



wwPDB X-ray Structure Validation Summary Report ⓘ

May 16, 2020 – 10:05 pm BST

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

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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

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

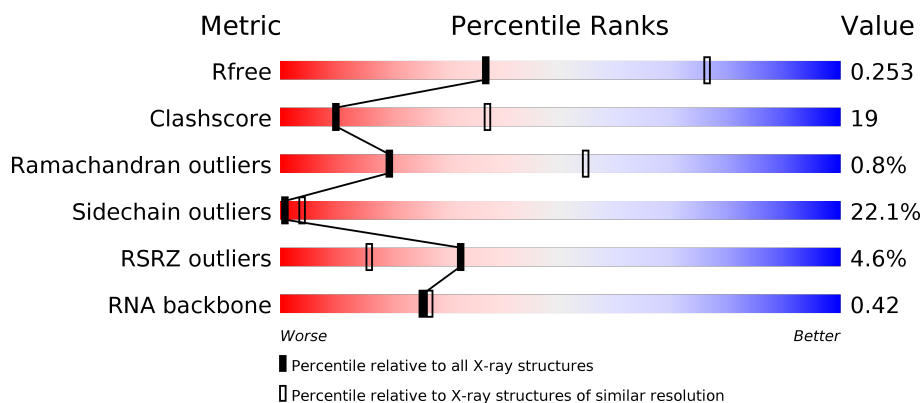
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION


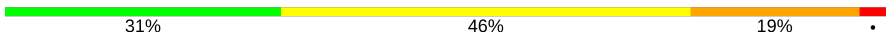


The reported resolution of this entry is 3.10 Å.

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.



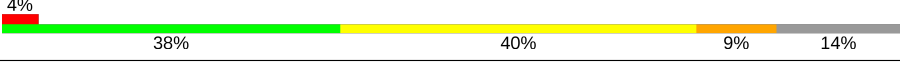
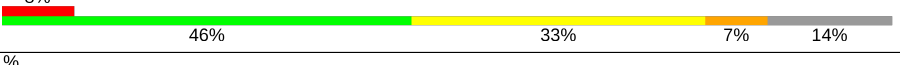

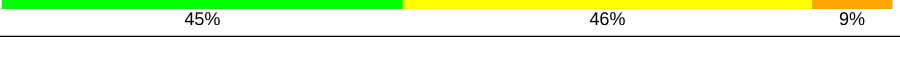



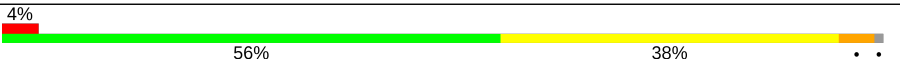

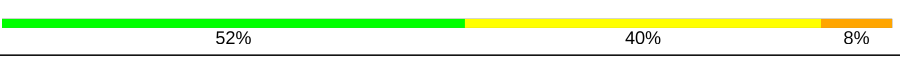

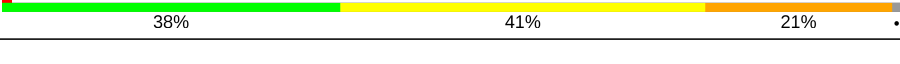

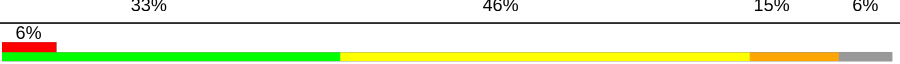





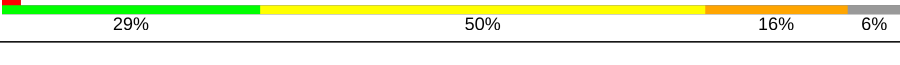
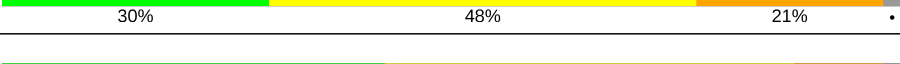




Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1094 (3.10-3.10)
Clashscore	141614	1184 (3.10-3.10)
Ramachandran outliers	138981	1141 (3.10-3.10)
Sidechain outliers	138945	1141 (3.10-3.10)
RSRZ outliers	127900	1067 (3.10-3.10)
RNA backbone	3102	1116 (3.40-2.80)

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

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

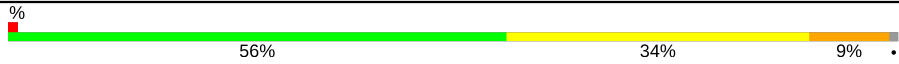
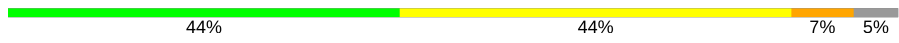
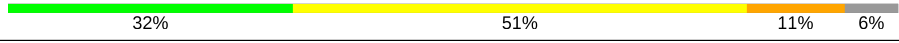
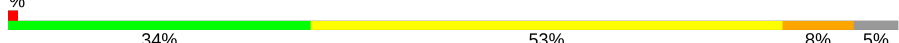
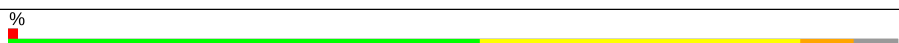
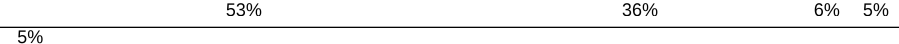

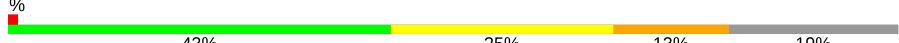

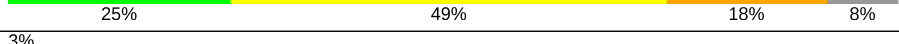
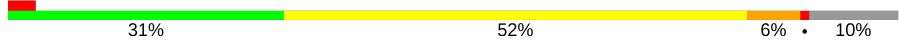

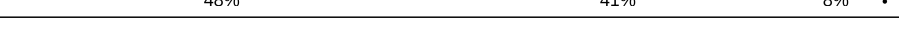
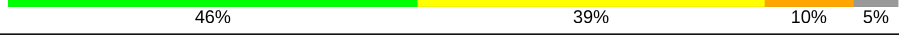
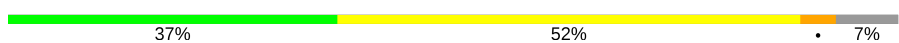
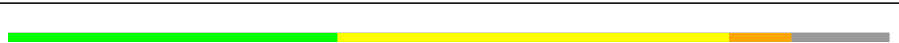




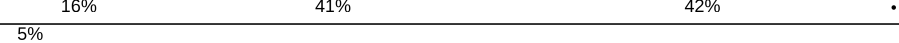



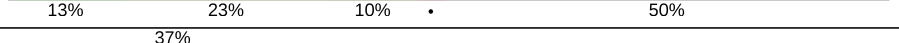
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Mol	Chain	Length	Quality of chain
3	22	239	
3	2E	239	
4	32	209	
4	3E	209	
5	42	162	
5	4E	162	
6	52	101	
6	5E	101	
7	62	156	
7	6E	156	
8	72	138	
8	7E	138	
9	82	128	
9	8E	128	
10	1A	105	
10	1I	105	
11	2A	129	
11	2I	129	
12	3A	132	
12	3I	132	
13	4A	126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

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


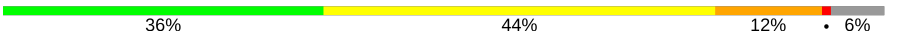
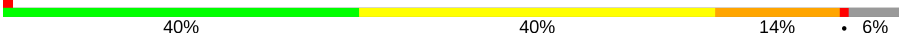



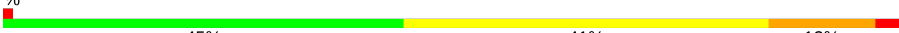







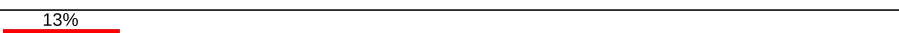




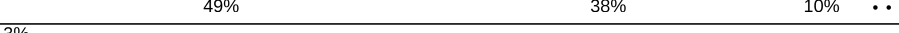

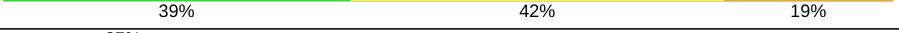



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Mol	Chain	Length	Quality of chain
29	79	229	
30	11	276	
30	19	276	
31	21	206	
31	29	206	
32	31	210	
32	39	210	
33	41	182	
33	49	182	
34	51	180	
34	59	180	
35	61	148	
35	69	148	
36	38	173	
37	15	140	
37	58	140	
38	25	122	
38	68	122	
39	35	150	
39	78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



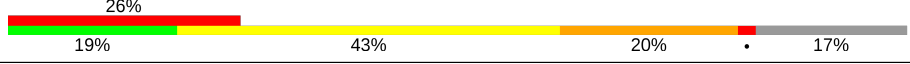
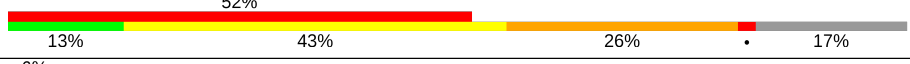
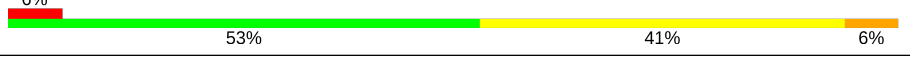
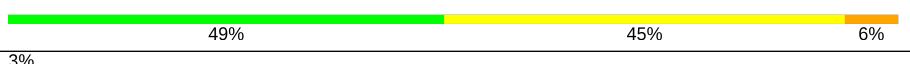
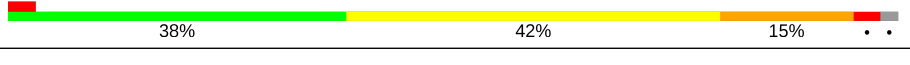

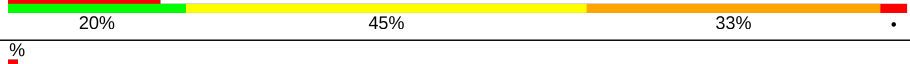
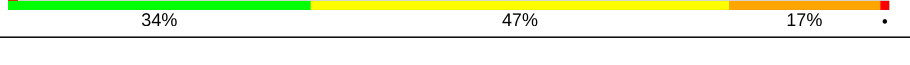
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Mol	Chain	Length	Quality of chain
42	A8	112	
43	75	146	
43	B8	146	
44	85	118	
44	C8	118	
45	95	101	
45	D8	101	
46	A5	113	
46	E8	113	
47	B5	96	
47	F8	96	
48	C5	110	
48	G8	110	
49	D5	206	
49	H8	206	
50	E5	85	
50	I8	85	
51	F5	98	
51	J8	98	
52	G5	72	
52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

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

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
26	PSU	5K	32	-	-	-	X
62	MG	1H	3343[A]	-	-	-	X
62	MG	1H	3343[B]	-	-	-	X
63	SF4	3E	302	-	-	X	-

2 Entry composition [i](#)

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 (three-letter code: K) (formula: K) (labeled as "Ligand of Interest" by author).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
61	45	1	Total	K	0	0
			1	1		
61	BA	1	Total	K	0	0
			1	1		
61	32	1	Total	K	0	0
			1	1		
61	13	51	Total	K	0	0
			51	51		
61	1J	1	Total	K	0	0
			1	1		
61	BI	1	Total	K	0	0
			1	1		
61	16	3	Total	K	0	0
			3	3		
61	21	1	Total	K	0	0
			1	1		
61	31	2	Total	K	0	0
			2	2		
61	4I	1	Total	K	0	0
			1	1		
61	5A	1	Total	K	0	0
			1	1		
61	52	1	Total	K	0	0
			1	1		
61	5E	1	Total	K	0	0
			1	1		
61	29	1	Total	K	0	0
			1	1		
61	2K	3	Total	K	0	0
			3	3		
61	4A	1	Total	K	0	0
			1	1		
61	39	2	Total	K	0	0
			2	2		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
61	1G	36	Total 36	K 36	0	0
61	11	1	Total 1	K 1	0	0
61	1H	144	Total 145	K 145	0	1
61	88	1	Total 1	K 1	0	0
61	49	1	Total 1	K 1	0	0
61	14	106	Total 106	K 106	0	0
61	19	1	Total 1	K 1	0	0
61	2A	1	Total 1	K 1	0	0
61	1K	1	Total 1	K 1	0	0
61	41	1	Total 1	K 1	0	0

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
62	14	294	Total 295	Mg 295	0	1
62	P8	1	Total 1	Mg 1	0	0
62	32	1	Total 1	Mg 1	0	0
62	13	119	Total 120	Mg 120	0	1
62	1J	4	Total 4	Mg 4	0	0
62	C8	1	Total 1	Mg 1	0	0
62	4L	1	Total 1	Mg 1	0	0
62	16	12	Total 12	Mg 12	0	0
62	42	1	Total 1	Mg 1	0	0

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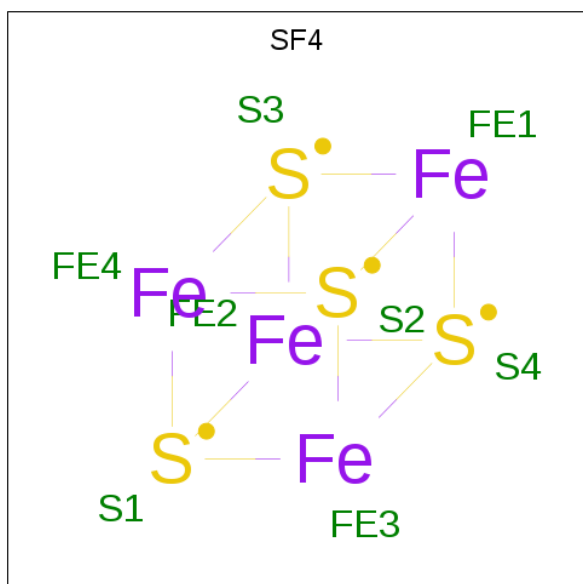
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
62	M5	2	Total 2	Mg 2	0	0
62	21	2	Total 2	Mg 2	0	0
62	31	1	Total 1	Mg 1	0	0
62	Q8	1	Total 2	Mg 2	0	1
62	L8	1	Total 1	Mg 1	0	0
62	I8	1	Total 1	Mg 1	0	0
62	29	2	Total 2	Mg 2	0	0
62	2K	2	Total 2	Mg 2	0	0
62	J8	1	Total 1	Mg 1	0	0
62	39	1	Total 1	Mg 1	0	0
62	1G	100	Total 102	Mg 102	0	2
62	11	1	Total 1	Mg 1	0	0
62	1H	433	Total 439	Mg 439	0	6
62	7I	1	Total 1	Mg 1	0	0
62	N8	1	Total 1	Mg 1	0	0
62	6E	1	Total 1	Mg 1	0	0
62	78	2	Total 2	Mg 2	0	0
62	3E	1	Total 1	Mg 1	0	0
62	F8	1	Total 1	Mg 1	0	0
62	O8	1	Total 1	Mg 1	0	0
62	41	1	Total 1	Mg 1	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
62	2L	3	Total	Mg	0	0
			3	3		

- Molecule 63 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe₄S₄).



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

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
64	5A	1	Total	Zn	0	0
			1	1		
64	5I	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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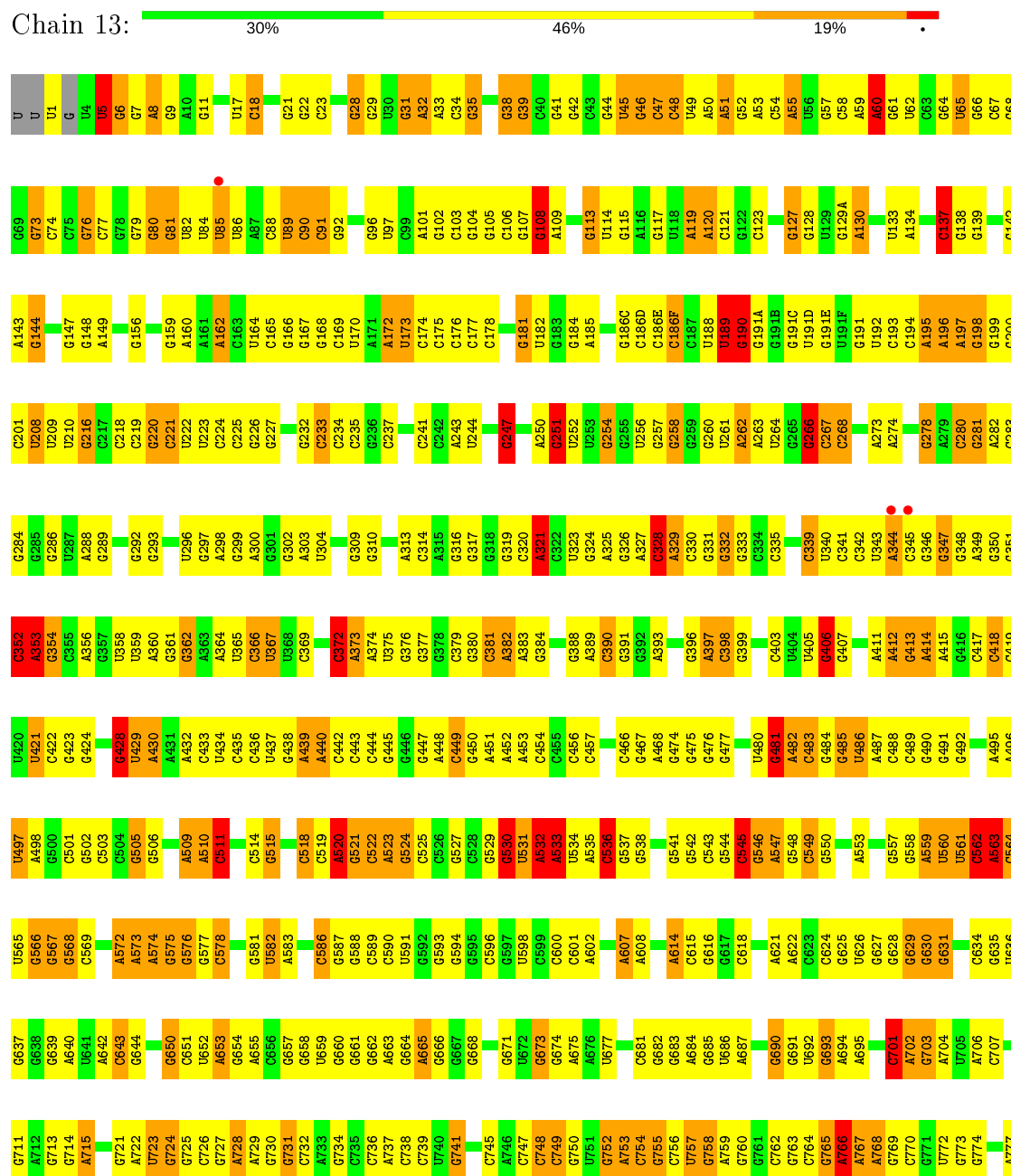
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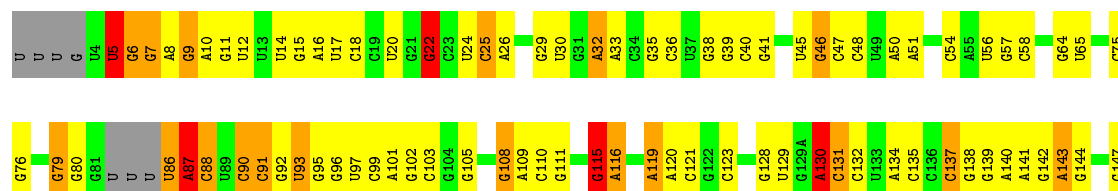
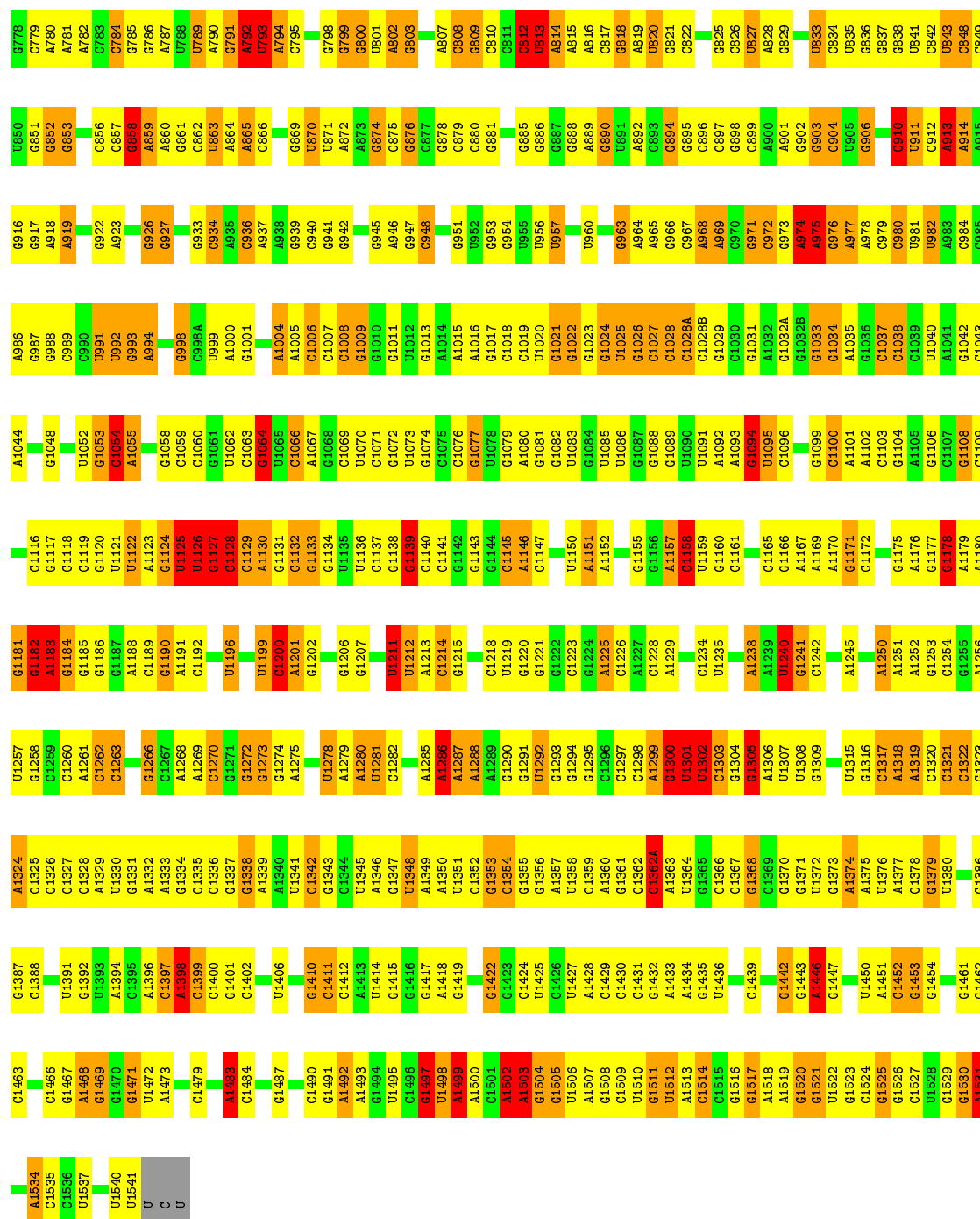
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65	M5	6	Total	O	0	0
			6	6		

3 Residue-property plots

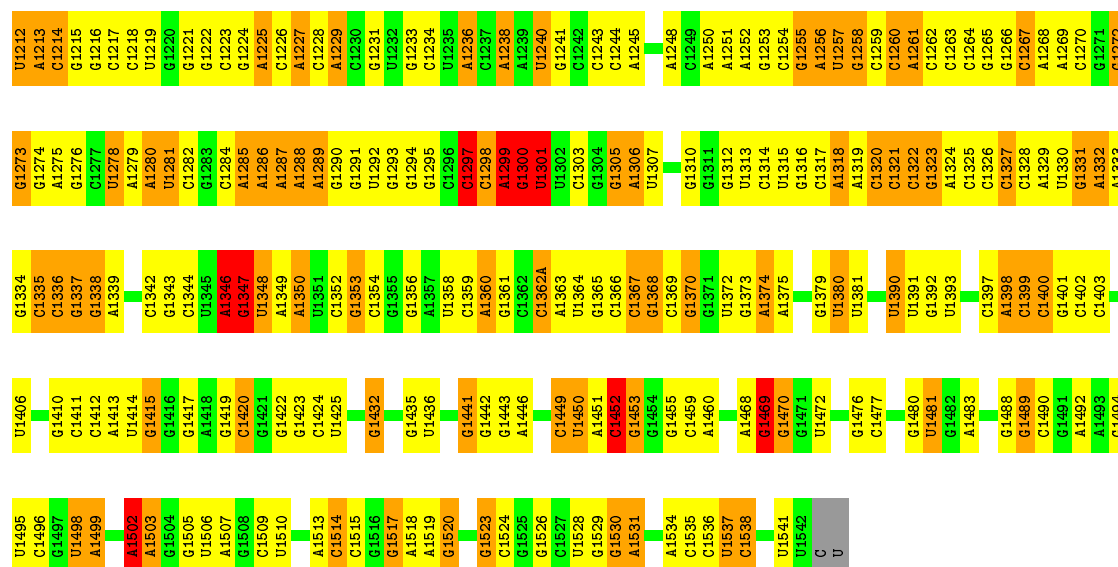
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are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

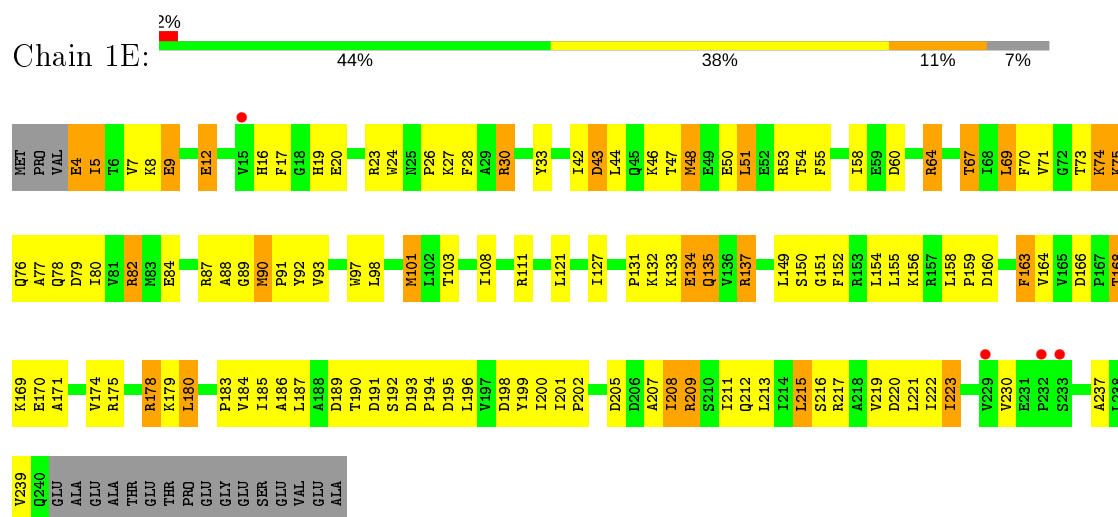




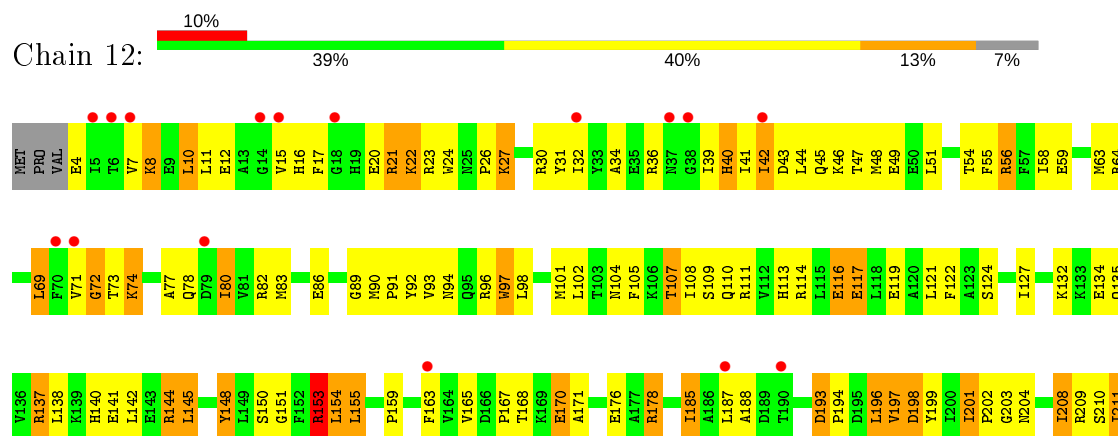
A1146	G1084	G1017	U955	G881	C912	G742	C601	U531	C449	A374		U208	G148
G1147	G1085	C1018	U956	C882	U913	U743	A602	A532	G450	U375	A303	U209	A149
U1148	U1086	C1019	U957	C883	A814	C744	A607	A533	A451	G376	U304	U210	C150
C1149		U1020	A958	U884	A815	C745	A608	U534	A452	G377	G305	G216	A151
A1150		G1021	A959	G885	A816	C746		A535	A453		G306	C217	A152
A1151		G1022	U960	G886	C817	C747		C536		G388		C218	C153
A1152		G1023	U961	G887	G818	C748	A614	G537	C457	A389		C219	C154
C1153		U1024	C962		A819	C749	C615	G538	C458	C390	G309		C155
A1154	A1092	U1025	U963	G890	U820	C750	G616	A539	G464	G391	G310	U222	G156
G1155	A1093	C1026	A964	U891	G821	U751	G617	A540	A465	G392	C311	U223	G157
G1156	G1094	C1027	A965	A892	C822	G752	G618	G541	C466	A393	C312	C224	C224
U1095	U1095	C1028	G966	G893	G823	A753	U619	G542	G467		G316	C225	G158
A1157	C1028A	C967	G967	G894	C824	C754	G620	C543	A468	G396	G317	C226	G159
U1159	C1028B	A968	G968	G895	G825	G755	A621	G544	G474	A397			A160
G1160	G1029	A969	C970	C896	C826	C756	A622	C545	G475	C398	A321	G230	C163
C1161	C970	C971	C897	C897	U827	U757	C623	G546	G476		C322	G231	U164
C1162	G1032A	G972	G972	G898	A828	A759	G624	A547	G477	C401	U323	G232	C165
	G1032B	G973	G973	G899	G829	A759	G625		A478	G402	G324	C233	G166
A1167	G1033	A974	G974	A900	U830	G760	U626	G550		C403	A325	C234	G167
A1169	G1034	A975	A975	A901	U831		G627		G481		G326	C235	G168
A1170	A1035	G976	G976	G902	C832	G763	G628	C554	A482	G406	A327		G169
G1171	G1036	A977	A977	G903	U833	C764	G629	C555	C483	G407	C328	U244	C174
C1172	C1037	A978	A978	G904	C834	G765	G630	C556	G484	A408	A329	G247	C175
	G1038	U978	U978	U905	U835	A766	G631	G557	G485	G409		G250	C176
G1175	C1039	C979	C979	G906	G836	A767	A632	G558	U486	G410	G332	G251	C177
A1176	U1040	C980	C980	A907	G837	A768		A559	A487	A411	G333	G252	G178
G1177	A1041	U981	U981	A908	G838	G769	G635	U560	C488	A412		G253	U180
C1178	G1042	A982	A982	A909	U841	C770	U636	U561	G489	G413	C336	U257	G181
A1179		A983	A983	C910	C842		G637	C562	G490	A414	C337	G258	U182
	A1046	C984	C984	U911	U843	G774	G638	A563	U494	A415	A338	G259	G183
G1181	G1047	C985	C985	C912	C848	G775	G639	C564		G416	C339	G265	U184
G1182	G1048	A986	A986	A913	C849	G776	A640		A495	C417	U340	G266	G185
A1183	U1049	G987	G987	A914	U850	A777	U641	G567	A496	C418	G341	G267	G186
G1184	G1050	G988	G988	A915	G851	G778	U646	G568	U497	C419	U342	G268	C187
G1185	C1051	C989	C989		G852	G779	C647			U420	U343		C188
G1186	U1052	C990	C990	A919	G853	A780	C647	A572	C501	U421	A344	U261	C189
G1187	G1053	U991	U991	U920	G854	A781	G650	A573	G502	G422	C345	A262	C186A
A1188	C1054	U992	U992	U921	G855	A782	C651	A574	C503	G423	G346	A263	C186B
C1189	A1055	G993	G993	G922	C856	C783	U652	G576	G504	G424	G347	U264	G186C
					C857	C784	A653	G577	G505	G425		G265	C186D
G1192	G1058	U997	U997	G925	G858	G786	G658	U582	C507	U427	G350	G266	
G1193	C1060	C998A	C998A	G926	A859	A787	U659	U583	C508	G428	C352	C269	U188
U1194	G1061	U999	U999	G927	A860		G660	G584	A509	U429	A353	A270	U189
C1195	U1062	A1000	A1000	C934	G861	A790	G661	G585	A510	A430	G354	C271	G190
U1196	C1063	G1001	G1001	A935			G662	G586	C511	A431		A272	G191A
G1197	G1064	G1002	G1002	C936	A865	G791	G663	C586	U512	A432	U358	A273	
G1198	U1065	A1003	A1003	A938	C866	A792	G664	G587	C513	C433	U359		U191E
U1199	C1066	A1004	A1004	G939	G867	A793	A665	G588	C513	U434	A360	C277	U191F
C1200	A1067	C1005	C1005		G868	C795	G666	C589	U516	C435	G361	G278	G191
A1201		G942	G942	G942	G869	C796	G667	C590	G517		G362	A279	U192
G1202	G1072	C1007	C1007	G943		G800	G667	U591	C518	G438	A363	C280	U193
C1203	U1073	C1008	C1008	A946	A872	U801	G668	G592	C519	A439	C366	G281	C194
A1204	G1074	G1009	G1009	G947	A873	C901	U669	G593	C519	A440	U367		A195
U1205		G1010	G1010	C948	G874	A807	G670	G594	G524	C442		U287	A196
G1206	G1077	G1011	G1011	A949	C875	A807	G671	G595	C525	C443		A288	A197
G1207	U1078				G876	C808	U672	C596	C526	C444		G289	G198
C1208	G1079	A1014	A1014	G953	C877	G809	U673	C599	G527	G445		G290	G199
		A1015	A1015	G954		C810	G674	C600	G530			A298	G200
		A1016	A1016			C811	G741			A448		G299	C201

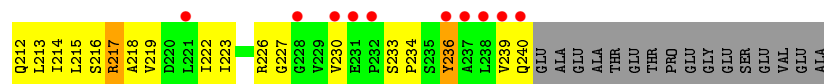


• Molecule 2: 30S ribosomal protein S2

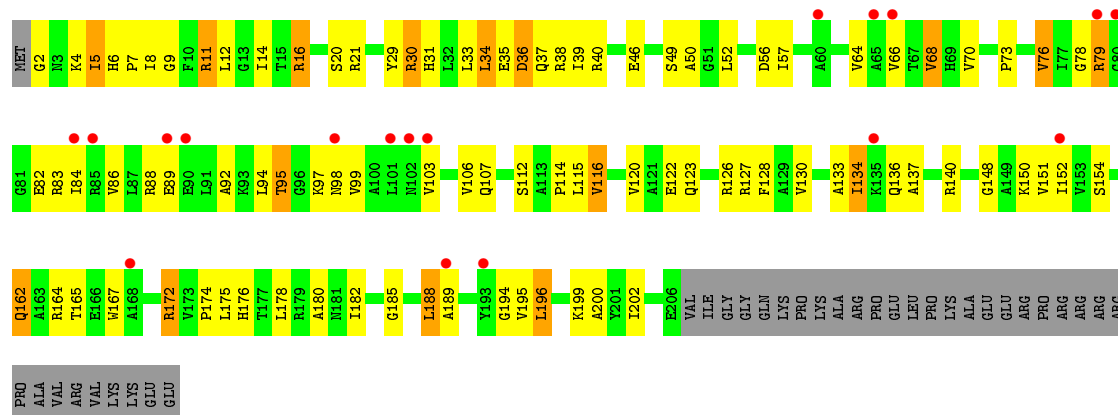


• Molecule 2: 30S ribosomal protein S2

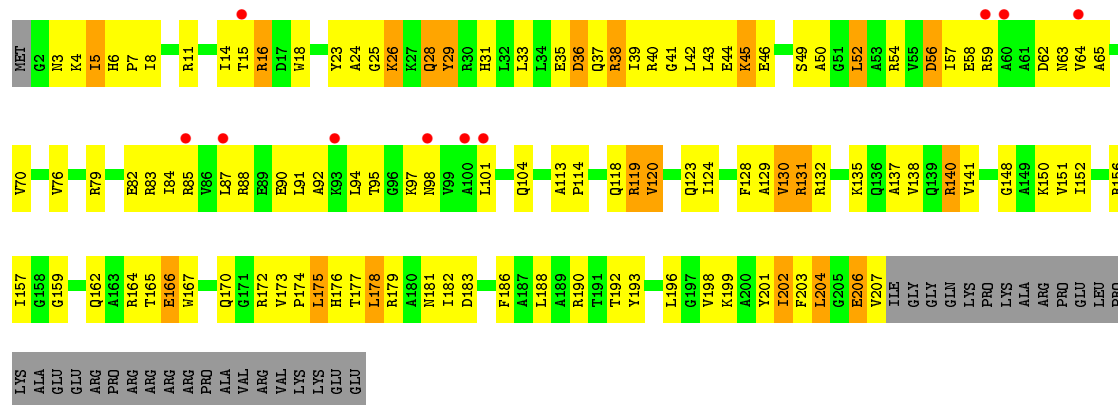




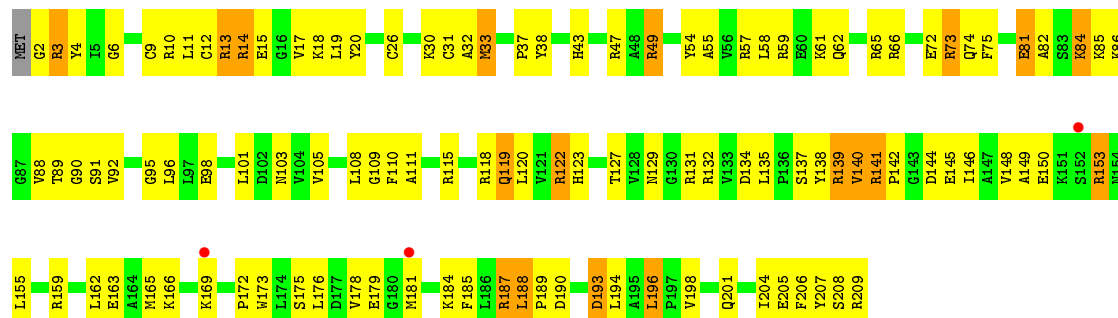
• Molecule 3: 30S ribosomal protein S3



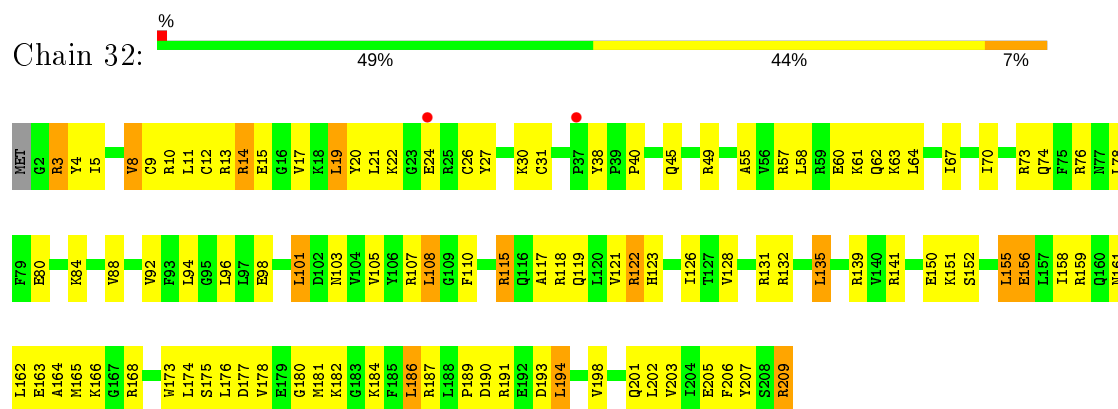
• Molecule 3: 30S ribosomal protein S3



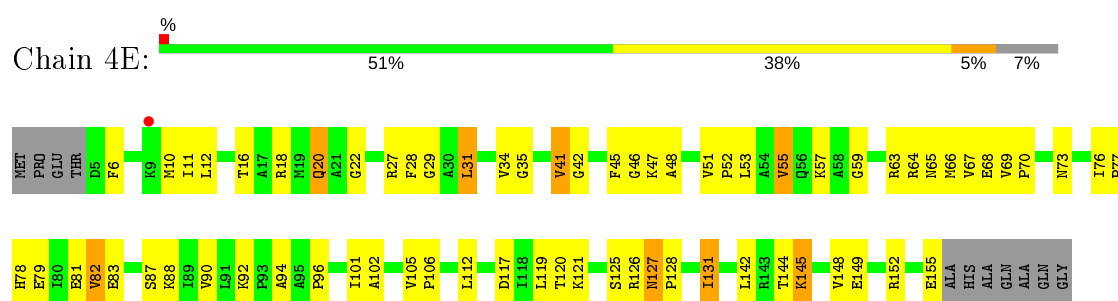
• Molecule 4: 30S ribosomal protein S4



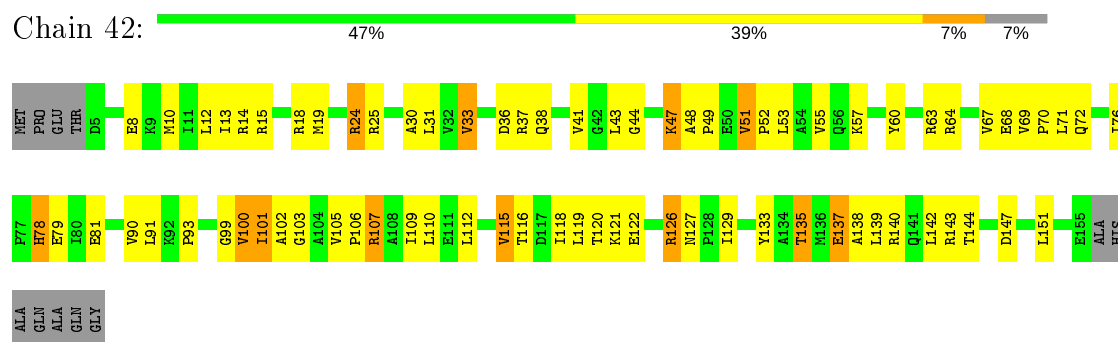
- Molecule 4: 30S ribosomal protein S4



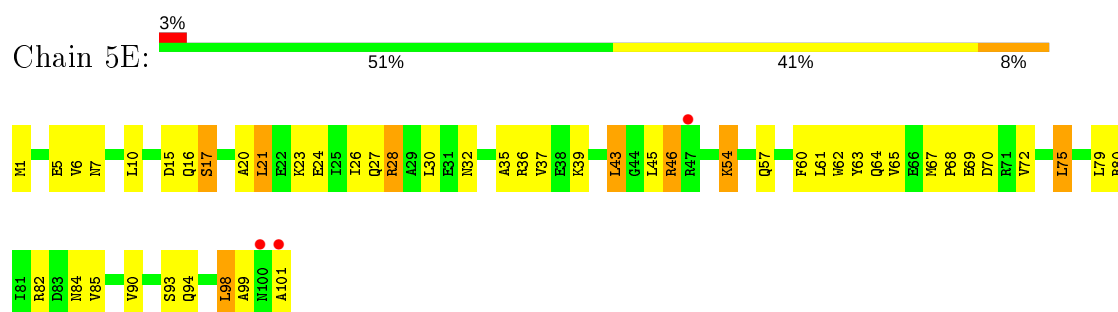
- Molecule 5: 30S ribosomal protein S5



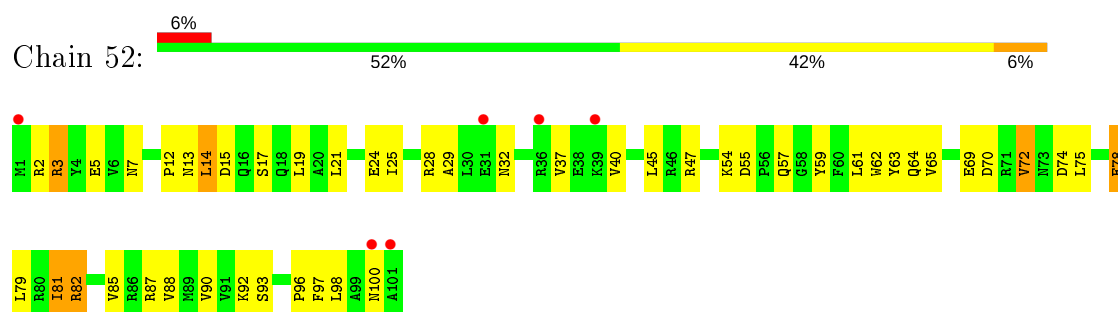
- Molecule 5: 30S ribosomal protein S5



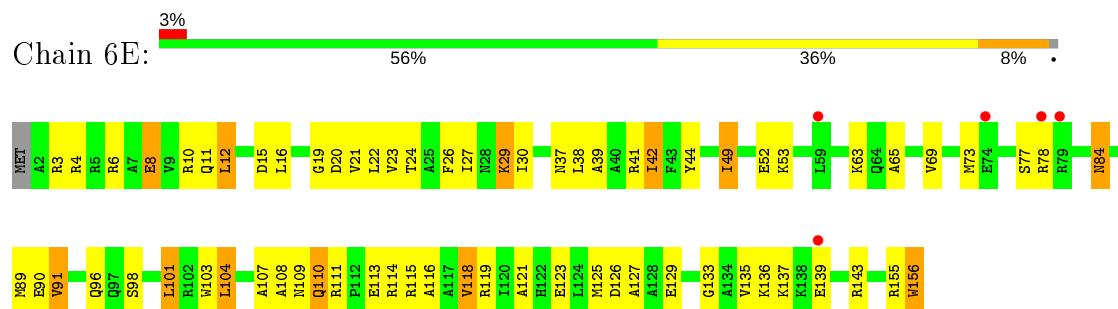
- Molecule 6: 30S ribosomal protein S6



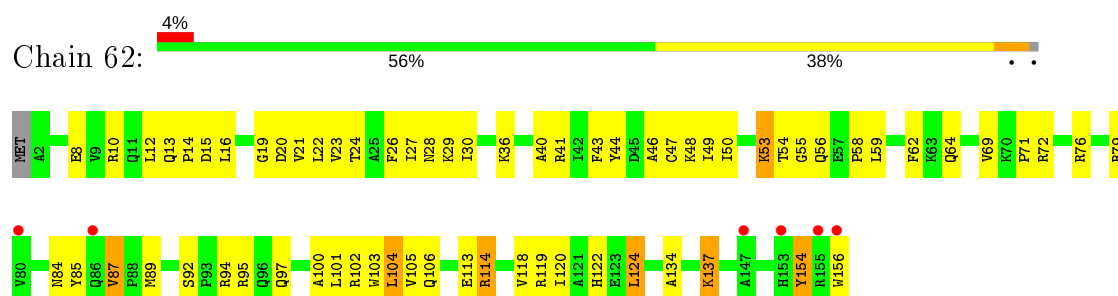
- Molecule 6: 30S ribosomal protein S6



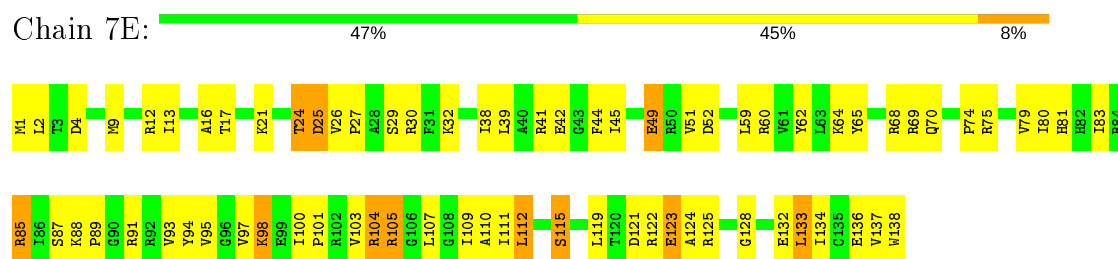
- Molecule 7: 30S ribosomal protein S7



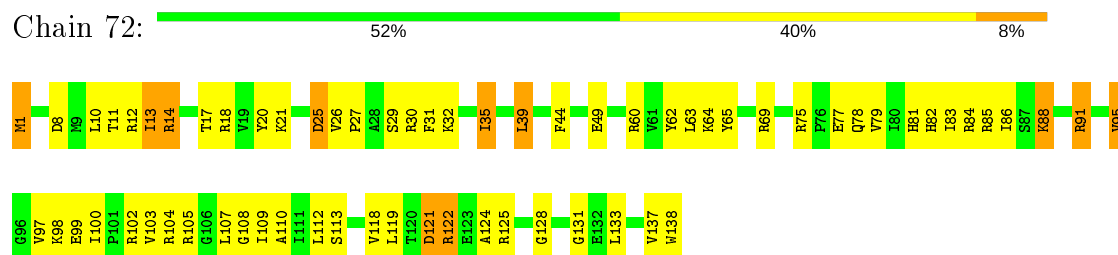
- Molecule 7: 30S ribosomal protein S7



- Molecule 8: 30S ribosomal protein S8



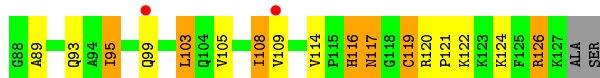
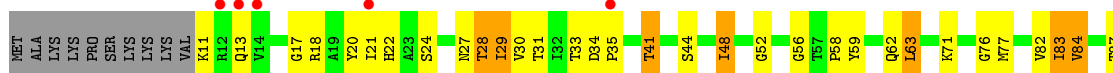
- Molecule 8: 30S ribosomal protein S8



- Chain 2I:
-
- | Category | Percentage |
|----------|------------|
| NET | 2% |
| ALA | 50% |
| LVS | 34% |
| PRO | 5% |
| SER | 10% |
| LVS | 2% |
| VAL | 2% |
| K11 | 2% |
| K12 | 2% |
| Q13 | 2% |
| V14 | 2% |
| A15 | 2% |
| S16 | 2% |
| G17 | 2% |
| R18 | 2% |
| A19 | 2% |
| Y20 | 2% |
| I21 | 2% |
| M27 | 2% |
| F28 | 2% |
| I29 | 2% |
| V30 | 2% |
| T31 | 2% |
| I32 | 2% |
| T33 | 2% |
| D34 | 2% |
| P35 | 2% |
| N38 | 2% |
| P39 | 2% |
| I40 | 2% |
| T41 | 2% |
| I43 | 2% |
| K51 | 2% |
| R54 | 2% |
| K55 | 2% |
| G56 | 2% |
| P57 | 2% |
| T58 | 2% |
| Y59 | 2% |
| A60 | 2% |
| D67 | 2% |
| K71 | 2% |
| M77 | 2% |
| Q78 | 2% |
| S79 | 2% |
| V80 | 2% |
| D81 | 2% |
| V82 | 2% |
| T83 | 2% |



- Molecule 11: 30S ribosomal protein S11



- Molecule 12: 30S ribosomal protein S12



- Molecule 12: 30S ribosomal protein S12

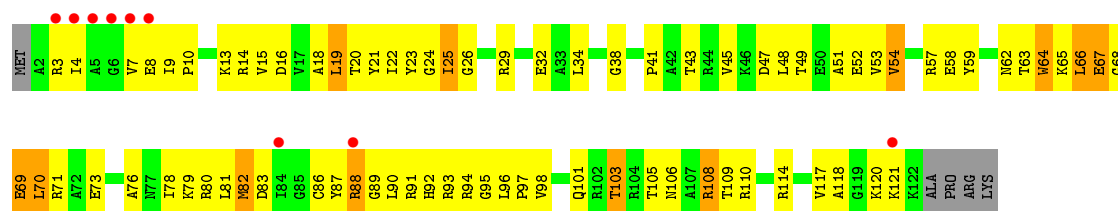


- Molecule 13: 30S ribosomal protein S13



- Molecule 13: 30S ribosomal protein S13





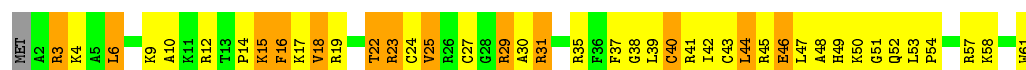
- Molecule 14: 30S ribosomal protein S14 type Z

Chain 5I: 43% 46% 10%



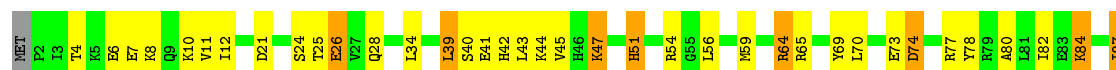
- Molecule 14: 30S ribosomal protein S14 type Z

Chain 5A: 30% 48% 21%



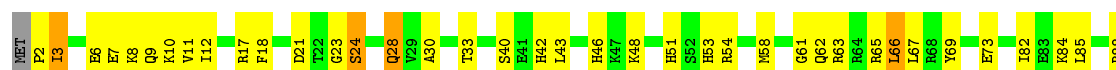
- Molecule 15: 30S ribosomal protein S15

Chain 6I: 56% 34% 9%



- Molecule 15: 30S ribosomal protein S15

Chain 6A: 56% 38% 6%

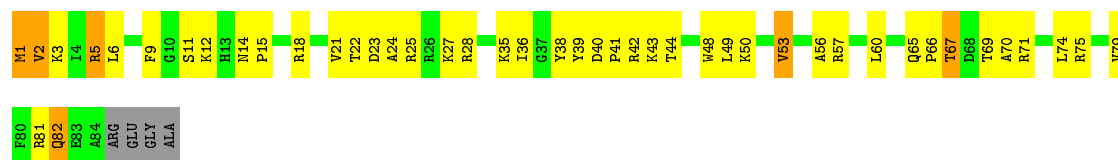


- Molecule 16: 30S ribosomal protein S16

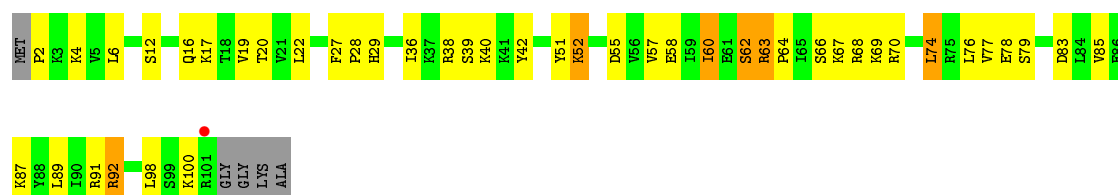
Chain 7I: 32% 51% 11% 6%



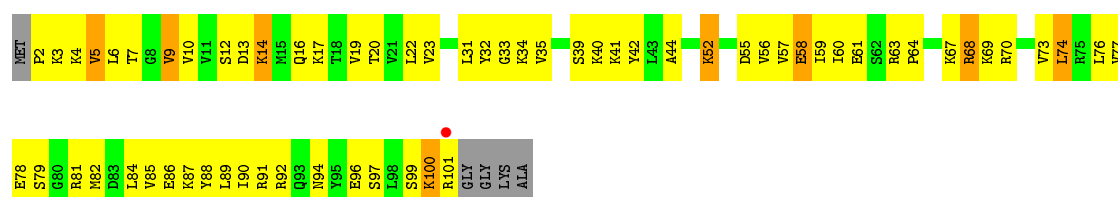
• Molecule 16: 30S ribosomal protein S16

Chain 7A: 

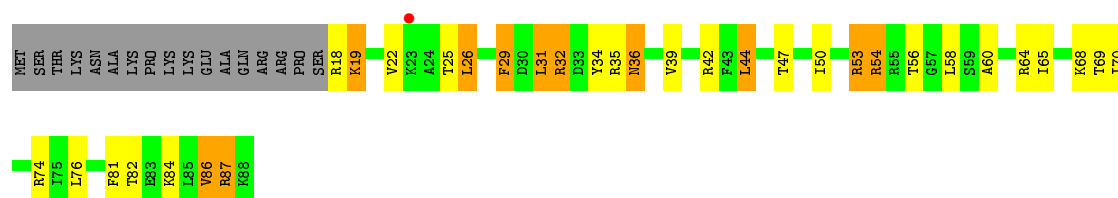
• Molecule 17: 30S ribosomal protein S17

Chain 8I: 

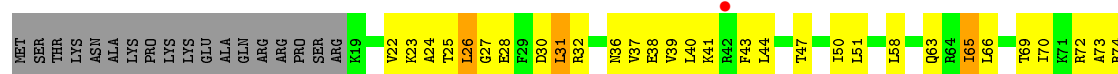
• Molecule 17: 30S ribosomal protein S17

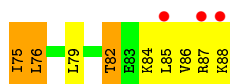
Chain 8A: 

• Molecule 18: 30S ribosomal protein S18

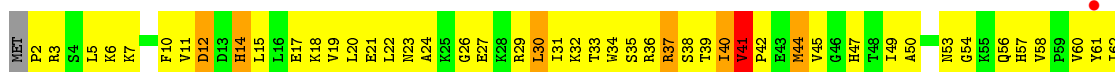
Chain 9I: 

• Molecule 18: 30S ribosomal protein S18

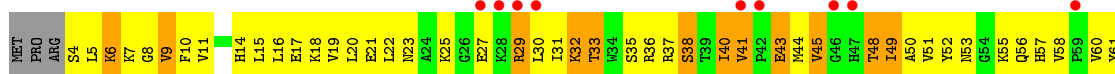
Chain 9A: 



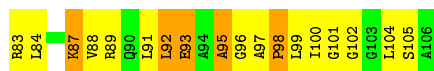
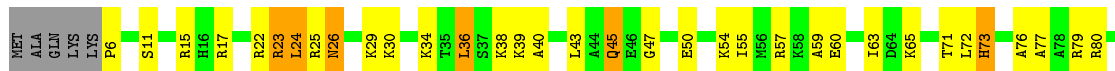
- Molecule 19: 30S ribosomal protein S19



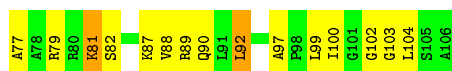
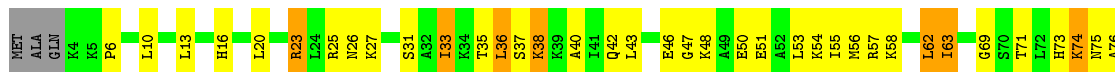
- Molecule 19: 30S ribosomal protein S19



- Molecule 20: 30S ribosomal protein S20

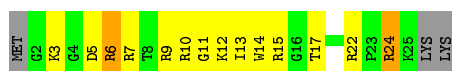


- Molecule 20: 30S ribosomal protein S20

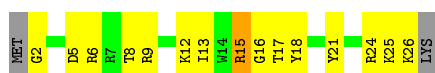


- Molecule 21: 30S ribosomal protein Thx

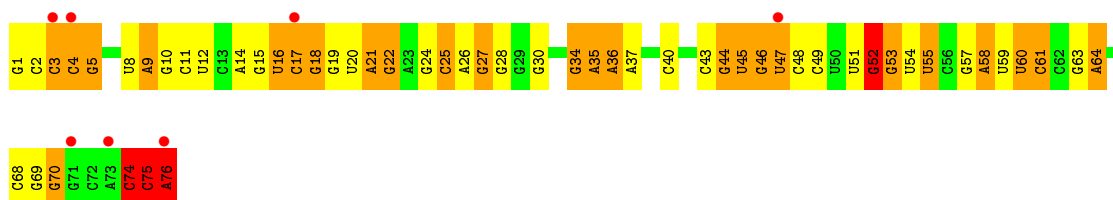
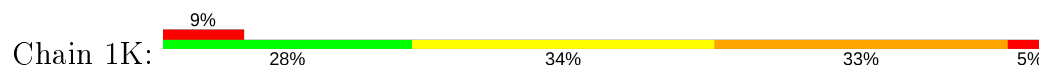




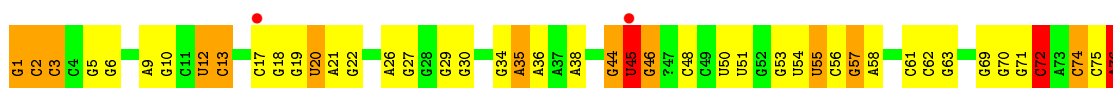
- Molecule 21: 30S ribosomal protein Thx



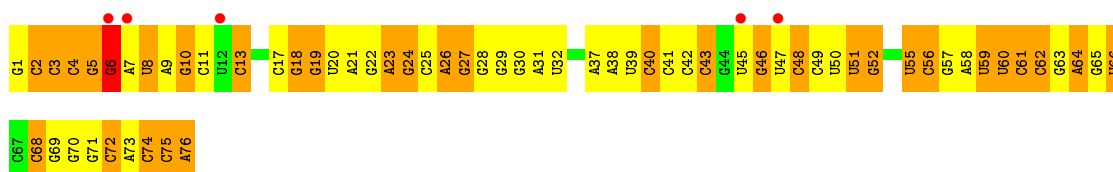
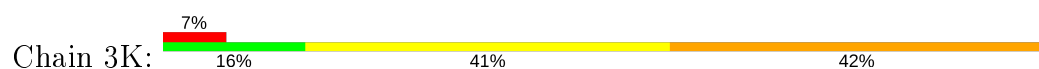
- Molecule 22: E. coli tRNAPhe



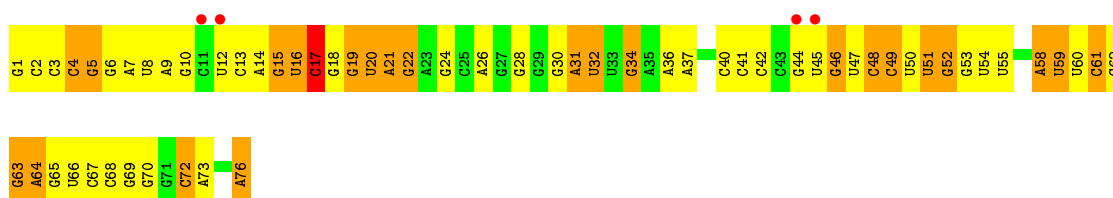
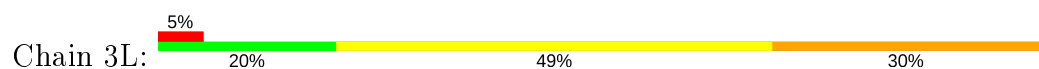
- Molecule 23: E. coli tRNAPhe



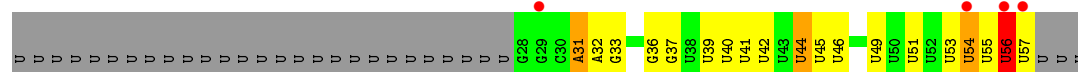
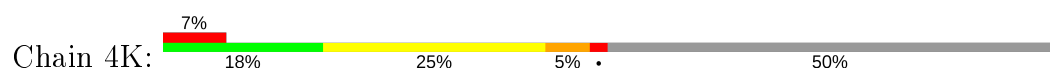
- Molecule 24: E. coli tRNAPhe



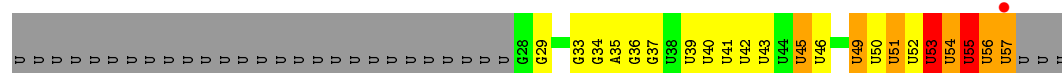
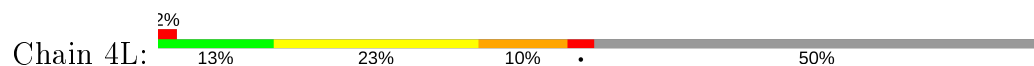
- Molecule 24: E. coli tRNAPhe



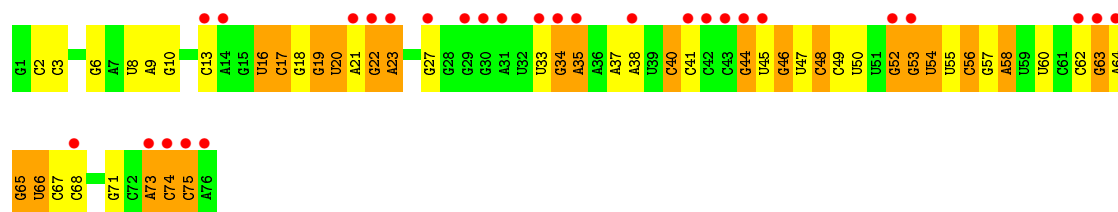
- Molecule 25: mRNA



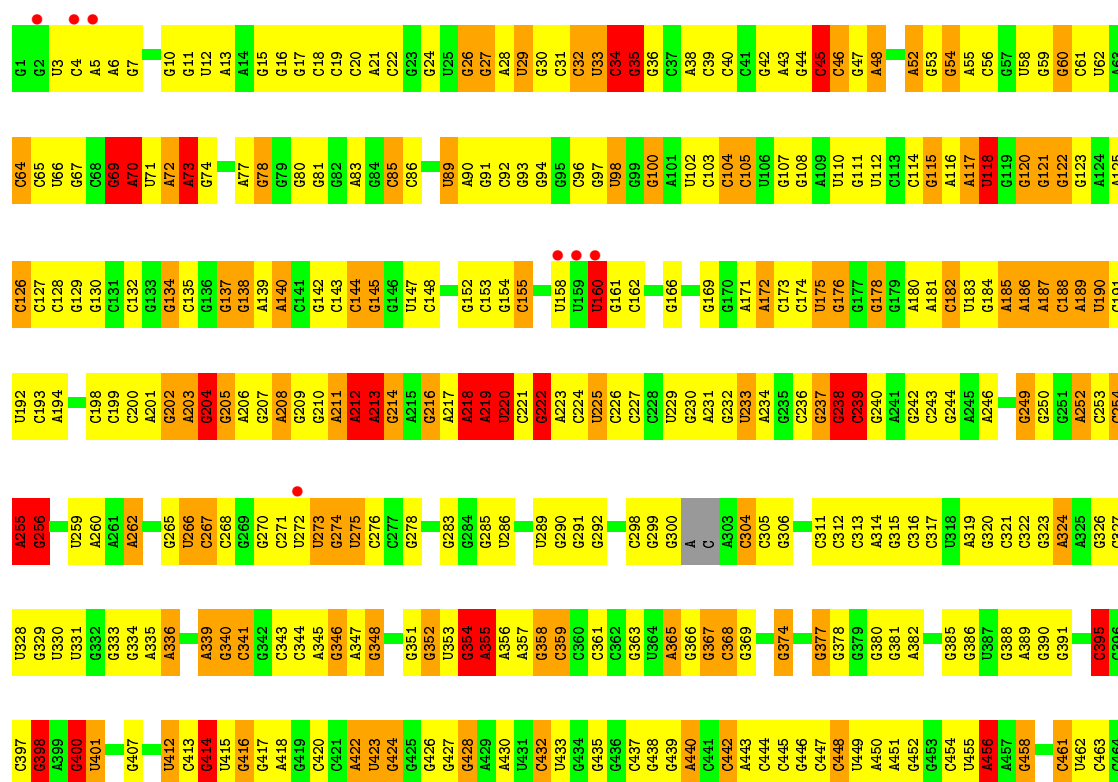
• Molecule 25: mRNA



• Molecule 26: E. coli tRNAPhe



• Molecule 27: 23S ribosomal RNA



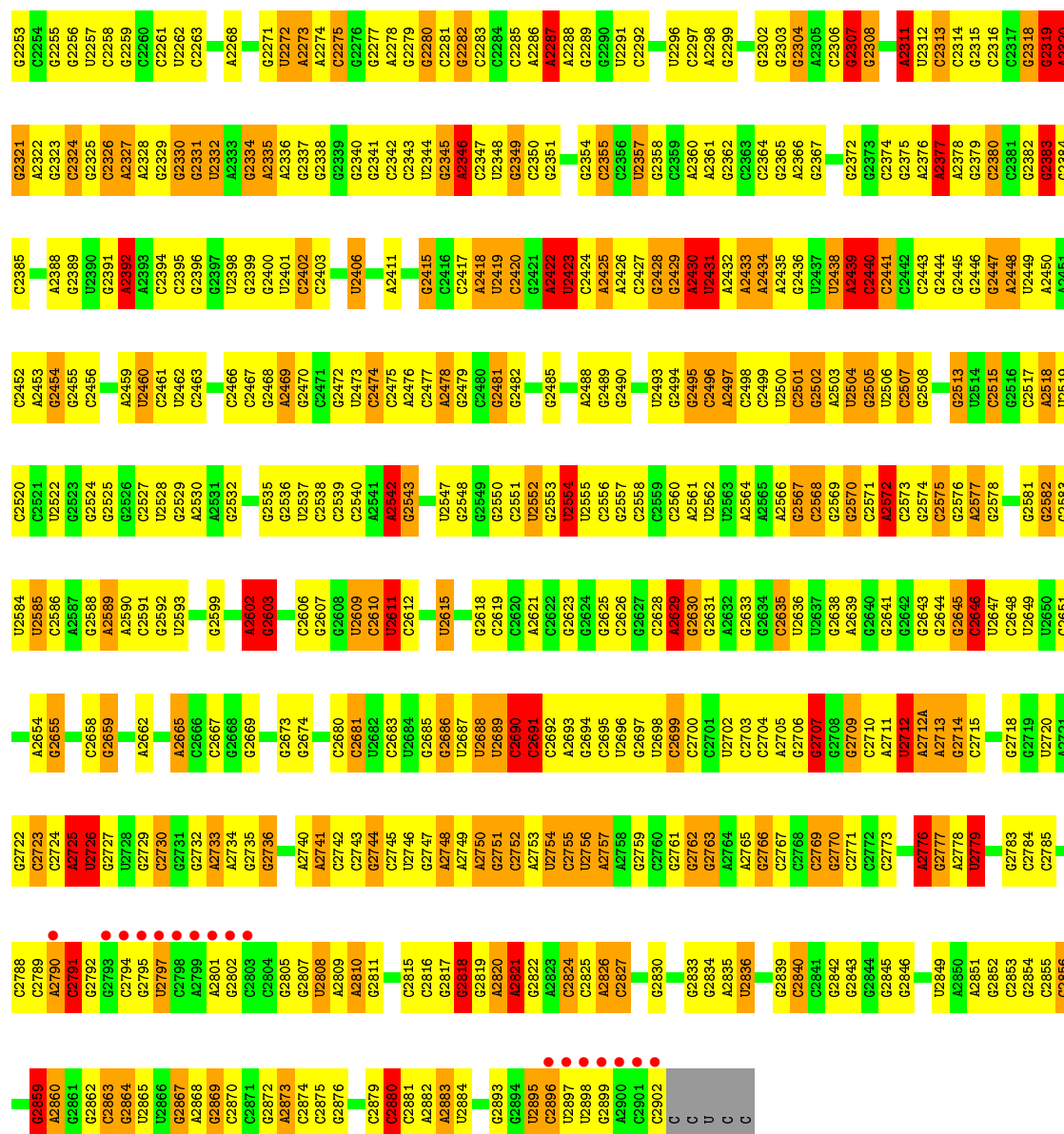
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	G1290		G1161	A1101	C1038		C904	G840	C780	G716	A653	U590	U630	G469
U1360	G1291	G1229		G1102	C1039	C905	C905	A841	G781	G717	G654	A591	A470	A471
C1362	G1292	G1230	C1168	G1103	G1040	G975	U906	G842	A782	A718	G655	U592	G632	C471
U1363	A1293	G1231	G1169	A1104	G1041	U976	G907	C843	A783	C719	G656	U593	A533	C472
	A1294	G1232	G1170	U1105	C1042	C977	U908	C844	A784	C720	A657	G584	G634	G473
	G1295	G1233	C1171	G1106	A1043	G978	A909	C845	C785	G721		A595	C635	A474
G1366	U1296	U1234	G1172	U1107	G1044	A979	G910	G846	G786	G722	C660	A596	C636	U475
C1367	G1297	A1235	A1173	U1108	C1045	G980	A911	G847	G787	A723	C661	G597	U537	A476
A1368	C1298	G1236	A1174	G1109	U1046	C981	A912	A848	U788	A724	C662	C598	G638	G477
A1369	G1299	G1237	A1175	G1110	A1047	C982	G913	G849	G789	A725	A663	A599	A639	C478
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G1371		G1239	U1177	U	G1049	G984	U916		G791	C727	U665	G601	A541	C480
U1372		A1240	G1178	G985	G1050	G985	G917	G853	G792	G728	C666	A602	C542	A481
U1373		G1241		G986	C1051	A918	A918	C854	G793	G729	C667	G603	C543	A482
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G1375	G1306	G1243	G1182	A	C1053	G988		G856	U795	C731	A669	C605	U545	A484
U1376	G1307	G1244	G1183	A	C1054	U989	G923	G857	G796	G732	A670	G606	G546	G485
G1377	C1308	U1245	G1184	G1118	C1055	G990	G924	U858	C797	A733	C671	G607	G547	U486
A1378	G1309	G1246	G1185	G1119	A1056	A991	U925	U859	A798	G734	A672	G608	G548	
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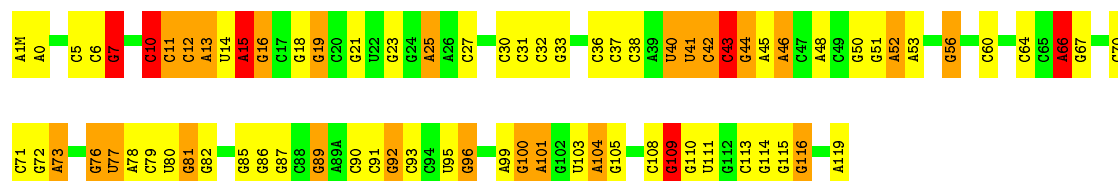
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	G1163	U	G1030	C967	C598	A836			C584		G447	C365	C297
	G1164	A	G1031	G968	C599	A837			C585		U448		G298
G1238	U1165	A	A1032	U969	A899	C838			C586		A449		
U1240	G1166	U	U1033	U970	A900	U839			C587		C450	U373	G301
A1241	U1167	A	G1034	C970	A901	C840			U588		G451	A374	C302
A1242	G1168	G	U1035	G971	C902	A841			C589		C452		U303
G1243	G1169	C1100	G1036	G972	C903	G842			A590		C453	G304	G304
G1244	G1170	U1101	G1037	A973	C904	G843			C591		A454	U305	U305
	G1171	A1102		G974	U905	C844			G592		C455	U306	U306
	G1173	A1103	C1040	C974A	G906	A845			C527		C456	G307	G307
G1247	U1174	G	G1041	C976	U907	C846			C528		A457	G308	G308
G1249	U1175	U1105	G1042			U847			A529		G458	G309	G309
G1250	G1176		C1043		A910	C848			G530		U459	A310	A310
C1251	A1177		A1044	A920	A911	C849			C601		A460	A390	A311
G1252	G1178	G1109	A1045	A921	G912	C846			G602		C461	G391	G312
A1253	C1179	A1111	A1046	C982	U913	U847			A603		C462	C392	C313
A1254	G1180	G1112	G1047	A983	C914	G848			G604		G463	C393	C314
U1255	C1181	U1113	A1048		C915	A849			C605		U464	A394	G315
G1256	G1114	G1114	C1049	C956	G916	C850			A536		G465	U395	C316
C1257	G1183	G1115	A1050	G987	A917	U851			U607		G467	G397	G317
G1258	G1184	C1116		A988	A918	U851			A608		G468	C319	C319
G1259	C1185		G1053	G989	A919	G854			G544		G469	A401	A320
G1260	G1186	G1122	A1054	A990	G919	C855			C546		A470	A402	G321
	G1187		G1055	C991	U922	C856			A547		U403	A322	A322
	G1190	A1126	G1056	C992	C923	C857			A548		A472	C404	G323
G1264	G1191	G1125	A1057	G993	C924	U858			G549		U405	U405	A324
A1265	G1192	G1126	U1058	C994	C924	G859			G550		G406	G406	G325
G1266		A1129	G1059	C995	G928	U860			G551		G407		
U1267		U1130	U1060	A996	G929	A861			C546		A479	U328	U328
A1268	G1195	G1131	U1061	G997	U930	G864			A547		A480	G329	G329
A1269		A1132	G1062	C998	G931	G864			A471		A412	A330	A330
G1270	U1198	U1133	C	U999	G932	A865			U613		U475		
G1271		C1135	U	A1000	A933	A866			G545				
A1272	C1202	G1136	U	A1001	A802	C867			G552		A479		
U1273	G1203	G1137	A	G1002	U868	U868			U553		A480		
A1274	A1204	G1138	U	G1003	A804	G869			U554		A412		
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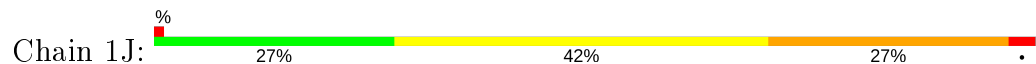


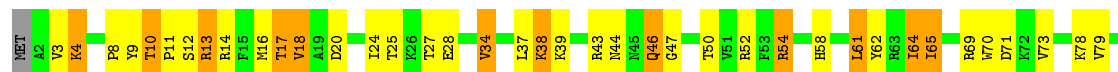
• Molecule 28: 5S ribosomal RNA

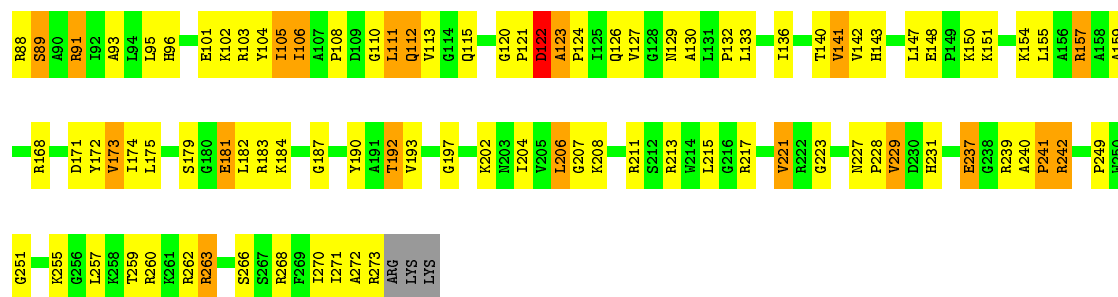
Chain 16: 36% 39% 20% 5%



• Molecule 28: 5S ribosomal RNA

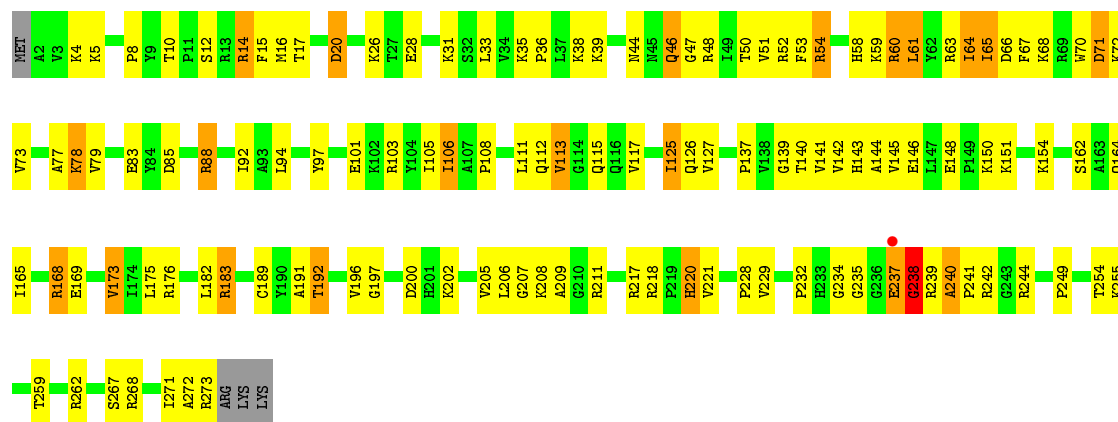






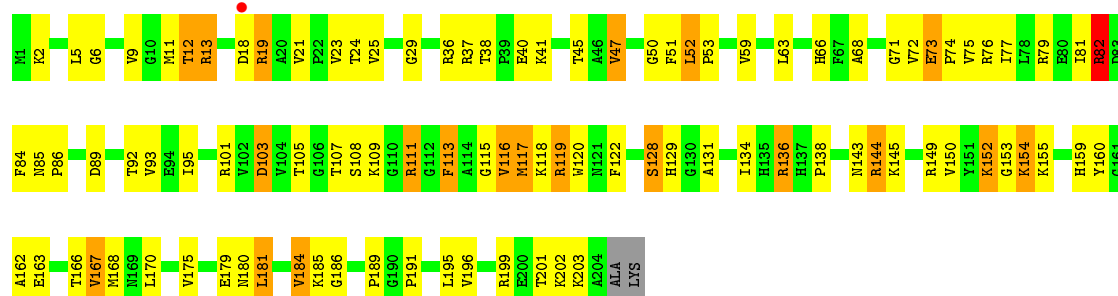
• Molecule 30: 50S ribosomal protein L2

Chain 19: 53% 37% 8%



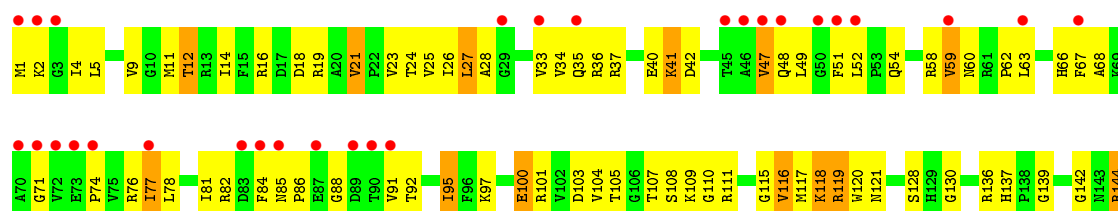
• Molecule 31: 50S ribosomal protein L3

Chain 21: 51% 38% 10%



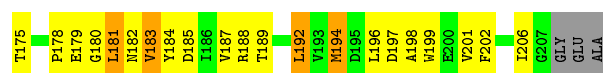
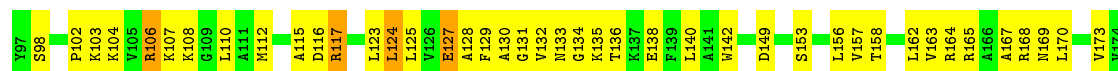
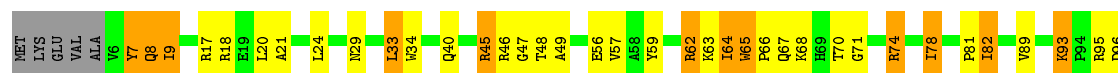
• Molecule 31: 50S ribosomal protein L3

Chain 29: 16% 46% 44% 9%

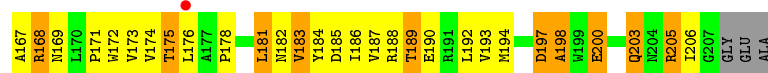
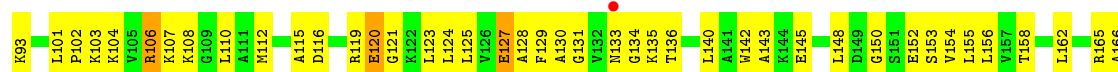
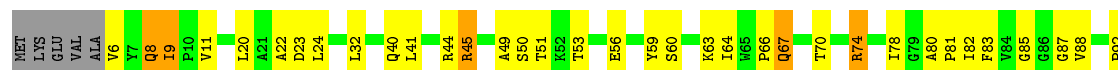




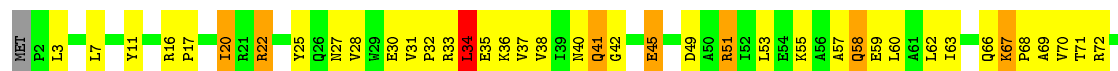
- Molecule 32: 50S ribosomal protein L4



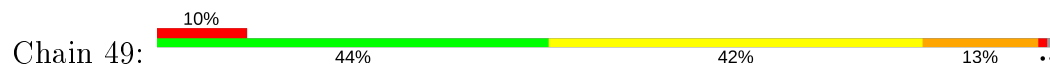
- Molecule 32: 50S ribosomal protein L4

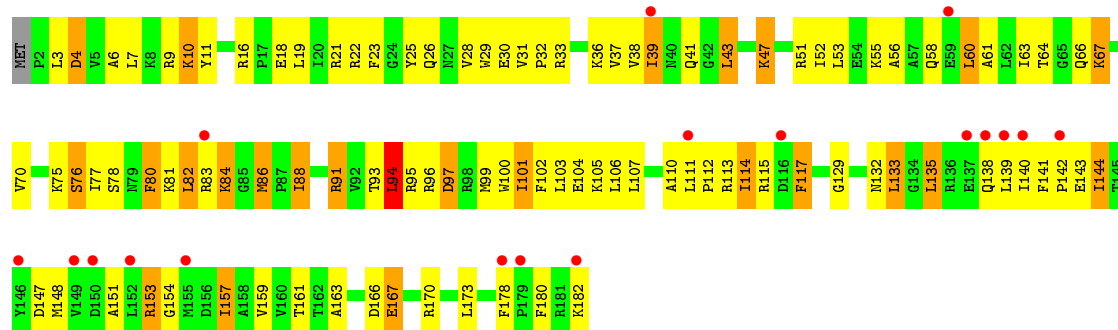


- Molecule 33: 50S ribosomal protein L5

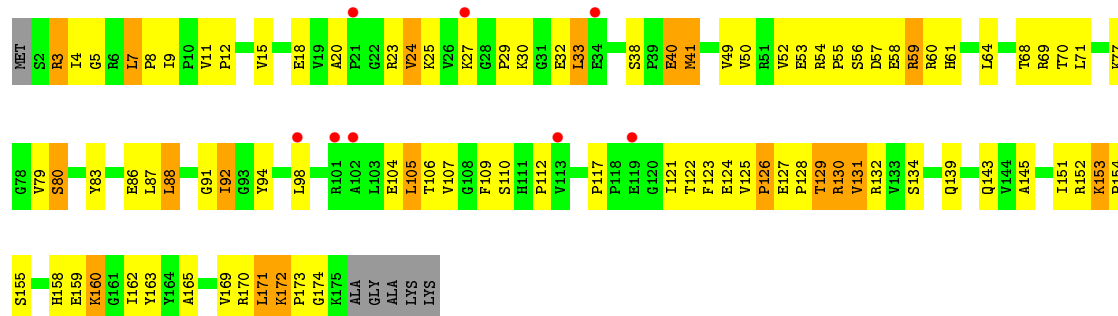


- Molecule 33: 50S ribosomal protein L5

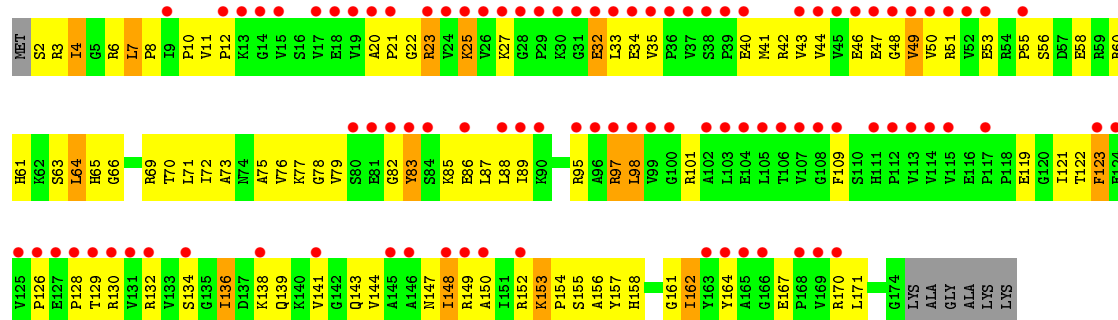
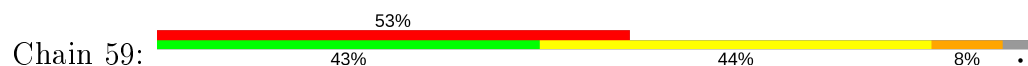




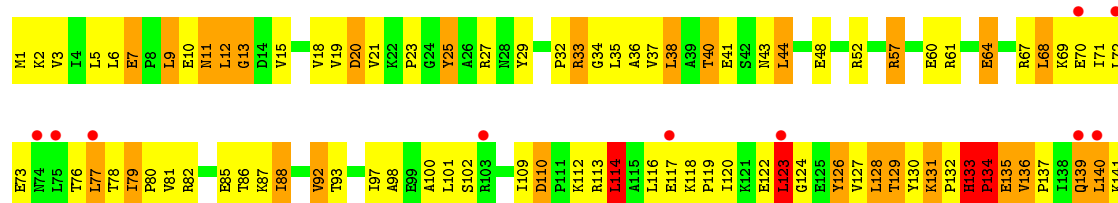
• Molecule 34: 50S ribosomal protein L6



• Molecule 34: 50S ribosomal protein L6

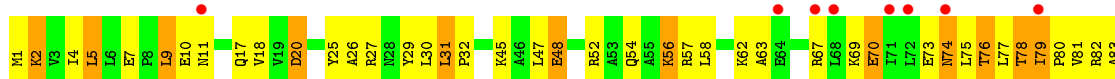


• Molecule 35: 50S ribosomal protein L9

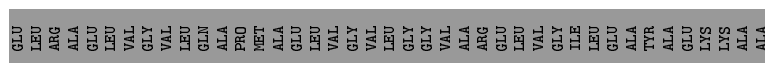
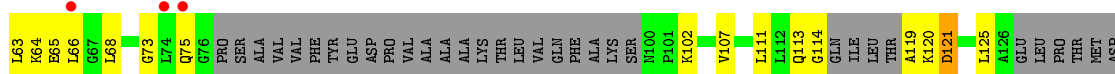
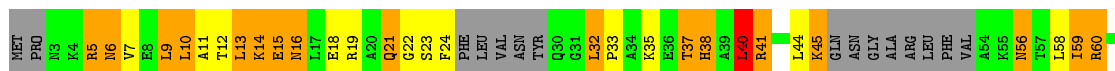
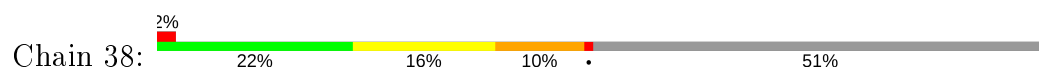




- Molecule 35: 50S ribosomal protein L9



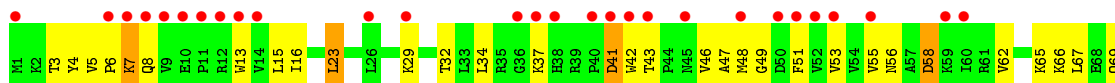
- Molecule 36: 50S ribosomal protein L10



- Molecule 37: 50S ribosomal protein L13

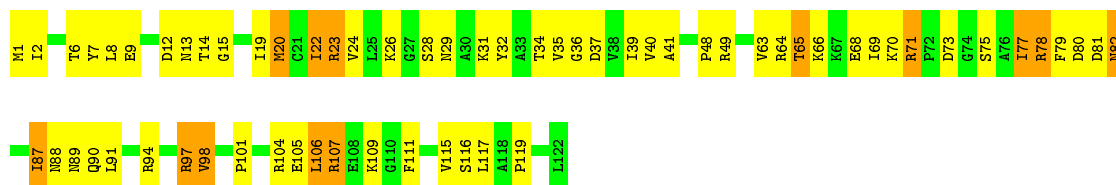


- Molecule 37: 50S ribosomal protein L13



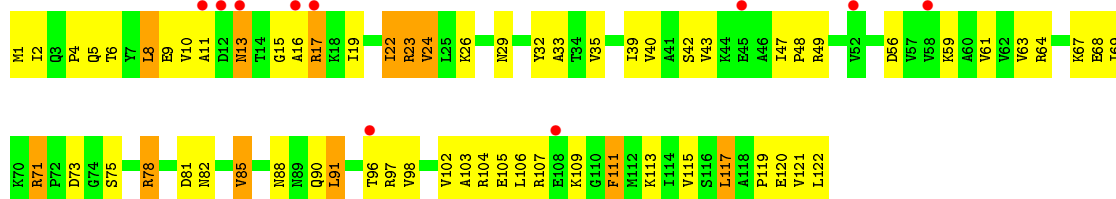
- Molecule 38: 50S ribosomal protein L14

Chain 68: 



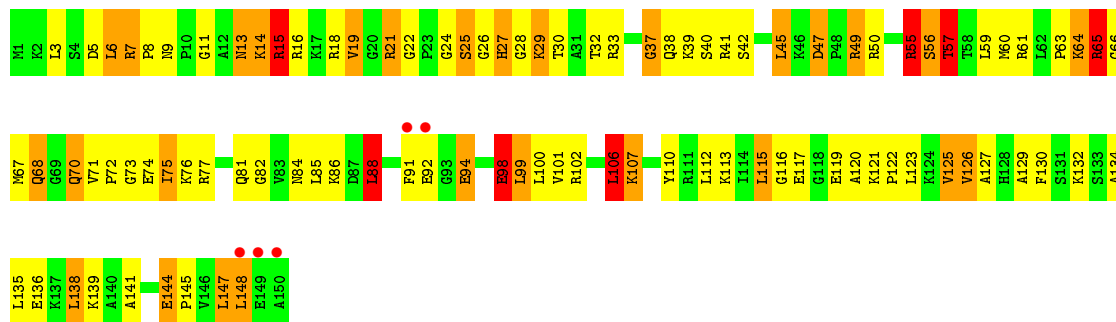
- Molecule 38: 50S ribosomal protein L14

Chain 25: 



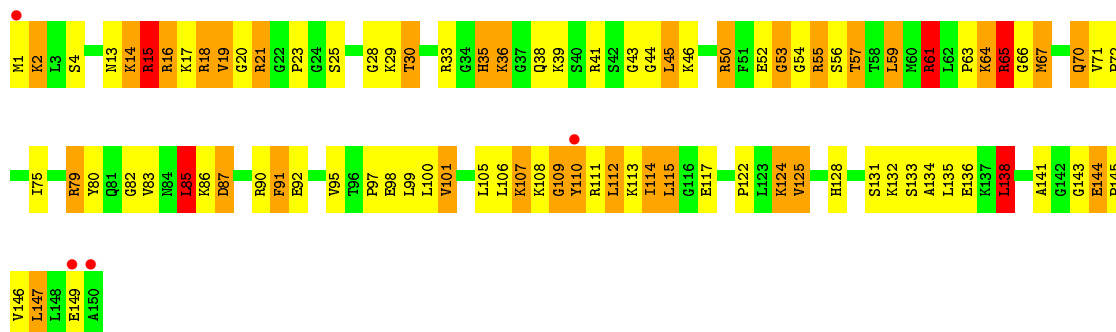
- Molecule 39: 50S ribosomal protein L15

Chain 78: 

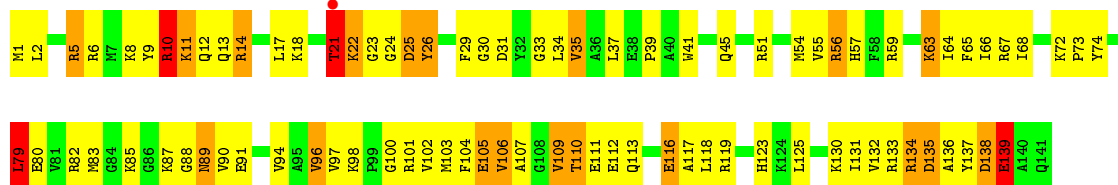


- Molecule 39: 50S ribosomal protein L15

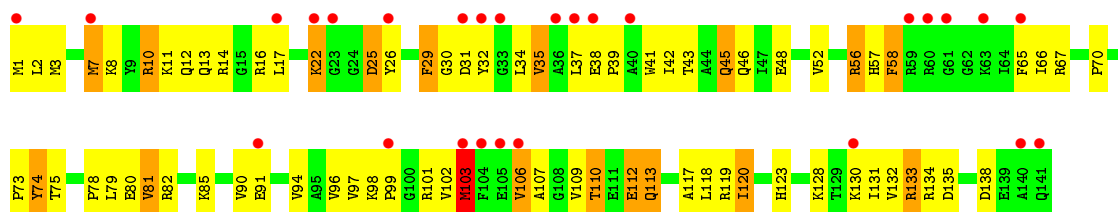
Chain 35: 



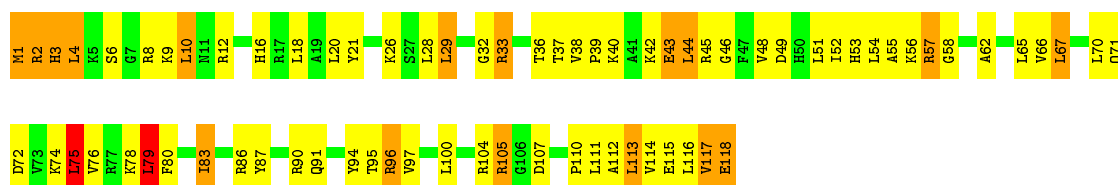
- Molecule 40: 50S ribosomal protein L16



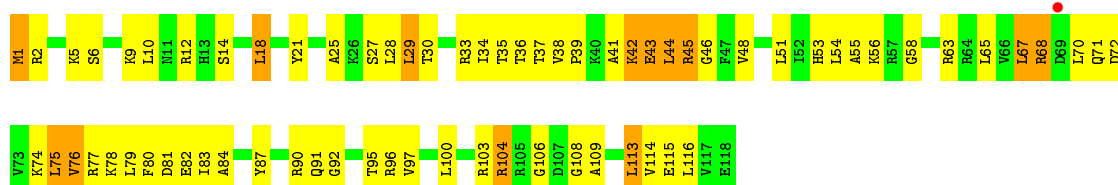
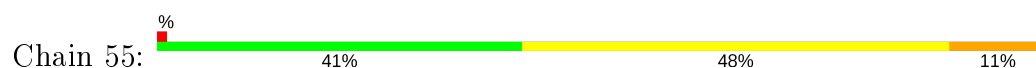
• Molecule 40: 50S ribosomal protein L16



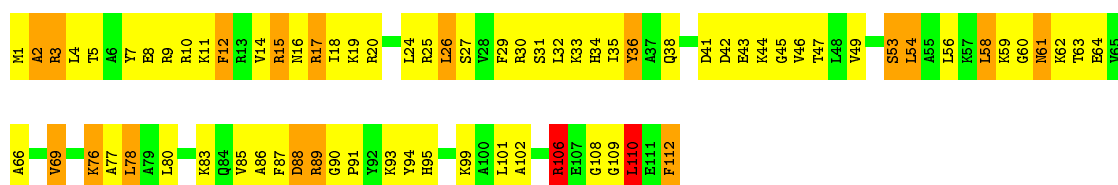
• Molecule 41: 50S ribosomal protein L17



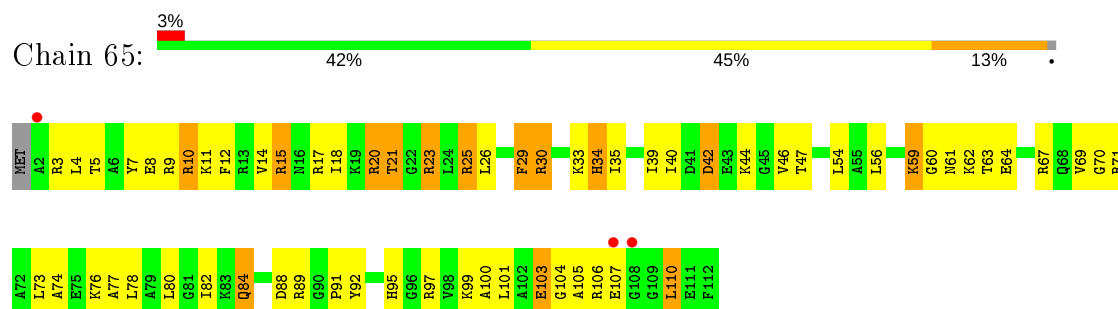
• Molecule 41: 50S ribosomal protein L17



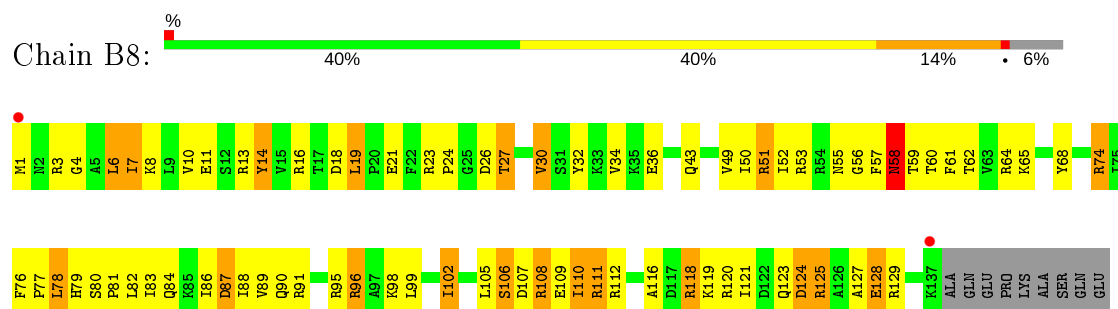
• Molecule 42: 50S ribosomal protein L18



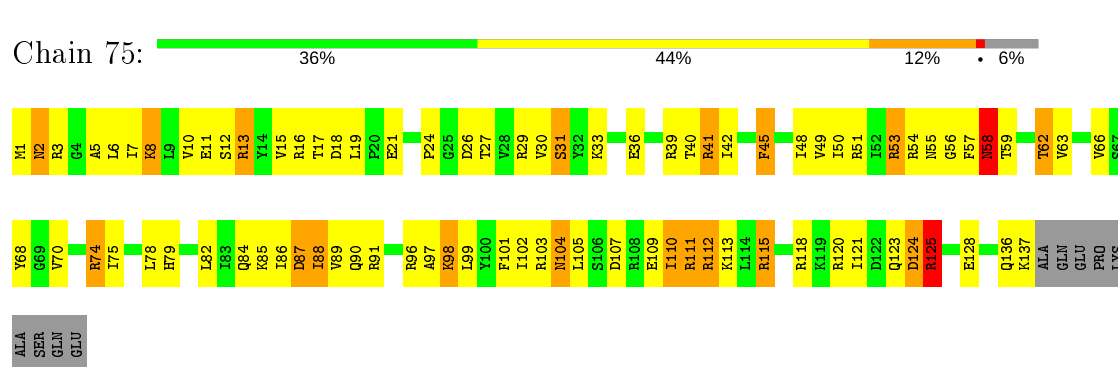
- Molecule 42: 50S ribosomal protein L18



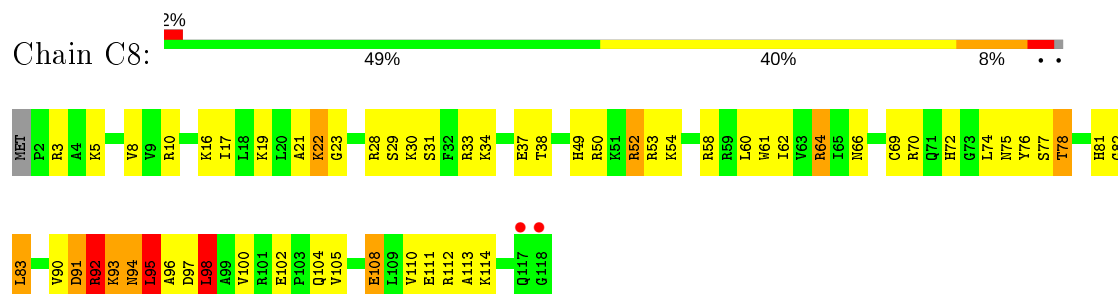
- Molecule 43: 50S ribosomal protein L19



- Molecule 43: 50S ribosomal protein L19

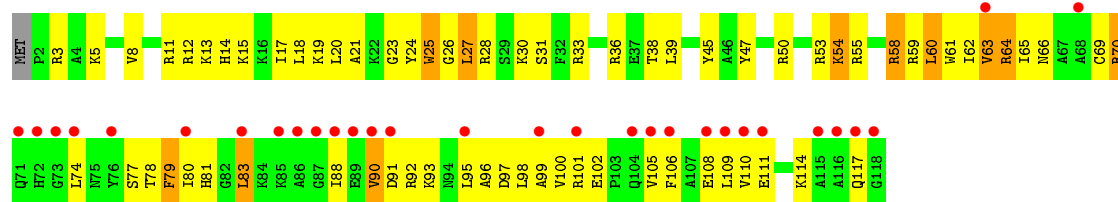


- Molecule 44: 50S ribosomal protein L20

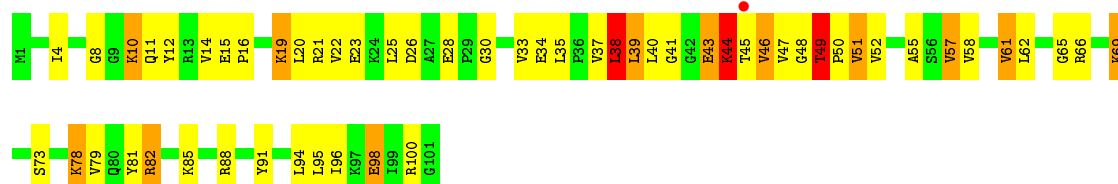


- Molecule 44: 50S ribosomal protein L20

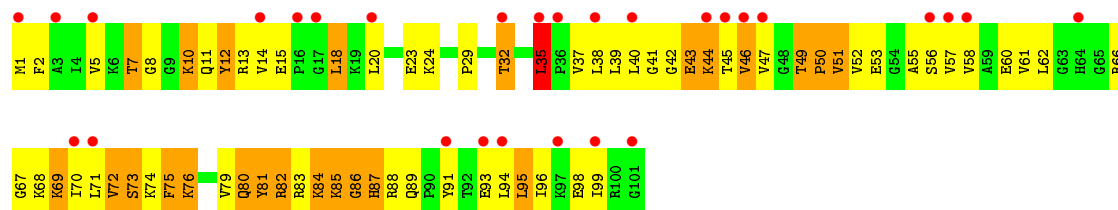




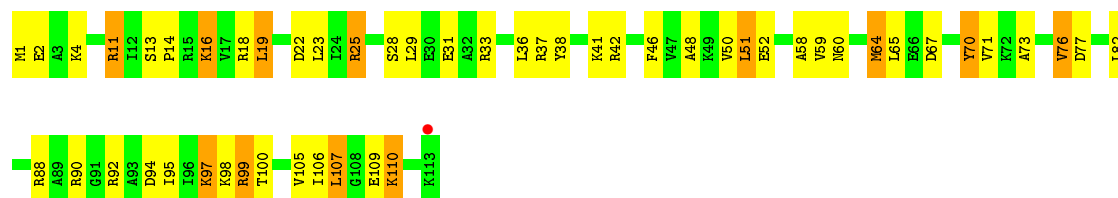
• Molecule 45: 50S ribosomal protein L21



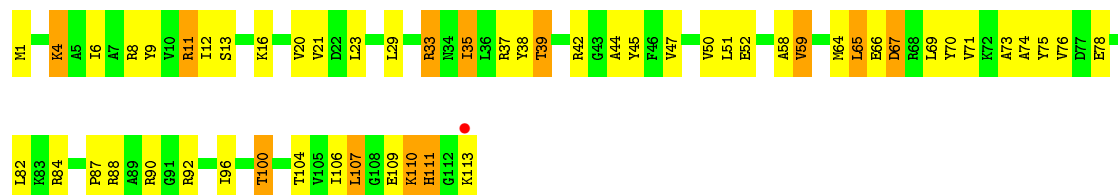
• Molecule 45: 50S ribosomal protein L21



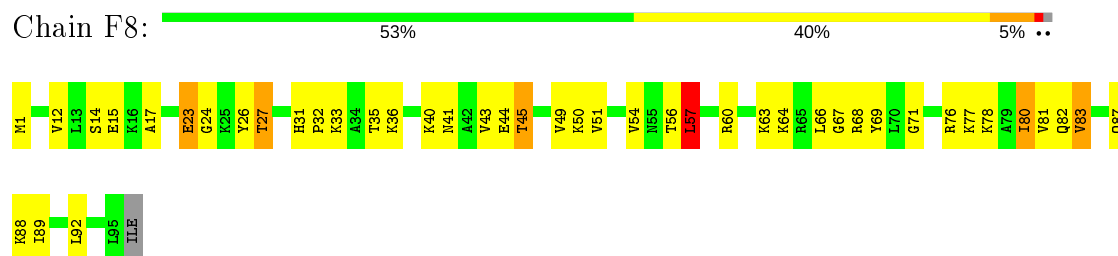
• Molecule 46: 50S ribosomal protein L22



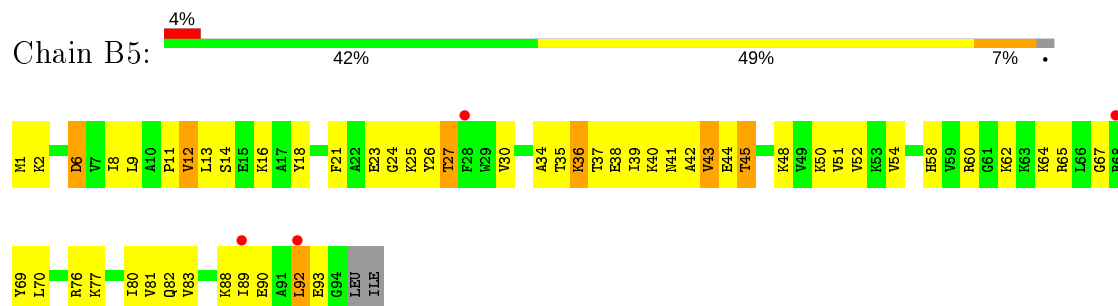
• Molecule 46: 50S ribosomal protein L22



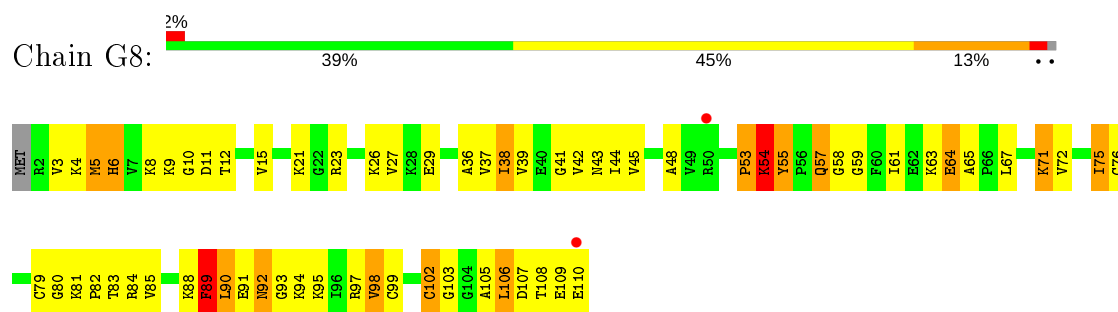
- Molecule 47: 50S ribosomal protein L23



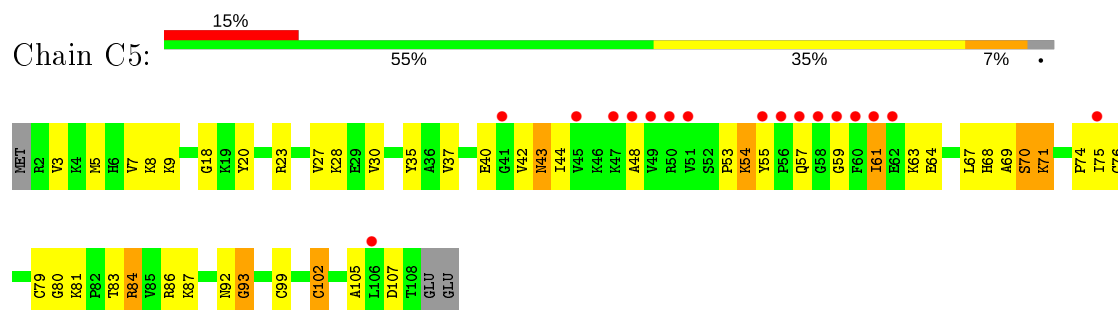
- Molecule 47: 50S ribosomal protein L23



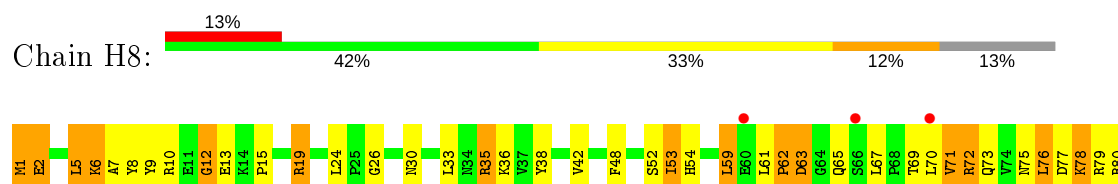
- Molecule 48: 50S ribosomal protein L24

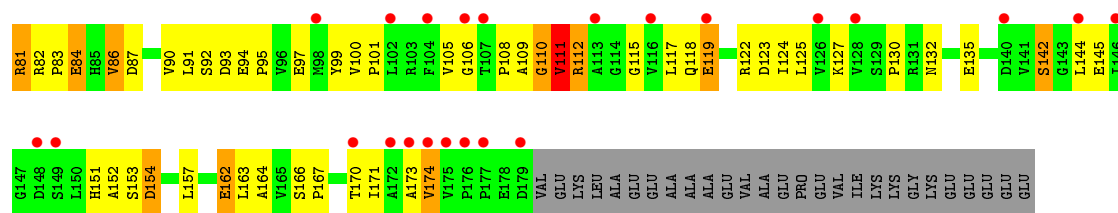


- Molecule 48: 50S ribosomal protein L24

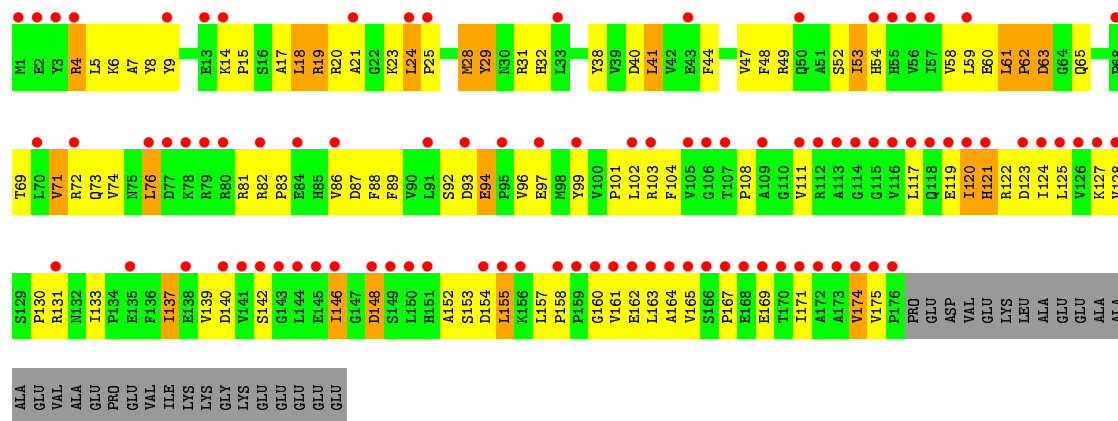
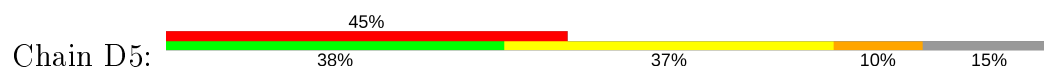


- Molecule 49: 50S ribosomal protein L25

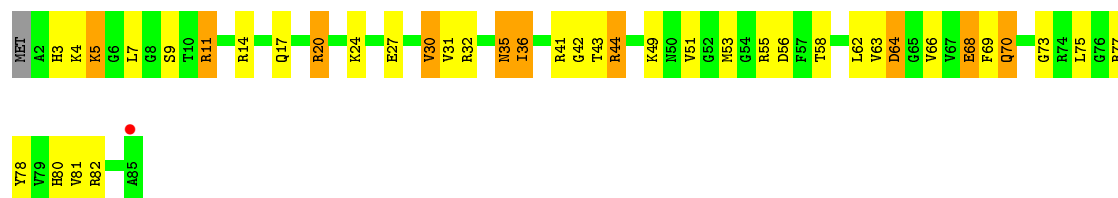




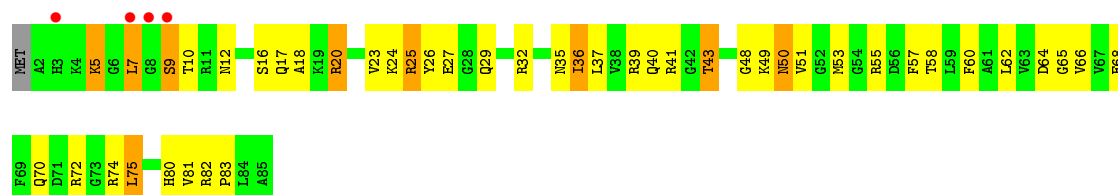
• Molecule 49: 50S ribosomal protein L25



• Molecule 50: 50S ribosomal protein L27

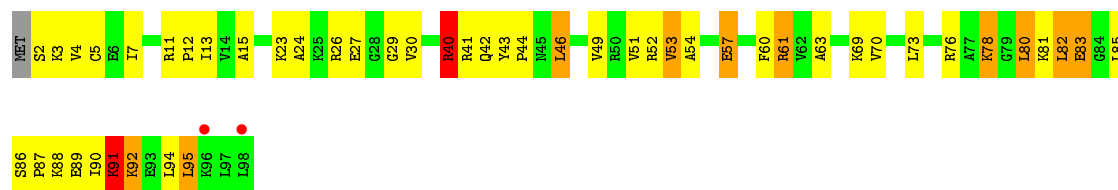


• Molecule 50: 50S ribosomal protein L27

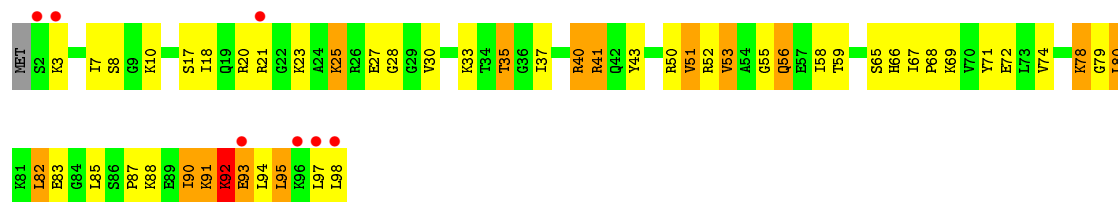


• Molecule 51: 50S ribosomal protein L28





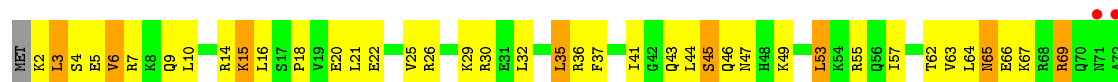
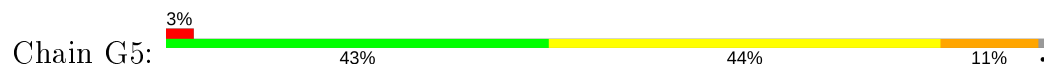
- Molecule 51: 50S ribosomal protein L28



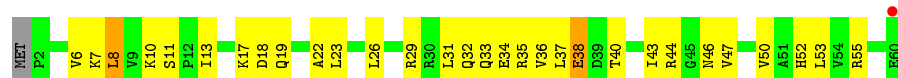
- Molecule 52: 50S ribosomal protein L29



- Molecule 52: 50S ribosomal protein L29



- Molecule 53: 50S ribosomal protein L30

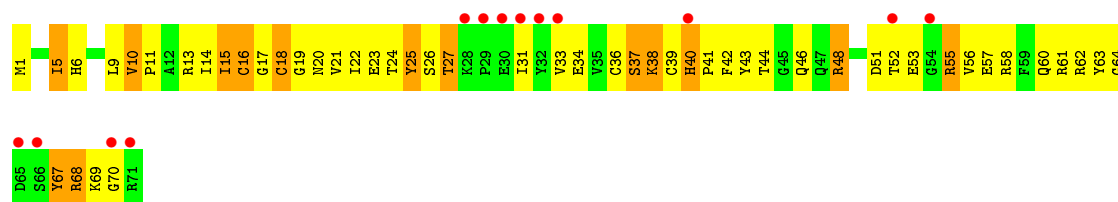


- Molecule 53: 50S ribosomal protein L30

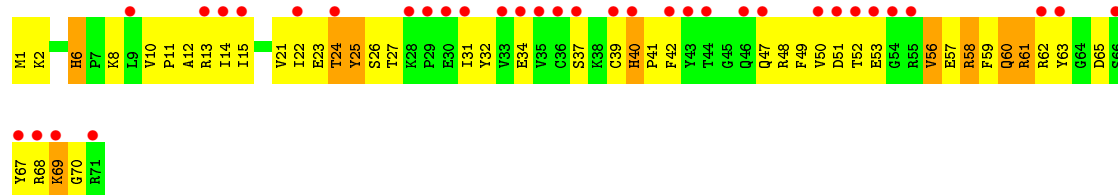


- Molecule 54: 50S ribosomal protein L31

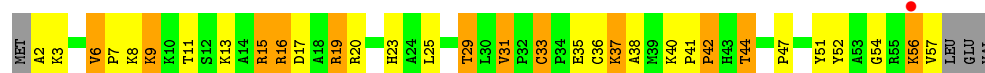




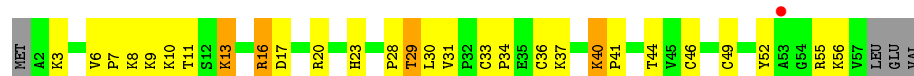
- Molecule 54: 50S ribosomal protein L31



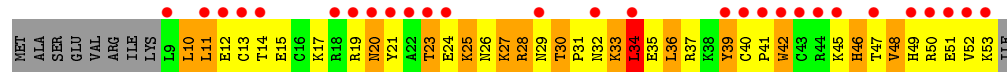
- Molecule 55: 50S ribosomal protein L32



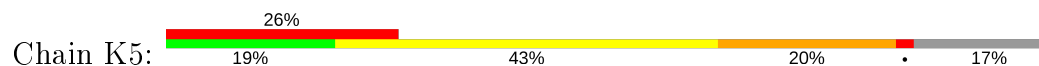
- Molecule 55: 50S ribosomal protein L32



- Molecule 56: 50S ribosomal protein L33



- Molecule 56: 50S ribosomal protein L33



- Molecule 57: 50S ribosomal protein L34

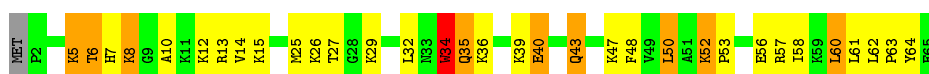




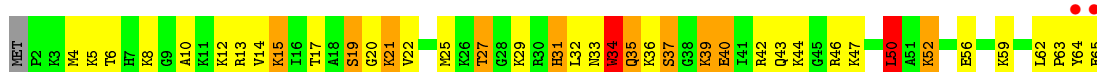
- Molecule 57: 50S ribosomal protein L34



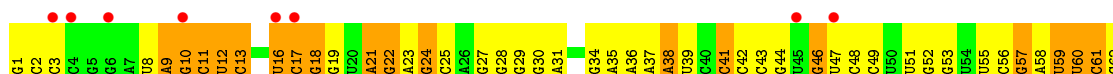
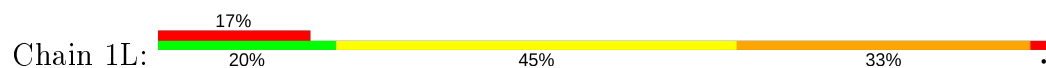
- Molecule 58: 50S ribosomal protein L35



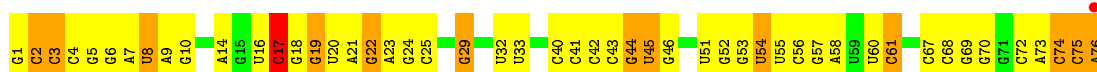
- Molecule 58: 50S ribosomal protein L35



- Molecule 59: E. coli tRNAPhe



- Molecule 60: E. coli tRNAPhe



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 – 3.00	Depositor EDS
% Data completeness (in resolution range)	99.7 (223.10-3.10) 99.8 (223.10-3.00)	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 0.196 , 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)	0.27 , 67.8	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: MA6, MIA, SF4, 0TD, 2MA, 2MG, 3AU, UR3, M2G, 7MG, 5MU, ZN, 5MC, K, OMC, MG, OMG, H2U, OMU, 4OC, 4SU, PSU

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	13	0.79	8/36175 (0.0%)	1.40	445/56452 (0.8%)
1	1G	0.69	1/36106 (0.0%)	1.30	264/56346 (0.5%)
2	12	0.36	0/1959	0.61	1/2642 (0.0%)
2	1E	0.38	0/1959	0.59	1/2642 (0.0%)
3	22	0.37	0/1636	0.60	0/2205
3	2E	0.44	0/1629	0.61	0/2195
4	32	0.48	0/1732	0.62	1/2318 (0.0%)
4	3E	0.49	0/1732	0.64	0/2318
5	42	0.46	0/1171	0.64	0/1576
5	4E	0.54	1/1171 (0.1%)	0.64	0/1576
6	52	0.47	0/855	0.65	0/1154
6	5E	0.49	0/855	0.62	0/1154
7	62	0.43	0/1275	0.54	0/1709
7	6E	0.47	0/1275	0.57	0/1709
8	72	0.39	0/1135	0.62	0/1527
8	7E	0.49	0/1135	0.67	0/1527
9	82	0.36	0/1022	0.56	0/1371
9	8E	0.44	0/1022	0.58	0/1371
10	1A	0.41	0/814	0.63	0/1095
10	1I	0.43	0/814	0.64	0/1095
11	2A	0.42	0/888	0.58	0/1198
11	2I	0.48	0/879	0.62	0/1187
12	3A	0.50	0/982	0.71	1/1313 (0.1%)
12	3I	0.61	0/982	0.80	1/1313 (0.1%)
13	4A	0.38	0/974	0.59	0/1303
13	4I	0.44	0/956	0.65	0/1281
14	5A	0.43	0/500	0.65	0/664
14	5I	0.51	0/500	0.66	0/664
15	6A	0.44	0/744	0.56	0/992
15	6I	0.49	0/744	0.65	0/992
16	7A	0.50	0/721	0.63	0/970

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

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

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

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

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

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

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

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

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

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

There are no chirality outliers.

5 of 105 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	2E	11	ARG	Peptide
12	3I	101	VAL	Peptide
12	3I	115	SER	Peptide
12	3I	44	LYS	Peptide
5	4E	20	GLN	Peptide

5.2 Too-close contacts ⓘ

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

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

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

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

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

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

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

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 19.

The worst 5 of 9273 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:14:1780:A:OP1	65:14:3511:HOH:O	1.75	1.02
27:14:676:A:H8	27:14:2069:G:H21	1.08	1.02
27:1H:1066:U:HO2'	27:1H:1068:A:H2	1.07	1.00
27:14:249:C:OP1	65:14:3512:HOH:O	1.80	1.00
1:13:1422:G:H5''	38:68:48:PRO:HB3	1.43	0.99

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

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:5K:75:C:O2'	27:1H:100:G:O6[1_455]	1.97	0.23

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	12	235/256 (92%)	188 (80%)	45 (19%)	2 (1%)	17	52
2	1E	235/256 (92%)	176 (75%)	58 (25%)	1 (0%)	34	69
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%)	22	57
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%)	19	54
9	8E	125/128 (98%)	106 (85%)	18 (14%)	1 (1%)	19	54
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%)	3	16
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%)	17	52
14	5A	58/61 (95%)	44 (76%)	13 (22%)	1 (2%)	9	36

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
14	5I	58/61 (95%)	46 (79%)	11 (19%)	1 (2%)	9	36
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%)	13	44
20	BA	101/106 (95%)	80 (79%)	20 (20%)	1 (1%)	15	49
20	BI	99/106 (93%)	81 (82%)	17 (17%)	1 (1%)	15	49
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%)	8	33
30	19	270/276 (98%)	237 (88%)	29 (11%)	4 (2%)	10	39
31	21	202/206 (98%)	185 (92%)	16 (8%)	1 (0%)	29	64
31	29	202/206 (98%)	171 (85%)	31 (15%)	0	100	100
32	31	200/210 (95%)	177 (88%)	20 (10%)	3 (2%)	10	39
32	39	200/210 (95%)	168 (84%)	30 (15%)	2 (1%)	15	49
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%)	13	44
34	59	171/180 (95%)	122 (71%)	48 (28%)	1 (1%)	25	59
35	61	143/148 (97%)	105 (73%)	34 (24%)	4 (3%)	5	25
35	69	144/148 (97%)	109 (76%)	35 (24%)	0	100	100
36	38	74/173 (43%)	43 (58%)	29 (39%)	2 (3%)	5	25
37	15	136/140 (97%)	113 (83%)	22 (16%)	1 (1%)	22	57

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
37	58	136/140 (97%)	108 (79%)	25 (18%)	3 (2%)	6	29
38	25	120/122 (98%)	107 (89%)	13 (11%)	0	100	100
38	68	120/122 (98%)	106 (88%)	13 (11%)	1 (1%)	19	54
39	35	148/150 (99%)	104 (70%)	38 (26%)	6 (4%)	3	16
39	78	148/150 (99%)	113 (76%)	29 (20%)	6 (4%)	3	16
40	45	139/141 (99%)	105 (76%)	32 (23%)	2 (1%)	11	40
40	88	144/141 (102%)	109 (76%)	30 (21%)	5 (4%)	3	20
41	55	116/118 (98%)	98 (84%)	17 (15%)	1 (1%)	17	52
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%)	8	34
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%)	9	36
45	95	99/101 (98%)	70 (71%)	26 (26%)	3 (3%)	4	23
45	D8	99/101 (98%)	82 (83%)	15 (15%)	2 (2%)	7	31
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%)	8	33
48	G8	107/110 (97%)	80 (75%)	22 (21%)	5 (5%)	2	14
49	D5	174/206 (84%)	125 (72%)	47 (27%)	2 (1%)	14	46
49	H8	177/206 (86%)	127 (72%)	48 (27%)	2 (1%)	14	46
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%)	14	46
51	J8	95/98 (97%)	74 (78%)	20 (21%)	1 (1%)	14	46
52	G5	69/72 (96%)	60 (87%)	8 (12%)	1 (1%)	11	40
52	K8	70/72 (97%)	61 (87%)	8 (11%)	1 (1%)	11	40

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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%)	4	24
54	M8	69/71 (97%)	38 (55%)	28 (41%)	3 (4%)	2	16
55	J5	54/60 (90%)	45 (83%)	8 (15%)	1 (2%)	8	33
55	N8	54/60 (90%)	44 (82%)	9 (17%)	1 (2%)	8	33
56	K5	43/54 (80%)	22 (51%)	21 (49%)	0	100	100
56	O8	43/54 (80%)	28 (65%)	13 (30%)	2 (5%)	2	14
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%)	19	54

5 of 99 Ramachandran outliers are listed below:

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

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	12	205/220 (93%)	156 (76%)	49 (24%)	0	2
2	1E	205/220 (93%)	162 (79%)	43 (21%)	1	5
3	22	160/188 (85%)	124 (78%)	36 (22%)	1	3
3	2E	159/188 (85%)	122 (77%)	37 (23%)	1	3

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	32	180/181 (99%)	146 (81%)	34 (19%)	1	6
4	3E	180/181 (99%)	141 (78%)	39 (22%)	1	4
5	42	116/123 (94%)	96 (83%)	20 (17%)	2	9
5	4E	116/123 (94%)	95 (82%)	21 (18%)	1	7
6	52	90/90 (100%)	76 (84%)	14 (16%)	2	11
6	5E	90/90 (100%)	76 (84%)	14 (16%)	2	11
7	62	126/127 (99%)	105 (83%)	21 (17%)	2	9
7	6E	126/127 (99%)	99 (79%)	27 (21%)	1	4
8	72	119/119 (100%)	98 (82%)	21 (18%)	2	8
8	7E	119/119 (100%)	101 (85%)	18 (15%)	3	12
9	82	97/99 (98%)	67 (69%)	30 (31%)	0	0
9	8E	97/99 (98%)	73 (75%)	24 (25%)	0	2
10	1A	89/92 (97%)	69 (78%)	20 (22%)	1	3
10	1I	89/92 (97%)	68 (76%)	21 (24%)	1	2
11	2A	89/99 (90%)	69 (78%)	20 (22%)	1	3
11	2I	88/99 (89%)	74 (84%)	14 (16%)	2	11
12	3A	103/108 (95%)	77 (75%)	26 (25%)	0	1
12	3I	103/108 (95%)	83 (81%)	20 (19%)	1	6
13	4A	97/101 (96%)	77 (79%)	20 (21%)	1	5
13	4I	95/101 (94%)	70 (74%)	25 (26%)	0	1
14	5A	49/50 (98%)	35 (71%)	14 (29%)	0	1
14	5I	49/50 (98%)	37 (76%)	12 (24%)	0	2
15	6A	79/80 (99%)	73 (92%)	6 (8%)	13	41
15	6I	79/80 (99%)	64 (81%)	15 (19%)	1	6
16	7A	72/74 (97%)	59 (82%)	13 (18%)	1	7
16	7I	72/74 (97%)	58 (81%)	14 (19%)	1	6
17	8A	95/97 (98%)	80 (84%)	15 (16%)	2	11
17	8I	95/97 (98%)	83 (87%)	12 (13%)	4	18
18	9A	61/77 (79%)	47 (77%)	14 (23%)	1	3
18	9I	62/77 (80%)	47 (76%)	15 (24%)	0	2
19	AA	73/80 (91%)	50 (68%)	23 (32%)	0	0

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
19	AI	73/80 (91%)	52 (71%)	21 (29%)	0	1
20	BA	75/82 (92%)	65 (87%)	10 (13%)	4	16
20	BI	75/82 (92%)	63 (84%)	12 (16%)	2	11
21	1B	20/22 (91%)	17 (85%)	3 (15%)	3	12
21	1F	19/22 (86%)	17 (90%)	2 (10%)	7	26
29	71	111/181 (61%)	95 (86%)	16 (14%)	3	14
29	79	111/181 (61%)	97 (87%)	14 (13%)	4	18
30	11	214/218 (98%)	171 (80%)	43 (20%)	1	5
30	19	214/218 (98%)	172 (80%)	42 (20%)	1	6
31	21	164/166 (99%)	133 (81%)	31 (19%)	1	6
31	29	164/166 (99%)	132 (80%)	32 (20%)	1	6
32	31	161/166 (97%)	130 (81%)	31 (19%)	1	6
32	39	161/166 (97%)	130 (81%)	31 (19%)	1	6
33	41	155/156 (99%)	119 (77%)	36 (23%)	1	3
33	49	155/156 (99%)	114 (74%)	41 (26%)	0	1
34	51	145/148 (98%)	113 (78%)	32 (22%)	1	4
34	59	144/148 (97%)	115 (80%)	29 (20%)	1	5
35	61	122/124 (98%)	86 (70%)	36 (30%)	0	1
35	69	122/124 (98%)	88 (72%)	34 (28%)	0	1
36	38	66/135 (49%)	39 (59%)	27 (41%)	0	0
37	15	117/119 (98%)	94 (80%)	23 (20%)	1	6
37	58	117/119 (98%)	83 (71%)	34 (29%)	0	1
38	25	100/100 (100%)	79 (79%)	21 (21%)	1	5
38	68	100/100 (100%)	76 (76%)	24 (24%)	0	2
39	35	116/116 (100%)	71 (61%)	45 (39%)	0	0
39	78	116/116 (100%)	83 (72%)	33 (28%)	0	1
40	45	111/111 (100%)	88 (79%)	23 (21%)	1	5
40	88	113/111 (102%)	88 (78%)	25 (22%)	1	4
41	55	101/101 (100%)	80 (79%)	21 (21%)	1	5
41	98	101/101 (100%)	74 (73%)	27 (27%)	0	1
42	65	87/88 (99%)	68 (78%)	19 (22%)	1	4

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

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
58	M5	52/55 (94%)	42 (81%)	10 (19%)	1	6
58	Q8	52/55 (94%)	41 (79%)	11 (21%)	1	5
All	All	9889/10493 (94%)	7700 (78%)	2189 (22%)	1	4

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

Mol	Chain	Res	Type
49	H8	132	ASN
4	32	73	ARG
47	B5	62	LYS
51	J8	41	ARG
57	P8	41	ARG

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

Mol	Chain	Res	Type
4	32	123	HIS
18	9A	63	GLN
52	G5	46	GLN
10	1A	13	HIS
32	39	169	ASN

5.3.3 RNA ⓘ

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

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

5 of 2571 RNA backbone outliers are listed below:

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

5 of 262 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
27	1H	2042	A
1	1G	130	A
27	14	2210	G
27	1H	2190	U
27	1H	2579	A

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	OMG	14	2251	60,61,27	18,26,27	5.43	7 (38%)	20,38,41	5.29	7 (35%)
27	5MC	14	1962	61,27	15,22,23	2.90	5 (33%)	19,32,35	1.02	1 (5%)
59	PSU	1L	32	59	17,21,22	1.03	1 (5%)	20,30,33	3.49	6 (30%)
24	PSU	3K	39	24	17,21,22	1.02	1 (5%)	20,30,33	3.24	6 (30%)
23	4SU	2K	8	23	14,21,22	3.06	2 (14%)	15,30,33	1.18	2 (13%)
27	PSU	1H	2618	27	17,21,22	1.54	4 (23%)	20,30,33	3.34	8 (40%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
27	PSU	1H	1934	27	17,21,22	1.07	1 (5%)	20,30,33	3.00	6 (30%)
27	5MU	1H	1938	27	15,22,23	2.09	3 (20%)	16,32,35	1.46	2 (12%)
1	PSU	1G	516	1,62	17,21,22	1.13	1 (5%)	20,30,33	3.49	6 (30%)
1	2MG	13	1207	1,61	19,26,27	4.46	8 (42%)	21,38,41	2.62	6 (28%)
26	PSU	5K	39	26	17,21,22	1.11	1 (5%)	20,30,33	3.33	6 (30%)
27	OMG	1H	2264	61,27,23	18,26,27	5.32	6 (33%)	20,38,41	5.64	8 (40%)
22	PSU	1K	55	22	17,21,22	1.00	1 (5%)	20,30,33	3.25	8 (40%)
60	PSU	2L	32	60	17,21,22	1.27	3 (17%)	20,30,33	3.00	6 (30%)
23	H2U	2K	16	23	18,21,22	1.88	4 (22%)	21,30,33	1.90	5 (23%)
27	OMU	1H	2565	62,27	14,22,23	2.25	5 (35%)	14,31,34	0.88	1 (7%)
24	PSU	3L	39	24	17,21,22	1.05	1 (5%)	20,30,33	3.35	6 (30%)
23	H2U	2K	20	23	18,21,22	2.11	4 (22%)	21,30,33	1.98	4 (19%)
27	OMC	1H	1943	61,27	15,22,23	2.20	5 (33%)	17,31,34	1.60	3 (17%)
1	7MG	1G	527	1,61	22,26,27	3.44	6 (27%)	28,39,42	2.49	10 (35%)
1	MA6	1G	1518	1	19,26,27	1.14	2 (10%)	18,38,41	2.56	2 (11%)
27	5MU	1H	1962	61,27	15,22,23	1.99	3 (20%)	16,32,35	2.54	3 (18%)
23	PSU	2K	55	23	17,21,22	0.97	2 (11%)	20,30,33	3.18	5 (25%)
22	PSU	1K	32	61,22	17,21,22	0.97	1 (5%)	20,30,33	3.68	5 (25%)
59	PSU	1L	39	59	17,21,22	1.39	3 (17%)	20,30,33	3.11	7 (35%)
1	5MC	1G	1400	1	15,22,23	3.38	5 (33%)	19,32,35	1.44	3 (15%)
26	PSU	5K	55	26	17,21,22	1.07	1 (5%)	20,30,33	3.24	6 (30%)
27	5MU	14	1915	27	15,22,23	2.19	3 (20%)	16,32,35	1.99	3 (18%)
12	0TD	3I	89	12	4,9,10	1.40	0	3,11,13	3.44	1 (33%)
23	3AU	2K	47	23	14,28,29	3.10	4 (28%)	15,40,43	1.07	1 (6%)
27	5MC	14	1942	27	15,22,23	3.19	5 (33%)	19,32,35	1.40	3 (15%)
27	2MA	14	2503	61,62,27	17,25,26	3.08	5 (29%)	19,37,40	1.95	4 (21%)
22	5MU	1K	54	22	15,22,23	2.14	3 (20%)	16,32,35	1.74	2 (12%)
26	5MU	5K	54	26	15,22,23	2.16	3 (20%)	16,32,35	1.73	2 (12%)
27	PSU	14	1917	27	17,21,22	1.22	2 (11%)	20,30,33	3.49	6 (30%)
27	5MC	1H	1985	61,27	15,22,23	3.14	5 (33%)	19,32,35	1.78	4 (21%)
27	PSU	14	1911	27	17,21,22	1.04	1 (5%)	20,30,33	3.34	5 (25%)
24	PSU	3K	32	24	17,21,22	0.94	1 (5%)	20,30,33	3.28	6 (30%)
26	MIA	5K	37	26	24,31,32	2.56	4 (16%)	26,44,47	3.34	11 (42%)
60	4SU	2L	8	60	14,21,22	3.20	2 (14%)	15,30,33	1.32	2 (13%)
27	5MU	14	1939	61,27	15,22,23	2.07	3 (20%)	16,32,35	1.98	2 (12%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	5MC	1G	1404	1	15,22,23	2.97	5 (33%)	19,32,35	1.24	1 (5%)
22	7MG	1K	46	22	22,26,27	3.42	6 (27%)	28,39,42	2.44	10 (35%)
26	H2U	5K	20	26,28	18,21,22	2.32	4 (22%)	21,30,33	1.88	5 (23%)
26	PSU	5K	32	26	17,21,22	1.12	2 (11%)	20,30,33	3.36	6 (30%)
1	MA6	13	1519	1	19,26,27	0.95	1 (5%)	18,38,41	3.24	3 (16%)
26	4SU	5K	8	26	14,21,22	3.11	2 (14%)	15,30,33	1.19	2 (13%)
60	PSU	2L	39	60	17,21,22	0.98	1 (5%)	20,30,33	3.21	7 (35%)
60	7MG	2L	46	60	22,26,27	3.46	7 (31%)	28,39,42	2.53	13 (46%)
23	PSU	2K	32	23	17,21,22	1.23	3 (17%)	20,30,33	3.08	7 (35%)
1	5MC	1G	967	1	15,22,23	3.15	5 (33%)	19,32,35	1.36	3 (15%)
1	5MC	1G	1407	1	15,22,23	2.92	5 (33%)	19,32,35	1.39	2 (10%)
1	7MG	13	527	1,61	22,26,27	3.46	7 (31%)	28,39,42	2.58	11 (39%)
1	5MC	13	1400	1	15,22,23	3.24	5 (33%)	19,32,35	1.43	3 (15%)
1	PSU	13	516	1,62	17,21,22	0.95	1 (5%)	20,30,33	3.27	5 (25%)
1	M2G	1G	966	1	20,27,28	4.14	6 (30%)	22,40,43	1.58	6 (27%)
22	PSU	1K	39	22	17,21,22	1.17	2 (11%)	20,30,33	3.04	6 (30%)
1	MA6	1G	1519	1	19,26,27	1.08	2 (10%)	18,38,41	2.87	2 (11%)
24	PSU	3L	32	24	17,21,22	1.18	2 (11%)	20,30,33	3.43	7 (35%)
27	2MA	1H	2516	61,27	17,25,26	2.80	6 (35%)	19,37,40	2.33	6 (31%)
27	OMC	14	1920	27	15,22,23	2.23	4 (26%)	17,31,34	1.20	2 (11%)
22	4SU	1K	8	22	14,21,22	3.20	2 (14%)	15,30,33	1.28	2 (13%)
24	MIA	3K	37	24,25	24,31,32	2.51	4 (16%)	26,44,47	3.26	11 (42%)
23	7MG	2K	46	23	22,26,27	3.54	6 (27%)	28,39,42	2.46	10 (35%)
1	M2G	13	966	1	20,27,28	3.79	7 (35%)	22,40,43	1.74	7 (31%)
27	5MC	1H	1965	27	15,22,23	2.84	5 (33%)	19,32,35	1.47	3 (15%)
12	0TD	3A	89	1,12	4,9,10	1.27	0	3,11,13	1.43	1 (33%)
23	MIA	2K	37	23	24,31,32	2.37	4 (16%)	26,44,47	2.56	10 (38%)
1	4OC	1G	1402	1,62	16,23,24	2.77	6 (37%)	17,32,35	2.46	1 (5%)
60	5MU	2L	54	60	15,22,23	2.13	3 (20%)	16,32,35	1.73	2 (12%)
1	UR3	13	1498	1	14,22,23	2.56	3 (21%)	15,32,35	1.27	3 (20%)
27	OMU	14	2552	62,27	14,22,23	2.72	5 (35%)	14,31,34	0.93	1 (7%)
24	MIA	3L	37	24	24,31,32	2.55	4 (16%)	26,44,47	3.40	11 (42%)
23	5MU	2K	54	23	15,22,23	2.08	3 (20%)	16,32,35	1.89	2 (12%)
60	H2U	2L	16	60	18,21,22	2.10	4 (22%)	21,30,33	1.94	5 (23%)
59	5MU	1L	54	59	15,22,23	2.13	3 (20%)	16,32,35	1.69	2 (12%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	5MC	13	1407	1	15,22,23	2.81	5 (33%)	19,32,35	1.42	4 (21%)
1	5MC	13	967	1	15,22,23	3.28	5 (33%)	19,32,35	1.47	4 (21%)
23	PSU	2K	39	23	17,21,22	1.20	3 (17%)	20,30,33	3.03	6 (30%)
27	PSU	14	2605	27	17,21,22	1.28	3 (17%)	20,30,33	3.32	8 (40%)
59	MIA	1L	37	59	24,31,32	2.29	3 (12%)	26,44,47	3.02	9 (34%)
1	2MG	1G	1207	1	19,26,27	4.77	7 (36%)	21,38,41	2.18	7 (33%)
26	H2U	5K	16	26	18,21,22	2.15	4 (22%)	21,30,33	1.97	5 (23%)
1	5MC	13	1404	1	15,22,23	2.63	5 (33%)	19,32,35	1.57	3 (15%)
22	MIA	1K	37	22	24,31,32	2.23	3 (12%)	26,44,47	3.01	8 (30%)
60	MIA	2L	37	60	24,31,32	2.30	3 (12%)	26,44,47	2.80	8 (30%)
1	MA6	13	1518	1	19,26,27	0.95	0	18,38,41	2.75	2 (11%)
1	4OC	13	1402	1,62	16,23,24	3.01	6 (37%)	17,32,35	1.34	1 (5%)
60	3AU	2L	47	60	14,28,29	2.92	4 (28%)	15,40,43	0.92	1 (6%)
60	PSU	2L	55	60	17,21,22	1.12	1 (5%)	20,30,33	3.46	6 (30%)
1	UR3	1G	1498	1	14,22,23	2.64	4 (28%)	15,32,35	1.11	1 (6%)
27	PSU	1H	1940	27	17,21,22	1.55	3 (17%)	20,30,33	3.69	6 (30%)

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	OMG	14	2251	60,61,27	-	0/5/27/28	0/3/3/3
27	5MC	14	1962	61,27	-	2/5/25/26	0/2/2/2
59	PSU	1L	32	59	-	0/7/25/26	0/2/2/2
24	PSU	3K	39	24	-	0/7/25/26	0/2/2/2
23	4SU	2K	8	23	-	0/5/25/26	0/2/2/2
27	PSU	1H	2618	27	-	0/7/25/26	0/2/2/2
27	PSU	1H	1934	27	-	0/7/25/26	0/2/2/2
27	5MU	1H	1938	27	-	3/5/25/26	0/2/2/2
1	PSU	1G	516	1,62	-	0/7/25/26	0/2/2/2
1	2MG	13	1207	1,61	-	0/5/27/28	0/3/3/3
26	PSU	5K	39	26	-	0/7/25/26	0/2/2/2
27	OMG	1H	2264	61,27,23	-	0/5/27/28	0/3/3/3
22	PSU	1K	55	22	-	2/7/25/26	0/2/2/2
60	PSU	2L	32	60	-	0/7/25/26	0/2/2/2
23	H2U	2K	16	23	-	0/7/38/39	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
27	OMU	1H	2565	62,27	-	0/7/27/28	0/2/2/2
24	PSU	3L	39	24	-	0/7/25/26	0/2/2/2
23	H2U	2K	20	23	-	5/7/38/39	0/2/2/2
27	OMC	1H	1943	61,27	-	0/7/27/28	0/2/2/2
1	7MG	1G	527	1,61	-	2/7/37/38	0/3/3/3
1	MA6	1G	1518	1	-	5/7/29/30	0/3/3/3
27	5MU	1H	1962	61,27	-	4/5/25/26	0/2/2/2
23	PSU	2K	55	23	-	3/7/25/26	0/2/2/2
22	PSU	1K	32	61,22	-	0/7/25/26	0/2/2/2
59	PSU	1L	39	59	-	0/7/25/26	0/2/2/2
1	5MC	1G	1400	1	-	2/5/25/26	0/2/2/2
26	PSU	5K	55	26	-	3/7/25/26	0/2/2/2
27	5MU	14	1915	27	-	0/5/25/26	0/2/2/2
12	0TD	3I	89	12	-	1/3/12/14	-
23	3AU	2K	47	23	-	7/10/34/35	0/2/2/2
27	5MC	14	1942	27	-	0/5/25/26	0/2/2/2
27	2MA	14	2503	61,62,27	-	1/3/25/26	0/3/3/3
22	5MU	1K	54	22	-	0/5/25/26	0/2/2/2
26	5MU	5K	54	26	-	2/5/25/26	0/2/2/2
27	PSU	14	1917	27	-	0/7/25/26	0/2/2/2
27	5MC	1H	1985	61,27	-	2/5/25/26	0/2/2/2
27	PSU	14	1911	27	-	0/7/25/26	0/2/2/2
24	PSU	3K	32	24	-	2/7/25/26	0/2/2/2
26	MIA	5K	37	26	-	6/11/33/34	0/3/3/3
60	4SU	2L	8	60	-	2/5/25/26	0/2/2/2
27	5MU	14	1939	61,27	-	2/5/25/26	0/2/2/2
1	5MC	1G	1404	1	-	0/5/25/26	0/2/2/2
22	7MG	1K	46	22	-	2/7/37/38	0/3/3/3
26	H2U	5K	20	26,28	-	5/7/38/39	0/2/2/2
26	PSU	5K	32	26	-	0/7/25/26	0/2/2/2
1	MA6	13	1519	1	-	3/7/29/30	0/3/3/3
26	4SU	5K	8	26	-	2/5/25/26	0/2/2/2
60	PSU	2L	39	60	-	0/7/25/26	0/2/2/2
60	7MG	2L	46	60	-	2/7/37/38	0/3/3/3
23	PSU	2K	32	23	-	0/7/25/26	0/2/2/2
1	5MC	1G	967	1	-	0/5/25/26	0/2/2/2
1	5MC	1G	1407	1	-	0/5/25/26	0/2/2/2
1	7MG	13	527	1,61	-	2/7/37/38	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	5MC	13	1400	1	-	0/5/25/26	0/2/2/2
1	PSU	13	516	1,62	-	0/7/25/26	0/2/2/2
1	M2G	1G	966	1	-	0/7/29/30	0/3/3/3
22	PSU	1K	39	22	-	0/7/25/26	0/2/2/2
1	MA6	1G	1519	1	-	2/7/29/30	0/3/3/3
24	PSU	3L	32	24	-	3/7/25/26	0/2/2/2
27	2MA	1H	2516	61,27	-	1/3/25/26	0/3/3/3
27	OMC	14	1920	27	-	1/7/27/28	0/2/2/2
22	4SU	1K	8	22	-	1/5/25/26	0/2/2/2
24	MIA	3K	37	24,25	-	8/11/33/34	0/3/3/3
23	7MG	2K	46	23	-	0/7/37/38	0/3/3/3
1	M2G	13	966	1	-	0/7/29/30	0/3/3/3
27	5MC	1H	1965	27	-	0/5/25/26	0/2/2/2
12	0TD	3A	89	1,12	-	2/3/12/14	-
23	MIA	2K	37	23	-	3/11/33/34	0/3/3/3
1	4OC	1G	1402	1,62	-	2/9/29/30	0/2/2/2
60	5MU	2L	54	60	-	2/5/25/26	0/2/2/2
1	UR3	13	1498	1	-	2/5/25/26	0/2/2/2
27	OMU	14	2552	62,27	-	4/7/27/28	0/2/2/2
24	MIA	3L	37	24	-	4/11/33/34	0/3/3/3
23	5MU	2K	54	23	-	0/5/25/26	0/2/2/2
60	H2U	2L	16	60	-	0/7/38/39	0/2/2/2
59	5MU	1L	54	59	-	0/5/25/26	0/2/2/2
1	5MC	13	1407	1	-	0/5/25/26	0/2/2/2
1	5MC	13	967	1	-	0/5/25/26	0/2/2/2
23	PSU	2K	39	23	-	0/7/25/26	0/2/2/2
27	PSU	14	2605	27	-	0/7/25/26	0/2/2/2
59	MIA	1L	37	59	-	2/11/33/34	0/3/3/3
1	2MG	1G	1207	1	-	2/5/27/28	0/3/3/3
26	H2U	5K	16	26	-	3/7/38/39	0/2/2/2
1	5MC	13	1404	1	-	0/5/25/26	0/2/2/2
22	MIA	1K	37	22	-	4/11/33/34	0/3/3/3
60	MIA	2L	37	60	-	4/11/33/34	0/3/3/3
1	MA6	13	1518	1	-	0/7/29/30	0/3/3/3
1	4OC	13	1402	1,62	-	2/9/29/30	0/2/2/2
60	3AU	2L	47	60	-	5/10/34/35	0/2/2/2
60	PSU	2L	55	60	-	0/7/25/26	0/2/2/2
1	UR3	1G	1498	1	-	0/5/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
27	PSU	1H	1940	27	-	0/7/25/26	0/2/2/2

The worst 5 of 321 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	1G	1207	2MG	C2-N2	15.57	1.47	1.34
27	14	2251	OMG	C4-N3	14.90	1.59	1.35
27	1H	2264	OMG	C4-N3	14.66	1.58	1.35
27	14	2251	OMG	C8-N7	-13.98	1.09	1.34
1	13	1207	2MG	C2-N2	13.81	1.45	1.34

The worst 5 of 447 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	1H	2264	OMG	C6-C5-C4	-17.19	104.39	120.80
27	14	2251	OMG	C6-C5-C4	-15.66	105.85	120.80
22	1K	32	PSU	N1-C2-N3	-13.03	118.07	128.43
1	13	1519	MA6	N1-C6-N6	-12.51	103.89	117.06
1	1G	516	PSU	N1-C2-N3	-12.33	118.62	128.43

There are no chirality outliers.

5 of 129 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
27	1H	1938	5MU	C2'-C1'-N1-C6
27	1H	1938	5MU	C3'-C4'-C5'-O5'
23	2K	20	H2U	C3'-C4'-C5'-O5'
23	2K	20	H2U	O4'-C1'-N1-C6
1	1G	1518	MA6	C5-C6-N6-C9

There are no ring outliers.

55 monomers are involved in 98 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
27	14	2251	OMG	2	0
27	14	1962	5MC	2	0
24	3K	39	PSU	1	0
27	1H	1938	5MU	1	0
1	1G	516	PSU	1	0
1	13	1207	2MG	1	0
27	1H	2264	OMG	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
22	1K	55	PSU	4	0
60	2L	32	PSU	1	0
27	1H	2565	OMU	3	0
23	2K	20	H2U	1	0
27	1H	1943	OMC	2	0
1	1G	1518	MA6	2	0
27	1H	1962	5MU	1	0
23	2K	55	PSU	1	0
59	1L	39	PSU	1	0
1	1G	1400	5MC	1	0
26	5K	55	PSU	1	0
27	14	1915	5MU	1	0
27	14	1942	5MC	1	0
27	14	2503	2MA	2	0
22	1K	54	5MU	1	0
26	5K	54	5MU	1	0
27	1H	1985	5MC	1	0
27	14	1911	PSU	1	0
26	5K	37	MIA	1	0
60	2L	8	4SU	2	0
27	14	1939	5MU	3	0
22	1K	46	7MG	4	0
26	5K	20	H2U	1	0
1	13	1519	MA6	2	0
1	1G	967	5MC	2	0
1	13	1400	5MC	1	0
1	1G	1519	MA6	4	0
24	3L	32	PSU	1	0
27	1H	2516	2MA	3	0
24	3K	37	MIA	2	0
23	2K	46	7MG	1	0
1	13	966	M2G	1	0
12	3A	89	0TD	3	0
1	1G	1402	4OC	2	0
60	2L	54	5MU	4	0
1	13	1498	UR3	4	0
27	14	2552	OMU	4	0
24	3L	37	MIA	2	0
23	2K	54	5MU	2	0
1	13	967	5MC	1	0
59	1L	37	MIA	2	0
1	1G	1207	2MG	3	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
26	5K	16	H2U	4	0
22	1K	37	MIA	1	0
1	13	1518	MA6	2	0
1	13	1402	4OC	1	0
1	1G	1498	UR3	3	0
27	1H	1940	PSU	1	0

5.5 Carbohydrates [i](#)

There are no carbohydrates 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	32	303	4	0,12,12	0.00	-	-		
63	SF4	3E	302	4	0,12,12	0.00	-	-		

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
63	SF4	32	303	4	-	-	0/6/5/5
63	SF4	3E	302	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	32	303	SF4	1	0
63	3E	302	SF4	3	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%)	-0.60	3 (0%) 95 90	28, 69, 150, 240	0
1	1G	1501/1522 (98%)	-0.63	1 (0%) 95 92	38, 81, 144, 248	0
2	12	237/256 (92%)	0.60	26 (10%) 5 2	85, 134, 165, 184	0
2	1E	237/256 (92%)	0.16	4 (1%) 70 49	67, 105, 147, 160	0
3	22	206/239 (86%)	0.24	10 (4%) 29 14	81, 109, 137, 144	0
3	2E	205/239 (85%)	0.62	18 (8%) 10 4	62, 81, 122, 145	0
4	32	208/209 (99%)	-0.05	2 (0%) 82 67	58, 74, 95, 120	0
4	3E	208/209 (99%)	0.01	3 (1%) 75 56	58, 77, 99, 108	0
5	42	151/162 (93%)	-0.14	0 100 100	67, 84, 102, 133	0
5	4E	151/162 (93%)	-0.11	1 (0%) 87 75	50, 67, 90, 113	0
6	52	101/101 (100%)	0.58	6 (5%) 22 10	53, 74, 90, 111	0
6	5E	101/101 (100%)	0.36	3 (2%) 50 27	50, 73, 89, 106	0
7	62	155/156 (99%)	0.42	6 (3%) 39 20	78, 93, 131, 152	0
7	6E	155/156 (99%)	0.17	5 (3%) 47 25	66, 85, 109, 117	0
8	72	138/138 (100%)	-0.27	0 100 100	64, 85, 96, 105	0
8	7E	138/138 (100%)	-0.45	0 100 100	55, 72, 85, 97	0
9	82	127/128 (99%)	-0.43	1 (0%) 86 72	78, 115, 132, 137	0
9	8E	127/128 (99%)	-0.37	0 100 100	57, 102, 119, 123	0
10	1A	99/105 (94%)	-0.11	3 (3%) 50 27	86, 123, 142, 144	0
10	1I	99/105 (94%)	0.28	6 (6%) 21 9	52, 105, 131, 135	0
11	2A	117/129 (90%)	0.60	7 (5%) 21 10	50, 77, 104, 140	0
11	2I	116/129 (89%)	0.41	3 (2%) 56 33	42, 69, 94, 119	0
12	3A	124/132 (93%)	0.84	20 (16%) 1 1	49, 69, 95, 149	0
12	3I	124/132 (93%)	0.44	6 (4%) 30 14	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%)	0.36	9 (7%) 14 5	81, 118, 131, 141	0
13	4I	119/126 (94%)	-0.14	2 (1%) 70 49	57, 92, 109, 118	0
14	5A	60/61 (98%)	-0.19	0 100 100	83, 97, 121, 126	0
14	5I	60/61 (98%)	-0.31	0 100 100	61, 71, 85, 99	0
15	6A	88/89 (98%)	-0.05	0 100 100	53, 75, 94, 100	0
15	6I	88/89 (98%)	-0.20	1 (1%) 80 64	44, 66, 90, 98	0
16	7A	84/88 (95%)	-0.71	0 100 100	59, 68, 86, 124	0
16	7I	83/88 (94%)	-0.67	0 100 100	63, 76, 99, 127	0
17	8A	100/105 (95%)	-0.06	1 (1%) 82 67	57, 77, 94, 110	0
17	8I	100/105 (95%)	-0.26	1 (1%) 82 67	53, 69, 81, 87	0
18	9A	70/88 (79%)	0.54	4 (5%) 23 11	60, 75, 104, 126	0
18	9I	71/88 (80%)	0.23	1 (1%) 75 56	54, 69, 110, 127	0
19	AA	86/93 (92%)	0.92	17 (19%) 1 0	105, 131, 158, 170	0
19	AI	84/93 (90%)	0.16	3 (3%) 42 22	72, 96, 114, 119	0
20	BA	103/106 (97%)	-0.49	0 100 100	65, 84, 109, 116	0
20	BI	101/106 (95%)	-0.45	0 100 100	65, 83, 111, 123	0
21	1B	25/27 (92%)	-0.54	0 100 100	94, 109, 123, 127	0
21	1F	24/27 (88%)	-0.62	0 100 100	74, 85, 99, 110	0
22	1K	69/76 (90%)	0.65	7 (10%) 7 2	51, 163, 204, 219	0
23	2K	66/76 (86%)	-0.14	2 (3%) 50 27	33, 59, 81, 131	0
24	3K	73/76 (96%)	0.44	5 (6%) 17 7	35, 200, 222, 230	0
24	3L	73/76 (96%)	0.19	4 (5%) 25 11	49, 197, 229, 238	0
25	4K	30/60 (50%)	0.53	4 (13%) 3 1	43, 130, 219, 232	0
25	4L	30/60 (50%)	-0.04	1 (3%) 46 24	61, 148, 218, 223	0
26	5K	68/76 (89%)	1.84	28 (41%) 0 0	80, 154, 180, 197	0
27	14	2865/2917 (98%)	-0.38	29 (1%) 82 67	27, 59, 194, 252	0
27	1H	2879/2917 (98%)	-0.32	28 (0%) 82 67	13, 37, 171, 243	0
28	16	122/122 (100%)	-0.53	0 100 100	37, 55, 74, 146	0
28	1J	121/122 (99%)	-0.50	1 (0%) 86 72	65, 90, 118, 175	0
29	71	135/229 (58%)	1.92	50 (37%) 0 0	113, 202, 228, 236	0
29	79	135/229 (58%)	0.91	27 (20%) 1 0	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%)	-0.12	0 100 100	14, 32, 47, 68	0
30	19	272/276 (98%)	0.07	1 (0%) 92 84	25, 45, 61, 73	0
31	21	204/206 (99%)	0.23	1 (0%) 91 81	16, 46, 74, 97	0
31	29	204/206 (99%)	0.78	32 (15%) 2 1	38, 72, 98, 111	0
32	31	202/210 (96%)	-0.26	0 100 100	13, 43, 72, 99	0
32	39	202/210 (96%)	0.09	2 (0%) 82 67	30, 65, 95, 109	0
33	41	181/182 (99%)	-0.04	0 100 100	50, 66, 95, 111	0
33	49	181/182 (99%)	0.76	18 (9%) 7 2	82, 99, 124, 132	0
34	51	174/180 (96%)	0.27	8 (4%) 32 16	53, 76, 96, 117	0
34	59	173/180 (96%)	2.84	95 (54%) 0 0	135, 183, 220, 240	0
35	61	145/148 (97%)	0.60	10 (6%) 16 7	43, 96, 112, 126	0
35	69	146/148 (98%)	0.39	12 (8%) 11 4	52, 93, 116, 129	0
36	38	84/173 (48%)	-0.09	3 (3%) 42 22	116, 159, 172, 180	0
37	15	138/140 (98%)	1.52	44 (31%) 0 0	51, 84, 109, 119	0
37	58	138/140 (98%)	-0.03	3 (2%) 62 41	29, 46, 80, 92	0
38	25	122/122 (100%)	0.81	10 (8%) 11 4	43, 65, 83, 95	0
38	68	122/122 (100%)	0.25	0 100 100	21, 40, 54, 64	0
39	35	150/150 (100%)	0.15	4 (2%) 54 31	35, 77, 106, 122	0
39	78	150/150 (100%)	-0.02	5 (3%) 46 24	19, 46, 81, 121	0
40	45	141/141 (100%)	1.13	27 (19%) 1 0	47, 85, 114, 163	0
40	88	141/141 (100%)	-0.15	1 (0%) 87 75	25, 45, 68, 91	0
41	55	118/118 (100%)	-0.06	1 (0%) 86 72	38, 57, 78, 93	0
41	98	118/118 (100%)	-0.48	0 100 100	24, 42, 61, 73	0
42	65	111/112 (99%)	-0.16	3 (2%) 54 31	63, 89, 122, 132	0
42	A8	112/112 (100%)	-0.11	0 100 100	41, 55, 75, 94	0
43	75	137/146 (93%)	-0.24	0 100 100	57, 73, 145, 164	0
43	B8	137/146 (93%)	0.01	2 (1%) 73 54	32, 53, 104, 138	0
44	85	117/118 (99%)	0.96	30 (25%) 0 0	41, 78, 120, 134	0
44	C8	117/118 (99%)	-0.43	2 (1%) 70 49	20, 37, 63, 93	0
45	95	101/101 (100%)	1.44	28 (27%) 0 0	41, 94, 109, 125	0
45	D8	101/101 (100%)	-0.17	1 (0%) 82 67	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%)	0.15	1 (0%) 84 69	37, 50, 93, 124	0
46	E8	113/113 (100%)	-0.40	1 (0%) 84 69	25, 35, 63, 104	0
47	B5	94/96 (97%)	0.20	4 (4%) 35 17	40, 58, 79, 106	0
47	F8	95/96 (98%)	-0.47	0 100 100	23, 36, 54, 74	0
48	C5	107/110 (97%)	0.98	17 (15%) 1 1	61, 81, 130, 140	0
48	G8	109/110 (99%)	-0.20	2 (1%) 68 47	44, 71, 118, 137	0
49	D5	176/206 (85%)	2.55	93 (52%) 0 0	89, 130, 206, 210	0
49	H8	179/206 (86%)	0.81	26 (14%) 2 1	47, 85, 160, 171	0
50	E5	84/85 (98%)	0.27	4 (4%) 30 14	44, 65, 88, 110	0
50	I8	84/85 (98%)	-0.24	1 (1%) 79 61	21, 38, 63, 81	0
51	F5	97/98 (98%)	0.40	7 (7%) 15 6	37, 57, 98, 111	0
51	J8	97/98 (98%)	0.16	2 (2%) 63 43	20, 41, 88, 114	0
52	G5	71/72 (98%)	0.01	2 (2%) 53 30	49, 69, 96, 122	0
52	K8	72/72 (100%)	-0.31	0 100 100	30, 47, 64, 82	0
53	H5	59/60 (98%)	1.33	16 (27%) 0 0	57, 76, 119, 122	0
53	L8	59/60 (98%)	-0.10	1 (1%) 70 49	30, 44, 74, 93	0
54	I5	71/71 (100%)	2.26	35 (49%) 0 0	104, 142, 169, 174	0
54	M8	71/71 (100%)	1.03	13 (18%) 1 0	72, 115, 152, 158	0
55	J5	56/60 (93%)	0.33	1 (1%) 68 47	35, 63, 121, 129	0
55	N8	56/60 (93%)	-0.28	1 (1%) 68 47	18, 47, 108, 114	0
56	K5	45/54 (83%)	1.51	14 (31%) 0 0	103, 136, 163, 169	0
56	O8	45/54 (83%)	2.85	28 (62%) 0 0	73, 103, 134, 144	0
57	L5	49/49 (100%)	0.02	3 (6%) 21 9	28, 35, 77, 88	0
57	P8	49/49 (100%)	-0.45	0 100 100	15, 20, 50, 71	0
58	M5	64/65 (98%)	0.10	2 (3%) 49 26	41, 51, 76, 94	0
58	Q8	64/65 (98%)	-0.39	0 100 100	21, 31, 41, 62	0
59	1L	72/76 (94%)	0.74	13 (18%) 1 0	80, 196, 235, 239	0
60	2L	67/76 (88%)	-0.12	1 (1%) 73 54	52, 82, 113, 145	0
All	All	21491/22459 (95%)	-0.01	990 (4%) 32 16	13, 69, 169, 252	0

The worst 5 of 990 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
49	D5	106	GLY	15.3
34	59	124	GLU	12.2
27	14	2798	C	12.2
27	14	2797	U	11.7
27	14	2799	A	10.7

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

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
26	PSU	5K	32	20/21	0.73	0.55	152,165,171,173	0
22	4SU	1K	8	20/21	0.73	0.22	181,183,191,193	0
26	H2U	5K	16	20/21	0.78	0.30	121,137,151,153	0
26	PSU	5K	39	20/21	0.79	0.32	116,146,158,158	0
26	H2U	5K	20	20/21	0.80	0.18	119,139,156,163	0
22	PSU	1K	55	20/21	0.81	0.17	123,134,149,150	0
26	PSU	5K	55	20/21	0.81	0.32	115,127,149,152	0
26	5MU	5K	54	21/22	0.85	0.36	129,137,141,145	0
59	5MU	1L	54	21/22	0.85	0.22	139,160,167,169	0
22	7MG	1K	46	24/25	0.85	0.22	180,185,193,198	0
60	H2U	2L	16	20/21	0.86	0.22	100,112,131,139	0
26	4SU	5K	8	20/21	0.86	0.28	147,151,156,157	0
24	PSU	3K	32	20/21	0.86	0.20	111,117,123,125	0
24	PSU	3K	39	20/21	0.88	0.23	100,112,118,119	0
24	PSU	3L	32	20/21	0.88	0.23	116,119,126,129	0
26	MIA	5K	37	29/30	0.89	0.42	89,114,142,145	0
23	H2U	2K	16	20/21	0.89	0.25	67,90,114,126	0
60	3AU	2L	47	27/28	0.91	0.20	95,125,138,141	0
60	5MU	2L	54	21/22	0.92	0.26	75,85,99,108	0
24	MIA	3L	37	29/30	0.92	0.26	81,113,120,124	0
24	PSU	3L	39	20/21	0.92	0.17	97,111,120,122	0
60	7MG	2L	46	24/25	0.92	0.15	89,104,121,126	0
1	2MG	1G	1207	24/25	0.92	0.13	91,101,104,108	0
59	PSU	1L	32	20/21	0.92	0.11	96,104,118,121	0
22	5MU	1K	54	21/22	0.92	0.25	94,115,123,126	0
60	PSU	2L	55	20/21	0.92	0.14	77,82,88,89	0
23	H2U	2K	20	20/21	0.93	0.18	88,97,110,111	0
24	MIA	3K	37	29/30	0.93	0.25	95,112,116,117	0
23	PSU	2K	55	20/21	0.94	0.13	60,67,80,86	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
1	PSU	1G	516	20/21	0.94	0.12	71,76,78,79	0
59	MIA	1L	37	29/30	0.94	0.17	68,80,95,96	0
27	5MU	14	1915	21/22	0.94	0.17	63,72,80,88	0
12	0TD	3A	89	10/11	0.94	0.20	65,69,72,77	0
12	0TD	3I	89	10/11	0.94	0.26	44,46,56,71	0
60	4SU	2L	8	20/21	0.94	0.13	70,83,90,90	0
60	PSU	2L	39	20/21	0.95	0.15	59,68,72,72	0
23	3AU	2K	47	27/28	0.95	0.18	62,95,113,114	0
23	5MU	2K	54	21/22	0.95	0.14	64,68,76,78	0
23	7MG	2K	46	24/25	0.95	0.20	56,62,98,99	0
1	7MG	1G	527	24/25	0.95	0.17	60,65,70,73	0
27	PSU	1H	1940	20/21	0.95	0.18	35,44,54,54	0
27	5MC	1H	1965	21/22	0.96	0.17	27,33,36,42	0
27	5MU	1H	1938	21/22	0.96	0.14	45,48,54,64	0
1	4OC	1G	1402	22/23	0.96	0.13	46,57,61,71	0
22	PSU	1K	32	20/21	0.96	0.14	65,70,79,85	0
59	PSU	1L	39	20/21	0.96	0.11	77,98,110,110	0
1	5MC	1G	967	21/22	0.96	0.12	61,68,76,86	0
1	PSU	13	516	20/21	0.96	0.13	50,55,58,60	0
22	PSU	1K	39	20/21	0.96	0.16	50,67,75,75	0
1	MA6	1G	1519	24/25	0.96	0.20	44,54,57,58	0
1	5MC	1G	1404	21/22	0.96	0.16	44,49,55,59	0
27	OMC	14	1920	21/22	0.96	0.17	54,60,62,64	0
60	MIA	2L	37	29/30	0.96	0.14	64,69,80,85	0
1	5MC	1G	1400	21/22	0.96	0.16	52,64,70,72	0
60	PSU	2L	32	20/21	0.96	0.14	68,73,80,80	0
27	PSU	14	1917	20/21	0.96	0.11	53,60,67,70	0
1	5MC	1G	1407	21/22	0.97	0.17	43,49,53,60	0
23	MIA	2K	37	29/30	0.97	0.20	41,47,63,67	0
1	7MG	13	527	24/25	0.97	0.17	42,50,56,63	0
1	5MC	13	1400	21/22	0.97	0.20	38,45,51,56	0
27	5MC	14	1942	21/22	0.97	0.19	47,57,61,71	0
1	M2G	1G	966	25/26	0.97	0.13	59,67,76,77	0
27	PSU	1H	1934	20/21	0.97	0.16	36,42,47,51	0
27	OMG	14	2251	24/25	0.97	0.18	35,40,44,46	0
1	5MC	13	967	21/22	0.97	0.18	43,50,56,59	0
23	PSU	2K	39	20/21	0.97	0.20	39,48,57,59	0
27	PSU	14	2605	20/21	0.97	0.21	29,33,41,51	0
27	PSU	1H	2618	20/21	0.97	0.17	17,19,24,24	0
27	PSU	14	1911	20/21	0.97	0.13	51,59,64,64	0
1	MA6	1G	1518	24/25	0.97	0.15	52,57,60,62	0
1	5MC	13	1404	21/22	0.97	0.18	26,29,41,43	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
22	MIA	1K	37	29/30	0.97	0.19	43,49,58,62	0
1	2MG	13	1207	24/25	0.97	0.13	57,64,68,69	0
23	PSU	2K	32	20/21	0.97	0.16	45,50,57,58	0
1	M2G	13	966	25/26	0.97	0.19	40,46,57,61	0
1	UR3	1G	1498	21/22	0.97	0.17	40,49,53,55	0
27	OMU	1H	2565	21/22	0.97	0.20	19,22,26,36	0
1	MA6	13	1519	24/25	0.98	0.18	28,31,33,33	0
23	4SU	2K	8	20/21	0.98	0.16	42,48,57,62	0
27	2MA	14	2503	23/24	0.98	0.19	28,32,36,41	0
27	5MU	1H	1962	21/22	0.98	0.17	20,23,30,41	0
27	5MU	14	1939	21/22	0.98	0.18	34,40,44,51	0
27	2MA	1H	2516	23/24	0.98	0.19	13,17,24,26	0
1	UR3	13	1498	21/22	0.98	0.20	29,33,42,43	0
27	OMU	14	2552	21/22	0.98	0.19	37,42,47,58	0
27	OMG	1H	2264	24/25	0.98	0.17	19,23,25,26	0
1	MA6	13	1518	24/25	0.98	0.17	27,32,35,38	0
1	4OC	13	1402	22/23	0.98	0.18	29,37,42,46	0
27	OMC	1H	1943	21/22	0.98	0.17	34,37,43,46	0
27	5MC	1H	1985	21/22	0.98	0.17	24,30,34,37	0
27	5MC	14	1962	21/22	0.98	0.20	38,45,53,58	0
1	5MC	13	1407	21/22	0.98	0.20	29,32,37,40	0

6.3 Carbohydrates ⓘ

There are no carbohydrates 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(\AA^2)	Q<0.9
62	MG	13	1764	1/1	0.59	0.07	86,86,86,86	0
62	MG	1H	3555	1/1	0.61	0.10	56,56,56,56	0
62	MG	1H	3576	1/1	0.65	0.07	69,69,69,69	0
62	MG	14	3336	1/1	0.66	0.15	78,78,78,78	0
62	MG	1H	3343[A]	1/1	0.66	0.88	55,55,55,55	1
62	MG	1H	3343[B]	1/1	0.66	0.88	68,68,68,68	1
62	MG	1H	3569	1/1	0.70	0.06	62,62,62,62	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
62	MG	13	1722	1/1	0.70	0.12	52,52,52,52	0
62	MG	1G	1714	1/1	0.70	0.08	88,88,88,88	0
61	K	13	1611	1/1	0.70	0.12	114,114,114,114	0
62	MG	1G	1698	1/1	0.71	0.29	66,66,66,66	0
62	MG	O8	101	1/1	0.71	0.21	60,60,60,60	0
62	MG	14	3221	1/1	0.72	0.16	52,52,52,52	0
61	K	14	3053	1/1	0.73	0.12	102,102,102,102	0
62	MG	1G	1661	1/1	0.73	0.38	79,79,79,79	0
61	K	14	3097	1/1	0.73	0.11	91,91,91,91	0
61	K	14	3012	1/1	0.73	0.20	117,117,117,117	0
62	MG	1H	3282	1/1	0.74	0.21	49,49,49,49	0
62	MG	1H	3549	1/1	0.74	0.08	60,60,60,60	0
62	MG	14	3260	1/1	0.74	0.25	84,84,84,84	0
62	MG	1H	3364	1/1	0.74	0.24	58,58,58,58	0
62	MG	1H	3331	1/1	0.74	0.21	54,54,54,54	0
62	MG	13	1662	1/1	0.74	0.21	54,54,54,54	0
62	MG	1G	1733	1/1	0.74	0.07	81,81,81,81	0
62	MG	13	1690	1/1	0.74	0.11	51,51,51,51	0
61	K	1H	3005	1/1	0.75	0.17	100,100,100,100	0
62	MG	M5	101	1/1	0.75	0.11	84,84,84,84	0
62	MG	1H	3211	1/1	0.75	0.16	56,56,56,56	0
62	MG	1H	3340	1/1	0.76	0.24	48,48,48,48	0
62	MG	14	3125	1/1	0.76	0.17	60,60,60,60	0
62	MG	1H	3305	1/1	0.76	0.32	41,41,41,41	0
62	MG	14	3317	1/1	0.77	0.11	40,40,40,40	0
61	K	32	301	1/1	0.77	0.09	104,104,104,104	0
62	MG	1H	3391	1/1	0.77	0.14	20,20,20,20	0
62	MG	1G	1678	1/1	0.77	0.30	54,54,54,54	0
62	MG	1H	3312	1/1	0.77	0.28	39,39,39,39	0
62	MG	14	3375	1/1	0.77	0.09	84,84,84,84	0
62	MG	14	3187	1/1	0.77	0.31	51,51,51,51	0
62	MG	14	3173	1/1	0.77	0.18	66,66,66,66	0
62	MG	1H	3294	1/1	0.78	0.14	59,59,59,59	0
62	MG	1G	1653	1/1	0.78	0.18	53,53,53,53	0
62	MG	1G	1711	1/1	0.78	0.11	97,97,97,97	0
62	MG	13	1698	1/1	0.78	0.32	84,84,84,84	0
62	MG	14	3249	1/1	0.78	0.17	62,62,62,62	0
61	K	13	1608	1/1	0.78	0.11	89,89,89,89	0
61	K	1H	3020	1/1	0.79	0.14	65,65,65,65	0
61	K	1H	3140	1/1	0.79	0.14	62,62,62,62	0
62	MG	14	3280	1/1	0.79	0.09	45,45,45,45	0
62	MG	1H	3359	1/1	0.79	0.28	62,62,62,62	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
62	MG	13	1692	1/1	0.79	0.24	51,51,51,51	0
62	MG	1H	3272	1/1	0.79	0.37	55,55,55,55	0
62	MG	1H	3290	1/1	0.79	0.13	38,38,38,38	0
61	K	49	201	1/1	0.80	0.18	108,108,108,108	0
62	MG	1H	3550	1/1	0.80	0.06	64,64,64,64	0
62	MG	1H	3285	1/1	0.80	0.30	43,43,43,43	0
62	MG	1G	1690	1/1	0.80	0.35	74,74,74,74	0
62	MG	1H	3541	1/1	0.80	0.07	66,66,66,66	0
61	K	1G	1631	1/1	0.80	0.26	86,86,86,86	0
62	MG	14	3309	1/1	0.80	0.11	26,26,26,26	0
61	K	1G	1605	1/1	0.80	0.07	92,92,92,92	0
62	MG	14	3244	1/1	0.81	0.19	64,64,64,64	0
62	MG	13	1679	1/1	0.81	0.28	45,45,45,45	0
61	K	1G	1602	1/1	0.81	0.19	104,104,104,104	0
61	K	39	302	1/1	0.81	0.20	74,74,74,74	0
62	MG	14	3149	1/1	0.81	0.27	37,37,37,37	0
62	MG	13	1672	1/1	0.81	0.24	49,49,49,49	0
62	MG	1G	1707	1/1	0.81	0.12	62,62,62,62	0
62	MG	13	1738	1/1	0.82	0.09	86,86,86,86	0
62	MG	14	3268	1/1	0.82	0.16	36,36,36,36	0
62	MG	14	3230	1/1	0.82	0.11	54,54,54,54	0
62	MG	1H	3563	1/1	0.82	0.10	75,75,75,75	0
61	K	29	301	1/1	0.82	0.09	86,86,86,86	0
62	MG	13	1770	1/1	0.82	0.12	71,71,71,71	0
62	MG	13	1755	1/1	0.82	0.07	83,83,83,83	0
62	MG	14	3181	1/1	0.82	0.22	49,49,49,49	0
62	MG	1H	3544	1/1	0.82	0.06	63,63,63,63	0
62	MG	1H	3539	1/1	0.82	0.12	66,66,66,66	0
62	MG	14	3391	1/1	0.82	0.06	81,81,81,81	0
62	MG	1H	3512	1/1	0.82	0.15	39,39,39,39	0
61	K	14	3065	1/1	0.82	0.17	55,55,55,55	0
62	MG	14	3332	1/1	0.82	0.09	54,54,54,54	0
62	MG	14	3399	1/1	0.82	0.07	106,106,106,106	0
62	MG	1H	3461	1/1	0.83	0.14	20,20,20,20	0
62	MG	1H	3279	1/1	0.83	0.24	32,32,32,32	0
62	MG	1H	3330	1/1	0.83	0.20	45,45,45,45	0
61	K	1G	1627	1/1	0.83	0.11	92,92,92,92	0
62	MG	1H	3453	1/1	0.83	0.14	20,20,20,20	0
62	MG	13	1665	1/1	0.83	0.22	51,51,51,51	0
62	MG	1H	3551	1/1	0.83	0.07	45,45,45,45	0
62	MG	1G	1736	1/1	0.83	0.11	62,62,62,62	0
62	MG	1G	1718	1/1	0.83	0.07	39,39,39,39	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
62	MG	13	1707	1/1	0.83	0.27	58,58,58,58	0
62	MG	1H	3500	1/1	0.83	0.11	63,63,63,63	0
62	MG	1G	1688	1/1	0.83	0.21	65,65,65,65	0
62	MG	1H	3493	1/1	0.83	0.08	27,27,27,27	0
61	K	5A	101	1/1	0.83	0.08	82,82,82,82	0
62	MG	1H	3281	1/1	0.83	0.36	49,49,49,49	0
61	K	1G	1609	1/1	0.83	0.08	91,91,91,91	0
62	MG	1H	3295	1/1	0.83	0.17	29,29,29,29	0
61	K	1G	1614	1/1	0.83	0.09	86,86,86,86	0
61	K	14	3064	1/1	0.83	0.11	87,87,87,87	0
62	MG	14	3278	1/1	0.83	0.22	49,49,49,49	0
62	MG	14	3275	1/1	0.84	0.14	42,42,42,42	0
61	K	1H	3002	1/1	0.84	0.12	73,73,73,73	0
62	MG	1H	3450	1/1	0.84	0.07	52,52,52,52	0
62	MG	13	1741	1/1	0.84	0.09	109,109,109,109	0
62	MG	14	3310	1/1	0.84	0.10	25,25,25,25	0
62	MG	1H	3372	1/1	0.84	0.17	31,31,31,31	0
62	MG	14	3394	1/1	0.84	0.13	61,61,61,61	0
62	MG	14	3360	1/1	0.84	0.16	37,37,37,37	0
62	MG	1H	3242	1/1	0.84	0.14	37,37,37,37	0
61	K	13	1648	1/1	0.84	0.09	71,71,71,71	0
61	K	14	3034	1/1	0.84	0.13	86,86,86,86	0
61	K	1H	3004	1/1	0.85	0.15	88,88,88,88	0
62	MG	14	3122	1/1	0.85	0.22	49,49,49,49	0
62	MG	14	3380	1/1	0.85	0.14	76,76,76,76	0
62	MG	13	1715	1/1	0.85	0.24	60,60,60,60	0
62	MG	14	3267	1/1	0.85	0.13	44,44,44,44	0
62	MG	13	1709[B]	1/1	0.85	0.41	45,45,45,45	1
61	K	1G	1632	1/1	0.85	0.07	78,78,78,78	0
61	K	14	3040	1/1	0.85	0.10	93,93,93,93	0
62	MG	1H	3517	1/1	0.85	0.16	26,26,26,26	0
62	MG	1G	1709	1/1	0.85	0.07	73,73,73,73	0
62	MG	14	3124	1/1	0.85	0.13	58,58,58,58	0
62	MG	1H	3496	1/1	0.85	0.08	48,48,48,48	0
62	MG	1H	3311	1/1	0.85	0.16	47,47,47,47	0
62	MG	1G	1689	1/1	0.85	0.21	57,57,57,57	0
62	MG	14	3231	1/1	0.85	0.14	39,39,39,39	0
62	MG	13	1709[A]	1/1	0.85	0.41	40,40,40,40	1
62	MG	1H	3245	1/1	0.86	0.31	50,50,50,50	0
62	MG	1H	3227	1/1	0.86	0.19	29,29,29,29	0
61	K	14	3088	1/1	0.86	0.09	98,98,98,98	0
61	K	13	1649	1/1	0.86	0.10	81,81,81,81	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
61	K	1G	1607	1/1	0.86	0.14	87,87,87,87	0
62	MG	1H	3429	1/1	0.86	0.18	29,29,29,29	0
62	MG	1H	3457	1/1	0.86	0.20	25,25,25,25	0
61	K	1H	3044	1/1	0.86	0.22	92,92,92,92	0
61	K	14	3067	1/1	0.86	0.21	70,70,70,70	0
62	MG	14	3341	1/1	0.86	0.14	35,35,35,35	0
61	K	1H	3032	1/1	0.86	0.15	54,54,54,54	0
61	K	1G	1601	1/1	0.86	0.13	115,115,115,115	0
62	MG	13	1766	1/1	0.86	0.06	64,64,64,64	0
61	K	14	3052	1/1	0.86	0.09	76,76,76,76	0
62	MG	14	3166	1/1	0.86	0.13	58,58,58,58	0
62	MG	14	3120	1/1	0.86	0.15	44,44,44,44	0
62	MG	1G	1691	1/1	0.86	0.29	64,64,64,64	0
62	MG	1H	3213	1/1	0.86	0.17	25,25,25,25	0
62	MG	14	3164	1/1	0.86	0.17	48,48,48,48	0
62	MG	1H	3153	1/1	0.86	0.19	45,45,45,45	0
62	MG	1H	3254	1/1	0.86	0.20	29,29,29,29	0
62	MG	1H	3553	1/1	0.86	0.08	60,60,60,60	0
62	MG	1H	3431	1/1	0.86	0.07	46,46,46,46	0
62	MG	13	1677	1/1	0.86	0.21	42,42,42,42	0
62	MG	13	1750	1/1	0.86	0.10	52,52,52,52	0
61	K	14	3013	1/1	0.86	0.28	84,84,84,84	0
62	MG	1G	1687	1/1	0.86	0.10	67,67,67,67	0
62	MG	1H	3174	1/1	0.86	0.29	60,60,60,60	0
62	MG	1G	1716	1/1	0.86	0.06	70,70,70,70	0
61	K	14	3038	1/1	0.86	0.12	92,92,92,92	0
62	MG	14	3326	1/1	0.86	0.11	40,40,40,40	0
62	MG	13	1753	1/1	0.86	0.08	69,69,69,69	0
62	MG	1H	3514	1/1	0.86	0.14	53,53,53,53	0
62	MG	1H	3516	1/1	0.87	0.13	21,21,21,21	0
61	K	1H	3091	1/1	0.87	0.09	64,64,64,64	0
62	MG	13	1725	1/1	0.87	0.30	58,58,58,58	0
61	K	13	1603	1/1	0.87	0.08	75,75,75,75	0
61	K	13	1615	1/1	0.87	0.09	90,90,90,90	0
62	MG	1G	1731	1/1	0.87	0.09	81,81,81,81	0
62	MG	14	3242	1/1	0.87	0.18	65,65,65,65	0
62	MG	14	3201	1/1	0.87	0.22	49,49,49,49	0
62	MG	1H	3300	1/1	0.87	0.41	59,59,59,59	0
62	MG	1H	3417	1/1	0.87	0.08	61,61,61,61	0
62	MG	1H	3376	1/1	0.87	0.19	54,54,54,54	0
62	MG	13	1702	1/1	0.87	0.21	60,60,60,60	0
62	MG	1H	3190	1/1	0.87	0.28	32,32,32,32	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
62	MG	1H	3489	1/1	0.87	0.11	57,57,57,57	0
61	K	14	3091	1/1	0.87	0.15	78,78,78,78	0
62	MG	14	3270	1/1	0.87	0.14	66,66,66,66	0
62	MG	14	3263	1/1	0.87	0.25	60,60,60,60	0
62	MG	1G	1679	1/1	0.87	0.10	62,62,62,62	0
62	MG	14	3118	1/1	0.87	0.23	58,58,58,58	0
62	MG	1H	3422	1/1	0.87	0.13	29,29,29,29	0
62	MG	14	3256	1/1	0.87	0.18	67,67,67,67	0
62	MG	14	3305	1/1	0.87	0.06	40,40,40,40	0
62	MG	1H	3552	1/1	0.87	0.15	85,85,85,85	0
62	MG	14	3354	1/1	0.87	0.12	30,30,30,30	0
62	MG	1G	1724	1/1	0.87	0.08	82,82,82,82	0
62	MG	1H	3325	1/1	0.87	0.27	50,50,50,50	0
62	MG	1G	1734	1/1	0.87	0.12	94,94,94,94	0
62	MG	1H	3209	1/1	0.87	0.31	52,52,52,52	0
62	MG	14	3327	1/1	0.87	0.07	36,36,36,36	0
62	MG	14	3215	1/1	0.87	0.22	45,45,45,45	0
61	K	1G	1623	1/1	0.87	0.10	95,95,95,95	0
62	MG	14	3161	1/1	0.87	0.14	47,47,47,47	0
62	MG	1G	1659	1/1	0.87	0.38	64,64,64,64	0
62	MG	14	3176	1/1	0.87	0.27	69,69,69,69	0
62	MG	1H	3452	1/1	0.87	0.07	68,68,68,68	0
62	MG	1H	3466	1/1	0.87	0.14	22,22,22,22	0
61	K	1H	3036	1/1	0.87	0.20	60,60,60,60	0
62	MG	14	3228	1/1	0.87	0.15	58,58,58,58	0
62	MG	13	1761	1/1	0.87	0.08	86,86,86,86	0
62	MG	1G	1677	1/1	0.88	0.20	57,57,57,57	0
62	MG	1H	3328[B]	1/1	0.88	0.44	27,27,27,27	1
62	MG	1H	3373	1/1	0.88	0.29	43,43,43,43	0
61	K	1K	101	1/1	0.88	0.09	83,83,83,83	0
61	K	14	3007	1/1	0.88	0.12	64,64,64,64	0
62	MG	1H	3334	1/1	0.88	0.18	43,43,43,43	0
62	MG	13	1673	1/1	0.88	0.28	55,55,55,55	0
62	MG	14	3217	1/1	0.88	0.14	69,69,69,69	0
62	MG	1G	1715	1/1	0.88	0.12	39,39,39,39	0
62	MG	1H	3327	1/1	0.88	0.15	40,40,40,40	0
62	MG	1H	3298	1/1	0.88	0.15	28,28,28,28	0
62	MG	14	3331	1/1	0.88	0.10	51,51,51,51	0
62	MG	1H	3413	1/1	0.88	0.08	49,49,49,49	0
62	MG	1H	3481	1/1	0.88	0.11	21,21,21,21	0
61	K	1H	3040[A]	1/1	0.88	0.31	46,46,46,46	1
62	MG	13	1684	1/1	0.88	0.34	73,73,73,73	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
62	MG	1H	3162	1/1	0.88	0.32	58,58,58,58	0
62	MG	1H	3264	1/1	0.88	0.32	55,55,55,55	0
62	MG	14	3387	1/1	0.88	0.11	45,45,45,45	0
62	MG	1H	3186	1/1	0.88	0.38	55,55,55,55	0
61	K	1H	3040[B]	1/1	0.88	0.31	43,43,43,43	1
62	MG	1H	3561	1/1	0.88	0.08	38,38,38,38	0
62	MG	1H	3179	1/1	0.88	0.21	30,30,30,30	0
62	MG	1G	1644	1/1	0.88	0.17	59,59,59,59	0
61	K	13	1609	1/1	0.88	0.10	57,57,57,57	0
62	MG	1H	3567	1/1	0.88	0.10	24,24,24,24	0
62	MG	1H	3328[A]	1/1	0.88	0.44	22,22,22,22	1
62	MG	14	3195	1/1	0.88	0.20	53,53,53,53	0
62	MG	14	3233	1/1	0.88	0.21	52,52,52,52	0
62	MG	14	3188	1/1	0.88	0.15	56,56,56,56	0
62	MG	14	3303	1/1	0.88	0.06	58,58,58,58	0
61	K	1H	3131	1/1	0.88	0.14	63,63,63,63	0
62	MG	14	3225	1/1	0.88	0.13	47,47,47,47	0
62	MG	1H	3437	1/1	0.88	0.08	51,51,51,51	0
62	MG	14	3186	1/1	0.88	0.27	49,49,49,49	0
62	MG	1H	3259	1/1	0.88	0.20	46,46,46,46	0
62	MG	1G	1730	1/1	0.88	0.09	78,78,78,78	0
62	MG	1G	1674	1/1	0.88	0.24	122,122,122,122	0
62	MG	14	3182	1/1	0.88	0.23	62,62,62,62	0
62	MG	1H	3202	1/1	0.88	0.23	45,45,45,45	0
61	K	14	3004	1/1	0.88	0.14	81,81,81,81	0
62	MG	13	1720	1/1	0.88	0.24	64,64,64,64	0
62	MG	1H	3161	1/1	0.88	0.31	55,55,55,55	0
62	MG	1H	3474	1/1	0.88	0.17	24,24,24,24	0
62	MG	1H	3361	1/1	0.88	0.28	57,57,57,57	0
62	MG	1H	3326	1/1	0.88	0.30	60,60,60,60	0
61	K	14	3006	1/1	0.88	0.14	106,106,106,106	0
62	MG	13	1655	1/1	0.88	0.28	51,51,51,51	0
61	K	1H	3142	1/1	0.88	0.22	78,78,78,78	0
62	MG	13	1680	1/1	0.88	0.31	49,49,49,49	0
62	MG	1G	1657	1/1	0.88	0.30	53,53,53,53	0
61	K	13	1605	1/1	0.88	0.08	81,81,81,81	0
61	K	14	3080	1/1	0.88	0.10	79,79,79,79	0
61	K	14	3037	1/1	0.88	0.06	60,60,60,60	0
61	K	13	1650	1/1	0.88	0.16	97,97,97,97	0
62	MG	13	1704	1/1	0.89	0.29	56,56,56,56	0
62	MG	1H	3366	1/1	0.89	0.12	40,40,40,40	0
62	MG	14	3386	1/1	0.89	0.15	61,61,61,61	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
62	MG	1G	1720	1/1	0.89	0.16	73,73,73,73	0
62	MG	14	3294	1/1	0.89	0.09	51,51,51,51	0
61	K	14	3098	1/1	0.89	0.13	67,67,67,67	0
62	MG	14	3337	1/1	0.89	0.03	83,83,83,83	0
62	MG	1G	1696	1/1	0.89	0.37	52,52,52,52	0
61	K	14	3079	1/1	0.89	0.17	81,81,81,81	0
62	MG	1H	3329	1/1	0.89	0.31	63,63,63,63	0
62	MG	14	3190	1/1	0.89	0.14	77,77,77,77	0
62	MG	14	3240	1/1	0.89	0.29	57,57,57,57	0
62	MG	1H	3221	1/1	0.89	0.18	34,34,34,34	0
62	MG	14	3261	1/1	0.89	0.13	43,43,43,43	0
62	MG	1G	1697	1/1	0.89	0.29	63,63,63,63	0
62	MG	1G	1692	1/1	0.89	0.36	72,72,72,72	0
62	MG	13	1678	1/1	0.89	0.28	38,38,38,38	0
62	MG	14	3384	1/1	0.89	0.05	47,47,47,47	0
61	K	13	1643	1/1	0.89	0.07	76,76,76,76	0
62	MG	14	3325	1/1	0.89	0.10	30,30,30,30	0
62	MG	1H	3299	1/1	0.89	0.12	47,47,47,47	0
62	MG	1H	3473	1/1	0.89	0.15	19,19,19,19	0
62	MG	1H	3275	1/1	0.89	0.30	44,44,44,44	0
62	MG	16	214	1/1	0.89	0.06	57,57,57,57	0
62	MG	14	3290	1/1	0.89	0.08	36,36,36,36	0
61	K	14	3086	1/1	0.89	0.10	65,65,65,65	0
62	MG	14	3239	1/1	0.89	0.28	66,66,66,66	0
62	MG	1H	3477	1/1	0.89	0.15	28,28,28,28	0
62	MG	1H	3424	1/1	0.89	0.18	42,42,42,42	0
61	K	1H	3072	1/1	0.89	0.14	53,53,53,53	0
62	MG	1H	3238	1/1	0.89	0.16	39,39,39,39	0
62	MG	14	3381	1/1	0.89	0.10	56,56,56,56	0
62	MG	1H	3199	1/1	0.89	0.26	34,34,34,34	0
62	MG	78	201	1/1	0.89	0.24	38,38,38,38	0
62	MG	14	3388	1/1	0.89	0.07	91,91,91,91	0
62	MG	1G	1669	1/1	0.89	0.42	60,60,60,60	0
62	MG	14	3396	1/1	0.89	0.09	66,66,66,66	0
62	MG	1H	3183	1/1	0.89	0.17	47,47,47,47	0
62	MG	14	3148	1/1	0.89	0.13	43,43,43,43	0
62	MG	14	3312	1/1	0.89	0.12	38,38,38,38	0
62	MG	1G	1728	1/1	0.89	0.06	50,50,50,50	0
62	MG	1H	3303	1/1	0.89	0.17	46,46,46,46	0
62	MG	14	3291	1/1	0.89	0.07	58,58,58,58	0
62	MG	14	3295	1/1	0.89	0.11	50,50,50,50	0
62	MG	14	3383	1/1	0.89	0.09	51,51,51,51	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
62	MG	1H	3287	1/1	0.89	0.17	37,37,37,37	0
62	MG	1H	3165	1/1	0.89	0.21	40,40,40,40	0
62	MG	1H	3352	1/1	0.90	0.19	43,43,43,43	0
62	MG	1H	3345[A]	1/1	0.90	0.48	23,23,23,23	1
62	MG	1G	1683[A]	1/1	0.90	0.58	51,51,51,51	1
61	K	14	3072	1/1	0.90	0.08	85,85,85,85	0
62	MG	13	1732	1/1	0.90	0.07	51,51,51,51	0
62	MG	14	3241	1/1	0.90	0.14	59,59,59,59	0
62	MG	1H	3255	1/1	0.90	0.24	47,47,47,47	0
62	MG	1H	3419	1/1	0.90	0.10	27,27,27,27	0
62	MG	14	3235	1/1	0.90	0.17	50,50,50,50	0
62	MG	21	303	1/1	0.90	0.10	33,33,33,33	0
62	MG	1H	3375	1/1	0.90	0.30	36,36,36,36	0
61	K	1H	3041	1/1	0.90	0.15	68,68,68,68	0
62	MG	1H	3554	1/1	0.90	0.06	77,77,77,77	0
62	MG	1H	3380	1/1	0.90	0.32	44,44,44,44	0
62	MG	14	3167	1/1	0.90	0.18	38,38,38,38	0
62	MG	13	1727	1/1	0.90	0.13	60,60,60,60	0
62	MG	14	3362	1/1	0.90	0.05	68,68,68,68	0
62	MG	1H	3451	1/1	0.90	0.05	82,82,82,82	0
61	K	16	202	1/1	0.90	0.08	74,74,74,74	0
61	K	1H	3129	1/1	0.90	0.22	60,60,60,60	0
62	MG	1G	1695	1/1	0.90	0.23	72,72,72,72	0
62	MG	1H	3239	1/1	0.90	0.15	26,26,26,26	0
62	MG	13	1710	1/1	0.90	0.16	52,52,52,52	0
62	MG	1H	3367	1/1	0.90	0.18	35,35,35,35	0
62	MG	1G	1683[B]	1/1	0.90	0.58	45,45,45,45	1
62	MG	1H	3548	1/1	0.90	0.12	32,32,32,32	0
62	MG	14	3197	1/1	0.90	0.20	48,48,48,48	0
62	MG	14	3208	1/1	0.90	0.25	58,58,58,58	0
62	MG	1H	3180	1/1	0.90	0.17	43,43,43,43	0
62	MG	1H	3572	1/1	0.90	0.11	25,25,25,25	0
62	MG	1H	3237	1/1	0.90	0.18	38,38,38,38	0
62	MG	1H	3522	1/1	0.90	0.09	49,49,49,49	0
62	MG	13	1699	1/1	0.90	0.12	43,43,43,43	0
61	K	14	3102	1/1	0.90	0.07	76,76,76,76	0
62	MG	14	3248	1/1	0.90	0.31	60,60,60,60	0
62	MG	14	3194	1/1	0.90	0.21	54,54,54,54	0
61	K	14	3045	1/1	0.90	0.18	83,83,83,83	0
61	K	1H	3027	1/1	0.90	0.10	63,63,63,63	0
62	MG	1H	3345[B]	1/1	0.90	0.48	24,24,24,24	1
62	MG	14	3352	1/1	0.90	0.13	63,63,63,63	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
62	MG	1G	1721	1/1	0.90	0.08	45,45,45,45	0
62	MG	1H	3363	1/1	0.90	0.13	56,56,56,56	0
62	MG	14	3250	1/1	0.90	0.12	38,38,38,38	0
62	MG	1H	3151	1/1	0.90	0.26	41,41,41,41	0
62	MG	14	3350	1/1	0.90	0.10	39,39,39,39	0
62	MG	1H	3263	1/1	0.90	0.11	36,36,36,36	0
62	MG	1H	3542	1/1	0.90	0.08	33,33,33,33	0
62	MG	13	1695	1/1	0.90	0.14	66,66,66,66	0
62	MG	1H	3323	1/1	0.90	0.29	52,52,52,52	0
62	MG	14	3145	1/1	0.90	0.18	49,49,49,49	0
62	MG	14	3382	1/1	0.90	0.06	52,52,52,52	0
62	MG	14	3154	1/1	0.90	0.18	50,50,50,50	0
62	MG	1H	3535	1/1	0.90	0.07	64,64,64,64	0
62	MG	13	1734	1/1	0.90	0.06	41,41,41,41	0
62	MG	14	3137	1/1	0.90	0.15	49,49,49,49	0
61	K	1G	1634	1/1	0.90	0.10	62,62,62,62	0
62	MG	14	3142	1/1	0.90	0.25	51,51,51,51	0
62	MG	1G	1671	1/1	0.90	0.35	46,46,46,46	0
62	MG	1H	3556	1/1	0.90	0.12	47,47,47,47	0
62	MG	16	210	1/1	0.90	0.26	62,62,62,62	0
62	MG	13	1703	1/1	0.90	0.22	49,49,49,49	0
62	MG	13	1719	1/1	0.90	0.34	63,63,63,63	0
62	MG	1H	3220	1/1	0.90	0.35	50,50,50,50	0
62	MG	13	1708	1/1	0.90	0.26	60,60,60,60	0
62	MG	1H	3438	1/1	0.90	0.13	74,74,74,74	0
62	MG	1H	3336	1/1	0.90	0.40	45,45,45,45	0
62	MG	1H	3497	1/1	0.90	0.08	55,55,55,55	0
62	MG	1G	1725	1/1	0.90	0.08	69,69,69,69	0
61	K	13	1651	1/1	0.90	0.15	81,81,81,81	0
62	MG	1G	1660	1/1	0.90	0.32	46,46,46,46	0
62	MG	14	3389	1/1	0.90	0.07	45,45,45,45	0
62	MG	6E	201	1/1	0.90	0.34	62,62,62,62	0
61	K	1H	3134	1/1	0.91	0.17	54,54,54,54	0
61	K	2A	201	1/1	0.91	0.07	70,70,70,70	0
62	MG	14	3226	1/1	0.91	0.16	55,55,55,55	0
62	MG	1H	3440	1/1	0.91	0.10	62,62,62,62	0
62	MG	14	3372	1/1	0.91	0.11	64,64,64,64	0
62	MG	14	3272	1/1	0.91	0.20	61,61,61,61	0
62	MG	1H	3488	1/1	0.91	0.10	35,35,35,35	0
62	MG	1H	3482	1/1	0.91	0.10	45,45,45,45	0
62	MG	1H	3148	1/1	0.91	0.30	35,35,35,35	0
62	MG	14	3265	1/1	0.91	0.16	34,34,34,34	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
62	MG	1H	3320[A]	1/1	0.91	0.38	8,8,8,8	1
61	K	1J	201	1/1	0.91	0.10	81,81,81,81	0
62	MG	13	1701	1/1	0.91	0.21	69,69,69,69	0
62	MG	1G	1686	1/1	0.91	0.40	75,75,75,75	0
61	K	13	1623	1/1	0.91	0.09	56,56,56,56	0
62	MG	14	3116	1/1	0.91	0.22	32,32,32,32	0
62	MG	1H	3528	1/1	0.91	0.10	50,50,50,50	0
62	MG	16	207	1/1	0.91	0.21	43,43,43,43	0
62	MG	13	1671	1/1	0.91	0.24	49,49,49,49	0
62	MG	1G	1705	1/1	0.91	0.10	73,73,73,73	0
61	K	1H	3099	1/1	0.91	0.10	59,59,59,59	0
61	K	14	3014	1/1	0.91	0.20	80,80,80,80	0
62	MG	1H	3540	1/1	0.91	0.06	50,50,50,50	0
62	MG	14	3369	1/1	0.91	0.08	76,76,76,76	0
62	MG	14	3277	1/1	0.91	0.14	61,61,61,61	0
61	K	1H	3138	1/1	0.91	0.10	62,62,62,62	0
62	MG	14	3143	1/1	0.91	0.12	39,39,39,39	0
62	MG	14	3308	1/1	0.91	0.06	77,77,77,77	0
62	MG	14	3202	1/1	0.91	0.21	42,42,42,42	0
62	MG	13	1756	1/1	0.91	0.08	63,63,63,63	0
62	MG	1H	3320[B]	1/1	0.91	0.38	9,9,9,9	1
62	MG	14	3223	1/1	0.91	0.16	40,40,40,40	0
62	MG	14	3216	1/1	0.91	0.18	51,51,51,51	0
61	K	BI	201	1/1	0.91	0.08	108,108,108,108	0
62	MG	1H	3321	1/1	0.91	0.24	36,36,36,36	0
61	K	14	3035	1/1	0.91	0.12	83,83,83,83	0
62	MG	13	1757	1/1	0.91	0.12	50,50,50,50	0
61	K	13	1631	1/1	0.91	0.12	58,58,58,58	0
62	MG	14	3264	1/1	0.91	0.13	45,45,45,45	0
61	K	13	1645	1/1	0.91	0.10	72,72,72,72	0
62	MG	1H	3370	1/1	0.91	0.41	61,61,61,61	0
61	K	13	1646	1/1	0.91	0.16	63,63,63,63	0
61	K	1H	3051	1/1	0.91	0.07	49,49,49,49	0
62	MG	1G	1699	1/1	0.91	0.25	62,62,62,62	0
62	MG	1H	3428	1/1	0.91	0.09	23,23,23,23	0
61	K	1H	3095	1/1	0.91	0.09	58,58,58,58	0
62	MG	16	209	1/1	0.91	0.40	59,59,59,59	0
62	MG	1H	3454	1/1	0.91	0.12	23,23,23,23	0
62	MG	14	3209	1/1	0.91	0.13	53,53,53,53	0
62	MG	14	3178	1/1	0.91	0.30	53,53,53,53	0
61	K	1G	1618	1/1	0.91	0.14	79,79,79,79	0
62	MG	13	1763	1/1	0.91	0.06	64,64,64,64	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
62	MG	1G	1666	1/1	0.91	0.33	46,46,46,46	0
62	MG	1H	3201	1/1	0.91	0.18	45,45,45,45	0
61	K	13	1619	1/1	0.91	0.29	58,58,58,58	0
61	K	1H	3023	1/1	0.91	0.12	63,63,63,63	0
62	MG	14	3299	1/1	0.91	0.05	48,48,48,48	0
62	MG	1H	3335	1/1	0.91	0.28	40,40,40,40	0
62	MG	13	1758	1/1	0.91	0.07	76,76,76,76	0
61	K	14	3099	1/1	0.91	0.06	67,67,67,67	0
62	MG	2K	104	1/1	0.92	0.35	48,48,48,48	0
61	K	13	1642	1/1	0.92	0.12	93,93,93,93	0
62	MG	14	3321	1/1	0.92	0.12	26,26,26,26	0
62	MG	13	1705	1/1	0.92	0.21	56,56,56,56	0
62	MG	16	213	1/1	0.92	0.08	41,41,41,41	0
61	K	1G	1625	1/1	0.92	0.06	108,108,108,108	0
62	MG	1G	1647	1/1	0.92	0.29	55,55,55,55	0
62	MG	13	1694	1/1	0.92	0.30	57,57,57,57	0
61	K	14	3061	1/1	0.92	0.08	63,63,63,63	0
62	MG	13	1700	1/1	0.92	0.15	47,47,47,47	0
62	MG	14	3281	1/1	0.92	0.15	25,25,25,25	0
62	MG	1H	3207	1/1	0.92	0.24	38,38,38,38	0
62	MG	1H	3529	1/1	0.92	0.19	54,54,54,54	0
62	MG	1H	3480	1/1	0.92	0.15	18,18,18,18	0
61	K	1H	3048	1/1	0.92	0.11	72,72,72,72	0
62	MG	39	303	1/1	0.92	0.26	54,54,54,54	0
62	MG	1H	3276	1/1	0.92	0.20	44,44,44,44	0
62	MG	14	3262	1/1	0.92	0.19	41,41,41,41	0
62	MG	1H	3240	1/1	0.92	0.21	39,39,39,39	0
62	MG	1H	3394	1/1	0.92	0.14	11,11,11,11	0
62	MG	1H	3362	1/1	0.92	0.27	64,64,64,64	0
61	K	1G	1604	1/1	0.92	0.07	91,91,91,91	0
62	MG	13	1742	1/1	0.92	0.06	60,60,60,60	0
62	MG	14	3370	1/1	0.92	0.11	44,44,44,44	0
61	K	13	1610	1/1	0.92	0.15	103,103,103,103	0
62	MG	1H	3164	1/1	0.92	0.17	58,58,58,58	0
62	MG	1H	3332	1/1	0.92	0.38	48,48,48,48	0
62	MG	13	1658	1/1	0.92	0.21	36,36,36,36	0
62	MG	1H	3266	1/1	0.92	0.16	39,39,39,39	0
62	MG	1H	3157	1/1	0.92	0.22	49,49,49,49	0
62	MG	14	3349	1/1	0.92	0.08	48,48,48,48	0
62	MG	13	1664	1/1	0.92	0.25	57,57,57,57	0
62	MG	14	3189	1/1	0.92	0.10	50,50,50,50	0
61	K	1H	3110	1/1	0.92	0.09	60,60,60,60	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
62	MG	1G	1727	1/1	0.92	0.08	59,59,59,59	0
62	MG	1H	3564	1/1	0.92	0.16	25,25,25,25	0
62	MG	13	1751	1/1	0.92	0.13	75,75,75,75	0
62	MG	1H	3416	1/1	0.92	0.04	69,69,69,69	0
62	MG	14	3334	1/1	0.92	0.08	33,33,33,33	0
62	MG	1H	3381	1/1	0.92	0.23	39,39,39,39	0
62	MG	14	3282	1/1	0.92	0.09	48,48,48,48	0
62	MG	1H	3333	1/1	0.92	0.27	50,50,50,50	0
62	MG	1H	3302	1/1	0.92	0.13	29,29,29,29	0
62	MG	1H	3558	1/1	0.92	0.07	56,56,56,56	0
62	MG	13	1767	1/1	0.92	0.12	70,70,70,70	0
61	K	1H	3050	1/1	0.92	0.29	53,53,53,53	0
62	MG	1H	3189	1/1	0.92	0.20	41,41,41,41	0
61	K	1H	3123	1/1	0.92	0.08	50,50,50,50	0
61	K	1G	1616	1/1	0.92	0.15	86,86,86,86	0
61	K	1H	3126	1/1	0.92	0.13	86,86,86,86	0
62	MG	1H	3377	1/1	0.92	0.24	26,26,26,26	0
62	MG	1H	3225	1/1	0.92	0.24	37,37,37,37	0
62	MG	14	3165	1/1	0.92	0.20	45,45,45,45	0
62	MG	14	3232	1/1	0.92	0.16	63,63,63,63	0
62	MG	16	205	1/1	0.92	0.23	46,46,46,46	0
61	K	14	3041	1/1	0.92	0.14	66,66,66,66	0
61	K	14	3048	1/1	0.92	0.16	67,67,67,67	0
62	MG	14	3119	1/1	0.92	0.22	49,49,49,49	0
62	MG	1G	1649	1/1	0.92	0.29	74,74,74,74	0
62	MG	1H	3547	1/1	0.92	0.06	52,52,52,52	0
62	MG	13	1749	1/1	0.92	0.15	52,52,52,52	0
62	MG	14	3109	1/1	0.92	0.17	41,41,41,41	0
62	MG	1H	3185	1/1	0.92	0.20	40,40,40,40	0
62	MG	1H	3495	1/1	0.92	0.06	48,48,48,48	0
62	MG	16	206	1/1	0.92	0.15	52,52,52,52	0
62	MG	13	1714	1/1	0.92	0.29	83,83,83,83	0
62	MG	1G	1663[A]	1/1	0.92	0.45	29,29,29,29	1
61	K	13	1638	1/1	0.92	0.09	56,56,56,56	0
62	MG	14	3180	1/1	0.92	0.15	59,59,59,59	0
62	MG	1H	3508	1/1	0.92	0.12	22,22,22,22	0
62	MG	1H	3520	1/1	0.92	0.08	37,37,37,37	0
62	MG	14	3212	1/1	0.92	0.23	44,44,44,44	0
62	MG	1H	3346	1/1	0.92	0.24	55,55,55,55	0
62	MG	14	3185	1/1	0.92	0.21	51,51,51,51	0
62	MG	1H	3358	1/1	0.92	0.26	41,41,41,41	0
61	K	1H	3022	1/1	0.92	0.10	66,66,66,66	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
62	MG	1G	1663[B]	1/1	0.92	0.45	30,30,30,30	1
62	MG	13	1768	1/1	0.92	0.07	78,78,78,78	0
62	MG	13	1654	1/1	0.92	0.23	42,42,42,42	0
62	MG	14	3136	1/1	0.92	0.18	59,59,59,59	0
62	MG	1H	3390	1/1	0.92	0.10	26,26,26,26	0
62	MG	14	3274	1/1	0.92	0.15	54,54,54,54	0
61	K	1G	1608	1/1	0.92	0.08	80,80,80,80	0
62	MG	4L	101	1/1	0.92	0.25	79,79,79,79	0
62	MG	1G	1708	1/1	0.92	0.09	101,101,101,101	0
62	MG	1H	3475	1/1	0.92	0.11	40,40,40,40	0
62	MG	13	1706	1/1	0.92	0.16	46,46,46,46	0
62	MG	1H	3159	1/1	0.92	0.25	44,44,44,44	0
62	MG	14	3314	1/1	0.92	0.12	28,28,28,28	0
61	K	14	3024	1/1	0.92	0.08	52,52,52,52	0
61	K	1H	3135	1/1	0.92	0.15	82,82,82,82	0
62	MG	1H	3485	1/1	0.92	0.05	29,29,29,29	0
62	MG	13	1717	1/1	0.92	0.33	62,62,62,62	0
62	MG	14	3279	1/1	0.92	0.13	22,22,22,22	0
62	MG	1H	3506	1/1	0.92	0.16	15,15,15,15	0
62	MG	14	3373	1/1	0.92	0.10	68,68,68,68	0
61	K	1H	3081	1/1	0.92	0.17	49,49,49,49	0
61	K	14	3105	1/1	0.92	0.11	91,91,91,91	0
62	MG	1H	3163	1/1	0.93	0.39	55,55,55,55	0
62	MG	14	3397	1/1	0.93	0.18	75,75,75,75	0
62	MG	1H	3204	1/1	0.93	0.21	29,29,29,29	0
61	K	1H	3070	1/1	0.93	0.07	46,46,46,46	0
62	MG	1H	3434	1/1	0.93	0.06	46,46,46,46	0
61	K	14	3033	1/1	0.93	0.10	52,52,52,52	0
62	MG	16	204	1/1	0.93	0.26	39,39,39,39	0
62	MG	14	3374	1/1	0.93	0.11	30,30,30,30	0
62	MG	31	303	1/1	0.93	0.16	37,37,37,37	0
62	MG	1H	3269	1/1	0.93	0.13	33,33,33,33	0
62	MG	1H	3258	1/1	0.93	0.41	52,52,52,52	0
61	K	1H	3082	1/1	0.93	0.11	46,46,46,46	0
62	MG	1H	3523	1/1	0.93	0.10	32,32,32,32	0
62	MG	1H	3409	1/1	0.93	0.21	14,14,14,14	0
62	MG	14	3343	1/1	0.93	0.10	50,50,50,50	0
62	MG	1H	3169	1/1	0.93	0.26	15,15,15,15	0
61	K	1G	1617	1/1	0.93	0.08	63,63,63,63	0
62	MG	1G	1658	1/1	0.93	0.27	46,46,46,46	0
61	K	2K	103	1/1	0.93	0.07	79,79,79,79	0
62	MG	1H	3449	1/1	0.93	0.16	15,15,15,15	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
62	MG	14	3365	1/1	0.93	0.10	28,28,28,28	0
61	K	1H	3026	1/1	0.93	0.17	88,88,88,88	0
62	MG	13	1687	1/1	0.93	0.27	50,50,50,50	0
61	K	1H	3107	1/1	0.93	0.12	44,44,44,44	0
62	MG	14	3390	1/1	0.93	0.07	79,79,79,79	0
62	MG	1G	1702	1/1	0.93	0.09	64,64,64,64	0
62	MG	1H	3160	1/1	0.93	0.24	29,29,29,29	0
61	K	1H	3125	1/1	0.93	0.15	64,64,64,64	0
62	MG	14	3313	1/1	0.93	0.08	33,33,33,33	0
62	MG	1H	3565	1/1	0.93	0.14	25,25,25,25	0
62	MG	13	1747	1/1	0.93	0.13	32,32,32,32	0
61	K	14	3003	1/1	0.93	0.13	100,100,100,100	0
62	MG	14	3174	1/1	0.93	0.20	38,38,38,38	0
62	MG	1H	3296	1/1	0.93	0.15	32,32,32,32	0
62	MG	14	3400	1/1	0.93	0.06	63,63,63,63	0
62	MG	1G	1712	1/1	0.93	0.04	81,81,81,81	0
62	MG	1H	3233	1/1	0.93	0.17	51,51,51,51	0
62	MG	1J	203	1/1	0.93	0.20	48,48,48,48	0
61	K	14	3076	1/1	0.93	0.09	86,86,86,86	0
62	MG	1H	3515	1/1	0.93	0.12	40,40,40,40	0
61	K	13	1620	1/1	0.93	0.07	87,87,87,87	0
62	MG	3E	301	1/1	0.93	0.06	82,82,82,82	0
61	K	1H	3111	1/1	0.93	0.08	51,51,51,51	0
62	MG	1H	3318	1/1	0.93	0.10	56,56,56,56	0
62	MG	1H	3499	1/1	0.93	0.10	32,32,32,32	0
62	MG	1H	3205	1/1	0.93	0.27	33,33,33,33	0
61	K	1H	3073	1/1	0.93	0.09	56,56,56,56	0
62	MG	1H	3171	1/1	0.93	0.29	30,30,30,30	0
62	MG	1H	3339	1/1	0.93	0.14	55,55,55,55	0
62	MG	1H	3278	1/1	0.93	0.25	28,28,28,28	0
62	MG	1H	3479	1/1	0.93	0.13	18,18,18,18	0
62	MG	1G	1726	1/1	0.93	0.14	49,49,49,49	0
61	K	14	3039	1/1	0.93	0.14	61,61,61,61	0
61	K	13	1614	1/1	0.93	0.23	71,71,71,71	0
61	K	5E	201	1/1	0.93	0.08	76,76,76,76	0
62	MG	1H	3293	1/1	0.93	0.37	40,40,40,40	0
62	MG	14	3353	1/1	0.93	0.10	62,62,62,62	0
61	K	1H	3119	1/1	0.93	0.15	46,46,46,46	0
62	MG	14	3269	1/1	0.93	0.26	68,68,68,68	0
61	K	1G	1612	1/1	0.93	0.07	58,58,58,58	0
62	MG	1H	3383	1/1	0.93	0.20	18,18,18,18	0
61	K	21	301	1/1	0.93	0.10	62,62,62,62	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
62	MG	1H	3308	1/1	0.93	0.11	27,27,27,27	0
62	MG	1H	3243	1/1	0.93	0.32	41,41,41,41	0
62	MG	1H	3566	1/1	0.93	0.16	37,37,37,37	0
62	MG	1H	3546	1/1	0.93	0.06	61,61,61,61	0
62	MG	13	1736	1/1	0.93	0.11	44,44,44,44	0
62	MG	1H	3246	1/1	0.93	0.24	35,35,35,35	0
62	MG	13	1681	1/1	0.93	0.26	44,44,44,44	0
62	MG	14	3159	1/1	0.93	0.33	56,56,56,56	0
62	MG	1G	1667	1/1	0.93	0.23	42,42,42,42	0
62	MG	1H	3455	1/1	0.93	0.17	11,11,11,11	0
62	MG	1H	3543	1/1	0.93	0.12	48,48,48,48	0
61	K	14	3070	1/1	0.93	0.06	92,92,92,92	0
62	MG	1H	3286	1/1	0.93	0.32	48,48,48,48	0
61	K	1H	3108	1/1	0.93	0.16	76,76,76,76	0
62	MG	13	1686	1/1	0.93	0.10	34,34,34,34	0
62	MG	13	1711	1/1	0.93	0.28	55,55,55,55	0
61	K	13	1602	1/1	0.93	0.14	72,72,72,72	0
62	MG	13	1723	1/1	0.93	0.36	60,60,60,60	0
62	MG	1H	3545	1/1	0.93	0.07	45,45,45,45	0
62	MG	14	3366	1/1	0.93	0.09	55,55,55,55	0
62	MG	1H	3192	1/1	0.93	0.21	37,37,37,37	0
62	MG	C8	201	1/1	0.93	0.20	44,44,44,44	0
62	MG	1H	3355	1/1	0.93	0.17	57,57,57,57	0
62	MG	1H	3562	1/1	0.93	0.13	31,31,31,31	0
62	MG	1H	3315	1/1	0.93	0.32	43,43,43,43	0
62	MG	1H	3248	1/1	0.93	0.34	34,34,34,34	0
62	MG	1H	3313	1/1	0.93	0.09	44,44,44,44	0
61	K	1G	1635	1/1	0.93	0.27	91,91,91,91	0
61	K	1H	3006	1/1	0.93	0.11	44,44,44,44	0
62	MG	1H	3271	1/1	0.93	0.20	47,47,47,47	0
62	MG	1H	3265	1/1	0.93	0.11	48,48,48,48	0
61	K	1H	3105	1/1	0.93	0.12	50,50,50,50	0
62	MG	1H	3537	1/1	0.93	0.07	54,54,54,54	0
62	MG	1H	3155[A]	1/1	0.93	0.43	19,19,19,19	1
62	MG	13	1733	1/1	0.93	0.08	62,62,62,62	0
62	MG	1H	3155[B]	1/1	0.93	0.43	22,22,22,22	1
61	K	13	1606	1/1	0.93	0.12	57,57,57,57	0
62	MG	14	3138	1/1	0.93	0.17	31,31,31,31	0
62	MG	1H	3421	1/1	0.93	0.06	36,36,36,36	0
61	K	1H	3030	1/1	0.93	0.08	73,73,73,73	0
62	MG	1H	3392	1/1	0.93	0.07	51,51,51,51	0
62	MG	1H	3526	1/1	0.94	0.11	21,21,21,21	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
61	K	1H	3047	1/1	0.94	0.15	74,74,74,74	0
61	K	2K	101	1/1	0.94	0.20	62,62,62,62	0
62	MG	1H	3465	1/1	0.94	0.10	21,21,21,21	0
62	MG	14	3364	1/1	0.94	0.10	36,36,36,36	0
62	MG	1H	3426	1/1	0.94	0.20	12,12,12,12	0
61	K	1H	3038	1/1	0.94	0.24	56,56,56,56	0
62	MG	14	3379	1/1	0.94	0.07	43,43,43,43	0
62	MG	13	1729	1/1	0.94	0.05	61,61,61,61	0
62	MG	1H	3252	1/1	0.94	0.29	42,42,42,42	0
62	MG	13	1657	1/1	0.94	0.24	38,38,38,38	0
61	K	14	3081	1/1	0.94	0.09	54,54,54,54	0
62	MG	14	3357	1/1	0.94	0.08	48,48,48,48	0
62	MG	14	3234	1/1	0.94	0.21	55,55,55,55	0
62	MG	14	3107	1/1	0.94	0.17	33,33,33,33	0
62	MG	1G	1685	1/1	0.94	0.13	51,51,51,51	0
62	MG	13	1713	1/1	0.94	0.28	46,46,46,46	0
62	MG	13	1769	1/1	0.94	0.13	54,54,54,54	0
62	MG	1G	1670	1/1	0.94	0.15	57,57,57,57	0
62	MG	1G	1735	1/1	0.94	0.06	88,88,88,88	0
61	K	45	201	1/1	0.94	0.22	90,90,90,90	0
62	MG	P8	101	1/1	0.94	0.19	35,35,35,35	0
61	K	1H	3109	1/1	0.94	0.10	57,57,57,57	0
61	K	14	3022	1/1	0.94	0.10	50,50,50,50	0
61	K	1H	3045	1/1	0.94	0.10	59,59,59,59	0
62	MG	14	3306	1/1	0.94	0.10	32,32,32,32	0
62	MG	1H	3307	1/1	0.94	0.12	25,25,25,25	0
62	MG	14	3207	1/1	0.94	0.30	62,62,62,62	0
62	MG	1H	3443	1/1	0.94	0.08	42,42,42,42	0
62	MG	1H	3365	1/1	0.94	0.17	58,58,58,58	0
62	MG	1G	1710	1/1	0.94	0.06	59,59,59,59	0
62	MG	1G	1676	1/1	0.94	0.18	71,71,71,71	0
62	MG	41	202	1/1	0.94	0.15	55,55,55,55	0
62	MG	14	3170	1/1	0.94	0.23	54,54,54,54	0
62	MG	14	3175[A]	1/1	0.94	0.25	39,39,39,39	1
62	MG	14	3348	1/1	0.94	0.10	30,30,30,30	0
62	MG	1J	202	1/1	0.94	0.08	83,83,83,83	0
62	MG	1H	3476	1/1	0.94	0.15	15,15,15,15	0
62	MG	1G	1651	1/1	0.94	0.18	43,43,43,43	0
62	MG	1G	1701	1/1	0.94	0.10	45,45,45,45	0
62	MG	1H	3527	1/1	0.94	0.06	26,26,26,26	0
62	MG	13	1760	1/1	0.94	0.05	65,65,65,65	0
61	K	1H	3046	1/1	0.94	0.20	72,72,72,72	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
61	K	1H	3144	1/1	0.94	0.21	56,56,56,56	0
62	MG	1H	3503	1/1	0.94	0.12	29,29,29,29	0
62	MG	13	1691	1/1	0.94	0.26	50,50,50,50	0
62	MG	7I	101	1/1	0.94	0.15	71,71,71,71	0
62	MG	14	3340	1/1	0.94	0.11	26,26,26,26	0
61	K	13	1607	1/1	0.94	0.08	65,65,65,65	0
62	MG	14	3318	1/1	0.94	0.12	35,35,35,35	0
62	MG	1H	3184	1/1	0.94	0.26	40,40,40,40	0
61	K	13	1647	1/1	0.94	0.13	50,50,50,50	0
61	K	1H	3058	1/1	0.94	0.11	43,43,43,43	0
62	MG	14	3237	1/1	0.94	0.09	96,96,96,96	0
62	MG	1H	3214	1/1	0.94	0.32	41,41,41,41	0
61	K	14	3083	1/1	0.94	0.08	70,70,70,70	0
62	MG	14	3361	1/1	0.94	0.10	48,48,48,48	0
62	MG	1H	3478	1/1	0.94	0.07	44,44,44,44	0
61	K	13	1622	1/1	0.94	0.06	61,61,61,61	0
62	MG	14	3184	1/1	0.94	0.19	48,48,48,48	0
62	MG	1H	3222	1/1	0.94	0.27	32,32,32,32	0
62	MG	14	3213	1/1	0.94	0.11	40,40,40,40	0
61	K	1H	3122	1/1	0.94	0.07	65,65,65,65	0
62	MG	1H	3532	1/1	0.94	0.05	56,56,56,56	0
62	MG	1H	3369	1/1	0.94	0.31	46,46,46,46	0
62	MG	13	1721	1/1	0.94	0.13	99,99,99,99	0
61	K	2K	102	1/1	0.94	0.15	58,58,58,58	0
62	MG	1H	3200	1/1	0.94	0.25	36,36,36,36	0
62	MG	1H	3433	1/1	0.94	0.15	51,51,51,51	0
62	MG	2L	101	1/1	0.94	0.08	58,58,58,58	0
62	MG	13	1666	1/1	0.94	0.34	46,46,46,46	0
61	K	13	1640	1/1	0.94	0.07	60,60,60,60	0
62	MG	1H	3513	1/1	0.94	0.06	30,30,30,30	0
62	MG	N8	101	1/1	0.94	0.19	41,41,41,41	0
61	K	1H	3024	1/1	0.94	0.11	59,59,59,59	0
61	K	1H	3010	1/1	0.94	0.11	66,66,66,66	0
62	MG	1H	3224	1/1	0.94	0.23	35,35,35,35	0
61	K	14	3087	1/1	0.94	0.11	74,74,74,74	0
62	MG	14	3271	1/1	0.94	0.21	51,51,51,51	0
61	K	13	1630	1/1	0.94	0.07	66,66,66,66	0
61	K	13	1604	1/1	0.94	0.09	82,82,82,82	0
62	MG	1H	3341	1/1	0.94	0.19	24,24,24,24	0
62	MG	14	3377	1/1	0.94	0.05	59,59,59,59	0
62	MG	16	215	1/1	0.94	0.09	52,52,52,52	0
62	MG	14	3330	1/1	0.94	0.10	39,39,39,39	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
61	K	13	1621	1/1	0.94	0.07	61,61,61,61	0
62	MG	14	3224	1/1	0.94	0.12	36,36,36,36	0
62	MG	13	1718	1/1	0.94	0.30	55,55,55,55	0
62	MG	13	1730	1/1	0.94	0.09	76,76,76,76	0
62	MG	1H	3314	1/1	0.94	0.19	41,41,41,41	0
61	K	14	3047	1/1	0.94	0.11	74,74,74,74	0
62	MG	14	3284	1/1	0.94	0.06	34,34,34,34	0
62	MG	32	302	1/1	0.94	0.09	79,79,79,79	0
62	MG	1H	3348	1/1	0.94	0.18	30,30,30,30	0
61	K	14	3104	1/1	0.94	0.08	75,75,75,75	0
62	MG	14	3315	1/1	0.94	0.09	39,39,39,39	0
61	K	4A	201	1/1	0.94	0.09	96,96,96,96	0
61	K	13	1644	1/1	0.94	0.14	74,74,74,74	0
62	MG	14	3220	1/1	0.94	0.09	46,46,46,46	0
62	MG	1H	3398	1/1	0.94	0.05	52,52,52,52	0
62	MG	14	3392	1/1	0.94	0.16	75,75,75,75	0
62	MG	14	3276	1/1	0.94	0.13	52,52,52,52	0
61	K	88	201	1/1	0.94	0.14	57,57,57,57	0
62	MG	1H	3349	1/1	0.94	0.23	48,48,48,48	0
62	MG	14	3351	1/1	0.94	0.11	55,55,55,55	0
62	MG	1G	1700	1/1	0.94	0.28	52,52,52,52	0
61	K	1H	3011	1/1	0.94	0.10	59,59,59,59	0
62	MG	14	3131	1/1	0.94	0.15	43,43,43,43	0
61	K	1H	3088	1/1	0.94	0.06	50,50,50,50	0
61	K	13	1635	1/1	0.94	0.11	95,95,95,95	0
62	MG	14	3175[B]	1/1	0.94	0.25	36,36,36,36	1
62	MG	14	3293	1/1	0.94	0.10	60,60,60,60	0
62	MG	1H	3270	1/1	0.94	0.12	42,42,42,42	0
61	K	1G	1611	1/1	0.94	0.10	86,86,86,86	0
62	MG	14	3359	1/1	0.94	0.10	33,33,33,33	0
62	MG	1H	3181	1/1	0.94	0.23	36,36,36,36	0
62	MG	1G	1723	1/1	0.94	0.14	59,59,59,59	0
61	K	1H	3114	1/1	0.94	0.16	55,55,55,55	0
62	MG	1H	3351	1/1	0.94	0.38	79,79,79,79	0
62	MG	1H	3344	1/1	0.94	0.24	39,39,39,39	0
61	K	14	3020	1/1	0.94	0.08	64,64,64,64	0
62	MG	14	3199	1/1	0.94	0.22	66,66,66,66	0
62	MG	1H	3490	1/1	0.94	0.08	32,32,32,32	0
61	K	14	3009	1/1	0.94	0.18	64,64,64,64	0
62	MG	14	3376	1/1	0.94	0.07	54,54,54,54	0
62	MG	14	3311	1/1	0.95	0.13	31,31,31,31	0
61	K	1H	3101	1/1	0.95	0.08	49,49,49,49	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
61	K	14	3029	1/1	0.95	0.14	81,81,81,81	0
62	MG	1H	3251	1/1	0.95	0.28	39,39,39,39	0
62	MG	1H	3483	1/1	0.95	0.07	36,36,36,36	0
62	MG	1H	3399	1/1	0.95	0.11	24,24,24,24	0
61	K	1H	3080	1/1	0.95	0.11	45,45,45,45	0
61	K	52	201	1/1	0.95	0.05	76,76,76,76	0
62	MG	14	3393	1/1	0.95	0.11	63,63,63,63	0
61	K	1H	3121	1/1	0.95	0.12	62,62,62,62	0
62	MG	1G	1729	1/1	0.95	0.09	67,67,67,67	0
61	K	13	1616	1/1	0.95	0.09	75,75,75,75	0
62	MG	13	1744	1/1	0.95	0.13	19,19,19,19	0
61	K	1H	3136	1/1	0.95	0.12	54,54,54,54	0
61	K	1H	3124	1/1	0.95	0.08	64,64,64,64	0
62	MG	14	3259	1/1	0.95	0.18	42,42,42,42	0
62	MG	14	3257	1/1	0.95	0.34	65,65,65,65	0
62	MG	1H	3212	1/1	0.95	0.13	44,44,44,44	0
61	K	1H	3052	1/1	0.95	0.15	52,52,52,52	0
62	MG	14	3247	1/1	0.95	0.09	47,47,47,47	0
62	MG	2L	103	1/1	0.95	0.21	45,45,45,45	0
62	MG	1H	3289	1/1	0.95	0.30	35,35,35,35	0
62	MG	1H	3310	1/1	0.95	0.14	18,18,18,18	0
62	MG	13	1688	1/1	0.95	0.28	56,56,56,56	0
62	MG	1H	3353	1/1	0.95	0.30	33,33,33,33	0
61	K	1H	3009	1/1	0.95	0.12	64,64,64,64	0
62	MG	14	3168	1/1	0.95	0.24	37,37,37,37	0
62	MG	14	3292	1/1	0.95	0.15	29,29,29,29	0
62	MG	1H	3274	1/1	0.95	0.10	31,31,31,31	0
62	MG	2L	102	1/1	0.95	0.27	56,56,56,56	0
62	MG	13	1696	1/1	0.95	0.30	64,64,64,64	0
62	MG	14	3304	1/1	0.95	0.05	63,63,63,63	0
62	MG	1G	1703	1/1	0.95	0.09	81,81,81,81	0
62	MG	1H	3316	1/1	0.95	0.18	60,60,60,60	0
62	MG	14	3356	1/1	0.95	0.09	36,36,36,36	0
62	MG	14	3163	1/1	0.95	0.19	31,31,31,31	0
61	K	13	1636	1/1	0.95	0.08	70,70,70,70	0
62	MG	13	1697	1/1	0.95	0.31	45,45,45,45	0
62	MG	14	3229	1/1	0.95	0.12	48,48,48,48	0
61	K	1H	3097	1/1	0.95	0.09	25,25,25,25	0
62	MG	14	3339	1/1	0.95	0.11	29,29,29,29	0
62	MG	14	3367	1/1	0.95	0.05	70,70,70,70	0
62	MG	14	3320	1/1	0.95	0.11	25,25,25,25	0
61	K	1H	3012	1/1	0.95	0.07	51,51,51,51	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
61	K	1H	3137	1/1	0.95	0.15	63,63,63,63	0
62	MG	1G	1713	1/1	0.95	0.07	120,120,120,120	0
62	MG	1H	3494	1/1	0.95	0.06	43,43,43,43	0
62	MG	1G	1694	1/1	0.95	0.15	43,43,43,43	0
62	MG	1H	3197	1/1	0.95	0.14	30,30,30,30	0
62	MG	1H	3557	1/1	0.95	0.11	22,22,22,22	0
62	MG	14	3298	1/1	0.95	0.12	32,32,32,32	0
62	MG	1H	3425	1/1	0.95	0.11	16,16,16,16	0
62	MG	1H	3182	1/1	0.95	0.24	49,49,49,49	0
62	MG	14	3183	1/1	0.95	0.25	30,30,30,30	0
62	MG	1H	3244	1/1	0.95	0.23	34,34,34,34	0
61	K	14	3096	1/1	0.95	0.07	70,70,70,70	0
61	K	1H	3015	1/1	0.95	0.14	44,44,44,44	0
62	MG	1H	3292	1/1	0.95	0.10	32,32,32,32	0
62	MG	1H	3196	1/1	0.95	0.20	40,40,40,40	0
62	MG	1H	3420	1/1	0.95	0.16	20,20,20,20	0
62	MG	14	3121	1/1	0.95	0.31	47,47,47,47	0
61	K	14	3055	1/1	0.95	0.39	65,65,65,65	0
62	MG	J8	101	1/1	0.95	0.24	32,32,32,32	0
62	MG	1H	3463	1/1	0.95	0.12	17,17,17,17	0
61	K	1H	3098	1/1	0.95	0.10	41,41,41,41	0
62	MG	1H	3524	1/1	0.95	0.13	16,16,16,16	0
62	MG	Q8	101[A]	1/1	0.95	0.37	13,13,13,13	1
61	K	14	3106	1/1	0.95	0.29	68,68,68,68	0
61	K	13	1625	1/1	0.95	0.09	77,77,77,77	0
62	MG	1H	3491	1/1	0.95	0.12	42,42,42,42	0
62	MG	13	1716	1/1	0.95	0.13	37,37,37,37	0
61	K	13	1627	1/1	0.95	0.14	46,46,46,46	0
62	MG	14	3191	1/1	0.95	0.10	34,34,34,34	0
62	MG	14	3146	1/1	0.95	0.21	49,49,49,49	0
61	K	1H	3049	1/1	0.95	0.12	55,55,55,55	0
62	MG	1H	3573	1/1	0.95	0.09	40,40,40,40	0
61	K	14	3069	1/1	0.95	0.09	56,56,56,56	0
62	MG	1H	3357	1/1	0.95	0.19	28,28,28,28	0
62	MG	1J	204	1/1	0.95	0.27	64,64,64,64	0
62	MG	1H	3149	1/1	0.95	0.30	40,40,40,40	0
61	K	14	3051	1/1	0.95	0.09	65,65,65,65	0
62	MG	1H	3152	1/1	0.95	0.10	36,36,36,36	0
62	MG	14	3342	1/1	0.95	0.10	32,32,32,32	0
62	MG	13	1652	1/1	0.95	0.23	43,43,43,43	0
61	K	1H	3120	1/1	0.95	0.12	60,60,60,60	0
62	MG	1G	1682	1/1	0.95	0.31	41,41,41,41	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
62	MG	1H	3262	1/1	0.95	0.42	46,46,46,46	0
62	MG	1H	3280	1/1	0.95	0.12	86,86,86,86	0
62	MG	14	3115	1/1	0.95	0.14	42,42,42,42	0
61	K	1H	3039	1/1	0.95	0.15	54,54,54,54	0
62	MG	14	3171	1/1	0.95	0.21	55,55,55,55	0
62	MG	14	3319	1/1	0.95	0.07	27,27,27,27	0
62	MG	13	1689	1/1	0.95	0.29	53,53,53,53	0
62	MG	1H	3501	1/1	0.95	0.17	57,57,57,57	0
62	MG	14	3324	1/1	0.95	0.09	43,43,43,43	0
62	MG	1H	3253	1/1	0.95	0.39	41,41,41,41	0
62	MG	14	3111	1/1	0.95	0.16	32,32,32,32	0
61	K	14	3082	1/1	0.95	0.08	80,80,80,80	0
61	K	13	1639	1/1	0.95	0.08	66,66,66,66	0
62	MG	1H	3219	1/1	0.95	0.33	31,31,31,31	0
61	K	14	3085	1/1	0.95	0.10	62,62,62,62	0
62	MG	1H	3445	1/1	0.95	0.09	50,50,50,50	0
62	MG	14	3140	1/1	0.95	0.13	47,47,47,47	0
61	K	1H	3096	1/1	0.95	0.19	52,52,52,52	0
62	MG	1H	3533	1/1	0.95	0.07	49,49,49,49	0
62	MG	1H	3235	1/1	0.95	0.13	42,42,42,42	0
62	MG	1G	1664	1/1	0.95	0.26	40,40,40,40	0
62	MG	16	208	1/1	0.95	0.20	44,44,44,44	0
62	MG	Q8	101[B]	1/1	0.95	0.37	11,11,11,11	1
62	MG	13	1674	1/1	0.95	0.21	75,75,75,75	0
62	MG	1G	1643	1/1	0.95	0.20	62,62,62,62	0
62	MG	1H	3505	1/1	0.95	0.10	16,16,16,16	0
61	K	1G	1622	1/1	0.95	0.08	74,74,74,74	0
62	MG	14	3385	1/1	0.95	0.06	58,58,58,58	0
61	K	14	3073	1/1	0.95	0.07	60,60,60,60	0
62	MG	1H	3448	1/1	0.95	0.09	57,57,57,57	0
62	MG	13	1728	1/1	0.95	0.10	60,60,60,60	0
62	MG	14	3117	1/1	0.95	0.10	49,49,49,49	0
61	K	13	1641	1/1	0.95	0.08	84,84,84,84	0
62	MG	1H	3322	1/1	0.95	0.17	23,23,23,23	0
61	K	13	1601	1/1	0.95	0.10	67,67,67,67	0
62	MG	1H	3382	1/1	0.95	0.17	13,13,13,13	0
61	K	14	3049	1/1	0.95	0.06	49,49,49,49	0
62	MG	1G	1719	1/1	0.95	0.25	66,66,66,66	0
62	MG	14	3329	1/1	0.95	0.08	28,28,28,28	0
61	K	1H	3112	1/1	0.95	0.14	48,48,48,48	0
61	K	1H	3094	1/1	0.95	0.17	51,51,51,51	0
62	MG	1H	3177	1/1	0.95	0.30	29,29,29,29	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
62	MG	1H	3436	1/1	0.95	0.06	57,57,57,57	0
62	MG	14	3162	1/1	0.95	0.13	46,46,46,46	0
62	MG	14	3335	1/1	0.95	0.05	70,70,70,70	0
62	MG	13	1759	1/1	0.95	0.06	52,52,52,52	0
61	K	1H	3084	1/1	0.95	0.14	47,47,47,47	0
62	MG	14	3395	1/1	0.95	0.09	25,25,25,25	0
61	K	14	3017	1/1	0.95	0.21	52,52,52,52	0
62	MG	1H	3223	1/1	0.95	0.20	30,30,30,30	0
61	K	1H	3061	1/1	0.95	0.08	43,43,43,43	0
62	MG	14	3289	1/1	0.95	0.14	51,51,51,51	0
61	K	14	3018	1/1	0.95	0.07	65,65,65,65	0
62	MG	13	1667	1/1	0.95	0.20	29,29,29,29	0
61	K	1H	3035	1/1	0.95	0.25	52,52,52,52	0
62	MG	42	201	1/1	0.96	0.18	70,70,70,70	0
62	MG	14	3222	1/1	0.96	0.20	57,57,57,57	0
62	MG	1H	3430	1/1	0.96	0.10	54,54,54,54	0
62	MG	14	3296	1/1	0.96	0.09	35,35,35,35	0
62	MG	1G	1640	1/1	0.96	0.39	51,51,51,51	0
62	MG	1H	3156	1/1	0.96	0.39	33,33,33,33	0
61	K	1H	3042	1/1	0.96	0.10	54,54,54,54	0
61	K	19	301	1/1	0.96	0.15	52,52,52,52	0
61	K	14	3056	1/1	0.96	0.13	56,56,56,56	0
62	MG	1H	3560	1/1	0.96	0.16	13,13,13,13	0
62	MG	14	3300	1/1	0.96	0.07	61,61,61,61	0
61	K	1G	1636	1/1	0.96	0.10	78,78,78,78	0
61	K	14	3095	1/1	0.96	0.06	64,64,64,64	0
62	MG	14	3139	1/1	0.96	0.15	41,41,41,41	0
61	K	14	3062	1/1	0.96	0.13	76,76,76,76	0
62	MG	1H	3291	1/1	0.96	0.20	47,47,47,47	0
61	K	1H	3115	1/1	0.96	0.07	52,52,52,52	0
61	K	14	3103	1/1	0.96	0.10	70,70,70,70	0
62	MG	14	3254	1/1	0.96	0.18	62,62,62,62	0
62	MG	1H	3356	1/1	0.96	0.17	43,43,43,43	0
61	K	14	3002	1/1	0.96	0.06	69,69,69,69	0
62	MG	1H	3462	1/1	0.96	0.09	27,27,27,27	0
61	K	1H	3031	1/1	0.96	0.07	39,39,39,39	0
62	MG	1H	3158	1/1	0.96	0.22	57,57,57,57	0
61	K	1H	3085	1/1	0.96	0.07	39,39,39,39	0
62	MG	1G	1681	1/1	0.96	0.28	45,45,45,45	0
62	MG	1G	1673	1/1	0.96	0.13	50,50,50,50	0
62	MG	1H	3459	1/1	0.96	0.10	15,15,15,15	0
62	MG	14	3322	1/1	0.96	0.09	41,41,41,41	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
61	K	1G	1603	1/1	0.96	0.21	62,62,62,62	0
62	MG	1H	3273	1/1	0.96	0.25	61,61,61,61	0
62	MG	14	3252	1/1	0.96	0.17	42,42,42,42	0
62	MG	1H	3471	1/1	0.96	0.07	56,56,56,56	0
62	MG	1H	3531	1/1	0.96	0.07	21,21,21,21	0
61	K	14	3015	1/1	0.96	0.07	47,47,47,47	0
62	MG	1H	3228	1/1	0.96	0.27	31,31,31,31	0
62	MG	1H	3435	1/1	0.96	0.05	46,46,46,46	0
61	K	1H	3054	1/1	0.96	0.10	27,27,27,27	0
62	MG	14	3227	1/1	0.96	0.14	38,38,38,38	0
62	MG	14	3211	1/1	0.96	0.23	58,58,58,58	0
61	K	14	3074	1/1	0.96	0.13	73,73,73,73	0
62	MG	1G	1645	1/1	0.96	0.19	62,62,62,62	0
61	K	1H	3037	1/1	0.96	0.24	70,70,70,70	0
62	MG	1H	3470	1/1	0.96	0.14	24,24,24,24	0
61	K	1H	3034	1/1	0.96	0.16	66,66,66,66	0
62	MG	14	3238	1/1	0.96	0.14	44,44,44,44	0
62	MG	1G	1668	1/1	0.96	0.33	69,69,69,69	0
62	MG	1H	3208	1/1	0.96	0.12	37,37,37,37	0
61	K	14	3084	1/1	0.96	0.07	73,73,73,73	0
62	MG	14	3198	1/1	0.96	0.14	33,33,33,33	0
61	K	1G	1628	1/1	0.96	0.14	76,76,76,76	0
62	MG	1G	1648	1/1	0.96	0.25	67,67,67,67	0
61	K	1H	3143	1/1	0.96	0.09	71,71,71,71	0
62	MG	13	1731	1/1	0.96	0.14	38,38,38,38	0
61	K	14	3026	1/1	0.96	0.09	35,35,35,35	0
61	K	1H	3067	1/1	0.96	0.10	53,53,53,53	0
62	MG	1G	1646	1/1	0.96	0.22	66,66,66,66	0
62	MG	1H	3577	1/1	0.96	0.10	37,37,37,37	0
61	K	13	1634	1/1	0.96	0.07	90,90,90,90	0
62	MG	1H	3525	1/1	0.96	0.09	15,15,15,15	0
61	K	1G	1620	1/1	0.96	0.10	83,83,83,83	0
61	K	14	3010	1/1	0.96	0.08	58,58,58,58	0
62	MG	1H	3195	1/1	0.96	0.25	37,37,37,37	0
62	MG	13	1661	1/1	0.96	0.23	39,39,39,39	0
62	MG	13	1765	1/1	0.96	0.09	73,73,73,73	0
62	MG	1H	3283	1/1	0.96	0.31	44,44,44,44	0
62	MG	1H	3427	1/1	0.96	0.04	36,36,36,36	0
61	K	14	3078	1/1	0.96	0.08	81,81,81,81	0
61	K	1H	3113	1/1	0.96	0.12	30,30,30,30	0
62	MG	1H	3173	1/1	0.96	0.20	28,28,28,28	0
61	K	13	1624	1/1	0.96	0.10	59,59,59,59	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
62	MG	14	3302	1/1	0.96	0.13	29,29,29,29	0
62	MG	14	3113	1/1	0.96	0.19	36,36,36,36	0
62	MG	1H	3444	1/1	0.96	0.12	23,23,23,23	0
61	K	14	3043	1/1	0.96	0.11	80,80,80,80	0
62	MG	14	3218	1/1	0.96	0.13	60,60,60,60	0
62	MG	14	3204	1/1	0.96	0.17	38,38,38,38	0
62	MG	1H	3261	1/1	0.96	0.07	44,44,44,44	0
62	MG	1H	3538	1/1	0.96	0.14	27,27,27,27	0
62	MG	1H	3247	1/1	0.96	0.26	21,21,21,21	0
62	MG	1H	3206	1/1	0.96	0.20	25,25,25,25	0
61	K	1H	3128	1/1	0.96	0.08	64,64,64,64	0
61	K	14	3100	1/1	0.96	0.13	71,71,71,71	0
61	K	1H	3064	1/1	0.96	0.10	34,34,34,34	0
62	MG	1G	1732	1/1	0.96	0.07	83,83,83,83	0
62	MG	14	3108	1/1	0.96	0.19	59,59,59,59	0
61	K	1H	3016	1/1	0.96	0.08	63,63,63,63	0
61	K	1H	3029	1/1	0.96	0.08	85,85,85,85	0
62	MG	1H	3319	1/1	0.96	0.21	50,50,50,50	0
62	MG	1G	1638	1/1	0.96	0.21	46,46,46,46	0
62	MG	1H	3256	1/1	0.96	0.19	40,40,40,40	0
62	MG	M5	102	1/1	0.96	0.12	58,58,58,58	0
62	MG	1H	3176[A]	1/1	0.96	0.26	21,21,21,21	1
62	MG	1H	3441	1/1	0.96	0.07	61,61,61,61	0
62	MG	1H	3231	1/1	0.96	0.29	43,43,43,43	0
61	K	14	3060	1/1	0.96	0.08	45,45,45,45	0
62	MG	1H	3511	1/1	0.96	0.11	26,26,26,26	0
61	K	14	3030	1/1	0.96	0.07	63,63,63,63	0
62	MG	14	3110	1/1	0.96	0.17	35,35,35,35	0
62	MG	1H	3568	1/1	0.96	0.06	34,34,34,34	0
61	K	14	3028	1/1	0.96	0.10	45,45,45,45	0
61	K	1H	3079	1/1	0.96	0.17	37,37,37,37	0
62	MG	1H	3226	1/1	0.96	0.40	40,40,40,40	0
62	MG	14	3152	1/1	0.96	0.18	32,32,32,32	0
62	MG	1H	3360	1/1	0.96	0.11	28,28,28,28	0
62	MG	1J	205	1/1	0.96	0.10	68,68,68,68	0
62	MG	1H	3317	1/1	0.96	0.34	52,52,52,52	0
62	MG	1H	3502	1/1	0.96	0.09	25,25,25,25	0
62	MG	1H	3395	1/1	0.96	0.14	23,23,23,23	0
62	MG	1H	3530	1/1	0.96	0.10	21,21,21,21	0
61	K	13	1626	1/1	0.96	0.09	73,73,73,73	0
62	MG	1H	3387	1/1	0.96	0.09	16,16,16,16	0
62	MG	1G	1652	1/1	0.96	0.20	17,17,17,17	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
62	MG	14	3301	1/1	0.96	0.12	38,38,38,38	0
62	MG	1H	3468	1/1	0.96	0.11	24,24,24,24	0
62	MG	1H	3176[B]	1/1	0.96	0.26	20,20,20,20	1
62	MG	14	3251	1/1	0.96	0.19	45,45,45,45	0
61	K	1H	3104	1/1	0.96	0.09	42,42,42,42	0
62	MG	14	3169	1/1	0.96	0.18	33,33,33,33	0
61	K	14	3066	1/1	0.96	0.07	64,64,64,64	0
62	MG	14	3288	1/1	0.96	0.12	39,39,39,39	0
61	K	14	3093	1/1	0.96	0.05	53,53,53,53	0
62	MG	1G	1680	1/1	0.96	0.26	50,50,50,50	0
62	MG	14	3205	1/1	0.96	0.28	51,51,51,51	0
62	MG	14	3246	1/1	0.96	0.10	35,35,35,35	0
61	K	1G	1633	1/1	0.96	0.05	76,76,76,76	0
62	MG	1H	3509	1/1	0.96	0.13	27,27,27,27	0
61	K	13	1618	1/1	0.96	0.07	85,85,85,85	0
62	MG	1H	3277	1/1	0.96	0.25	42,42,42,42	0
61	K	1H	3063	1/1	0.96	0.15	47,47,47,47	0
61	K	14	3016	1/1	0.96	0.08	44,44,44,44	0
62	MG	1H	3456	1/1	0.96	0.24	14,14,14,14	0
62	MG	14	3141	1/1	0.96	0.16	26,26,26,26	0
62	MG	14	3144	1/1	0.96	0.13	36,36,36,36	0
61	K	14	3027	1/1	0.96	0.18	54,54,54,54	0
62	MG	14	3236	1/1	0.96	0.30	50,50,50,50	0
61	K	14	3075	1/1	0.97	0.06	36,36,36,36	0
61	K	13	1632	1/1	0.97	0.12	79,79,79,79	0
62	MG	1H	3216	1/1	0.97	0.27	34,34,34,34	0
61	K	14	3021	1/1	0.97	0.11	41,41,41,41	0
61	K	1H	3014	1/1	0.97	0.11	60,60,60,60	0
61	K	BA	201	1/1	0.97	0.06	72,72,72,72	0
62	MG	14	3156	1/1	0.97	0.21	34,34,34,34	0
61	K	14	3089	1/1	0.97	0.04	64,64,64,64	0
61	K	1G	1624	1/1	0.97	0.07	60,60,60,60	0
62	MG	1H	3400	1/1	0.97	0.15	20,20,20,20	0
62	MG	1H	3411	1/1	0.97	0.12	20,20,20,20	0
62	MG	13	1752	1/1	0.97	0.08	47,47,47,47	0
62	MG	13	1660	1/1	0.97	0.16	39,39,39,39	0
62	MG	1H	3379	1/1	0.97	0.38	47,47,47,47	0
61	K	1H	3007	1/1	0.97	0.07	55,55,55,55	0
62	MG	1G	1654	1/1	0.97	0.30	50,50,50,50	0
62	MG	14	3398	1/1	0.97	0.09	47,47,47,47	0
62	MG	1H	3301	1/1	0.97	0.20	41,41,41,41	0
62	MG	13	1712	1/1	0.97	0.24	43,43,43,43	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
62	MG	1H	3460	1/1	0.97	0.14	11,11,11,11	0
62	MG	14	3346	1/1	0.97	0.12	52,52,52,52	0
62	MG	1G	1665	1/1	0.97	0.09	50,50,50,50	0
61	K	1H	3132	1/1	0.97	0.19	87,87,87,87	0
62	MG	1H	3167	1/1	0.97	0.24	20,20,20,20	0
62	MG	13	1745	1/1	0.97	0.07	39,39,39,39	0
62	MG	14	3338	1/1	0.97	0.07	34,34,34,34	0
62	MG	1H	3403	1/1	0.97	0.14	27,27,27,27	0
62	MG	14	3345	1/1	0.97	0.07	48,48,48,48	0
61	K	14	3094	1/1	0.97	0.11	86,86,86,86	0
62	MG	I8	101	1/1	0.97	0.18	26,26,26,26	0
62	MG	1H	3492	1/1	0.97	0.08	63,63,63,63	0
62	MG	1H	3284	1/1	0.97	0.15	36,36,36,36	0
62	MG	1H	3570	1/1	0.97	0.06	50,50,50,50	0
62	MG	1H	3342	1/1	0.97	0.29	27,27,27,27	0
62	MG	16	211	1/1	0.97	0.08	57,57,57,57	0
62	MG	14	3347	1/1	0.97	0.12	27,27,27,27	0
62	MG	14	3196	1/1	0.97	0.12	59,59,59,59	0
62	MG	1H	3178	1/1	0.97	0.18	17,17,17,17	0
61	K	14	3011	1/1	0.97	0.13	80,80,80,80	0
62	MG	1G	1656	1/1	0.97	0.32	58,58,58,58	0
62	MG	1G	1672	1/1	0.97	0.21	66,66,66,66	0
62	MG	1H	3229	1/1	0.97	0.33	43,43,43,43	0
61	K	1H	3043	1/1	0.97	0.12	58,58,58,58	0
62	MG	14	3114	1/1	0.97	0.08	33,33,33,33	0
62	MG	14	3130	1/1	0.97	0.07	38,38,38,38	0
62	MG	2K	105	1/1	0.97	0.06	45,45,45,45	0
62	MG	14	3133	1/1	0.97	0.22	39,39,39,39	0
62	MG	13	1675	1/1	0.97	0.24	49,49,49,49	0
62	MG	1H	3414	1/1	0.97	0.13	39,39,39,39	0
62	MG	14	3371	1/1	0.97	0.10	32,32,32,32	0
62	MG	14	3245	1/1	0.97	0.22	36,36,36,36	0
62	MG	14	3129	1/1	0.97	0.15	34,34,34,34	0
62	MG	1H	3368	1/1	0.97	0.28	44,44,44,44	0
61	K	1H	3127	1/1	0.97	0.07	47,47,47,47	0
62	MG	1H	3412	1/1	0.97	0.15	16,16,16,16	0
61	K	1G	1630	1/1	0.97	0.10	80,80,80,80	0
62	MG	1H	3487	1/1	0.97	0.07	41,41,41,41	0
61	K	1H	3013	1/1	0.97	0.20	81,81,81,81	0
61	K	1H	3071	1/1	0.97	0.10	42,42,42,42	0
62	MG	13	1746	1/1	0.97	0.12	37,37,37,37	0
62	MG	1H	3217	1/1	0.97	0.34	31,31,31,31	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
62	MG	14	3134	1/1	0.97	0.22	34,34,34,34	0
62	MG	1H	3397	1/1	0.97	0.14	17,17,17,17	0
62	MG	1H	3519	1/1	0.97	0.25	25,25,25,25	0
61	K	1H	3100	1/1	0.97	0.10	44,44,44,44	0
62	MG	14	3355	1/1	0.97	0.08	39,39,39,39	0
62	MG	1H	3405	1/1	0.97	0.07	16,16,16,16	0
62	MG	13	1693	1/1	0.97	0.31	61,61,61,61	0
61	K	14	3032	1/1	0.97	0.14	53,53,53,53	0
61	K	13	1629	1/1	0.97	0.08	50,50,50,50	0
61	K	13	1613	1/1	0.97	0.10	76,76,76,76	0
62	MG	1H	3393	1/1	0.97	0.11	17,17,17,17	0
61	K	14	3005	1/1	0.97	0.12	82,82,82,82	0
62	MG	13	1653	1/1	0.97	0.23	67,67,67,67	0
61	K	13	1633	1/1	0.97	0.13	55,55,55,55	0
62	MG	1H	3464	1/1	0.97	0.15	23,23,23,23	0
62	MG	14	3112	1/1	0.97	0.14	44,44,44,44	0
62	MG	1H	3215	1/1	0.97	0.20	40,40,40,40	0
62	MG	1H	3571	1/1	0.97	0.15	26,26,26,26	0
62	MG	1G	1684	1/1	0.97	0.15	79,79,79,79	0
62	MG	1G	1675	1/1	0.97	0.15	65,65,65,65	0
61	K	14	3057	1/1	0.97	0.07	54,54,54,54	0
61	K	1H	3118	1/1	0.97	0.15	56,56,56,56	0
62	MG	1H	3407	1/1	0.97	0.14	16,16,16,16	0
62	MG	29	303	1/1	0.97	0.08	28,28,28,28	0
62	MG	1H	3210	1/1	0.97	0.23	38,38,38,38	0
62	MG	1H	3507	1/1	0.97	0.11	17,17,17,17	0
62	MG	14	3179	1/1	0.97	0.20	32,32,32,32	0
62	MG	14	3158	1/1	0.97	0.26	49,49,49,49	0
62	MG	1H	3288	1/1	0.97	0.17	44,44,44,44	0
62	MG	1H	3267	1/1	0.97	0.13	53,53,53,53	0
62	MG	14	3150	1/1	0.97	0.17	29,29,29,29	0
62	MG	1H	3338	1/1	0.97	0.13	43,43,43,43	0
61	K	1G	1626	1/1	0.97	0.07	67,67,67,67	0
61	K	1G	1610	1/1	0.97	0.10	68,68,68,68	0
62	MG	1H	3350	1/1	0.97	0.22	25,25,25,25	0
61	K	1H	3093	1/1	0.97	0.09	42,42,42,42	0
61	K	14	3077	1/1	0.97	0.12	73,73,73,73	0
61	K	1G	1615	1/1	0.97	0.07	60,60,60,60	0
62	MG	1G	1706	1/1	0.97	0.11	43,43,43,43	0
62	MG	1H	3304	1/1	0.97	0.25	38,38,38,38	0
61	K	1H	3057	1/1	0.97	0.08	23,23,23,23	0
62	MG	1H	3147	1/1	0.97	0.23	54,54,54,54	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
62	MG	1H	3166	1/1	0.97	0.14	41,41,41,41	0
62	MG	1H	3257	1/1	0.97	0.20	40,40,40,40	0
62	MG	14	3203	1/1	0.97	0.30	45,45,45,45	0
62	MG	14	3132	1/1	0.97	0.20	53,53,53,53	0
62	MG	13	1743	1/1	0.97	0.10	54,54,54,54	0
62	MG	1H	3518	1/1	0.97	0.09	37,37,37,37	0
61	K	1H	3025	1/1	0.97	0.10	53,53,53,53	0
62	MG	1H	3187	1/1	0.97	0.19	30,30,30,30	0
62	MG	14	3316	1/1	0.97	0.08	34,34,34,34	0
61	K	1G	1613	1/1	0.97	0.06	63,63,63,63	0
61	K	1G	1606	1/1	0.97	0.21	61,61,61,61	0
62	MG	1H	3324	1/1	0.97	0.24	12,12,12,12	0
61	K	14	3071	1/1	0.97	0.09	77,77,77,77	0
61	K	14	3025	1/1	0.97	0.05	50,50,50,50	0
62	MG	14	3193	1/1	0.97	0.16	40,40,40,40	0
61	K	1H	3053	1/1	0.97	0.13	25,25,25,25	0
62	MG	13	1754	1/1	0.97	0.09	35,35,35,35	0
61	K	31	301	1/1	0.97	0.09	48,48,48,48	0
62	MG	1H	3306	1/1	0.97	0.12	34,34,34,34	0
62	MG	1H	3236	1/1	0.97	0.32	43,43,43,43	0
62	MG	1G	1642	1/1	0.97	0.18	45,45,45,45	0
62	MG	1G	1639	1/1	0.97	0.25	69,69,69,69	0
62	MG	13	1685	1/1	0.97	0.27	45,45,45,45	0
61	K	14	3042	1/1	0.97	0.09	51,51,51,51	0
62	MG	78	202	1/1	0.97	0.10	30,30,30,30	0
61	K	1H	3103	1/1	0.97	0.14	33,33,33,33	0
62	MG	1H	3230	1/1	0.97	0.34	39,39,39,39	0
61	K	14	3031	1/1	0.97	0.10	29,29,29,29	0
62	MG	14	3333	1/1	0.97	0.07	62,62,62,62	0
62	MG	1H	3297	1/1	0.97	0.17	40,40,40,40	0
62	MG	14	3206	1/1	0.97	0.12	55,55,55,55	0
62	MG	1H	3510	1/1	0.97	0.11	19,19,19,19	0
62	MG	13	1683	1/1	0.97	0.17	39,39,39,39	0
62	MG	14	3378	1/1	0.97	0.03	57,57,57,57	0
62	MG	1H	3484	1/1	0.97	0.16	16,16,16,16	0
62	MG	14	3210	1/1	0.97	0.15	47,47,47,47	0
62	MG	1H	3559	1/1	0.97	0.17	15,15,15,15	0
62	MG	14	3255	1/1	0.97	0.14	63,63,63,63	0
62	MG	1H	3575	1/1	0.97	0.14	17,17,17,17	0
61	K	14	3068	1/1	0.97	0.07	61,61,61,61	0
62	MG	14	3363	1/1	0.97	0.10	26,26,26,26	0
62	MG	1H	3504	1/1	0.97	0.17	20,20,20,20	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
61	K	1H	3130	1/1	0.97	0.13	61,61,61,61	0
62	MG	L8	101	1/1	0.97	0.18	38,38,38,38	0
62	MG	1H	3432	1/1	0.97	0.09	55,55,55,55	0
62	MG	1H	3232	1/1	0.97	0.22	43,43,43,43	0
62	MG	1H	3374	1/1	0.97	0.10	28,28,28,28	0
61	K	1H	3086	1/1	0.97	0.06	66,66,66,66	0
62	MG	13	1748	1/1	0.97	0.14	38,38,38,38	0
61	K	1H	3117	1/1	0.97	0.17	57,57,57,57	0
61	K	1H	3021	1/1	0.97	0.23	78,78,78,78	0
62	MG	1G	1655	1/1	0.97	0.16	58,58,58,58	0
62	MG	13	1659	1/1	0.97	0.12	56,56,56,56	0
62	MG	1H	3146	1/1	0.97	0.22	38,38,38,38	0
62	MG	1H	3260	1/1	0.97	0.09	24,24,24,24	0
61	K	1G	1621	1/1	0.97	0.05	76,76,76,76	0
62	MG	1H	3354	1/1	0.97	0.18	29,29,29,29	0
62	MG	1H	3193	1/1	0.97	0.21	40,40,40,40	0
62	MG	14	3153	1/1	0.97	0.21	51,51,51,51	0
62	MG	13	1682	1/1	0.97	0.33	33,33,33,33	0
61	K	1H	3028	1/1	0.97	0.09	87,87,87,87	0
61	K	14	3058	1/1	0.97	0.09	85,85,85,85	0
61	K	1H	3139	1/1	0.97	0.14	64,64,64,64	0
62	MG	14	3358	1/1	0.97	0.14	51,51,51,51	0
62	MG	1H	3309	1/1	0.97	0.07	52,52,52,52	0
62	MG	1H	3439	1/1	0.98	0.12	53,53,53,53	0
62	MG	1H	3249	1/1	0.98	0.20	31,31,31,31	0
62	MG	13	1726	1/1	0.98	0.20	46,46,46,46	0
61	K	1H	3092	1/1	0.98	0.09	37,37,37,37	0
61	K	1H	3069	1/1	0.98	0.11	16,16,16,16	0
62	MG	14	3328	1/1	0.98	0.11	25,25,25,25	0
62	MG	13	1724	1/1	0.98	0.25	43,43,43,43	0
62	MG	14	3214	1/1	0.98	0.33	66,66,66,66	0
62	MG	1H	3467	1/1	0.98	0.12	44,44,44,44	0
62	MG	1H	3534	1/1	0.98	0.10	27,27,27,27	0
62	MG	14	3200	1/1	0.98	0.26	52,52,52,52	0
61	K	1G	1629	1/1	0.98	0.11	88,88,88,88	0
62	MG	1H	3469	1/1	0.98	0.15	13,13,13,13	0
61	K	14	3023	1/1	0.98	0.07	60,60,60,60	0
61	K	1H	3133	1/1	0.98	0.14	61,61,61,61	0
62	MG	1H	3442	1/1	0.98	0.12	56,56,56,56	0
61	K	14	3101	1/1	0.98	0.07	76,76,76,76	0
62	MG	14	3135	1/1	0.98	0.16	47,47,47,47	0
61	K	1H	3076	1/1	0.98	0.16	50,50,50,50	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
62	MG	14	3285	1/1	0.98	0.05	30,30,30,30	0
62	MG	1H	3446	1/1	0.98	0.06	48,48,48,48	0
62	MG	14	3157	1/1	0.98	0.18	34,34,34,34	0
62	MG	1H	3574	1/1	0.98	0.17	24,24,24,24	0
62	MG	1H	3203	1/1	0.98	0.20	26,26,26,26	0
61	K	14	3092	1/1	0.98	0.09	106,106,106,106	0
62	MG	1G	1650	1/1	0.98	0.30	68,68,68,68	0
61	K	1H	3077	1/1	0.98	0.12	47,47,47,47	0
62	MG	1H	3145	1/1	0.98	0.23	17,17,17,17	0
62	MG	1H	3536	1/1	0.98	0.11	23,23,23,23	0
62	MG	1H	3170	1/1	0.98	0.24	18,18,18,18	0
62	MG	14	3253	1/1	0.98	0.14	47,47,47,47	0
61	K	1H	3008	1/1	0.98	0.08	65,65,65,65	0
61	K	1H	3066	1/1	0.98	0.18	27,27,27,27	0
62	MG	1H	3472	1/1	0.98	0.11	17,17,17,17	0
62	MG	1H	3385	1/1	0.98	0.14	20,20,20,20	0
62	MG	16	212	1/1	0.98	0.11	36,36,36,36	0
61	K	1H	3141	1/1	0.98	0.19	41,41,41,41	0
61	K	1H	3018	1/1	0.98	0.16	51,51,51,51	0
62	MG	21	302	1/1	0.98	0.08	14,14,14,14	0
62	MG	13	1656	1/1	0.98	0.14	49,49,49,49	0
62	MG	14	3323	1/1	0.98	0.08	56,56,56,56	0
62	MG	14	3286	1/1	0.98	0.12	25,25,25,25	0
62	MG	1H	3371	1/1	0.98	0.06	31,31,31,31	0
62	MG	1H	3175	1/1	0.98	0.23	31,31,31,31	0
62	MG	1H	3418	1/1	0.98	0.10	29,29,29,29	0
62	MG	1H	3268	1/1	0.98	0.11	34,34,34,34	0
62	MG	1H	3194	1/1	0.98	0.14	14,14,14,14	0
62	MG	13	1737	1/1	0.98	0.12	65,65,65,65	0
62	MG	14	3177	1/1	0.98	0.05	45,45,45,45	0
62	MG	14	3155	1/1	0.98	0.23	38,38,38,38	0
61	K	16	203	1/1	0.98	0.07	44,44,44,44	0
62	MG	13	1739	1/1	0.98	0.13	30,30,30,30	0
62	MG	13	1735	1/1	0.98	0.10	35,35,35,35	0
61	K	1H	3078	1/1	0.98	0.08	45,45,45,45	0
61	K	14	3059	1/1	0.98	0.09	48,48,48,48	0
62	MG	14	3258	1/1	0.98	0.16	34,34,34,34	0
62	MG	1H	3486	1/1	0.98	0.11	36,36,36,36	0
62	MG	1H	3498	1/1	0.98	0.09	24,24,24,24	0
62	MG	1H	3404	1/1	0.98	0.09	43,43,43,43	0
62	MG	1H	3250	1/1	0.98	0.25	38,38,38,38	0
62	MG	1H	3150	1/1	0.98	0.27	25,25,25,25	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
62	MG	1H	3234	1/1	0.98	0.32	39,39,39,39	0
62	MG	1H	3410	1/1	0.98	0.12	16,16,16,16	0
62	MG	1G	1637	1/1	0.98	0.19	55,55,55,55	0
61	K	14	3044	1/1	0.98	0.14	69,69,69,69	0
62	MG	14	3243	1/1	0.98	0.18	54,54,54,54	0
61	K	13	1637	1/1	0.98	0.17	64,64,64,64	0
62	MG	1H	3447	1/1	0.98	0.07	19,19,19,19	0
61	K	41	201	1/1	0.98	0.14	67,67,67,67	0
62	MG	1H	3458	1/1	0.98	0.16	21,21,21,21	0
62	MG	1H	3218	1/1	0.98	0.24	28,28,28,28	0
62	MG	1G	1722	1/1	0.98	0.10	46,46,46,46	0
61	K	1H	3075	1/1	0.98	0.09	28,28,28,28	0
62	MG	1G	1641	1/1	0.98	0.30	64,64,64,64	0
61	K	1H	3106	1/1	0.98	0.18	59,59,59,59	0
62	MG	14	3273	1/1	0.98	0.14	37,37,37,37	0
61	K	14	3063	1/1	0.98	0.09	57,57,57,57	0
61	K	1H	3060	1/1	0.98	0.09	34,34,34,34	0
61	K	1H	3056	1/1	0.98	0.08	37,37,37,37	0
62	MG	1H	3521	1/1	0.98	0.17	14,14,14,14	0
62	MG	1H	3168	1/1	0.98	0.24	15,15,15,15	0
62	MG	F8	101	1/1	0.98	0.11	32,32,32,32	0
62	MG	14	3127	1/1	0.98	0.16	30,30,30,30	0
61	K	16	201	1/1	0.98	0.06	55,55,55,55	0
62	MG	1H	3378	1/1	0.98	0.10	28,28,28,28	0
61	K	1H	3068	1/1	0.98	0.18	29,29,29,29	0
62	MG	1H	3406	1/1	0.98	0.09	14,14,14,14	0
62	MG	1H	3191	1/1	0.98	0.19	24,24,24,24	0
61	K	39	301	1/1	0.98	0.05	75,75,75,75	0
61	K	31	302	1/1	0.98	0.03	45,45,45,45	0
62	MG	14	3283	1/1	0.98	0.08	21,21,21,21	0
61	K	1H	3090	1/1	0.98	0.10	55,55,55,55	0
62	MG	1G	1693	1/1	0.98	0.17	40,40,40,40	0
62	MG	1H	3347	1/1	0.98	0.16	38,38,38,38	0
62	MG	13	1740	1/1	0.98	0.08	33,33,33,33	0
62	MG	13	1676	1/1	0.98	0.28	53,53,53,53	0
62	MG	29	302	1/1	0.98	0.18	38,38,38,38	0
61	K	13	1612	1/1	0.98	0.11	50,50,50,50	0
62	MG	13	1669	1/1	0.98	0.18	34,34,34,34	0
62	MG	1H	3389	1/1	0.98	0.07	13,13,13,13	0
61	K	1H	3102	1/1	0.98	0.08	51,51,51,51	0
62	MG	13	1668	1/1	0.98	0.18	31,31,31,31	0
62	MG	14	3126	1/1	0.98	0.18	27,27,27,27	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
61	K	1H	3017	1/1	0.98	0.26	56,56,56,56	0
62	MG	14	3172	1/1	0.98	0.23	26,26,26,26	0
62	MG	1G	1704	1/1	0.98	0.05	66,66,66,66	0
61	K	14	3019	1/1	0.98	0.09	40,40,40,40	0
61	K	1H	3074	1/1	0.98	0.09	34,34,34,34	0
61	K	1H	3087	1/1	0.98	0.09	31,31,31,31	0
61	K	14	3001	1/1	0.98	0.06	76,76,76,76	0
61	K	1H	3062	1/1	0.98	0.12	27,27,27,27	0
61	K	1H	3019	1/1	0.98	0.07	60,60,60,60	0
61	K	1G	1619	1/1	0.98	0.10	74,74,74,74	0
62	MG	1H	3384	1/1	0.98	0.14	11,11,11,11	0
61	K	4I	201	1/1	0.98	0.10	71,71,71,71	0
62	MG	1H	3396	1/1	0.98	0.15	16,16,16,16	0
62	MG	13	1762	1/1	0.98	0.08	52,52,52,52	0
61	K	1H	3059	1/1	0.98	0.08	19,19,19,19	0
62	MG	1H	3415	1/1	0.98	0.18	16,16,16,16	0
62	MG	1H	3188	1/1	0.98	0.28	20,20,20,20	0
62	MG	13	1663	1/1	0.98	0.24	47,47,47,47	0
62	MG	1H	3337	1/1	0.98	0.12	23,23,23,23	0
62	MG	14	3147	1/1	0.98	0.25	40,40,40,40	0
61	K	1H	3116	1/1	0.98	0.04	61,61,61,61	0
62	MG	13	1670	1/1	0.98	0.13	42,42,42,42	0
61	K	14	3046	1/1	0.98	0.09	54,54,54,54	0
61	K	1H	3055	1/1	0.98	0.08	31,31,31,31	0
62	MG	1H	3423	1/1	0.98	0.11	35,35,35,35	0
62	MG	14	3123	1/1	0.98	0.04	36,36,36,36	0
62	MG	1H	3388	1/1	0.98	0.11	15,15,15,15	0
61	K	14	3008	1/1	0.98	0.18	47,47,47,47	0
61	K	1H	3003	1/1	0.98	0.10	56,56,56,56	0
61	K	11	301	1/1	0.98	0.08	31,31,31,31	0
61	K	14	3090	1/1	0.99	0.07	64,64,64,64	0
62	MG	1G	1662	1/1	0.99	0.27	51,51,51,51	0
61	K	14	3054	1/1	0.99	0.06	58,58,58,58	0
61	K	13	1628	1/1	0.99	0.09	51,51,51,51	0
61	K	14	3050	1/1	0.99	0.05	63,63,63,63	0
62	MG	1H	3172	1/1	0.99	0.30	31,31,31,31	0
61	K	14	3036	1/1	0.99	0.14	41,41,41,41	0
61	K	1H	3083	1/1	0.99	0.11	54,54,54,54	0
63	SF4	3E	302	8/8	0.99	0.16	56,57,68,71	0
62	MG	1H	3241	1/1	0.99	0.28	30,30,30,30	0
62	MG	1H	3386	1/1	0.99	0.10	31,31,31,31	0
62	MG	1G	1717	1/1	0.99	0.09	67,67,67,67	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
64	ZN	5I	101	1/1	0.99	0.12	70,70,70,70	0
61	K	1H	3001	1/1	0.99	0.07	48,48,48,48	0
62	MG	14	3160	1/1	0.99	0.12	38,38,38,38	0
62	MG	14	3287	1/1	0.99	0.06	39,39,39,39	0
62	MG	14	3128	1/1	0.99	0.26	28,28,28,28	0
62	MG	14	3219	1/1	0.99	0.14	33,33,33,33	0
62	MG	14	3297	1/1	0.99	0.09	28,28,28,28	0
62	MG	14	3192	1/1	0.99	0.20	41,41,41,41	0
62	MG	14	3344	1/1	0.99	0.08	31,31,31,31	0
61	K	13	1617	1/1	0.99	0.17	50,50,50,50	0
62	MG	14	3151	1/1	0.99	0.15	26,26,26,26	0
62	MG	1H	3154	1/1	0.99	0.23	26,26,26,26	0
62	MG	1H	3408	1/1	0.99	0.09	29,29,29,29	0
61	K	1H	3065	1/1	0.99	0.11	30,30,30,30	0
62	MG	14	3368	1/1	0.99	0.12	29,29,29,29	0
62	MG	1H	3198	1/1	0.99	0.12	20,20,20,20	0
62	MG	11	302	1/1	0.99	0.08	14,14,14,14	0
62	MG	1H	3401	1/1	0.99	0.09	16,16,16,16	0
64	ZN	5A	102	1/1	0.99	0.12	82,82,82,82	0
62	MG	14	3266	1/1	0.99	0.11	38,38,38,38	0
62	MG	14	3307	1/1	0.99	0.11	36,36,36,36	0
63	SF4	32	303	8/8	0.99	0.14	57,68,76,85	0
61	K	1H	3033	1/1	0.99	0.17	36,36,36,36	0
61	K	1H	3089	1/1	0.99	0.12	36,36,36,36	0
62	MG	1H	3402	1/1	1.00	0.09	23,23,23,23	0

6.5 Other polymers

There are no such residues in this entry.