



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 20, 2026 – 03:41 AM UTC

PDB ID : 6QNQ / pdb_00006qnq
Title : 70S ribosome initiation complex (IC) with experimentally assigned potassium ions
Authors : Rozov, A.; Khusainov, I.; Yusupov, M.; Yusupova, G.
Deposited on : 2019-02-11
Resolution : 3.50 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

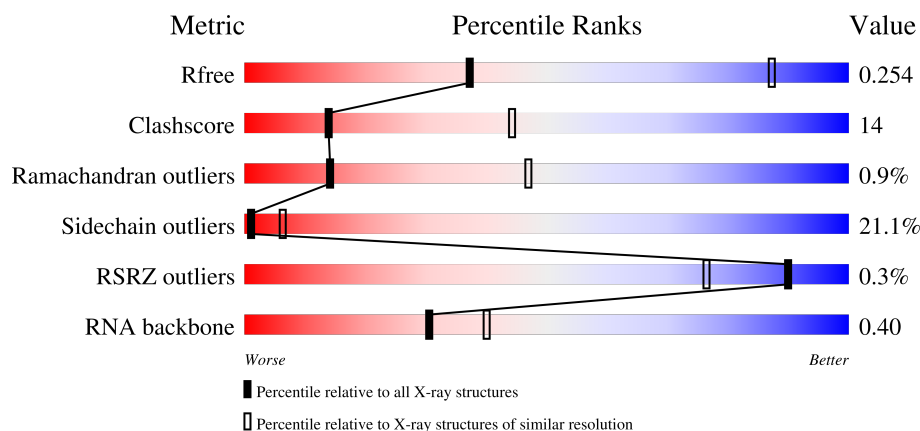
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.50 Å.

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



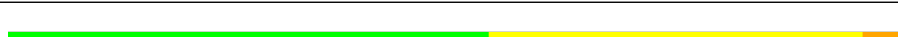
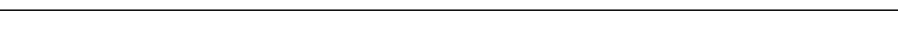
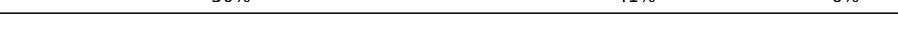
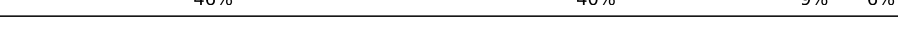
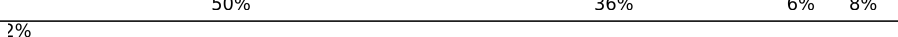
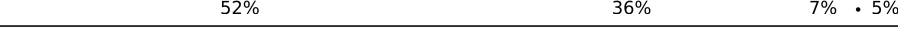
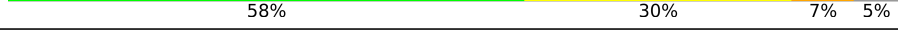
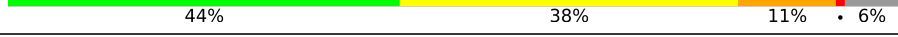
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1085 (3.54-3.46)
Clashscore	190562	1140 (3.54-3.46)
Ramachandran outliers	187476	1113 (3.54-3.46)
Sidechain outliers	187428	1114 (3.54-3.46)
RSRZ outliers	180081	1084 (3.54-3.46)
RNA backbone	3983	1010 (3.98-3.02)

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

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

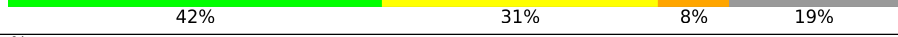
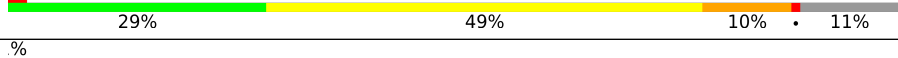
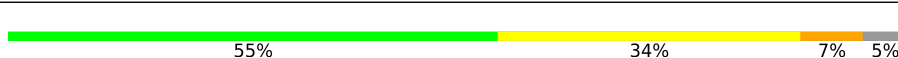
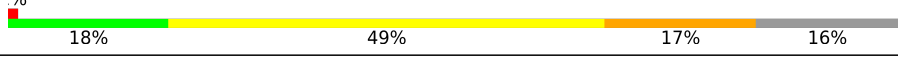
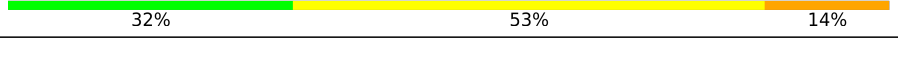
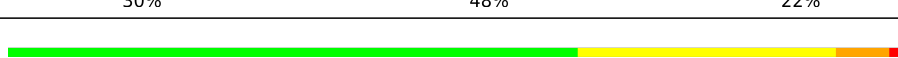
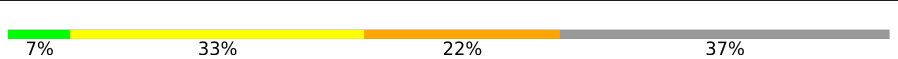
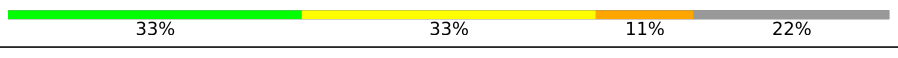
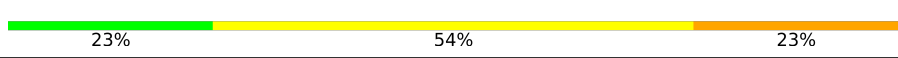
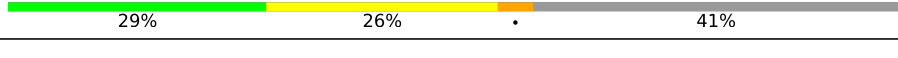
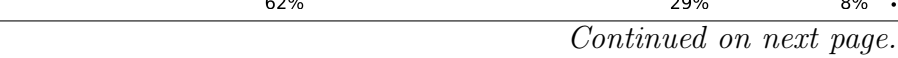
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Mol	Chain	Length	Quality of chain
3	22	239	
3	2E	239	
4	32	209	
4	3E	209	
5	42	162	
5	4E	162	
6	52	101	
6	5E	101	
7	62	156	
7	6E	156	
8	72	138	
8	7E	138	
9	82	128	
9	8E	128	
10	1A	105	
10	1I	105	
11	2A	129	
11	2I	129	
12	3A	132	
12	3I	132	
13	4A	126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

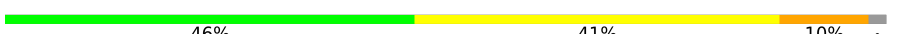
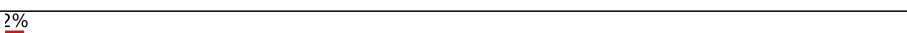
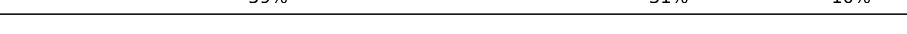
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Mol	Chain	Length	Quality of chain
15	6I	89	
16	7A	88	
16	7I	88	
17	8A	105	
17	8I	105	
18	9A	88	
18	9I	88	
19	AA	93	
19	AI	93	
20	BA	106	
20	BI	106	
21	1B	27	
21	1F	27	
22	1K	77	
22	3K	77	
22	3L	77	
23	2K	77	
24	4K	27	
24	4L	27	
25	14	2917	
25	1H	2917	
26	16	122	
26	1J	122	
27	7I	229	
28	11	276	

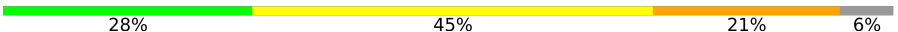
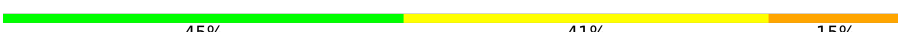
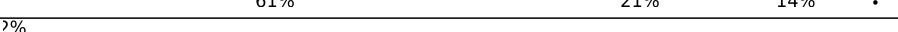
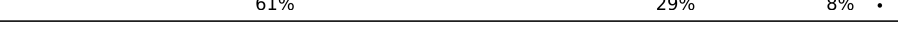
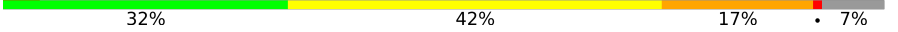
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Mol	Chain	Length	Quality of chain
28	19	276	 55% 38% 7% .
29	21	206	 61% 29% 9% .
29	29	206	 55% 34% 9% .
30	31	210	 55% 33% 8% .
30	39	210	 46% 41% 10% .
31	41	182	 52% 39% 9% .
31	49	182	 52% 37% 10% ..
32	51	180	 48% 38% 11% .
32	59	180	 49% 38% 10% .
33	61	148	 42% 39% 16% ..
33	69	148	 50% 38% 11% .
34	38	173	 35% 32% 12% . 20%
35	15	140	 59% 34% 5% .
35	58	140	 53% 35% 10% ..
36	25	122	 59% 31% 10% .
36	68	122	 60% 37% .
37	35	150	 42% 41% 15% ..
37	78	150	 50% 32% 16% ..
38	45	141	 50% 38% 11% ..
38	88	141	 58% 32% 9% .
39	55	118	 58% 35% 7% .
39	98	118	 55% 33% 12% .
40	65	112	 45% 48% 6% .
40	A8	112	 50% 38% 12% .
41	75	146	 36% 43% 14% 6% .

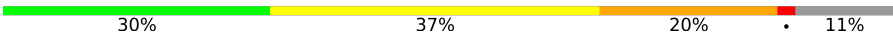
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Mol	Chain	Length	Quality of chain
41	B8	146	
42	85	118	
42	C8	118	
43	95	101	
43	D8	101	
44	A5	113	
44	E8	113	
45	B5	96	
45	F8	96	
46	C5	110	
46	G8	110	
47	D5	206	
47	H8	206	
48	E5	85	
48	I8	85	
49	F5	96	
49	J8	96	
50	G5	72	
50	K8	72	
51	H5	60	
51	L8	60	
52	I5	71	
52	M8	71	
53	J5	60	
53	N8	60	

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Mol	Chain	Length	Quality of chain
54	K5	54	
54	O8	54	
55	L5	49	
55	P8	49	
56	M5	65	
56	Q8	65	
57	2L	77	

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
60	SF4	32	303	-	-	X	-

2 Entry composition

There are 62 unique types of molecules in this entry. The entry contains 300507 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	1506	Total	C	N	O	P	0	0	0
			32387	14423	5999	10459	1506			
1	1G	1510	Total	C	N	O	P	0	0	0
			32470	14460	6012	10488	1510			

- 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	236	Total	C	N	O	S	0	0	0
			1915	1223	343	344	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	154	Total	C	N	O	S	0	0	0
			1178	743	221	210	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	149	Total	C	N	O	S	0	0	0
			1217	759	242	210	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	124	Total	C	N	O		0	0	0
			983	624	190	169				
9	82	127	Total	C	N	O	S	0	0	0
			1002	635	193	173	1			

- 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	117	Total	C	N	O	S	0	0	0
			864	537	162	162	3			
11	2A	119	Total	C	N	O	S	0	0	0
			889	554	169	163	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	118	Total	C	N	O	S	0	0	0
			937	579	193	163	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
			485	309	101	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	99	Total	C	N	O	S	0	0	0
			819	525	150	142	2			

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
19	AI	86	Total	C	N	O	S	0	0	0
			688	438	128	120	2			
19	AA	83	Total	C	N	O	S	0	0	0
			665	424	122	117	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	25	Total	C	N	O	0	0	0
			217	134	52	31			
21	1B	25	Total	C	N	O	0	0	0
			217	134	52	31			

- Molecule 22 is a RNA chain called E. coli tRNA^{fMet}.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
22	1K	65	Total	C	N	O	P	0	0	0
			1385	618	249	454	64			
22	3K	77	Total	C	N	O	P	0	0	0
			1640	732	297	535	76			
22	3L	77	Total	C	N	O	P	0	0	0
			1640	732	297	535	76			

- Molecule 23 is a RNA chain called E. coli tRNA^{fMet}.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
23	2K	77	Total	C	N	O	P	S	0	0	0
			1643	735	297	534	76	1			

- Molecule 24 is a RNA chain called mRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
24	4K	17	Total	C	N	O	P	0	0	0
			373	168	79	109	17			
24	4L	21	Total	C	N	O	P	0	0	0
			463	208	99	135	21			

- Molecule 25 is a RNA chain called 23S ribosomal RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
25	1H	2879	Total	C	N	O	P	0	0	0
			62010	27605	11592	19935	2878			
25	14	2879	Total	C	N	O	P	0	0	0
			62013	27604	11596	19934	2879			

- Molecule 26 is a RNA chain called 5S ribosomal RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
26	16	120	Total	C	N	O	P	0	0	0
			2573	1146	476	832	119			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
26	1J	122	Total	C	N	O	P	0	0	0
			2617	1166	486	844	121			

- Molecule 27 is a protein called 50S ribosomal protein L1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
27	71	135	Total	C	N	O	S	0	0	0
			1049	662	197	189	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
28	11	274	Total	C	N	O	S	0	0	0
			2125	1341	422	359	3			
28	19	274	Total	C	N	O	S	0	0	0
			2124	1341	421	359	3			

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
30	31	202	Total	C	N	O	S	0	0	0
			1585	1011	297	275	2			
30	39	206	Total	C	N	O	S	0	0	0
			1619	1033	302	281	3			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
31	41	181	Total	C	N	O	S	0	0	0
			1473	942	268	259	4			
31	49	181	Total	C	N	O	S	0	0	0
			1473	942	268	259	4			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
32	51	174	Total	C	N	O	S	0	0	0
			1336	848	251	236	1			
32	59	174	Total	C	N	O	S	0	0	0
			1336	848	251	236	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
33	61	146	Total	C	N	O	S	0	0	0
			1136	726	201	208	1			
33	69	146	Total	C	N	O	S	0	0	0
			1136	726	201	208	1			

- Molecule 34 is a protein called 50S ribosomal protein L10.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
34	38	139	Total	C	N	O	S	0	0	0
			1056	672	187	195	2			

- Molecule 35 is a protein called 50S ribosomal protein L13.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
35	58	138	Total	C	N	O	S	0	0	0
			1104	712	206	182	4			
35	15	138	Total	C	N	O	S	0	0	0
			1104	712	206	182	4			

- Molecule 36 is a protein called 50S ribosomal protein L14.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
36	68	122	Total	C	N	O	S	0	0	0
			932	588	171	169	4			
36	25	122	Total	C	N	O	S	0	0	0
			932	588	171	169	4			

- Molecule 37 is a protein called 50S ribosomal protein L15.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
37	78	148	Total	C	N	O	S	0	0	0
			1130	704	230	193	3			
37	35	147	Total	C	N	O	S	0	0	0
			1122	698	229	192	3			

- Molecule 38 is a protein called 50S ribosomal protein L16.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
38	88	141	Total	C	N	O	S	0	0	0
			1121	715	212	187	7			
38	45	140	Total	C	N	O	S	0	0	0
			1112	710	210	185	7			

- Molecule 39 is a protein called 50S ribosomal protein L17.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
39	98	118	Total	C	N	O	S	0	0	0
			967	604	203	159	1			
39	55	118	Total	C	N	O	S	0	0	0
			967	604	203	159	1			

- Molecule 40 is a protein called 50S ribosomal protein L18.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
40	A8	111	Total	C	N	O	0	0	0
			881	556	176	149			
40	65	111	Total	C	N	O	0	0	0
			881	556	176	149			

- Molecule 41 is a protein called 50S ribosomal protein L19.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
41	B8	137	Total	C	N	O	S	0	0	0
			1141	710	234	196	1			
41	75	137	Total	C	N	O	S	0	0	0
			1141	710	234	196	1			

- Molecule 42 is a protein called 50S ribosomal protein L20.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
42	C8	117	Total	C	N	O	S	0	0	0
			963	610	202	150	1			
42	85	117	Total	C	N	O	S	0	0	0
			963	610	202	150	1			

- Molecule 43 is a protein called 50S ribosomal protein L21.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
43	D8	100	Total	C	N	O	S	0	0	0
			774	499	141	133	1			
43	95	101	Total	C	N	O	S	0	0	0
			778	501	142	134	1			

- Molecule 44 is a protein called 50S ribosomal protein L22.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
44	E8	113	Total	C	N	O	S	0	0	0
			899	566	177	154	2			
44	A5	112	Total	C	N	O	S	0	0	0
			890	560	175	153	2			

- Molecule 45 is a protein called 50S ribosomal protein L23.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
45	F8	95	Total	C	N	O	S	0	0	0
			747	485	135	126	1			
45	B5	93	Total	C	N	O		0	0	0
			730	474	132	124				

- Molecule 46 is a protein called 50S ribosomal protein L24.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
46	G8	107	Total	C	N	O	S	0	0	0
			805	517	151	132	5			
46	C5	109	Total	C	N	O	S	0	0	0
			825	528	153	139	5			

- Molecule 47 is a protein called 50S ribosomal protein L25.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
47	H8	174	Total	C	N	O	S	0	0	0
			1390	887	250	250	3			
47	D5	176	Total	C	N	O	S	0	0	0
			1404	897	252	252	3			

- Molecule 48 is a protein called 50S ribosomal protein L27.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
48	I8	77	Total	C	N	O	S	0	0	0
			611	378	129	103	1			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
48	E5	79	Total	C	N	O	S	0	0	0
			623	386	131	105	1			

- Molecule 49 is a protein called 50S ribosomal protein L28.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
49	J8	96	Total	C	N	O	S	0	0	0
			754	474	149	129	2			
49	F5	92	Total	C	N	O	S	0	0	0
			721	451	144	125	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
50	K8	71	Total	C	N	O	S	0	0	0
			590	367	119	103	1			
50	G5	69	Total	C	N	O	S	0	0	0
			580	358	118	103	1			

- Molecule 51 is a protein called 50S ribosomal protein L30.

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

- Molecule 52 is a protein called 50S ribosomal protein L31.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
52	M8	66	Total	C	N	O	S	0	0	0
			533	335	96	97	5			
52	I5	71	Total	C	N	O	S	0	0	0
			580	364	108	103	5			

- Molecule 53 is a protein called 50S ribosomal protein L32.

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

- Molecule 54 is a protein called 50S ribosomal protein L33.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
54	O8	49	Total	C	N	O	S	0	0	0
			424	264	87	69	4			
54	K5	48	Total	C	N	O	S	0	0	0
			417	259	86	68	4			

- Molecule 55 is a protein called 50S ribosomal protein L34.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
55	P8	48	Total	C	N	O	S	0	0	0
			418	257	104	55	2			
55	L5	48	Total	C	N	O	S	0	0	0
			418	257	104	55	2			

- Molecule 56 is a protein called 50S ribosomal protein L35.

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

- Molecule 57 is a RNA chain called E. coli tRNA^{fMet}.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
57	2L	77	Total	C	N	O	P	S	0	0
			1643	735	297	534	76	1		

- Molecule 58 is POTASSIUM ION (CCD ID: K) (formula: K) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
58	13	37	Total	K	0	1
			38	38		
58	5E	1	Total	K	0	0
			1	1		
58	5I	1	Total	K	0	0
			1	1		
58	8I	1	Total	K	0	0
			1	1		
58	1H	121	Total	K	0	1
			122	122		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
58	16	2	Total 2	K 2	0	0
58	11	1	Total 1	K 1	0	0
58	21	1	Total 1	K 1	0	0
58	31	2	Total 2	K 2	0	0
58	41	2	Total 2	K 2	0	0
58	1G	25	Total 25	K 25	0	0
58	32	1	Total 1	K 1	0	0
58	52	1	Total 1	K 1	0	0
58	3A	1	Total 1	K 1	0	0
58	BA	1	Total 1	K 1	0	0
58	14	94	Total 94	K 94	0	0
58	19	1	Total 1	K 1	0	0
58	29	2	Total 2	K 2	0	0
58	39	1	Total 1	K 1	0	0

- Molecule 59 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

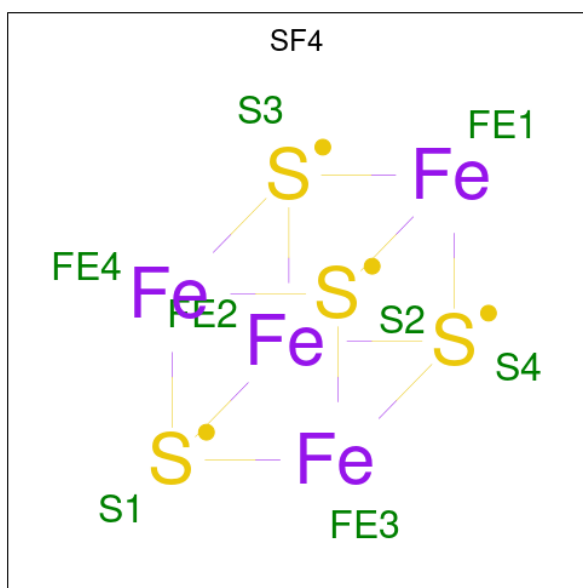
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
59	13	111	Total 111	Mg 111	0	0
59	3E	1	Total 1	Mg 1	0	0
59	8E	1	Total 1	Mg 1	0	0
59	4I	1	Total 1	Mg 1	0	0
59	7I	1	Total 1	Mg 1	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
59	BI	2	Total 2	Mg 2	0	0
59	2K	1	Total 1	Mg 1	0	0
59	1H	404	Total 405	Mg 405	0	1
59	16	8	Total 8	Mg 8	0	0
59	21	2	Total 2	Mg 2	0	0
59	41	1	Total 1	Mg 1	0	0
59	78	1	Total 1	Mg 1	0	0
59	D8	3	Total 3	Mg 3	0	0
59	G8	1	Total 1	Mg 1	0	0
59	I8	2	Total 2	Mg 2	0	0
59	J8	1	Total 1	Mg 1	0	0
59	N8	1	Total 1	Mg 1	0	0
59	Q8	1	Total 1	Mg 1	0	0
59	1G	102	Total 102	Mg 102	0	0
59	32	1	Total 1	Mg 1	0	0
59	2L	2	Total 2	Mg 2	0	0
59	14	312	Total 312	Mg 312	0	0
59	1J	5	Total 5	Mg 5	0	0
59	29	2	Total 2	Mg 2	0	0
59	55	1	Total 1	Mg 1	0	0
59	E5	1	Total 1	Mg 1	0	0

- Molecule 60 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe_4S_4).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
60	3E	1	Total	Fe	S	0	0
			8	4	4		
60	32	1	Total	Fe	S	0	0
			8	4	4		

- Molecule 61 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
61	5I	1	Total	Zn	0	0
			1	1		
61	5A	1	Total	Zn	0	0
			1	1		

- Molecule 62 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
62	13	190	Total	O	0	0
			190	190		
62	3E	2	Total	O	0	0
			2	2		
62	3I	1	Total	O	0	0
			1	1		
62	4I	2	Total	O	0	0
			2	2		
62	5I	1	Total	O	0	0
			1	1		

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
62	6I	1	Total O 1 1	0	0
62	7I	3	Total O 3 3	0	0
62	BI	4	Total O 4 4	0	0
62	3K	1	Total O 1 1	0	0
62	4K	2	Total O 2 2	0	0
62	1H	983	Total O 983 983	0	0
62	16	12	Total O 12 12	0	0
62	11	10	Total O 10 10	0	0
62	21	5	Total O 5 5	0	0
62	31	6	Total O 6 6	0	0
62	58	1	Total O 1 1	0	0
62	78	6	Total O 6 6	0	0
62	98	1	Total O 1 1	0	0
62	B8	2	Total O 2 2	0	0
62	C8	2	Total O 2 2	0	0
62	F8	2	Total O 2 2	0	0
62	G8	1	Total O 1 1	0	0
62	I8	5	Total O 5 5	0	0
62	J8	3	Total O 3 3	0	0
62	Q8	1	Total O 1 1	0	0
62	1G	268	Total O 268 268	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
62	32	4	Total 4	O 4	0	0
62	42	1	Total 1	O 1	0	0
62	3A	1	Total 1	O 1	0	0
62	7A	5	Total 5	O 5	0	0
62	BA	1	Total 1	O 1	0	0
62	2L	6	Total 6	O 6	0	0
62	4L	4	Total 4	O 4	0	0
62	14	681	Total 681	O 681	0	0
62	1J	16	Total 16	O 16	0	0
62	19	12	Total 12	O 12	0	0
62	29	3	Total 3	O 3	0	0
62	39	3	Total 3	O 3	0	0
62	35	3	Total 3	O 3	0	0
62	55	2	Total 2	O 2	0	0
62	75	1	Total 1	O 1	0	0
62	85	1	Total 1	O 1	0	0
62	B5	2	Total 2	O 2	0	0
62	C5	2	Total 2	O 2	0	0
62	F5	1	Total 1	O 1	0	0
62	G5	1	Total 1	O 1	0	0
62	L5	1	Total 1	O 1	0	0

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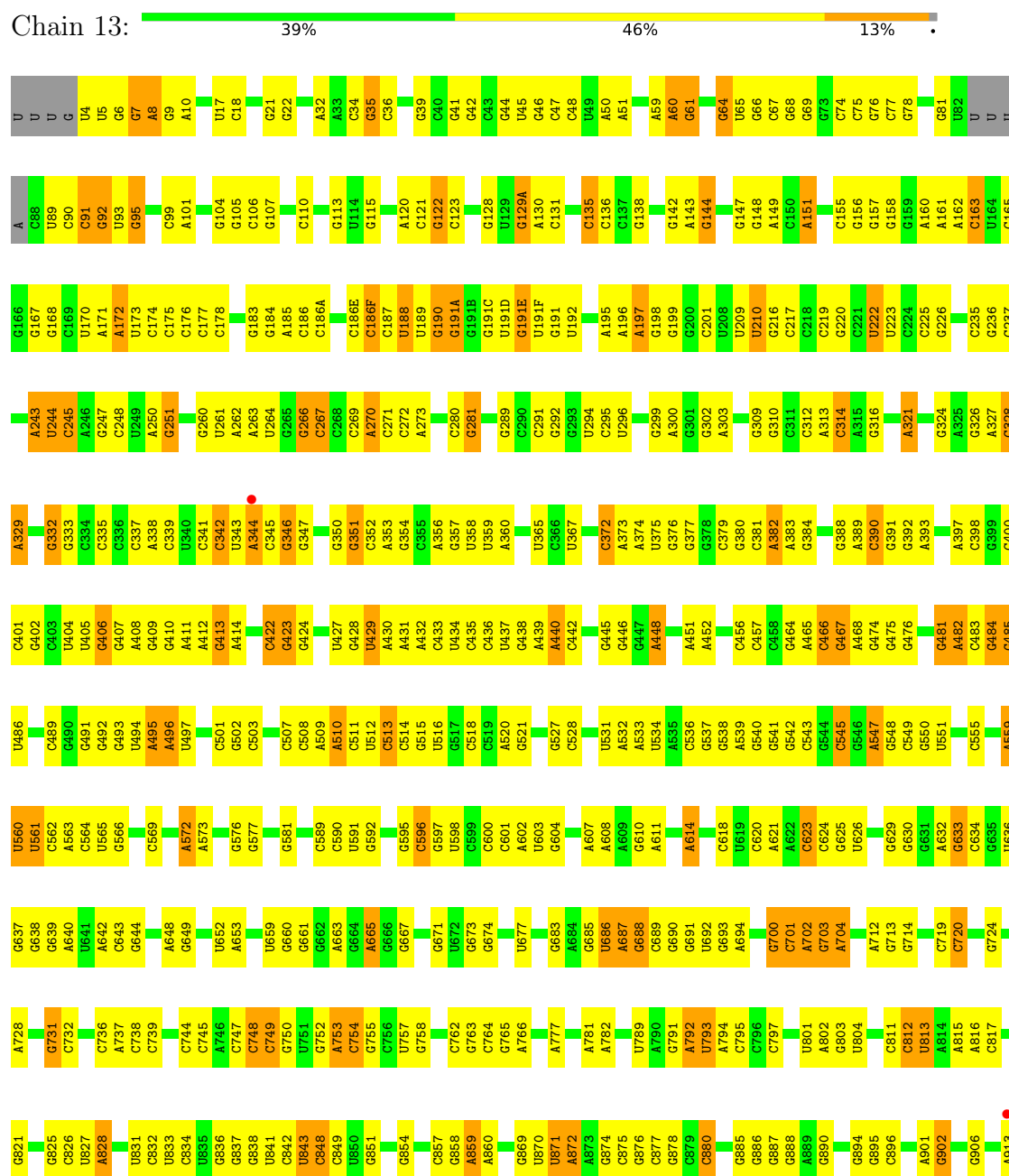
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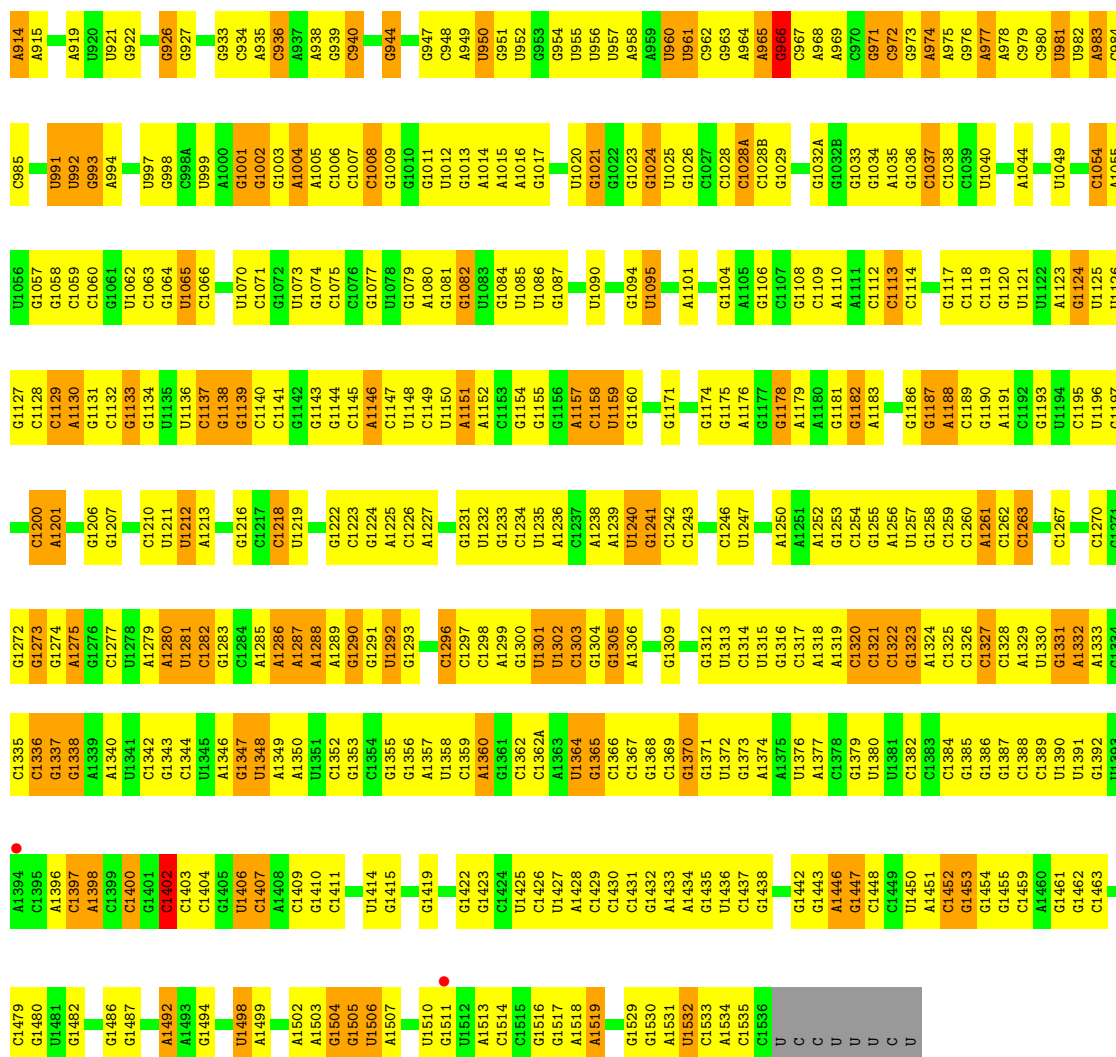
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
62	M5	1	Total	O	0	0
			1	1		

3 Residue-property plots [i](#)

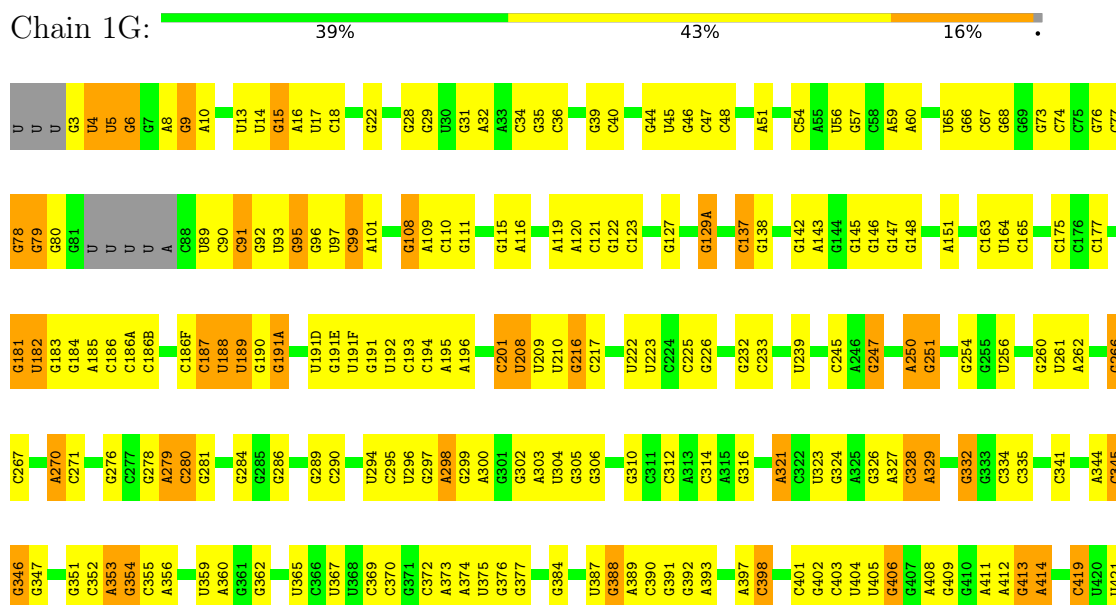
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

• Molecule 1: 16S ribosomal RNA



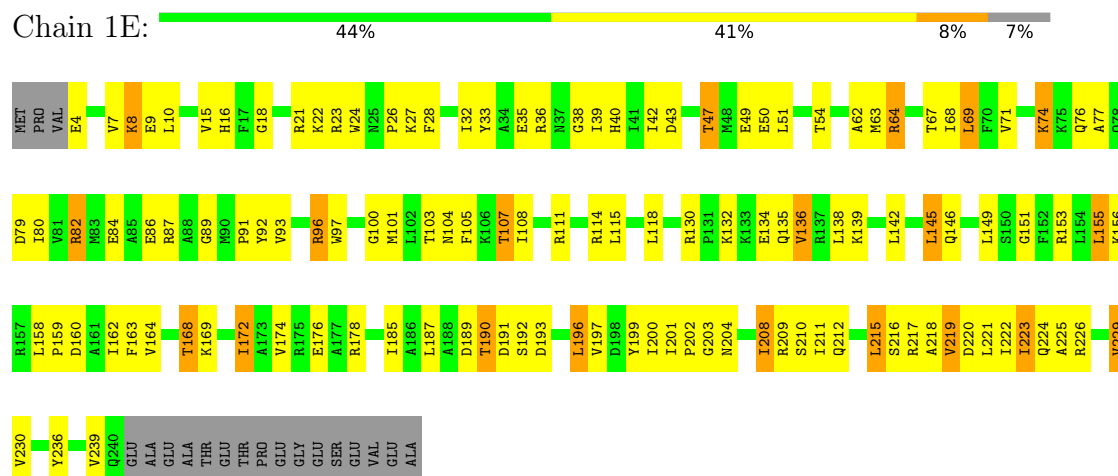


• Molecule 1: 16S ribosomal RNA

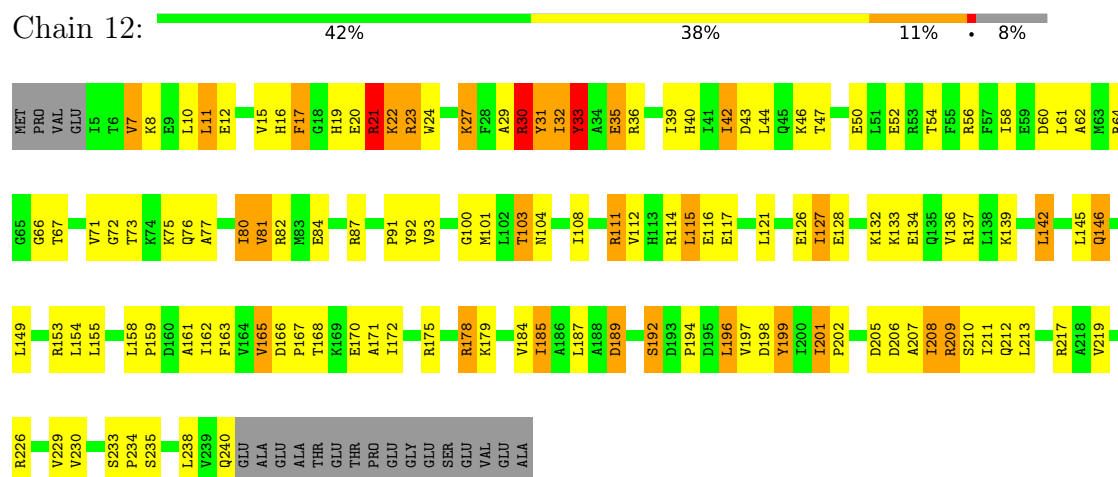


U1481	U1380	A1318	A1252	A1188	U1126	U1062	G1001	C932	G758	A694	G587	A509	C422
G1482	U1381	A1319	G1253	C1169	U1127	C1063	G1002	G933	C762	G695	G587	A510	G423
A1483	G1387	C1320	G1254	G1190	C1128	G1064	G1003	C934	C763	U686	G595	C511	G424
	C1388	C1321	G1255	G1191	C1129	A1005	A1004	A935	G764	A687	G596	U516	G425
C1490	C1389	G1323	U1257	C1195	A1130	C1066	A1006	A937	C765	C689	U598	G517	G426
G1491	U1392	A1324	G1258	U1196	G1131	A1067	C1007	G942	A766	C690	C599	C518	U429
A1492	U1393	C1325	C1259	G1197	C1132	C1068	C1008	U943	A767	G691	C601	C519	A430
U1498	A1394	C1327	G1198	U1199	G1134	C1069	G1009	U944	A768	G692	G601	A520	A435
A1499	C1395	C1328	C1200	C1071	U1135	U1070	G1010	A946	C769	G693	G601	G521	C435
	A1396	A1201	G1072	U1073	U1136	G1072	G1011	G947	G770	C701	A607	C522	
A1502	C1397	U1330	G1266	U1202	C1137	U1073	A1014	C948	G773	A702	A608	G527	A439
A1503	A1398	G1331	C1267	C1203	G1138	G1074	A1015		G774	G703	G610		A440
G1504	C1399	A1332	A1268	A1204	G1139	C1075	G1016	G951	A777	A704		A532	C442
G1505	C1400	A1333	A1269	U1205	C1140	C1076	A1017	U952	G778	A533	C613	A533	G445
U1506	G1401	G1334	C1270	G1206	C1141	G1077	G1018	G953	C779	C707	A614	U534	G446
A1507	C1402	C1335	G1271	G1207	G1142	U1078	C1019	G954	A780	C708	C615	A535	G447
G1508	C1403	C1336	G1272	C1208	G1143	A1080	U1020	U955	C781	G709	G616	C536	A448
C1509	G1404	G1337	G1273	G1215	G1144	G1081	G1023	U956	C782	G710	G617	G537	
U1510	G1405	C1342	G1274	U1211	C1145	G1082	U1024	U957	G785	G714	C618	G538	A452
G1511	U1406	G1343	A1275	A1212	A1146	U1083	U1025		G786	A715	U619	A539	A453
A1512	C1407	C1344	G1276	A1213	C1147	G1084	G1026	U960	A790	G716	C620	G540	
A1513		U1345	C1277	G1214	U1148	U1085	G1027	U961	G791	A717	A621	G541	C457
C1514		A1346	U1278	G1215	U1149	U1086	C1028	G963	A792	G718	C624	C543	C458
C1515		G1347	A1279	G1216	U1150	G1087	C1028A	A964	A793	C719		G544	G464
G1516		U1348	A1280	C1217	A1151	U1088	C1028B	A965	A794	C720	G627	C545	A465
G1517	A1413	C1349	U1281	C1218	G1154	G1089	G1029	A966	C806	C628	G627	C546	C466
A1518	G1414	A1349	C1282	U1219	G1155	U1090	G1030	G966	A807	G629	G628	A547	G467
A1519	G1415	A1350	G1283	U1220	G1156	U1091	G1031	A968	U801	A722	G630	G548	A468
G1520	G1416	U1351	C1284	G1221	G1157	A1092	G1032	A969	A802	U723		G549	G474
G1521	G1417	C1352	A1285	G1222	A1157	U1093	A1033	C970	G803	G724			C475
	A1418	G1353	A1286	C1223	U1158	G1094	G1032A	G971	C806	A728	U636	U552	G476
	G1419	C1354	A1287	U1224	U1159	U1095	G1033B	G972	A807	A729	G637	A553	G477
G1529	G1422	G1355	A1288	A1225	G1160	C1096	G1033	C973	C807	G730	C643	C554	A478
A1531	G1423	A1357	U1289	C1226	C1161	C1097	G1034	G885	A815	C738	U652	C555	U486
U1532	A1434	U1358	G1290	A1227	C1162	G1098	A1035	A974	C810	G739	A653	A563	C489
C1533	G1435	C1359	G1291	C1228	C1163	G1099	G1036	A975	G811	U740	C856	G567	G490
A1534	U1436	A1360	U1292	A1229	G1164	C1100	C1037	A976	C812	C735		G568	U494
C1535	C1437	G1361	G1294	G1230	C1165	A1101	C1038	A977	U813	C736	U646	A572	A495
C1536		C1362	G1295	U1232	G1166	G1104	C1039	A978	A814	A737	C647	A573	A496
U1537	G1442	A1363	C1296	U1235	A1167	A1105	G1042	C979	A815	C738	C644	A574	U497
	G1443	U1364	C1297	A1236	U1170	G1106	A1043	U981	A816	C739	A655	G575	A498
	G1446	G1365	C1298	A1237	G1171	G1109	A1044	U982	C817	U741		G576	C501
		C1366	A1299	C1238	G1174	A1110	C1045	A983	U818	G742		G577	G502
	U1450	G1367	U1301	A1239	G1175	A1111	A1046	A986	U820	U743	G661	A578	C503
	A1451	C1368	U1302	U1240	A1176	C1112	G1047	G987	C821	C744	A663	A579	C504
C1452	G1452	C1369	C1303	G1241	G1177	C1113	U1049	G988	C822	C745	G664	A574	U497
G1453	G1453	G1370	G1304	C1242	G1178	C1114	G1050	C989	C823		A665	G575	A498
		G1371	G1305	C1243	A1179	C1115	C1051	C990	C824	C746		G576	G500
	G1454	U1372	A1306	C1244	A1180	G1116	U1052	U991	G668	C749		G577	C501
		G1373		A1245	G1181	G1117	G1053	U992	U751	G750	G668	G577	C502
	G1454	A1374	G1309	G1246	G1182	C1118	C1054	G993	G829	G752	G673	G581	C503
	G1454	U1375		U1247	A1183	C1119	U1055	A994	C832	A753	G674	U582	C504
	C1465	U1376	C1314	A1248	G1184	U1122	U1056	G927	C832	C754	A675	A583	G505
	G1466	A1377	U1315	C1249	G1185	U1123	G1057	G928	C833	C755		G584	G506
	G1467	G1378	G1316	A1250	G1186	G1124	G1058	G929	U834	C756	G682	G584	C507
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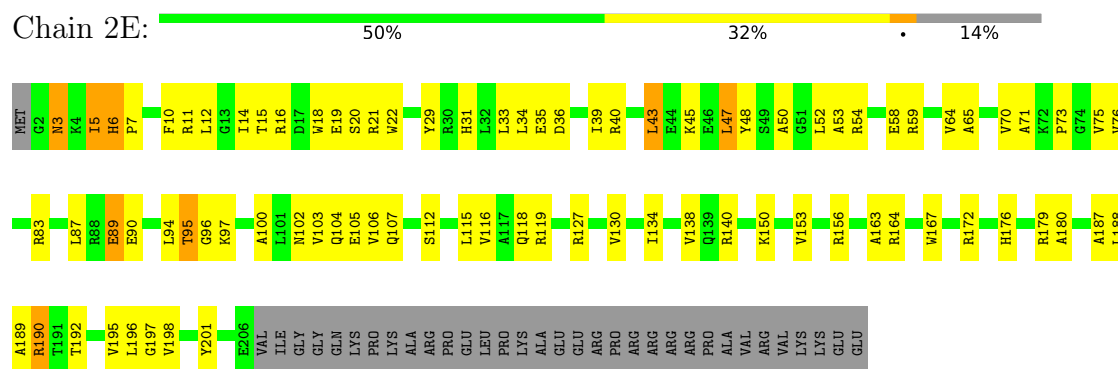
- Molecule 2: 30S ribosomal protein S2



- Molecule 2: 30S ribosomal protein S2



- Molecule 3: 30S ribosomal protein S3

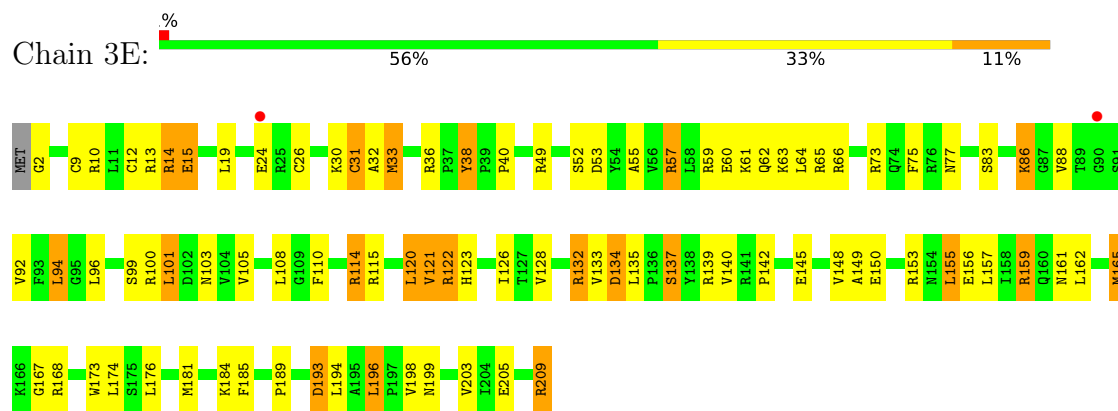


- Molecule 3: 30S ribosomal protein S3

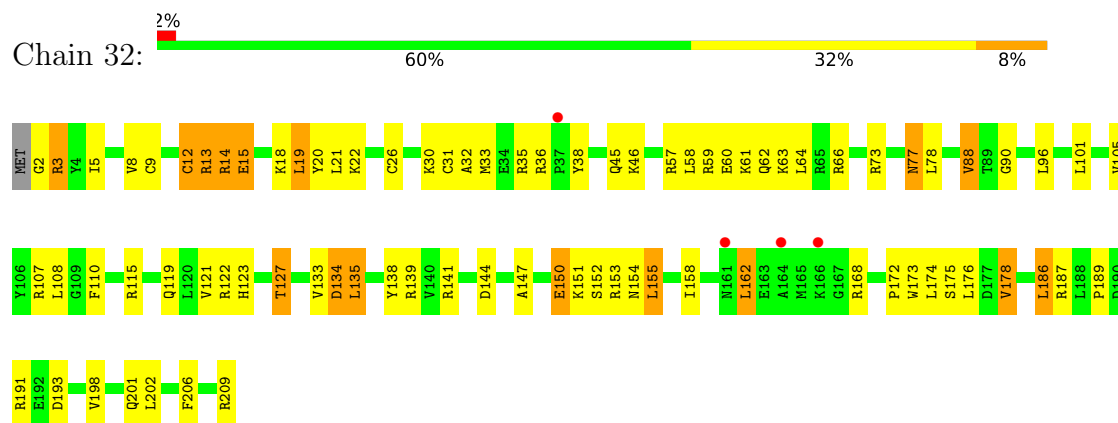




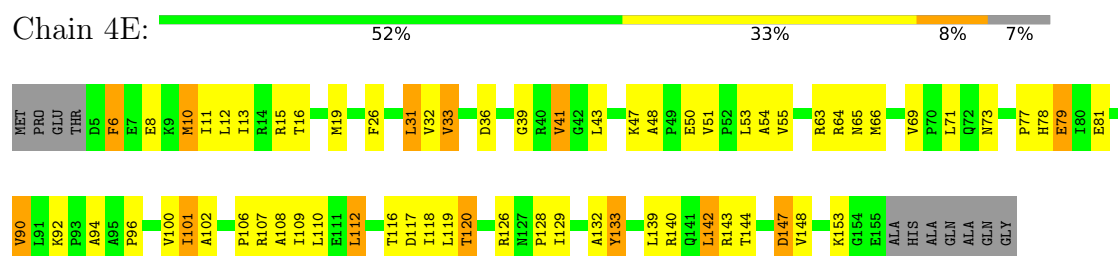
• Molecule 4: 30S ribosomal protein S4



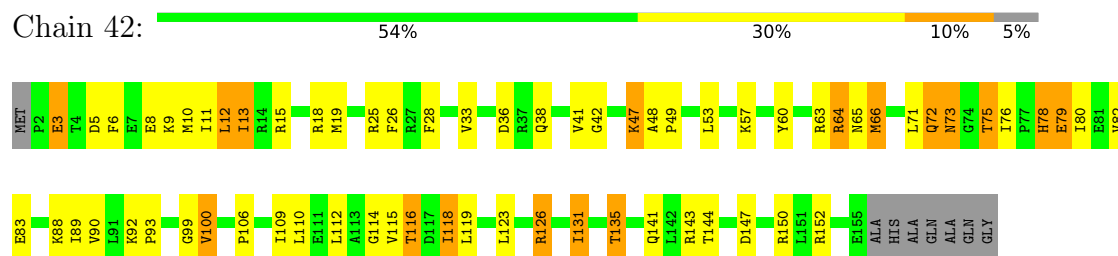
• Molecule 4: 30S ribosomal protein S4



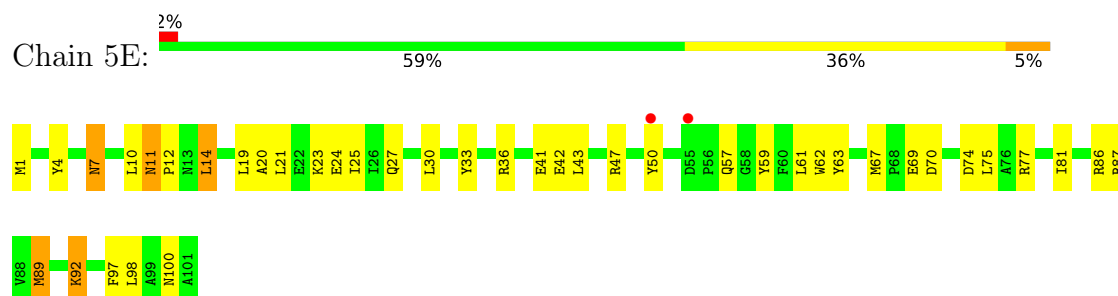
• Molecule 5: 30S ribosomal protein S5



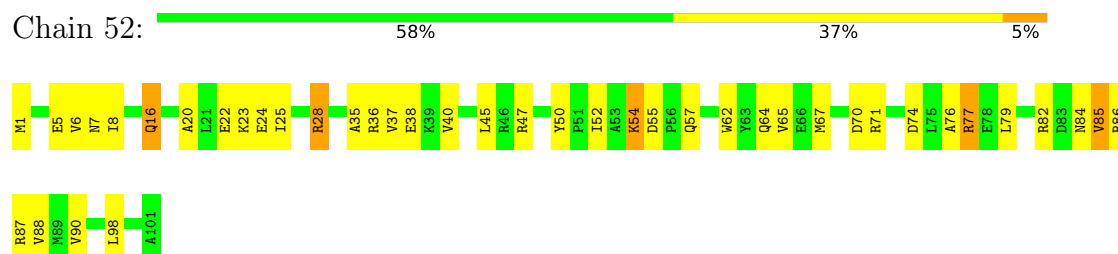
- Molecule 5: 30S ribosomal protein S5



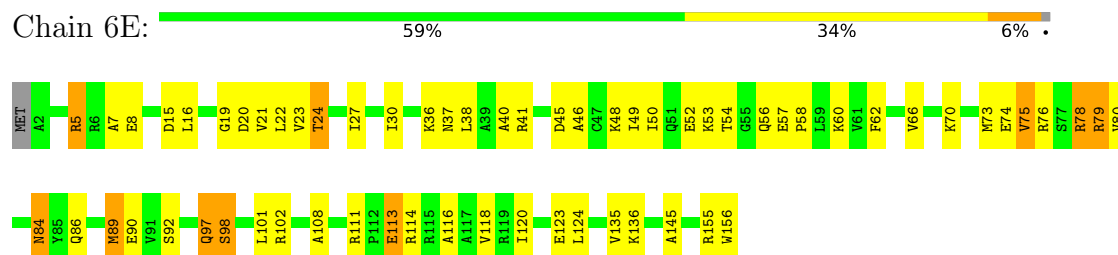
- Molecule 6: 30S ribosomal protein S6



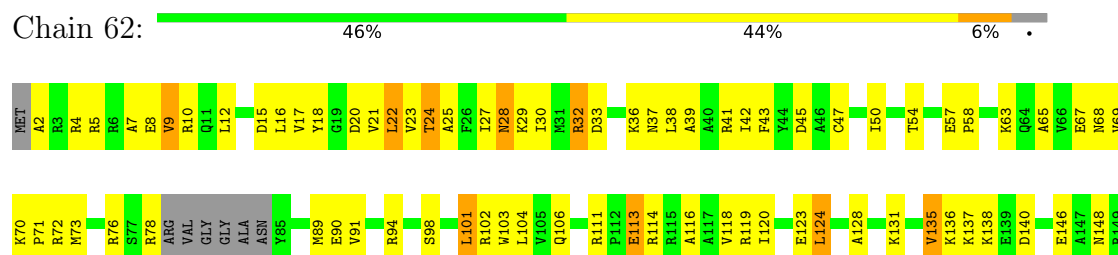
- Molecule 6: 30S ribosomal protein S6



- Molecule 7: 30S ribosomal protein S7



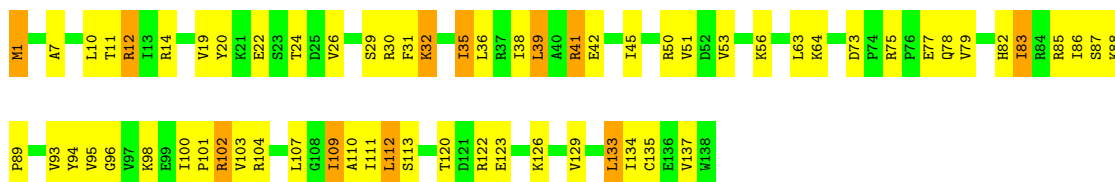
- Molecule 7: 30S ribosomal protein S7





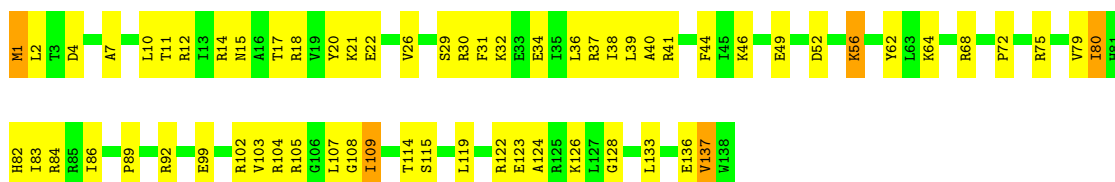
- Molecule 8: 30S ribosomal protein S8

Chain 7E: 53% 39% 8%



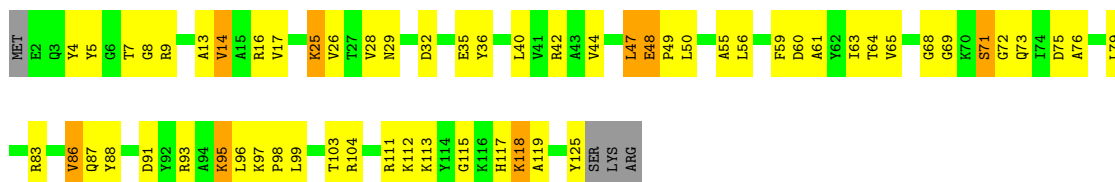
- Molecule 8: 30S ribosomal protein S8

Chain 72: 54% 42% 4%



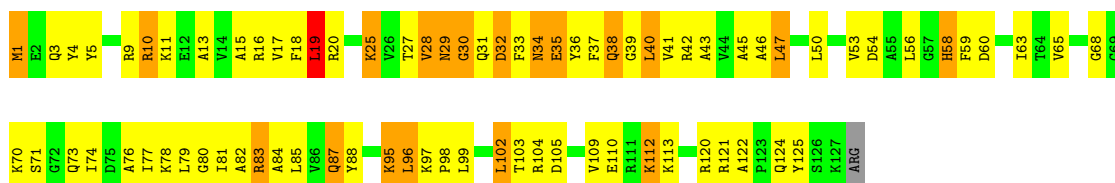
- Molecule 9: 30S ribosomal protein S9

Chain 8E: 50% 41% 6%



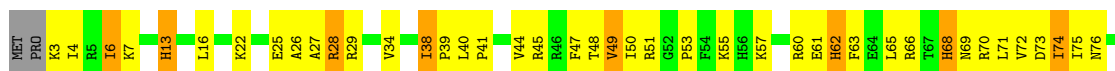
- Molecule 9: 30S ribosomal protein S9

Chain 82: 38% 46% 15% 1%



- Molecule 10: 30S ribosomal protein S10

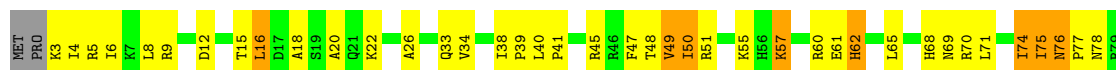
Chain 1I: 48% 38% 9% 5%





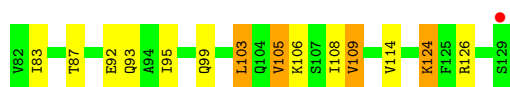
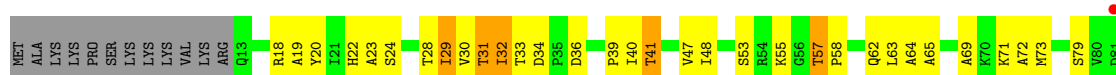
• Molecule 10: 30S ribosomal protein S10

Chain 1A: 46% 40% 9% 6%



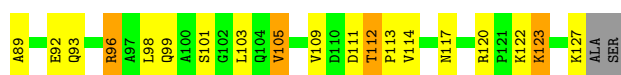
• Molecule 11: 30S ribosomal protein S11

Chain 2I: 2% 55% 29% 7% 9%



• Molecule 11: 30S ribosomal protein S11

Chain 2A: 50% 36% 6% 8%



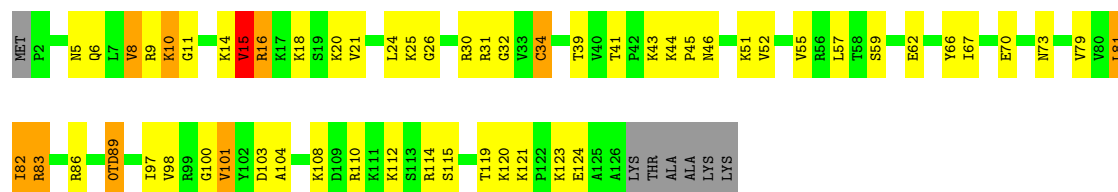
• Molecule 12: 30S ribosomal protein S12

Chain 3I: 58% 30% 7% 5%

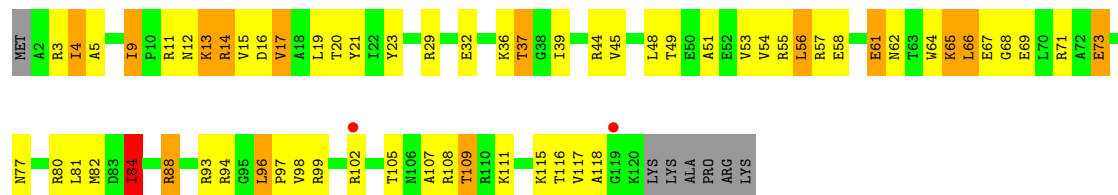
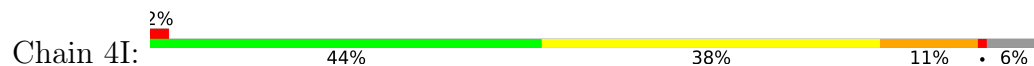


• Molecule 12: 30S ribosomal protein S12

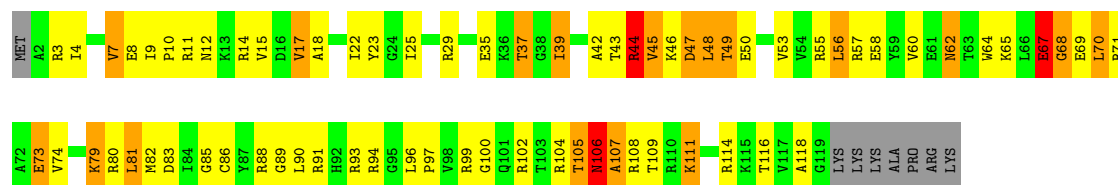
Chain 3A: 52% 36% 7% 5%



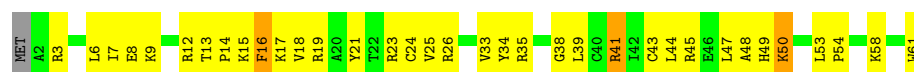
- Molecule 13: 30S ribosomal protein S13



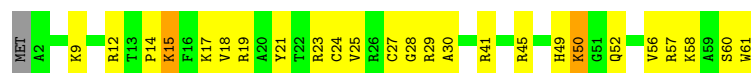
- Molecule 13: 30S ribosomal protein S13



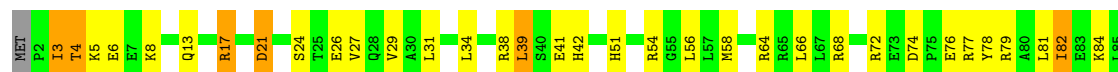
- Molecule 14: 30S ribosomal protein S14 type Z



- Molecule 14: 30S ribosomal protein S14 type Z



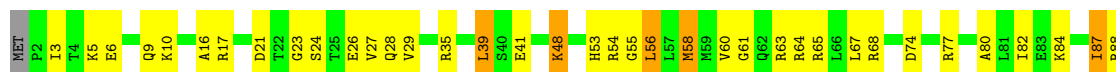
- Molecule 15: 30S ribosomal protein S15





- Molecule 15: 30S ribosomal protein S15

Chain 6A: 57% 36% 6%



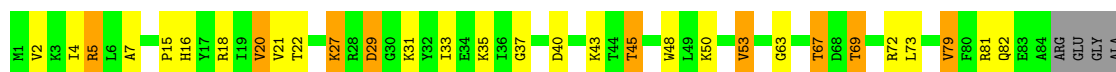
- Molecule 16: 30S ribosomal protein S16

Chain 7I: 51% 36% 7% 6%



- Molecule 16: 30S ribosomal protein S16

Chain 7A: 61% 24% 10% 5%



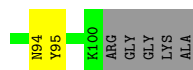
- Molecule 17: 30S ribosomal protein S17

Chain 8I: 2% 57% 32% 6% 5%

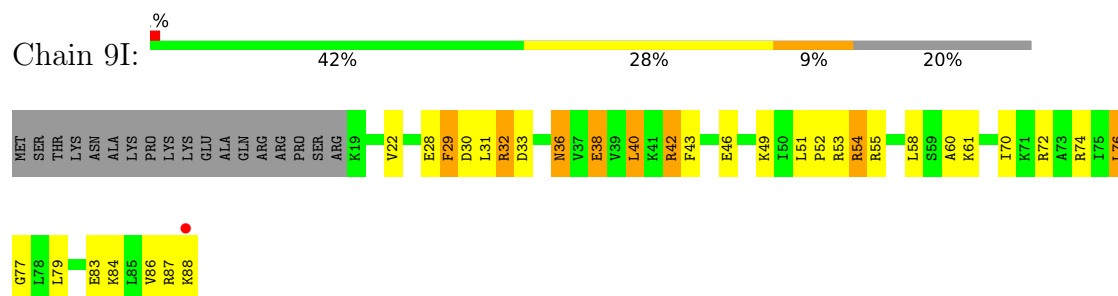


- Molecule 17: 30S ribosomal protein S17

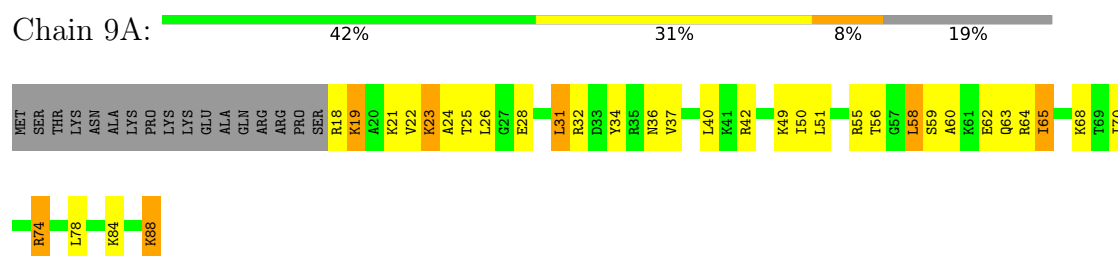
Chain 8A: 54% 36% 6%



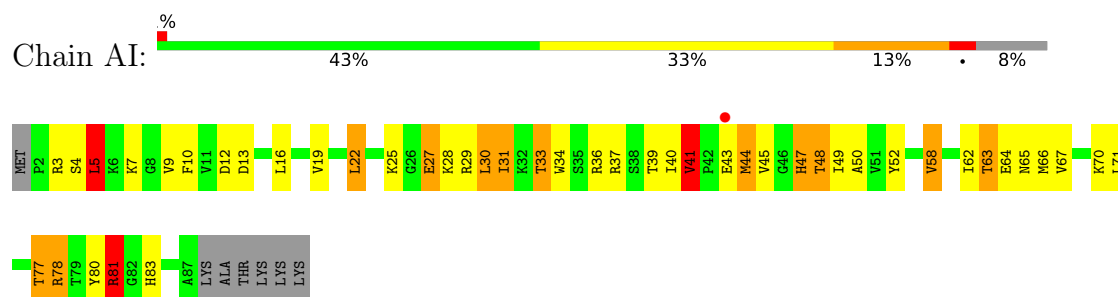
• Molecule 18: 30S ribosomal protein S18



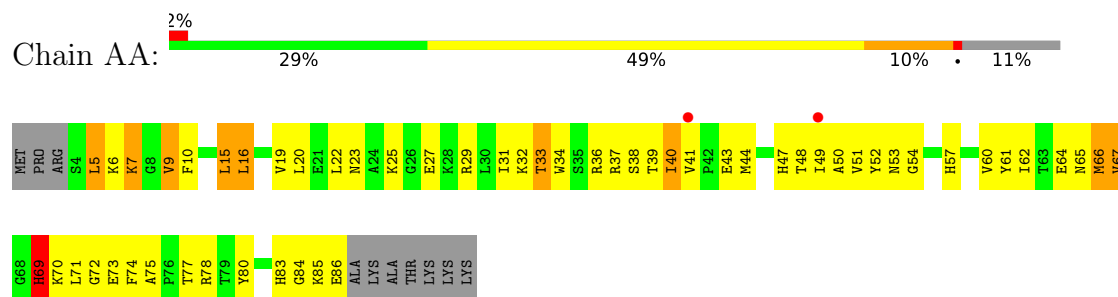
• Molecule 18: 30S ribosomal protein S18



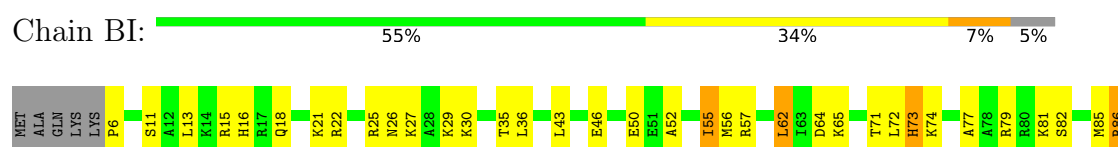
• Molecule 19: 30S ribosomal protein S19



• Molecule 19: 30S ribosomal protein S19



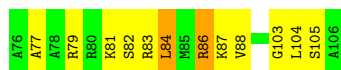
• Molecule 20: 30S ribosomal protein S20





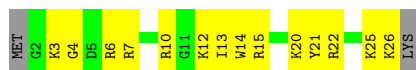
- Molecule 20: 30S ribosomal protein S20

Chain BA: 49% 41% 8%



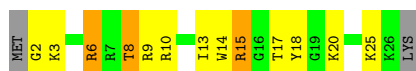
- Molecule 21: 30S ribosomal protein Thx

Chain 1F: 41% 52% 7%



- Molecule 21: 30S ribosomal protein Thx

Chain 1B: 44% 37% 11% 7%



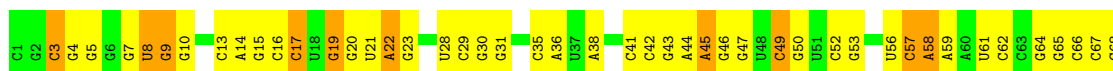
- Molecule 22: E. coli tRNA^{fMet}

Chain 1K: 18% 49% 17% 16%



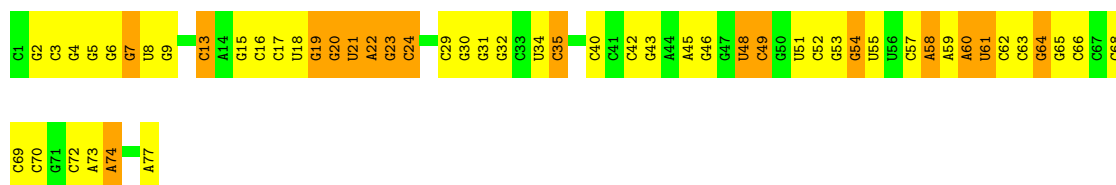
- Molecule 22: E. coli tRNA^{fMet}

Chain 3K: 32% 53% 14%



- Molecule 22: E. coli tRNA^{fMet}

Chain 3L: 30% 48% 22%



- Molecule 23: E. coli tRNAfMet

Chain 2K: 64% 29% 6% .



- Molecule 24: mRNA

Chain 4K: 7% 33% 22% 37%



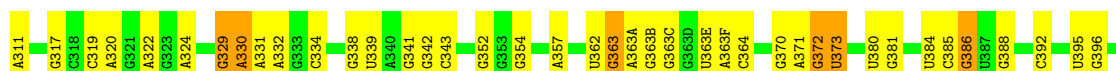
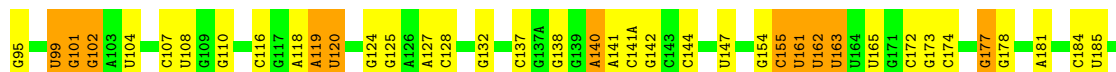
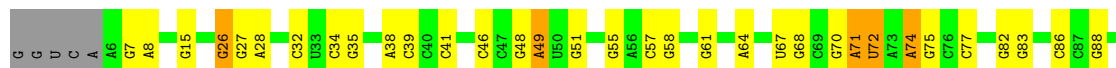
- Molecule 24: mRNA

Chain 4L: 33% 33% 11% 22%



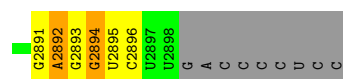
- Molecule 25: 23S ribosomal RNA

Chain 1H: 47% 39% 12% .



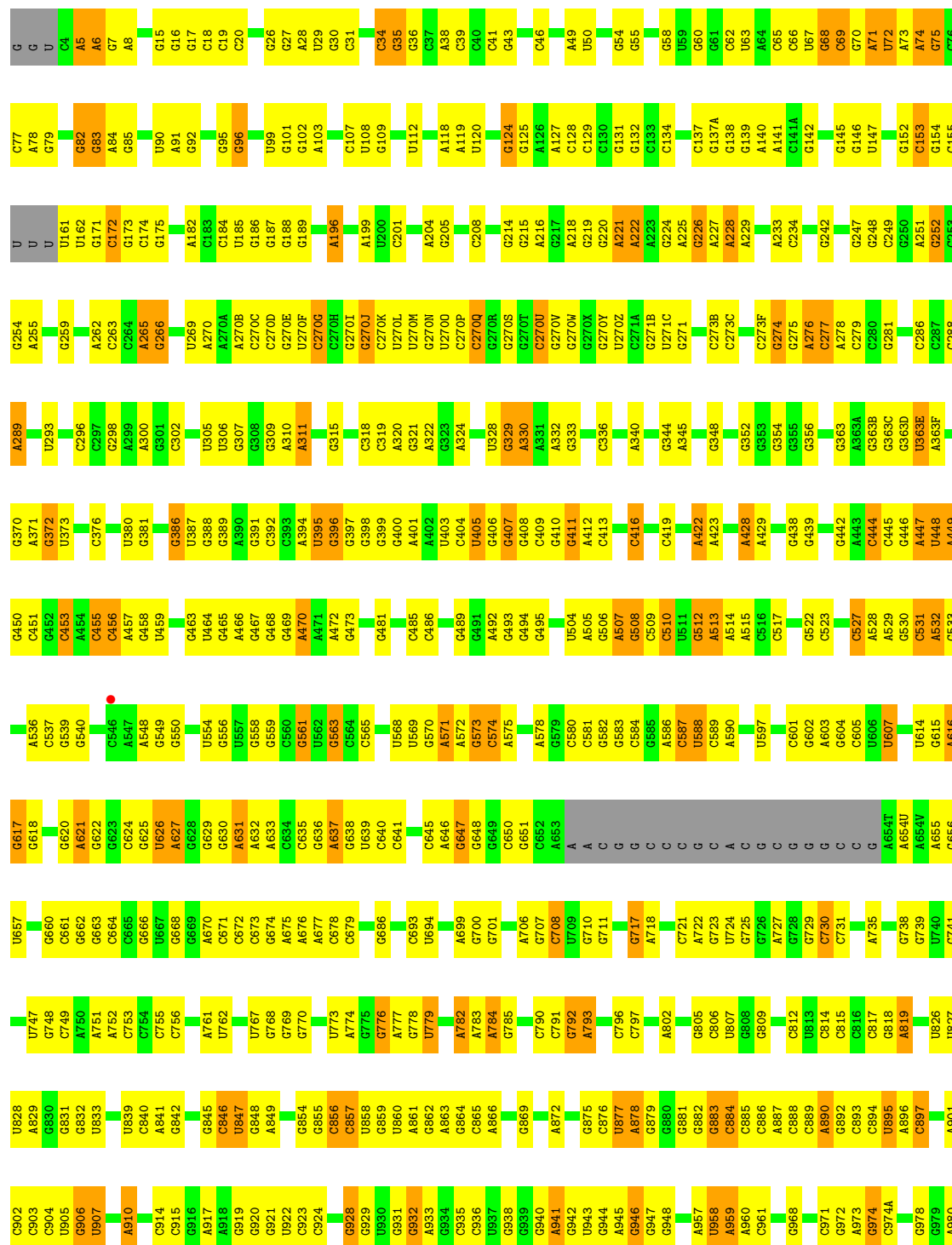




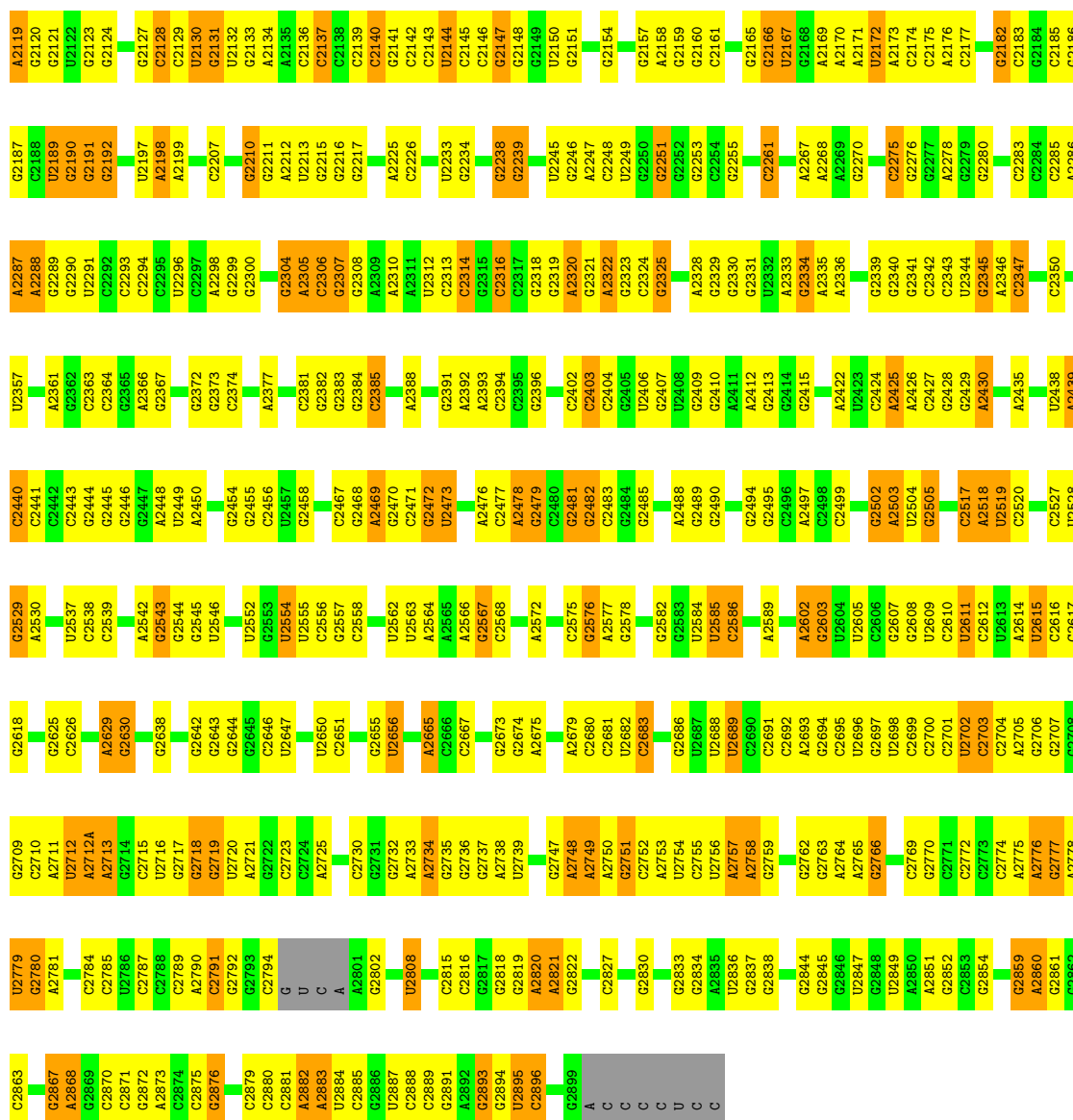


● Molecule 25: 23S ribosomal RNA

Chain 14: 44% 42% 14%

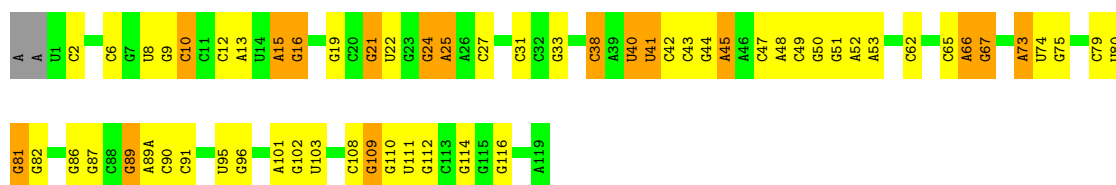


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A2054	G1964	A1791	G1695	G1595	A1427	A1349	G1271	G1188	G1120	C1052	A983
C2055	C1965	G1792	G1695	A1510	C1428	U1352	G1272	U1189	G1122	G1053	A984
G2056	A1966	C1793	U1697	C1598	G1429	A1353	A1272	G1190	G1055	A1054	C985
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A2058	G1882	C1795	A1698	A1603	U1431	G1358	A1278	G1192	A1057	U1058	A990
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U2113	C2043	G1860	A1783	G1678	A1495	C1413	G1337	U1253	G1176	C1043	C1043
A2114	G2046	U1864	A1784	C1686	A1496	G1416	G1343	U1254	G1178	G1110	G1110
G2115	U1955	U1865	A1785	G1687	C1502	C1417	G1344	U1255	C1179	A1045	A1045
G2116	C1957	G1869	A1787	U1688	G1502	C1418	G1345	G1256	G1180	A1046	A1046
A2117	G2050	U1870	C1788	A1689	G1502	C1419	G1346	C1257	C1181	U1113	U1113
U2118	A2051	C1870	G1788	A1699	C1505	A1419	G1346	G1259	G1183	A1048	A1048



• Molecule 26: 5S ribosomal RNA

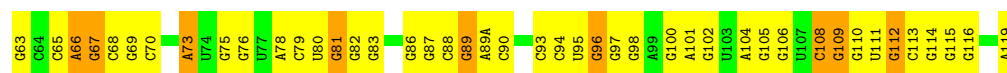
Chain 16: 49% 36% 13%



• Molecule 26: 5S ribosomal RNA

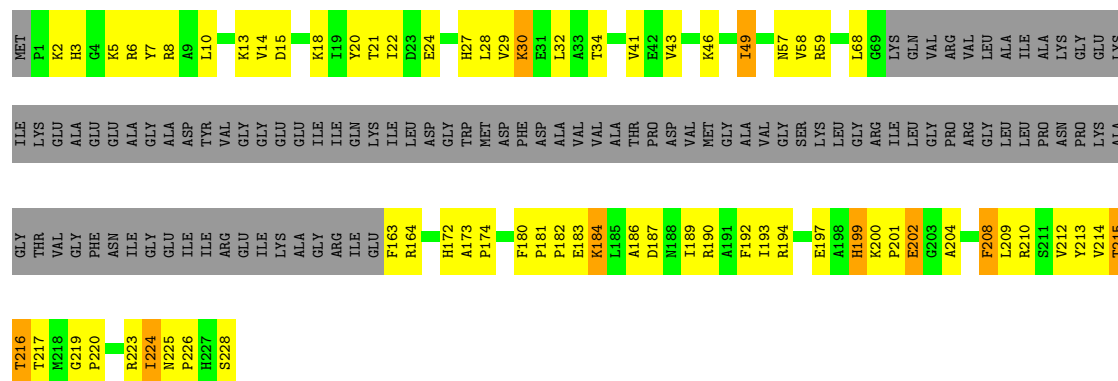
Chain 1J: 23% 54% 23%





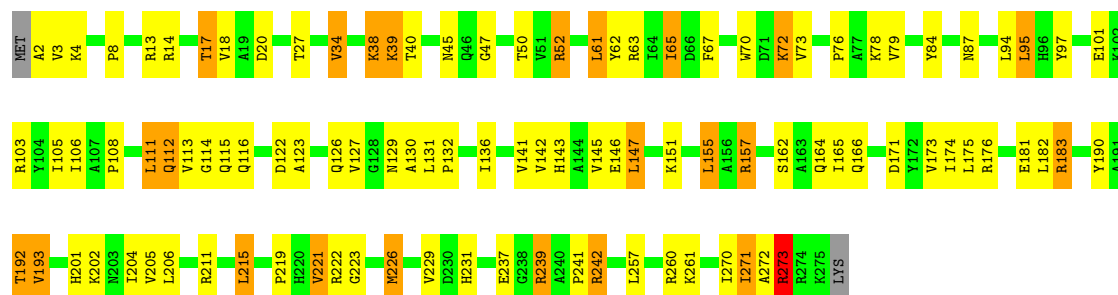
• Molecule 27: 50S ribosomal protein L1

Chain 71: 29% 26% 41%



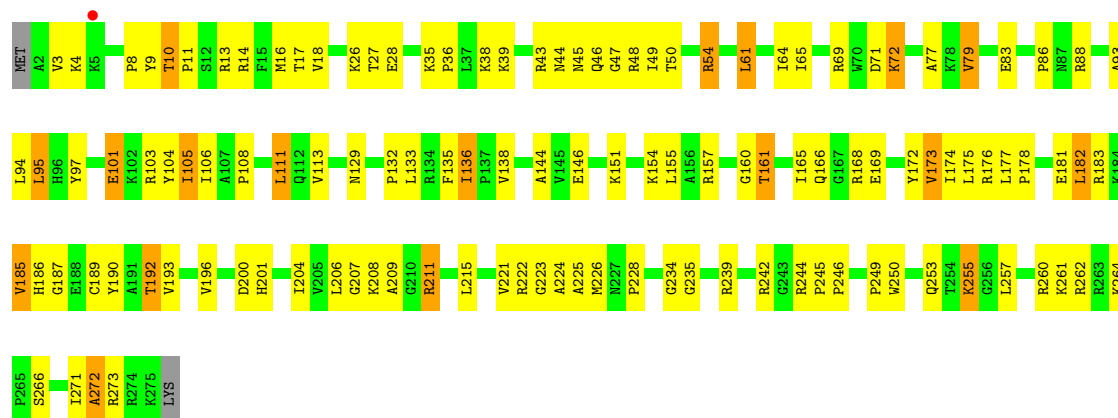
• Molecule 28: 50S ribosomal protein L2

Chain 11: 62% 29% 8%



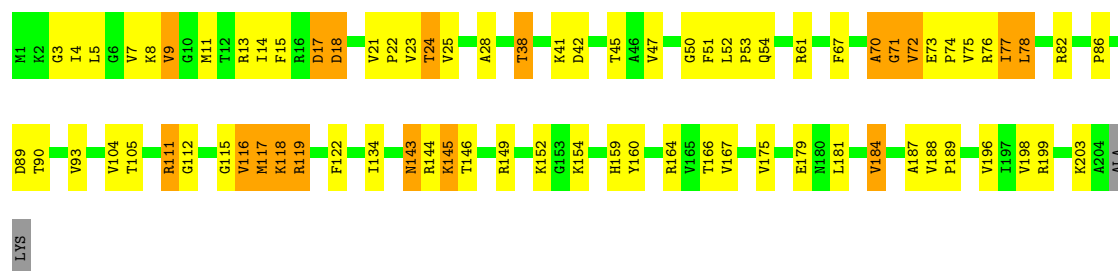
• Molecule 28: 50S ribosomal protein L2

Chain 19: 55% 38% 7%



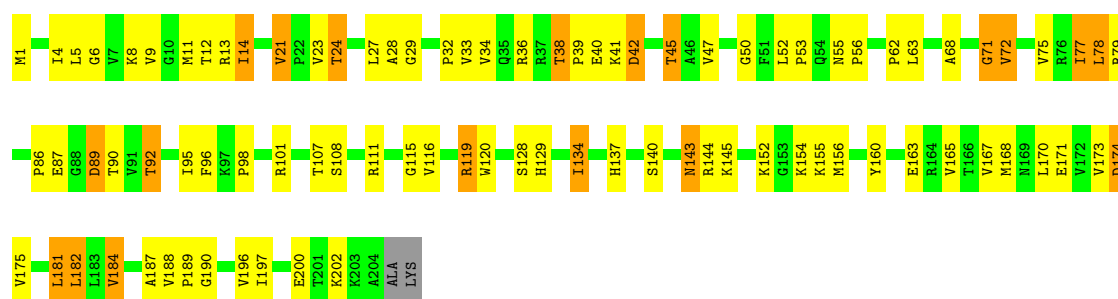
• Molecule 29: 50S ribosomal protein L3

Chain 21:  61% 29% 9% .



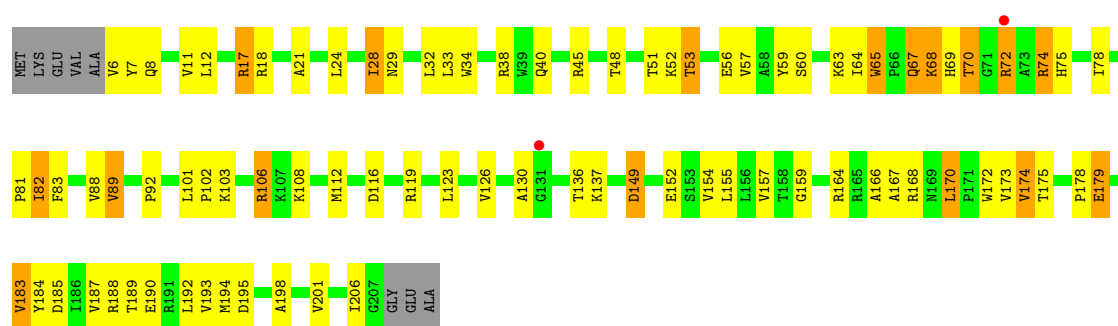
- Molecule 29: 50S ribosomal protein L3

Chain 29:  55% 34% 9% .

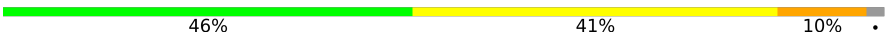


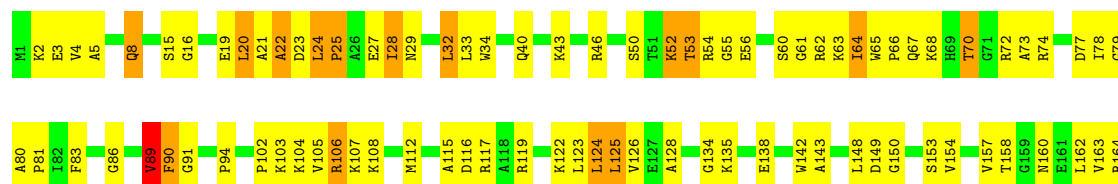
- Molecule 30: 50S ribosomal protein L4

Chain 31:  55% 33% 8% .



- Molecule 30: 50S ribosomal protein L4

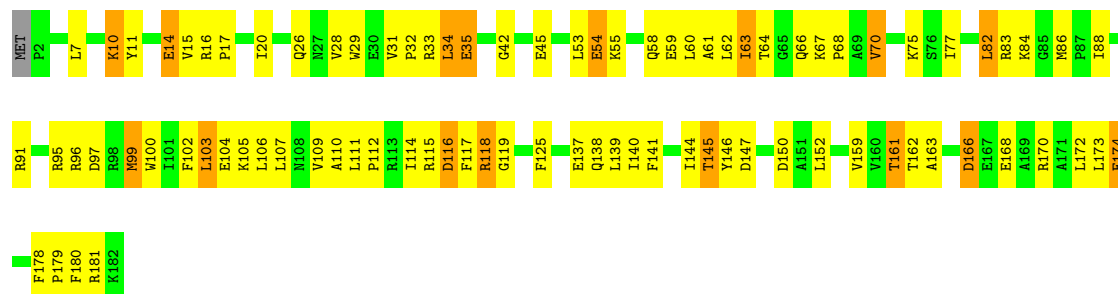
Chain 39:  46% 41% 10% .





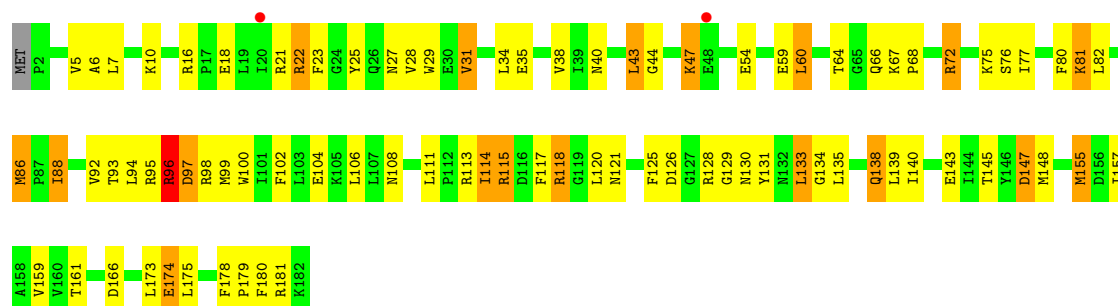
• Molecule 31: 50S ribosomal protein L5

Chain 41: 52% 39% 9% .



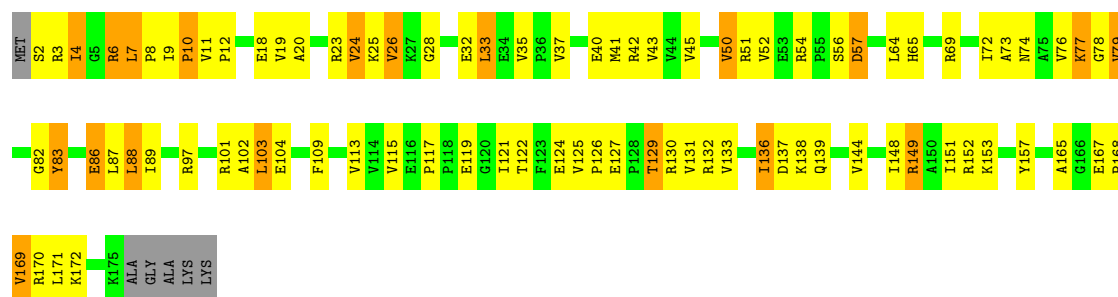
• Molecule 31: 50S ribosomal protein L5

Chain 49: 52% 37% 10% ..



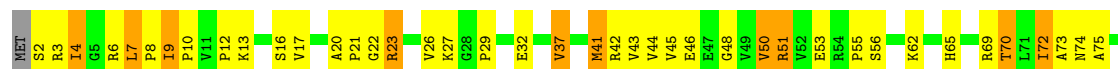
• Molecule 32: 50S ribosomal protein L6

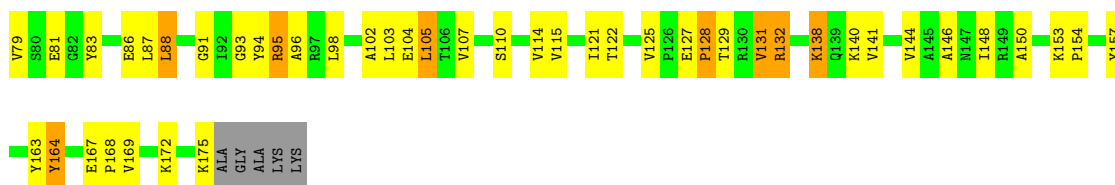
Chain 51: 48% 38% 11% .



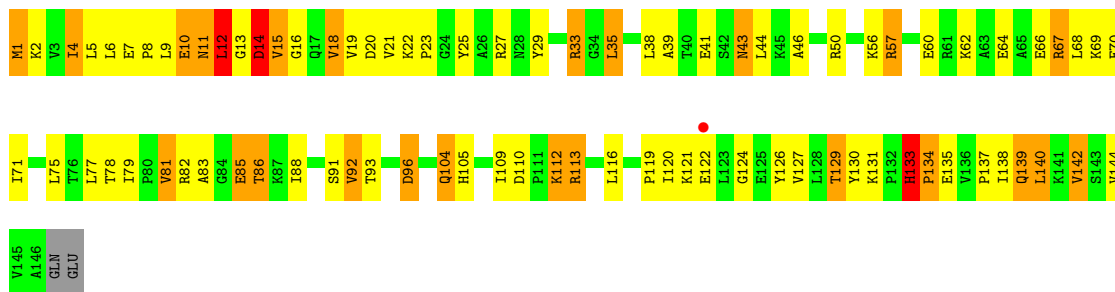
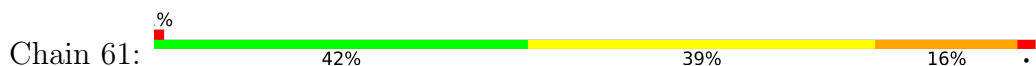
• Molecule 32: 50S ribosomal protein L6

Chain 59: 49% 38% 10% .

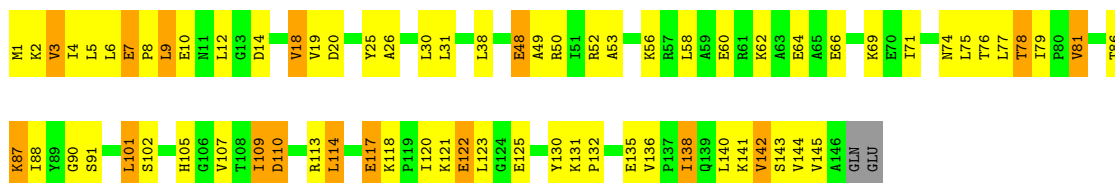




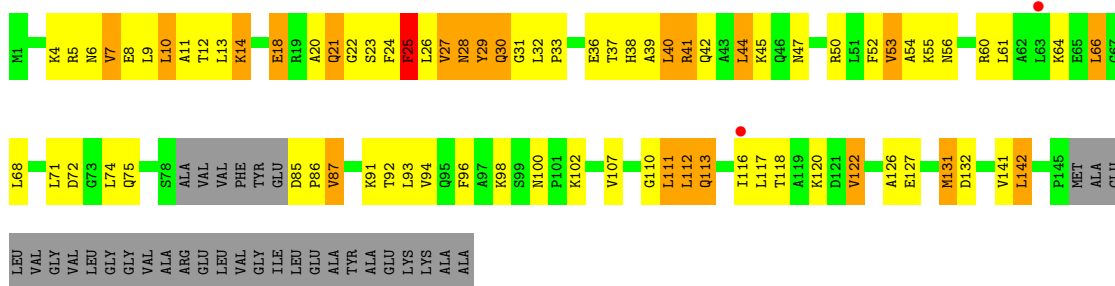
- Molecule 33: 50S ribosomal protein L9



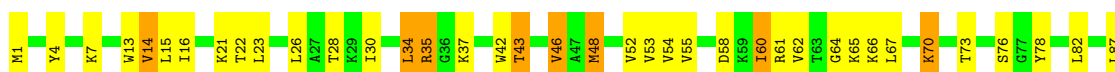
- Molecule 33: 50S ribosomal protein L9

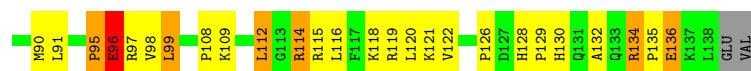


- Molecule 34: 50S ribosomal protein L10



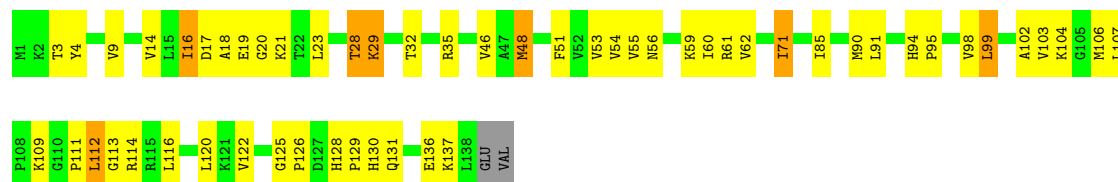
- Molecule 35: 50S ribosomal protein L13





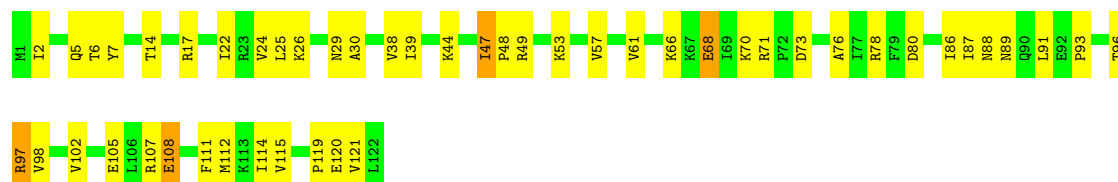
• Molecule 35: 50S ribosomal protein L13

Chain 15: 59% 34% 5% •



• Molecule 36: 50S ribosomal protein L14

Chain 68: 60% 37% •



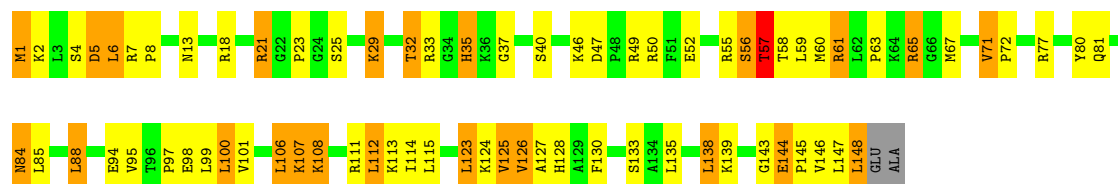
• Molecule 36: 50S ribosomal protein L14

Chain 25: 2% 59% 31% 10%



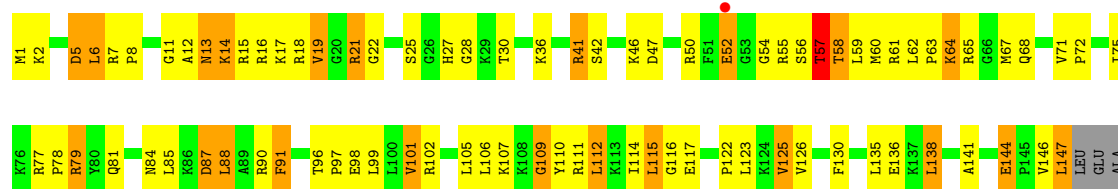
• Molecule 37: 50S ribosomal protein L15

Chain 78: 50% 32% 16% ••



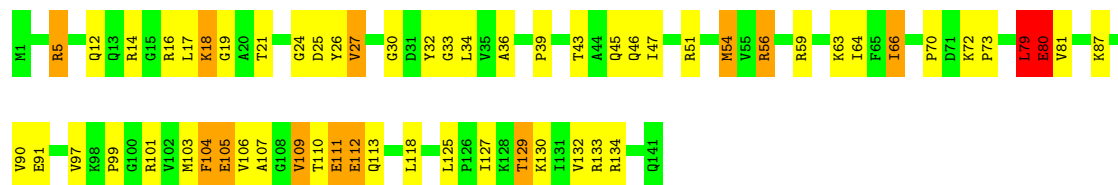
• Molecule 37: 50S ribosomal protein L15

Chain 35: 42% 41% 15% ••



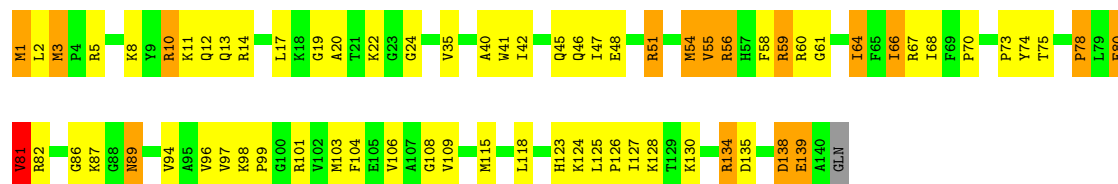
• Molecule 38: 50S ribosomal protein L16

Chain 88: 58% 32% 9% .



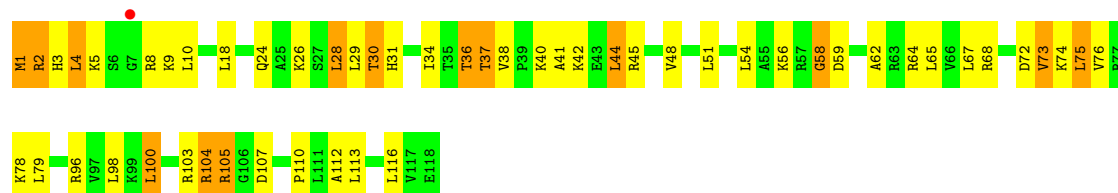
• Molecule 38: 50S ribosomal protein L16

Chain 45: 50% 38% 11% ..



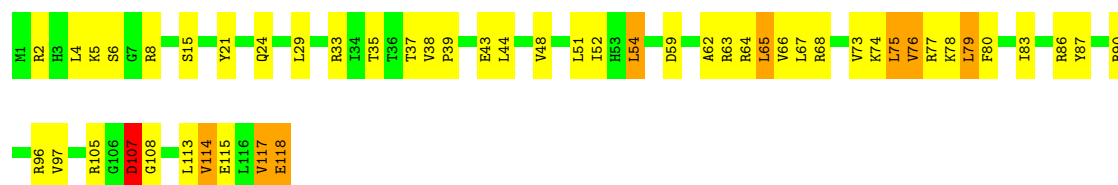
• Molecule 39: 50S ribosomal protein L17

Chain 98: % 55% 33% 12%



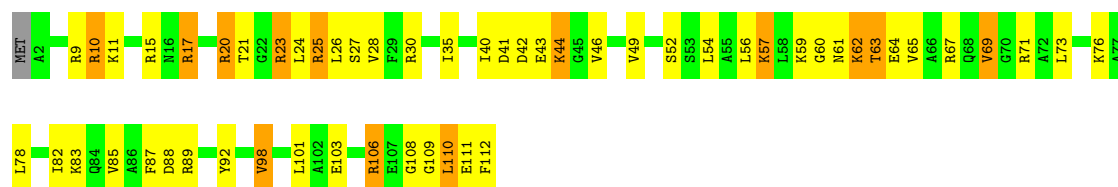
• Molecule 39: 50S ribosomal protein L17

Chain 55: 58% 35% 7% .



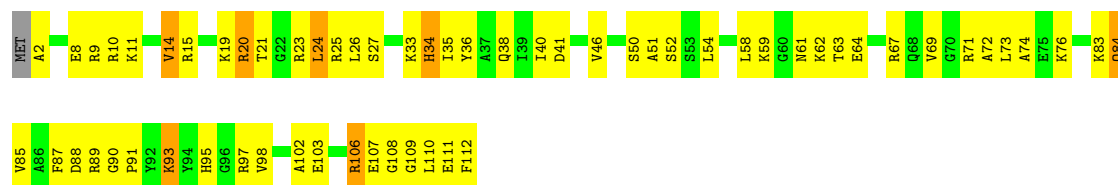
• Molecule 40: 50S ribosomal protein L18

Chain A8:  50% 38% 12% .

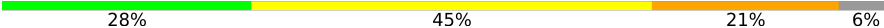


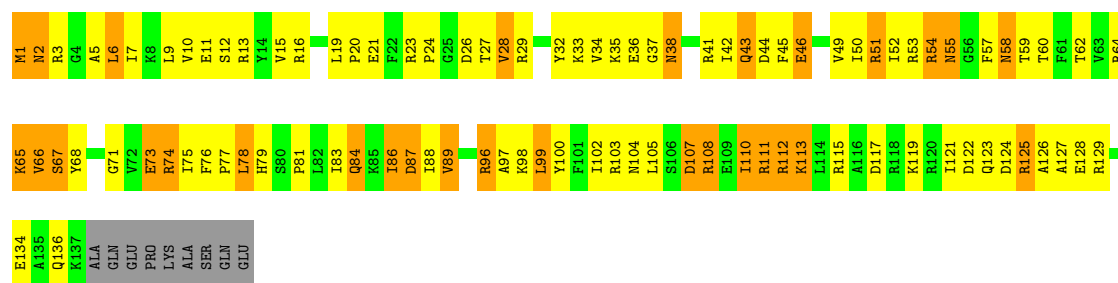
- Molecule 40: 50S ribosomal protein L18

Chain 65:  45% 48% 6% .



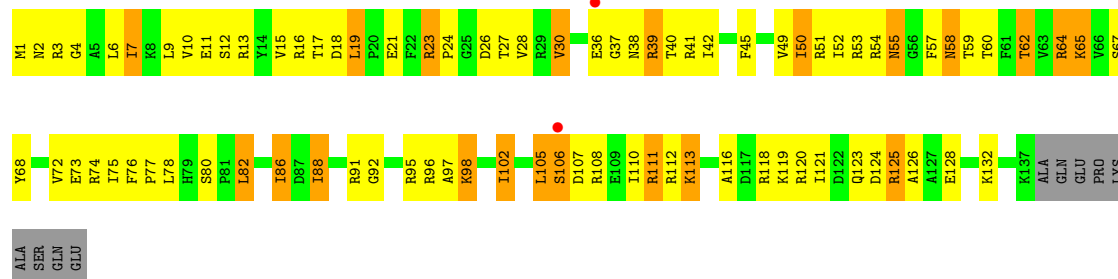
- Molecule 41: 50S ribosomal protein L19

Chain B8:  28% 45% 21% 6% .



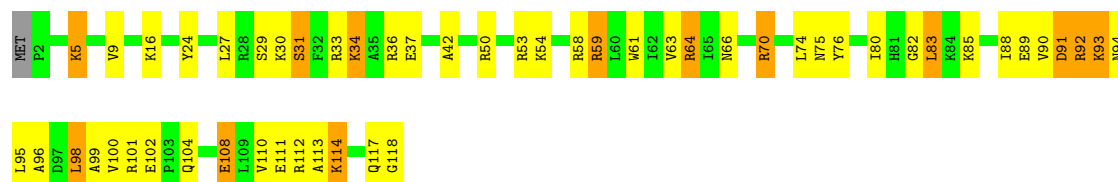
- Molecule 41: 50S ribosomal protein L19

Chain 75:  36% 43% 14% 6% .



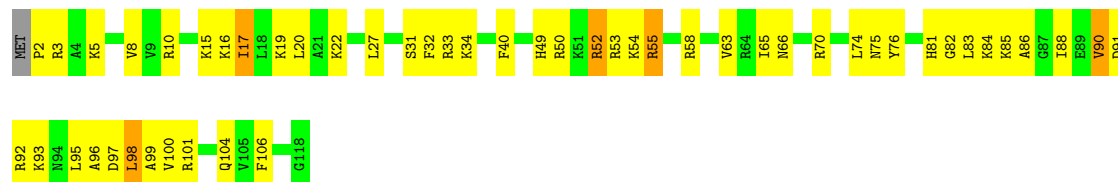
- Molecule 42: 50S ribosomal protein L20

Chain C8:  54% 34% 11% .



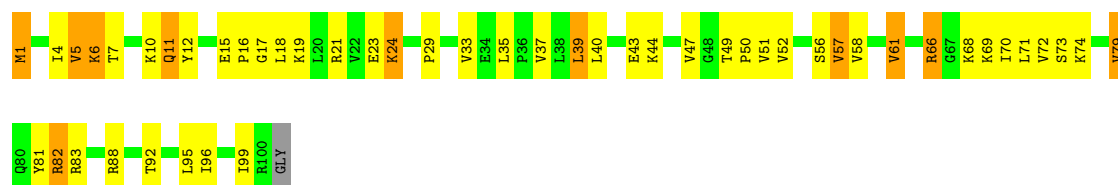
- Molecule 42: 50S ribosomal protein L20

Chain 85: 56% 39% . .



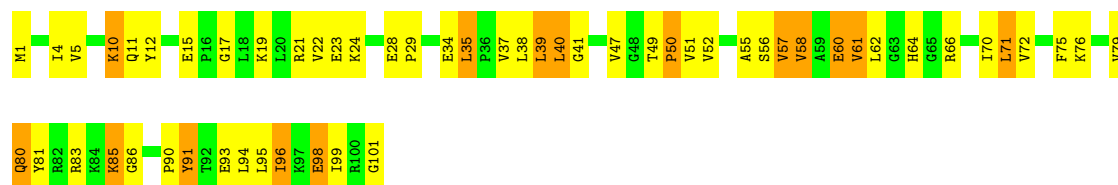
- Molecule 43: 50S ribosomal protein L21

Chain D8: 50% 39% 11% .



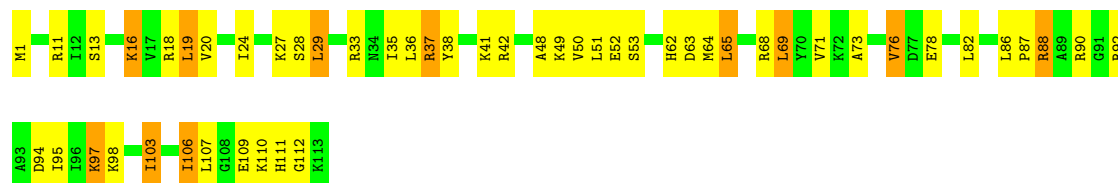
- Molecule 43: 50S ribosomal protein L21

Chain 95: 45% 41% 15%



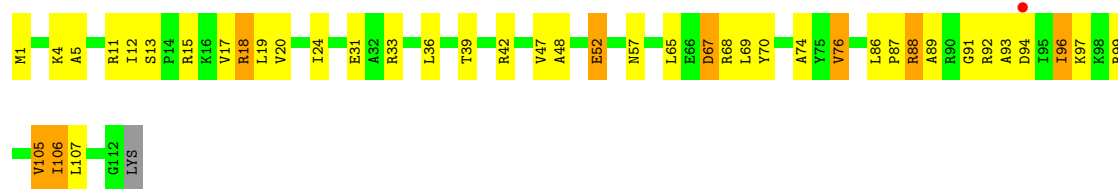
- Molecule 44: 50S ribosomal protein L22

Chain E8: 55% 35% 10%



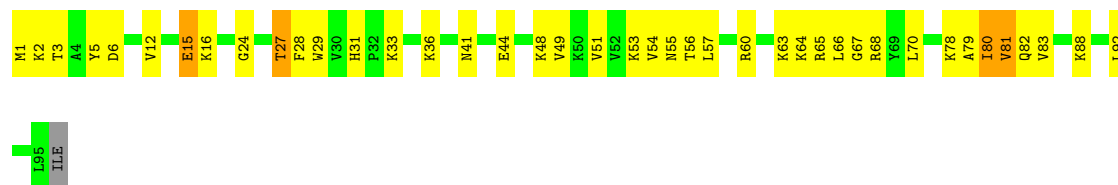
- Molecule 44: 50S ribosomal protein L22

Chain A5: 62% 30% 7% .



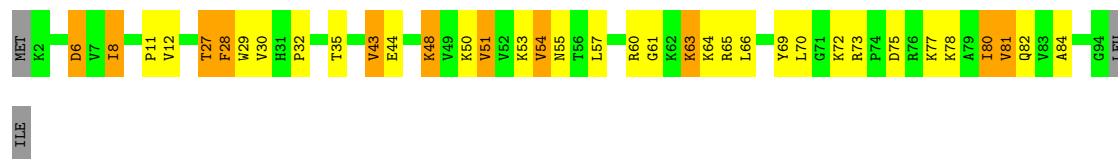
- Molecule 45: 50S ribosomal protein L23

Chain F8: 56% 39% ..



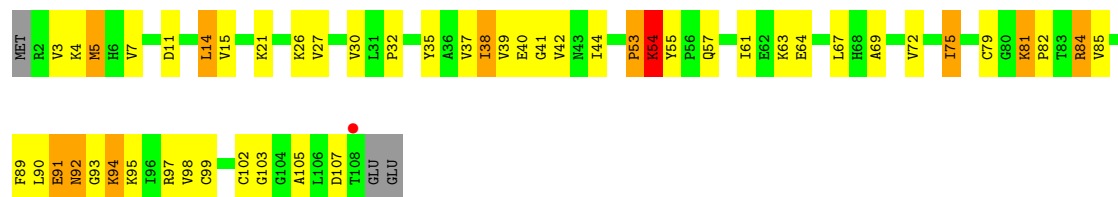
- Molecule 45: 50S ribosomal protein L23

Chain B5: 59% 26% 11% .



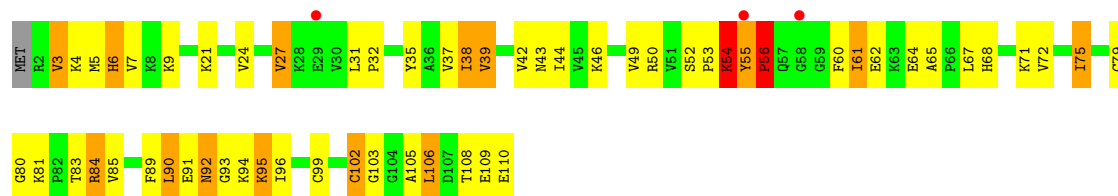
- Molecule 46: 50S ribosomal protein L24

Chain G8: 52% 35% 9% ..

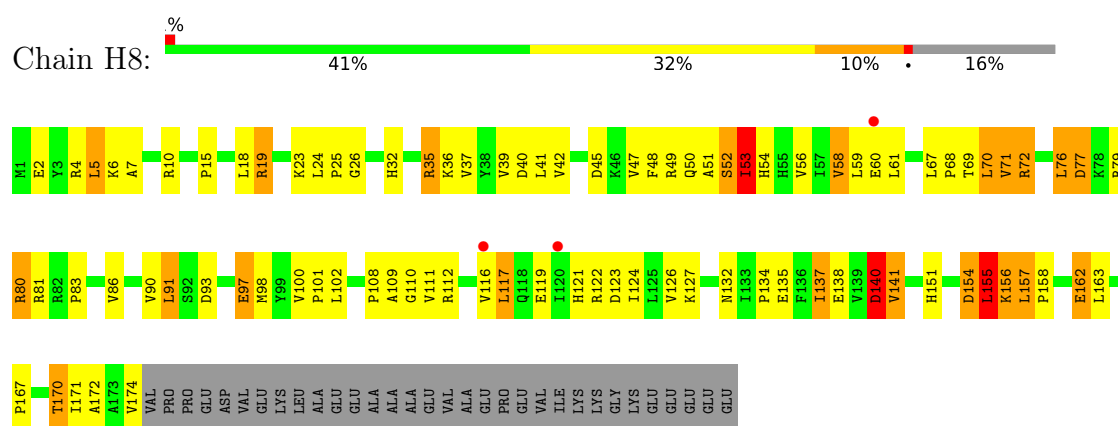


- Molecule 46: 50S ribosomal protein L24

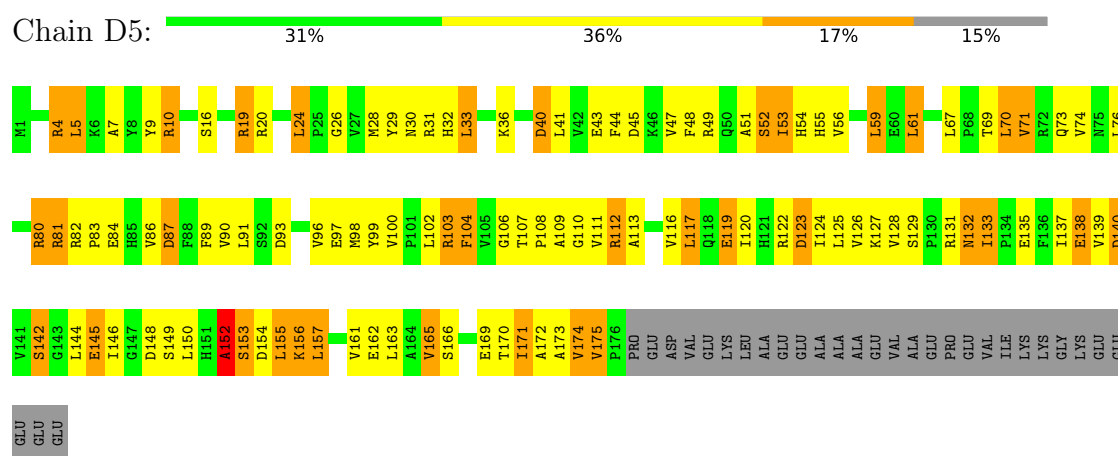
Chain C5: 3% 46% 38% 13% ..



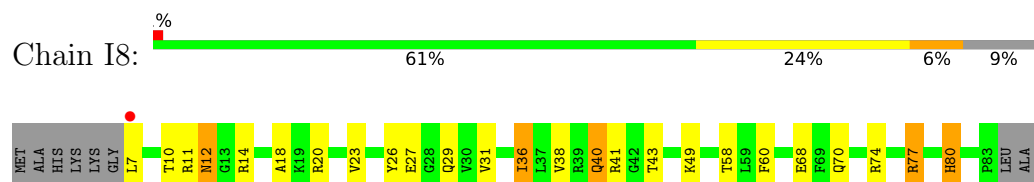
- Molecule 47: 50S ribosomal protein L25



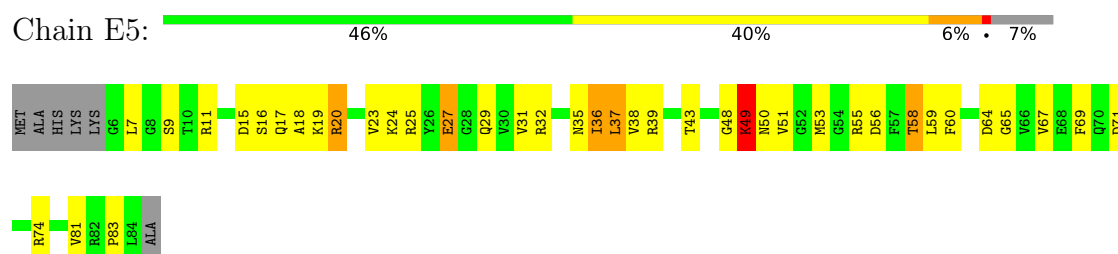
- Molecule 47: 50S ribosomal protein L25



- Molecule 48: 50S ribosomal protein L27

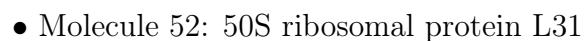
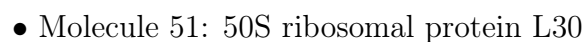
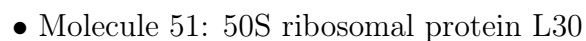
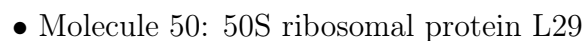
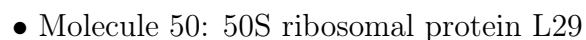
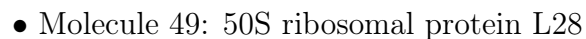


- Molecule 48: 50S ribosomal protein L27



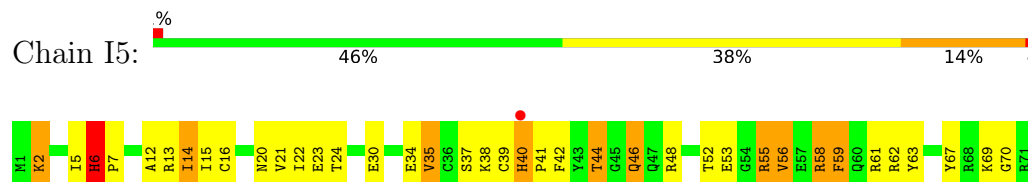
- Molecule 49: 50S ribosomal protein L28



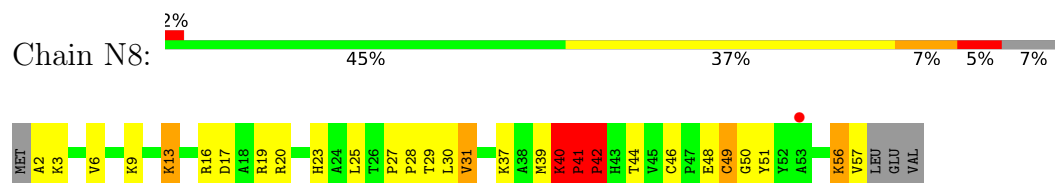


GLY
ARG

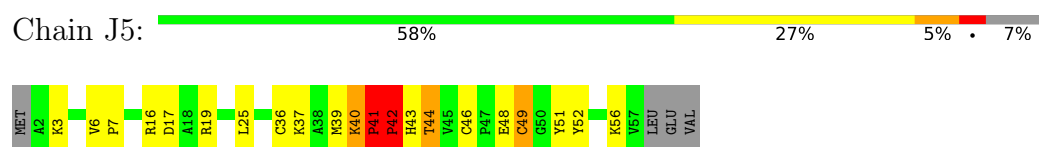
- Molecule 52: 50S ribosomal protein L31



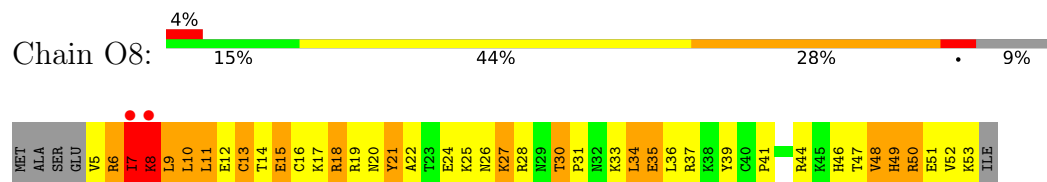
- Molecule 53: 50S ribosomal protein L32



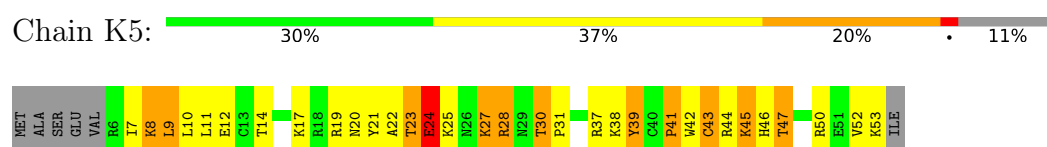
- Molecule 53: 50S ribosomal protein L32



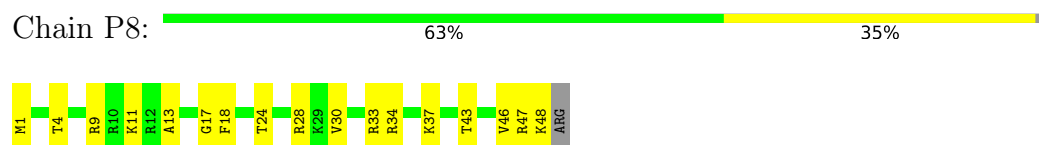
- Molecule 54: 50S ribosomal protein L33



- Molecule 54: 50S ribosomal protein L33



- Molecule 55: 50S ribosomal protein L34



- Molecule 55: 50S ribosomal protein L34

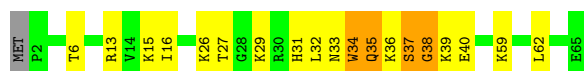




- Molecule 56: 50S ribosomal protein L35



- Molecule 56: 50S ribosomal protein L35



- Molecule 57: E. coli tRNA^{fMet}



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	210.46Å 452.18Å 626.12Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	226.09 – 3.50 226.09 – 3.50	Depositor EDS
% Data completeness (in resolution range)	100.0 (226.09-3.50) 100.0 (226.09-3.50)	Depositor EDS
R_{merge}	0.28	Depositor
R_{sym}	0.18	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.34 (at 3.01Å)	Xtriage
Refinement program	PHENIX 1.13_2998	Depositor
R, R_{free}	0.187 , 0.251 0.198 , 0.254	Depositor DCC
R_{free} test set	22133 reflections (1.88%)	wwPDB-VP
Wilson B-factor (Å ²)	71.7	Xtriage
Anisotropy	0.113	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.26 , 60.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.40$, $\langle L^2 \rangle = 0.22$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	300507	wwPDB-VP
Average B, all atoms (Å ²)	96.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.33% 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: OMC, 2MG, OMG, PSU, 4OC, UR3, ZN, K, 5MC, MG, 4SU, 5MU, 2MA, OMU, M2G, 0TD, H2U, SF4, MA6, 7MG

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	0.17	1/35952 (0.0%)	0.39	0/56107
1	1G	0.16	1/36044 (0.0%)	0.40	3/56250 (0.0%)
2	12	0.19	0/1950	0.47	0/2630
2	1E	0.18	0/1959	0.44	0/2642
3	22	0.19	0/1636	0.50	0/2205
3	2E	0.18	0/1629	0.45	0/2195
4	32	0.17	0/1732	0.45	0/2318
4	3E	0.21	0/1732	0.45	0/2318
5	42	0.21	0/1195	0.45	0/1609
5	4E	0.16	0/1171	0.41	0/1576
6	52	0.15	0/855	0.40	0/1154
6	5E	0.15	0/855	0.39	0/1154
7	62	0.16	0/1235	0.44	0/1654
7	6E	0.14	0/1275	0.38	0/1709
8	72	0.16	0/1135	0.39	0/1527
8	7E	0.18	0/1135	0.46	0/1527
9	82	0.22	0/1021	0.64	0/1371
9	8E	0.17	0/1002	0.47	0/1346
10	1A	0.18	0/814	0.50	0/1095
10	1I	0.16	0/814	0.43	0/1095
11	2A	0.18	0/904	0.46	0/1219
11	2I	0.16	0/879	0.39	0/1188
12	3A	0.17	0/982	0.53	0/1313
12	3I	0.21	0/982	0.52	0/1313
13	4A	0.20	0/947	0.58	0/1270
13	4I	0.21	0/956	0.54	1/1281 (0.1%)
14	5A	0.16	0/494	0.49	0/657
14	5I	0.20	0/500	0.63	2/664 (0.3%)
15	6A	0.15	0/744	0.38	0/992
15	6I	0.16	0/744	0.35	0/992
16	7A	0.18	0/721	0.45	0/970

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
16	7I	0.17	0/716	0.44	0/963
17	8A	0.18	0/832	0.39	0/1113
17	8I	0.15	0/847	0.40	0/1131
18	9A	0.17	0/589	0.43	0/782
18	9I	0.17	0/578	0.42	0/768
19	AA	0.19	0/679	0.51	0/913
19	AI	0.20	0/703	0.59	0/945
20	BA	0.17	0/778	0.50	1/1028 (0.1%)
20	BI	0.18	0/768	0.60	3/1014 (0.3%)
21	1B	0.20	0/221	0.47	0/288
21	1F	0.17	0/221	0.43	0/288
22	1K	0.14	0/1547	0.38	0/2411
22	3K	0.13	0/1832	0.32	0/2855
22	3L	0.14	0/1832	0.33	0/2855
23	2K	0.19	0/1696	0.33	0/2644
24	4K	0.16	0/421	0.37	0/655
24	4L	0.14	0/523	0.38	0/815
25	14	0.18	0/69194	0.40	3/108015 (0.0%)
25	1H	0.20	0/69191	0.42	4/108008 (0.0%)
26	16	0.17	0/2878	0.38	0/4490
26	1J	0.15	0/2928	0.37	0/4568
27	7I	0.19	0/1072	0.44	0/1447
28	11	0.23	0/2175	0.55	0/2933
28	19	0.20	0/2173	0.49	2/2928 (0.1%)
29	21	0.20	0/1592	0.46	0/2149
29	29	0.19	0/1592	0.47	0/2149
30	31	0.22	0/1620	0.48	0/2194
30	39	0.21	0/1654	0.55	0/2239
31	41	0.18	0/1498	0.50	0/2016
31	49	0.18	0/1498	0.50	0/2016
32	51	0.20	0/1362	0.54	0/1841
32	59	0.27	1/1362 (0.1%)	0.47	0/1841
33	61	0.21	0/1151	0.64	0/1558
33	69	0.20	0/1151	0.56	0/1558
34	38	0.23	0/1069	0.66	0/1444
35	15	0.17	0/1131	0.42	0/1525
35	58	0.21	0/1131	0.51	0/1525
36	25	0.19	0/942	0.48	0/1269
36	68	0.19	0/942	0.47	0/1269
37	35	0.25	0/1139	0.70	0/1514
37	78	0.25	0/1147	0.73	1/1525 (0.1%)
38	45	0.22	0/1133	0.53	0/1515
38	88	0.23	0/1142	0.60	1/1527 (0.1%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
39	55	0.26	1/981 (0.1%)	0.50	0/1312
39	98	0.20	0/981	0.55	0/1312
40	65	0.21	0/891	0.53	0/1187
40	A8	0.22	0/891	0.63	0/1187
41	75	0.50	1/1155 (0.1%)	0.72	0/1542
41	B8	0.46	0/1155	0.68	0/1542
42	85	0.22	0/981	0.54	0/1306
42	C8	0.20	0/981	0.45	0/1306
43	95	0.24	0/789	0.61	0/1057
43	D8	0.22	0/785	0.52	0/1052
44	A5	0.19	0/901	0.47	0/1209
44	E8	0.22	0/910	0.51	0/1220
45	B5	0.20	0/744	0.45	0/1000
45	F8	0.20	0/761	0.44	0/1021
46	C5	0.25	0/838	0.66	0/1121
46	G8	0.21	0/818	0.60	0/1094
47	D5	0.26	0/1435	0.69	2/1947 (0.1%)
47	H8	0.23	0/1420	0.62	0/1925
48	E5	0.19	0/631	0.51	0/841
48	I8	0.19	0/619	0.49	0/825
49	F5	0.21	0/728	0.49	0/967
49	J8	0.37	1/761 (0.1%)	0.60	0/1010
50	G5	0.18	0/582	0.45	0/771
50	K8	0.19	0/592	0.55	0/784
51	H5	0.17	0/473	0.44	0/635
51	L8	0.19	0/473	0.40	0/635
52	I5	0.26	0/593	0.71	0/795
52	M8	0.24	0/545	0.75	2/733 (0.3%)
53	J5	0.22	0/448	0.49	0/606
53	N8	0.33	1/448 (0.2%)	0.57	0/606
54	K5	0.29	0/424	1.08	6/565 (1.1%)
54	O8	0.30	0/431	0.83	2/575 (0.3%)
55	L5	0.20	0/426	0.45	0/561
55	P8	0.24	0/426	0.48	0/561
56	M5	0.18	0/514	0.45	0/679
56	Q8	0.20	0/514	0.41	0/679
57	2L	0.18	0/1718	0.35	0/2678
All	All	0.19	7/321407 (0.0%)	0.44	33/480718 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
2	12	0	4
4	32	0	1
7	6E	0	1
12	3A	0	1
12	3I	0	2
13	4A	0	4
19	AA	0	1
19	AI	0	3
20	BA	0	1
20	BI	0	1
28	11	0	1
29	21	0	2
29	29	0	1
31	41	0	1
31	49	0	1
32	51	0	2
33	61	0	4
33	69	0	1
34	38	0	4
37	35	0	3
37	78	0	3
38	45	0	3
38	88	0	1
41	B8	0	1
42	85	0	1
43	95	0	1
45	B5	0	1
46	G8	0	2
47	D5	0	6
47	H8	0	4
48	E5	0	1
49	J8	0	2
50	K8	0	1
52	I5	0	1
52	M8	0	4
53	J5	0	2
53	N8	0	3
54	K5	0	4
54	O8	0	1
All	All	0	81

The worst 5 of 7 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
41	75	106	SER	CA-C	8.11	1.63	1.52
32	59	167	GLU	C-O	-6.74	1.20	1.23
49	J8	67	ILE	CA-CB	6.60	1.57	1.54
1	1G	1498	UR3	O3'-P	5.83	1.62	1.56
1	13	1498	UR3	O3'-P	5.79	1.62	1.56

The worst 5 of 33 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	K5	30	THR	CA-C-N	8.01	146.22	127.00
54	K5	30	THR	C-N-CA	8.01	146.22	127.00
54	K5	30	THR	C-N-CD	-7.70	103.66	120.60
37	78	35	HIS	N-CA-C	7.30	121.14	111.28
20	BA	6	PRO	N-CA-CB	6.75	110.46	103.38

There are no chirality outliers.

5 of 81 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
12	3I	23	ALA	Peptide
12	3I	44	LYS	Peptide
7	6E	5	ARG	Peptide
19	AI	41	VAL	Peptide
19	AI	5	LEU	Peptide

5.2 Too-close contacts [i](#)

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	32387	0	16370	693	0
1	1G	32470	0	16411	755	0
2	12	1915	0	1969	85	0
2	1E	1924	0	1975	71	0
3	22	1612	0	1677	63	0
3	2E	1605	0	1668	52	0
4	32	1702	0	1766	64	0
4	3E	1702	0	1766	68	0
5	42	1178	0	1234	41	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	4E	1155	0	1213	39	0
6	52	842	0	857	28	0
6	5E	842	0	857	21	0
7	62	1217	0	1256	55	0
7	6E	1256	0	1296	36	0
8	72	1115	0	1177	42	0
8	7E	1115	0	1177	41	0
9	82	1002	0	1025	79	0
9	8E	983	0	1006	49	0
10	1A	801	0	849	35	0
10	1I	801	0	849	43	0
11	2A	889	0	916	34	0
11	2I	864	0	878	24	0
12	3A	977	0	1061	36	0
12	3I	977	0	1061	30	0
13	4A	937	0	995	60	0
13	4I	946	0	1008	43	0
14	5A	485	0	519	25	0
14	5I	491	0	530	32	0
15	6A	733	0	771	23	0
15	6I	733	0	771	19	0
16	7A	705	0	725	20	0
16	7I	700	0	720	27	0
17	8A	819	0	880	26	0
17	8I	834	0	904	27	0
18	9A	584	0	657	27	0
18	9I	573	0	644	29	0
19	AA	665	0	684	61	0
19	AI	688	0	710	43	0
20	BA	776	0	857	32	0
20	BI	766	0	854	30	0
21	1B	217	0	234	14	0
21	1F	217	0	234	13	0
22	1K	1385	0	705	38	0
22	3K	1640	0	837	30	0
22	3L	1640	0	837	36	0
23	2K	1643	0	847	17	0
24	4K	373	0	186	8	0
24	4L	463	0	230	7	0
25	14	62013	0	31255	1097	0
25	1H	62010	0	31252	1057	0
26	16	2573	0	1305	35	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
26	1J	2617	0	1328	78	0
27	71	1049	0	1071	52	0
28	11	2125	0	2199	64	0
28	19	2124	0	2197	91	0
29	21	1559	0	1618	49	0
29	29	1559	0	1617	58	0
30	31	1585	0	1632	73	0
30	39	1619	0	1674	82	0
31	41	1473	0	1535	64	0
31	49	1473	0	1535	65	0
32	51	1336	0	1418	58	0
32	59	1336	0	1418	48	0
33	61	1136	0	1223	43	0
33	69	1136	0	1223	40	0
34	38	1056	0	1119	50	0
35	15	1104	0	1180	33	0
35	58	1104	0	1180	42	0
36	25	932	0	996	33	0
36	68	932	0	996	33	0
37	35	1122	0	1206	78	0
37	78	1130	0	1217	65	0
38	45	1112	0	1171	57	0
38	88	1121	0	1179	35	0
39	55	967	0	1033	43	0
39	98	967	0	1033	32	0
40	65	881	0	943	47	0
40	A8	881	0	943	37	0
41	75	1141	0	1202	76	0
41	B8	1141	0	1202	89	0
42	85	963	0	1022	52	0
42	C8	963	0	1021	44	0
43	95	778	0	852	46	0
43	D8	774	0	849	32	0
44	A5	890	0	951	22	0
44	E8	899	0	964	30	0
45	B5	730	0	780	27	0
45	F8	747	0	805	27	0
46	C5	825	0	898	47	0
46	G8	805	0	881	27	0
47	D5	1404	0	1437	81	0
47	H8	1390	0	1421	60	0
48	E5	623	0	645	30	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
48	I8	611	0	631	23	0
49	F5	721	0	791	24	0
49	J8	754	0	838	25	0
50	G5	580	0	629	16	0
50	K8	590	0	643	25	0
51	H5	468	0	518	12	0
51	L8	468	0	518	15	0
52	I5	580	0	577	30	0
52	M8	533	0	526	33	0
53	J5	434	0	454	15	0
53	N8	434	0	454	29	0
54	K5	417	0	441	20	0
54	O8	424	0	450	36	0
55	L5	418	0	467	17	0
55	P8	418	0	467	10	0
56	M5	506	0	567	15	0
56	Q8	506	0	567	18	0
57	2L	1643	0	845	25	0
58	11	1	0	0	0	0
58	13	38	0	0	0	0
58	14	94	0	0	0	0
58	16	2	0	0	0	0
58	19	1	0	0	0	0
58	1G	25	0	0	0	0
58	1H	122	0	0	0	0
58	21	1	0	0	0	0
58	29	2	0	0	0	0
58	31	2	0	0	0	0
58	32	1	0	0	0	0
58	39	1	0	0	0	0
58	3A	1	0	0	0	0
58	41	2	0	0	0	0
58	52	1	0	0	0	0
58	5E	1	0	0	0	0
58	5I	1	0	0	0	0
58	8I	1	0	0	0	0
58	BA	1	0	0	0	0
59	13	111	0	0	0	0
59	14	312	0	0	0	0
59	16	8	0	0	0	0
59	1G	102	0	0	0	0
59	1H	405	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
59	1J	5	0	0	0	0
59	21	2	0	0	0	0
59	29	2	0	0	0	0
59	2K	1	0	0	0	0
59	2L	2	0	0	0	0
59	32	1	0	0	0	0
59	3E	1	0	0	0	0
59	41	1	0	0	0	0
59	4I	1	0	0	0	0
59	55	1	0	0	0	0
59	78	1	0	0	0	0
59	7I	1	0	0	0	0
59	8E	1	0	0	0	0
59	BI	2	0	0	0	0
59	D8	3	0	0	0	0
59	E5	1	0	0	0	0
59	G8	1	0	0	0	0
59	I8	2	0	0	0	0
59	J8	1	0	0	0	0
59	N8	1	0	0	0	0
59	Q8	1	0	0	0	0
60	32	8	0	0	2	0
60	3E	8	0	0	1	0
61	5A	1	0	0	0	0
61	5I	1	0	0	0	0
62	11	10	0	0	1	0
62	13	190	0	0	11	0
62	14	681	0	0	72	0
62	16	12	0	0	2	0
62	19	12	0	0	4	0
62	1G	268	0	0	18	0
62	1H	983	0	0	113	0
62	1J	16	0	0	4	0
62	21	5	0	0	0	0
62	29	3	0	0	0	0
62	2L	6	0	0	0	0
62	31	6	0	0	0	0
62	32	4	0	0	0	0
62	35	3	0	0	1	0
62	39	3	0	0	0	0
62	3A	1	0	0	0	0
62	3E	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
62	3I	1	0	0	0	0
62	3K	1	0	0	0	0
62	42	1	0	0	0	0
62	4I	2	0	0	0	0
62	4K	2	0	0	0	0
62	4L	4	0	0	0	0
62	55	2	0	0	0	0
62	58	1	0	0	0	0
62	5I	1	0	0	0	0
62	6I	1	0	0	0	0
62	75	1	0	0	0	0
62	78	6	0	0	1	0
62	7A	5	0	0	0	0
62	7I	3	0	0	1	0
62	85	1	0	0	0	0
62	98	1	0	0	0	0
62	B5	2	0	0	0	0
62	B8	2	0	0	0	0
62	BA	1	0	0	0	0
62	BI	4	0	0	1	0
62	C5	2	0	0	0	0
62	C8	2	0	0	0	0
62	F5	1	0	0	0	0
62	F8	2	0	0	0	0
62	G5	1	0	0	0	0
62	G8	1	0	0	0	0
62	I8	5	0	0	0	0
62	J8	3	0	0	0	0
62	L5	1	0	0	0	0
62	M5	1	0	0	0	0
62	Q8	1	0	0	0	0
All	All	300507	0	201662	6882	0

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 14.

The worst 5 of 6882 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)
28:19:182:LEU:H	28:19:272:ALA:HB3	1.30	0.97
1:13:1129:C:H5'	1:13:1130:A:H5'	1.47	0.96

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:1H:1053:C:H42	25:1H:1106:G:H1	1.12	0.95
25:14:2245:U:H5'	25:14:2246:G:H5'	1.47	0.95
1:1G:73:G:H1	1:1G:97:U:H3	1.10	0.94

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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	234/256 (91%)	193 (82%)	36 (15%)	5 (2%)	5	31
2	1E	235/256 (92%)	200 (85%)	35 (15%)	0	100	100
3	22	204/239 (85%)	161 (79%)	41 (20%)	2 (1%)	12	44
3	2E	203/239 (85%)	172 (85%)	31 (15%)	0	100	100
4	32	206/209 (99%)	188 (91%)	18 (9%)	0	100	100
4	3E	206/209 (99%)	190 (92%)	16 (8%)	0	100	100
5	42	152/162 (94%)	134 (88%)	18 (12%)	0	100	100
5	4E	149/162 (92%)	140 (94%)	9 (6%)	0	100	100
6	52	99/101 (98%)	94 (95%)	5 (5%)	0	100	100
6	5E	99/101 (98%)	91 (92%)	8 (8%)	0	100	100
7	62	145/156 (93%)	122 (84%)	21 (14%)	2 (1%)	9	38
7	6E	153/156 (98%)	140 (92%)	13 (8%)	0	100	100
8	72	136/138 (99%)	125 (92%)	11 (8%)	0	100	100
8	7E	136/138 (99%)	123 (90%)	13 (10%)	0	100	100
9	82	125/128 (98%)	90 (72%)	29 (23%)	6 (5%)	2	16
9	8E	122/128 (95%)	107 (88%)	15 (12%)	0	100	100
10	1A	97/105 (92%)	79 (81%)	18 (19%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
10	1I	97/105 (92%)	84 (87%)	13 (13%)	0	100	100
11	2A	117/129 (91%)	100 (86%)	16 (14%)	1 (1%)	14	47
11	2I	115/129 (89%)	108 (94%)	7 (6%)	0	100	100
12	3A	122/132 (92%)	101 (83%)	18 (15%)	3 (2%)	4	28
12	3I	122/132 (92%)	102 (84%)	19 (16%)	1 (1%)	16	49
13	4A	116/126 (92%)	79 (68%)	31 (27%)	6 (5%)	1	14
13	4I	117/126 (93%)	99 (85%)	16 (14%)	2 (2%)	7	35
14	5A	58/61 (95%)	49 (84%)	8 (14%)	1 (2%)	7	35
14	5I	58/61 (95%)	48 (83%)	9 (16%)	1 (2%)	7	35
15	6A	86/89 (97%)	81 (94%)	5 (6%)	0	100	100
15	6I	86/89 (97%)	77 (90%)	9 (10%)	0	100	100
16	7A	82/88 (93%)	76 (93%)	6 (7%)	0	100	100
16	7I	81/88 (92%)	73 (90%)	8 (10%)	0	100	100
17	8A	97/105 (92%)	91 (94%)	6 (6%)	0	100	100
17	8I	98/105 (93%)	92 (94%)	6 (6%)	0	100	100
18	9A	69/88 (78%)	62 (90%)	7 (10%)	0	100	100
18	9I	68/88 (77%)	61 (90%)	7 (10%)	0	100	100
19	AA	81/93 (87%)	56 (69%)	25 (31%)	0	100	100
19	AI	84/93 (90%)	68 (81%)	15 (18%)	1 (1%)	10	41
20	BA	101/106 (95%)	89 (88%)	12 (12%)	0	100	100
20	BI	99/106 (93%)	85 (86%)	13 (13%)	1 (1%)	12	44
21	1B	23/27 (85%)	19 (83%)	4 (17%)	0	100	100
21	1F	23/27 (85%)	19 (83%)	4 (17%)	0	100	100
27	7I	131/229 (57%)	118 (90%)	13 (10%)	0	100	100
28	11	272/276 (99%)	247 (91%)	24 (9%)	1 (0%)	30	62
28	19	270/276 (98%)	244 (90%)	26 (10%)	0	100	100
29	21	202/206 (98%)	177 (88%)	23 (11%)	2 (1%)	12	44
29	29	202/206 (98%)	183 (91%)	18 (9%)	1 (0%)	24	57
30	31	200/210 (95%)	174 (87%)	25 (12%)	1 (0%)	24	57
30	39	204/210 (97%)	166 (81%)	34 (17%)	4 (2%)	6	32
31	41	179/182 (98%)	144 (80%)	33 (18%)	2 (1%)	11	43

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
31	49	179/182 (98%)	141 (79%)	35 (20%)	3 (2%)	7	35
32	51	172/180 (96%)	139 (81%)	31 (18%)	2 (1%)	10	41
32	59	172/180 (96%)	131 (76%)	39 (23%)	2 (1%)	10	41
33	61	144/148 (97%)	112 (78%)	30 (21%)	2 (1%)	9	38
33	69	144/148 (97%)	113 (78%)	30 (21%)	1 (1%)	18	51
34	38	135/173 (78%)	75 (56%)	57 (42%)	3 (2%)	5	30
35	15	136/140 (97%)	121 (89%)	15 (11%)	0	100	100
35	58	136/140 (97%)	110 (81%)	23 (17%)	3 (2%)	5	30
36	25	120/122 (98%)	105 (88%)	15 (12%)	0	100	100
36	68	120/122 (98%)	110 (92%)	10 (8%)	0	100	100
37	35	145/150 (97%)	109 (75%)	35 (24%)	1 (1%)	18	51
37	78	146/150 (97%)	110 (75%)	33 (23%)	3 (2%)	5	31
38	45	138/141 (98%)	111 (80%)	26 (19%)	1 (1%)	18	51
38	88	139/141 (99%)	105 (76%)	32 (23%)	2 (1%)	9	38
39	55	116/118 (98%)	107 (92%)	8 (7%)	1 (1%)	14	47
39	98	116/118 (98%)	105 (90%)	9 (8%)	2 (2%)	7	35
40	65	109/112 (97%)	88 (81%)	21 (19%)	0	100	100
40	A8	109/112 (97%)	84 (77%)	24 (22%)	1 (1%)	14	47
41	75	135/146 (92%)	107 (79%)	27 (20%)	1 (1%)	18	51
41	B8	135/146 (92%)	113 (84%)	22 (16%)	0	100	100
42	85	115/118 (98%)	99 (86%)	15 (13%)	1 (1%)	14	47
42	C8	115/118 (98%)	106 (92%)	8 (7%)	1 (1%)	14	47
43	95	99/101 (98%)	78 (79%)	20 (20%)	1 (1%)	12	44
43	D8	98/101 (97%)	83 (85%)	15 (15%)	0	100	100
44	A5	110/113 (97%)	104 (94%)	6 (6%)	0	100	100
44	E8	111/113 (98%)	99 (89%)	12 (11%)	0	100	100
45	B5	91/96 (95%)	77 (85%)	14 (15%)	0	100	100
45	F8	93/96 (97%)	85 (91%)	8 (9%)	0	100	100
46	C5	107/110 (97%)	82 (77%)	22 (21%)	3 (3%)	4	26
46	G8	105/110 (96%)	79 (75%)	24 (23%)	2 (2%)	6	33
47	D5	174/206 (84%)	114 (66%)	55 (32%)	5 (3%)	3	26

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
47	H8	172/206 (84%)	123 (72%)	45 (26%)	4 (2%)	5	30
48	E5	77/85 (91%)	65 (84%)	12 (16%)	0	100	100
48	I8	75/85 (88%)	65 (87%)	10 (13%)	0	100	100
49	F5	90/96 (94%)	75 (83%)	15 (17%)	0	100	100
49	J8	94/96 (98%)	75 (80%)	16 (17%)	3 (3%)	3	24
50	G5	67/72 (93%)	58 (87%)	9 (13%)	0	100	100
50	K8	69/72 (96%)	56 (81%)	11 (16%)	2 (3%)	3	26
51	H5	57/60 (95%)	53 (93%)	4 (7%)	0	100	100
51	L8	57/60 (95%)	52 (91%)	5 (9%)	0	100	100
52	I5	69/71 (97%)	40 (58%)	28 (41%)	1 (1%)	9	38
52	M8	64/71 (90%)	32 (50%)	30 (47%)	2 (3%)	3	25
53	J5	54/60 (90%)	42 (78%)	10 (18%)	2 (4%)	2	21
53	N8	54/60 (90%)	45 (83%)	7 (13%)	2 (4%)	2	21
54	K5	46/54 (85%)	21 (46%)	22 (48%)	3 (6%)	1	11
54	O8	47/54 (87%)	27 (57%)	17 (36%)	3 (6%)	1	11
55	L5	46/49 (94%)	46 (100%)	0	0	100	100
55	P8	46/49 (94%)	45 (98%)	1 (2%)	0	100	100
56	M5	62/65 (95%)	53 (86%)	7 (11%)	2 (3%)	3	24
56	Q8	62/65 (95%)	58 (94%)	4 (6%)	0	100	100
All	All	11633/12452 (93%)	9754 (84%)	1771 (15%)	108 (1%)	14	47

5 of 108 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
14	5I	16	PHE
35	58	96	GLU
39	98	3	HIS
47	H8	53	ILE
49	J8	30	VAL

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	204/220 (93%)	148 (72%)	56 (28%)	0	3
2	1E	205/220 (93%)	162 (79%)	43 (21%)	1	6
3	22	160/188 (85%)	115 (72%)	45 (28%)	0	3
3	2E	159/188 (85%)	133 (84%)	26 (16%)	2	14
4	32	180/181 (99%)	156 (87%)	24 (13%)	4	20
4	3E	180/181 (99%)	148 (82%)	32 (18%)	2	10
5	42	119/123 (97%)	88 (74%)	31 (26%)	0	3
5	4E	116/123 (94%)	92 (79%)	24 (21%)	1	6
6	52	90/90 (100%)	83 (92%)	7 (8%)	11	36
6	5E	90/90 (100%)	73 (81%)	17 (19%)	1	9
7	62	123/127 (97%)	102 (83%)	21 (17%)	2	12
7	6E	126/127 (99%)	102 (81%)	24 (19%)	1	8
8	72	119/119 (100%)	99 (83%)	20 (17%)	2	13
8	7E	119/119 (100%)	93 (78%)	26 (22%)	1	6
9	82	97/99 (98%)	76 (78%)	21 (22%)	1	6
9	8E	95/99 (96%)	79 (83%)	16 (17%)	2	13
10	1A	89/92 (97%)	70 (79%)	19 (21%)	1	6
10	1I	89/92 (97%)	73 (82%)	16 (18%)	2	10
11	2A	91/99 (92%)	73 (80%)	18 (20%)	1	7
11	2I	88/99 (89%)	70 (80%)	18 (20%)	1	7
12	3A	103/108 (95%)	82 (80%)	21 (20%)	1	7
12	3I	103/108 (95%)	86 (84%)	17 (16%)	2	13
13	4A	94/101 (93%)	66 (70%)	28 (30%)	0	2
13	4I	95/101 (94%)	67 (70%)	28 (30%)	0	2
14	5A	48/50 (96%)	46 (96%)	2 (4%)	26	52
14	5I	49/50 (98%)	41 (84%)	8 (16%)	2	14
15	6A	79/80 (99%)	66 (84%)	13 (16%)	2	13
15	6I	79/80 (99%)	66 (84%)	13 (16%)	2	13
16	7A	72/74 (97%)	61 (85%)	11 (15%)	3	16
16	7I	72/74 (97%)	59 (82%)	13 (18%)	2	10

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
17	8A	93/97 (96%)	80 (86%)	13 (14%)	3	19
17	8I	95/97 (98%)	83 (87%)	12 (13%)	4	21
18	9A	62/77 (80%)	48 (77%)	14 (23%)	1	5
18	9I	61/77 (79%)	49 (80%)	12 (20%)	1	8
19	AA	72/80 (90%)	56 (78%)	16 (22%)	1	5
19	AI	74/80 (92%)	55 (74%)	19 (26%)	0	3
20	BA	75/82 (92%)	63 (84%)	12 (16%)	2	14
20	BI	75/82 (92%)	62 (83%)	13 (17%)	2	11
21	1B	20/22 (91%)	14 (70%)	6 (30%)	0	2
21	1F	20/22 (91%)	19 (95%)	1 (5%)	22	48
27	71	111/181 (61%)	95 (86%)	16 (14%)	3	18
28	11	214/218 (98%)	166 (78%)	48 (22%)	1	5
28	19	213/218 (98%)	181 (85%)	32 (15%)	3	17
29	21	164/166 (99%)	134 (82%)	30 (18%)	2	10
29	29	164/166 (99%)	134 (82%)	30 (18%)	2	10
30	31	161/166 (97%)	135 (84%)	26 (16%)	2	14
30	39	165/166 (99%)	135 (82%)	30 (18%)	2	10
31	41	155/156 (99%)	130 (84%)	25 (16%)	2	14
31	49	155/156 (99%)	126 (81%)	29 (19%)	1	9
32	51	145/148 (98%)	114 (79%)	31 (21%)	1	6
32	59	145/148 (98%)	114 (79%)	31 (21%)	1	6
33	61	122/124 (98%)	80 (66%)	42 (34%)	0	2
33	69	122/124 (98%)	91 (75%)	31 (25%)	0	3
34	38	112/135 (83%)	77 (69%)	35 (31%)	0	2
35	15	117/119 (98%)	98 (84%)	19 (16%)	2	14
35	58	117/119 (98%)	88 (75%)	29 (25%)	1	4
36	25	100/100 (100%)	80 (80%)	20 (20%)	1	7
36	68	100/100 (100%)	84 (84%)	16 (16%)	2	14
37	35	114/116 (98%)	82 (72%)	32 (28%)	0	3
37	78	115/116 (99%)	88 (76%)	27 (24%)	1	4
38	45	110/111 (99%)	89 (81%)	21 (19%)	1	8

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
38	88	111/111 (100%)	88 (79%)	23 (21%)	1	6
39	55	101/101 (100%)	83 (82%)	18 (18%)	2	10
39	98	101/101 (100%)	78 (77%)	23 (23%)	1	5
40	65	87/88 (99%)	73 (84%)	14 (16%)	2	14
40	A8	87/88 (99%)	61 (70%)	26 (30%)	0	2
41	75	120/127 (94%)	90 (75%)	30 (25%)	0	4
41	B8	120/127 (94%)	75 (62%)	45 (38%)	0	1
42	85	93/94 (99%)	77 (83%)	16 (17%)	2	12
42	C8	93/94 (99%)	73 (78%)	20 (22%)	1	6
43	95	82/82 (100%)	59 (72%)	23 (28%)	0	3
43	D8	82/82 (100%)	54 (66%)	28 (34%)	0	2
44	A5	91/92 (99%)	71 (78%)	20 (22%)	1	5
44	E8	92/92 (100%)	69 (75%)	23 (25%)	0	4
45	B5	74/78 (95%)	61 (82%)	13 (18%)	2	11
45	F8	76/78 (97%)	60 (79%)	16 (21%)	1	6
46	C5	88/91 (97%)	58 (66%)	30 (34%)	0	2
46	G8	85/91 (93%)	63 (74%)	22 (26%)	0	3
47	D5	155/179 (87%)	112 (72%)	43 (28%)	0	3
47	H8	153/179 (86%)	116 (76%)	37 (24%)	1	4
48	E5	63/67 (94%)	51 (81%)	12 (19%)	1	8
48	I8	62/67 (92%)	54 (87%)	8 (13%)	4	21
49	F5	77/81 (95%)	56 (73%)	21 (27%)	0	3
49	J8	81/81 (100%)	71 (88%)	10 (12%)	4	22
50	G5	64/67 (96%)	48 (75%)	16 (25%)	0	4
50	K8	64/67 (96%)	42 (66%)	22 (34%)	0	2
51	H5	51/52 (98%)	45 (88%)	6 (12%)	5	23
51	L8	51/52 (98%)	39 (76%)	12 (24%)	1	4
52	I5	63/63 (100%)	43 (68%)	20 (32%)	0	2
52	M8	59/63 (94%)	43 (73%)	16 (27%)	0	3
53	J5	48/52 (92%)	38 (79%)	10 (21%)	1	6
53	N8	48/52 (92%)	37 (77%)	11 (23%)	1	5

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
54	K5	47/52 (90%)	34 (72%)	13 (28%)	0	3
54	O8	48/52 (92%)	28 (58%)	20 (42%)	0	0
55	L5	41/42 (98%)	33 (80%)	8 (20%)	1	8
55	P8	41/42 (98%)	36 (88%)	5 (12%)	5	22
56	M5	52/55 (94%)	46 (88%)	6 (12%)	5	24
56	Q8	52/55 (94%)	46 (88%)	6 (12%)	5	24
All	All	9804/10308 (95%)	7736 (79%)	2068 (21%)	1	6

5 of 2068 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
44	A5	18	ARG
46	C5	95	LYS
44	A5	1	MET
41	B8	6	LEU
40	A8	35	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 69 such sidechains are listed below:

Mol	Chain	Res	Type
29	29	132	HIS
30	39	40	GLN
47	D5	151	HIS
28	11	227	ASN
28	11	220	HIS

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	13	1504/1522 (98%)	361 (24%)	47 (3%)
1	1G	1508/1522 (99%)	398 (26%)	53 (3%)
22	1K	64/77 (83%)	20 (31%)	2 (3%)
22	3K	76/77 (98%)	23 (30%)	0
22	3L	76/77 (98%)	31 (40%)	2 (2%)
23	2K	76/77 (98%)	9 (11%)	1 (1%)
24	4K	16/27 (59%)	10 (62%)	2 (12%)
24	4L	20/27 (74%)	8 (40%)	1 (5%)
25	14	2876/2917 (98%)	759 (26%)	50 (1%)

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Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
25	1H	2874/2917 (98%)	676 (23%)	63 (2%)
26	16	119/122 (97%)	28 (23%)	2 (1%)
26	1J	121/122 (99%)	40 (33%)	3 (2%)
57	2L	76/77 (98%)	11 (14%)	0
All	All	9406/9561 (98%)	2374 (25%)	226 (2%)

5 of 2374 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	13	5	U
1	13	6	G
1	13	7	G
1	13	8	A
1	13	32	A

5 of 226 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
26	16	24	G
25	14	2859	G
1	1G	872	A
25	14	2776	A
25	14	1647	G

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

59 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
25	OMC	1H	1920	25	19,22,23	1.76	4 (21%)	25,31,34	1.07	4 (16%)
1	M2G	1G	966	1	24,27,28	2.90	8 (33%)	33,40,43	1.71	7 (21%)
25	PSU	1H	2605	25	18,21,22	1.17	2 (11%)	21,30,33	2.13	5 (23%)
25	OMG	14	2251	57,25,58	23,26,27	5.12	11 (47%)	32,38,41	4.73	18 (56%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
25	2MA	1H	2503	59,25,58	22,25,26	3.57	7 (31%)	32,37,40	2.35	9 (28%)
23	H2U	2K	21	23	18,21,22	2.17	4 (22%)	19,30,33	1.64	3 (15%)
57	OMC	2L	33	57	19,22,23	1.82	4 (21%)	25,31,34	1.09	3 (12%)
25	5MC	1H	1942	25	19,22,23	3.83	8 (42%)	26,32,35	1.04	2 (7%)
57	5MU	2L	55	57	19,22,23	3.98	5 (26%)	27,32,35	3.24	10 (37%)
25	OMU	1H	2552	59,25	19,22,23	2.96	8 (42%)	25,31,34	1.88	5 (20%)
1	MA6	1G	1519	1	23,26,27	1.43	5 (21%)	33,38,41	2.71	12 (36%)
25	PSU	1H	1917	25	18,21,22	1.19	1 (5%)	21,30,33	1.97	4 (19%)
1	4OC	13	1402	1	20,23,24	3.12	8 (40%)	25,32,35	0.87	1 (4%)
1	5MC	13	1407	1	19,22,23	4.09	8 (42%)	26,32,35	1.04	1 (3%)
1	PSU	13	516	59,1	18,21,22	1.19	1 (5%)	21,30,33	1.75	4 (19%)
25	5MU	1H	1939	25,58	19,22,23	3.81	5 (26%)	27,32,35	3.70	8 (29%)
1	5MC	1G	1407	1	19,22,23	4.09	8 (42%)	26,32,35	1.10	2 (7%)
1	PSU	1G	516	59,1	18,21,22	1.19	1 (5%)	21,30,33	1.89	4 (19%)
23	PSU	2K	56	23	18,21,22	1.17	1 (5%)	21,30,33	1.95	5 (23%)
25	5MU	14	1939	25,58	19,22,23	3.78	5 (26%)	27,32,35	3.42	9 (33%)
25	5MU	14	1915	25	19,22,23	4.05	5 (26%)	27,32,35	3.28	9 (33%)
1	MA6	13	1518	1	23,26,27	1.49	5 (21%)	33,38,41	2.71	12 (36%)
25	5MC	14	1962	25	19,22,23	4.13	8 (42%)	26,32,35	1.41	5 (19%)
25	PSU	14	2605	25	18,21,22	1.18	1 (5%)	21,30,33	1.82	3 (14%)
12	0TD	3A	89	12	8,9,10	1.43	0	6,11,13	3.19	3 (50%)
1	4OC	1G	1402	1	20,23,24	2.97	8 (40%)	25,32,35	1.15	1 (4%)
1	MA6	1G	1518	1	23,26,27	1.50	5 (21%)	33,38,41	2.61	11 (33%)
25	PSU	14	1911	25	18,21,22	1.14	1 (5%)	21,30,33	1.73	4 (19%)
57	4SU	2L	8	57	18,21,22	1.85	3 (16%)	25,30,33	1.98	4 (16%)
1	5MC	13	1400	1	19,22,23	4.28	8 (42%)	26,32,35	1.08	2 (7%)
23	7MG	2K	47	23	23,26,27	3.14	8 (34%)	27,39,42	2.77	9 (33%)
25	OMC	14	1920	25	19,22,23	1.78	4 (21%)	25,31,34	0.84	1 (4%)
1	7MG	13	527	58,1	23,26,27	3.12	8 (34%)	27,39,42	2.83	9 (33%)
57	PSU	2L	56	57	18,21,22	1.21	1 (5%)	21,30,33	1.92	4 (19%)
1	7MG	1G	527	58,1	23,26,27	3.10	8 (34%)	27,39,42	2.83	9 (33%)
25	2MA	14	2503	59,25,58	22,25,26	3.68	8 (36%)	32,37,40	2.26	11 (34%)
25	OMG	1H	2251	25,58,23	23,26,27	5.07	11 (47%)	32,38,41	4.75	16 (50%)
1	5MC	1G	1400	1	19,22,23	4.14	8 (42%)	26,32,35	1.08	2 (7%)
1	UR3	13	1498	1	19,22,23	2.84	7 (36%)	26,32,35	1.72	4 (15%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
57	7MG	2L	47	57	23,26,27	3.09	8 (34%)	27,39,42	2.81	9 (33%)
1	UR3	1G	1498	1	19,22,23	2.84	7 (36%)	26,32,35	1.83	4 (15%)
1	5MC	13	1404	1	19,22,23	4.12	8 (42%)	26,32,35	1.12	2 (7%)
1	5MC	1G	1404	1	19,22,23	4.17	8 (42%)	26,32,35	1.00	2 (7%)
25	OMU	14	2552	59,25	19,22,23	3.05	8 (42%)	25,31,34	2.02	5 (20%)
25	5MC	14	1942	25	19,22,23	4.09	8 (42%)	26,32,35	1.07	2 (7%)
23	5MU	2K	55	23	19,22,23	3.99	5 (26%)	27,32,35	3.19	8 (29%)
23	OMC	2K	33	23	19,22,23	1.80	3 (15%)	25,31,34	1.03	2 (8%)
25	5MU	1H	1915	25	19,22,23	4.02	5 (26%)	27,32,35	3.30	10 (37%)
12	0TD	3I	89	12	8,9,10	1.28	0	6,11,13	2.92	3 (50%)
1	2MG	1G	1207	1	23,26,27	3.13	8 (34%)	33,38,41	2.17	8 (24%)
1	MA6	13	1519	1	23,26,27	1.49	5 (21%)	33,38,41	2.66	11 (33%)
23	4SU	2K	8	23	18,21,22	1.87	3 (16%)	25,30,33	2.45	5 (20%)
25	PSU	14	1917	25	18,21,22	1.10	1 (5%)	21,30,33	1.95	5 (23%)
1	2MG	13	1207	1	23,26,27	3.04	8 (34%)	33,38,41	2.29	13 (39%)
25	5MC	1H	1962	25,58	19,22,23	4.14	8 (42%)	26,32,35	1.06	1 (3%)
1	5MC	1G	967	1	19,22,23	4.17	8 (42%)	26,32,35	1.04	2 (7%)
1	M2G	13	966	1	24,27,28	2.99	8 (33%)	33,40,43	1.68	6 (18%)
25	PSU	1H	1911	25	18,21,22	1.14	1 (5%)	21,30,33	1.84	4 (19%)
1	5MC	13	967	1	19,22,23	4.13	8 (42%)	26,32,35	1.02	2 (7%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
25	OMC	1H	1920	25	-	2/9/27/28	0/2/2/2
1	M2G	1G	966	1	-	0/11/29/30	0/3/3/3
25	PSU	1H	2605	25	-	2/7/25/26	0/2/2/2
25	OMG	14	2251	57,25,58	-	0/9/27/28	0/3/3/3
25	2MA	1H	2503	59,25,58	-	3/7/25/26	0/3/3/3
23	H2U	2K	21	23	-	4/7/38/39	0/2/2/2
57	OMC	2L	33	57	-	3/9/27/28	0/2/2/2
25	5MC	1H	1942	25	-	0/7/25/26	0/2/2/2
57	5MU	2L	55	57	-	0/7/25/26	0/2/2/2
25	OMU	1H	2552	59,25	-	0/9/27/28	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	MA6	1G	1519	1	-	3/11/29/30	0/3/3/3
25	PSU	1H	1917	25	-	1/7/25/26	0/2/2/2
1	4OC	13	1402	1	-	2/9/29/30	0/2/2/2
1	5MC	13	1407	1	-	0/7/25/26	0/2/2/2
1	PSU	13	516	59,1	-	0/7/25/26	0/2/2/2
25	5MU	1H	1939	25,58	-	0/7/25/26	0/2/2/2
1	5MC	1G	1407	1	-	0/7/25/26	0/2/2/2
1	PSU	1G	516	59,1	-	0/7/25/26	0/2/2/2
23	PSU	2K	56	23	-	2/7/25/26	0/2/2/2
25	5MU	14	1939	25,58	-	0/7/25/26	0/2/2/2
25	5MU	14	1915	25	-	3/7/25/26	0/2/2/2
1	MA6	13	1518	1	-	0/11/29/30	0/3/3/3
25	5MC	14	1962	25	-	2/7/25/26	0/2/2/2
25	PSU	14	2605	25	-	0/7/25/26	0/2/2/2
12	0TD	3A	89	12	-	5/7/12/14	-
1	4OC	1G	1402	1	-	2/9/29/30	0/2/2/2
1	MA6	1G	1518	1	-	2/11/29/30	0/3/3/3
25	PSU	14	1911	25	-	0/7/25/26	0/2/2/2
57	4SU	2L	8	57	-	3/7/25/26	0/2/2/2
1	5MC	13	1400	1	-	2/7/25/26	0/2/2/2
23	7MG	2K	47	23	-	2/7/37/38	0/3/3/3
25	OMC	14	1920	25	-	2/9/27/28	0/2/2/2
1	7MG	13	527	58,1	-	2/7/37/38	0/3/3/3
57	PSU	2L	56	57	-	0/7/25/26	0/2/2/2
1	7MG	1G	527	58,1	-	3/7/37/38	0/3/3/3
25	2MA	14	2503	59,25,58	-	0/7/25/26	0/3/3/3
25	OMG	1H	2251	25,58,23	-	1/9/27/28	0/3/3/3
1	5MC	1G	1400	1	-	2/7/25/26	0/2/2/2
1	UR3	13	1498	1	-	0/7/25/26	0/2/2/2
57	7MG	2L	47	57	-	3/7/37/38	0/3/3/3
1	UR3	1G	1498	1	-	0/7/25/26	0/2/2/2
1	5MC	13	1404	1	-	0/7/25/26	0/2/2/2
1	5MC	1G	1404	1	-	0/7/25/26	0/2/2/2
25	OMU	14	2552	59,25	-	1/9/27/28	0/2/2/2
25	5MC	14	1942	25	-	0/7/25/26	0/2/2/2
23	5MU	2K	55	23	-	0/7/25/26	0/2/2/2
23	OMC	2K	33	23	-	1/9/27/28	0/2/2/2
25	5MU	1H	1915	25	-	0/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
12	0TD	3I	89	12	-	3/7/12/14	-
1	2MG	1G	1207	1	-	0/9/27/28	0/3/3/3
1	MA6	13	1519	1	-	4/11/29/30	0/3/3/3
23	4SU	2K	8	23	-	0/7/25/26	0/2/2/2
25	PSU	14	1917	25	-	0/7/25/26	0/2/2/2
1	2MG	13	1207	1	-	1/9/27/28	0/3/3/3
25	5MC	1H	1962	25,58	-	2/7/25/26	0/2/2/2
1	5MC	1G	967	1	-	0/7/25/26	0/2/2/2
1	M2G	13	966	1	-	1/11/29/30	0/3/3/3
25	PSU	1H	1911	25	-	0/7/25/26	0/2/2/2
1	5MC	13	967	1	-	2/7/25/26	0/2/2/2

The worst 5 of 329 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	14	1915	5MU	C2-N1	13.36	1.59	1.38
25	1H	1915	5MU	C2-N1	13.12	1.59	1.38
57	2L	55	5MU	C2-N1	13.00	1.58	1.38
23	2K	55	5MU	C2-N1	12.97	1.58	1.38
25	1H	1939	5MU	C2-N1	12.34	1.57	1.38

The worst 5 of 339 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	1H	1939	5MU	C5-C4-N3	11.63	125.43	115.32
25	1H	2251	OMG	C6-C5-N7	11.24	150.75	130.29
25	14	1939	5MU	C5-C4-N3	11.05	124.93	115.32
25	14	2251	OMG	C6-C5-N7	10.94	150.20	130.29
25	1H	1915	5MU	C5-C4-N3	10.50	124.45	115.32

There are no chirality outliers.

5 of 71 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
12	3I	89	0TD	SB-CB-CG-OD2
12	3I	89	0TD	SB-CB-CG-OD1
12	3A	89	0TD	CA-CB-SB-CSB
1	13	1402	4OC	O4'-C4'-C5'-O5'
1	1G	1402	4OC	O4'-C4'-C5'-O5'

There are no ring outliers.

31 monomers are involved in 51 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
25	1H	1920	OMC	3	0
25	14	2251	OMG	3	0
23	2K	21	H2U	2	0
57	2L	33	OMC	1	0
25	1H	2552	OMU	1	0
1	1G	1519	MA6	1	0
1	13	1402	4OC	1	0
1	13	1407	5MC	1	0
25	1H	1939	5MU	1	0
25	14	1939	5MU	1	0
25	14	1962	5MC	1	0
12	3A	89	0TD	1	0
1	1G	1402	4OC	2	0
1	1G	1518	MA6	2	0
25	14	1911	PSU	1	0
57	2L	8	4SU	3	0
25	14	1920	OMC	1	0
25	14	2503	2MA	4	0
25	1H	2251	OMG	3	0
1	1G	1400	5MC	1	0
1	13	1498	UR3	1	0
1	1G	1498	UR3	2	0
1	1G	1404	5MC	2	0
25	14	1942	5MC	1	0
23	2K	55	5MU	2	0
23	2K	33	OMC	2	0
12	3I	89	0TD	1	0
1	1G	1207	2MG	3	0
1	13	1519	MA6	1	0
1	13	966	M2G	1	0
25	1H	1911	PSU	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 1272 ligands modelled in this entry, 1270 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	$\# Z > 2$
60	SF4	3E	302	-	0,12,12	-	-	-		
60	SF4	32	303	-	0,12,12	-	-	-		

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
60	SF4	3E	302	-	-	-	0/6/5/5
60	SF4	32	303	-	-	-	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 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
60	3E	302	SF4	1	0
60	32	303	SF4	2	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	1494/1522 (98%)	-0.49	4 (0%) 90 76	40, 102, 169, 228	0
1	1G	1498/1522 (98%)	-0.53	1 (0%) 92 86	53, 104, 169, 213	0
2	12	236/256 (92%)	-0.20	0 100 100	114, 155, 171, 178	0
2	1E	237/256 (92%)	-0.26	0 100 100	108, 143, 167, 181	0
3	22	206/239 (86%)	0.09	2 (0%) 79 56	110, 131, 163, 182	0
3	2E	205/239 (85%)	-0.33	0 100 100	95, 124, 157, 172	0
4	32	208/209 (99%)	0.11	4 (1%) 66 41	78, 99, 120, 133	0
4	3E	208/209 (99%)	-0.03	2 (0%) 79 56	83, 112, 134, 144	0
5	42	154/162 (95%)	-0.09	0 100 100	86, 105, 134, 174	0
5	4E	151/162 (93%)	-0.20	0 100 100	77, 103, 130, 152	0
6	52	101/101 (100%)	-0.29	0 100 100	78, 103, 117, 125	0
6	5E	101/101 (100%)	0.16	2 (1%) 65 39	72, 104, 117, 140	0
7	62	149/156 (95%)	-0.22	0 100 100	110, 132, 151, 159	0
7	6E	155/156 (99%)	-0.14	0 100 100	99, 115, 145, 161	0
8	72	138/138 (100%)	-0.32	0 100 100	83, 107, 123, 128	0
8	7E	138/138 (100%)	-0.27	0 100 100	84, 106, 120, 126	0
9	82	127/128 (99%)	-0.31	0 100 100	104, 154, 173, 185	0
9	8E	124/128 (96%)	-0.38	0 100 100	84, 139, 155, 167	0
10	1A	99/105 (94%)	-0.05	0 100 100	111, 147, 169, 180	0
10	1I	99/105 (94%)	-0.26	0 100 100	93, 151, 166, 170	0
11	2A	119/129 (92%)	-0.28	0 100 100	87, 109, 142, 171	0
11	2I	117/129 (90%)	0.04	2 (1%) 69 43	63, 94, 129, 162	0
12	3A	124/132 (93%)	-0.13	0 100 100	71, 88, 113, 157	0
12	3I	124/132 (93%)	-0.21	0 100 100	62, 81, 111, 156	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
13	4A	118/126 (93%)	-0.01	0 100 100	108, 146, 166, 175	0
13	4I	119/126 (94%)	0.17	2 (1%) 69 43	81, 123, 139, 150	0
14	5A	60/61 (98%)	0.01	0 100 100	114, 131, 142, 149	0
14	5I	60/61 (98%)	-0.22	0 100 100	101, 118, 129, 135	0
15	6A	88/89 (98%)	-0.31	0 100 100	72, 98, 121, 128	0
15	6I	88/89 (98%)	-0.24	1 (1%) 78 54	65, 98, 120, 127	0
16	7A	84/88 (95%)	-0.30	0 100 100	75, 88, 106, 142	0
16	7I	83/88 (94%)	-0.16	0 100 100	95, 107, 130, 157	0
17	8A	99/105 (94%)	-0.23	0 100 100	77, 92, 108, 114	0
17	8I	100/105 (95%)	0.01	2 (2%) 65 39	75, 98, 113, 120	0
18	9A	71/88 (80%)	-0.30	0 100 100	86, 107, 135, 146	0
18	9I	70/88 (79%)	0.04	1 (1%) 73 48	78, 100, 127, 152	0
19	AA	83/93 (89%)	0.26	2 (2%) 59 35	120, 151, 166, 171	0
19	AI	86/93 (92%)	0.32	1 (1%) 76 52	102, 130, 148, 155	0
20	BA	103/106 (97%)	-0.22	0 100 100	82, 98, 125, 137	0
20	BI	101/106 (95%)	-0.21	0 100 100	92, 110, 130, 137	0
21	1B	25/27 (92%)	-0.22	0 100 100	123, 140, 157, 165	0
21	1F	25/27 (92%)	-0.43	0 100 100	104, 117, 136, 147	0
22	1K	65/77 (84%)	0.61	1 (1%) 72 47	88, 119, 149, 174	59 (90%)
22	3K	77/77 (100%)	-0.12	0 100 100	71, 198, 220, 236	0
22	3L	77/77 (100%)	-0.41	0 100 100	87, 216, 245, 255	0
23	2K	71/77 (92%)	-0.51	0 100 100	54, 91, 130, 147	0
24	4K	17/27 (62%)	-0.03	0 100 100	75, 132, 206, 207	0
24	4L	21/27 (77%)	-0.22	0 100 100	88, 171, 227, 232	0
25	14	2868/2917 (98%)	-0.59	2 (0%) 92 86	40, 79, 193, 238	0
25	1H	2868/2917 (98%)	-0.70	5 (0%) 91 82	27, 61, 173, 226	0
26	16	120/122 (98%)	-0.71	0 100 100	66, 93, 111, 146	0
26	1J	122/122 (100%)	-0.56	0 100 100	94, 132, 160, 193	0
27	7I	135/229 (58%)	-0.00	0 100 100	117, 180, 198, 211	0
28	11	274/276 (99%)	-0.26	0 100 100	29, 47, 70, 96	0
28	19	274/276 (99%)	-0.04	1 (0%) 88 72	39, 66, 86, 100	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
29	21	204/206 (99%)	-0.35	0 100 100	34, 74, 110, 127	0
29	29	204/206 (99%)	-0.21	0 100 100	47, 80, 111, 120	0
30	31	202/210 (96%)	-0.32	2 (0%) 79 56	31, 68, 110, 127	0
30	39	206/210 (98%)	-0.09	0 100 100	46, 91, 152, 177	0
31	41	181/182 (99%)	0.07	0 100 100	82, 103, 138, 149	0
31	49	181/182 (99%)	0.08	2 (1%) 78 54	118, 146, 161, 184	0
32	51	174/180 (96%)	-0.11	0 100 100	72, 98, 118, 136	0
32	59	174/180 (96%)	-0.02	0 100 100	115, 155, 176, 187	0
33	61	146/148 (98%)	0.15	1 (0%) 84 63	60, 109, 130, 140	0
33	69	146/148 (98%)	0.07	0 100 100	79, 120, 142, 156	0
34	38	139/173 (80%)	0.39	2 (1%) 73 48	156, 193, 210, 232	0
35	15	138/140 (98%)	-0.09	0 100 100	68, 102, 129, 140	0
35	58	138/140 (98%)	-0.18	0 100 100	56, 76, 118, 127	0
36	25	122/122 (100%)	0.07	3 (2%) 58 35	53, 75, 93, 103	0
36	68	122/122 (100%)	-0.33	0 100 100	45, 65, 85, 105	0
37	35	147/150 (98%)	-0.35	1 (0%) 84 63	51, 96, 127, 150	0
37	78	148/150 (98%)	-0.41	0 100 100	32, 72, 102, 123	0
38	45	140/141 (99%)	-0.14	0 100 100	72, 99, 127, 138	0
38	88	141/141 (100%)	-0.13	0 100 100	46, 73, 106, 128	0
39	55	118/118 (100%)	-0.26	0 100 100	48, 71, 99, 122	0
39	98	118/118 (100%)	-0.14	1 (0%) 82 60	40, 69, 94, 116	0
40	65	111/112 (99%)	-0.41	0 100 100	103, 125, 139, 148	0
40	A8	111/112 (99%)	-0.14	0 100 100	75, 93, 115, 127	0
41	75	137/146 (93%)	-0.12	2 (1%) 72 47	68, 84, 137, 157	0
41	B8	137/146 (93%)	-0.26	0 100 100	61, 81, 134, 164	0
42	85	117/118 (99%)	-0.25	0 100 100	57, 90, 147, 158	0
42	C8	117/118 (99%)	-0.36	0 100 100	37, 63, 101, 120	0
43	95	101/101 (100%)	0.05	0 100 100	53, 123, 143, 159	0
43	D8	100/101 (99%)	-0.10	0 100 100	41, 90, 118, 134	0
44	A5	112/113 (99%)	-0.28	1 (0%) 81 58	52, 66, 100, 144	0
44	E8	113/113 (100%)	-0.44	0 100 100	40, 55, 97, 140	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
45	B5	93/96 (96%)	-0.09	0 100 100	58, 77, 106, 124	0
45	F8	95/96 (98%)	-0.40	0 100 100	42, 56, 85, 99	0
46	C5	109/110 (99%)	0.30	3 (2%) 55 32	73, 102, 120, 128	0
46	G8	107/110 (97%)	-0.19	1 (0%) 81 58	62, 87, 135, 148	0
47	D5	176/206 (85%)	-0.11	0 100 100	117, 145, 178, 186	0
47	H8	174/206 (84%)	0.29	3 (1%) 69 43	79, 118, 177, 192	0
48	E5	79/85 (92%)	-0.66	0 100 100	70, 90, 113, 160	0
48	I8	77/85 (90%)	-0.41	1 (1%) 75 50	49, 67, 93, 114	0
49	F5	92/96 (95%)	0.06	2 (2%) 62 37	54, 79, 115, 130	0
49	J8	96/96 (100%)	0.02	2 (2%) 63 38	41, 66, 117, 150	0
50	G5	69/72 (95%)	-0.11	0 100 100	69, 95, 121, 145	0
50	K8	71/72 (98%)	-0.14	2 (2%) 55 32	45, 69, 89, 110	0
51	H5	59/60 (98%)	-0.24	0 100 100	70, 97, 146, 169	0
51	L8	59/60 (98%)	-0.34	0 100 100	49, 71, 105, 114	0
52	I5	71/71 (100%)	0.23	1 (1%) 73 48	147, 178, 194, 204	0
52	M8	66/71 (92%)	0.49	3 (4%) 38 20	114, 141, 171, 192	0
53	J5	56/60 (93%)	0.04	0 100 100	50, 76, 143, 153	0
53	N8	56/60 (93%)	-0.19	1 (1%) 67 42	35, 75, 145, 151	0
54	K5	48/54 (88%)	0.01	0 100 100	128, 165, 181, 188	0
54	O8	49/54 (90%)	0.39	2 (4%) 41 22	106, 140, 158, 162	0
55	L5	48/49 (97%)	-0.38	0 100 100	41, 51, 82, 94	0
55	P8	48/49 (97%)	-0.62	0 100 100	26, 35, 71, 76	0
56	M5	64/65 (98%)	-0.64	0 100 100	59, 73, 98, 119	0
56	Q8	64/65 (98%)	-0.59	0 100 100	38, 53, 74, 95	0
57	2L	72/77 (93%)	-0.55	1 (1%) 73 48	67, 113, 154, 178	0
All	All	21207/22013 (96%)	-0.33	72 (0%) 90 76	26, 95, 171, 255	59 (0%)

The worst 5 of 72 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
54	O8	7	ILE	3.7
13	4I	119	GLY	3.6
30	31	131	GLY	3.5

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Mol	Chain	Res	Type	RSRZ
25	1H	1538	G	3.4
17	8I	98	LEU	3.3

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

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
25	5MU	14	1915	21/22	0.80	0.08	116,128,139,153	0
23	5MU	2K	55	21/22	0.83	0.08	103,113,125,145	0
57	5MU	2L	55	21/22	0.84	0.06	119,129,134,137	0
57	4SU	2L	8	20/21	0.85	0.07	120,131,140,141	0
23	H2U	2K	21	20/21	0.85	0.11	117,140,147,150	0
23	PSU	2K	56	20/21	0.86	0.07	92,104,120,124	0
57	PSU	2L	56	20/21	0.87	0.06	123,128,134,135	0
1	5MC	1G	967	21/22	0.88	0.07	92,107,118,120	0
57	7MG	2L	47	24/25	0.89	0.06	114,141,151,162	0
25	PSU	14	1911	20/21	0.89	0.07	86,94,118,121	0
25	5MU	1H	1915	21/22	0.89	0.08	75,91,102,116	0
1	2MG	13	1207	24/25	0.90	0.11	100,112,118,119	0
1	7MG	13	527	24/25	0.90	0.10	71,80,86,92	0
23	7MG	2K	47	24/25	0.90	0.08	96,105,114,126	0
1	PSU	1G	516	20/21	0.91	0.06	98,102,108,110	0
12	0TD	3I	89	10/11	0.91	0.10	81,87,92,107	0
1	2MG	1G	1207	24/25	0.91	0.06	115,120,125,127	0
1	M2G	1G	966	25/26	0.91	0.07	87,107,115,124	0
23	OMC	2K	33	21/22	0.91	0.08	77,82,89,101	0
1	5MC	1G	1404	21/22	0.92	0.10	77,85,89,91	0
57	OMC	2L	33	21/22	0.92	0.08	91,100,107,111	0
1	5MC	13	967	21/22	0.92	0.09	71,82,94,99	0
1	5MC	1G	1400	21/22	0.92	0.07	81,92,98,102	0
25	PSU	14	1917	20/21	0.92	0.08	87,104,109,110	0
25	OMC	14	1920	21/22	0.93	0.08	73,91,99,102	0
1	5MC	1G	1407	21/22	0.93	0.10	75,80,85,98	0
12	0TD	3A	89	10/11	0.93	0.11	89,95,100,105	0
25	PSU	1H	1917	20/21	0.94	0.08	65,76,90,91	0
1	M2G	13	966	25/26	0.94	0.08	68,77,90,94	0
1	4OC	1G	1402	22/23	0.94	0.07	71,84,91,99	0
25	5MC	14	1962	21/22	0.94	0.08	59,67,76,83	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
1	5MC	13	1404	21/22	0.94	0.10	54,59,69,79	0
1	PSU	13	516	20/21	0.94	0.05	84,95,98,98	0
1	7MG	1G	527	24/25	0.94	0.09	88,99,101,102	0
1	UR3	1G	1498	21/22	0.94	0.10	65,76,83,86	0
1	5MC	13	1400	21/22	0.94	0.08	58,74,79,86	0
25	5MC	1H	1942	21/22	0.95	0.09	39,50,56,61	0
25	5MC	14	1942	21/22	0.95	0.09	62,71,82,90	0
1	MA6	1G	1519	24/25	0.95	0.12	64,79,84,86	0
25	2MA	14	2503	23/24	0.95	0.10	39,50,63,79	0
1	4OC	13	1402	22/23	0.95	0.09	61,71,79,84	0
1	UR3	13	1498	21/22	0.95	0.11	44,62,69,73	0
25	OMC	1H	1920	21/22	0.95	0.08	60,66,70,72	0
1	5MC	13	1407	21/22	0.95	0.09	53,59,65,67	0
25	5MU	1H	1939	21/22	0.95	0.12	36,41,48,50	0
25	OMG	14	2251	24/25	0.96	0.07	51,57,64,69	0
25	2MA	1H	2503	23/24	0.96	0.09	30,38,48,59	0
1	MA6	13	1518	24/25	0.96	0.10	50,57,61,62	0
25	OMU	1H	2552	21/22	0.96	0.08	37,45,51,53	0
25	PSU	1H	2605	20/21	0.96	0.09	35,40,48,53	0
25	PSU	14	2605	20/21	0.96	0.08	42,52,74,77	0
23	4SU	2K	8	20/21	0.96	0.06	85,91,97,101	0
1	MA6	1G	1518	24/25	0.96	0.09	68,78,82,84	0
25	PSU	1H	1911	20/21	0.96	0.08	50,63,72,74	0
25	5MC	1H	1962	21/22	0.96	0.08	50,57,61,66	0
1	MA6	13	1519	24/25	0.96	0.12	51,56,62,64	0
25	OMU	14	2552	21/22	0.97	0.08	48,55,62,67	0
25	5MU	14	1939	21/22	0.97	0.08	44,52,57,62	0
25	OMG	1H	2251	24/25	0.98	0.05	36,43,49,53	0

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
58	K	1H	3072	1/1	0.40	0.12	100,100,100,100	0
59	MG	1H	3326[A]	1/1	0.47	0.37	58,58,58,58	1
59	MG	1H	3326[B]	1/1	0.47	0.37	55,55,55,55	1
59	MG	14	3174	1/1	0.51	0.24	78,78,78,78	0
58	K	16	202	1/1	0.56	0.12	116,116,116,116	0
59	MG	1G	1656	1/1	0.57	0.25	100,100,100,100	0
58	K	1H	3010	1/1	0.57	0.11	93,93,93,93	0
59	MG	1H	3239	1/1	0.59	0.26	83,83,83,83	0
59	MG	13	1682	1/1	0.61	0.19	101,101,101,101	0
59	MG	1G	1665	1/1	0.62	0.23	84,84,84,84	0
59	MG	1H	3140	1/1	0.63	0.26	82,82,82,82	0
59	MG	14	3211	1/1	0.63	0.23	64,64,64,64	0
58	K	13	1635	1/1	0.64	0.18	104,104,104,104	0
59	MG	13	1710	1/1	0.64	0.19	97,97,97,97	0
58	K	14	3088	1/1	0.64	0.13	101,101,101,101	0
59	MG	1G	1648	1/1	0.64	0.30	83,83,83,83	0
59	MG	1H	3231	1/1	0.66	0.21	67,67,67,67	0
59	MG	1G	1628	1/1	0.67	0.23	92,92,92,92	0
59	MG	13	1688	1/1	0.67	0.20	83,83,83,83	0
58	K	1H	3016	1/1	0.68	0.09	114,114,114,114	0
58	K	13	1636	1/1	0.69	0.09	136,136,136,136	0
59	MG	16	205	1/1	0.69	0.22	84,84,84,84	0
59	MG	14	3254	1/1	0.69	0.24	71,71,71,71	0
58	K	5E	201	1/1	0.70	0.17	113,113,113,113	0
58	K	1H	3014	1/1	0.70	0.20	84,84,84,84	0
58	K	1G	1604	1/1	0.71	0.11	111,111,111,111	0
59	MG	14	3246	1/1	0.71	0.15	76,76,76,76	0
59	MG	1G	1661	1/1	0.71	0.17	114,114,114,114	0
58	K	1H	3052	1/1	0.72	0.12	127,127,127,127	0
59	MG	1G	1635	1/1	0.72	0.21	80,80,80,80	0
58	K	3A	201	1/1	0.73	0.12	93,93,93,93	0
59	MG	13	1693	1/1	0.73	0.18	78,78,78,78	0
59	MG	14	3196	1/1	0.73	0.20	90,90,90,90	0
59	MG	14	3202	1/1	0.73	0.13	84,84,84,84	0
58	K	41	202	1/1	0.73	0.09	128,128,128,128	0
58	K	1H	3044	1/1	0.73	0.07	82,82,82,82	0
59	MG	1H	3158	1/1	0.73	0.18	89,89,89,89	0
58	K	14	3042	1/1	0.74	0.09	83,83,83,83	0
58	K	14	3069	1/1	0.74	0.08	89,89,89,89	0
58	K	1G	1605	1/1	0.74	0.10	92,92,92,92	0
59	MG	1H	3221	1/1	0.74	0.28	77,77,77,77	0
59	MG	1G	1662	1/1	0.74	0.17	74,74,74,74	0
59	MG	13	1695	1/1	0.74	0.23	76,76,76,76	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
59	MG	13	1696	1/1	0.75	0.16	80,80,80,80	0
58	K	13	1626	1/1	0.75	0.12	99,99,99,99	0
58	K	14	3005	1/1	0.75	0.12	91,91,91,91	0
59	MG	1H	3310	1/1	0.75	0.23	78,78,78,78	0
58	K	1G	1606	1/1	0.75	0.08	102,102,102,102	0
59	MG	1H	3174	1/1	0.76	0.10	71,71,71,71	0
59	MG	1G	1649	1/1	0.76	0.17	85,85,85,85	0
59	MG	14	3197	1/1	0.76	0.17	60,60,60,60	0
58	K	8I	201	1/1	0.76	0.09	104,104,104,104	0
59	MG	13	1686	1/1	0.76	0.22	95,95,95,95	0
59	MG	14	3218	1/1	0.76	0.17	66,66,66,66	0
58	K	1H	3079	1/1	0.76	0.08	114,114,114,114	0
59	MG	1H	3159	1/1	0.76	0.18	68,68,68,68	0
59	MG	1H	3284	1/1	0.77	0.23	66,66,66,66	0
58	K	52	201	1/1	0.77	0.12	116,116,116,116	0
58	K	1G	1601	1/1	0.77	0.11	102,102,102,102	0
58	K	13	1613	1/1	0.78	0.08	100,100,100,100	0
59	MG	1G	1627	1/1	0.78	0.21	88,88,88,88	0
59	MG	13	1652	1/1	0.78	0.23	95,95,95,95	0
58	K	14	3055	1/1	0.78	0.07	116,116,116,116	0
58	K	13	1610	1/1	0.78	0.09	114,114,114,114	0
58	K	14	3075	1/1	0.78	0.09	116,116,116,116	0
59	MG	14	3137	1/1	0.79	0.11	83,83,83,83	0
58	K	14	3049	1/1	0.79	0.11	103,103,103,103	0
59	MG	1H	3244	1/1	0.79	0.12	52,52,52,52	0
59	MG	1G	1652	1/1	0.79	0.14	94,94,94,94	0
59	MG	16	207	1/1	0.79	0.23	88,88,88,88	0
59	MG	1H	3213	1/1	0.79	0.11	73,73,73,73	0
59	MG	3E	301	1/1	0.79	0.23	84,84,84,84	0
59	MG	1H	3139	1/1	0.79	0.25	76,76,76,76	0
59	MG	1G	1666	1/1	0.79	0.19	77,77,77,77	0
59	MG	1H	3207	1/1	0.80	0.09	56,56,56,56	0
59	MG	13	1709	1/1	0.80	0.19	85,85,85,85	0
58	K	14	3058	1/1	0.80	0.20	84,84,84,84	0
59	MG	1G	1663	1/1	0.80	0.24	73,73,73,73	0
59	MG	1G	1664	1/1	0.80	0.25	73,73,73,73	0
59	MG	13	1687	1/1	0.80	0.17	75,75,75,75	0
58	K	13	1606	1/1	0.80	0.09	87,87,87,87	0
59	MG	1H	3188	1/1	0.80	0.20	84,84,84,84	0
59	MG	14	3267	1/1	0.80	0.21	92,92,92,92	0
59	MG	1H	3285	1/1	0.81	0.27	66,66,66,66	0
59	MG	1H	3304	1/1	0.81	0.22	69,69,69,69	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
58	K	1G	1615	1/1	0.81	0.14	106,106,106,106	0
59	MG	13	1685	1/1	0.81	0.26	85,85,85,85	0
58	K	1H	3099	1/1	0.81	0.11	81,81,81,81	0
59	MG	1J	202	1/1	0.81	0.15	69,69,69,69	0
59	MG	13	1645	1/1	0.82	0.10	71,71,71,71	0
58	K	13	1618	1/1	0.82	0.11	90,90,90,90	0
59	MG	13	1678	1/1	0.82	0.18	79,79,79,79	0
59	MG	13	1698	1/1	0.82	0.25	67,67,67,67	0
59	MG	13	1701	1/1	0.82	0.25	72,72,72,72	0
58	K	14	3008	1/1	0.82	0.08	88,88,88,88	0
58	K	14	3033	1/1	0.82	0.14	84,84,84,84	0
59	MG	1H	3238	1/1	0.82	0.27	82,82,82,82	0
58	K	13	1620	1/1	0.82	0.06	115,115,115,115	0
59	MG	BI	201	1/1	0.82	0.11	108,108,108,108	0
59	MG	14	3220	1/1	0.82	0.07	53,53,53,53	0
59	MG	1H	3133	1/1	0.82	0.15	55,55,55,55	0
58	K	14	3076	1/1	0.82	0.07	89,89,89,89	0
58	K	13	1607	1/1	0.82	0.10	90,90,90,90	0
59	MG	13	1691	1/1	0.82	0.18	88,88,88,88	0
58	K	1H	3038	1/1	0.83	0.07	86,86,86,86	0
59	MG	1H	3325	1/1	0.83	0.26	65,65,65,65	0
59	MG	13	1663	1/1	0.83	0.24	68,68,68,68	0
59	MG	13	1676	1/1	0.83	0.14	53,53,53,53	0
58	K	14	3026	1/1	0.83	0.10	109,109,109,109	0
59	MG	14	3209	1/1	0.83	0.20	72,72,72,72	0
59	MG	13	1699	1/1	0.83	0.23	68,68,68,68	0
58	K	13	1633	1/1	0.83	0.06	108,108,108,108	0
59	MG	13	1707	1/1	0.83	0.15	65,65,65,65	0
59	MG	14	3233	1/1	0.83	0.14	80,80,80,80	0
59	MG	1G	1630	1/1	0.83	0.18	64,64,64,64	0
59	MG	1H	3309	1/1	0.83	0.13	56,56,56,56	0
59	MG	14	3265	1/1	0.83	0.26	67,67,67,67	0
59	MG	14	3096	1/1	0.83	0.12	59,59,59,59	0
59	MG	14	3131	1/1	0.83	0.24	66,66,66,66	0
59	MG	14	3136	1/1	0.84	0.16	77,77,77,77	0
59	MG	13	1656	1/1	0.84	0.21	73,73,73,73	0
59	MG	14	3142	1/1	0.84	0.18	62,62,62,62	0
58	K	14	3081	1/1	0.84	0.10	89,89,89,89	0
59	MG	14	3185	1/1	0.84	0.17	76,76,76,76	0
59	MG	14	3192	1/1	0.84	0.14	63,63,63,63	0
59	MG	1H	3316	1/1	0.84	0.21	59,59,59,59	0
59	MG	7I	101	1/1	0.84	0.16	124,124,124,124	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
59	MG	1G	1660	1/1	0.84	0.22	79,79,79,79	0
58	K	14	3083	1/1	0.84	0.08	119,119,119,119	0
58	K	13	1637	1/1	0.84	0.08	123,123,123,123	0
58	K	14	3092	1/1	0.84	0.08	83,83,83,83	0
58	K	29	302	1/1	0.84	0.07	89,89,89,89	0
58	K	14	3039	1/1	0.84	0.09	94,94,94,94	0
58	K	13	1634	1/1	0.84	0.08	111,111,111,111	0
59	MG	14	3250	1/1	0.84	0.25	84,84,84,84	0
59	MG	14	3252	1/1	0.84	0.23	75,75,75,75	0
59	MG	13	1655	1/1	0.84	0.12	80,80,80,80	0
59	MG	14	3103	1/1	0.84	0.17	82,82,82,82	0
59	MG	14	3124	1/1	0.84	0.06	63,63,63,63	0
59	MG	14	3268	1/1	0.84	0.12	79,79,79,79	0
59	MG	1H	3180	1/1	0.84	0.17	72,72,72,72	0
59	MG	1G	1676	1/1	0.85	0.19	81,81,81,81	0
59	MG	1H	3317	1/1	0.85	0.25	63,63,63,63	0
59	MG	1H	3323	1/1	0.85	0.29	73,73,73,73	0
59	MG	14	3115	1/1	0.85	0.19	46,46,46,46	0
59	MG	13	1674	1/1	0.85	0.11	92,92,92,92	0
58	K	BA	201	1/1	0.85	0.12	96,96,96,96	0
58	K	1H	3117	1/1	0.85	0.11	85,85,85,85	0
58	K	1H	3009	1/1	0.85	0.13	97,97,97,97	0
59	MG	1H	3223	1/1	0.85	0.12	64,64,64,64	0
59	MG	1H	3229	1/1	0.85	0.08	51,51,51,51	0
58	K	14	3019	1/1	0.85	0.16	81,81,81,81	0
58	K	13	1627	1/1	0.85	0.07	91,91,91,91	0
58	K	13	1630	1/1	0.85	0.08	82,82,82,82	0
59	MG	1G	1646	1/1	0.85	0.16	107,107,107,107	0
58	K	13	1605	1/1	0.85	0.07	94,94,94,94	0
59	MG	1H	3252	1/1	0.85	0.18	72,72,72,72	0
59	MG	1G	1651	1/1	0.85	0.24	63,63,63,63	0
59	MG	1H	3276	1/1	0.85	0.23	63,63,63,63	0
58	K	1H	3020	1/1	0.85	0.12	105,105,105,105	0
59	MG	1G	1658	1/1	0.85	0.21	76,76,76,76	0
59	MG	14	3243	1/1	0.85	0.26	74,74,74,74	0
58	K	1H	3082	1/1	0.85	0.05	80,80,80,80	0
59	MG	1H	3289	1/1	0.85	0.16	75,75,75,75	0
58	K	1H	3033	1/1	0.85	0.10	94,94,94,94	0
59	MG	14	3253	1/1	0.85	0.21	52,52,52,52	0
58	K	1H	3110	1/1	0.85	0.10	111,111,111,111	0
58	K	1H	3112	1/1	0.85	0.09	87,87,87,87	0
59	MG	14	3266	1/1	0.85	0.18	74,74,74,74	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
59	MG	1H	3312	1/1	0.85	0.14	70,70,70,70	0
59	MG	13	1671	1/1	0.85	0.17	65,65,65,65	0
59	MG	1G	1672	1/1	0.85	0.20	63,63,63,63	0
59	MG	1G	1643	1/1	0.86	0.08	56,56,56,56	0
59	MG	13	1697	1/1	0.86	0.14	70,70,70,70	0
58	K	1G	1617	1/1	0.86	0.07	94,94,94,94	0
58	K	1H	3091	1/1	0.86	0.14	62,62,62,62	0
59	MG	1H	3308	1/1	0.86	0.17	55,55,55,55	0
59	MG	13	1679	1/1	0.86	0.12	89,89,89,89	0
58	K	14	3027	1/1	0.86	0.10	97,97,97,97	0
59	MG	14	3199	1/1	0.86	0.10	105,105,105,105	0
59	MG	14	3201	1/1	0.86	0.18	68,68,68,68	0
58	K	13	1628	1/1	0.86	0.07	103,103,103,103	0
59	MG	1H	3215	1/1	0.86	0.28	65,65,65,65	0
59	MG	13	1653	1/1	0.86	0.16	74,74,74,74	0
59	MG	1H	3321	1/1	0.86	0.16	55,55,55,55	0
58	K	1H	3101	1/1	0.86	0.08	60,60,60,60	0
59	MG	1H	3227	1/1	0.86	0.20	58,58,58,58	0
59	MG	8E	201	1/1	0.86	0.16	49,49,49,49	0
59	MG	4I	201	1/1	0.86	0.25	84,84,84,84	0
59	MG	1H	3327	1/1	0.86	0.28	72,72,72,72	0
58	K	41	201	1/1	0.86	0.11	114,114,114,114	0
59	MG	14	3095	1/1	0.86	0.19	57,57,57,57	0
59	MG	13	1690	1/1	0.86	0.20	77,77,77,77	0
58	K	14	3047	1/1	0.86	0.08	97,97,97,97	0
59	MG	13	1665	1/1	0.86	0.15	50,50,50,50	0
58	K	1H	3018	1/1	0.86	0.07	93,93,93,93	0
59	MG	1G	1634	1/1	0.86	0.17	110,110,110,110	0
59	MG	14	3269	1/1	0.86	0.17	79,79,79,79	0
58	K	14	3091	1/1	0.86	0.10	103,103,103,103	0
59	MG	14	3190	1/1	0.87	0.14	81,81,81,81	0
59	MG	1H	3236	1/1	0.87	0.12	54,54,54,54	0
58	K	1H	3113[B]	1/1	0.87	0.17	39,39,39,39	1
58	K	14	3036	1/1	0.87	0.08	85,85,85,85	0
59	MG	1H	3243	1/1	0.87	0.22	94,94,94,94	0
59	MG	1H	3336	1/1	0.87	0.15	54,54,54,54	0
58	K	13	1614	1/1	0.87	0.12	103,103,103,103	0
59	MG	14	3203	1/1	0.87	0.13	85,85,85,85	0
58	K	1H	3120	1/1	0.87	0.11	79,79,79,79	0
59	MG	1G	1671	1/1	0.87	0.26	79,79,79,79	0
59	MG	1H	3170	1/1	0.87	0.13	47,47,47,47	0
58	K	1H	3096	1/1	0.87	0.14	75,75,75,75	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
58	K	1H	3069	1/1	0.87	0.06	74,74,74,74	0
58	K	14	3052	1/1	0.87	0.06	105,105,105,105	0
59	MG	1H	3203	1/1	0.87	0.12	52,52,52,52	0
58	K	1H	3019	1/1	0.87	0.08	78,78,78,78	0
58	K	1H	3102	1/1	0.87	0.06	94,94,94,94	0
58	K	1H	3040	1/1	0.87	0.18	111,111,111,111	0
58	K	14	3070	1/1	0.87	0.08	95,95,95,95	0
58	K	13	1604	1/1	0.87	0.07	90,90,90,90	0
58	K	1H	3113[A]	1/1	0.87	0.17	45,45,45,45	1
59	MG	14	3155	1/1	0.87	0.15	57,57,57,57	0
59	MG	14	3162	1/1	0.87	0.20	58,58,58,58	0
59	MG	13	1670	1/1	0.87	0.17	72,72,72,72	0
59	MG	14	3270	1/1	0.87	0.12	57,57,57,57	0
59	MG	1H	3138	1/1	0.87	0.22	66,66,66,66	0
59	MG	1H	3278	1/1	0.88	0.22	68,68,68,68	0
59	MG	1H	3282	1/1	0.88	0.12	48,48,48,48	0
59	MG	1H	3184	1/1	0.88	0.19	65,65,65,65	0
59	MG	1G	1637	1/1	0.88	0.17	77,77,77,77	0
59	MG	14	3150	1/1	0.88	0.17	63,63,63,63	0
59	MG	14	3154	1/1	0.88	0.19	72,72,72,72	0
59	MG	1G	1639	1/1	0.88	0.19	55,55,55,55	0
58	K	1G	1622	1/1	0.88	0.07	118,118,118,118	0
59	MG	14	3167	1/1	0.88	0.19	60,60,60,60	0
58	K	39	301	1/1	0.88	0.08	107,107,107,107	0
59	MG	14	3179	1/1	0.88	0.20	66,66,66,66	0
59	MG	14	3183	1/1	0.88	0.17	63,63,63,63	0
59	MG	14	3184	1/1	0.88	0.19	73,73,73,73	0
58	K	1H	3034	1/1	0.88	0.07	83,83,83,83	0
59	MG	1H	3211	1/1	0.88	0.21	47,47,47,47	0
59	MG	1G	1650	1/1	0.88	0.17	65,65,65,65	0
58	K	31	302	1/1	0.88	0.06	90,90,90,90	0
58	K	1H	3092	1/1	0.88	0.07	70,70,70,70	0
59	MG	14	3198	1/1	0.88	0.18	63,63,63,63	0
59	MG	1G	1655	1/1	0.88	0.20	67,67,67,67	0
58	K	14	3074	1/1	0.88	0.08	94,94,94,94	0
59	MG	1H	3315	1/1	0.88	0.30	70,70,70,70	0
59	MG	13	1689	1/1	0.88	0.09	80,80,80,80	0
58	K	14	3001	1/1	0.88	0.10	87,87,87,87	0
59	MG	1H	3318	1/1	0.88	0.19	85,85,85,85	0
58	K	14	3041	1/1	0.88	0.12	54,54,54,54	0
58	K	1G	1609	1/1	0.88	0.12	113,113,113,113	0
59	MG	14	3225	1/1	0.88	0.09	62,62,62,62	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
59	MG	14	3226	1/1	0.88	0.10	49,49,49,49	0
59	MG	1H	3235	1/1	0.88	0.14	62,62,62,62	0
59	MG	14	3235	1/1	0.88	0.16	61,61,61,61	0
58	K	14	3082	1/1	0.88	0.14	76,76,76,76	0
59	MG	1G	1667	1/1	0.88	0.16	60,60,60,60	0
59	MG	1G	1670	1/1	0.88	0.19	60,60,60,60	0
58	K	1H	3025	1/1	0.88	0.05	100,100,100,100	0
58	K	14	3017	1/1	0.88	0.12	107,107,107,107	0
59	MG	1G	1674	1/1	0.88	0.18	50,50,50,50	0
59	MG	14	3263	1/1	0.88	0.23	66,66,66,66	0
58	K	14	3051	1/1	0.88	0.08	93,93,93,93	0
59	MG	2L	102	1/1	0.88	0.11	132,132,132,132	0
59	MG	1H	3389	1/1	0.88	0.12	38,38,38,38	0
59	MG	13	1677	1/1	0.88	0.11	63,63,63,63	0
58	K	1H	3012	1/1	0.88	0.09	80,80,80,80	0
59	MG	1H	3259	1/1	0.88	0.14	59,59,59,59	0
59	MG	13	1702	1/1	0.88	0.22	62,62,62,62	0
59	MG	14	3160	1/1	0.89	0.13	73,73,73,73	0
59	MG	13	1661	1/1	0.89	0.12	42,42,42,42	0
59	MG	13	1662	1/1	0.89	0.17	67,67,67,67	0
59	MG	14	3171	1/1	0.89	0.07	71,71,71,71	0
58	K	14	3079	1/1	0.89	0.09	112,112,112,112	0
58	K	14	3003	1/1	0.89	0.08	86,86,86,86	0
59	MG	13	1669	1/1	0.89	0.16	53,53,53,53	0
58	K	1H	3001	1/1	0.89	0.06	88,88,88,88	0
59	MG	13	1704	1/1	0.89	0.13	53,53,53,53	0
58	K	1H	3097	1/1	0.89	0.08	69,69,69,69	0
58	K	14	3084	1/1	0.89	0.08	75,75,75,75	0
59	MG	1H	3319	1/1	0.89	0.14	55,55,55,55	0
58	K	14	3085	1/1	0.89	0.05	94,94,94,94	0
58	K	14	3086	1/1	0.89	0.14	97,97,97,97	0
59	MG	1H	3324	1/1	0.89	0.20	59,59,59,59	0
58	K	1H	3063	1/1	0.89	0.07	55,55,55,55	0
58	K	14	3089	1/1	0.89	0.07	97,97,97,97	0
59	MG	1G	1668	1/1	0.89	0.24	55,55,55,55	0
58	K	13	1608	1/1	0.89	0.08	96,96,96,96	0
59	MG	13	1683	1/1	0.89	0.10	55,55,55,55	0
59	MG	14	3214	1/1	0.89	0.25	57,57,57,57	0
58	K	14	3022	1/1	0.89	0.07	92,92,92,92	0
59	MG	1H	3134	1/1	0.89	0.23	59,59,59,59	0
58	K	1G	1619	1/1	0.89	0.09	79,79,79,79	0
59	MG	1G	1690	1/1	0.89	0.08	109,109,109,109	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
58	K	14	3067	1/1	0.89	0.07	90,90,90,90	0
59	MG	D8	202	1/1	0.89	0.08	52,52,52,52	0
59	MG	D8	203	1/1	0.89	0.12	55,55,55,55	0
59	MG	1H	3253	1/1	0.89	0.15	53,53,53,53	0
59	MG	13	1642	1/1	0.89	0.19	59,59,59,59	0
59	MG	14	3251	1/1	0.89	0.21	52,52,52,52	0
59	MG	1H	3263	1/1	0.89	0.18	33,33,33,33	0
58	K	1H	3037	1/1	0.89	0.07	77,77,77,77	0
58	K	13	1629	1/1	0.89	0.06	92,92,92,92	0
59	MG	14	3262	1/1	0.89	0.17	45,45,45,45	0
59	MG	1H	3280	1/1	0.89	0.15	64,64,64,64	0
59	MG	1H	3161	1/1	0.89	0.15	32,32,32,32	0
59	MG	14	3145	1/1	0.89	0.17	86,86,86,86	0
59	MG	14	3149	1/1	0.89	0.18	46,46,46,46	0
58	K	1H	3017	1/1	0.89	0.06	94,94,94,94	0
59	MG	14	3153	1/1	0.89	0.12	68,68,68,68	0
58	K	1H	3043	1/1	0.89	0.07	82,82,82,82	0
59	MG	14	3315	1/1	0.89	0.07	84,84,84,84	0
58	K	1H	3031	1/1	0.89	0.07	96,96,96,96	0
59	MG	E5	101	1/1	0.89	0.05	36,36,36,36	0
58	K	14	3066	1/1	0.90	0.13	80,80,80,80	0
59	MG	1G	1654	1/1	0.90	0.18	58,58,58,58	0
59	MG	14	3176	1/1	0.90	0.23	67,67,67,67	0
58	K	1H	3027	1/1	0.90	0.13	91,91,91,91	0
58	K	31	301	1/1	0.90	0.08	60,60,60,60	0
59	MG	1H	3217	1/1	0.90	0.14	52,52,52,52	0
58	K	1G	1620	1/1	0.90	0.07	101,101,101,101	0
58	K	1H	3029	1/1	0.90	0.06	104,104,104,104	0
58	K	1G	1625	1/1	0.90	0.10	106,106,106,106	0
58	K	13	1625	1/1	0.90	0.07	94,94,94,94	0
59	MG	1H	3126	1/1	0.90	0.23	53,53,53,53	0
59	MG	1H	3131	1/1	0.90	0.16	42,42,42,42	0
58	K	14	3078	1/1	0.90	0.20	98,98,98,98	0
58	K	1H	3032	1/1	0.90	0.09	58,58,58,58	0
58	K	14	3040	1/1	0.90	0.13	72,72,72,72	0
58	K	13	1609	1/1	0.90	0.10	91,91,91,91	0
59	MG	1H	3332	1/1	0.90	0.29	59,59,59,59	0
59	MG	1H	3335	1/1	0.90	0.13	50,50,50,50	0
59	MG	1G	1673	1/1	0.90	0.22	73,73,73,73	0
58	K	1H	3084	1/1	0.90	0.07	77,77,77,77	0
59	MG	1H	3248	1/1	0.90	0.12	47,47,47,47	0
59	MG	1H	3142	1/1	0.90	0.13	71,71,71,71	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
59	MG	13	1666	1/1	0.90	0.07	83,83,83,83	0
58	K	1H	3088	1/1	0.90	0.07	74,74,74,74	0
58	K	14	3048	1/1	0.90	0.10	101,101,101,101	0
59	MG	14	3239	1/1	0.90	0.21	66,66,66,66	0
58	K	14	3004	1/1	0.90	0.08	55,55,55,55	0
59	MG	14	3105	1/1	0.90	0.20	36,36,36,36	0
59	MG	1H	3172	1/1	0.90	0.15	48,48,48,48	0
59	MG	1G	1629	1/1	0.90	0.09	69,69,69,69	0
58	K	13	1615	1/1	0.90	0.05	91,91,91,91	0
58	K	1H	3054	1/1	0.90	0.10	68,68,68,68	0
59	MG	1H	3181	1/1	0.90	0.19	41,41,41,41	0
59	MG	14	3141	1/1	0.90	0.17	60,60,60,60	0
59	MG	13	1703	1/1	0.90	0.25	69,69,69,69	0
58	K	14	3014	1/1	0.90	0.06	82,82,82,82	0
59	MG	1G	1640	1/1	0.90	0.20	53,53,53,53	0
59	MG	1H	3291	1/1	0.90	0.13	62,62,62,62	0
59	MG	1G	1645	1/1	0.90	0.17	40,40,40,40	0
59	MG	1H	3295	1/1	0.90	0.09	46,46,46,46	0
59	MG	1H	3297	1/1	0.90	0.19	52,52,52,52	0
59	MG	1H	3191	1/1	0.90	0.27	72,72,72,72	0
59	MG	14	3375	1/1	0.90	0.09	57,57,57,57	0
59	MG	14	3377	1/1	0.90	0.08	70,70,70,70	0
59	MG	13	1705	1/1	0.90	0.20	60,60,60,60	0
59	MG	29	304	1/1	0.90	0.19	62,62,62,62	0
58	K	1H	3060	1/1	0.90	0.15	55,55,55,55	0
59	MG	1H	3484	1/1	0.91	0.08	47,47,47,47	0
59	MG	14	3188	1/1	0.91	0.12	54,54,54,54	0
59	MG	16	203	1/1	0.91	0.12	57,57,57,57	0
59	MG	1H	3199	1/1	0.91	0.11	60,60,60,60	0
59	MG	14	3193	1/1	0.91	0.11	63,63,63,63	0
59	MG	1H	3132	1/1	0.91	0.20	58,58,58,58	0
59	MG	D8	201	1/1	0.91	0.14	71,71,71,71	0
59	MG	1H	3204	1/1	0.91	0.20	51,51,51,51	0
59	MG	1H	3283	1/1	0.91	0.17	58,58,58,58	0
59	MG	13	1643	1/1	0.91	0.11	76,76,76,76	0
59	MG	1H	3208	1/1	0.91	0.27	52,52,52,52	0
59	MG	1G	1696	1/1	0.91	0.07	129,129,129,129	0
59	MG	14	3206	1/1	0.91	0.16	67,67,67,67	0
58	K	1H	3081	1/1	0.91	0.13	66,66,66,66	0
59	MG	1H	3290	1/1	0.91	0.21	51,51,51,51	0
59	MG	14	3213	1/1	0.91	0.30	58,58,58,58	0
59	MG	1G	1633	1/1	0.91	0.14	65,65,65,65	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
59	MG	14	3217	1/1	0.91	0.17	59,59,59,59	0
59	MG	1H	3212	1/1	0.91	0.07	57,57,57,57	0
58	K	32	301	1/1	0.91	0.10	133,133,133,133	0
59	MG	14	3113	1/1	0.91	0.24	51,51,51,51	0
58	K	13	1602	1/1	0.91	0.07	113,113,113,113	0
59	MG	14	3231	1/1	0.91	0.08	48,48,48,48	0
59	MG	14	3118	1/1	0.91	0.13	53,53,53,53	0
58	K	14	3023	1/1	0.91	0.11	93,93,93,93	0
59	MG	1H	3218	1/1	0.91	0.11	53,53,53,53	0
58	K	14	3025	1/1	0.91	0.07	97,97,97,97	0
59	MG	14	3244	1/1	0.91	0.18	46,46,46,46	0
59	MG	1H	3150	1/1	0.91	0.11	76,76,76,76	0
59	MG	14	3247	1/1	0.91	0.17	60,60,60,60	0
59	MG	14	3139	1/1	0.91	0.19	46,46,46,46	0
59	MG	1H	3151	1/1	0.91	0.26	54,54,54,54	0
59	MG	1H	3156	1/1	0.91	0.15	55,55,55,55	0
58	K	1G	1610	1/1	0.91	0.07	95,95,95,95	0
58	K	1G	1613	1/1	0.91	0.06	96,96,96,96	0
59	MG	14	3260	1/1	0.91	0.19	56,56,56,56	0
59	MG	14	3261	1/1	0.91	0.14	75,75,75,75	0
58	K	1H	3003	1/1	0.91	0.05	76,76,76,76	0
58	K	1H	3109	1/1	0.91	0.08	54,54,54,54	0
58	K	1G	1618	1/1	0.91	0.10	102,102,102,102	0
58	K	1H	3118	1/1	0.91	0.18	89,89,89,89	0
59	MG	13	1692	1/1	0.91	0.15	70,70,70,70	0
59	MG	1H	3246	1/1	0.91	0.13	58,58,58,58	0
58	K	14	3093	1/1	0.91	0.09	72,72,72,72	0
59	MG	14	3169	1/1	0.91	0.12	57,57,57,57	0
59	MG	1H	3183	1/1	0.91	0.18	49,49,49,49	0
59	MG	14	3350	1/1	0.91	0.20	69,69,69,69	0
58	K	1H	3035	1/1	0.91	0.09	98,98,98,98	0
59	MG	1H	3257	1/1	0.91	0.09	49,49,49,49	0
59	MG	14	3381	1/1	0.91	0.10	77,77,77,77	0
59	MG	14	3387	1/1	0.91	0.07	45,45,45,45	0
59	MG	14	3389	1/1	0.91	0.09	69,69,69,69	0
59	MG	1J	201	1/1	0.91	0.07	131,131,131,131	0
59	MG	1H	3186	1/1	0.91	0.23	50,50,50,50	0
59	MG	29	303	1/1	0.91	0.14	37,37,37,37	0
58	K	14	3013	1/1	0.91	0.06	98,98,98,98	0
58	K	1H	3111	1/1	0.91	0.11	75,75,75,75	0
58	K	1H	3089	1/1	0.92	0.09	50,50,50,50	0
59	MG	1H	3273	1/1	0.92	0.06	49,49,49,49	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
59	MG	1H	3274	1/1	0.92	0.10	56,56,56,56	0
59	MG	13	1711	1/1	0.92	0.15	48,48,48,48	0
59	MG	16	206	1/1	0.92	0.12	62,62,62,62	0
59	MG	14	3200	1/1	0.92	0.09	102,102,102,102	0
59	MG	13	1712	1/1	0.92	0.12	50,50,50,50	0
59	MG	1G	1691	1/1	0.92	0.08	84,84,84,84	0
59	MG	13	1741	1/1	0.92	0.06	106,106,106,106	0
59	MG	13	1680	1/1	0.92	0.18	71,71,71,71	0
59	MG	14	3208	1/1	0.92	0.07	61,61,61,61	0
58	K	29	301	1/1	0.92	0.09	56,56,56,56	0
58	K	14	3061	1/1	0.92	0.06	103,103,103,103	0
59	MG	14	3101	1/1	0.92	0.09	61,61,61,61	0
59	MG	14	3102	1/1	0.92	0.08	57,57,57,57	0
59	MG	13	1684	1/1	0.92	0.14	56,56,56,56	0
59	MG	1H	3288	1/1	0.92	0.09	51,51,51,51	0
59	MG	14	3106	1/1	0.92	0.18	34,34,34,34	0
59	MG	14	3222	1/1	0.92	0.07	57,57,57,57	0
58	K	14	3064	1/1	0.92	0.15	70,70,70,70	0
59	MG	13	1640	1/1	0.92	0.13	72,72,72,72	0
59	MG	14	3228	1/1	0.92	0.16	88,88,88,88	0
58	K	1H	3119	1/1	0.92	0.08	92,92,92,92	0
59	MG	14	3120	1/1	0.92	0.08	44,44,44,44	0
58	K	13	1624	1/1	0.92	0.11	83,83,83,83	0
59	MG	14	3129	1/1	0.92	0.08	44,44,44,44	0
59	MG	14	3240	1/1	0.92	0.12	59,59,59,59	0
58	K	1H	3053	1/1	0.92	0.12	63,63,63,63	0
58	K	1G	1624	1/1	0.92	0.07	116,116,116,116	0
59	MG	14	3245	1/1	0.92	0.22	64,64,64,64	0
59	MG	1H	3305	1/1	0.92	0.18	57,57,57,57	0
59	MG	1G	1642	1/1	0.92	0.19	59,59,59,59	0
59	MG	14	3140	1/1	0.92	0.18	45,45,45,45	0
58	K	1H	3093	1/1	0.92	0.06	79,79,79,79	0
58	K	13	1631	1/1	0.92	0.08	93,93,93,93	0
59	MG	14	3143	1/1	0.92	0.16	72,72,72,72	0
58	K	1H	3015	1/1	0.92	0.07	80,80,80,80	0
59	MG	14	3256	1/1	0.92	0.24	64,64,64,64	0
59	MG	14	3258	1/1	0.92	0.12	37,37,37,37	0
58	K	1H	3026	1/1	0.92	0.13	62,62,62,62	0
59	MG	1H	3313	1/1	0.92	0.12	52,52,52,52	0
59	MG	1H	3145	1/1	0.92	0.13	32,32,32,32	0
58	K	13	1612[B]	1/1	0.92	0.25	23,23,23,23	1
58	K	1H	3028	1/1	0.92	0.07	50,50,50,50	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
59	MG	14	3159	1/1	0.92	0.17	53,53,53,53	0
58	K	1H	3073	1/1	0.92	0.10	47,47,47,47	0
58	K	14	3046	1/1	0.92	0.14	68,68,68,68	0
58	K	1H	3075	1/1	0.92	0.07	81,81,81,81	0
59	MG	1H	3322	1/1	0.92	0.16	60,60,60,60	0
59	MG	1H	3242	1/1	0.92	0.15	57,57,57,57	0
58	K	13	1612[A]	1/1	0.92	0.25	35,35,35,35	1
59	MG	1H	3168	1/1	0.92	0.22	46,46,46,46	0
59	MG	14	3177	1/1	0.92	0.14	64,64,64,64	0
59	MG	14	3378	1/1	0.92	0.09	71,71,71,71	0
59	MG	14	3178	1/1	0.92	0.10	36,36,36,36	0
58	K	1H	3041	1/1	0.92	0.10	66,66,66,66	0
58	K	14	3050	1/1	0.92	0.09	81,81,81,81	0
58	K	1H	3030	1/1	0.92	0.10	86,86,86,86	0
59	MG	13	1706	1/1	0.92	0.20	63,63,63,63	0
58	K	5I	101	1/1	0.92	0.09	129,129,129,129	0
58	K	1H	3045	1/1	0.92	0.06	72,72,72,72	0
59	MG	1H	3352	1/1	0.92	0.07	59,59,59,59	0
59	MG	1H	3179	1/1	0.93	0.09	51,51,51,51	0
58	K	14	3010	1/1	0.93	0.06	53,53,53,53	0
59	MG	14	3191	1/1	0.93	0.20	45,45,45,45	0
58	K	1H	3057	1/1	0.93	0.05	43,43,43,43	0
58	K	1H	3013	1/1	0.93	0.06	83,83,83,83	0
59	MG	1H	3261	1/1	0.93	0.22	49,49,49,49	0
59	MG	1H	3262	1/1	0.93	0.12	49,49,49,49	0
58	K	1G	1608	1/1	0.93	0.07	113,113,113,113	0
59	MG	1H	3268	1/1	0.93	0.16	50,50,50,50	0
59	MG	BI	202	1/1	0.93	0.07	94,94,94,94	0
59	MG	1H	3122	1/1	0.93	0.18	29,29,29,29	0
59	MG	1G	1711	1/1	0.93	0.06	104,104,104,104	0
59	MG	1G	1716	1/1	0.93	0.07	107,107,107,107	0
59	MG	1H	3125	1/1	0.93	0.15	41,41,41,41	0
58	K	13	1616	1/1	0.93	0.04	96,96,96,96	0
59	MG	41	203	1/1	0.93	0.13	40,40,40,40	0
59	MG	14	3100	1/1	0.93	0.07	47,47,47,47	0
59	MG	1H	3279	1/1	0.93	0.20	74,74,74,74	0
59	MG	1H	3129	1/1	0.93	0.16	34,34,34,34	0
58	K	14	3021	1/1	0.93	0.07	47,47,47,47	0
59	MG	N8	101	1/1	0.93	0.10	56,56,56,56	0
59	MG	14	3219	1/1	0.93	0.12	45,45,45,45	0
58	K	1H	3011	1/1	0.93	0.04	61,61,61,61	0
59	MG	14	3110	1/1	0.93	0.19	48,48,48,48	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
59	MG	14	3112	1/1	0.93	0.06	55,55,55,55	0
59	MG	13	1675	1/1	0.93	0.10	91,91,91,91	0
59	MG	14	3114	1/1	0.93	0.15	57,57,57,57	0
58	K	1H	3090	1/1	0.93	0.06	65,65,65,65	0
59	MG	1H	3137	1/1	0.93	0.14	42,42,42,42	0
59	MG	14	3234	1/1	0.93	0.34	67,67,67,67	0
59	MG	13	1700	1/1	0.93	0.11	63,63,63,63	0
58	K	14	3024	1/1	0.93	0.07	57,57,57,57	0
59	MG	14	3126	1/1	0.93	0.12	69,69,69,69	0
59	MG	14	3242	1/1	0.93	0.18	44,44,44,44	0
58	K	1H	3048	1/1	0.93	0.05	67,67,67,67	0
59	MG	1H	3293	1/1	0.93	0.10	55,55,55,55	0
59	MG	14	3135	1/1	0.93	0.17	42,42,42,42	0
59	MG	13	1647	1/1	0.93	0.15	59,59,59,59	0
59	MG	1H	3219	1/1	0.93	0.15	50,50,50,50	0
59	MG	1H	3301	1/1	0.93	0.12	59,59,59,59	0
59	MG	13	1650	1/1	0.93	0.06	73,73,73,73	0
59	MG	1H	3222	1/1	0.93	0.18	67,67,67,67	0
59	MG	1H	3306	1/1	0.93	0.14	44,44,44,44	0
59	MG	1G	1647	1/1	0.93	0.10	80,80,80,80	0
59	MG	1H	3307	1/1	0.93	0.09	39,39,39,39	0
59	MG	14	3257	1/1	0.93	0.15	48,48,48,48	0
59	MG	13	1681	1/1	0.93	0.13	76,76,76,76	0
58	K	14	3054	1/1	0.93	0.04	77,77,77,77	0
58	K	1G	1616	1/1	0.93	0.05	89,89,89,89	0
59	MG	1H	3157	1/1	0.93	0.12	62,62,62,62	0
59	MG	1G	1653	1/1	0.93	0.19	52,52,52,52	0
59	MG	14	3264	1/1	0.93	0.16	55,55,55,55	0
59	MG	1H	3233	1/1	0.93	0.14	59,59,59,59	0
59	MG	13	1708	1/1	0.93	0.18	59,59,59,59	0
58	K	1H	3039	1/1	0.93	0.05	81,81,81,81	0
59	MG	14	3165	1/1	0.93	0.14	70,70,70,70	0
59	MG	1G	1657	1/1	0.93	0.12	74,74,74,74	0
59	MG	1H	3160	1/1	0.93	0.16	29,29,29,29	0
59	MG	14	3170	1/1	0.93	0.12	52,52,52,52	0
59	MG	14	3341	1/1	0.93	0.10	52,52,52,52	0
59	MG	1G	1659	1/1	0.93	0.13	72,72,72,72	0
59	MG	14	3172	1/1	0.93	0.15	72,72,72,72	0
59	MG	14	3173	1/1	0.93	0.28	64,64,64,64	0
58	K	13	1601	1/1	0.93	0.07	87,87,87,87	0
59	MG	1H	3241	1/1	0.93	0.12	39,39,39,39	0
59	MG	14	3386	1/1	0.93	0.10	82,82,82,82	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
59	MG	1H	3167	1/1	0.93	0.05	33,33,33,33	0
59	MG	13	1658	1/1	0.93	0.13	35,35,35,35	0
59	MG	13	1660	1/1	0.93	0.15	60,60,60,60	0
59	MG	14	3182	1/1	0.93	0.12	42,42,42,42	0
58	K	1H	3023	1/1	0.93	0.07	68,68,68,68	0
58	K	1H	3055	1/1	0.93	0.04	40,40,40,40	0
59	MG	55	201	1/1	0.93	0.15	59,59,59,59	0
59	MG	1H	3249	1/1	0.93	0.15	53,53,53,53	0
59	MG	1H	3196	1/1	0.94	0.06	42,42,42,42	0
59	MG	14	3210	1/1	0.94	0.19	45,45,45,45	0
58	K	1G	1603	1/1	0.94	0.16	79,79,79,79	0
58	K	13	1623	1/1	0.94	0.10	121,121,121,121	0
59	MG	1H	3320	1/1	0.94	0.19	43,43,43,43	0
59	MG	14	3215	1/1	0.94	0.13	45,45,45,45	0
58	K	1H	3021	1/1	0.94	0.06	78,78,78,78	0
59	MG	14	3134	1/1	0.94	0.08	67,67,67,67	0
59	MG	1H	3143	1/1	0.94	0.18	63,63,63,63	0
59	MG	13	1648	1/1	0.94	0.10	61,61,61,61	0
59	MG	1H	3209	1/1	0.94	0.16	33,33,33,33	0
59	MG	14	3224	1/1	0.94	0.04	53,53,53,53	0
59	MG	1H	3269	1/1	0.94	0.17	54,54,54,54	0
59	MG	1H	3210	1/1	0.94	0.09	50,50,50,50	0
59	MG	1H	3147	1/1	0.94	0.09	19,19,19,19	0
58	K	1H	3103	1/1	0.94	0.05	65,65,65,65	0
58	K	1H	3107	1/1	0.94	0.05	82,82,82,82	0
59	MG	1H	3334	1/1	0.94	0.16	55,55,55,55	0
59	MG	14	3148	1/1	0.94	0.11	58,58,58,58	0
59	MG	14	3237	1/1	0.94	0.11	58,58,58,58	0
59	MG	1H	3214	1/1	0.94	0.10	26,26,26,26	0
58	K	14	3030	1/1	0.94	0.07	56,56,56,56	0
59	MG	14	3151	1/1	0.94	0.14	57,57,57,57	0
59	MG	1H	3281	1/1	0.94	0.08	93,93,93,93	0
58	K	14	3032	1/1	0.94	0.07	61,61,61,61	0
59	MG	1H	3393	1/1	0.94	0.08	44,44,44,44	0
59	MG	1H	3415	1/1	0.94	0.07	94,94,94,94	0
59	MG	1H	3474	1/1	0.94	0.07	47,47,47,47	0
59	MG	1H	3477	1/1	0.94	0.08	43,43,43,43	0
58	K	14	3012	1/1	0.94	0.05	91,91,91,91	0
59	MG	1H	3518	1/1	0.94	0.07	40,40,40,40	0
58	K	14	3056	1/1	0.94	0.04	57,57,57,57	0
59	MG	16	204	1/1	0.94	0.13	80,80,80,80	0
58	K	14	3057	1/1	0.94	0.05	68,68,68,68	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
58	K	13	1603	1/1	0.94	0.07	117,117,117,117	0
59	MG	1H	3165	1/1	0.94	0.14	30,30,30,30	0
58	K	14	3060	1/1	0.94	0.04	67,67,67,67	0
59	MG	1G	1683	1/1	0.94	0.12	90,90,90,90	0
59	MG	1G	1685	1/1	0.94	0.09	87,87,87,87	0
58	K	1H	3047	1/1	0.94	0.14	37,37,37,37	0
59	MG	13	1664	1/1	0.94	0.17	53,53,53,53	0
59	MG	14	3181	1/1	0.94	0.07	46,46,46,46	0
58	K	14	3063	1/1	0.94	0.06	84,84,84,84	0
59	MG	1H	3173	1/1	0.94	0.09	57,57,57,57	0
58	K	1H	3024	1/1	0.94	0.08	56,56,56,56	0
59	MG	1H	3177	1/1	0.94	0.14	54,54,54,54	0
58	K	13	1622	1/1	0.94	0.05	73,73,73,73	0
59	MG	14	3289	1/1	0.94	0.08	53,53,53,53	0
59	MG	1H	3240	1/1	0.94	0.21	52,52,52,52	0
59	MG	14	3325	1/1	0.94	0.09	81,81,81,81	0
59	MG	14	3099	1/1	0.94	0.10	32,32,32,32	0
59	MG	14	3347	1/1	0.94	0.09	57,57,57,57	0
59	MG	1G	1632	1/1	0.94	0.09	109,109,109,109	0
59	MG	14	3357	1/1	0.94	0.17	95,95,95,95	0
58	K	14	3094	1/1	0.94	0.05	111,111,111,111	0
59	MG	14	3195	1/1	0.94	0.11	64,64,64,64	0
58	K	1H	3086	1/1	0.94	0.09	79,79,79,79	0
59	MG	14	3379	1/1	0.94	0.12	42,42,42,42	0
58	K	14	3068	1/1	0.94	0.10	48,48,48,48	0
59	MG	1G	1636	1/1	0.94	0.10	89,89,89,89	0
58	K	14	3044	1/1	0.94	0.08	95,95,95,95	0
59	MG	1G	1638	1/1	0.94	0.15	43,43,43,43	0
59	MG	14	3398	1/1	0.94	0.09	63,63,63,63	0
59	MG	14	3406	1/1	0.94	0.08	55,55,55,55	0
59	MG	13	1638	1/1	0.94	0.12	58,58,58,58	0
58	K	1H	3042	1/1	0.94	0.14	62,62,62,62	0
59	MG	1H	3190	1/1	0.94	0.18	49,49,49,49	0
59	MG	14	3205	1/1	0.94	0.09	37,37,37,37	0
58	K	14	3073	1/1	0.94	0.10	81,81,81,81	0
59	MG	1G	1644	1/1	0.94	0.15	55,55,55,55	0
59	MG	1G	1725	1/1	0.95	0.06	97,97,97,97	0
59	MG	1G	1727	1/1	0.95	0.05	93,93,93,93	0
59	MG	2L	101	1/1	0.95	0.11	55,55,55,55	0
58	K	14	3077	1/1	0.95	0.12	72,72,72,72	0
59	MG	13	1733	1/1	0.95	0.09	117,117,117,117	0
59	MG	13	1738	1/1	0.95	0.09	91,91,91,91	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
59	MG	14	3207	1/1	0.95	0.17	58,58,58,58	0
59	MG	1H	3287	1/1	0.95	0.21	43,43,43,43	0
59	MG	16	210	1/1	0.95	0.08	98,98,98,98	0
58	K	14	3009	1/1	0.95	0.06	69,69,69,69	0
59	MG	78	201	1/1	0.95	0.06	32,32,32,32	0
59	MG	1H	3164	1/1	0.95	0.09	45,45,45,45	0
59	MG	13	1651	1/1	0.95	0.12	51,51,51,51	0
59	MG	1H	3225	1/1	0.95	0.21	58,58,58,58	0
58	K	14	3053	1/1	0.95	0.06	63,63,63,63	0
59	MG	1H	3294	1/1	0.95	0.13	35,35,35,35	0
58	K	14	3031	1/1	0.95	0.05	78,78,78,78	0
59	MG	1H	3296	1/1	0.95	0.10	50,50,50,50	0
58	K	1H	3108	1/1	0.95	0.09	86,86,86,86	0
59	MG	14	3223	1/1	0.95	0.08	53,53,53,53	0
58	K	13	1621	1/1	0.95	0.05	59,59,59,59	0
59	MG	14	3119	1/1	0.95	0.10	51,51,51,51	0
58	K	14	3034	1/1	0.95	0.06	49,49,49,49	0
59	MG	14	3121	1/1	0.95	0.06	43,43,43,43	0
59	MG	2K	101	1/1	0.95	0.16	42,42,42,42	0
59	MG	14	3232	1/1	0.95	0.23	69,69,69,69	0
58	K	14	3035	1/1	0.95	0.12	62,62,62,62	0
59	MG	1H	3178	1/1	0.95	0.18	34,34,34,34	0
58	K	14	3059	1/1	0.95	0.10	73,73,73,73	0
58	K	1H	3064	1/1	0.95	0.07	49,49,49,49	0
58	K	14	3037	1/1	0.95	0.06	60,60,60,60	0
58	K	14	3090	1/1	0.95	0.06	65,65,65,65	0
58	K	1H	3066	1/1	0.95	0.06	80,80,80,80	0
59	MG	1H	3314	1/1	0.95	0.14	49,49,49,49	0
59	MG	1H	3245	1/1	0.95	0.14	41,41,41,41	0
58	K	1G	1612	1/1	0.95	0.09	101,101,101,101	0
59	MG	1H	3247	1/1	0.95	0.18	44,44,44,44	0
59	MG	13	1668	1/1	0.95	0.09	41,41,41,41	0
59	MG	14	3248	1/1	0.95	0.05	41,41,41,41	0
59	MG	14	3249	1/1	0.95	0.08	54,54,54,54	0
59	MG	1H	3136	1/1	0.95	0.19	37,37,37,37	0
58	K	14	3065	1/1	0.95	0.07	92,92,92,92	0
59	MG	1H	3193	1/1	0.95	0.09	43,43,43,43	0
59	MG	1H	3254	1/1	0.95	0.13	50,50,50,50	0
58	K	1H	3100	1/1	0.95	0.10	78,78,78,78	0
59	MG	1H	3258	1/1	0.95	0.11	48,48,48,48	0
58	K	1H	3002	1/1	0.95	0.04	71,71,71,71	0
59	MG	1H	3260	1/1	0.95	0.12	43,43,43,43	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
59	MG	1H	3200	1/1	0.95	0.10	67,67,67,67	0
58	K	1H	3050	1/1	0.95	0.09	70,70,70,70	0
59	MG	1H	3328	1/1	0.95	0.19	61,61,61,61	0
59	MG	1H	3141	1/1	0.95	0.11	37,37,37,37	0
59	MG	1H	3265	1/1	0.95	0.23	63,63,63,63	0
58	K	14	3002	1/1	0.95	0.06	90,90,90,90	0
58	K	1G	1602	1/1	0.95	0.18	70,70,70,70	0
59	MG	1H	3347	1/1	0.95	0.09	50,50,50,50	0
58	K	14	3072	1/1	0.95	0.04	89,89,89,89	0
59	MG	13	1641	1/1	0.95	0.12	90,90,90,90	0
59	MG	1H	3275	1/1	0.95	0.23	60,60,60,60	0
59	MG	14	3175	1/1	0.95	0.23	59,59,59,59	0
58	K	1H	3061	1/1	0.95	0.09	47,47,47,47	0
59	MG	1H	3419	1/1	0.95	0.09	43,43,43,43	0
59	MG	14	3340	1/1	0.95	0.07	74,74,74,74	0
59	MG	1G	1669	1/1	0.95	0.05	72,72,72,72	0
59	MG	1H	3426	1/1	0.95	0.11	68,68,68,68	0
59	MG	14	3348	1/1	0.95	0.09	102,102,102,102	0
59	MG	1H	3427	1/1	0.95	0.08	41,41,41,41	0
59	MG	1H	3461	1/1	0.95	0.08	33,33,33,33	0
59	MG	1H	3466	1/1	0.95	0.07	34,34,34,34	0
58	K	1H	3106	1/1	0.95	0.10	92,92,92,92	0
59	MG	1H	3153	1/1	0.95	0.11	44,44,44,44	0
59	MG	14	3186	1/1	0.95	0.09	48,48,48,48	0
59	MG	14	3380	1/1	0.95	0.09	70,70,70,70	0
59	MG	1G	1677	1/1	0.95	0.04	76,76,76,76	0
59	MG	14	3189	1/1	0.95	0.17	26,26,26,26	0
58	K	1H	3095	1/1	0.95	0.06	44,44,44,44	0
59	MG	1H	3493	1/1	0.95	0.13	63,63,63,63	0
59	MG	14	3394	1/1	0.95	0.08	82,82,82,82	0
59	MG	14	3395	1/1	0.95	0.08	50,50,50,50	0
59	MG	1G	1686	1/1	0.95	0.06	94,94,94,94	0
59	MG	14	3399	1/1	0.95	0.07	55,55,55,55	0
59	MG	14	3401	1/1	0.95	0.13	89,89,89,89	0
59	MG	1H	3514	1/1	0.95	0.07	88,88,88,88	0
59	MG	14	3194	1/1	0.95	0.05	64,64,64,64	0
59	MG	1H	3515	1/1	0.95	0.13	90,90,90,90	0
58	K	14	3028	1/1	0.95	0.06	56,56,56,56	0
59	MG	1H	3522	1/1	0.95	0.11	102,102,102,102	0
59	MG	1H	3216	1/1	0.95	0.12	45,45,45,45	0
59	MG	1G	1722	1/1	0.95	0.05	97,97,97,97	0
59	MG	1H	3388	1/1	0.96	0.08	38,38,38,38	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
58	K	1H	3046	1/1	0.96	0.10	50,50,50,50	0
58	K	1H	3058	1/1	0.96	0.03	56,56,56,56	0
59	MG	1H	3394	1/1	0.96	0.06	38,38,38,38	0
59	MG	1H	3399	1/1	0.96	0.08	54,54,54,54	0
59	MG	13	1739	1/1	0.96	0.05	97,97,97,97	0
58	K	14	3006	1/1	0.96	0.12	62,62,62,62	0
59	MG	1G	1675	1/1	0.96	0.11	54,54,54,54	0
59	MG	13	1654	1/1	0.96	0.12	36,36,36,36	0
58	K	1H	3076	1/1	0.96	0.05	86,86,86,86	0
59	MG	1G	1678	1/1	0.96	0.06	71,71,71,71	0
59	MG	1H	3437	1/1	0.96	0.16	49,49,49,49	0
59	MG	1H	3450	1/1	0.96	0.05	91,91,91,91	0
59	MG	1H	3163	1/1	0.96	0.14	40,40,40,40	0
59	MG	1H	3220	1/1	0.96	0.07	45,45,45,45	0
58	K	1H	3005	1/1	0.96	0.05	67,67,67,67	0
59	MG	1H	3475	1/1	0.96	0.08	91,91,91,91	0
59	MG	1G	1702	1/1	0.96	0.11	87,87,87,87	0
59	MG	1G	1704	1/1	0.96	0.04	110,110,110,110	0
59	MG	1G	1710	1/1	0.96	0.08	70,70,70,70	0
59	MG	1H	3476	1/1	0.96	0.08	42,42,42,42	0
58	K	14	3087	1/1	0.96	0.03	84,84,84,84	0
59	MG	1G	1718	1/1	0.96	0.05	91,91,91,91	0
59	MG	14	3212	1/1	0.96	0.19	34,34,34,34	0
59	MG	1H	3481	1/1	0.96	0.07	43,43,43,43	0
59	MG	1H	3483	1/1	0.96	0.12	75,75,75,75	0
58	K	1H	3006	1/1	0.96	0.03	59,59,59,59	0
59	MG	1H	3492	1/1	0.96	0.06	67,67,67,67	0
59	MG	1H	3286	1/1	0.96	0.20	52,52,52,52	0
59	MG	1H	3498	1/1	0.96	0.08	37,37,37,37	0
59	MG	1H	3508	1/1	0.96	0.19	78,78,78,78	0
59	MG	14	3221	1/1	0.96	0.19	52,52,52,52	0
59	MG	14	3097	1/1	0.96	0.14	38,38,38,38	0
59	MG	14	3098	1/1	0.96	0.12	38,38,38,38	0
59	MG	1H	3224	1/1	0.96	0.17	51,51,51,51	0
58	K	14	3011	1/1	0.96	0.05	56,56,56,56	0
58	K	1H	3022	1/1	0.96	0.08	51,51,51,51	0
59	MG	1H	3228	1/1	0.96	0.11	48,48,48,48	0
59	MG	14	3229	1/1	0.96	0.17	65,65,65,65	0
58	K	1G	1621	1/1	0.96	0.04	74,74,74,74	0
59	MG	14	3104	1/1	0.96	0.14	29,29,29,29	0
59	MG	1H	3292	1/1	0.96	0.14	54,54,54,54	0
59	MG	1H	3230	1/1	0.96	0.09	38,38,38,38	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
59	MG	14	3107	1/1	0.96	0.11	40,40,40,40	0
59	MG	14	3108	1/1	0.96	0.11	62,62,62,62	0
58	K	1H	3007	1/1	0.96	0.12	54,54,54,54	0
58	K	14	3015	1/1	0.96	0.09	52,52,52,52	0
59	MG	14	3241	1/1	0.96	0.14	34,34,34,34	0
59	MG	1H	3234	1/1	0.96	0.14	33,33,33,33	0
59	MG	21	303	1/1	0.96	0.14	30,30,30,30	0
59	MG	1H	3176	1/1	0.96	0.14	32,32,32,32	0
59	MG	1H	3298	1/1	0.96	0.13	23,23,23,23	0
59	MG	1H	3300	1/1	0.96	0.10	31,31,31,31	0
59	MG	1H	3127	1/1	0.96	0.22	54,54,54,54	0
59	MG	1H	3302	1/1	0.96	0.16	41,41,41,41	0
59	MG	1H	3237	1/1	0.96	0.15	51,51,51,51	0
59	MG	Q8	101	1/1	0.96	0.08	32,32,32,32	0
59	MG	1G	1626	1/1	0.96	0.12	72,72,72,72	0
58	K	1G	1623	1/1	0.96	0.04	126,126,126,126	0
59	MG	14	3132	1/1	0.96	0.05	47,47,47,47	0
59	MG	13	1667	1/1	0.96	0.15	39,39,39,39	0
59	MG	14	3255	1/1	0.96	0.14	52,52,52,52	0
58	K	14	3018	1/1	0.96	0.06	71,71,71,71	0
58	K	1H	3085	1/1	0.96	0.04	64,64,64,64	0
58	K	1H	3116	1/1	0.96	0.04	80,80,80,80	0
59	MG	14	3138	1/1	0.96	0.13	40,40,40,40	0
59	MG	1H	3135	1/1	0.96	0.05	50,50,50,50	0
59	MG	1H	3311	1/1	0.96	0.21	57,57,57,57	0
58	K	1H	3036	1/1	0.96	0.05	55,55,55,55	0
59	MG	13	1673	1/1	0.96	0.12	56,56,56,56	0
58	K	1H	3067	1/1	0.96	0.05	49,49,49,49	0
59	MG	14	3144	1/1	0.96	0.06	50,50,50,50	0
58	K	1H	3008	1/1	0.96	0.12	61,61,61,61	0
59	MG	14	3146	1/1	0.96	0.05	30,30,30,30	0
59	MG	14	3147	1/1	0.96	0.08	54,54,54,54	0
59	MG	1H	3192	1/1	0.96	0.08	49,49,49,49	0
59	MG	14	3277	1/1	0.96	0.08	53,53,53,53	0
59	MG	14	3278	1/1	0.96	0.08	43,43,43,43	0
58	K	1H	3105	1/1	0.96	0.05	60,60,60,60	0
59	MG	14	3293	1/1	0.96	0.06	91,91,91,91	0
59	MG	14	3308	1/1	0.96	0.06	80,80,80,80	0
59	MG	1G	1641	1/1	0.96	0.14	53,53,53,53	0
59	MG	14	3317	1/1	0.96	0.05	94,94,94,94	0
59	MG	14	3324	1/1	0.96	0.06	62,62,62,62	0
59	MG	1H	3194	1/1	0.96	0.17	45,45,45,45	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
59	MG	14	3332	1/1	0.96	0.04	110,110,110,110	0
59	MG	14	3338	1/1	0.96	0.06	73,73,73,73	0
58	K	1G	1611	1/1	0.96	0.06	94,94,94,94	0
58	K	16	201	1/1	0.96	0.06	102,102,102,102	0
59	MG	14	3344	1/1	0.96	0.13	89,89,89,89	0
59	MG	13	1646	1/1	0.96	0.07	59,59,59,59	0
59	MG	14	3157	1/1	0.96	0.10	57,57,57,57	0
59	MG	1H	3201	1/1	0.96	0.11	48,48,48,48	0
59	MG	1H	3202	1/1	0.96	0.13	46,46,46,46	0
59	MG	14	3366	1/1	0.96	0.06	77,77,77,77	0
58	K	13	1632	1/1	0.96	0.06	83,83,83,83	0
59	MG	14	3376	1/1	0.96	0.09	61,61,61,61	0
58	K	14	3080	1/1	0.96	0.03	94,94,94,94	0
59	MG	1H	3148	1/1	0.96	0.10	39,39,39,39	0
59	MG	1H	3149	1/1	0.96	0.14	29,29,29,29	0
59	MG	1H	3264	1/1	0.96	0.15	47,47,47,47	0
58	K	14	3029	1/1	0.96	0.05	68,68,68,68	0
59	MG	14	3385	1/1	0.96	0.05	63,63,63,63	0
59	MG	1H	3267	1/1	0.96	0.06	60,60,60,60	0
59	MG	1H	3333	1/1	0.96	0.13	50,50,50,50	0
59	MG	13	1714	1/1	0.96	0.04	106,106,106,106	0
59	MG	14	3391	1/1	0.96	0.06	62,62,62,62	0
59	MG	14	3392	1/1	0.96	0.08	69,69,69,69	0
59	MG	13	1732	1/1	0.96	0.08	81,81,81,81	0
59	MG	1H	3271	1/1	0.96	0.17	45,45,45,45	0
59	MG	1H	3341	1/1	0.96	0.09	31,31,31,31	0
59	MG	1H	3272	1/1	0.96	0.09	60,60,60,60	0
59	MG	1H	3350	1/1	0.96	0.07	26,26,26,26	0
59	MG	14	3402	1/1	0.96	0.04	123,123,123,123	0
59	MG	1H	3154	1/1	0.96	0.17	31,31,31,31	0
59	MG	1H	3359	1/1	0.96	0.07	55,55,55,55	0
59	MG	1H	3363	1/1	0.96	0.07	32,32,32,32	0
59	MG	1H	3369	1/1	0.96	0.06	52,52,52,52	0
59	MG	1H	3373	1/1	0.96	0.07	39,39,39,39	0
59	MG	1H	3377	1/1	0.96	0.06	44,44,44,44	0
59	MG	14	3187	1/1	0.96	0.12	41,41,41,41	0
58	K	1H	3114	1/1	0.97	0.04	58,58,58,58	0
59	MG	14	3116	1/1	0.97	0.11	41,41,41,41	0
58	K	1H	3071	1/1	0.97	0.08	65,65,65,65	0
59	MG	1H	3404	1/1	0.97	0.05	65,65,65,65	0
58	K	1H	3004	1/1	0.97	0.13	66,66,66,66	0
59	MG	1H	3175	1/1	0.97	0.10	34,34,34,34	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
59	MG	1H	3421	1/1	0.97	0.05	80,80,80,80	0
59	MG	14	3125	1/1	0.97	0.10	45,45,45,45	0
59	MG	14	3227	1/1	0.97	0.12	41,41,41,41	0
59	MG	1H	3424	1/1	0.97	0.06	84,84,84,84	0
58	K	1G	1614	1/1	0.97	0.06	100,100,100,100	0
59	MG	14	3230	1/1	0.97	0.13	44,44,44,44	0
58	K	1H	3094	1/1	0.97	0.05	65,65,65,65	0
59	MG	1H	3432	1/1	0.97	0.11	73,73,73,73	0
59	MG	13	1725	1/1	0.97	0.04	116,116,116,116	0
59	MG	1H	3438	1/1	0.97	0.07	36,36,36,36	0
59	MG	1H	3447	1/1	0.97	0.04	98,98,98,98	0
59	MG	14	3236	1/1	0.97	0.11	41,41,41,41	0
59	MG	13	1728	1/1	0.97	0.04	106,106,106,106	0
59	MG	1H	3454	1/1	0.97	0.06	42,42,42,42	0
59	MG	1H	3266	1/1	0.97	0.05	40,40,40,40	0
58	K	1H	3083	1/1	0.97	0.05	43,43,43,43	0
59	MG	1H	3473	1/1	0.97	0.08	27,27,27,27	0
58	K	1H	3077	1/1	0.97	0.05	49,49,49,49	0
59	MG	13	1736	1/1	0.97	0.05	100,100,100,100	0
59	MG	1H	3226	1/1	0.97	0.04	42,42,42,42	0
58	K	14	3071	1/1	0.97	0.09	75,75,75,75	0
59	MG	1H	3479	1/1	0.97	0.07	47,47,47,47	0
59	MG	1H	3480	1/1	0.97	0.06	58,58,58,58	0
59	MG	13	1694	1/1	0.97	0.09	43,43,43,43	0
59	MG	1H	3144	1/1	0.97	0.08	38,38,38,38	0
59	MG	13	1672	1/1	0.97	0.11	24,24,24,24	0
59	MG	1H	3487	1/1	0.97	0.04	85,85,85,85	0
59	MG	14	3152	1/1	0.97	0.10	69,69,69,69	0
59	MG	1H	3488	1/1	0.97	0.05	83,83,83,83	0
59	MG	1H	3490	1/1	0.97	0.06	53,53,53,53	0
59	MG	13	1742	1/1	0.97	0.05	94,94,94,94	0
59	MG	14	3156	1/1	0.97	0.12	55,55,55,55	0
59	MG	1H	3232	1/1	0.97	0.21	40,40,40,40	0
59	MG	14	3259	1/1	0.97	0.05	45,45,45,45	0
59	MG	14	3158	1/1	0.97	0.12	35,35,35,35	0
59	MG	1H	3495	1/1	0.97	0.12	80,80,80,80	0
59	MG	13	1744	1/1	0.97	0.04	107,107,107,107	0
59	MG	1H	3500	1/1	0.97	0.08	45,45,45,45	0
59	MG	14	3163	1/1	0.97	0.06	48,48,48,48	0
59	MG	14	3164	1/1	0.97	0.08	70,70,70,70	0
58	K	1H	3121	1/1	0.97	0.03	66,66,66,66	0
59	MG	14	3166	1/1	0.97	0.14	37,37,37,37	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
59	MG	1H	3509	1/1	0.97	0.05	101,101,101,101	0
59	MG	1H	3511	1/1	0.97	0.05	93,93,93,93	0
59	MG	1H	3512	1/1	0.97	0.07	61,61,61,61	0
59	MG	14	3273	1/1	0.97	0.06	46,46,46,46	0
59	MG	14	3274	1/1	0.97	0.07	30,30,30,30	0
59	MG	14	3276	1/1	0.97	0.09	44,44,44,44	0
59	MG	1H	3513	1/1	0.97	0.05	105,105,105,105	0
58	K	14	3020	1/1	0.97	0.04	72,72,72,72	0
59	MG	14	3288	1/1	0.97	0.15	79,79,79,79	0
59	MG	1H	3195	1/1	0.97	0.12	51,51,51,51	0
59	MG	14	3291	1/1	0.97	0.16	64,64,64,64	0
59	MG	1G	1684	1/1	0.97	0.07	75,75,75,75	0
59	MG	14	3297	1/1	0.97	0.05	44,44,44,44	0
59	MG	14	3299	1/1	0.97	0.06	57,57,57,57	0
59	MG	1H	3516	1/1	0.97	0.10	60,60,60,60	0
59	MG	14	3310	1/1	0.97	0.07	27,27,27,27	0
59	MG	14	3312	1/1	0.97	0.09	87,87,87,87	0
59	MG	1H	3517	1/1	0.97	0.05	55,55,55,55	0
58	K	1H	3104	1/1	0.97	0.04	53,53,53,53	0
59	MG	14	3320	1/1	0.97	0.09	90,90,90,90	0
59	MG	14	3322	1/1	0.97	0.04	93,93,93,93	0
59	MG	14	3323	1/1	0.97	0.06	47,47,47,47	0
59	MG	1H	3521	1/1	0.97	0.05	113,113,113,113	0
59	MG	1G	1695	1/1	0.97	0.04	97,97,97,97	0
59	MG	14	3327	1/1	0.97	0.06	66,66,66,66	0
59	MG	14	3328	1/1	0.97	0.05	66,66,66,66	0
59	MG	1H	3198	1/1	0.97	0.10	82,82,82,82	0
59	MG	1G	1697	1/1	0.97	0.04	81,81,81,81	0
59	MG	1G	1699	1/1	0.97	0.07	101,101,101,101	0
59	MG	1H	3524	1/1	0.97	0.06	35,35,35,35	0
58	K	1H	3070	1/1	0.97	0.04	54,54,54,54	0
59	MG	1G	1706	1/1	0.97	0.04	96,96,96,96	0
59	MG	1G	1707	1/1	0.97	0.05	120,120,120,120	0
59	MG	1H	3329	1/1	0.97	0.14	73,73,73,73	0
58	K	1G	1607	1/1	0.97	0.03	93,93,93,93	0
59	MG	14	3359	1/1	0.97	0.10	94,94,94,94	0
59	MG	14	3361	1/1	0.97	0.05	71,71,71,71	0
58	K	14	3007	1/1	0.97	0.21	52,52,52,52	0
59	MG	14	3371	1/1	0.97	0.08	61,61,61,61	0
59	MG	14	3372	1/1	0.97	0.05	73,73,73,73	0
59	MG	13	1657	1/1	0.97	0.13	26,26,26,26	0
59	MG	1G	1720	1/1	0.97	0.05	106,106,106,106	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
58	K	11	301	1/1	0.97	0.04	47,47,47,47	0
59	MG	1G	1724	1/1	0.97	0.05	109,109,109,109	0
59	MG	21	301	1/1	0.97	0.05	34,34,34,34	0
59	MG	1H	3123	1/1	0.97	0.15	20,20,20,20	0
59	MG	1H	3337	1/1	0.97	0.07	37,37,37,37	0
59	MG	14	3383	1/1	0.97	0.07	71,71,71,71	0
59	MG	1H	3339	1/1	0.97	0.06	33,33,33,33	0
59	MG	1H	3340	1/1	0.97	0.07	29,29,29,29	0
59	MG	1H	3206	1/1	0.97	0.09	35,35,35,35	0
59	MG	1H	3344	1/1	0.97	0.06	21,21,21,21	0
59	MG	G8	201	1/1	0.97	0.06	89,89,89,89	0
59	MG	1H	3124	1/1	0.97	0.12	28,28,28,28	0
59	MG	14	3393	1/1	0.97	0.22	81,81,81,81	0
59	MG	13	1659	1/1	0.97	0.07	54,54,54,54	0
59	MG	1H	3351	1/1	0.97	0.06	33,33,33,33	0
59	MG	14	3397	1/1	0.97	0.05	46,46,46,46	0
58	K	21	302	1/1	0.97	0.06	66,66,66,66	0
58	K	14	3062	1/1	0.97	0.07	65,65,65,65	0
59	MG	1H	3250	1/1	0.97	0.05	47,47,47,47	0
59	MG	1H	3251	1/1	0.97	0.09	52,52,52,52	0
59	MG	1G	1631	1/1	0.97	0.10	49,49,49,49	0
59	MG	1H	3128	1/1	0.97	0.14	40,40,40,40	0
59	MG	13	1639	1/1	0.97	0.07	62,62,62,62	0
59	MG	1J	205	1/1	0.97	0.05	104,104,104,104	0
59	MG	1H	3130	1/1	0.97	0.14	28,28,28,28	0
58	K	1H	3098	1/1	0.97	0.07	67,67,67,67	0
59	MG	1H	3390	1/1	0.97	0.07	39,39,39,39	0
59	MG	1H	3303	1/1	0.97	0.15	41,41,41,41	0
59	MG	1H	3395	1/1	0.98	0.13	56,56,56,56	0
59	MG	16	208	1/1	0.98	0.04	63,63,63,63	0
59	MG	1H	3396	1/1	0.98	0.05	35,35,35,35	0
59	MG	1H	3397	1/1	0.98	0.06	29,29,29,29	0
59	MG	1H	3166	1/1	0.98	0.10	17,17,17,17	0
58	K	1H	3062	1/1	0.98	0.07	42,42,42,42	0
59	MG	1H	3406	1/1	0.98	0.04	95,95,95,95	0
59	MG	1H	3408	1/1	0.98	0.05	60,60,60,60	0
59	MG	1H	3410	1/1	0.98	0.04	86,86,86,86	0
59	MG	1H	3414	1/1	0.98	0.05	89,89,89,89	0
58	K	1H	3049	1/1	0.98	0.05	66,66,66,66	0
59	MG	I8	102	1/1	0.98	0.06	72,72,72,72	0
59	MG	J8	101	1/1	0.98	0.06	49,49,49,49	0
59	MG	1H	3416	1/1	0.98	0.08	59,59,59,59	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
59	MG	1H	3169	1/1	0.98	0.07	43,43,43,43	0
59	MG	1H	3420	1/1	0.98	0.05	95,95,95,95	0
59	MG	13	1740	1/1	0.98	0.04	105,105,105,105	0
58	K	1H	3087	1/1	0.98	0.03	76,76,76,76	0
58	K	1H	3078	1/1	0.98	0.09	61,61,61,61	0
59	MG	13	1743	1/1	0.98	0.04	105,105,105,105	0
59	MG	1H	3431	1/1	0.98	0.05	85,85,85,85	0
59	MG	14	3117	1/1	0.98	0.07	42,42,42,42	0
58	K	14	3038	1/1	0.98	0.11	63,63,63,63	0
59	MG	1H	3434	1/1	0.98	0.15	68,68,68,68	0
59	MG	13	1745	1/1	0.98	0.09	78,78,78,78	0
59	MG	13	1746	1/1	0.98	0.05	93,93,93,93	0
59	MG	14	3122	1/1	0.98	0.07	49,49,49,49	0
59	MG	1H	3439	1/1	0.98	0.06	55,55,55,55	0
59	MG	1H	3440	1/1	0.98	0.11	63,63,63,63	0
59	MG	1H	3441	1/1	0.98	0.10	51,51,51,51	0
59	MG	14	3128	1/1	0.98	0.08	35,35,35,35	0
59	MG	1H	3444	1/1	0.98	0.04	94,94,94,94	0
59	MG	14	3130	1/1	0.98	0.12	45,45,45,45	0
59	MG	1H	3446	1/1	0.98	0.04	92,92,92,92	0
59	MG	13	1747	1/1	0.98	0.03	91,91,91,91	0
59	MG	1H	3449	1/1	0.98	0.06	57,57,57,57	0
59	MG	13	1748	1/1	0.98	0.05	104,104,104,104	0
59	MG	1H	3330	1/1	0.98	0.04	45,45,45,45	0
59	MG	1H	3455	1/1	0.98	0.20	55,55,55,55	0
59	MG	1H	3457	1/1	0.98	0.04	35,35,35,35	0
59	MG	1H	3459	1/1	0.98	0.08	50,50,50,50	0
59	MG	1H	3460	1/1	0.98	0.04	62,62,62,62	0
59	MG	13	1644	1/1	0.98	0.04	49,49,49,49	0
59	MG	1H	3462	1/1	0.98	0.04	46,46,46,46	0
59	MG	1H	3465	1/1	0.98	0.06	39,39,39,39	0
59	MG	1H	3256	1/1	0.98	0.08	47,47,47,47	0
59	MG	1H	3467	1/1	0.98	0.05	67,67,67,67	0
59	MG	1H	3468	1/1	0.98	0.04	50,50,50,50	0
59	MG	1H	3470	1/1	0.98	0.10	45,45,45,45	0
59	MG	1H	3472	1/1	0.98	0.11	71,71,71,71	0
58	K	1H	3115	1/1	0.98	0.04	50,50,50,50	0
59	MG	14	3272	1/1	0.98	0.09	26,26,26,26	0
58	K	13	1619	1/1	0.98	0.03	77,77,77,77	0
58	K	1H	3065	1/1	0.98	0.06	43,43,43,43	0
59	MG	1H	3185	1/1	0.98	0.06	41,41,41,41	0
59	MG	1H	3338	1/1	0.98	0.06	35,35,35,35	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
59	MG	1H	3478	1/1	0.98	0.04	38,38,38,38	0
59	MG	14	3280	1/1	0.98	0.05	48,48,48,48	0
59	MG	14	3281	1/1	0.98	0.06	45,45,45,45	0
59	MG	14	3283	1/1	0.98	0.07	36,36,36,36	0
59	MG	14	3286	1/1	0.98	0.04	47,47,47,47	0
59	MG	14	3287	1/1	0.98	0.07	50,50,50,50	0
58	K	13	1611	1/1	0.98	0.03	79,79,79,79	0
59	MG	13	1713	1/1	0.98	0.04	83,83,83,83	0
59	MG	13	1649	1/1	0.98	0.10	101,101,101,101	0
59	MG	1H	3343	1/1	0.98	0.05	35,35,35,35	0
59	MG	14	3294	1/1	0.98	0.04	77,77,77,77	0
59	MG	13	1718	1/1	0.98	0.07	89,89,89,89	0
59	MG	1H	3486	1/1	0.98	0.05	54,54,54,54	0
59	MG	14	3302	1/1	0.98	0.04	52,52,52,52	0
59	MG	14	3303	1/1	0.98	0.05	73,73,73,73	0
59	MG	14	3304	1/1	0.98	0.05	38,38,38,38	0
59	MG	14	3305	1/1	0.98	0.08	69,69,69,69	0
59	MG	14	3306	1/1	0.98	0.06	49,49,49,49	0
59	MG	13	1719	1/1	0.98	0.05	112,112,112,112	0
59	MG	14	3309	1/1	0.98	0.04	85,85,85,85	0
59	MG	1H	3348	1/1	0.98	0.05	34,34,34,34	0
59	MG	1H	3349	1/1	0.98	0.05	28,28,28,28	0
59	MG	14	3313	1/1	0.98	0.05	89,89,89,89	0
59	MG	14	3314	1/1	0.98	0.05	91,91,91,91	0
59	MG	1H	3155	1/1	0.98	0.15	35,35,35,35	0
59	MG	13	1723	1/1	0.98	0.03	109,109,109,109	0
59	MG	14	3318	1/1	0.98	0.12	68,68,68,68	0
59	MG	1H	3494	1/1	0.98	0.04	78,78,78,78	0
59	MG	14	3168	1/1	0.98	0.04	37,37,37,37	0
58	K	19	301	1/1	0.98	0.15	61,61,61,61	0
58	K	14	3043	1/1	0.98	0.03	71,71,71,71	0
59	MG	1H	3499	1/1	0.98	0.12	68,68,68,68	0
59	MG	1H	3197	1/1	0.98	0.09	50,50,50,50	0
59	MG	1G	1679	1/1	0.98	0.07	64,64,64,64	0
59	MG	14	3331	1/1	0.98	0.07	58,58,58,58	0
59	MG	1G	1681	1/1	0.98	0.04	49,49,49,49	0
59	MG	14	3333	1/1	0.98	0.06	39,39,39,39	0
59	MG	14	3335	1/1	0.98	0.11	50,50,50,50	0
59	MG	1H	3501	1/1	0.98	0.03	78,78,78,78	0
59	MG	14	3339	1/1	0.98	0.04	77,77,77,77	0
59	MG	1H	3503	1/1	0.98	0.06	63,63,63,63	0
59	MG	1H	3504	1/1	0.98	0.13	85,85,85,85	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
59	MG	1H	3506	1/1	0.98	0.04	65,65,65,65	0
59	MG	1G	1688	1/1	0.98	0.04	82,82,82,82	0
59	MG	14	3180	1/1	0.98	0.15	40,40,40,40	0
59	MG	1G	1689	1/1	0.98	0.04	90,90,90,90	0
59	MG	14	3351	1/1	0.98	0.04	61,61,61,61	0
59	MG	14	3354	1/1	0.98	0.08	70,70,70,70	0
59	MG	14	3356	1/1	0.98	0.13	84,84,84,84	0
59	MG	13	1729	1/1	0.98	0.05	68,68,68,68	0
59	MG	1H	3370	1/1	0.98	0.06	38,38,38,38	0
59	MG	1G	1693	1/1	0.98	0.04	89,89,89,89	0
59	MG	14	3362	1/1	0.98	0.04	69,69,69,69	0
59	MG	14	3364	1/1	0.98	0.15	71,71,71,71	0
59	MG	1H	3371	1/1	0.98	0.04	35,35,35,35	0
59	MG	14	3368	1/1	0.98	0.10	40,40,40,40	0
59	MG	1H	3372	1/1	0.98	0.09	77,77,77,77	0
58	K	1H	3074	1/1	0.98	0.02	53,53,53,53	0
59	MG	14	3373	1/1	0.98	0.06	84,84,84,84	0
59	MG	14	3374	1/1	0.98	0.08	96,96,96,96	0
59	MG	1G	1698	1/1	0.98	0.08	103,103,103,103	0
59	MG	1H	3374	1/1	0.98	0.07	70,70,70,70	0
59	MG	1G	1700	1/1	0.98	0.07	108,108,108,108	0
59	MG	1H	3375	1/1	0.98	0.04	69,69,69,69	0
59	MG	1G	1703	1/1	0.98	0.04	93,93,93,93	0
58	K	14	3045	1/1	0.98	0.07	71,71,71,71	0
59	MG	1H	3380	1/1	0.98	0.05	61,61,61,61	0
59	MG	14	3382	1/1	0.98	0.07	77,77,77,77	0
59	MG	1H	3385	1/1	0.98	0.07	69,69,69,69	0
59	MG	14	3384	1/1	0.98	0.05	108,108,108,108	0
59	MG	1G	1709	1/1	0.98	0.05	102,102,102,102	0
59	MG	1H	3519	1/1	0.98	0.08	56,56,56,56	0
59	MG	1H	3520	1/1	0.98	0.05	70,70,70,70	0
59	MG	1G	1712	1/1	0.98	0.04	106,106,106,106	0
59	MG	14	3390	1/1	0.98	0.05	78,78,78,78	0
59	MG	1G	1713	1/1	0.98	0.05	80,80,80,80	0
59	MG	1G	1714	1/1	0.98	0.07	82,82,82,82	0
59	MG	1G	1715	1/1	0.98	0.06	92,92,92,92	0
59	MG	1H	3386	1/1	0.98	0.09	67,67,67,67	0
59	MG	1G	1717	1/1	0.98	0.05	88,88,88,88	0
59	MG	14	3396	1/1	0.98	0.05	51,51,51,51	0
59	MG	1H	3162	1/1	0.98	0.07	21,21,21,21	0
59	MG	1G	1719	1/1	0.98	0.05	101,101,101,101	0
59	MG	1H	3523	1/1	0.98	0.04	34,34,34,34	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
59	MG	14	3400	1/1	0.98	0.04	92,92,92,92	0
59	MG	1G	1721	1/1	0.98	0.04	88,88,88,88	0
59	MG	13	1735	1/1	0.98	0.04	57,57,57,57	0
59	MG	14	3405	1/1	0.98	0.09	45,45,45,45	0
59	MG	1G	1723	1/1	0.98	0.03	85,85,85,85	0
59	MG	1H	3277	1/1	0.98	0.11	18,18,18,18	0
59	MG	1H	3392	1/1	0.98	0.06	32,32,32,32	0
59	MG	1J	204	1/1	0.98	0.06	115,115,115,115	0
59	MG	1G	1726	1/1	0.98	0.04	98,98,98,98	0
58	K	1H	3056	1/1	0.98	0.04	43,43,43,43	0
59	MG	14	3216	1/1	0.98	0.07	42,42,42,42	0
59	MG	32	302	1/1	0.98	0.05	92,92,92,92	0
59	MG	13	1737	1/1	0.98	0.04	90,90,90,90	0
59	MG	1H	3270	1/1	0.99	0.09	37,37,37,37	0
59	MG	14	3271	1/1	0.99	0.04	52,52,52,52	0
59	MG	1H	3442	1/1	0.99	0.05	80,80,80,80	0
59	MG	16	209	1/1	0.99	0.07	75,75,75,75	0
59	MG	1G	1705	1/1	0.99	0.02	105,105,105,105	0
59	MG	14	3275	1/1	0.99	0.04	58,58,58,58	0
58	K	1H	3059	1/1	0.99	0.05	38,38,38,38	0
59	MG	1H	3445	1/1	0.99	0.08	42,42,42,42	0
59	MG	1G	1708	1/1	0.99	0.03	69,69,69,69	0
59	MG	14	3279	1/1	0.99	0.03	46,46,46,46	0
59	MG	1H	3299	1/1	0.99	0.10	34,34,34,34	0
59	MG	1H	3171	1/1	0.99	0.10	28,28,28,28	0
59	MG	14	3282	1/1	0.99	0.04	50,50,50,50	0
59	MG	1H	3448	1/1	0.99	0.04	61,61,61,61	0
59	MG	14	3285	1/1	0.99	0.04	43,43,43,43	0
59	MG	13	1730	1/1	0.99	0.05	79,79,79,79	0
59	MG	1H	3152	1/1	0.99	0.07	37,37,37,37	0
59	MG	1H	3451	1/1	0.99	0.10	63,63,63,63	0
59	MG	1H	3453	1/1	0.99	0.05	67,67,67,67	0
59	MG	14	3290	1/1	0.99	0.04	48,48,48,48	0
59	MG	I8	101	1/1	0.99	0.11	48,48,48,48	0
59	MG	14	3292	1/1	0.99	0.04	49,49,49,49	0
59	MG	1H	3376	1/1	0.99	0.04	29,29,29,29	0
59	MG	13	1731	1/1	0.99	0.06	92,92,92,92	0
59	MG	14	3295	1/1	0.99	0.08	51,51,51,51	0
59	MG	1H	3456	1/1	0.99	0.03	38,38,38,38	0
59	MG	14	3298	1/1	0.99	0.06	54,54,54,54	0
59	MG	1H	3379	1/1	0.99	0.03	67,67,67,67	0
59	MG	14	3300	1/1	0.99	0.05	41,41,41,41	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
59	MG	1H	3458	1/1	0.99	0.05	89,89,89,89	0
59	MG	1H	3331	1/1	0.99	0.24	55,55,55,55	0
59	MG	1H	3381	1/1	0.99	0.03	59,59,59,59	0
59	MG	1H	3382	1/1	0.99	0.06	36,36,36,36	0
59	MG	1H	3384	1/1	0.99	0.06	60,60,60,60	0
59	MG	14	3307	1/1	0.99	0.04	51,51,51,51	0
59	MG	1H	3463	1/1	0.99	0.03	40,40,40,40	0
59	MG	1H	3464	1/1	0.99	0.04	19,19,19,19	0
59	MG	13	1715	1/1	0.99	0.06	75,75,75,75	0
59	MG	14	3311	1/1	0.99	0.07	56,56,56,56	0
59	MG	13	1716	1/1	0.99	0.04	66,66,66,66	0
59	MG	13	1734	1/1	0.99	0.07	61,61,61,61	0
59	MG	13	1717	1/1	0.99	0.08	66,66,66,66	0
59	MG	1H	3469	1/1	0.99	0.06	87,87,87,87	0
59	MG	14	3316	1/1	0.99	0.09	53,53,53,53	0
58	K	1H	3051	1/1	0.99	0.03	58,58,58,58	0
59	MG	1H	3471	1/1	0.99	0.05	30,30,30,30	0
59	MG	14	3319	1/1	0.99	0.04	59,59,59,59	0
59	MG	1H	3391	1/1	0.99	0.07	31,31,31,31	0
59	MG	14	3321	1/1	0.99	0.05	51,51,51,51	0
58	K	13	1617	1/1	0.99	0.09	72,72,72,72	0
59	MG	1H	3255	1/1	0.99	0.05	36,36,36,36	0
59	MG	1H	3205	1/1	0.99	0.06	34,34,34,34	0
59	MG	14	3204	1/1	0.99	0.06	44,44,44,44	0
59	MG	14	3326	1/1	0.99	0.03	45,45,45,45	0
59	MG	13	1720	1/1	0.99	0.05	73,73,73,73	0
59	MG	1H	3182	1/1	0.99	0.02	47,47,47,47	0
59	MG	14	3329	1/1	0.99	0.13	70,70,70,70	0
59	MG	1H	3342	1/1	0.99	0.04	50,50,50,50	0
59	MG	1H	3398	1/1	0.99	0.08	74,74,74,74	0
59	MG	13	1721	1/1	0.99	0.07	68,68,68,68	0
59	MG	14	3334	1/1	0.99	0.05	48,48,48,48	0
59	MG	1H	3400	1/1	0.99	0.08	46,46,46,46	0
59	MG	14	3336	1/1	0.99	0.08	47,47,47,47	0
59	MG	14	3337	1/1	0.99	0.10	66,66,66,66	0
59	MG	14	3109	1/1	0.99	0.05	36,36,36,36	0
59	MG	1H	3402	1/1	0.99	0.04	63,63,63,63	0
59	MG	14	3111	1/1	0.99	0.02	44,44,44,44	0
59	MG	1H	3403	1/1	0.99	0.07	59,59,59,59	0
59	MG	14	3342	1/1	0.99	0.07	54,54,54,54	0
59	MG	14	3343	1/1	0.99	0.03	76,76,76,76	0
59	MG	13	1722	1/1	0.99	0.12	77,77,77,77	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
59	MG	14	3345	1/1	0.99	0.09	89,89,89,89	0
59	MG	14	3346	1/1	0.99	0.04	76,76,76,76	0
59	MG	1H	3345	1/1	0.99	0.04	24,24,24,24	0
59	MG	1H	3407	1/1	0.99	0.06	65,65,65,65	0
59	MG	14	3349	1/1	0.99	0.03	77,77,77,77	0
59	MG	1H	3489	1/1	0.99	0.08	76,76,76,76	0
59	MG	1H	3346	1/1	0.99	0.05	27,27,27,27	0
59	MG	14	3352	1/1	0.99	0.06	64,64,64,64	0
59	MG	14	3353	1/1	0.99	0.06	65,65,65,65	0
59	MG	1H	3491	1/1	0.99	0.10	51,51,51,51	0
59	MG	14	3355	1/1	0.99	0.08	64,64,64,64	0
59	MG	1H	3409	1/1	0.99	0.10	64,64,64,64	0
58	K	14	3016	1/1	0.99	0.04	72,72,72,72	0
59	MG	14	3358	1/1	0.99	0.04	35,35,35,35	0
59	MG	1H	3412	1/1	0.99	0.12	85,85,85,85	0
59	MG	14	3360	1/1	0.99	0.03	64,64,64,64	0
59	MG	1H	3413	1/1	0.99	0.08	42,42,42,42	0
59	MG	14	3123	1/1	0.99	0.02	47,47,47,47	0
59	MG	14	3363	1/1	0.99	0.03	85,85,85,85	0
59	MG	1H	3496	1/1	0.99	0.03	64,64,64,64	0
59	MG	14	3365	1/1	0.99	0.06	80,80,80,80	0
59	MG	1H	3497	1/1	0.99	0.04	83,83,83,83	0
59	MG	14	3367	1/1	0.99	0.05	52,52,52,52	0
59	MG	13	1724	1/1	0.99	0.05	80,80,80,80	0
59	MG	14	3369	1/1	0.99	0.12	43,43,43,43	0
59	MG	14	3370	1/1	0.99	0.04	56,56,56,56	0
59	MG	14	3127	1/1	0.99	0.05	41,41,41,41	0
59	MG	1H	3187	1/1	0.99	0.06	37,37,37,37	0
58	K	1H	3080	1/1	0.99	0.02	51,51,51,51	0
59	MG	1H	3417	1/1	0.99	0.05	44,44,44,44	0
59	MG	1H	3502	1/1	0.99	0.03	94,94,94,94	0
59	MG	1H	3418	1/1	0.99	0.04	58,58,58,58	0
59	MG	14	3133	1/1	0.99	0.10	50,50,50,50	0
59	MG	1H	3189	1/1	0.99	0.09	46,46,46,46	0
59	MG	1H	3505	1/1	0.99	0.03	34,34,34,34	0
59	MG	14	3238	1/1	0.99	0.04	42,42,42,42	0
59	MG	1H	3146	1/1	0.99	0.12	24,24,24,24	0
59	MG	1H	3507	1/1	0.99	0.06	45,45,45,45	0
59	MG	1H	3354	1/1	0.99	0.02	70,70,70,70	0
59	MG	1H	3422	1/1	0.99	0.05	43,43,43,43	0
59	MG	1H	3510	1/1	0.99	0.08	80,80,80,80	0
59	MG	1H	3423	1/1	0.99	0.04	33,33,33,33	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
59	MG	1H	3355	1/1	0.99	0.03	32,32,32,32	0
59	MG	1H	3425	1/1	0.99	0.06	42,42,42,42	0
59	MG	1G	1680	1/1	0.99	0.03	90,90,90,90	0
59	MG	1H	3358	1/1	0.99	0.04	43,43,43,43	0
59	MG	1G	1682	1/1	0.99	0.04	60,60,60,60	0
59	MG	13	1726	1/1	0.99	0.02	122,122,122,122	0
59	MG	1H	3428	1/1	0.99	0.02	55,55,55,55	0
59	MG	1H	3429	1/1	0.99	0.05	63,63,63,63	0
59	MG	1H	3430	1/1	0.99	0.04	79,79,79,79	0
59	MG	1G	1687	1/1	0.99	0.04	93,93,93,93	0
59	MG	1H	3360	1/1	0.99	0.04	39,39,39,39	0
59	MG	1H	3361	1/1	0.99	0.07	32,32,32,32	0
59	MG	1H	3433	1/1	0.99	0.13	44,44,44,44	0
59	MG	1H	3362	1/1	0.99	0.03	33,33,33,33	0
59	MG	1G	1692	1/1	0.99	0.06	97,97,97,97	0
59	MG	14	3403	1/1	0.99	0.03	75,75,75,75	0
59	MG	14	3404	1/1	0.99	0.04	34,34,34,34	0
59	MG	1H	3435	1/1	0.99	0.09	72,72,72,72	0
59	MG	1G	1694	1/1	0.99	0.04	62,62,62,62	0
59	MG	1H	3436	1/1	0.99	0.04	33,33,33,33	0
59	MG	1H	3525	1/1	0.99	0.06	46,46,46,46	0
59	MG	1J	203	1/1	0.99	0.04	105,105,105,105	0
59	MG	14	3161	1/1	0.99	0.13	44,44,44,44	0
59	MG	13	1727	1/1	0.99	0.03	47,47,47,47	0
59	MG	1H	3364	1/1	0.99	0.04	28,28,28,28	0
59	MG	1H	3367	1/1	0.99	0.07	61,61,61,61	0
58	K	1H	3068	1/1	0.99	0.08	37,37,37,37	0
59	MG	1G	1701	1/1	0.99	0.04	108,108,108,108	0
60	SF4	3E	302	8/8	0.99	0.05	78,87,103,104	0
60	SF4	32	303	8/8	0.99	0.07	73,95,102,116	0
61	ZN	5I	102	1/1	0.99	0.04	110,110,110,110	0
61	ZN	5A	101	1/1	0.99	0.04	115,115,115,115	0
59	MG	1H	3378	1/1	1.00	0.02	30,30,30,30	0
59	MG	1H	3443	1/1	1.00	0.08	61,61,61,61	0
59	MG	14	3301	1/1	1.00	0.06	53,53,53,53	0
59	MG	1H	3387	1/1	1.00	0.03	37,37,37,37	0
59	MG	14	3284	1/1	1.00	0.02	39,39,39,39	0
59	MG	1H	3366	1/1	1.00	0.01	44,44,44,44	0
59	MG	1H	3356	1/1	1.00	0.04	31,31,31,31	0
59	MG	1H	3368	1/1	1.00	0.01	20,20,20,20	0
59	MG	1H	3411	1/1	1.00	0.02	28,28,28,28	0
59	MG	1H	3357	1/1	1.00	0.02	34,34,34,34	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
59	MG	14	3388	1/1	1.00	0.07	53,53,53,53	0
59	MG	1H	3401	1/1	1.00	0.02	73,73,73,73	0
59	MG	1H	3383	1/1	1.00	0.04	54,54,54,54	0
59	MG	14	3330	1/1	1.00	0.01	48,48,48,48	0
59	MG	1H	3452	1/1	1.00	0.03	48,48,48,48	0
59	MG	1H	3353	1/1	1.00	0.07	53,53,53,53	0
59	MG	1H	3482	1/1	1.00	0.03	22,22,22,22	0
59	MG	1H	3365	1/1	1.00	0.03	40,40,40,40	0
59	MG	14	3296	1/1	1.00	0.03	44,44,44,44	0
59	MG	1H	3405	1/1	1.00	0.07	50,50,50,50	0
59	MG	1H	3485	1/1	1.00	0.03	27,27,27,27	0

6.5 Other polymers [i](#)

There are no such residues in this entry.