



wwPDB X-ray Structure Validation Summary Report ⓘ

Jun 24, 2024 – 09:41 PM EDT

PDB ID : 6QNQ
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	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.37.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

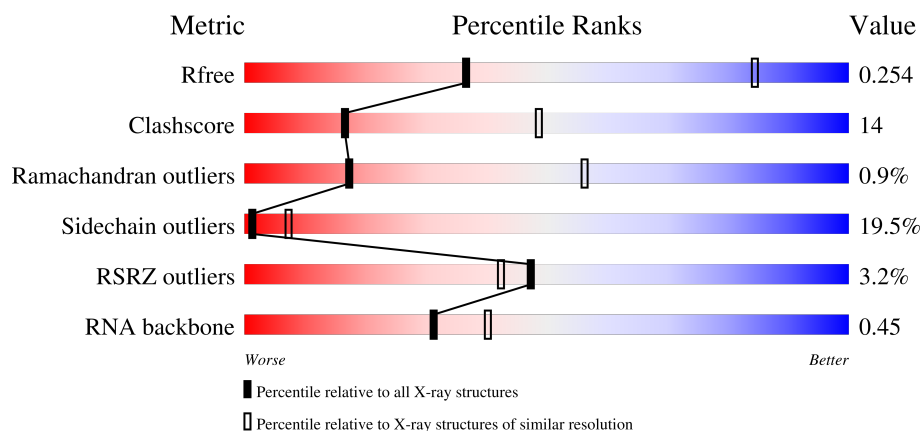
1 Overall quality at a glance

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}	130704	1659 (3.60-3.40)
Clashscore	141614	1036 (3.58-3.42)
Ramachandran outliers	138981	1005 (3.58-3.42)
Sidechain outliers	138945	1006 (3.58-3.42)
RSRZ outliers	127900	1559 (3.60-3.40)
RNA backbone	3102	1002 (4.00-3.00)

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	 40% 46% 12% ..
1	1G	1522	 40% 43% 16% ..
2	12	256	 7% 42% 40% 9% 8%
2	1E	256	 13% 45% 39% 9% 7%







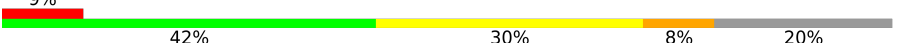

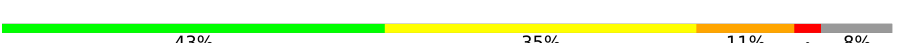


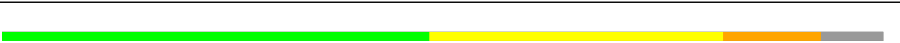
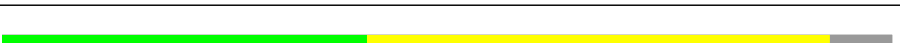
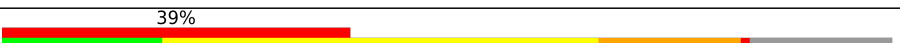
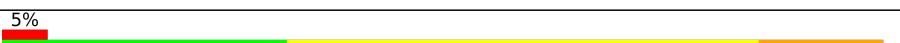

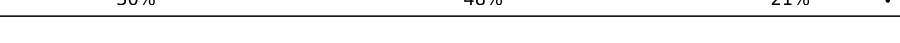
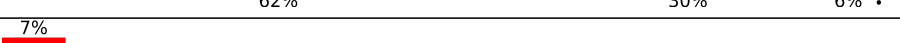
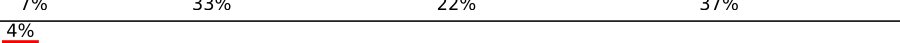
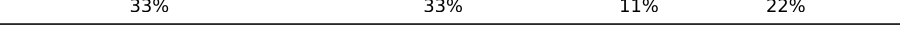



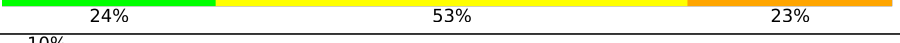

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Mol	Chain	Length	Quality of chain
3	22	239	
3	2E	239	
4	32	209	
4	3E	209	
5	42	162	
5	4E	162	
6	52	101	
6	5E	101	
7	62	156	
7	6E	156	
8	72	138	
8	7E	138	
9	82	128	
9	8E	128	
10	1A	105	
10	1I	105	
11	2A	129	
11	2I	129	
12	3A	132	
12	3I	132	
13	4A	126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





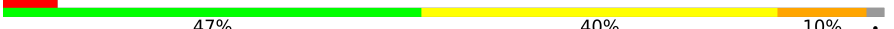

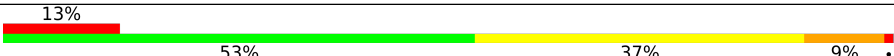


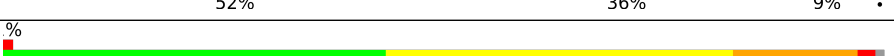
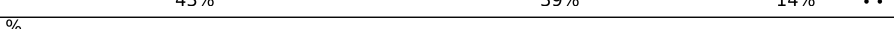

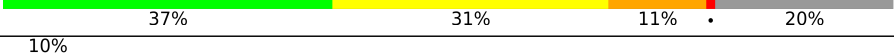



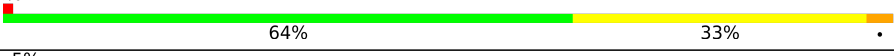
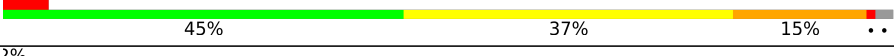





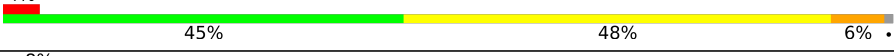

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Mol	Chain	Length	Quality of chain
15	6I	89	% 
16	7A	88	
16	7I	88	
17	8A	105	
17	8I	105	
18	9A	88	
18	9I	88	
19	AA	93	
19	AI	93	
20	BA	106	
20	BI	106	
21	1B	27	
21	1F	27	
22	1K	77	
22	3K	77	
22	3L	77	
23	2K	77	
24	4K	27	
24	4L	27	
25	14	2917	
25	1H	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	
29	21	206	
29	29	206	
30	31	210	
30	39	210	
31	41	182	
31	49	182	
32	51	180	
32	59	180	
33	61	148	
33	69	148	
34	38	173	
35	15	140	
35	58	140	
36	25	122	
36	68	122	
37	35	150	
37	78	150	
38	45	141	
38	88	141	
39	55	118	
39	98	118	
40	65	112	
40	A8	112	
41	75	146	

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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
58	K	13	1635	-	-	-	X
59	MG	1G	1648	-	-	-	X
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 (three-letter code: 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 (three-letter code: MG) (formula: Mg).

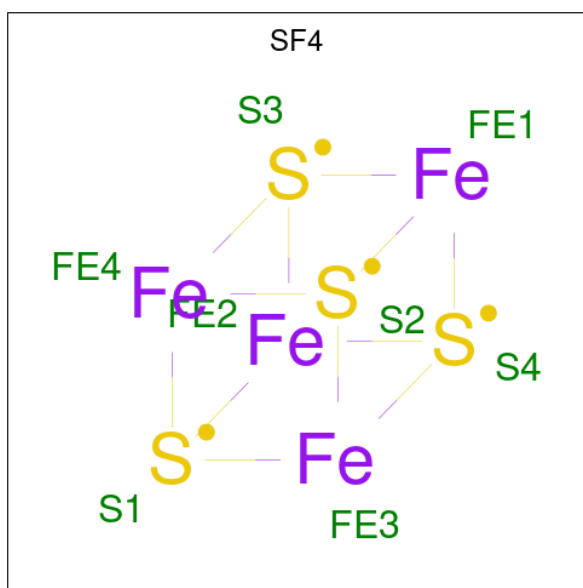
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
59	13	111	Total 111	Mg 111	0	0
59	3E	1	Total 1	Mg 1	0	0
59	8E	1	Total 1	Mg 1	0	0
59	4I	1	Total 1	Mg 1	0	0
59	7I	1	Total 1	Mg 1	0	0

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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 (three-letter code: 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 (three-letter code: 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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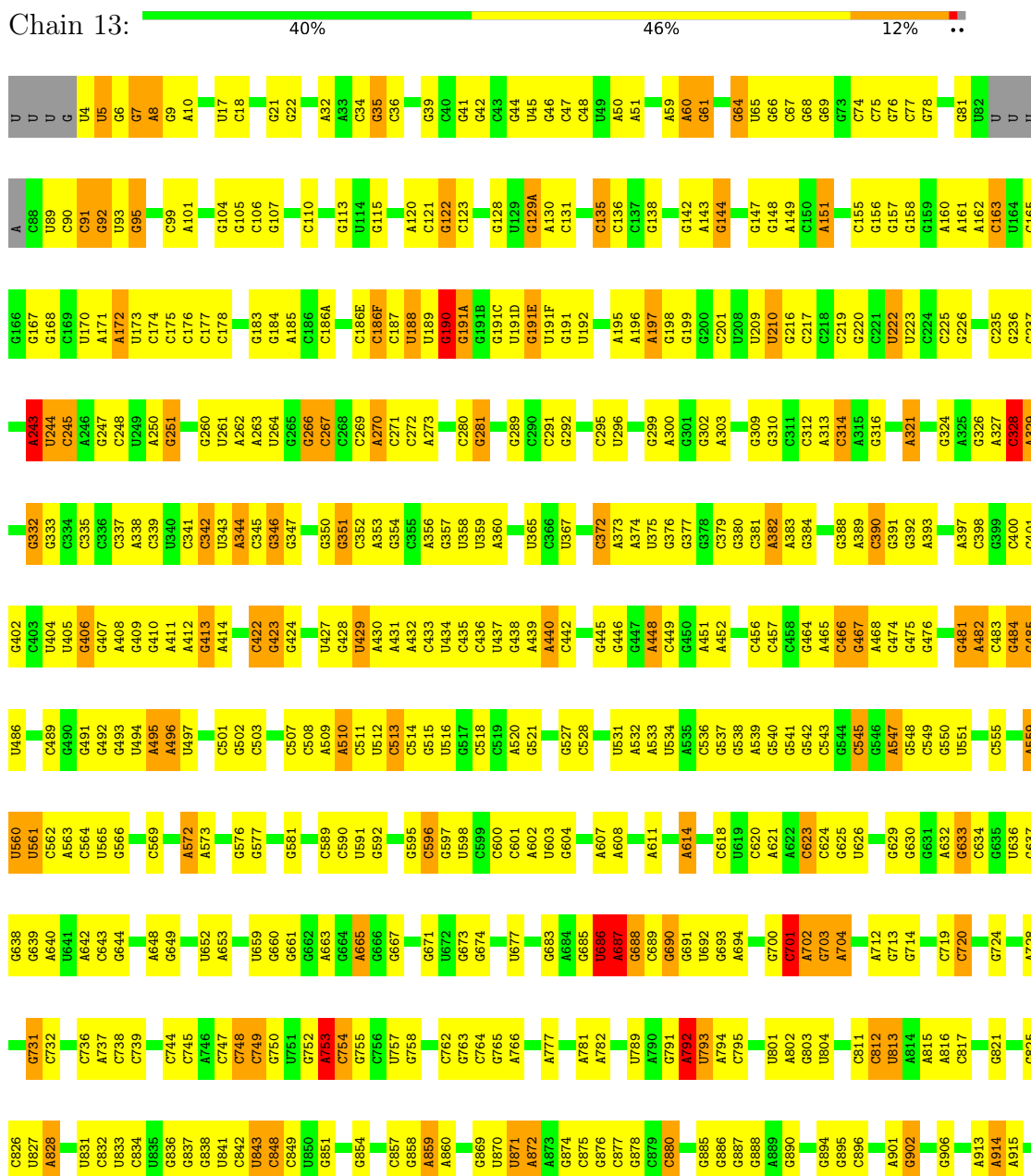
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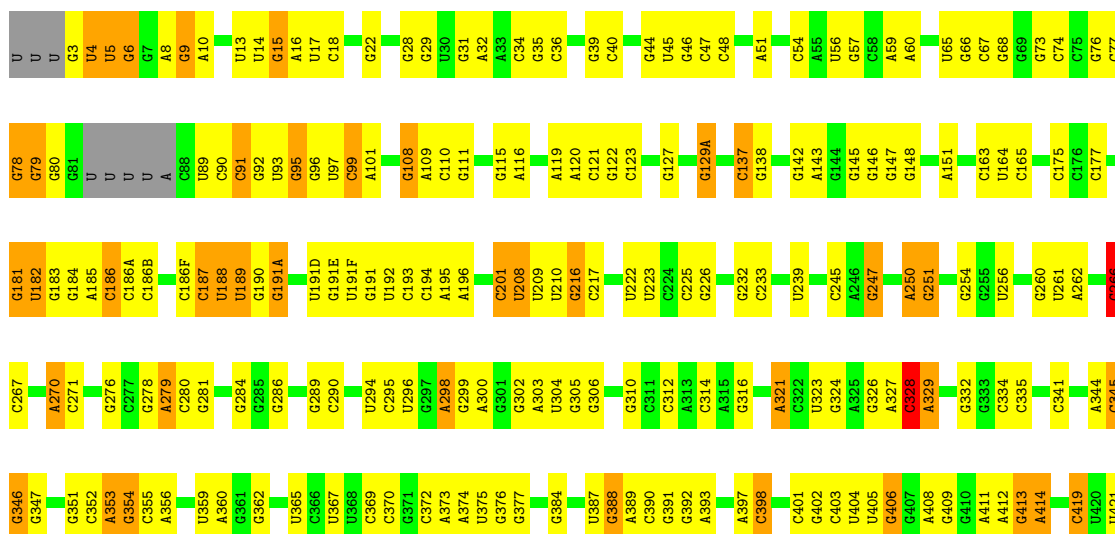
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
62	M5	1	Total	O	0	0
			1	1		

3 Residue-property plots

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.

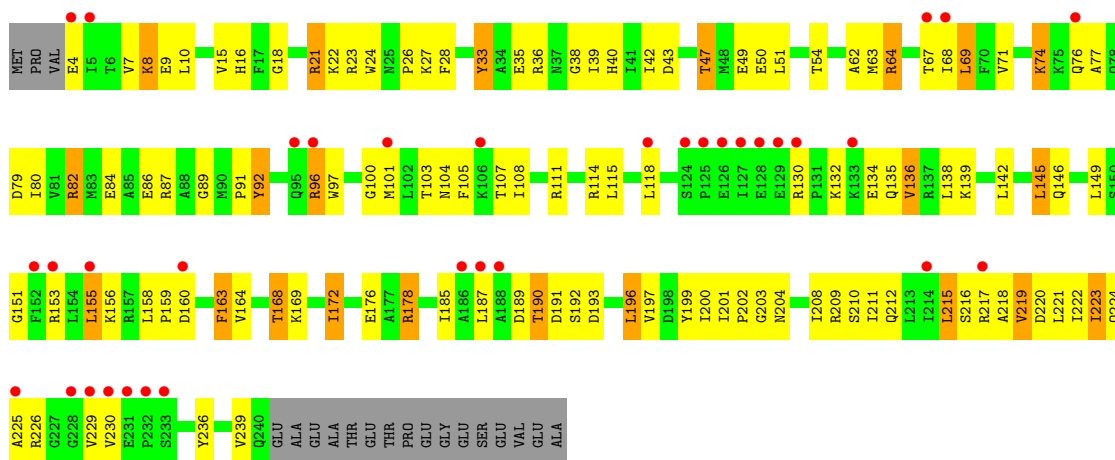
• Molecule 1: 16S ribosomal RNA



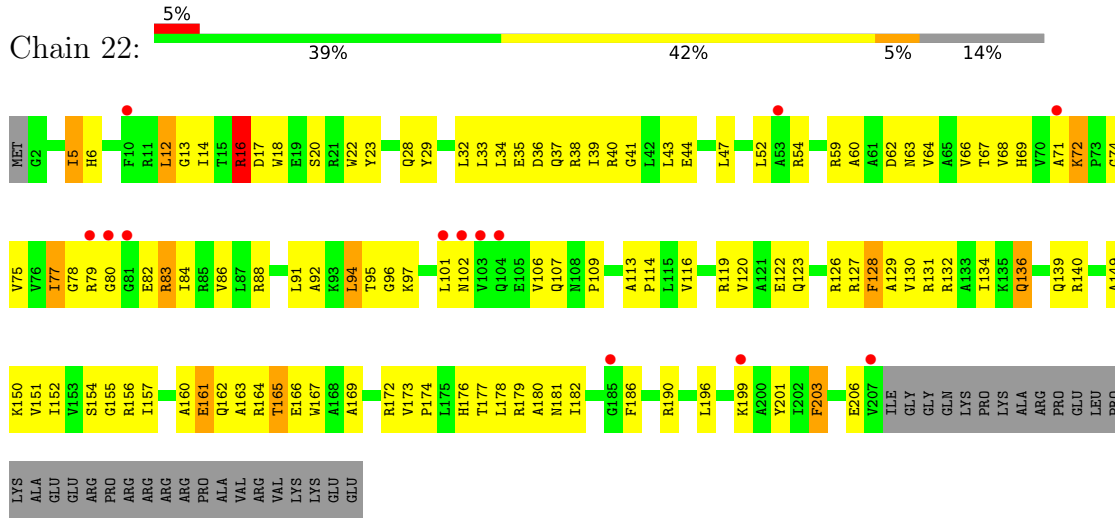


A1483	G1387	C1320	C1254	G1190	G1127	C1063	G1003	C934	U841	C762	A684	G587	A509	C422
G1490	C1388	C1321	G1255	U1194	C1128	G1064	A1004	A935	C842	G763	G685	G587	A510	G423
G1491	C1389	C1322	A1256	U1195	C1129	U1065	A1005	A936	U843	C764	U686	G595	C511	G424
A1492	G1392	A1324	U1257	U1196	A1130	C1066	C1006	A937	C848	G765	A687	G596	U516	G425
U1493	U1393	C1325	C1258	U1197	G1131	A1067	C1007	G942	C849	U598	G688	U597	G517	G426
A1499	G1395	C1326	C1260	G1198	G1133	U1069	C1008	U943	U850	A767	C689	C599	C518	U429
A1502	A1396	C1327	C1263	U1199	G1134	U1070	C1009	A946	G851	A768	G690	G600	C519	A430
A1503	C1397	A1329	G1266	C1200	U1135	C1071	G1010	A947	G852	C770	G691	C601	A520	C435
G1504	A1398	G1330	G1267	A1201	U1136	G1072	G1011	C948	G854	G773	A702	A607	C522	C436
G1505	C1399	G1331	C1268	C1203	C1137	U1073	A1014	G951	G858	A777	G703	A608	G527	A439
U1506	G1400	A1332	A1269	A1204	G1138	G1074	A1015	U952	A859	G778	A704	A609	A440	A442
A1507	G1401	A1333	A1270	U1205	C1140	C1076	G1017	U953	A860	U779	G707	G610	A532	G445
G1508	C1402	G1334	C1271	G1206	C1141	U1077	C1018	G954	G861	A780	C708	C613	A533	G446
A1509	C1404	C1336	G1272	G1207	G1142	G1078	C1019	U955	U870	G785	G709	A614	U534	G447
U1510	G1405	G1273	G1274	C1208	G1143	U1080	U1020	U956	U871	G786	G710	C615	A535	G448
G1511	U1406	A1275	A1276	U1211	G1144	G1081	G1023	U957	U872	C794	G714	C616	C536	A448
U1512	C1407	A1277	A1278	U1212	C1145	U1082	G1024	U960	A873	G795	A715	C617	C537	A452
A1513	G1342	G1278	G1279	U1213	C1146	U1083	U1025	U961	A874	G796	A716	C618	G538	A453
C1514	C1343	C1279	G1280	U1214	U1147	G1084	G1026	C962	U875	A797	A717	C619	A539	G457
C1515	C1344	U1277	A1279	G1215	U1148	U1085	G1027	C963	C874	G798	C718	C620	G540	G458
G1516	U1345	C1278	A1280	C1216	C1149	U1086	C1028	G964	C875	G799	G719	C621	G541	C457
U1517	A1346	A1279	A1281	U1217	U1150	G1087	G1028A	A965	G876	U793	G720	C624	C543	G459
A1518	G1347	G1280	U1281	C1218	A1151	U1088	C1028B	U966	C877	A794	G721	C625	C544	G464
A1519	U1348	C1282	C1283	U1219	G1154	U1090	G1029	G967	C878	U801	A722	C627	C545	A465
G1520	C1349	G1283	G1284	U1220	G1155	U1091	C1030	C968	C879	U802	G723	C628	A546	G466
G1521	U1349	C1277	A1284	G1221	C1156	A1092	G1031	A969	C880	A802	G724	C629	C547	G467
U1529	A1349	A1285	A1286	C1222	A1157	U1093	A1032	C970	C881	G803	G724	C630	G548	G474
G1530	G1354	C1287	A1287	G1223	C1158	G1094	G1032A	G971	C882	C806	A728	C631	U552	G475
A1531	C1355	A1288	A1289	U1224	U1159	U1095	G1032B	C972	C883	A807	A729	C632	A553	G476
C1532	G1356	G1289	G1290	C1225	G1160	C1096	G1033	G973	C884	C810	A730	C633	C554	G477
A1534	A1357	U1289	G1291	C1226	C1161	U1097	A1034	A975	U885	C811	G735	C634	C555	A482
C1535	C1358	G1292	U1292	C1228	G1163	G1098	A1035	A976	C904	C812	C736	C635	A559	C483
G1536	A1360	G1293	G1294	U1230	C1164	C1100	C1036	A977	C905	U813	A737	C636	U560	G484
U1537	G1361	G1295	G1296	U1231	C1165	A1101	C1037	A978	C906	U814	C738	C637	U561	U486
U1540	C1362	C1296	C1297	U1232	G1166	G1104	C1038	A979	C907	A815	U740	C638	C562	C489
U	A1362A	C1297	C1298	U1233	A1167	A1105	G1042	C980	C908	A816	G741	C639	U563	G490
U	A1363	C1297	C1298	U1234	A1169	G1106	G1043	C981	C909	A817	G742	C640	C564	G491
C	A1364	U1297	A1299	G1237	G1171	G1109	A1044	U982	C910	U818	G743	C641	U494	U494
U	G1365	A1299	G1300	C1237	G1174	A1110	C1045	A983	C912	U819	U744	C642	A495	A495
U	C1366	G1300	U1301	A1238	C1175	A1111	A1046	A986	C913	U820	C745	C643	A496	U497
U	C1367	U1302	U1303	A1239	A1176	A1112	G1047	A987	A913	C822	G746	C644	A497	A498
U	C1368	C1303	C1304	U1240	G1177	C1113	U1049	G988	A915	G823	A572	C645	A573	G500
U	C1369	G1304	G1305	G1242	G1178	C1114	G1050	C989	C824	C748	A574	C646	C501	C501
U	G1370	G1305	A1306	C1243	A1179	C1115	C1051	C990	U920	G749	G575	A665	C502	C503
U	G1373	A1306	G1309	C1244	A1180	C1116	U1052	U991	U921	G750	C576	A666	C504	C504
U	A1374	G1309	G1310	A1245	G1181	G1117	G1053	U992	G922	G751	G577	C668	C505	C505
U	U1375	C1314	C1315	U1246	A1183	C1118	C1054	A994	G926	A753	G673	C669	C506	C506
U	A1377	U1315	G1316	U1247	G1184	C1119	U1055	A995	G927	C754	G674	C670	C507	C507
U	C1378	G1316	G1317	U1248	G1185	C1120	U1056	C998A	G928	G755	A675	C671	G581	G581
U	G1379	A1250	C1317	A1251	G1186	A1123	G1057	U999	G929	C756	C672	C672	A582	A582
U	U1380	A1251	A1252	G1187	G1187	A1124	G1058	A1000	C932	C757	G673	C673	A583	A583
U	A1381	A1318	A1319	U1125	U1188	U1126	C1059	G1001	C932	G758	G683	C674	G584	G584
U	G1482	G1253	G1254	U1126	C1189	U1126	U1062	G1002	G933	G838	G683	C675	C586	C586

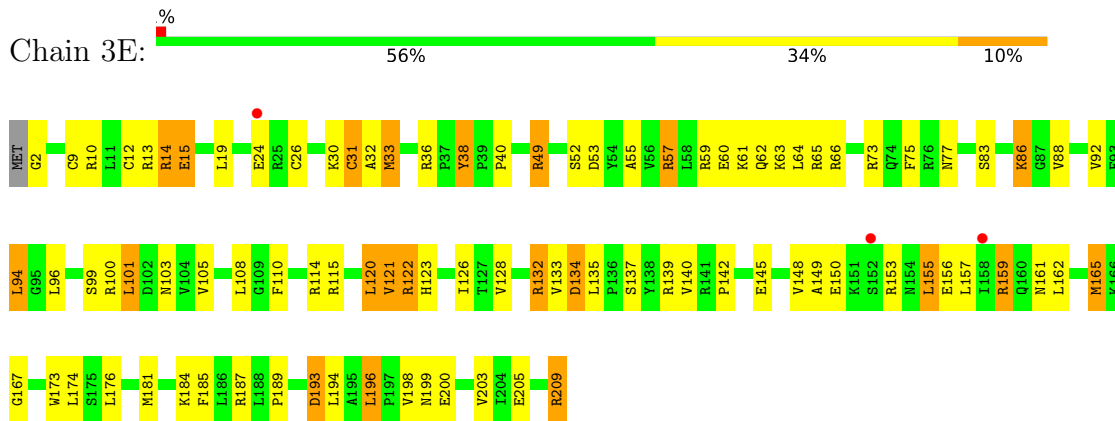
- Molecule 2: 30S ribosomal protein S2



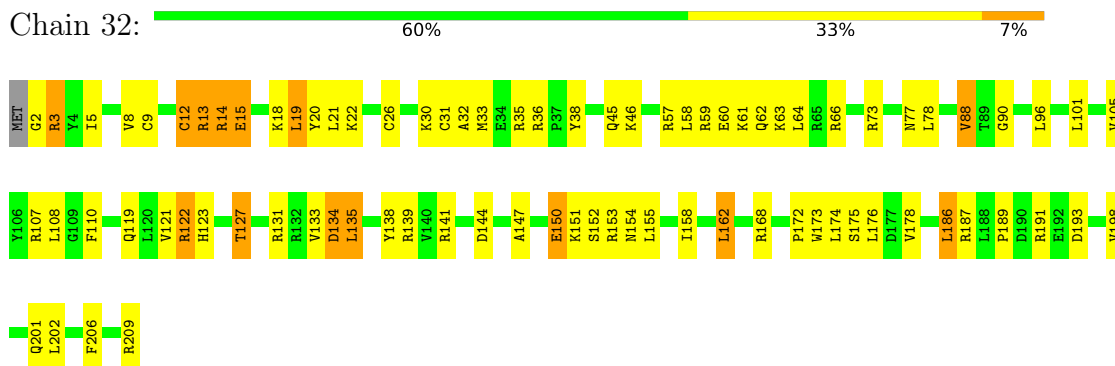
- Molecule 3: 30S ribosomal protein S3



- Molecule 4: 30S ribosomal protein S4

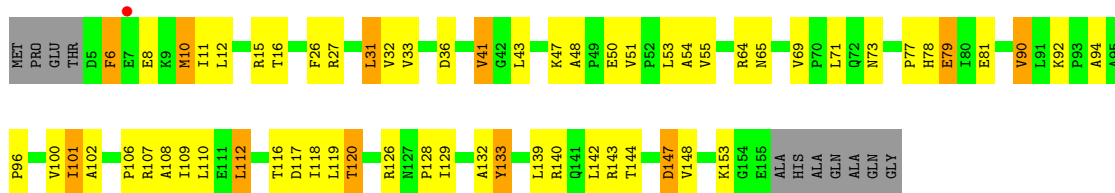


- Molecule 4: 30S ribosomal protein S4

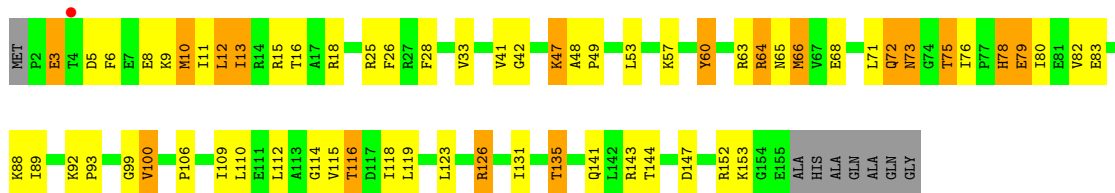


- Molecule 5: 30S ribosomal protein S5

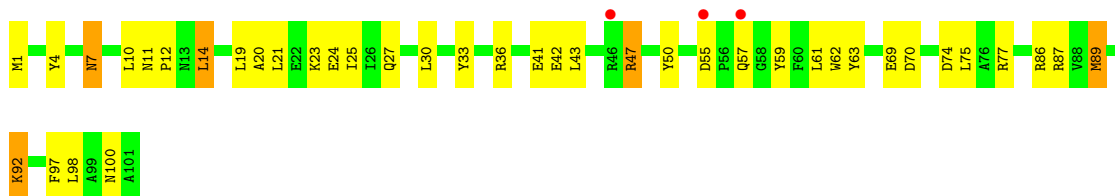




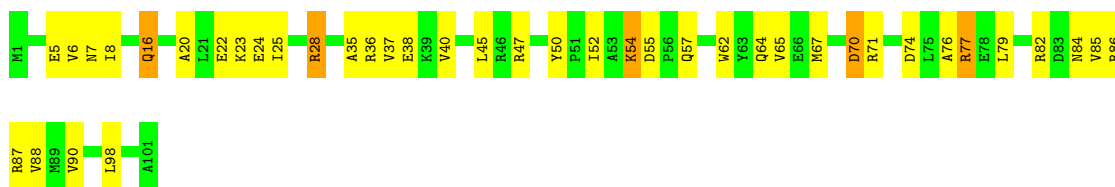
• Molecule 5: 30S ribosomal protein S5



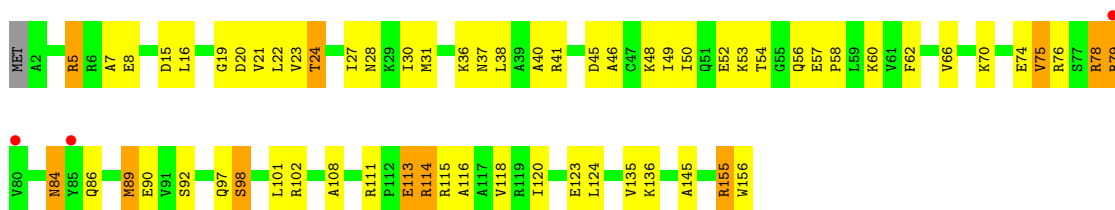
• Molecule 6: 30S ribosomal protein S6



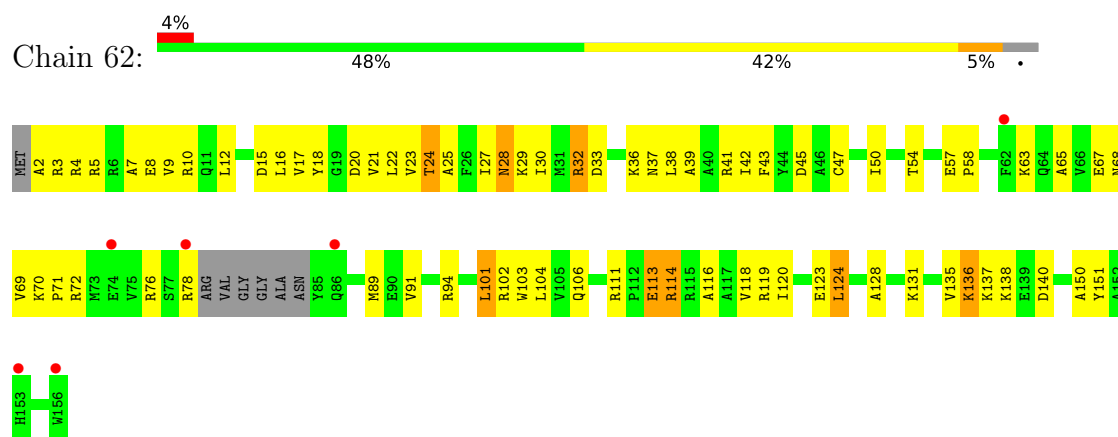
• Molecule 6: 30S ribosomal protein S6



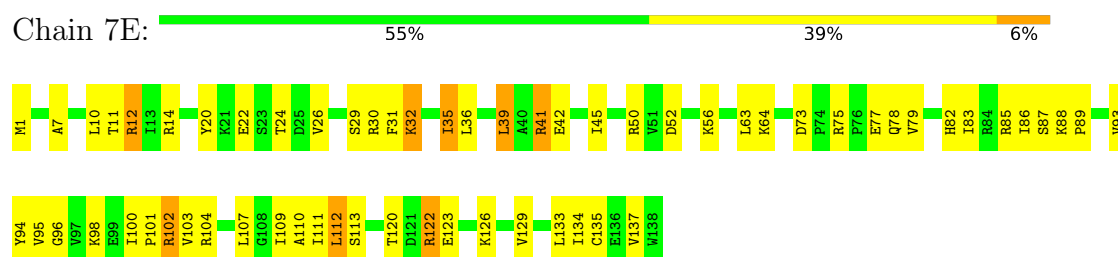
• Molecule 7: 30S ribosomal protein S7



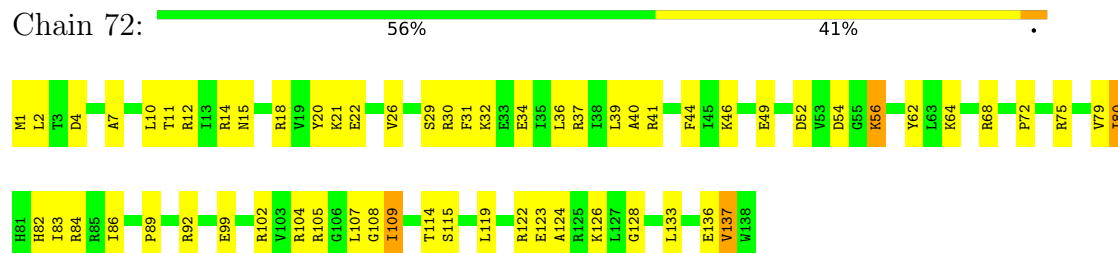
• Molecule 7: 30S ribosomal protein S7



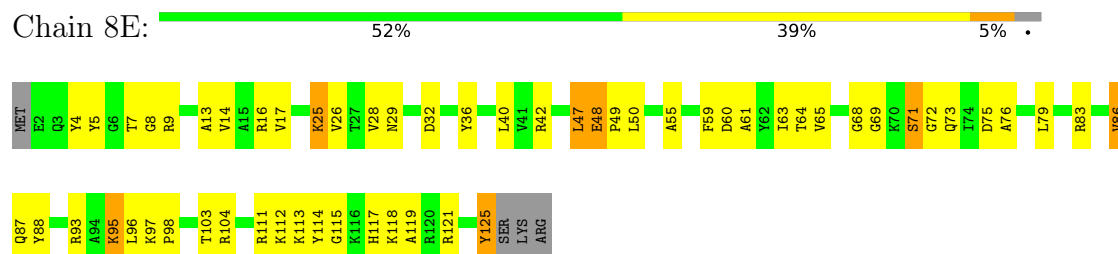
- Molecule 8: 30S ribosomal protein S8



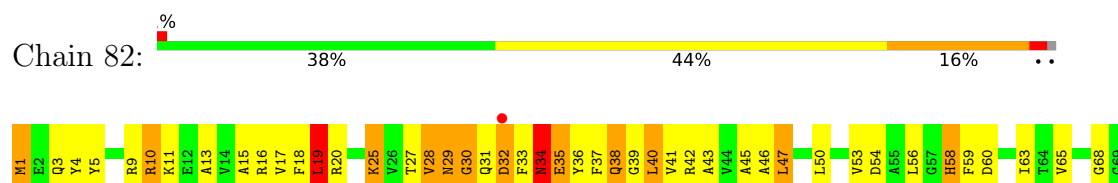
- Molecule 8: 30S ribosomal protein S8



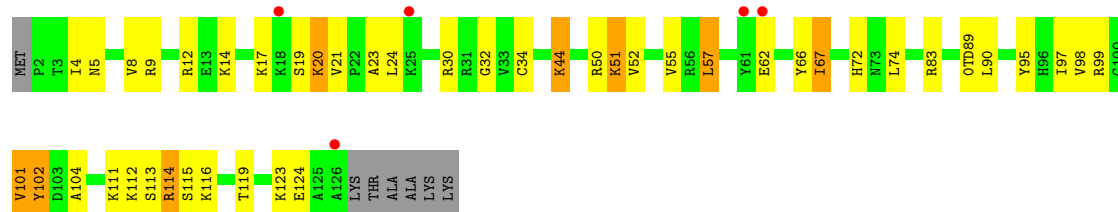
- Molecule 9: 30S ribosomal protein S9



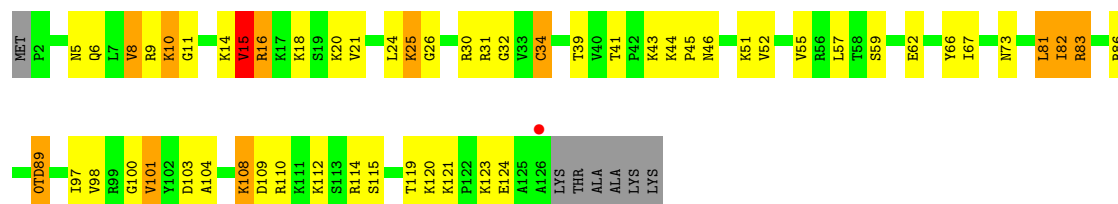
- Molecule 9: 30S ribosomal protein S9



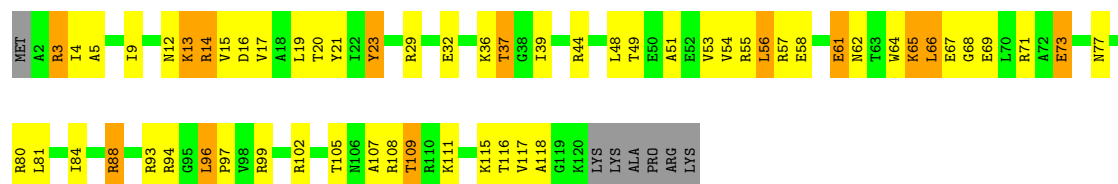




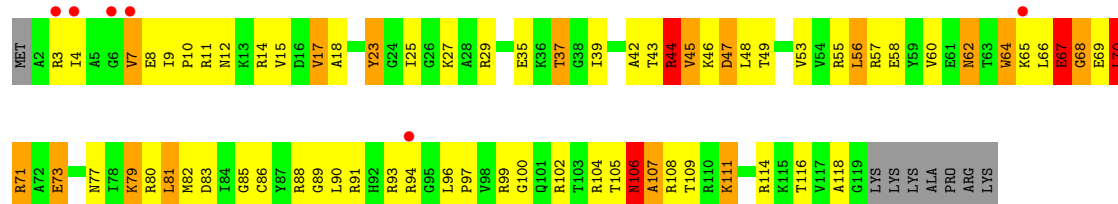
- Molecule 12: 30S ribosomal protein S12



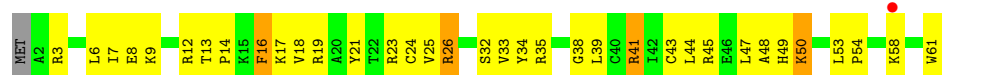
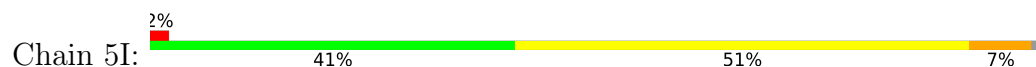
- Molecule 13: 30S ribosomal protein S13



- Molecule 13: 30S ribosomal protein S13

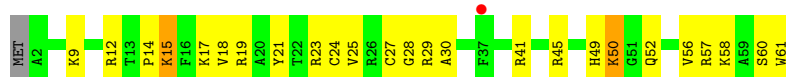


- Molecule 14: 30S ribosomal protein S14 type Z



- Molecule 14: 30S ribosomal protein S14 type Z

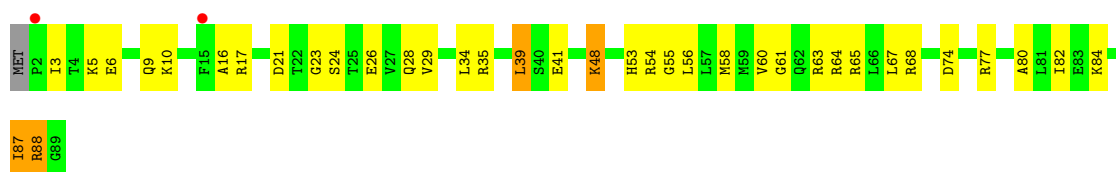




- Molecule 15: 30S ribosomal protein S15



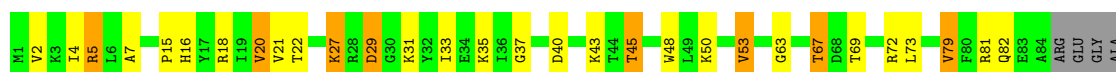
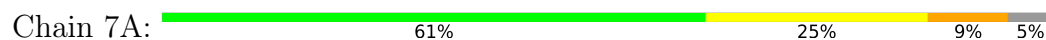
- Molecule 15: 30S ribosomal protein S15



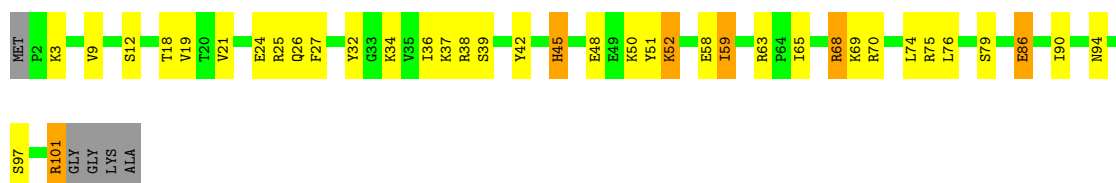
- Molecule 16: 30S ribosomal protein S16



- Molecule 16: 30S ribosomal protein S16

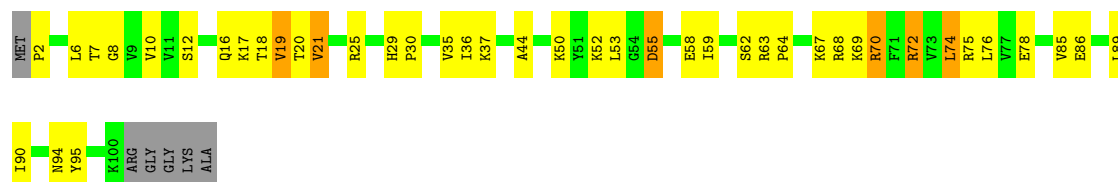


- Molecule 17: 30S ribosomal protein S17

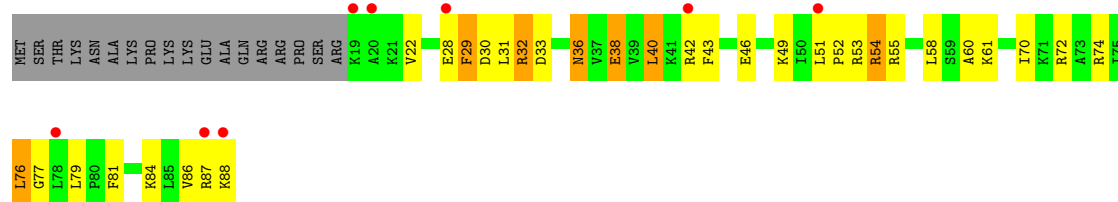
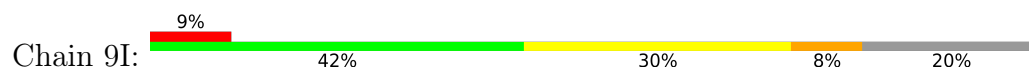


- Molecule 17: 30S ribosomal protein S17

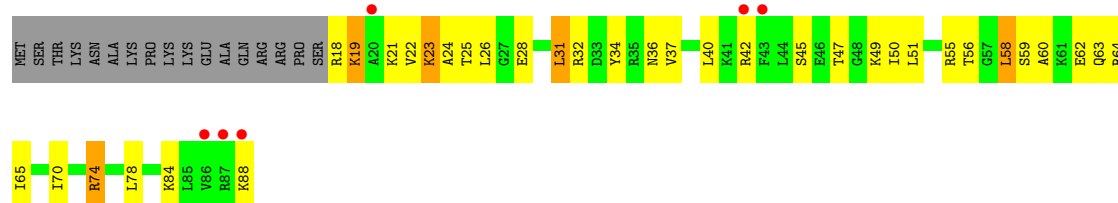
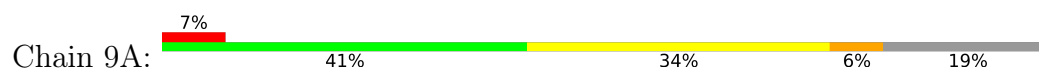




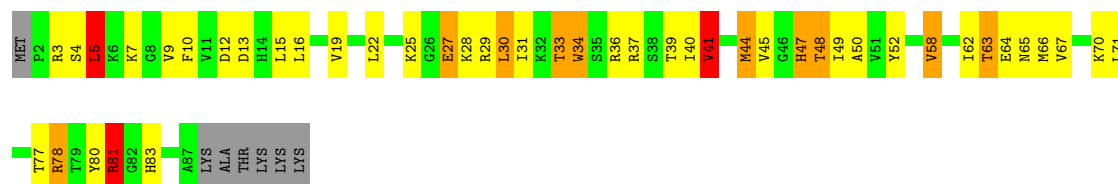
- Molecule 18: 30S ribosomal protein S18



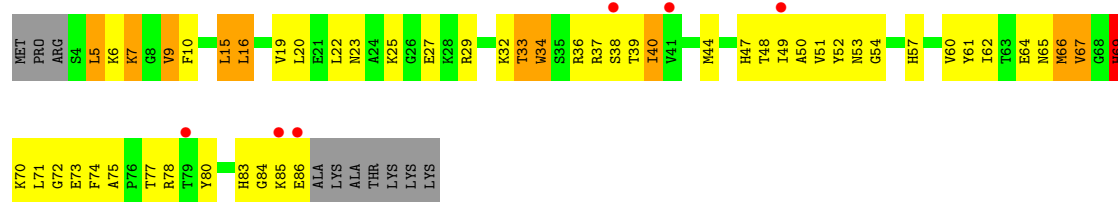
- Molecule 18: 30S ribosomal protein S18



- Molecule 19: 30S ribosomal protein S19

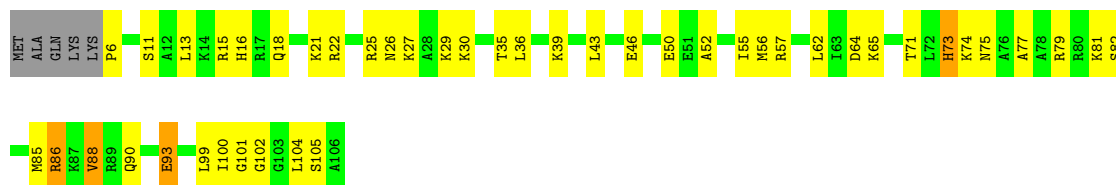


- Molecule 19: 30S ribosomal protein S19



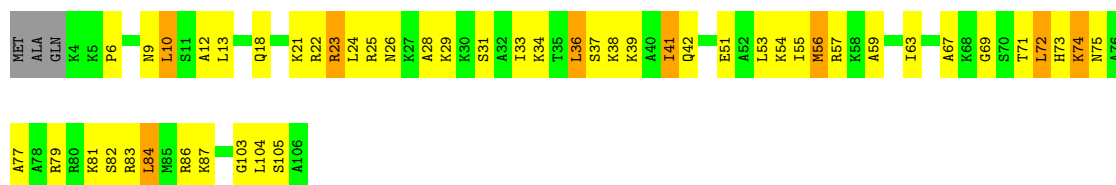
- Molecule 20: 30S ribosomal protein S20

Chain BI:  53% 39% 5%



- Molecule 20: 30S ribosomal protein S20

Chain BA:  51% 39% 8%



- Molecule 21: 30S ribosomal protein Thx

Chain 1F:  41% 52% 7%




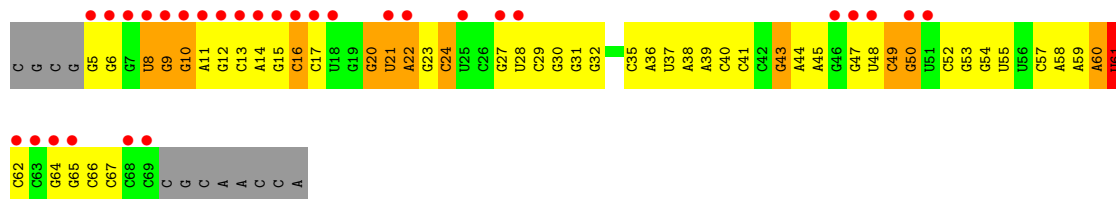
- Molecule 21: 30S ribosomal protein Thx

Chain 1B:  48% 33% 11% 7%



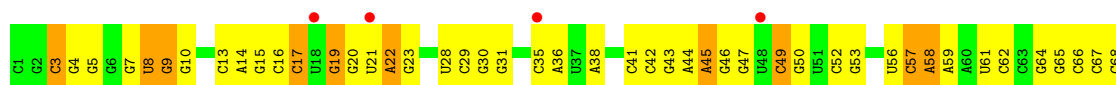
- Molecule 22: E. coli tRNA^{fMet}

Chain 1K:  39% 18% 49% 16% 16%



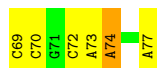
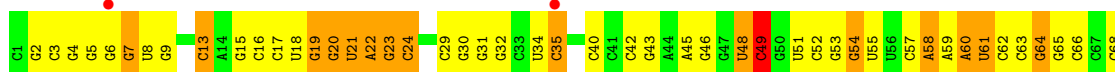
- Molecule 22: E. coli tRNA^{fMet}

Chain 3K:  5% 32% 53% 14%





- Molecule 22: E. coli tRNA^fMet



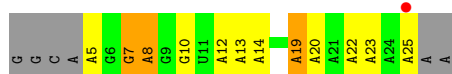
- Molecule 23: E. coli tRNA^fMet



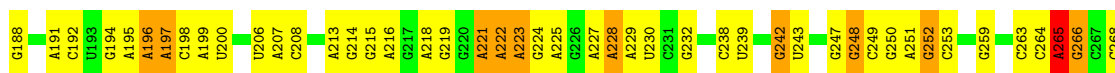
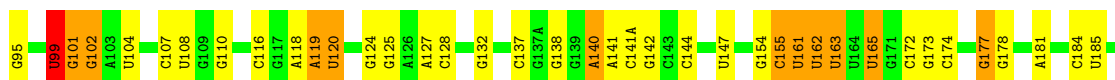
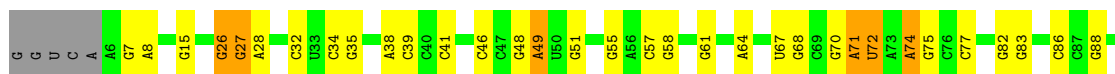
- Molecule 24: mRNA



- Molecule 24: mRNA

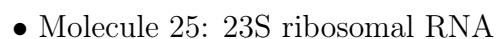


- Molecule 25: 23S ribosomal RNA



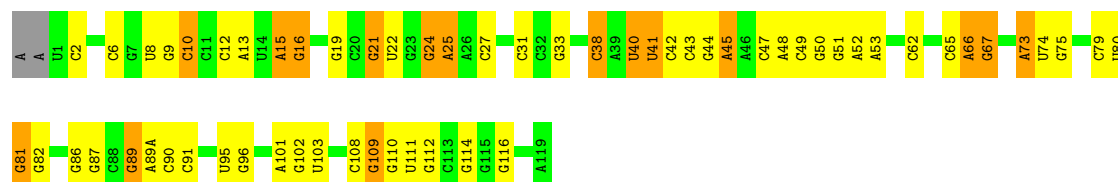
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A1241	G1151	U1066	U1066	G1002	C935	A781	G686	A637	A567	C485	U403	G318	C270C
G1242	G1152	A1067	G1068	G1003	C936	A782	G704	G638	U568	C486	U405	C319	C270D
G1243	G1153	U1068	A1069	C1004	G937	A783	G705	U639	G570	C487	U406	A320	C270E
A1331	A1155	G1069	A1070	C1005	U938	A784	G706	C640	A571	C488	G407	G321	U270F
G1332	A1156	G1071	G1071	C1006	G939	A872	G707	G641	A572	C489	G408	A322	C270G
G1333	U1165	C1072	G1072	C1007	G940	G873	G708	G642	G573	G496	G411	G323	C270H
G1334	C1166	C1073	C1073	C1008	A941	G874	C709	A643	A574	G500	A412	A324	G270I
G1335	U1167	A1074	G1074	A1009	U942	G875	G710	C644	A575	G501	A413	G329	U270L
A1264	U1168	G1075	C1075	A1010	U943	G876	G711	C645	A576	A503	C414	A330	U270M
U1255	G1169	A1076	U1076	G1011	G944	A792	U714	A653	U504	U504	C415	A331	G270N
G1256	G1170	C1077	C1077	A1012	G945	A793	U715	A654	A505	A505	C416	A332	U270O
G1257	G1171	U1078	U1078	C1013	G946	G796	U716	G654A	C580	C580	C417	A333	C270P
G1258	G1172	A1079	A1079	U1014	A953	G797	U717	G654B	C581	C581	C418	A334	C270Q
A1265	G1173	U1080	U1080	G1015	G954	G798	U718	G	C582	C582	U421	G339	C270R
A1266	A1174	U1081	U1081	G1016	C955	G799	U719	G	C583	C583	A422	A340	G270S
G1267	G1175	U1082	U1082	U1019	G956	G801	C720	C	A586	A586	U423	U339	G270T
U1268	G1176	U1083	U1083	A1020	G957	A802	C721	C	C587	C587	G424	A341	G270U
A1269	A1177	A1084	A1084	A1021	U958	G803	C722	C	C588	C588	U425	G342	G270V
C1178	C1178	A1085	A1085	G1022	A959	G804	U723	C	U588	U588	U426	G343	G270W
C1179	C1179	A1086	A1086	U1023	A960	G805	U724	C	C589	C589	A427	G344	G270X
C1180	C1180	G1087	G1087	G1024	C961	U810	U725	A	A590	A590	U428	G345	G270Y
G1271	G1271	A1088	A1088	G1025	G962	U811	G726	C	C591	C591	A432	G352	G271B
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G1283	G1195	A1095	A1095	U1035	C971	A820	U733	C	G604	G604	U442	U362	C273D
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C1293	C1207	U1104	U1104	G1039	C903	U824	G740	A654U	A609	A609	U446	G363C	G275
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G1298	U1211	G1106	G1106	G1041	G977	A826	G742	C558	A532	A532	A448	U384	C277
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G1310	A1226	C1114	C1114	C1049	C985	C856	G763	C566	G622	G622	A456	G381	A300
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G1410	G1239	U1121	U1121	U1056	C992	C857	G770	C573	G628	G628	A463	U388	G308
A1411	A1237	G1122	G1122	G1057	C993	U858	G771	G674	G629	G629	A464	U389	G309
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		U1141	U1141	U1061	G997	G862	G775	G680	A633	A633	A468	G396	
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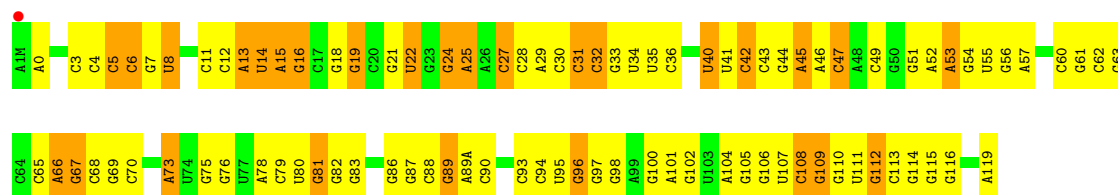


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G1817	G1732	G1733	G1632	G1540	U1454	C1376	A1302	G1218	G1144	G1071	C1004	G929	C857	G775
U1818	C1733	G1734	A1634	U1541	G1455	A1379	G1306	G1219	G1145	G1074	C1007	U930	G859	G776
A1819	C1735	G1735	G1635	G1542	G1455	G1380	A1307	A1220	A1148	C1075	C1008	G931	U860	A777
U1820	G1741	C1741	C1636	A1543	C1458	U1372	A1308	C1221	U1149	C1076	A1009	G932	U861	G778
G1822	C1742	G1742	A1637	C1544	G1459	G1383	A1309	C1222	C1150	A1077	A1010	G933	G862	U779
G1823	G1743	G1743	C1638	A1545A	A1461	A1384	G1310	C1223	G1151	A1080	G1011	G934	A863	A782
G1824	G1750	G1750	U1639	C1546	G1461	G1385	G1311	C1224	C1152	U1083	U1012	C935	G864	A783
A1825	U1825	C1640	C1640	C1547	C1467	G1386	U1312	C1225	C1153	A1084	C1013	U837	A866	A784
G1826	G1753	G1643	G1643	C1548	C1468	G1387	U1313	G1226	C1154	A1085	U1014	G938	G869	G785
C1827	C1754	G1644	G1644	C1550	A1469	C1388	U1314	G1229A	A1155	A1086	G1015	G939	C790	C790
A1829	G1755	G1645	G1645	A1558	G1470	G1389	C1315	C1230	A1156	G1087	G1016	G940	A872	C791
G1835	G1756	G1646	G1647	A1559	A1471	U1391	U1316	G1231	U1159	G1089	A1021	G942	G875	A793
C1836	U1757	C1648	C1648	G1560	G1475	U1395	C1317	G1232	G1160	U1090	G1022	G944	C876	C796
C1837	G1759	A1652	A1652	A1566	G1478	U1396	G1319	C1233	C1161	G1091	U1023	G945	U877	C797
G1839	G1762	G1653	G1653	A1567	U1478	G1401	A1321	A1241	G1163	A1096	A1027	G948	A802	A802
U1847	G1763	A1654	A1654	G1568	G1482	C1402	A1322	G1242	G1164	G1099	A1028	A957	G805	G805
A1848	G1764	C1657	C1658	A1569	G1483	C1403	U1323	G1243	U1165	C1100	A1029	U958	C806	C806
C1771	C1771	G1658	G1658	A1570	A1486	C1404	G1324	G1244	C1166	U1101	G1030	A959	U807	U807
G1772	G1772	A1665	A1665	U1578	G1487	U1405	U1326	A1247	G1170	G1089	G1031	A960	C884	C884
A1773	C1773	G1667	G1667	A1579	G1488	A1406	G1325	G1245	G1171	U1101	G1032	A961	C885	G808
U1775	U1775	G1667	G1667	A1580	U1489	C1407	U1329	G1246	G1172	C1102	A1033	C961	C886	G809
G1776	G1776	A1668	A1668	G1581	G1491	C1408	G1330	U1249	G1173	G1096	U1034	G968	A887	C812
A1853	A1854	C1668	C1668	C1582	G1492	G1410	G1332	G1251	U1175	U1105	U1035	C971	C888	C813
G1858	A1780	G1674	G1674	A1583	C1493	C1411	C1333	G1252	G1176	G1106	G1036	C972	A889	U813
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G1860	G1782	A1586	A1586	A1586	G1495	G1413	G1337	U1254	C1178	G1109	C1044	G974	C893	C815
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G1869	U1864	C1686	C1686	C1588	C1502	C1417	G1344	U1256	G1180	A1112	A1046	G978	U895	C817
C1870	A1786	G1687	G1687	A1591	C1502	C1417	G1344	C1257	C1181	G1112	A1046	G979	A896	A819
A1871	A1787	U1688	U1688	C1592	C1505	G1418	C1345	G1258	G1183	U1113	A1047	C978	C897	G818
A1872	C1788	A1689	A1689	G1593	C1505	U1420	G1346	G1259	G1183	G1114	A1048	G979	A896	U826
							G1347	G1260		G1115	C1049	A980	A901	U827

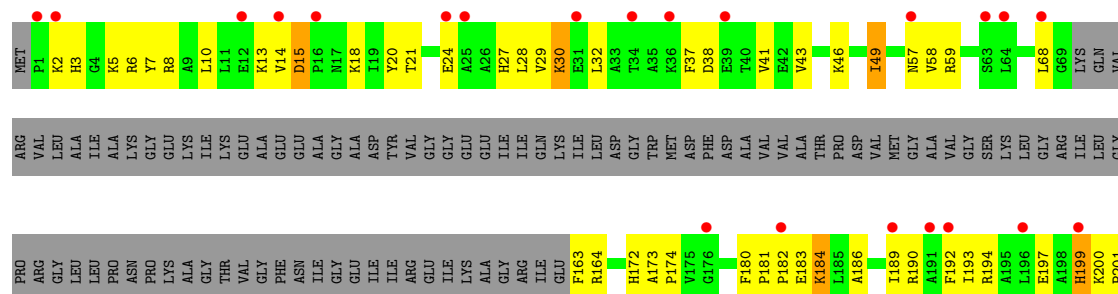
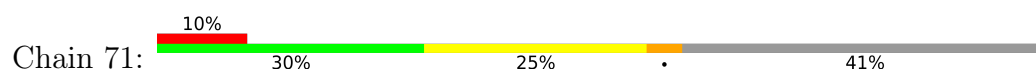




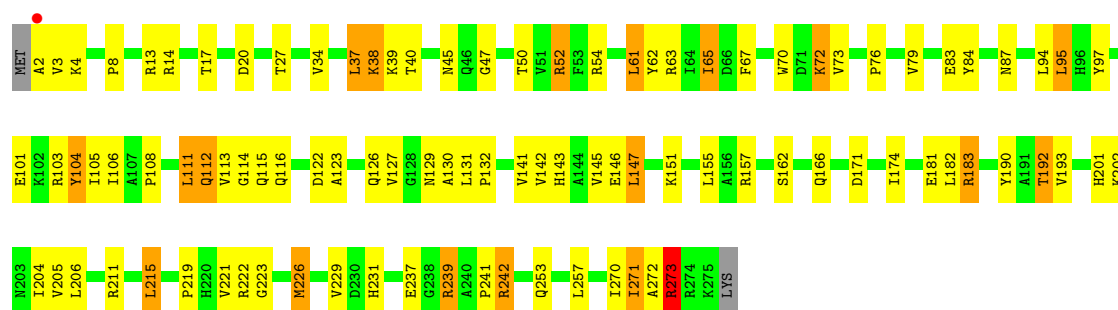
- Molecule 26: 5S ribosomal RNA



- Molecule 27: 50S ribosomal protein L1

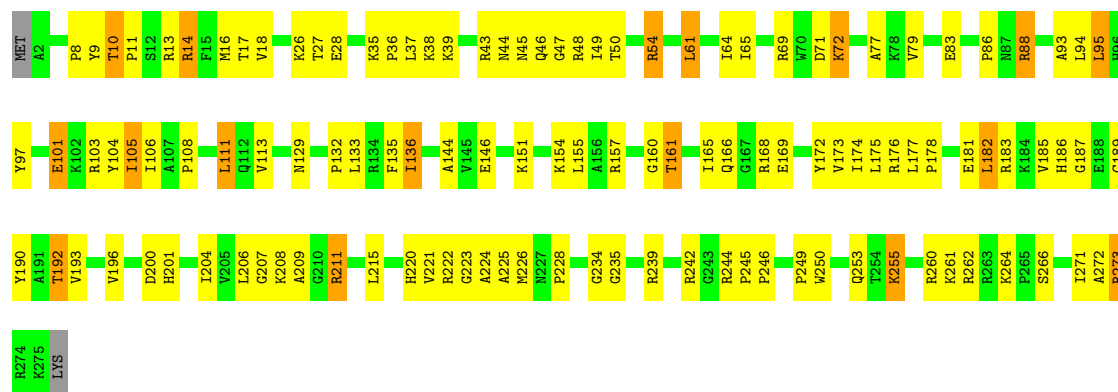


- Molecule 28: 50S ribosomal protein L2

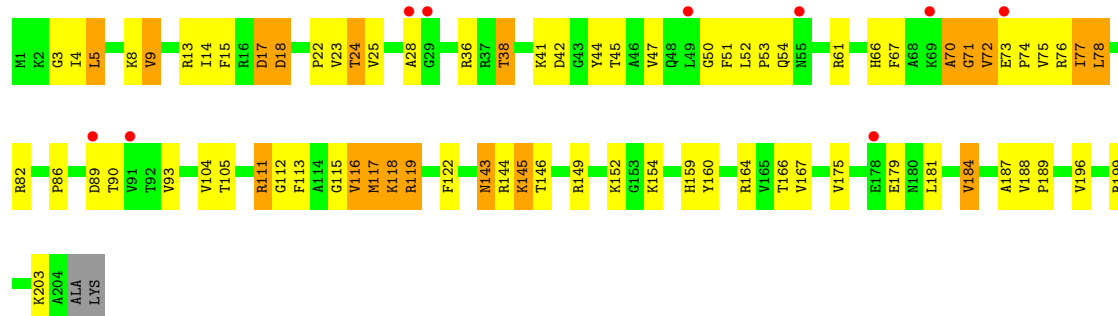


- Molecule 28: 50S ribosomal protein L2

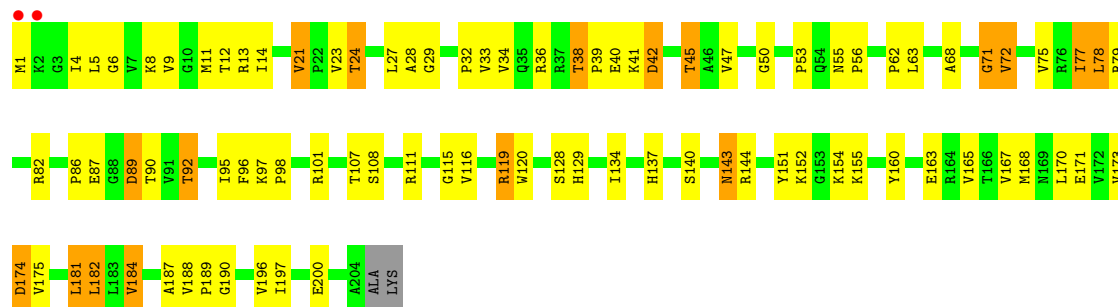




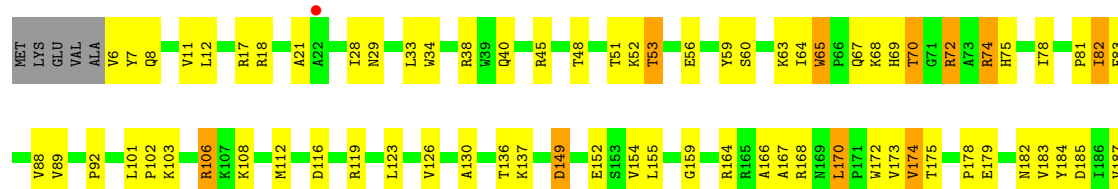
• Molecule 29: 50S ribosomal protein L3

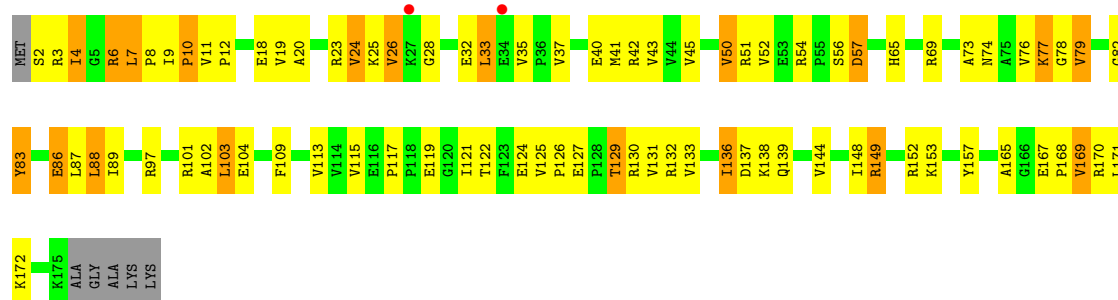


• Molecule 29: 50S ribosomal protein L3

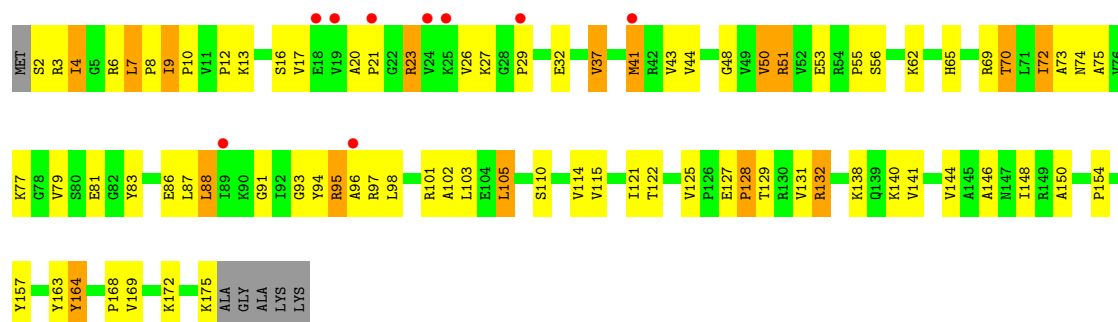


• Molecule 30: 50S ribosomal protein L4

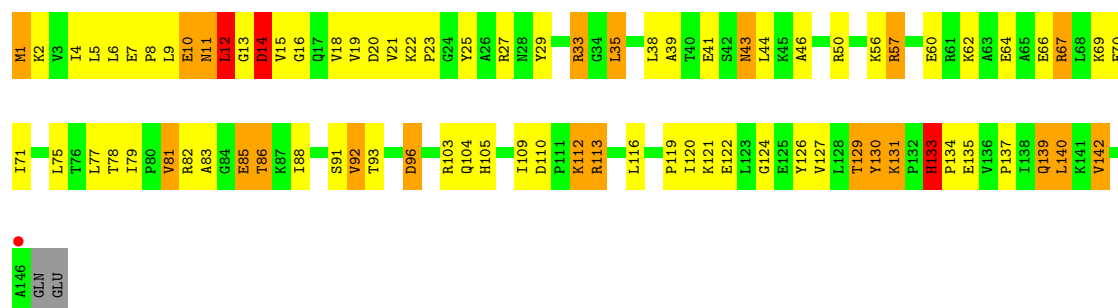




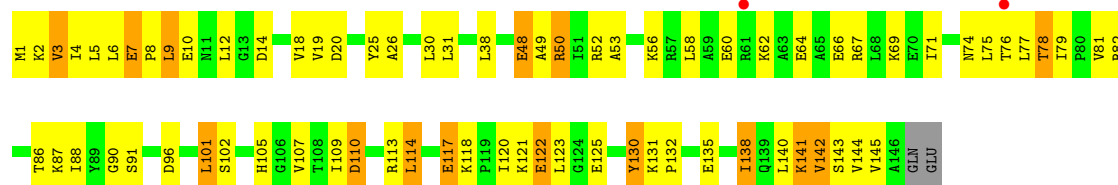
- Molecule 32: 50S ribosomal protein L6



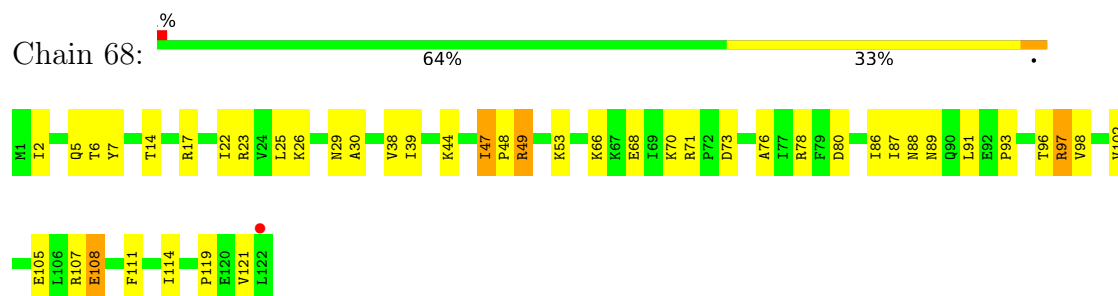
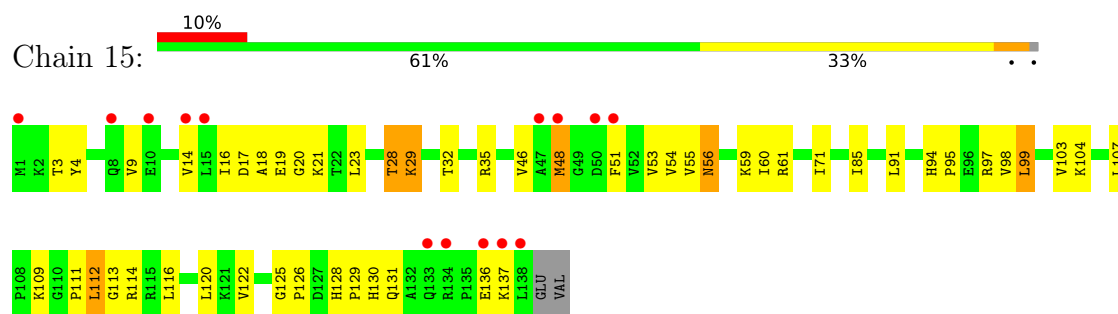
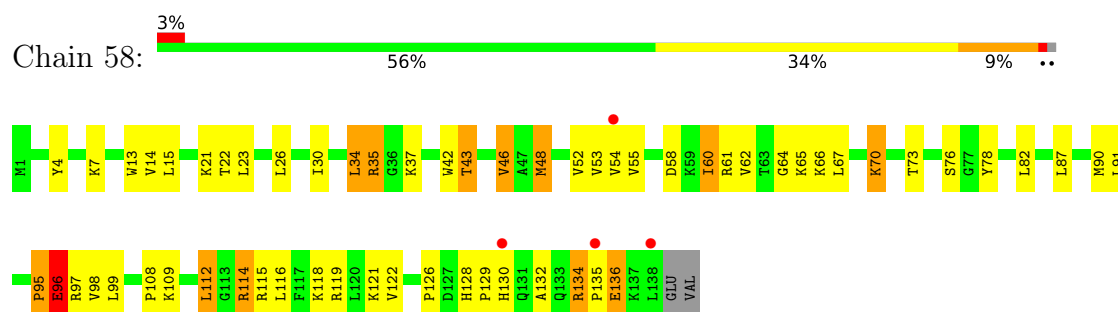
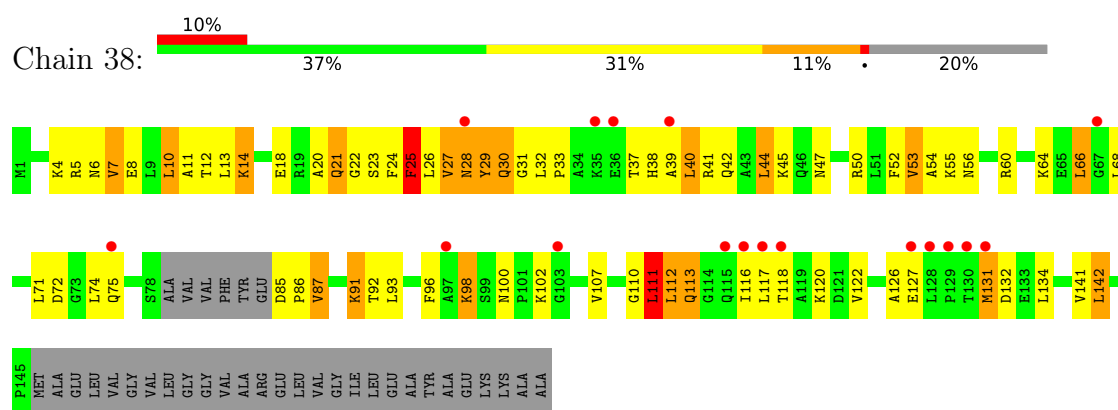
- Molecule 33: 50S ribosomal protein L9

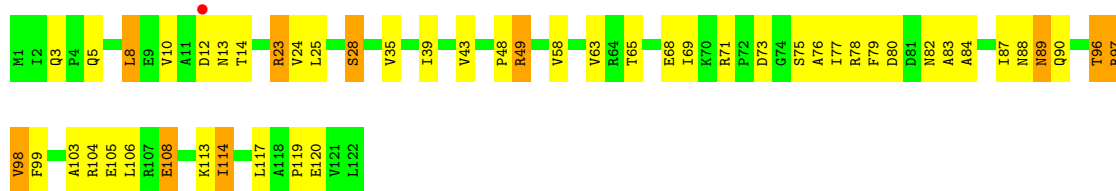


- Molecule 33: 50S ribosomal protein L9

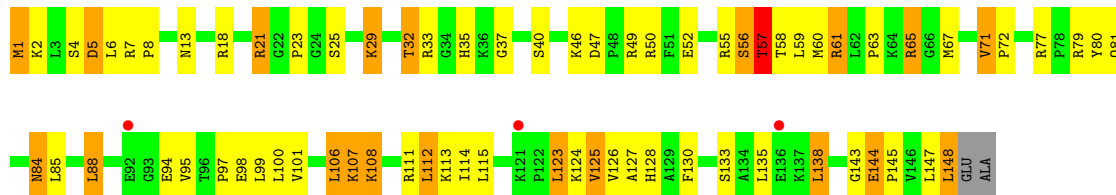


- Molecule 34: 50S ribosomal protein L10

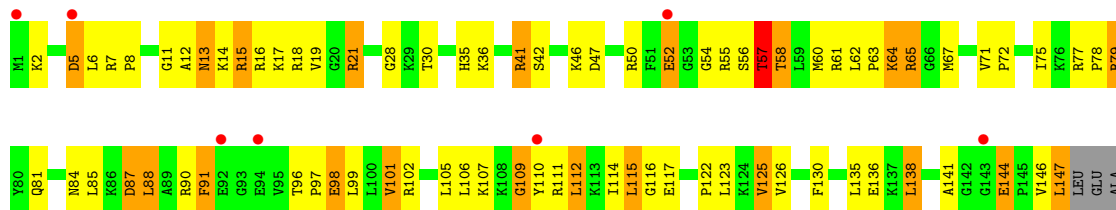




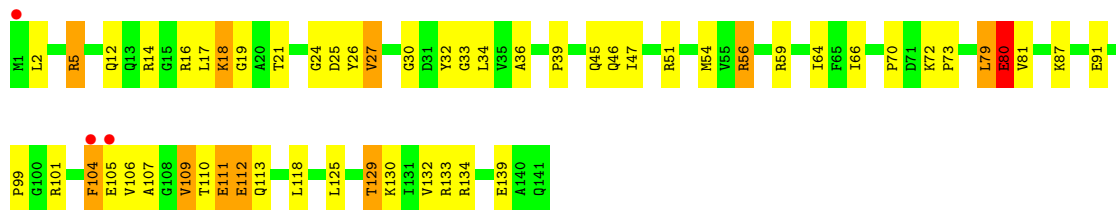
• Molecule 37: 50S ribosomal protein L15



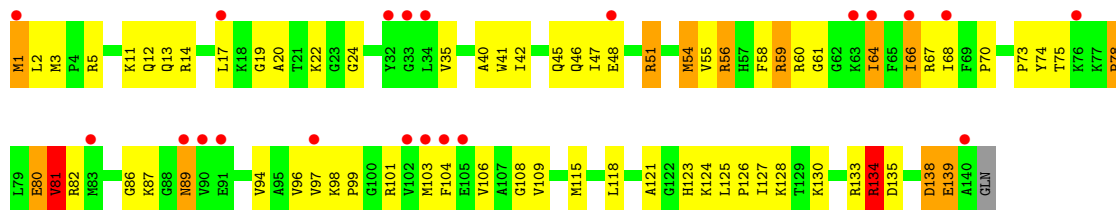
• Molecule 37: 50S ribosomal protein L15



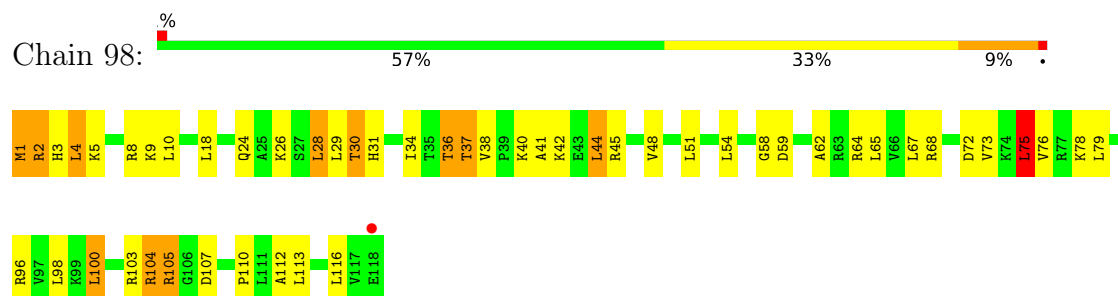
• Molecule 38: 50S ribosomal protein L16



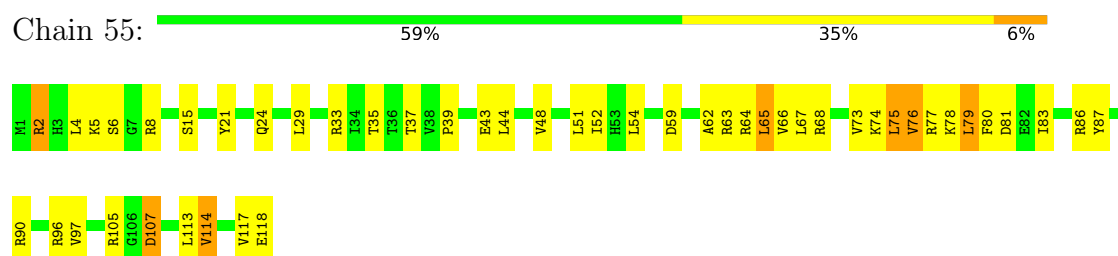
• Molecule 38: 50S ribosomal protein L16



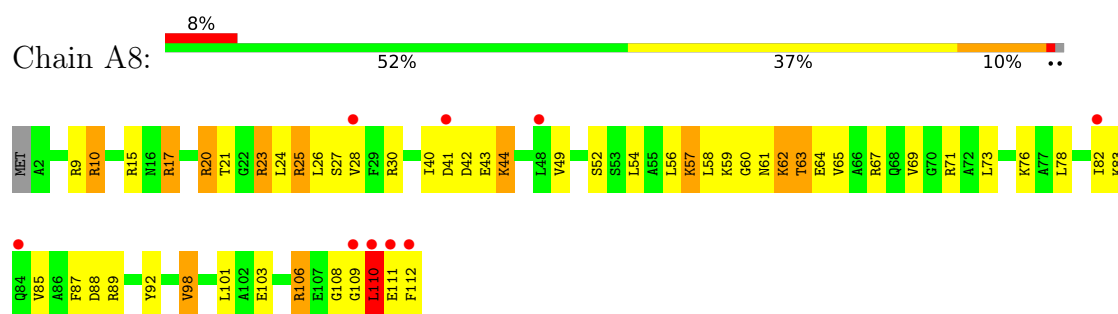
• Molecule 39: 50S ribosomal protein L17



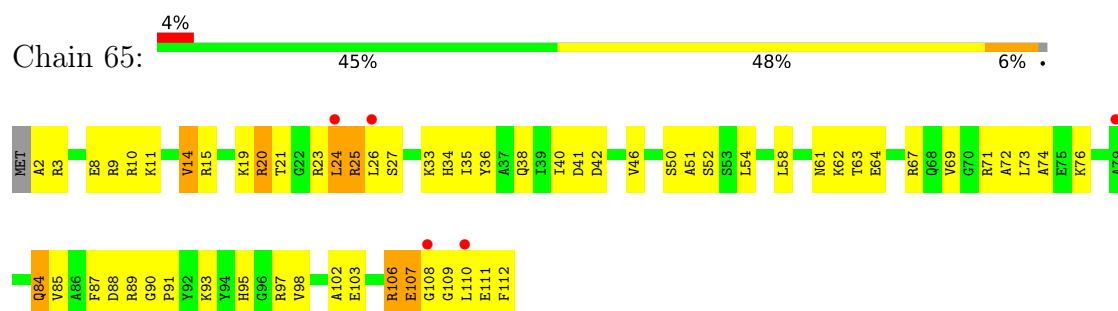
• Molecule 39: 50S ribosomal protein L17



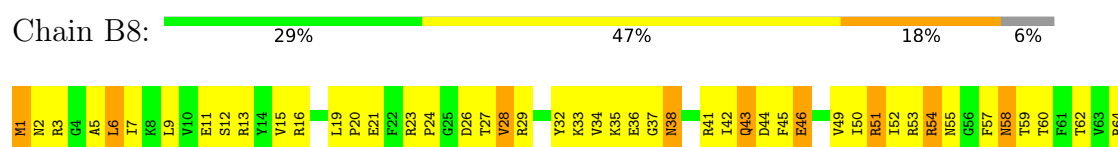
• Molecule 40: 50S ribosomal protein L18

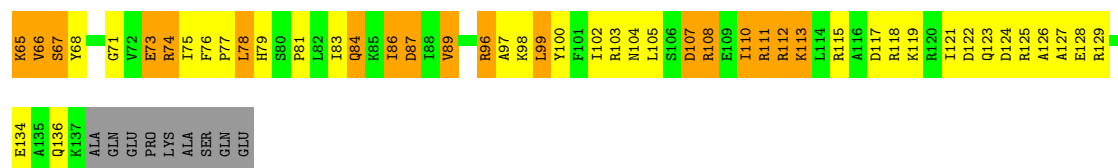


• Molecule 40: 50S ribosomal protein L18

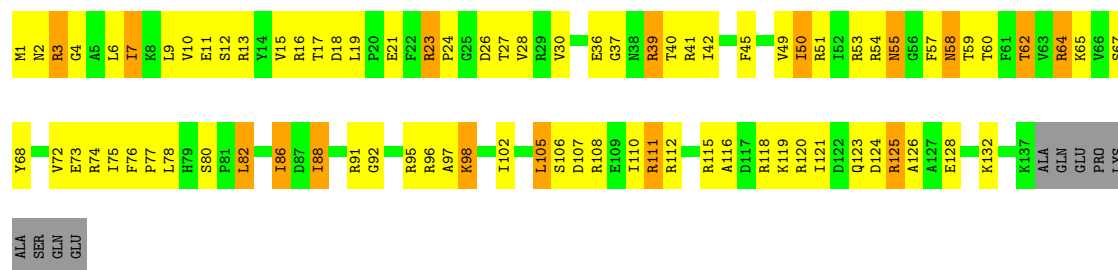


• Molecule 41: 50S ribosomal protein L19

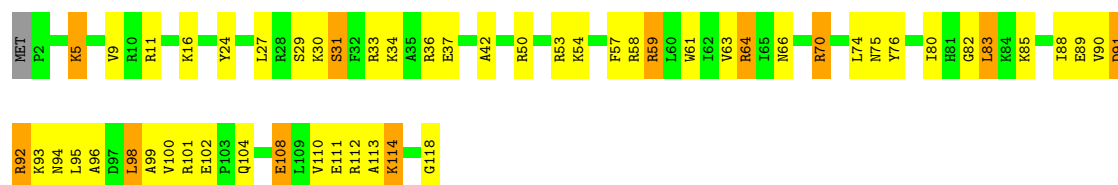




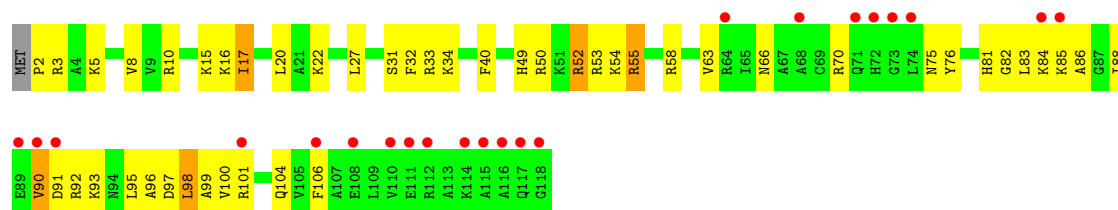
• Molecule 41: 50S ribosomal protein L19



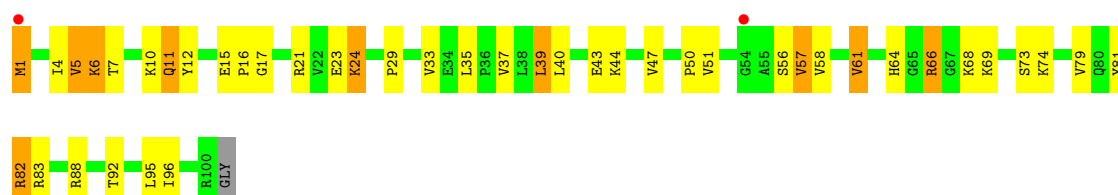
• Molecule 42: 50S ribosomal protein L20



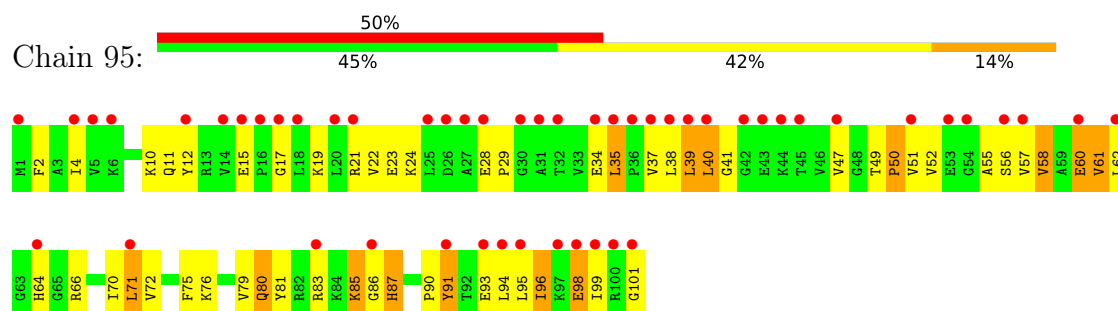
• Molecule 42: 50S ribosomal protein L20



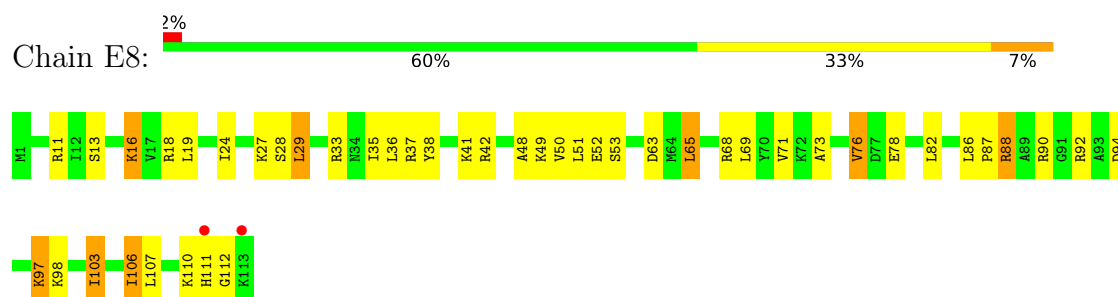
• Molecule 43: 50S ribosomal protein L21



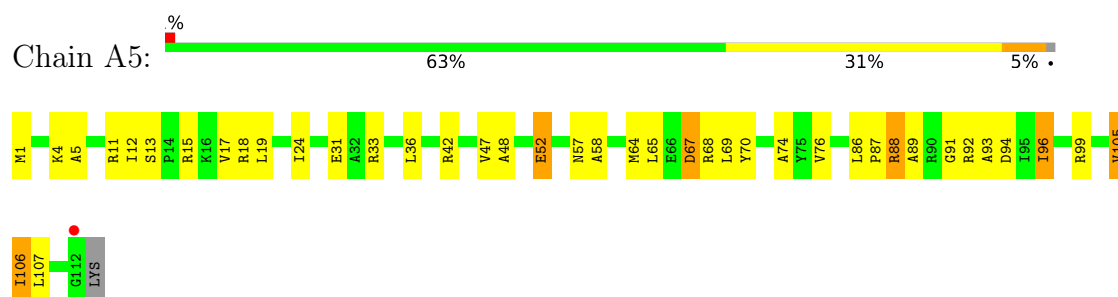
- Molecule 43: 50S ribosomal protein L21



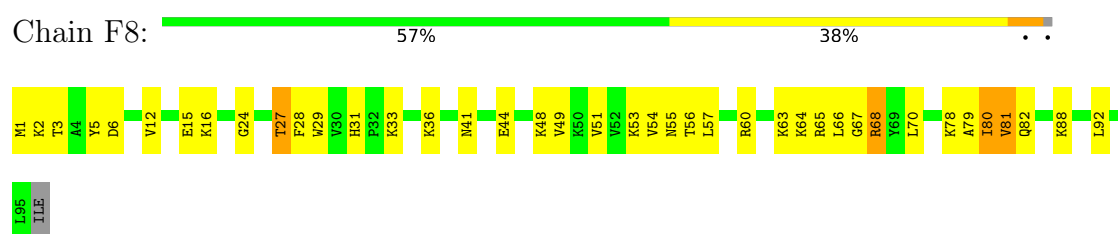
- Molecule 44: 50S ribosomal protein L22



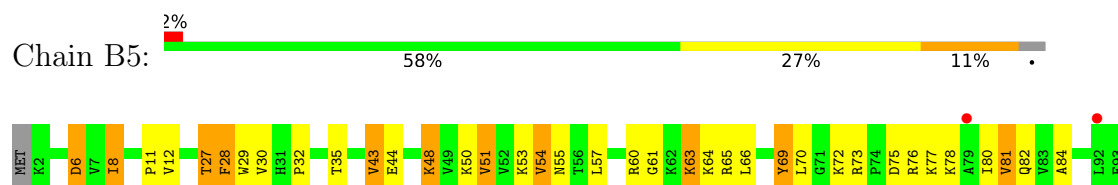
- Molecule 44: 50S ribosomal protein L22



- Molecule 45: 50S ribosomal protein L23



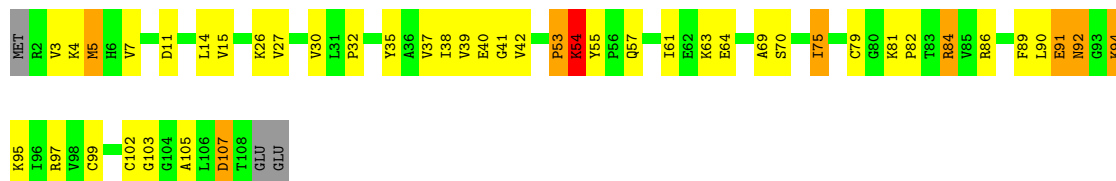
- Molecule 45: 50S ribosomal protein L23





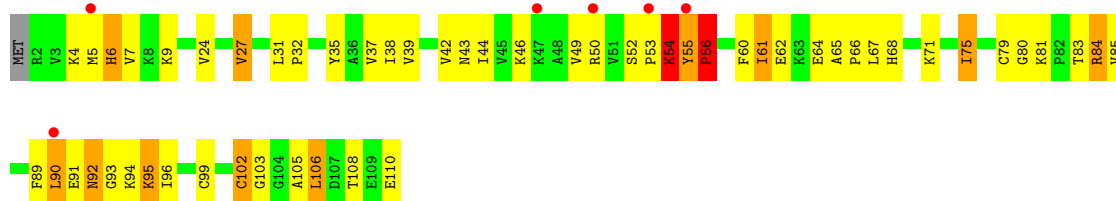
- Molecule 46: 50S ribosomal protein L24

Chain G8: 56% 33% 7% ..



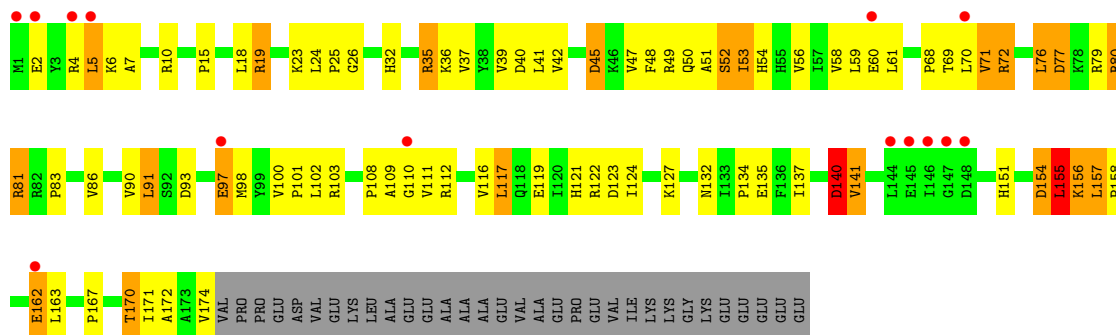
- Molecule 46: 50S ribosomal protein L24

Chain C5: 5% 49% 38% 10% ..



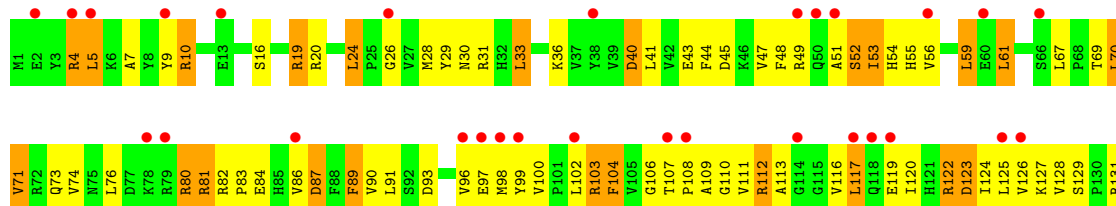
- Molecule 47: 50S ribosomal protein L25

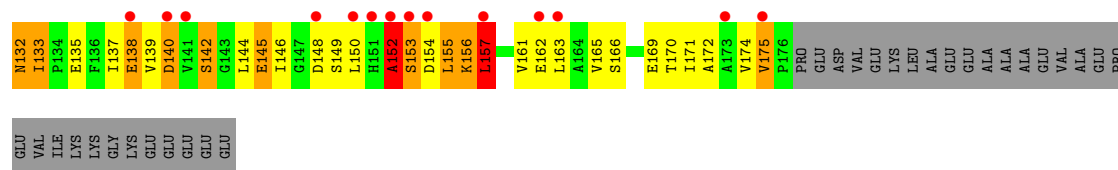
Chain H8: 7% 42% 32% 10% . 16%



- Molecule 47: 50S ribosomal protein L25

Chain D5: 21% 32% 36% 16% . 15%

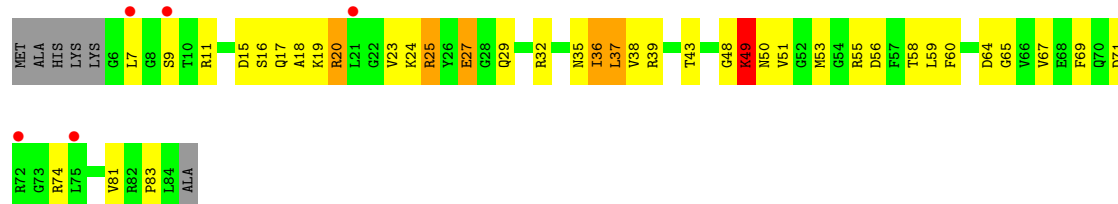




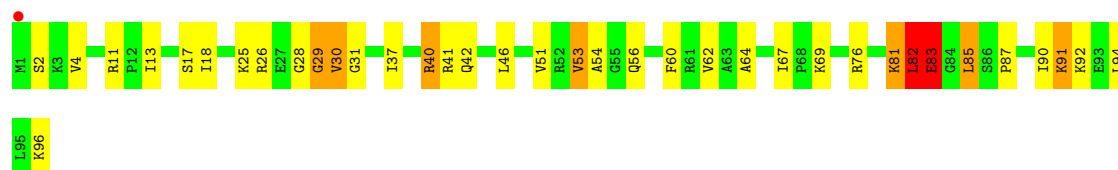
- Molecule 48: 50S ribosomal protein L27



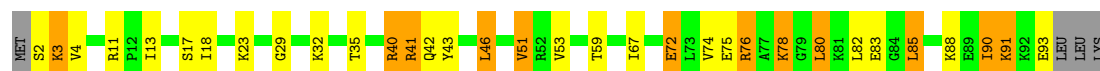
- Molecule 48: 50S ribosomal protein L27



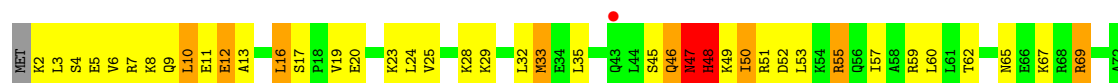
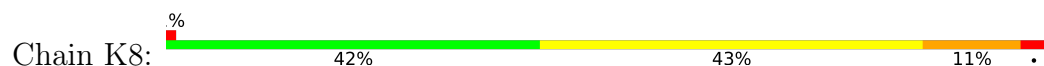
- Molecule 49: 50S ribosomal protein L28



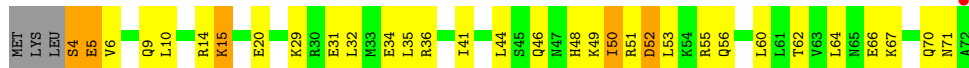
- Molecule 49: 50S ribosomal protein L28



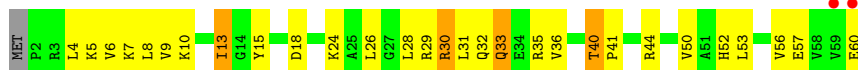
- Molecule 50: 50S ribosomal protein L29



- Molecule 50: 50S ribosomal protein L29



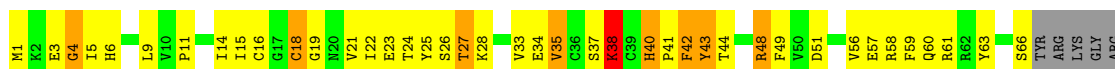
- Molecule 51: 50S ribosomal protein L30



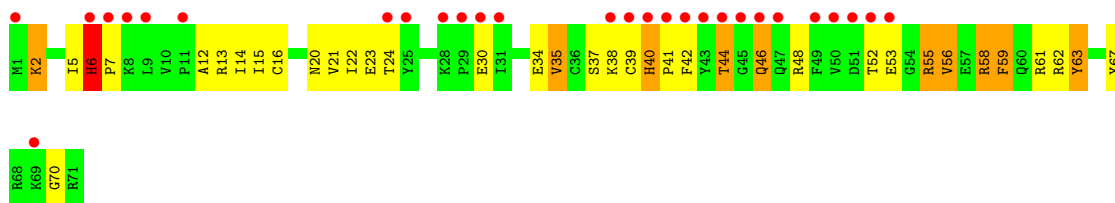
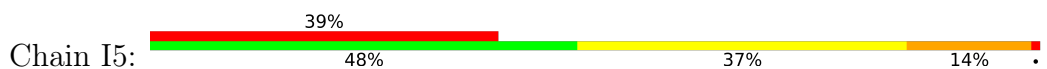
- Molecule 51: 50S ribosomal protein L30



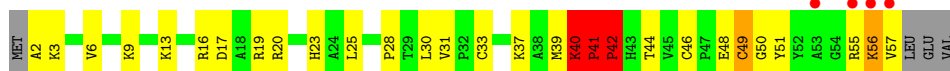
- Molecule 52: 50S ribosomal protein L31



- Molecule 52: 50S ribosomal protein L31

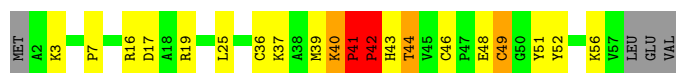


- Molecule 53: 50S ribosomal protein L32

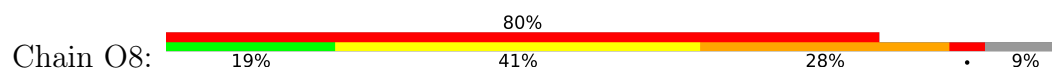


- Molecule 53: 50S ribosomal protein L32

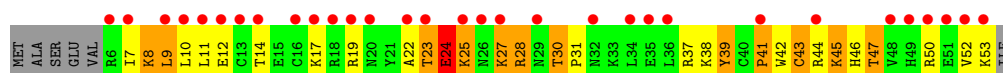




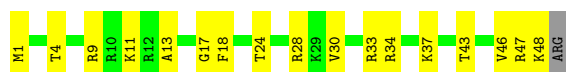
- Molecule 54: 50S ribosomal protein L33



- Molecule 54: 50S ribosomal protein L33



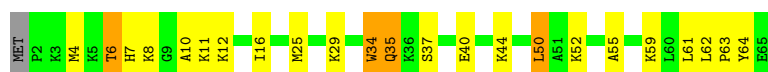
- Molecule 55: 50S ribosomal protein L34



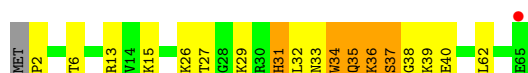
- Molecule 55: 50S ribosomal protein L34



- Molecule 56: 50S ribosomal protein L35

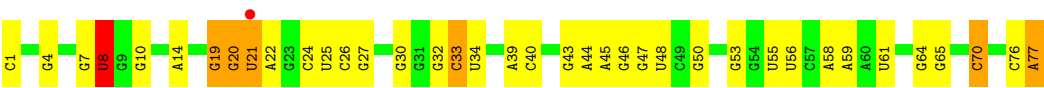


- Molecule 56: 50S ribosomal protein L35



- 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 – 3.00	Depositor EDS
% Data completeness (in resolution range)	100.0 (226.09-3.50) 100.0 (226.09-3.00)	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 0.196 , 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)	0.23 , 62.6	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	0.94	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: 7MG, 2MA, 0TD, H2U, PSU, OMU, MA6, 5MC, K, 4OC, 5MU, OMC, SF4, OMG, ZN, M2G, UR3, MG, 2MG, 4SU

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	0.28	0/35952	0.86	45/56107 (0.1%)
1	1G	0.27	0/36044	0.85	42/56250 (0.1%)
2	12	0.26	0/1950	0.50	0/2630
2	1E	0.27	0/1959	0.47	0/2642
3	22	0.26	0/1636	0.50	0/2205
3	2E	0.27	0/1629	0.47	0/2195
4	32	0.27	0/1732	0.46	0/2318
4	3E	0.28	0/1732	0.46	0/2318
5	42	0.29	0/1195	0.49	0/1609
5	4E	0.26	0/1171	0.46	0/1576
6	52	0.27	0/855	0.47	0/1154
6	5E	0.26	0/855	0.46	0/1154
7	62	0.26	0/1235	0.42	0/1654
7	6E	0.25	0/1275	0.43	0/1709
8	72	0.26	0/1135	0.45	0/1527
8	7E	0.26	0/1135	0.47	0/1527
9	82	0.29	0/1021	0.59	0/1371
9	8E	0.27	0/1002	0.48	0/1346
10	1A	0.26	0/814	0.53	0/1095
10	1I	0.25	0/814	0.48	0/1095
11	2A	0.27	0/904	0.49	0/1219
11	2I	0.27	0/879	0.47	0/1188
12	3A	0.27	0/982	0.53	0/1313
12	3I	0.27	0/982	0.56	0/1313
13	4A	0.25	0/947	0.57	1/1270 (0.1%)
13	4I	0.27	0/956	0.52	0/1281
14	5A	0.26	0/494	0.50	0/657
14	5I	0.29	0/500	0.55	0/664
15	6A	0.24	0/744	0.39	0/992
15	6I	0.25	0/744	0.41	0/992
16	7A	0.27	0/721	0.49	0/970

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
16	7I	0.27	0/716	0.48	0/963
17	8A	0.27	0/832	0.45	0/1113
17	8I	0.26	0/847	0.47	0/1131
18	9A	0.27	0/589	0.50	0/782
18	9I	0.27	0/578	0.48	0/768
19	AA	0.26	0/679	0.54	0/913
19	AI	0.27	0/703	0.62	0/945
20	BA	0.25	0/778	0.50	1/1028 (0.1%)
20	BI	0.27	0/768	0.55	1/1014 (0.1%)
21	1B	0.26	0/221	0.47	0/288
21	1F	0.24	0/221	0.45	0/288
22	1K	0.23	0/1547	0.85	1/2411 (0.0%)
22	3K	0.21	0/1832	0.79	0/2855
22	3L	0.23	0/1832	0.86	3/2855 (0.1%)
23	2K	0.27	0/1696	0.82	1/2644 (0.0%)
24	4K	0.26	0/421	0.81	0/655
24	4L	0.23	0/523	0.76	0/815
25	14	0.32	0/69194	0.88	63/108015 (0.1%)
25	1H	0.36	0/69191	0.90	76/108008 (0.1%)
26	16	0.29	0/2878	0.84	0/4490
26	1J	0.25	0/2928	0.83	0/4568
27	7I	0.26	0/1072	0.50	0/1447
28	11	0.31	0/2175	0.57	1/2933 (0.0%)
28	19	0.30	0/2173	0.52	0/2928
29	21	0.30	0/1592	0.50	0/2149
29	29	0.28	0/1592	0.53	0/2149
30	31	0.31	0/1620	0.51	0/2194
30	39	0.29	0/1654	0.54	0/2239
31	41	0.27	0/1498	0.51	0/2016
31	49	0.26	0/1498	0.51	0/2016
32	51	0.28	0/1362	0.55	0/1841
32	59	0.27	0/1362	0.49	0/1841
33	61	0.28	0/1151	0.64	0/1558
33	69	0.28	0/1151	0.55	0/1558
34	38	0.28	0/1069	0.65	1/1444 (0.1%)
35	15	0.26	0/1131	0.50	0/1525
35	58	0.30	0/1131	0.53	0/1525
36	25	0.30	0/942	0.55	0/1269
36	68	0.30	0/942	0.53	0/1269
37	35	0.31	0/1139	0.67	0/1514
37	78	0.32	0/1147	0.65	0/1525
38	45	0.29	0/1133	0.54	0/1515
38	88	0.31	0/1142	0.56	0/1527

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
39	55	0.27	0/981	0.52	0/1312
39	98	0.27	0/981	0.53	1/1312 (0.1%)
40	65	0.28	0/891	0.57	0/1187
40	A8	0.29	0/891	0.63	1/1187 (0.1%)
41	75	0.49	0/1155	0.68	0/1542
41	B8	0.52	0/1155	0.67	0/1542
42	85	0.29	0/981	0.49	0/1306
42	C8	0.29	0/981	0.48	0/1306
43	95	0.29	0/789	0.56	0/1057
43	D8	0.29	0/785	0.55	0/1052
44	A5	0.28	0/901	0.51	0/1209
44	E8	0.30	0/910	0.52	0/1220
45	B5	0.30	0/744	0.52	0/1000
45	F8	0.32	0/761	0.53	0/1021
46	C5	0.33	0/838	0.61	0/1121
46	G8	0.30	0/818	0.58	0/1094
47	D5	0.30	0/1435	0.62	2/1947 (0.1%)
47	H8	0.28	0/1420	0.58	0/1925
48	E5	0.28	0/631	0.53	0/841
48	I8	0.29	0/619	0.50	0/825
49	F5	0.29	0/728	0.56	0/967
49	J8	0.35	0/761	0.58	0/1010
50	G5	0.27	0/582	0.47	0/771
50	K8	0.27	0/592	0.54	0/784
51	H5	0.25	0/473	0.49	0/635
51	L8	0.27	0/473	0.49	0/635
52	I5	0.29	0/593	0.63	0/795
52	M8	0.28	0/545	0.61	0/733
53	J5	0.28	0/448	0.50	0/606
53	N8	0.31	0/448	0.52	0/606
54	K5	0.29	0/424	0.82	2/565 (0.4%)
54	O8	0.32	0/431	0.65	0/575
55	L5	0.28	0/426	0.44	0/561
55	P8	0.30	0/426	0.47	0/561
56	M5	0.27	0/514	0.50	0/679
56	Q8	0.28	0/514	0.48	0/679
57	2L	0.24	0/1718	0.78	0/2678
All	All	0.31	0/321407	0.80	242/480718 (0.1%)

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

There are no bond length outliers.

The worst 5 of 242 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	14	2403	C	C2-N3-C4	16.20	128.00	119.90
25	14	247	G	C2-N3-C4	16.16	119.98	111.90
25	14	2403	C	N1-C2-N3	10.27	126.39	119.20
1	13	1054	C	N1-C2-O2	9.19	124.42	118.90
1	1G	1322	C	N1-C2-O2	9.15	124.39	118.90

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	691	0
1	1G	32470	0	16411	750	0
2	12	1915	0	1969	84	0
2	1E	1924	0	1975	69	0
3	22	1612	0	1677	60	0
3	2E	1605	0	1668	52	0
4	32	1702	0	1766	64	0
4	3E	1702	0	1766	65	0
5	42	1178	0	1234	42	0
5	4E	1155	0	1213	36	0
6	52	842	0	857	27	0
6	5E	842	0	857	19	0
7	62	1217	0	1256	51	0
7	6E	1256	0	1296	38	0
8	72	1115	0	1177	42	0
8	7E	1115	0	1177	40	0
9	82	1002	0	1025	77	0
9	8E	983	0	1006	48	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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	23	0
12	3A	977	0	1061	36	0
12	3I	977	0	1061	28	0
13	4A	937	0	995	58	0
13	4I	946	0	1008	42	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	25	0
17	8A	819	0	880	27	0
17	8I	834	0	904	27	0
18	9A	584	0	657	28	0
18	9I	573	0	644	29	0
19	AA	665	0	684	57	0
19	AI	688	0	710	43	0
20	BA	776	0	857	32	0
20	BI	766	0	854	31	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	8	0
25	14	62013	0	31255	1102	0
25	1H	62010	0	31252	1054	0
26	16	2573	0	1305	35	0
26	1J	2617	0	1328	78	0
27	71	1049	0	1071	51	0
28	11	2125	0	2199	62	0
28	19	2124	0	2197	90	0
29	21	1559	0	1618	50	0
29	29	1559	0	1617	55	0
30	31	1585	0	1632	70	0
30	39	1619	0	1674	74	0
31	41	1473	0	1535	59	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
31	49	1473	0	1535	63	0
32	51	1336	0	1418	56	0
32	59	1336	0	1418	46	0
33	61	1136	0	1223	42	0
33	69	1136	0	1223	40	0
34	38	1056	0	1119	49	0
35	15	1104	0	1180	29	0
35	58	1104	0	1180	39	0
36	25	932	0	996	33	0
36	68	932	0	996	31	0
37	35	1122	0	1206	71	0
37	78	1130	0	1217	66	0
38	45	1112	0	1171	55	0
38	88	1121	0	1179	32	0
39	55	967	0	1033	41	0
39	98	967	0	1033	30	0
40	65	881	0	943	46	0
40	A8	881	0	943	36	0
41	75	1141	0	1202	73	0
41	B8	1141	0	1202	85	0
42	85	963	0	1022	48	0
42	C8	963	0	1021	42	0
43	95	778	0	852	46	0
43	D8	774	0	849	29	0
44	A5	890	0	951	23	0
44	E8	899	0	964	27	0
45	B5	730	0	780	27	0
45	F8	747	0	805	26	0
46	C5	825	0	898	46	0
46	G8	805	0	881	25	0
47	D5	1404	0	1437	74	0
47	H8	1390	0	1421	58	0
48	E5	623	0	645	31	0
48	I8	611	0	631	23	0
49	F5	721	0	791	23	0
49	J8	754	0	838	25	0
50	G5	580	0	629	17	0
50	K8	590	0	643	25	0
51	H5	468	0	518	12	0
51	L8	468	0	518	14	0
52	I5	580	0	577	29	0
52	M8	533	0	526	30	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
53	J5	434	0	454	15	0
53	N8	434	0	454	29	0
54	K5	417	0	441	19	0
54	O8	424	0	450	35	0
55	L5	418	0	467	17	0
55	P8	418	0	467	10	0
56	M5	506	0	567	14	0
56	Q8	506	0	567	19	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
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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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
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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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	6768	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 6768 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
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 ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	12	234/256 (91%)	193 (82%)	36 (15%)	5 (2%)	7	38
2	1E	235/256 (92%)	200 (85%)	35 (15%)	0	100	100
3	22	204/239 (85%)	161 (79%)	41 (20%)	2 (1%)	15	54
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%)	11	46
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	20
9	8E	122/128 (95%)	107 (88%)	15 (12%)	0	100	100
10	1A	97/105 (92%)	79 (81%)	18 (19%)	0	100	100
10	1I	97/105 (92%)	84 (87%)	13 (13%)	0	100	100
11	2A	117/129 (91%)	100 (86%)	16 (14%)	1 (1%)	17	56
11	2I	115/129 (89%)	108 (94%)	7 (6%)	0	100	100
12	3A	122/132 (92%)	101 (83%)	18 (15%)	3 (2%)	5	34
12	3I	122/132 (92%)	102 (84%)	19 (16%)	1 (1%)	19	58
13	4A	116/126 (92%)	79 (68%)	31 (27%)	6 (5%)	2	18
13	4I	117/126 (93%)	99 (85%)	16 (14%)	2 (2%)	9	42
14	5A	58/61 (95%)	49 (84%)	8 (14%)	1 (2%)	9	42

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
14	5I	58/61 (95%)	48 (83%)	9 (16%)	1 (2%)	9	42
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%)	13	50
20	BA	101/106 (95%)	89 (88%)	12 (12%)	0	100	100
20	BI	99/106 (93%)	85 (86%)	13 (13%)	1 (1%)	15	54
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%)	34	72
28	19	270/276 (98%)	244 (90%)	26 (10%)	0	100	100
29	21	202/206 (98%)	177 (88%)	23 (11%)	2 (1%)	15	54
29	29	202/206 (98%)	183 (91%)	18 (9%)	1 (0%)	29	68
30	31	200/210 (95%)	174 (87%)	25 (12%)	1 (0%)	29	68
30	39	204/210 (97%)	166 (81%)	34 (17%)	4 (2%)	7	39
31	41	179/182 (98%)	144 (80%)	33 (18%)	2 (1%)	14	52
31	49	179/182 (98%)	141 (79%)	35 (20%)	3 (2%)	9	42
32	51	172/180 (96%)	139 (81%)	31 (18%)	2 (1%)	13	50
32	59	172/180 (96%)	131 (76%)	39 (23%)	2 (1%)	13	50
33	61	144/148 (97%)	112 (78%)	30 (21%)	2 (1%)	11	46
33	69	144/148 (97%)	113 (78%)	30 (21%)	1 (1%)	22	61
34	38	135/173 (78%)	75 (56%)	57 (42%)	3 (2%)	6	37
35	15	136/140 (97%)	121 (89%)	15 (11%)	0	100	100
35	58	136/140 (97%)	110 (81%)	23 (17%)	3 (2%)	6	37

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
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%)	22	61
37	78	146/150 (97%)	110 (75%)	33 (23%)	3 (2%)	7	38
38	45	138/141 (98%)	111 (80%)	26 (19%)	1 (1%)	22	61
38	88	139/141 (99%)	105 (76%)	32 (23%)	2 (1%)	11	46
39	55	116/118 (98%)	107 (92%)	8 (7%)	1 (1%)	17	56
39	98	116/118 (98%)	105 (90%)	9 (8%)	2 (2%)	9	42
40	65	109/112 (97%)	88 (81%)	21 (19%)	0	100	100
40	A8	109/112 (97%)	84 (77%)	24 (22%)	1 (1%)	17	56
41	75	135/146 (92%)	107 (79%)	27 (20%)	1 (1%)	22	61
41	B8	135/146 (92%)	113 (84%)	22 (16%)	0	100	100
42	85	115/118 (98%)	99 (86%)	15 (13%)	1 (1%)	17	56
42	C8	115/118 (98%)	106 (92%)	8 (7%)	1 (1%)	17	56
43	95	99/101 (98%)	78 (79%)	20 (20%)	1 (1%)	15	54
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%)	5	32
46	G8	105/110 (96%)	79 (75%)	24 (23%)	2 (2%)	8	40
47	D5	174/206 (84%)	114 (66%)	55 (32%)	5 (3%)	4	31
47	H8	172/206 (84%)	123 (72%)	45 (26%)	4 (2%)	6	36
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%)	4	29
50	G5	67/72 (93%)	58 (87%)	9 (13%)	0	100	100
50	K8	69/72 (96%)	56 (81%)	11 (16%)	2 (3%)	4	31
51	H5	57/60 (95%)	53 (93%)	4 (7%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
51	L8	57/60 (95%)	52 (91%)	5 (9%)	0	100	100
52	I5	69/71 (97%)	40 (58%)	28 (41%)	1 (1%)	11	46
52	M8	64/71 (90%)	32 (50%)	30 (47%)	2 (3%)	4	30
53	J5	54/60 (90%)	42 (78%)	10 (18%)	2 (4%)	3	26
53	N8	54/60 (90%)	45 (83%)	7 (13%)	2 (4%)	3	26
54	K5	46/54 (85%)	21 (46%)	22 (48%)	3 (6%)	1	14
54	O8	47/54 (87%)	27 (57%)	17 (36%)	3 (6%)	1	14
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%)	4	29
56	Q8	62/65 (95%)	58 (94%)	4 (6%)	0	100	100
All	All	11633/12452 (93%)	9754 (84%)	1771 (15%)	108 (1%)	17	56

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%)	153 (75%)	51 (25%)	0	4
2	1E	205/220 (93%)	162 (79%)	43 (21%)	1	5
3	22	160/188 (85%)	118 (74%)	42 (26%)	0	3
3	2E	159/188 (85%)	131 (82%)	28 (18%)	2	10
4	32	180/181 (99%)	158 (88%)	22 (12%)	5	23

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	3E	180/181 (99%)	148 (82%)	32 (18%)	2	10
5	42	119/123 (97%)	90 (76%)	29 (24%)	0	4
5	4E	116/123 (94%)	94 (81%)	22 (19%)	1	8
6	52	90/90 (100%)	83 (92%)	7 (8%)	12	42
6	5E	90/90 (100%)	73 (81%)	17 (19%)	1	8
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%)	101 (85%)	18 (15%)	3	17
8	7E	119/119 (100%)	98 (82%)	21 (18%)	2	10
9	82	97/99 (98%)	73 (75%)	24 (25%)	0	4
9	8E	95/99 (96%)	82 (86%)	13 (14%)	3	20
10	1A	89/92 (97%)	69 (78%)	20 (22%)	1	4
10	1I	89/92 (97%)	76 (85%)	13 (15%)	3	18
11	2A	91/99 (92%)	78 (86%)	13 (14%)	3	19
11	2I	88/99 (89%)	73 (83%)	15 (17%)	2	12
12	3A	103/108 (95%)	81 (79%)	22 (21%)	1	5
12	3I	103/108 (95%)	89 (86%)	14 (14%)	3	20
13	4A	94/101 (93%)	67 (71%)	27 (29%)	0	3
13	4I	95/101 (94%)	72 (76%)	23 (24%)	0	4
14	5A	48/50 (96%)	46 (96%)	2 (4%)	30	63
14	5I	49/50 (98%)	39 (80%)	10 (20%)	1	6
15	6A	79/80 (99%)	67 (85%)	12 (15%)	3	17
15	6I	79/80 (99%)	69 (87%)	10 (13%)	4	22
16	7A	72/74 (97%)	62 (86%)	10 (14%)	3	20
16	7I	72/74 (97%)	57 (79%)	15 (21%)	1	6
17	8A	93/97 (96%)	78 (84%)	15 (16%)	2	14
17	8I	95/97 (98%)	85 (90%)	10 (10%)	7	31
18	9A	62/77 (80%)	51 (82%)	11 (18%)	2	10
18	9I	61/77 (79%)	51 (84%)	10 (16%)	2	13
19	AA	72/80 (90%)	55 (76%)	17 (24%)	1	4
19	AI	74/80 (92%)	57 (77%)	17 (23%)	1	4

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
20	BA	75/82 (92%)	64 (85%)	11 (15%)	3	18
20	BI	75/82 (92%)	63 (84%)	12 (16%)	2	14
21	1B	20/22 (91%)	15 (75%)	5 (25%)	0	4
21	1F	20/22 (91%)	19 (95%)	1 (5%)	24	58
27	71	111/181 (61%)	95 (86%)	16 (14%)	3	18
28	11	214/218 (98%)	176 (82%)	38 (18%)	2	10
28	19	213/218 (98%)	183 (86%)	30 (14%)	3	19
29	21	164/166 (99%)	134 (82%)	30 (18%)	1	8
29	29	164/166 (99%)	134 (82%)	30 (18%)	1	8
30	31	161/166 (97%)	143 (89%)	18 (11%)	6	27
30	39	165/166 (99%)	133 (81%)	32 (19%)	1	7
31	41	155/156 (99%)	127 (82%)	28 (18%)	1	9
31	49	155/156 (99%)	127 (82%)	28 (18%)	1	9
32	51	145/148 (98%)	116 (80%)	29 (20%)	1	7
32	59	145/148 (98%)	119 (82%)	26 (18%)	2	9
33	61	122/124 (98%)	84 (69%)	38 (31%)	0	2
33	69	122/124 (98%)	90 (74%)	32 (26%)	0	3
34	38	112/135 (83%)	80 (71%)	32 (29%)	0	3
35	15	117/119 (98%)	99 (85%)	18 (15%)	2	16
35	58	117/119 (98%)	93 (80%)	24 (20%)	1	6
36	25	100/100 (100%)	82 (82%)	18 (18%)	1	9
36	68	100/100 (100%)	87 (87%)	13 (13%)	4	21
37	35	114/116 (98%)	82 (72%)	32 (28%)	0	3
37	78	115/116 (99%)	92 (80%)	23 (20%)	1	7
38	45	110/111 (99%)	89 (81%)	21 (19%)	1	8
38	88	111/111 (100%)	91 (82%)	20 (18%)	1	9
39	55	101/101 (100%)	85 (84%)	16 (16%)	2	15
39	98	101/101 (100%)	79 (78%)	22 (22%)	1	5
40	65	87/88 (99%)	72 (83%)	15 (17%)	2	11
40	A8	87/88 (99%)	64 (74%)	23 (26%)	0	3
41	75	120/127 (94%)	94 (78%)	26 (22%)	1	5

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
41	B8	120/127 (94%)	78 (65%)	42 (35%)	0	1
42	85	93/94 (99%)	79 (85%)	14 (15%)	3	17
42	C8	93/94 (99%)	74 (80%)	19 (20%)	1	6
43	95	82/82 (100%)	60 (73%)	22 (27%)	0	3
43	D8	82/82 (100%)	61 (74%)	21 (26%)	0	3
44	A5	91/92 (99%)	76 (84%)	15 (16%)	2	13
44	E8	92/92 (100%)	73 (79%)	19 (21%)	1	6
45	B5	74/78 (95%)	60 (81%)	14 (19%)	1	8
45	F8	76/78 (97%)	60 (79%)	16 (21%)	1	5
46	C5	88/91 (97%)	63 (72%)	25 (28%)	0	3
46	G8	85/91 (93%)	70 (82%)	15 (18%)	2	10
47	D5	155/179 (87%)	114 (74%)	41 (26%)	0	3
47	H8	153/179 (86%)	119 (78%)	34 (22%)	1	5
48	E5	63/67 (94%)	52 (82%)	11 (18%)	2	10
48	I8	62/67 (92%)	52 (84%)	10 (16%)	2	14
49	F5	77/81 (95%)	56 (73%)	21 (27%)	0	3
49	J8	81/81 (100%)	69 (85%)	12 (15%)	3	17
50	G5	64/67 (96%)	50 (78%)	14 (22%)	1	5
50	K8	64/67 (96%)	46 (72%)	18 (28%)	0	3
51	H5	51/52 (98%)	46 (90%)	5 (10%)	8	33
51	L8	51/52 (98%)	40 (78%)	11 (22%)	1	5
52	I5	63/63 (100%)	44 (70%)	19 (30%)	0	2
52	M8	59/63 (94%)	45 (76%)	14 (24%)	1	4
53	J5	48/52 (92%)	39 (81%)	9 (19%)	1	8
53	N8	48/52 (92%)	38 (79%)	10 (21%)	1	6
54	K5	47/52 (90%)	33 (70%)	14 (30%)	0	2
54	O8	48/52 (92%)	28 (58%)	20 (42%)	0	0
55	L5	41/42 (98%)	33 (80%)	8 (20%)	1	7
55	P8	41/42 (98%)	36 (88%)	5 (12%)	5	23
56	M5	52/55 (94%)	46 (88%)	6 (12%)	5	26
56	Q8	52/55 (94%)	47 (90%)	5 (10%)	8	34

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	9804/10308 (95%)	7888 (80%)	1916 (20%)	1 7

5 of 1916 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
52	M8	27	THR
47	D5	24	LEU
7	62	151	TYR
46	C5	66	PRO
54	K5	23	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 21 such sidechains are listed below:

Mol	Chain	Res	Type
19	AA	23	ASN
30	39	40	GLN
42	85	81	HIS
31	49	66	GLN
28	19	227	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	13	1501/1522 (98%)	359 (23%)	47 (3%)
1	1G	1505/1522 (98%)	396 (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	2875/2917 (98%)	759 (26%)	50 (1%)
25	1H	2873/2917 (98%)	674 (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	9398/9561 (98%)	2368 (25%)	226 (2%)

5 of 2368 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 [i](#)

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	5MC	1H	1942	25	18,22,23	3.63	7 (38%)	26,32,35	1.06	2 (7%)
25	5MC	14	1962	25	18,22,23	3.82	7 (38%)	26,32,35	1.40	5 (19%)
57	4SU	2L	8	57	18,21,22	1.77	3 (16%)	26,30,33	1.94	4 (15%)
57	7MG	2L	47	57	22,26,27	3.10	6 (27%)	29,39,42	2.80	10 (34%)
12	0TD	3I	89	12	7,9,10	1.15	0	6,11,13	2.89	3 (50%)
23	5MU	2K	55	23	19,22,23	3.93	5 (26%)	28,32,35	3.17	8 (28%)
1	UR3	1G	1498	1	19,22,23	2.79	7 (36%)	26,32,35	1.56	3 (11%)
1	2MG	1G	1207	1	18,26,27	2.72	7 (38%)	16,38,41	1.30	2 (12%)
23	H2U	2K	21	23	18,21,22	2.11	4 (22%)	21,30,33	1.96	4 (19%)
57	PSU	2L	56	57	18,21,22	1.16	1 (5%)	22,30,33	1.78	4 (18%)
1	5MC	1G	967	1	18,22,23	3.84	7 (38%)	26,32,35	1.05	2 (7%)
1	MA6	13	1519	1	18,26,27	1.06	2 (11%)	19,38,41	2.47	2 (10%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
25	5MU	14	1939	58,25	19,22,23	3.73	5 (26%)	28,32,35	3.41	9 (32%)
1	M2G	1G	966	1	20,27,28	3.86	7 (35%)	22,40,43	1.24	4 (18%)
25	5MC	14	1942	25	18,22,23	3.79	7 (38%)	26,32,35	1.08	2 (7%)
23	OMC	2K	33	23	19,22,23	1.81	4 (21%)	26,31,34	1.01	2 (7%)
25	PSU	1H	2605	25	18,21,22	1.12	2 (11%)	22,30,33	1.98	5 (22%)
25	OMU	1H	2552	59,25	19,22,23	2.91	8 (42%)	26,31,34	1.76	5 (19%)
1	5MC	1G	1400	1	18,22,23	3.82	7 (38%)	26,32,35	1.10	2 (7%)
1	PSU	13	516	1,59	18,21,22	1.14	1 (5%)	22,30,33	1.63	3 (13%)
25	PSU	14	2605	25	18,21,22	1.14	1 (5%)	22,30,33	1.69	3 (13%)
25	PSU	14	1911	25	18,21,22	1.11	1 (5%)	22,30,33	1.60	4 (18%)
25	OMU	14	2552	59,25	19,22,23	3.00	8 (42%)	26,31,34	1.90	5 (19%)
1	MA6	1G	1518	1	18,26,27	0.99	2 (11%)	19,38,41	2.45	2 (10%)
1	7MG	1G	527	1,58	22,26,27	3.11	7 (31%)	29,39,42	2.81	10 (34%)
25	PSU	1H	1917	25	18,21,22	1.14	1 (5%)	22,30,33	1.82	4 (18%)
25	PSU	1H	1911	25	18,21,22	1.11	1 (5%)	22,30,33	1.70	4 (18%)
25	5MC	1H	1962	58,25	18,22,23	3.84	7 (38%)	26,32,35	1.08	1 (3%)
1	5MC	13	1407	1	18,22,23	3.77	7 (38%)	26,32,35	1.05	1 (3%)
25	OMG	1H	2251	58,23,25	18,26,27	5.28	9 (50%)	19,38,41	3.66	6 (31%)
23	4SU	2K	8	23	18,21,22	1.78	3 (16%)	26,30,33	2.37	5 (19%)
25	OMG	14	2251	58,57,25	18,26,27	5.34	9 (50%)	19,38,41	3.68	7 (36%)
1	2MG	13	1207	1	18,26,27	2.71	7 (38%)	16,38,41	1.40	3 (18%)
25	OMC	1H	1920	25	19,22,23	1.78	4 (21%)	26,31,34	1.04	3 (11%)
12	0TD	3A	89	12	7,9,10	1.34	0	6,11,13	3.17	3 (50%)
25	5MU	1H	1939	58,25	19,22,23	3.76	5 (26%)	28,32,35	3.70	8 (28%)
1	5MC	13	1404	1	18,22,23	3.75	7 (38%)	26,32,35	1.14	2 (7%)
1	5MC	13	967	1	18,22,23	3.79	7 (38%)	26,32,35	1.05	2 (7%)
25	OMC	14	1920	25	19,22,23	1.80	4 (21%)	26,31,34	0.84	0
57	5MU	2L	55	57	19,22,23	3.92	5 (26%)	28,32,35	3.22	10 (35%)
25	2MA	1H	2503	58,59,25	17,25,26	2.24	6 (35%)	17,37,40	1.23	2 (11%)
25	PSU	14	1917	25	18,21,22	1.06	1 (5%)	22,30,33	1.81	4 (18%)
1	4OC	13	1402	1	20,23,24	3.10	8 (40%)	26,32,35	0.86	1 (3%)
23	PSU	2K	56	23	18,21,22	1.12	1 (5%)	22,30,33	1.81	5 (22%)
1	UR3	13	1498	1	19,22,23	2.79	7 (36%)	26,32,35	1.45	3 (11%)
1	5MC	13	1400	1	18,22,23	3.90	7 (38%)	26,32,35	1.10	2 (7%)
1	5MC	1G	1404	1	18,22,23	3.82	7 (38%)	26,32,35	1.01	2 (7%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
25	2MA	14	2503	58,59,25	17,25,26	2.32	6 (35%)	17,37,40	1.27	3 (17%)
57	OMC	2L	33	57	19,22,23	1.83	4 (21%)	26,31,34	1.06	2 (7%)
1	M2G	13	966	1	20,27,28	3.98	7 (35%)	22,40,43	1.41	5 (22%)
1	5MC	1G	1407	1	18,22,23	3.84	7 (38%)	26,32,35	1.09	1 (3%)
25	5MU	1H	1915	25	19,22,23	3.95	5 (26%)	28,32,35	3.28	10 (35%)
1	7MG	13	527	1,58	22,26,27	3.14	6 (27%)	29,39,42	2.82	10 (34%)
1	MA6	13	1518	1	18,26,27	0.97	1 (5%)	19,38,41	2.57	2 (10%)
1	PSU	1G	516	1,59	18,21,22	1.14	1 (5%)	22,30,33	1.76	4 (18%)
25	5MU	14	1915	25	19,22,23	3.99	5 (26%)	28,32,35	3.26	9 (32%)
1	MA6	1G	1519	1	18,26,27	0.97	2 (11%)	19,38,41	2.68	2 (10%)
23	7MG	2K	47	23	22,26,27	3.16	7 (31%)	29,39,42	2.76	10 (34%)
1	4OC	1G	1402	1	20,23,24	2.95	8 (40%)	26,32,35	1.15	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	5MC	1H	1942	25	-	0/7/25/26	0/2/2/2
25	5MC	14	1962	25	-	2/7/25/26	0/2/2/2
57	4SU	2L	8	57	-	3/7/25/26	0/2/2/2
57	7MG	2L	47	57	-	3/7/37/38	0/3/3/3
12	0TD	3I	89	12	-	3/7/12/14	-
23	5MU	2K	55	23	-	0/7/25/26	0/2/2/2
1	UR3	1G	1498	1	-	0/7/25/26	0/2/2/2
1	2MG	1G	1207	1	-	0/5/27/28	0/3/3/3
23	H2U	2K	21	23	-	4/7/38/39	0/2/2/2
57	PSU	2L	56	57	-	0/7/25/26	0/2/2/2
1	5MC	1G	967	1	-	0/7/25/26	0/2/2/2
1	MA6	13	1519	1	-	5/7/29/30	0/3/3/3
25	5MU	14	1939	58,25	-	0/7/25/26	0/2/2/2
1	M2G	1G	966	1	-	0/7/29/30	0/3/3/3
25	5MC	14	1942	25	-	0/7/25/26	0/2/2/2
23	OMC	2K	33	23	-	1/9/27/28	0/2/2/2
25	PSU	1H	2605	25	-	2/7/25/26	0/2/2/2
25	OMU	1H	2552	59,25	-	0/9/27/28	0/2/2/2
1	5MC	1G	1400	1	-	2/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	PSU	13	516	1,59	-	0/7/25/26	0/2/2/2
25	PSU	14	2605	25	-	0/7/25/26	0/2/2/2
25	PSU	14	1911	25	-	0/7/25/26	0/2/2/2
25	OMU	14	2552	59,25	-	0/9/27/28	0/2/2/2
1	MA6	1G	1518	1	-	3/7/29/30	0/3/3/3
1	7MG	1G	527	1,58	-	3/7/37/38	0/3/3/3
25	PSU	1H	1917	25	-	1/7/25/26	0/2/2/2
25	PSU	1H	1911	25	-	0/7/25/26	0/2/2/2
25	5MC	1H	1962	58,25	-	2/7/25/26	0/2/2/2
1	5MC	13	1407	1	-	0/7/25/26	0/2/2/2
25	OMG	1H	2251	58,23,25	-	1/5/27/28	0/3/3/3
23	4SU	2K	8	23	-	0/7/25/26	0/2/2/2
25	OMG	14	2251	58,57,25	-	0/5/27/28	0/3/3/3
1	2MG	13	1207	1	-	1/5/27/28	0/3/3/3
25	OMC	1H	1920	25	-	2/9/27/28	0/2/2/2
12	0TD	3A	89	12	-	3/7/12/14	-
25	5MU	1H	1939	58,25	-	0/7/25/26	0/2/2/2
1	5MC	13	1404	1	-	0/7/25/26	0/2/2/2
1	5MC	13	967	1	-	2/7/25/26	0/2/2/2
25	OMC	14	1920	25	-	2/9/27/28	0/2/2/2
57	5MU	2L	55	57	-	0/7/25/26	0/2/2/2
25	2MA	1H	2503	58,59,25	-	3/3/25/26	0/3/3/3
25	PSU	14	1917	25	-	0/7/25/26	0/2/2/2
1	4OC	13	1402	1	-	2/9/29/30	0/2/2/2
23	PSU	2K	56	23	-	2/7/25/26	0/2/2/2
1	UR3	13	1498	1	-	0/7/25/26	0/2/2/2
1	5MC	13	1400	1	-	2/7/25/26	0/2/2/2
1	5MC	1G	1404	1	-	0/7/25/26	0/2/2/2
25	2MA	14	2503	58,59,25	-	1/3/25/26	0/3/3/3
57	OMC	2L	33	57	-	3/9/27/28	0/2/2/2
1	M2G	13	966	1	-	1/7/29/30	0/3/3/3
1	5MC	1G	1407	1	-	0/7/25/26	0/2/2/2
25	5MU	1H	1915	25	-	0/7/25/26	0/2/2/2
1	7MG	13	527	1,58	-	2/7/37/38	0/3/3/3
1	MA6	13	1518	1	-	0/7/29/30	0/3/3/3
1	PSU	1G	516	1,59	-	0/7/25/26	0/2/2/2
25	5MU	14	1915	25	-	3/7/25/26	0/2/2/2
1	MA6	1G	1519	1	-	3/7/29/30	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
23	7MG	2K	47	23	-	2/7/37/38	0/3/3/3
1	4OC	1G	1402	1	-	2/9/29/30	0/2/2/2

The worst 5 of 288 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	14	2251	OMG	C8-N7	-15.42	1.08	1.35
25	1H	2251	OMG	C8-N7	-15.11	1.09	1.35
1	13	966	M2G	C2-N3	13.12	1.46	1.30
25	14	1915	5MU	C2-N1	13.04	1.59	1.38
25	1H	1915	5MU	C2-N1	12.81	1.59	1.38

The worst 5 of 243 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	1H	1939	5MU	C5-C4-N3	11.86	125.43	115.31
25	14	1939	5MU	C5-C4-N3	11.27	124.93	115.31
25	1H	1915	5MU	C5-C4-N3	10.71	124.45	115.31
25	14	1915	5MU	C5-C4-N3	10.68	124.43	115.31
57	2L	55	5MU	C5-C4-N3	10.49	124.26	115.31

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	3A	89	0TD	CA-CB-SB-CSB
1	13	1402	4OC	O4'-C4'-C5'-O5'
1	1G	1402	4OC	O4'-C4'-C5'-O5'
1	1G	1402	4OC	C3'-C4'-C5'-O5'

There are no ring outliers.

29 monomers are involved in 50 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
25	14	1962	5MC	1	0
57	2L	8	4SU	3	0
23	2K	55	5MU	2	0
1	1G	1498	UR3	2	0
1	1G	1207	2MG	3	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
23	2K	21	H2U	2	0
1	13	1519	MA6	1	0
25	14	1942	5MC	2	0
23	2K	33	OMC	2	0
25	1H	2552	OMU	1	0
1	1G	1400	5MC	1	0
25	14	1911	PSU	1	0
1	1G	1518	MA6	2	0
25	1H	1911	PSU	1	0
1	13	1407	5MC	1	0
25	1H	2251	OMG	3	0
25	14	2251	OMG	3	0
25	1H	1920	OMC	3	0
12	3A	89	0TD	1	0
25	14	1920	OMC	2	0
1	13	1402	4OC	1	0
1	13	1498	UR3	1	0
1	1G	1404	5MC	1	0
25	14	2503	2MA	4	0
57	2L	33	OMC	1	0
1	13	966	M2G	1	0
25	1H	1915	5MU	1	0
1	1G	1519	MA6	1	0
1	1G	1402	4OC	2	0

5.5 Carbohydrates [i](#)

There are no monosaccharides 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%)	-0.89	0 100 100	40, 102, 169, 228	0
1	1G	1498/1522 (98%)	-0.88	0 100 100	53, 104, 169, 213	0
2	12	236/256 (92%)	0.62	18 (7%) 13 14	114, 155, 171, 178	0
2	1E	237/256 (92%)	0.79	34 (14%) 2 3	108, 143, 167, 181	0
3	22	206/239 (86%)	0.34	13 (6%) 20 18	110, 131, 163, 182	0
3	2E	205/239 (85%)	0.97	30 (14%) 2 3	95, 124, 157, 172	0
4	32	208/209 (99%)	-0.60	0 100 100	78, 99, 120, 133	0
4	3E	208/209 (99%)	-0.08	3 (1%) 75 69	83, 112, 134, 144	0
5	42	154/162 (95%)	-0.50	1 (0%) 89 86	86, 105, 134, 174	0
5	4E	151/162 (93%)	-0.03	1 (0%) 87 83	77, 103, 130, 152	0
6	52	101/101 (100%)	0.02	0 100 100	78, 103, 117, 125	0
6	5E	101/101 (100%)	-0.03	3 (2%) 50 44	72, 104, 117, 140	0
7	62	149/156 (95%)	0.22	6 (4%) 38 33	110, 132, 151, 159	0
7	6E	155/156 (99%)	-0.17	3 (1%) 66 61	99, 115, 145, 161	0
8	72	138/138 (100%)	-0.83	0 100 100	83, 107, 123, 128	0
8	7E	138/138 (100%)	-0.45	0 100 100	84, 106, 120, 126	0
9	82	127/128 (99%)	-0.28	1 (0%) 86 81	104, 154, 173, 185	0
9	8E	124/128 (96%)	-0.26	0 100 100	84, 139, 155, 167	0
10	1A	99/105 (94%)	0.43	8 (8%) 12 12	111, 147, 169, 180	0
10	1I	99/105 (94%)	0.56	12 (12%) 4 5	93, 151, 166, 170	0
11	2A	119/129 (92%)	0.50	5 (4%) 36 32	87, 109, 142, 171	0
11	2I	117/129 (90%)	0.60	8 (6%) 17 16	63, 94, 129, 162	0
12	3A	124/132 (93%)	-0.24	1 (0%) 86 81	71, 88, 113, 157	0
12	3I	124/132 (93%)	0.19	5 (4%) 38 33	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%)	-0.14	6 (5%) 28 25	108, 146, 166, 175	0
13	4I	119/126 (94%)	-0.78	0 100 100	81, 123, 139, 150	0
14	5A	60/61 (98%)	-0.23	1 (1%) 70 64	114, 131, 142, 149	0
14	5I	60/61 (98%)	-0.23	1 (1%) 70 64	101, 119, 129, 135	0
15	6A	88/89 (98%)	-0.29	2 (2%) 60 54	72, 98, 121, 128	0
15	6I	88/89 (98%)	-0.67	1 (1%) 80 75	65, 98, 120, 127	0
16	7A	84/88 (95%)	-0.96	0 100 100	75, 88, 106, 142	0
16	7I	83/88 (94%)	-0.93	0 100 100	95, 107, 130, 157	0
17	8A	99/105 (94%)	-0.74	0 100 100	77, 92, 108, 114	0
17	8I	100/105 (95%)	-0.62	0 100 100	75, 98, 113, 120	0
18	9A	71/88 (80%)	0.37	6 (8%) 10 11	86, 107, 135, 146	0
18	9I	70/88 (79%)	0.69	8 (11%) 5 6	78, 100, 127, 152	0
19	AA	83/93 (89%)	0.10	6 (7%) 15 15	120, 151, 166, 171	0
19	AI	86/93 (92%)	-0.65	0 100 100	102, 130, 148, 155	0
20	BA	103/106 (97%)	-0.72	0 100 100	82, 98, 125, 137	0
20	BI	101/106 (95%)	-0.89	0 100 100	92, 110, 130, 137	0
21	1B	25/27 (92%)	-0.61	0 100 100	123, 140, 157, 165	0
21	1F	25/27 (92%)	-0.86	0 100 100	104, 117, 136, 147	0
22	1K	65/77 (84%)	1.68	30 (46%) 0 0	107, 153, 175, 184	59 (90%)
22	3K	77/77 (100%)	-0.34	4 (5%) 27 24	71, 198, 220, 236	0
22	3L	77/77 (100%)	-0.12	2 (2%) 56 49	87, 216, 245, 255	0
23	2K	71/77 (92%)	-0.76	0 100 100	54, 91, 130, 147	0
24	4K	17/27 (62%)	0.30	2 (11%) 4 5	75, 132, 206, 207	0
24	4L	21/27 (77%)	0.01	1 (4%) 30 27	88, 171, 227, 232	0
25	14	2868/2917 (98%)	-0.83	7 (0%) 95 93	40, 79, 193, 238	0
25	1H	2868/2917 (98%)	-0.72	3 (0%) 95 95	27, 61, 173, 226	0
26	16	120/122 (98%)	-0.83	0 100 100	66, 93, 111, 146	0
26	1J	122/122 (100%)	-0.82	1 (0%) 86 81	94, 132, 160, 193	0
27	7I	135/229 (58%)	0.87	22 (16%) 1 2	117, 180, 198, 211	0
28	11	274/276 (99%)	-0.54	1 (0%) 92 90	29, 47, 70, 96	0
28	19	274/276 (99%)	-0.18	0 100 100	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%)	0.26	9 (4%) 34 30	34, 74, 110, 127	0
29	29	204/206 (99%)	-0.45	2 (0%) 82 77	47, 80, 111, 120	0
30	31	202/210 (96%)	-0.38	1 (0%) 91 88	31, 68, 110, 127	0
30	39	206/210 (98%)	0.31	12 (5%) 23 20	46, 91, 152, 177	0
31	41	181/182 (99%)	-0.54	0 100 100	82, 103, 138, 149	0
31	49	181/182 (99%)	0.92	23 (12%) 3 4	118, 146, 161, 184	0
32	51	174/180 (96%)	-0.33	2 (1%) 80 75	72, 98, 118, 136	0
32	59	174/180 (96%)	0.22	9 (5%) 27 24	115, 155, 176, 187	0
33	61	146/148 (98%)	-0.36	1 (0%) 87 83	60, 109, 130, 140	0
33	69	146/148 (98%)	0.02	2 (1%) 75 69	79, 120, 142, 156	0
34	38	139/173 (80%)	0.48	17 (12%) 4 5	156, 193, 210, 232	0
35	15	138/140 (98%)	0.71	14 (10%) 7 7	68, 102, 129, 140	0
35	58	138/140 (98%)	-0.02	4 (2%) 51 45	56, 76, 118, 127	0
36	25	122/122 (100%)	0.13	1 (0%) 86 81	53, 75, 93, 103	0
36	68	122/122 (100%)	0.03	1 (0%) 86 81	45, 65, 85, 105	0
37	35	147/150 (98%)	0.47	7 (4%) 30 27	51, 96, 127, 150	0
37	78	148/150 (98%)	-0.10	3 (2%) 65 60	32, 72, 102, 123	0
38	45	140/141 (99%)	0.88	21 (15%) 2 3	72, 99, 127, 138	0
38	88	141/141 (100%)	0.01	3 (2%) 63 58	46, 73, 106, 128	0
39	55	118/118 (100%)	-0.71	0 100 100	48, 71, 99, 122	0
39	98	118/118 (100%)	-0.18	1 (0%) 86 81	40, 69, 94, 116	0
40	65	111/112 (99%)	0.32	5 (4%) 33 29	103, 125, 139, 148	0
40	A8	111/112 (99%)	0.46	9 (8%) 12 12	75, 93, 115, 127	0
41	75	137/146 (93%)	-0.73	0 100 100	68, 84, 137, 157	0
41	B8	137/146 (93%)	-0.41	0 100 100	61, 81, 134, 164	0
42	85	117/118 (99%)	0.80	22 (18%) 1 1	57, 90, 147, 158	0
42	C8	117/118 (99%)	-0.58	0 100 100	37, 63, 101, 120	0
43	95	101/101 (100%)	2.27	51 (50%) 0 0	53, 123, 143, 159	0
43	D8	100/101 (99%)	-0.17	2 (2%) 65 60	41, 90, 118, 134	0
44	A5	112/113 (99%)	-0.42	1 (0%) 84 79	52, 66, 100, 144	0
44	E8	113/113 (100%)	-0.27	2 (1%) 68 62	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%)	-0.41	2 (2%) 62 56	58, 77, 106, 124	0
45	F8	95/96 (98%)	-0.41	0 100 100	42, 56, 85, 99	0
46	C5	109/110 (99%)	0.17	6 (5%) 25 22	73, 102, 120, 128	0
46	G8	107/110 (97%)	-0.46	0 100 100	62, 87, 135, 148	0
47	D5	176/206 (85%)	1.27	43 (24%) 0 0	117, 145, 178, 186	0
47	H8	174/206 (84%)	0.60	14 (8%) 12 12	79, 118, 177, 192	0
48	E5	79/85 (92%)	0.67	5 (6%) 20 18	70, 90, 113, 160	0
48	I8	77/85 (90%)	0.06	1 (1%) 77 71	49, 67, 93, 114	0
49	F5	92/96 (95%)	0.06	0 100 100	54, 79, 115, 130	0
49	J8	96/96 (100%)	-0.34	1 (1%) 82 77	41, 66, 117, 150	0
50	G5	69/72 (95%)	-0.40	1 (1%) 75 69	69, 95, 121, 145	0
50	K8	71/72 (98%)	-0.46	1 (1%) 75 69	45, 69, 89, 110	0
51	H5	59/60 (98%)	1.24	13 (22%) 0 0	70, 97, 146, 169	0
51	L8	59/60 (98%)	0.11	2 (3%) 45 40	49, 71, 105, 114	0
52	I5	71/71 (100%)	1.66	28 (39%) 0 0	147, 178, 194, 204	0
52	M8	66/71 (92%)	-0.35	0 100 100	114, 141, 171, 192	0
53	J5	56/60 (93%)	-0.33	0 100 100	50, 76, 143, 153	0
53	N8	56/60 (93%)	0.18	4 (7%) 16 15	35, 75, 145, 151	0
54	K5	48/54 (88%)	3.56	31 (64%) 0 0	128, 165, 181, 188	0
54	O8	49/54 (90%)	4.07	43 (87%) 0 0	106, 140, 158, 162	0
55	L5	48/49 (97%)	-0.37	0 100 100	41, 51, 82, 94	0
55	P8	48/49 (97%)	-0.68	0 100 100	26, 35, 71, 76	0
56	M5	64/65 (98%)	0.41	1 (1%) 72 66	59, 73, 98, 119	0
56	Q8	64/65 (98%)	-0.25	0 100 100	38, 53, 74, 95	0
57	2L	72/77 (93%)	-0.54	1 (1%) 75 69	67, 113, 154, 178	0
All	All	21207/22013 (96%)	-0.32	678 (3%) 47 42	26, 95, 171, 255	59 (0%)

The worst 5 of 678 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
11	2I	129	SER	11.5
27	71	1	PRO	10.6
54	O8	44	ARG	10.5

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Mol	Chain	Res	Type	RSRZ
54	K5	50	ARG	10.1
54	O8	42	TRP	10.1

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

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
23	H2U	2K	21	20/21	0.88	0.22	117,140,147,150	0
57	4SU	2L	8	20/21	0.88	0.12	120,131,140,141	0
25	5MU	14	1915	21/22	0.89	0.11	116,128,139,153	0
57	PSU	2L	56	20/21	0.90	0.10	123,128,134,135	0
12	0TD	3A	89	10/11	0.91	0.27	89,95,100,105	0
23	5MU	2K	55	21/22	0.91	0.12	103,113,125,145	0
23	PSU	2K	56	20/21	0.91	0.11	92,104,120,124	0
57	7MG	2L	47	24/25	0.92	0.15	114,141,151,162	0
1	PSU	1G	516	20/21	0.92	0.12	98,102,108,110	0
25	2MA	14	2503	23/24	0.93	0.17	39,50,63,79	0
1	2MG	13	1207	24/25	0.93	0.14	100,112,118,119	0
12	0TD	3I	89	10/11	0.93	0.25	81,87,92,107	0
57	5MU	2L	55	21/22	0.93	0.11	119,129,134,137	0
23	7MG	2K	47	24/25	0.93	0.13	96,105,114,126	0
1	MA6	1G	1519	24/25	0.94	0.16	64,79,84,86	0
1	M2G	1G	966	25/26	0.94	0.12	87,107,115,124	0
1	5MC	1G	967	21/22	0.94	0.09	92,107,118,120	0
1	7MG	1G	527	24/25	0.94	0.13	88,99,101,102	0
1	4OC	1G	1402	22/23	0.94	0.14	71,84,91,99	0
25	PSU	14	1911	20/21	0.94	0.10	86,94,118,121	0
1	7MG	13	527	24/25	0.95	0.14	71,80,86,92	0
25	PSU	1H	1917	20/21	0.95	0.10	65,76,90,91	0
25	PSU	14	1917	20/21	0.95	0.13	87,104,109,110	0
25	OMC	14	1920	21/22	0.95	0.17	73,91,99,102	0
25	5MC	14	1962	21/22	0.95	0.13	59,67,76,83	0
25	2MA	1H	2503	23/24	0.95	0.17	30,38,48,59	0
1	2MG	1G	1207	24/25	0.95	0.12	115,120,125,127	0
1	5MC	13	967	21/22	0.95	0.16	71,82,94,99	0
1	M2G	13	966	25/26	0.95	0.15	68,77,90,94	0
23	4SU	2K	8	20/21	0.95	0.12	85,91,97,101	0
25	5MU	1H	1915	21/22	0.95	0.12	75,91,102,116	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
1	5MC	13	1400	21/22	0.96	0.13	58,74,79,86	0
1	5MC	1G	1400	21/22	0.96	0.12	81,92,98,102	0
25	OMC	1H	1920	21/22	0.96	0.12	60,66,70,72	0
1	PSU	13	516	20/21	0.96	0.09	84,95,98,98	0
25	5MU	1H	1939	21/22	0.96	0.15	36,41,48,50	0
25	5MU	14	1939	21/22	0.96	0.15	44,52,57,62	0
25	5MC	1H	1942	21/22	0.96	0.14	39,50,56,61	0
25	5MC	14	1942	21/22	0.96	0.18	62,71,82,90	0
25	5MC	1H	1962	21/22	0.96	0.14	50,57,61,66	0
23	OMC	2K	33	21/22	0.96	0.13	77,82,89,101	0
25	OMG	14	2251	24/25	0.96	0.12	51,57,64,69	0
1	5MC	1G	1404	21/22	0.96	0.11	77,85,89,91	0
1	5MC	13	1407	21/22	0.96	0.13	53,59,65,67	0
25	OMU	1H	2552	21/22	0.96	0.18	37,45,51,53	0
25	PSU	1H	2605	20/21	0.96	0.15	35,40,48,53	0
25	PSU	14	2605	20/21	0.96	0.12	42,52,74,77	0
1	5MC	1G	1407	21/22	0.96	0.11	75,80,85,98	0
1	UR3	13	1498	21/22	0.96	0.16	44,62,69,73	0
1	UR3	1G	1498	21/22	0.96	0.14	65,76,83,86	0
1	MA6	13	1518	24/25	0.96	0.15	50,57,61,62	0
25	OMU	14	2552	21/22	0.97	0.14	48,55,62,67	0
1	5MC	13	1404	21/22	0.97	0.12	54,59,69,79	0
25	OMG	1H	2251	24/25	0.97	0.12	36,43,49,53	0
1	MA6	1G	1518	24/25	0.97	0.13	68,78,82,84	0
57	OMC	2L	33	21/22	0.97	0.12	91,100,107,111	0
25	PSU	1H	1911	20/21	0.97	0.12	50,63,72,74	0
1	MA6	13	1519	24/25	0.97	0.14	51,56,62,64	0
1	4OC	13	1402	22/23	0.97	0.15	61,71,79,84	0

6.3 Carbohydrates [i](#)

There are no monosaccharides 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(\AA^2)	Q<0.9
58	K	1H	3052	1/1	0.22	0.19	127,127,127,127	0
59	MG	14	3381	1/1	0.28	0.13	77,77,77,77	0
59	MG	7I	101	1/1	0.31	0.19	124,124,124,124	0
59	MG	14	3338	1/1	0.34	0.10	73,73,73,73	0
59	MG	14	3265	1/1	0.38	0.21	67,67,67,67	0
59	MG	14	3398	1/1	0.38	0.14	63,63,63,63	0
59	MG	1G	1696	1/1	0.44	0.11	129,129,129,129	0
59	MG	2L	102	1/1	0.44	0.12	132,132,132,132	0
58	K	5E	201	1/1	0.47	0.22	113,113,113,113	0
58	K	4I	202	1/1	0.52	0.16	128,128,128,128	0
59	MG	14	3402	1/1	0.53	0.06	123,123,123,123	0
59	MG	1H	3310	1/1	0.55	0.26	78,78,78,78	0
59	MG	1H	3188	1/1	0.55	0.28	84,84,84,84	0
59	MG	14	3380	1/1	0.57	0.10	70,70,70,70	0
59	MG	13	1733	1/1	0.57	0.15	117,117,117,117	0
59	MG	13	1741	1/1	0.57	0.08	106,106,106,106	0
59	MG	1G	1716	1/1	0.57	0.10	107,107,107,107	0
59	MG	14	3243	1/1	0.58	0.23	74,74,74,74	0
59	MG	1H	3430	1/1	0.60	0.08	79,79,79,79	0
59	MG	14	3389	1/1	0.60	0.14	69,69,69,69	0
59	MG	1G	1704	1/1	0.61	0.07	110,110,110,110	0
58	K	1G	1604	1/1	0.62	0.19	111,111,111,111	0
59	MG	1G	1648	1/1	0.62	0.42	83,83,83,83	0
58	K	32	301	1/1	0.63	0.07	133,133,133,133	0
59	MG	16	210	1/1	0.63	0.09	98,98,98,98	0
58	K	1G	1606	1/1	0.63	0.11	102,102,102,102	0
59	MG	1G	1691	1/1	0.63	0.11	84,84,84,84	0
59	MG	14	3378	1/1	0.64	0.13	71,71,71,71	0
58	K	14	3091	1/1	0.65	0.11	103,103,103,103	0
59	MG	1H	3435	1/1	0.65	0.10	72,72,72,72	0
59	MG	1G	1725	1/1	0.66	0.08	97,97,97,97	0
59	MG	1H	3467	1/1	0.66	0.13	67,67,67,67	0
59	MG	14	3240	1/1	0.66	0.09	59,59,59,59	0
59	MG	1H	3446	1/1	0.67	0.07	92,92,92,92	0
59	MG	1H	3514	1/1	0.67	0.08	88,88,88,88	0
58	K	1H	3110	1/1	0.68	0.22	111,111,111,111	0
59	MG	14	3308	1/1	0.68	0.12	80,80,80,80	0
58	K	1H	3079	1/1	0.68	0.22	114,114,114,114	0
59	MG	1H	3513	1/1	0.69	0.06	105,105,105,105	0
59	MG	13	1699	1/1	0.69	0.21	68,68,68,68	0
59	MG	1G	1671	1/1	0.69	0.35	79,79,79,79	0
59	MG	14	3293	1/1	0.69	0.05	91,91,91,91	0
58	K	13	1634	1/1	0.70	0.12	111,111,111,111	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
59	MG	14	3350	1/1	0.70	0.18	69,69,69,69	0
59	MG	14	3356	1/1	0.70	0.14	84,84,84,84	0
59	MG	14	3175	1/1	0.70	0.24	59,59,59,59	0
59	MG	13	1738	1/1	0.70	0.10	91,91,91,91	0
59	MG	1H	3522	1/1	0.70	0.12	102,102,102,102	0
59	MG	1H	3487	1/1	0.70	0.09	85,85,85,85	0
59	MG	1H	3498	1/1	0.70	0.18	37,37,37,37	0
59	MG	1G	1661	1/1	0.70	0.24	114,114,114,114	0
59	MG	14	3277	1/1	0.71	0.14	53,53,53,53	0
58	K	14	3042	1/1	0.71	0.16	83,83,83,83	0
59	MG	14	3202	1/1	0.71	0.15	84,84,84,84	0
59	MG	1H	3509	1/1	0.71	0.08	101,101,101,101	0
58	K	1H	3099	1/1	0.71	0.21	81,81,81,81	0
59	MG	14	3172	1/1	0.71	0.13	72,72,72,72	0
59	MG	1H	3363	1/1	0.72	0.13	32,32,32,32	0
58	K	5I	101	1/1	0.72	0.09	129,129,129,129	0
59	MG	1G	1663	1/1	0.72	0.26	73,73,73,73	0
59	MG	1H	3351	1/1	0.72	0.12	33,33,33,33	0
59	MG	1H	3492	1/1	0.73	0.09	67,67,67,67	0
58	K	1G	1613	1/1	0.73	0.09	96,96,96,96	0
59	MG	14	3274	1/1	0.73	0.12	30,30,30,30	0
59	MG	14	3275	1/1	0.73	0.07	58,58,58,58	0
59	MG	14	3174	1/1	0.73	0.21	78,78,78,78	0
59	MG	14	3370	1/1	0.73	0.12	56,56,56,56	0
59	MG	1G	1693	1/1	0.74	0.06	89,89,89,89	0
59	MG	1H	3424	1/1	0.74	0.14	84,84,84,84	0
59	MG	1H	3474	1/1	0.74	0.09	47,47,47,47	0
59	MG	1G	1709	1/1	0.74	0.12	102,102,102,102	0
59	MG	14	3306	1/1	0.74	0.12	49,49,49,49	0
59	MG	13	1744	1/1	0.74	0.07	107,107,107,107	0
59	MG	14	3392	1/1	0.74	0.08	69,69,69,69	0
59	MG	1H	3450	1/1	0.74	0.05	91,91,91,91	0
59	MG	1H	3457	1/1	0.74	0.12	35,35,35,35	0
59	MG	1J	202	1/1	0.74	0.16	69,69,69,69	0
58	K	39	301	1/1	0.75	0.07	107,107,107,107	0
59	MG	1H	3419	1/1	0.75	0.13	43,43,43,43	0
58	K	14	3036	1/1	0.75	0.10	85,85,85,85	0
59	MG	3E	301	1/1	0.75	0.15	84,84,84,84	0
59	MG	1G	1695	1/1	0.75	0.05	97,97,97,97	0
59	MG	13	1723	1/1	0.75	0.08	109,109,109,109	0
59	MG	13	1731	1/1	0.75	0.07	92,92,92,92	0
59	MG	1H	3515	1/1	0.75	0.10	90,90,90,90	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
58	K	16	202	1/1	0.75	0.11	116,116,116,116	0
59	MG	1H	3327	1/1	0.75	0.33	72,72,72,72	0
59	MG	1H	3337	1/1	0.75	0.09	37,37,37,37	0
58	K	13	1605	1/1	0.75	0.17	94,94,94,94	0
59	MG	1H	3215	1/1	0.76	0.27	65,65,65,65	0
59	MG	1H	3476	1/1	0.76	0.17	42,42,42,42	0
59	MG	1G	1703	1/1	0.76	0.06	93,93,93,93	0
59	MG	1H	3244	1/1	0.76	0.17	52,52,52,52	0
59	MG	14	3250	1/1	0.76	0.27	84,84,84,84	0
59	MG	1G	1707	1/1	0.76	0.10	120,120,120,120	0
59	MG	1H	3286	1/1	0.76	0.21	52,52,52,52	0
59	MG	1H	3397	1/1	0.76	0.14	29,29,29,29	0
59	MG	1H	3508	1/1	0.76	0.22	78,78,78,78	0
59	MG	13	1740	1/1	0.76	0.09	105,105,105,105	0
58	K	1H	3030	1/1	0.76	0.26	86,86,86,86	0
59	MG	1H	3472	1/1	0.76	0.09	71,71,71,71	0
59	MG	14	3300	1/1	0.77	0.11	41,41,41,41	0
59	MG	1H	3511	1/1	0.77	0.06	93,93,93,93	0
58	K	1H	3034	1/1	0.77	0.11	83,83,83,83	0
59	MG	1H	3418	1/1	0.77	0.06	58,58,58,58	0
59	MG	1G	1664	1/1	0.77	0.31	73,73,73,73	0
59	MG	1H	3486	1/1	0.78	0.10	54,54,54,54	0
59	MG	14	3134	1/1	0.78	0.09	67,67,67,67	0
59	MG	1H	3361	1/1	0.78	0.14	32,32,32,32	0
59	MG	14	3374	1/1	0.78	0.13	96,96,96,96	0
59	MG	14	3276	1/1	0.78	0.07	44,44,44,44	0
58	K	14	3083	1/1	0.78	0.17	119,119,119,119	0
59	MG	14	3288	1/1	0.78	0.13	79,79,79,79	0
59	MG	13	1734	1/1	0.78	0.07	61,61,61,61	0
59	MG	13	1710	1/1	0.78	0.37	97,97,97,97	0
59	MG	1G	1690	1/1	0.78	0.11	109,109,109,109	0
59	MG	1H	3301	1/1	0.78	0.18	59,59,59,59	0
59	MG	D8	203	1/1	0.78	0.18	55,55,55,55	0
59	MG	1J	205	1/1	0.78	0.05	104,104,104,104	0
58	K	1H	3094	1/1	0.79	0.14	65,65,65,65	0
58	K	13	1602	1/1	0.79	0.06	113,113,113,113	0
58	K	1H	3048	1/1	0.79	0.12	67,67,67,67	0
59	MG	1G	1722	1/1	0.79	0.07	97,97,97,97	0
59	MG	1H	3461	1/1	0.79	0.16	33,33,33,33	0
58	K	1G	1619	1/1	0.79	0.06	79,79,79,79	0
59	MG	1H	3347	1/1	0.79	0.20	50,50,50,50	0
58	K	1H	3117	1/1	0.79	0.21	85,85,85,85	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
59	MG	14	3361	1/1	0.79	0.06	71,71,71,71	0
58	K	1H	3013	1/1	0.79	0.11	83,83,83,83	0
59	MG	1H	3161	1/1	0.79	0.15	32,32,32,32	0
59	MG	13	1729	1/1	0.79	0.06	68,68,68,68	0
59	MG	1G	1685	1/1	0.79	0.07	87,87,87,87	0
59	MG	1H	3402	1/1	0.79	0.13	63,63,63,63	0
59	MG	14	3386	1/1	0.79	0.10	82,82,82,82	0
59	MG	1H	3211	1/1	0.79	0.21	47,47,47,47	0
59	MG	1H	3504	1/1	0.79	0.18	85,85,85,85	0
58	K	13	1606	1/1	0.79	0.08	87,87,87,87	0
59	MG	1H	3242	1/1	0.79	0.13	57,57,57,57	0
58	K	14	3055	1/1	0.79	0.14	116,116,116,116	0
58	K	14	3067	1/1	0.79	0.09	90,90,90,90	0
59	MG	1H	3222	1/1	0.80	0.28	67,67,67,67	0
59	MG	1G	1641	1/1	0.80	0.16	53,53,53,53	0
59	MG	1H	3480	1/1	0.80	0.10	58,58,58,58	0
59	MG	1H	3423	1/1	0.80	0.12	33,33,33,33	0
59	MG	14	3102	1/1	0.80	0.10	57,57,57,57	0
58	K	1G	1605	1/1	0.80	0.10	92,92,92,92	0
59	MG	1H	3489	1/1	0.80	0.06	76,76,76,76	0
59	MG	1H	3426	1/1	0.80	0.15	68,68,68,68	0
58	K	1G	1622	1/1	0.80	0.08	118,118,118,118	0
59	MG	14	3186	1/1	0.80	0.17	48,48,48,48	0
59	MG	1H	3284	1/1	0.80	0.20	66,66,66,66	0
59	MG	14	3234	1/1	0.80	0.23	67,67,67,67	0
58	K	1H	3088	1/1	0.80	0.13	74,74,74,74	0
59	MG	1H	3288	1/1	0.80	0.12	51,51,51,51	0
59	MG	1H	3380	1/1	0.80	0.11	61,61,61,61	0
59	MG	14	3251	1/1	0.80	0.17	52,52,52,52	0
59	MG	1H	3389	1/1	0.80	0.14	38,38,38,38	0
59	MG	1H	3465	1/1	0.80	0.14	39,39,39,39	0
59	MG	13	1700	1/1	0.80	0.19	63,63,63,63	0
58	K	13	1635	1/1	0.80	0.55	104,104,104,104	0
59	MG	1H	3311	1/1	0.80	0.29	57,57,57,57	0
59	MG	29	304	1/1	0.80	0.14	62,62,62,62	0
59	MG	1H	3318	1/1	0.81	0.35	85,85,85,85	0
59	MG	1H	3322	1/1	0.81	0.16	60,60,60,60	0
59	MG	1H	3503	1/1	0.81	0.08	63,63,63,63	0
59	MG	1H	3326[A]	1/1	0.81	0.46	58,58,58,58	1
59	MG	1H	3427	1/1	0.81	0.21	41,41,41,41	0
59	MG	1H	3326[B]	1/1	0.81	0.46	55,55,55,55	1
59	MG	1H	3434	1/1	0.81	0.13	68,68,68,68	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
59	MG	14	3321	1/1	0.81	0.11	51,51,51,51	0
58	K	14	3027	1/1	0.81	0.10	97,97,97,97	0
59	MG	14	3347	1/1	0.81	0.15	57,57,57,57	0
58	K	13	1608	1/1	0.81	0.15	96,96,96,96	0
59	MG	14	3351	1/1	0.81	0.10	61,61,61,61	0
59	MG	1H	3265	1/1	0.81	0.26	63,63,63,63	0
59	MG	1H	3282	1/1	0.81	0.16	48,48,48,48	0
59	MG	1H	3459	1/1	0.81	0.17	50,50,50,50	0
59	MG	14	3372	1/1	0.81	0.07	73,73,73,73	0
58	K	1H	3061	1/1	0.81	0.17	47,47,47,47	0
59	MG	1H	3170	1/1	0.81	0.16	47,47,47,47	0
58	K	14	3052	1/1	0.81	0.13	105,105,105,105	0
59	MG	1H	3471	1/1	0.81	0.13	30,30,30,30	0
59	MG	1H	3292	1/1	0.81	0.14	54,54,54,54	0
59	MG	14	3387	1/1	0.81	0.18	45,45,45,45	0
59	MG	1H	3296	1/1	0.81	0.08	50,50,50,50	0
58	K	1G	1601	1/1	0.81	0.09	102,102,102,102	0
59	MG	1H	3477	1/1	0.81	0.11	43,43,43,43	0
59	MG	1H	3404	1/1	0.81	0.14	65,65,65,65	0
59	MG	1H	3414	1/1	0.81	0.05	89,89,89,89	0
58	K	1H	3072	1/1	0.81	0.16	100,100,100,100	0
58	K	16	201	1/1	0.81	0.08	102,102,102,102	0
59	MG	14	3252	1/1	0.82	0.24	75,75,75,75	0
59	MG	BI	202	1/1	0.82	0.10	94,94,94,94	0
58	K	1H	3113[B]	1/1	0.82	0.16	39,39,39,39	1
59	MG	14	3103	1/1	0.82	0.12	82,82,82,82	0
58	K	14	3094	1/1	0.82	0.10	111,111,111,111	0
59	MG	14	3155	1/1	0.82	0.11	57,57,57,57	0
59	MG	14	3379	1/1	0.82	0.19	42,42,42,42	0
59	MG	1H	3177	1/1	0.82	0.15	54,54,54,54	0
59	MG	D8	201	1/1	0.82	0.14	71,71,71,71	0
59	MG	1H	3180	1/1	0.82	0.28	72,72,72,72	0
59	MG	1G	1628	1/1	0.82	0.36	92,92,92,92	0
59	MG	1H	3385	1/1	0.82	0.08	69,69,69,69	0
59	MG	1H	3325	1/1	0.82	0.20	65,65,65,65	0
59	MG	14	3327	1/1	0.82	0.09	66,66,66,66	0
58	K	14	3026	1/1	0.82	0.08	109,109,109,109	0
59	MG	1J	201	1/1	0.82	0.11	131,131,131,131	0
59	MG	13	1691	1/1	0.82	0.22	88,88,88,88	0
58	K	14	3075	1/1	0.82	0.28	116,116,116,116	0
58	K	1H	3113[A]	1/1	0.82	0.16	45,45,45,45	1
59	MG	13	1730	1/1	0.83	0.09	79,79,79,79	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
59	MG	1H	3278	1/1	0.83	0.29	68,68,68,68	0
59	MG	14	3323	1/1	0.83	0.09	47,47,47,47	0
58	K	1G	1609	1/1	0.83	0.12	113,113,113,113	0
59	MG	1H	3328	1/1	0.83	0.14	61,61,61,61	0
59	MG	13	1732	1/1	0.83	0.18	81,81,81,81	0
59	MG	1H	3344	1/1	0.83	0.12	21,21,21,21	0
59	MG	1G	1683	1/1	0.83	0.14	90,90,90,90	0
59	MG	1H	3285	1/1	0.83	0.28	66,66,66,66	0
59	MG	14	3233	1/1	0.83	0.14	80,80,80,80	0
59	MG	1H	3348	1/1	0.83	0.11	34,34,34,34	0
58	K	14	3079	1/1	0.83	0.08	112,112,112,112	0
59	MG	1H	3355	1/1	0.83	0.10	32,32,32,32	0
59	MG	13	1698	1/1	0.83	0.23	67,67,67,67	0
58	K	13	1625	1/1	0.83	0.06	94,94,94,94	0
59	MG	1H	3373	1/1	0.83	0.12	39,39,39,39	0
59	MG	1H	3203	1/1	0.83	0.21	52,52,52,52	0
59	MG	1H	3207	1/1	0.83	0.17	56,56,56,56	0
59	MG	1H	3520	1/1	0.83	0.14	70,70,70,70	0
58	K	14	3088	1/1	0.83	0.16	101,101,101,101	0
59	MG	13	1707	1/1	0.83	0.22	65,65,65,65	0
58	K	14	3089	1/1	0.83	0.09	97,97,97,97	0
59	MG	14	3289	1/1	0.83	0.10	53,53,53,53	0
59	MG	14	3291	1/1	0.83	0.12	64,64,64,64	0
59	MG	1G	1727	1/1	0.83	0.05	93,93,93,93	0
58	K	1H	3089	1/1	0.83	0.08	50,50,50,50	0
58	K	1H	3003	1/1	0.83	0.09	76,76,76,76	0
59	MG	14	3295	1/1	0.84	0.15	51,51,51,51	0
59	MG	1H	3523	1/1	0.84	0.10	34,34,34,34	0
58	K	1H	3008	1/1	0.84	0.15	61,61,61,61	0
58	K	31	301	1/1	0.84	0.11	60,60,60,60	0
59	MG	13	1718	1/1	0.84	0.06	89,89,89,89	0
59	MG	1H	3392	1/1	0.84	0.12	32,32,32,32	0
58	K	1H	3112	1/1	0.84	0.15	87,87,87,87	0
59	MG	14	3332	1/1	0.84	0.06	110,110,110,110	0
59	MG	1H	3231	1/1	0.84	0.40	67,67,67,67	0
59	MG	4I	201	1/1	0.84	0.21	84,84,84,84	0
58	K	1H	3009	1/1	0.84	0.17	97,97,97,97	0
59	MG	1H	3416	1/1	0.84	0.20	59,59,59,59	0
59	MG	BI	201	1/1	0.84	0.13	108,108,108,108	0
59	MG	1H	3275	1/1	0.84	0.20	60,60,60,60	0
59	MG	13	1662	1/1	0.84	0.19	67,67,67,67	0
59	MG	1G	1686	1/1	0.84	0.07	94,94,94,94	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
59	MG	13	1671	1/1	0.84	0.14	65,65,65,65	0
58	K	1H	3090	1/1	0.84	0.08	65,65,65,65	0
58	K	1H	3039	1/1	0.84	0.10	81,81,81,81	0
59	MG	1H	3428	1/1	0.84	0.09	55,55,55,55	0
59	MG	14	3254	1/1	0.84	0.13	71,71,71,71	0
59	MG	14	3384	1/1	0.84	0.06	108,108,108,108	0
59	MG	1H	3350	1/1	0.84	0.12	26,26,26,26	0
59	MG	14	3270	1/1	0.84	0.10	57,57,57,57	0
59	MG	1H	3178	1/1	0.84	0.17	34,34,34,34	0
58	K	13	1601	1/1	0.84	0.09	87,87,87,87	0
58	K	1G	1607	1/1	0.84	0.07	93,93,93,93	0
59	MG	1H	3449	1/1	0.84	0.08	57,57,57,57	0
59	MG	1G	1711	1/1	0.84	0.10	104,104,104,104	0
59	MG	1H	3200	1/1	0.84	0.14	67,67,67,67	0
59	MG	13	1739	1/1	0.84	0.06	97,97,97,97	0
59	MG	1H	3375	1/1	0.84	0.08	69,69,69,69	0
59	MG	1H	3431	1/1	0.85	0.07	85,85,85,85	0
59	MG	1G	1710	1/1	0.85	0.05	70,70,70,70	0
58	K	1H	3041	1/1	0.85	0.10	66,66,66,66	0
59	MG	1G	1712	1/1	0.85	0.07	106,106,106,106	0
59	MG	13	1695	1/1	0.85	0.22	76,76,76,76	0
58	K	13	1636	1/1	0.85	0.16	136,136,136,136	0
58	K	14	3001	1/1	0.85	0.13	87,87,87,87	0
59	MG	14	3368	1/1	0.85	0.15	40,40,40,40	0
59	MG	1H	3315	1/1	0.85	0.20	70,70,70,70	0
58	K	14	3012	1/1	0.85	0.07	91,91,91,91	0
59	MG	1H	3352	1/1	0.85	0.15	59,59,59,59	0
59	MG	14	3377	1/1	0.85	0.11	70,70,70,70	0
58	K	1H	3069	1/1	0.85	0.10	74,74,74,74	0
59	MG	13	1736	1/1	0.85	0.08	100,100,100,100	0
58	K	1G	1615	1/1	0.85	0.18	106,106,106,106	0
59	MG	14	3290	1/1	0.85	0.09	48,48,48,48	0
59	MG	1H	3470	1/1	0.85	0.09	45,45,45,45	0
59	MG	14	3173	1/1	0.85	0.27	64,64,64,64	0
59	MG	1H	3369	1/1	0.85	0.11	52,52,52,52	0
59	MG	14	3297	1/1	0.85	0.05	44,44,44,44	0
59	MG	13	1670	1/1	0.85	0.25	72,72,72,72	0
58	K	1H	3121	1/1	0.85	0.14	66,66,66,66	0
59	MG	1H	3235	1/1	0.85	0.18	62,62,62,62	0
59	MG	14	3310	1/1	0.85	0.11	27,27,27,27	0
59	MG	1H	3429	1/1	0.85	0.08	63,63,63,63	0
59	MG	21	301	1/1	0.85	0.08	34,34,34,34	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
59	MG	1H	3335	1/1	0.85	0.18	50,50,50,50	0
58	K	14	3082	1/1	0.86	0.20	76,76,76,76	0
59	MG	1G	1630	1/1	0.86	0.20	64,64,64,64	0
58	K	14	3031	1/1	0.86	0.05	78,78,78,78	0
58	K	1G	1624	1/1	0.86	0.12	116,116,116,116	0
59	MG	1G	1651	1/1	0.86	0.20	63,63,63,63	0
59	MG	14	3302	1/1	0.86	0.07	52,52,52,52	0
59	MG	14	3140	1/1	0.86	0.20	45,45,45,45	0
59	MG	14	3141	1/1	0.86	0.22	60,60,60,60	0
59	MG	14	3145	1/1	0.86	0.20	86,86,86,86	0
59	MG	14	3154	1/1	0.86	0.25	72,72,72,72	0
59	MG	1H	3484	1/1	0.86	0.14	47,47,47,47	0
58	K	1H	3086	1/1	0.86	0.18	79,79,79,79	0
58	K	14	3050	1/1	0.86	0.15	81,81,81,81	0
59	MG	13	1701	1/1	0.86	0.16	72,72,72,72	0
59	MG	1G	1681	1/1	0.86	0.09	49,49,49,49	0
59	MG	14	3181	1/1	0.86	0.17	46,46,46,46	0
59	MG	14	3185	1/1	0.86	0.27	76,76,76,76	0
59	MG	1H	3290	1/1	0.86	0.26	51,51,51,51	0
59	MG	14	3357	1/1	0.86	0.21	95,95,95,95	0
59	MG	14	3359	1/1	0.86	0.16	94,94,94,94	0
59	MG	14	3190	1/1	0.86	0.13	81,81,81,81	0
59	MG	1H	3496	1/1	0.86	0.08	64,64,64,64	0
59	MG	1H	3201	1/1	0.86	0.15	48,48,48,48	0
58	K	1H	3092	1/1	0.86	0.09	70,70,70,70	0
58	K	1H	3082	1/1	0.86	0.10	80,80,80,80	0
59	MG	14	3375	1/1	0.86	0.17	57,57,57,57	0
59	MG	13	1658	1/1	0.86	0.13	35,35,35,35	0
58	K	14	3013	1/1	0.86	0.08	98,98,98,98	0
59	MG	1H	3312	1/1	0.86	0.13	70,70,70,70	0
59	MG	1G	1697	1/1	0.86	0.09	81,81,81,81	0
59	MG	1H	3221	1/1	0.86	0.28	77,77,77,77	0
59	MG	14	3382	1/1	0.86	0.07	77,77,77,77	0
59	MG	14	3256	1/1	0.86	0.18	64,64,64,64	0
59	MG	13	1665	1/1	0.86	0.19	50,50,50,50	0
59	MG	14	3267	1/1	0.86	0.20	92,92,92,92	0
59	MG	1H	3319	1/1	0.86	0.11	55,55,55,55	0
59	MG	13	1669	1/1	0.86	0.13	53,53,53,53	0
59	MG	14	3394	1/1	0.86	0.10	82,82,82,82	0
59	MG	14	3395	1/1	0.86	0.12	50,50,50,50	0
58	K	1H	3084	1/1	0.86	0.11	77,77,77,77	0
59	MG	1H	3239	1/1	0.86	0.41	83,83,83,83	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
59	MG	1H	3133	1/1	0.86	0.18	55,55,55,55	0
59	MG	1H	3151	1/1	0.86	0.26	54,54,54,54	0
58	K	1H	3103	1/1	0.86	0.13	65,65,65,65	0
59	MG	1H	3167	1/1	0.86	0.17	33,33,33,33	0
59	MG	1H	3506	1/1	0.87	0.08	65,65,65,65	0
59	MG	1H	3391	1/1	0.87	0.11	31,31,31,31	0
59	MG	1G	1684	1/1	0.87	0.14	75,75,75,75	0
58	K	1H	3031	1/1	0.87	0.11	96,96,96,96	0
59	MG	1H	3341	1/1	0.87	0.20	31,31,31,31	0
59	MG	1H	3398	1/1	0.87	0.05	74,74,74,74	0
59	MG	13	1656	1/1	0.87	0.24	73,73,73,73	0
59	MG	13	1688	1/1	0.87	0.25	83,83,83,83	0
59	MG	14	3376	1/1	0.87	0.21	61,61,61,61	0
59	MG	1H	3518	1/1	0.87	0.11	40,40,40,40	0
59	MG	1H	3159	1/1	0.87	0.17	68,68,68,68	0
59	MG	13	1690	1/1	0.87	0.22	77,77,77,77	0
59	MG	1G	1700	1/1	0.87	0.11	108,108,108,108	0
58	K	14	3037	1/1	0.87	0.08	60,60,60,60	0
58	K	1H	3010	1/1	0.87	0.12	93,93,93,93	0
59	MG	1H	3323	1/1	0.87	0.34	73,73,73,73	0
59	MG	1H	3360	1/1	0.87	0.12	39,39,39,39	0
59	MG	1H	3324	1/1	0.87	0.34	59,59,59,59	0
59	MG	1H	3173	1/1	0.87	0.14	57,57,57,57	0
59	MG	13	1664	1/1	0.87	0.10	53,53,53,53	0
59	MG	1H	3371	1/1	0.87	0.10	35,35,35,35	0
58	K	13	1623	1/1	0.87	0.10	121,121,121,121	0
59	MG	1H	3374	1/1	0.87	0.06	70,70,70,70	0
59	MG	14	3344	1/1	0.87	0.13	89,89,89,89	0
59	MG	13	1666	1/1	0.87	0.16	83,83,83,83	0
58	K	13	1610	1/1	0.87	0.10	114,114,114,114	0
59	MG	1H	3333	1/1	0.87	0.10	50,50,50,50	0
59	MG	1H	3243	1/1	0.87	0.35	94,94,94,94	0
59	MG	1H	3466	1/1	0.88	0.14	34,34,34,34	0
59	MG	1H	3279	1/1	0.88	0.21	74,74,74,74	0
59	MG	14	3124	1/1	0.88	0.08	63,63,63,63	0
58	K	1G	1625	1/1	0.88	0.12	106,106,106,106	0
59	MG	1H	3283	1/1	0.88	0.10	58,58,58,58	0
59	MG	1G	1639	1/1	0.88	0.29	55,55,55,55	0
59	MG	1H	3139	1/1	0.88	0.31	76,76,76,76	0
58	K	1H	3002	1/1	0.88	0.06	71,71,71,71	0
59	MG	1H	3340	1/1	0.88	0.12	29,29,29,29	0
59	MG	14	3157	1/1	0.88	0.14	57,57,57,57	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
59	MG	14	3325	1/1	0.88	0.08	81,81,81,81	0
59	MG	1G	1659	1/1	0.88	0.10	72,72,72,72	0
59	MG	1H	3406	1/1	0.88	0.08	95,95,95,95	0
59	MG	1H	3212	1/1	0.88	0.14	57,57,57,57	0
58	K	14	3054	1/1	0.88	0.06	77,77,77,77	0
58	K	14	3029	1/1	0.88	0.10	68,68,68,68	0
58	K	14	3057	1/1	0.88	0.08	68,68,68,68	0
58	K	14	3063	1/1	0.88	0.11	84,84,84,84	0
59	MG	14	3353	1/1	0.88	0.05	65,65,65,65	0
59	MG	14	3188	1/1	0.88	0.13	54,54,54,54	0
59	MG	13	1726	1/1	0.88	0.04	122,122,122,122	0
59	MG	1H	3493	1/1	0.88	0.12	63,63,63,63	0
59	MG	14	3203	1/1	0.88	0.13	85,85,85,85	0
59	MG	14	3209	1/1	0.88	0.16	72,72,72,72	0
59	MG	1H	3309	1/1	0.88	0.15	56,56,56,56	0
59	MG	1H	3236	1/1	0.88	0.09	54,54,54,54	0
59	MG	1H	3500	1/1	0.88	0.18	45,45,45,45	0
59	MG	1H	3359	1/1	0.88	0.12	55,55,55,55	0
59	MG	14	3246	1/1	0.88	0.07	76,76,76,76	0
59	MG	1H	3238	1/1	0.88	0.33	82,82,82,82	0
59	MG	13	1653	1/1	0.88	0.23	74,74,74,74	0
58	K	13	1630	1/1	0.88	0.09	82,82,82,82	0
58	K	1H	3044	1/1	0.88	0.10	82,82,82,82	0
58	K	13	1614	1/1	0.88	0.18	103,103,103,103	0
59	MG	14	3261	1/1	0.88	0.12	75,75,75,75	0
59	MG	14	3262	1/1	0.88	0.13	45,45,45,45	0
59	MG	14	3385	1/1	0.88	0.13	63,63,63,63	0
59	MG	1H	3439	1/1	0.88	0.08	55,55,55,55	0
59	MG	1H	3257	1/1	0.88	0.11	49,49,49,49	0
59	MG	1H	3198	1/1	0.88	0.21	82,82,82,82	0
59	MG	1H	3271	1/1	0.88	0.14	45,45,45,45	0
59	MG	1H	3455	1/1	0.88	0.19	55,55,55,55	0
59	MG	1H	3377	1/1	0.88	0.09	44,44,44,44	0
59	MG	14	3396	1/1	0.88	0.10	51,51,51,51	0
58	K	14	3014	1/1	0.88	0.09	82,82,82,82	0
59	MG	14	3281	1/1	0.88	0.11	45,45,45,45	0
59	MG	14	3404	1/1	0.88	0.09	34,34,34,34	0
59	MG	1H	3525	1/1	0.88	0.07	46,46,46,46	0
59	MG	16	207	1/1	0.88	0.27	88,88,88,88	0
59	MG	1J	203	1/1	0.88	0.05	105,105,105,105	0
59	MG	1H	3276	1/1	0.88	0.22	63,63,63,63	0
59	MG	1H	3122	1/1	0.88	0.22	29,29,29,29	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
59	MG	55	201	1/1	0.88	0.19	59,59,59,59	0
59	MG	1H	3258	1/1	0.89	0.15	48,48,48,48	0
59	MG	13	1737	1/1	0.89	0.05	90,90,90,90	0
59	MG	N8	101	1/1	0.89	0.14	56,56,56,56	0
58	K	1H	3066	1/1	0.89	0.09	80,80,80,80	0
59	MG	1H	3329	1/1	0.89	0.17	73,73,73,73	0
59	MG	1G	1635	1/1	0.89	0.26	80,80,80,80	0
59	MG	14	3148	1/1	0.89	0.13	58,58,58,58	0
59	MG	14	3315	1/1	0.89	0.06	84,84,84,84	0
59	MG	1H	3475	1/1	0.89	0.08	91,91,91,91	0
59	MG	14	3322	1/1	0.89	0.06	93,93,93,93	0
59	MG	13	1696	1/1	0.89	0.18	80,80,80,80	0
58	K	29	301	1/1	0.89	0.08	56,56,56,56	0
59	MG	1G	1650	1/1	0.89	0.20	65,65,65,65	0
58	K	13	1607	1/1	0.89	0.08	90,90,90,90	0
59	MG	13	1742	1/1	0.89	0.07	94,94,94,94	0
58	K	14	3015	1/1	0.89	0.16	52,52,52,52	0
58	K	14	3017	1/1	0.89	0.18	107,107,107,107	0
59	MG	13	1706	1/1	0.89	0.22	63,63,63,63	0
59	MG	1H	3490	1/1	0.89	0.06	53,53,53,53	0
59	MG	1G	1676	1/1	0.89	0.24	81,81,81,81	0
58	K	1H	3016	1/1	0.89	0.14	114,114,114,114	0
59	MG	14	3195	1/1	0.89	0.16	64,64,64,64	0
59	MG	14	3358	1/1	0.89	0.07	35,35,35,35	0
59	MG	14	3200	1/1	0.89	0.22	102,102,102,102	0
58	K	13	1632	1/1	0.89	0.10	83,83,83,83	0
59	MG	1H	3219	1/1	0.89	0.15	50,50,50,50	0
59	MG	14	3369	1/1	0.89	0.17	43,43,43,43	0
59	MG	13	1715	1/1	0.89	0.09	75,75,75,75	0
59	MG	14	3371	1/1	0.89	0.06	61,61,61,61	0
59	MG	14	3225	1/1	0.89	0.12	62,62,62,62	0
58	K	14	3069	1/1	0.89	0.12	89,89,89,89	0
59	MG	1G	1688	1/1	0.89	0.06	82,82,82,82	0
59	MG	14	3239	1/1	0.89	0.15	66,66,66,66	0
59	MG	1H	3225	1/1	0.89	0.18	58,58,58,58	0
59	MG	1H	3230	1/1	0.89	0.15	38,38,38,38	0
59	MG	1H	3505	1/1	0.89	0.13	34,34,34,34	0
58	K	13	1627	1/1	0.89	0.12	91,91,91,91	0
58	K	14	3076	1/1	0.89	0.13	89,89,89,89	0
58	K	13	1629	1/1	0.89	0.07	92,92,92,92	0
58	K	14	3035	1/1	0.89	0.09	62,62,62,62	0
59	MG	1G	1702	1/1	0.89	0.08	87,87,87,87	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
59	MG	1H	3512	1/1	0.89	0.14	61,61,61,61	0
58	K	1H	3038	1/1	0.89	0.11	86,86,86,86	0
59	MG	14	3263	1/1	0.89	0.26	66,66,66,66	0
59	MG	1H	3240	1/1	0.89	0.19	52,52,52,52	0
59	MG	13	1680	1/1	0.89	0.21	71,71,71,71	0
59	MG	1H	3456	1/1	0.89	0.13	38,38,38,38	0
58	K	1H	3104	1/1	0.89	0.08	53,53,53,53	0
58	K	14	3002	1/1	0.89	0.07	90,90,90,90	0
59	MG	1H	3246	1/1	0.89	0.20	58,58,58,58	0
59	MG	1H	3524	1/1	0.89	0.11	35,35,35,35	0
59	MG	1G	1723	1/1	0.89	0.06	85,85,85,85	0
59	MG	1H	3463	1/1	0.89	0.12	40,40,40,40	0
59	MG	1H	3252	1/1	0.89	0.18	72,72,72,72	0
59	MG	1J	204	1/1	0.89	0.07	115,115,115,115	0
59	MG	1H	3390	1/1	0.89	0.16	39,39,39,39	0
59	MG	14	3100	1/1	0.89	0.12	47,47,47,47	0
58	K	1G	1610	1/1	0.89	0.10	95,95,95,95	0
59	MG	14	3214	1/1	0.90	0.21	57,57,57,57	0
59	MG	14	3222	1/1	0.90	0.07	57,57,57,57	0
59	MG	1H	3372	1/1	0.90	0.15	77,77,77,77	0
59	MG	14	3231	1/1	0.90	0.09	48,48,48,48	0
59	MG	1G	1714	1/1	0.90	0.13	82,82,82,82	0
58	K	14	3028	1/1	0.90	0.07	56,56,56,56	0
59	MG	1G	1717	1/1	0.90	0.06	88,88,88,88	0
59	MG	1H	3183	1/1	0.90	0.14	49,49,49,49	0
58	K	14	3008	1/1	0.90	0.07	88,88,88,88	0
59	MG	1H	3436	1/1	0.90	0.07	33,33,33,33	0
59	MG	1H	3192	1/1	0.90	0.14	49,49,49,49	0
59	MG	1H	3502	1/1	0.90	0.05	94,94,94,94	0
59	MG	1H	3379	1/1	0.90	0.07	67,67,67,67	0
59	MG	1H	3331	1/1	0.90	0.20	55,55,55,55	0
59	MG	1H	3196	1/1	0.90	0.15	42,42,42,42	0
59	MG	1G	1668	1/1	0.90	0.25	55,55,55,55	0
58	K	13	1637	1/1	0.90	0.09	123,123,123,123	0
59	MG	1H	3241	1/1	0.90	0.15	39,39,39,39	0
58	K	1G	1608	1/1	0.90	0.17	113,113,113,113	0
58	K	14	3065	1/1	0.90	0.06	92,92,92,92	0
59	MG	1H	3304	1/1	0.90	0.29	69,69,69,69	0
59	MG	14	3273	1/1	0.90	0.10	46,46,46,46	0
59	MG	14	3151	1/1	0.90	0.19	57,57,57,57	0
59	MG	1H	3345	1/1	0.90	0.10	24,24,24,24	0
58	K	1H	3033	1/1	0.90	0.08	94,94,94,94	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
59	MG	14	3156	1/1	0.90	0.10	55,55,55,55	0
59	MG	14	3279	1/1	0.90	0.06	46,46,46,46	0
59	MG	1H	3403	1/1	0.90	0.07	59,59,59,59	0
59	MG	13	1676	1/1	0.90	0.11	53,53,53,53	0
59	MG	1H	3153	1/1	0.90	0.18	44,44,44,44	0
58	K	1H	3018	1/1	0.90	0.09	93,93,93,93	0
59	MG	13	1685	1/1	0.90	0.31	85,85,85,85	0
59	MG	14	3391	1/1	0.90	0.09	62,62,62,62	0
59	MG	1H	3417	1/1	0.90	0.12	44,44,44,44	0
59	MG	14	3183	1/1	0.90	0.11	63,63,63,63	0
58	K	1H	3102	1/1	0.90	0.09	94,94,94,94	0
59	MG	13	1689	1/1	0.90	0.11	80,80,80,80	0
58	K	14	3049	1/1	0.90	0.12	103,103,103,103	0
59	MG	14	3399	1/1	0.90	0.10	55,55,55,55	0
58	K	1H	3001	1/1	0.90	0.07	88,88,88,88	0
59	MG	1H	3482	1/1	0.90	0.11	22,22,22,22	0
59	MG	14	3309	1/1	0.90	0.09	85,85,85,85	0
59	MG	14	3197	1/1	0.90	0.14	60,60,60,60	0
59	MG	1H	3362	1/1	0.90	0.10	33,33,33,33	0
59	MG	1H	3226	1/1	0.90	0.10	42,42,42,42	0
59	MG	1H	3227	1/1	0.90	0.20	58,58,58,58	0
59	MG	14	3208	1/1	0.90	0.09	61,61,61,61	0
58	K	1G	1616	1/1	0.90	0.06	89,89,89,89	0
59	MG	1H	3447	1/1	0.91	0.05	98,98,98,98	0
59	MG	1G	1687	1/1	0.91	0.08	93,93,93,93	0
59	MG	1H	3507	1/1	0.91	0.06	45,45,45,45	0
59	MG	1H	3386	1/1	0.91	0.11	67,67,67,67	0
59	MG	13	1713	1/1	0.91	0.05	83,83,83,83	0
59	MG	14	3193	1/1	0.91	0.08	63,63,63,63	0
59	MG	1H	3204	1/1	0.91	0.24	51,51,51,51	0
59	MG	14	3196	1/1	0.91	0.14	90,90,90,90	0
58	K	13	1628	1/1	0.91	0.14	103,103,103,103	0
58	K	1H	3035	1/1	0.91	0.10	98,98,98,98	0
59	MG	14	3201	1/1	0.91	0.11	68,68,68,68	0
59	MG	14	3340	1/1	0.91	0.13	74,74,74,74	0
59	MG	14	3341	1/1	0.91	0.13	52,52,52,52	0
59	MG	1H	3394	1/1	0.91	0.09	38,38,38,38	0
58	K	14	3085	1/1	0.91	0.08	94,94,94,94	0
59	MG	14	3348	1/1	0.91	0.17	102,102,102,102	0
59	MG	14	3206	1/1	0.91	0.11	67,67,67,67	0
58	K	1H	3005	1/1	0.91	0.11	67,67,67,67	0
59	MG	1H	3519	1/1	0.91	0.06	56,56,56,56	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
58	K	1H	3118	1/1	0.91	0.38	89,89,89,89	0
59	MG	1G	1706	1/1	0.91	0.05	96,96,96,96	0
58	K	1H	3024	1/1	0.91	0.08	56,56,56,56	0
58	K	14	3093	1/1	0.91	0.10	72,72,72,72	0
59	MG	14	3360	1/1	0.91	0.09	64,64,64,64	0
59	MG	1H	3468	1/1	0.91	0.09	50,50,50,50	0
59	MG	1H	3273	1/1	0.91	0.11	49,49,49,49	0
59	MG	16	204	1/1	0.91	0.25	80,80,80,80	0
59	MG	1H	3223	1/1	0.91	0.10	64,64,64,64	0
59	MG	1H	3415	1/1	0.91	0.09	94,94,94,94	0
58	K	14	3040	1/1	0.91	0.12	72,72,72,72	0
59	MG	14	3249	1/1	0.91	0.11	54,54,54,54	0
58	K	14	3022	1/1	0.91	0.05	92,92,92,92	0
59	MG	1H	3181	1/1	0.91	0.17	41,41,41,41	0
59	MG	1G	1724	1/1	0.91	0.10	109,109,109,109	0
58	K	1H	3040	1/1	0.91	0.33	111,111,111,111	0
59	MG	1H	3479	1/1	0.91	0.12	47,47,47,47	0
59	MG	1H	3366	1/1	0.91	0.09	44,44,44,44	0
59	MG	1H	3184	1/1	0.91	0.26	65,65,65,65	0
59	MG	1H	3370	1/1	0.91	0.13	38,38,38,38	0
59	MG	13	1735	1/1	0.91	0.04	57,57,57,57	0
58	K	14	3003	1/1	0.91	0.10	86,86,86,86	0
59	MG	14	3129	1/1	0.91	0.11	44,44,44,44	0
59	MG	1G	1649	1/1	0.91	0.14	85,85,85,85	0
59	MG	1H	3134	1/1	0.91	0.20	59,59,59,59	0
59	MG	1H	3138	1/1	0.91	0.29	66,66,66,66	0
59	MG	14	3143	1/1	0.91	0.15	72,72,72,72	0
59	MG	1G	1652	1/1	0.91	0.12	94,94,94,94	0
58	K	1H	3063	1/1	0.91	0.10	55,55,55,55	0
59	MG	14	3280	1/1	0.91	0.08	48,48,48,48	0
59	MG	1H	3291	1/1	0.91	0.17	62,62,62,62	0
59	MG	1H	3495	1/1	0.91	0.10	80,80,80,80	0
59	MG	1H	3336	1/1	0.91	0.16	54,54,54,54	0
59	MG	1H	3140	1/1	0.91	0.32	82,82,82,82	0
59	MG	1H	3438	1/1	0.91	0.10	36,36,36,36	0
59	MG	14	3169	1/1	0.91	0.08	57,57,57,57	0
59	MG	1H	3501	1/1	0.91	0.05	78,78,78,78	0
59	MG	1H	3382	1/1	0.91	0.16	36,36,36,36	0
59	MG	1H	3440	1/1	0.91	0.11	63,63,63,63	0
59	MG	1H	3442	1/1	0.91	0.08	80,80,80,80	0
59	MG	1H	3339	1/1	0.91	0.11	33,33,33,33	0
59	MG	13	1712	1/1	0.92	0.11	50,50,50,50	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
59	MG	1H	3237	1/1	0.92	0.29	51,51,51,51	0
58	K	14	3047	1/1	0.92	0.16	97,97,97,97	0
59	MG	13	1714	1/1	0.92	0.05	106,106,106,106	0
59	MG	1H	3332	1/1	0.92	0.20	59,59,59,59	0
58	K	14	3048	1/1	0.92	0.11	101,101,101,101	0
58	K	1H	3076	1/1	0.92	0.14	86,86,86,86	0
59	MG	14	3283	1/1	0.92	0.14	36,36,36,36	0
59	MG	1H	3516	1/1	0.92	0.07	60,60,60,60	0
59	MG	13	1721	1/1	0.92	0.06	68,68,68,68	0
58	K	1H	3020	1/1	0.92	0.19	105,105,105,105	0
59	MG	1H	3338	1/1	0.92	0.13	35,35,35,35	0
59	MG	1H	3174	1/1	0.92	0.08	71,71,71,71	0
58	K	14	3005	1/1	0.92	0.21	91,91,91,91	0
59	MG	1H	3248	1/1	0.92	0.12	47,47,47,47	0
58	K	1H	3106	1/1	0.92	0.13	92,92,92,92	0
58	K	13	1609	1/1	0.92	0.20	91,91,91,91	0
59	MG	14	3303	1/1	0.92	0.06	73,73,73,73	0
58	K	1H	3026	1/1	0.92	0.31	62,62,62,62	0
59	MG	14	3307	1/1	0.92	0.07	51,51,51,51	0
59	MG	1H	3259	1/1	0.92	0.12	59,59,59,59	0
59	MG	1H	3182	1/1	0.92	0.16	47,47,47,47	0
58	K	14	3058	1/1	0.92	0.22	84,84,84,84	0
59	MG	14	3312	1/1	0.92	0.09	87,87,87,87	0
59	MG	14	3314	1/1	0.92	0.04	91,91,91,91	0
58	K	14	3062	1/1	0.92	0.06	65,65,65,65	0
59	MG	1H	3452	1/1	0.92	0.10	48,48,48,48	0
59	MG	1H	3454	1/1	0.92	0.12	42,42,42,42	0
59	MG	1H	3186	1/1	0.92	0.20	50,50,50,50	0
59	MG	1G	1633	1/1	0.92	0.21	65,65,65,65	0
59	MG	1G	1634	1/1	0.92	0.33	110,110,110,110	0
58	K	1H	3085	1/1	0.92	0.12	64,64,64,64	0
59	MG	1H	3190	1/1	0.92	0.17	49,49,49,49	0
59	MG	1H	3191	1/1	0.92	0.41	72,72,72,72	0
59	MG	14	3176	1/1	0.92	0.21	67,67,67,67	0
58	K	13	1615	1/1	0.92	0.08	91,91,91,91	0
59	MG	14	3346	1/1	0.92	0.05	76,76,76,76	0
59	MG	1H	3194	1/1	0.92	0.21	45,45,45,45	0
59	MG	13	1679	1/1	0.92	0.13	89,89,89,89	0
58	K	13	1603	1/1	0.92	0.11	117,117,117,117	0
59	MG	1H	3199	1/1	0.92	0.16	60,60,60,60	0
59	MG	1G	1654	1/1	0.92	0.17	58,58,58,58	0
59	MG	13	1683	1/1	0.92	0.09	55,55,55,55	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
59	MG	1H	3289	1/1	0.92	0.21	75,75,75,75	0
59	MG	13	1684	1/1	0.92	0.14	56,56,56,56	0
58	K	1H	3011	1/1	0.92	0.08	61,61,61,61	0
58	K	1G	1614	1/1	0.92	0.12	100,100,100,100	0
59	MG	1H	3293	1/1	0.92	0.11	55,55,55,55	0
59	MG	14	3365	1/1	0.92	0.08	80,80,80,80	0
59	MG	14	3366	1/1	0.92	0.08	77,77,77,77	0
59	MG	1G	1673	1/1	0.92	0.29	73,73,73,73	0
58	K	1H	3119	1/1	0.92	0.11	92,92,92,92	0
59	MG	1H	3208	1/1	0.92	0.18	52,52,52,52	0
59	MG	1H	3478	1/1	0.92	0.08	38,38,38,38	0
59	MG	1H	3302	1/1	0.92	0.19	41,41,41,41	0
59	MG	14	3373	1/1	0.92	0.06	84,84,84,84	0
59	MG	14	3213	1/1	0.92	0.19	58,58,58,58	0
58	K	1H	3120	1/1	0.92	0.13	79,79,79,79	0
59	MG	1H	3305	1/1	0.92	0.25	57,57,57,57	0
59	MG	1H	3483	1/1	0.92	0.14	75,75,75,75	0
59	MG	14	3226	1/1	0.92	0.08	49,49,49,49	0
59	MG	1H	3388	1/1	0.92	0.14	38,38,38,38	0
59	MG	1H	3307	1/1	0.92	0.09	39,39,39,39	0
59	MG	13	1746	1/1	0.92	0.06	93,93,93,93	0
59	MG	14	3235	1/1	0.92	0.16	61,61,61,61	0
58	K	1H	3012	1/1	0.92	0.11	80,80,80,80	0
59	MG	1G	1694	1/1	0.92	0.10	62,62,62,62	0
59	MG	14	3242	1/1	0.92	0.16	44,44,44,44	0
58	K	13	1624	1/1	0.92	0.18	83,83,83,83	0
59	MG	14	3244	1/1	0.92	0.25	46,46,46,46	0
59	MG	14	3390	1/1	0.92	0.07	78,78,78,78	0
58	K	1H	3004	1/1	0.92	0.24	66,66,66,66	0
59	MG	1H	3396	1/1	0.92	0.11	35,35,35,35	0
59	MG	14	3393	1/1	0.92	0.25	81,81,81,81	0
59	MG	1H	3313	1/1	0.92	0.14	52,52,52,52	0
58	K	1H	3071	1/1	0.92	0.13	65,65,65,65	0
59	MG	1H	3316	1/1	0.92	0.20	59,59,59,59	0
58	K	41	201	1/1	0.92	0.20	114,114,114,114	0
59	MG	1G	1705	1/1	0.92	0.03	105,105,105,105	0
58	K	52	201	1/1	0.92	0.27	116,116,116,116	0
58	K	14	3092	1/1	0.92	0.08	83,83,83,83	0
59	MG	14	3406	1/1	0.92	0.07	55,55,55,55	0
58	K	14	3041	1/1	0.92	0.12	54,54,54,54	0
59	MG	1H	3228	1/1	0.92	0.11	48,48,48,48	0
58	K	13	1613	1/1	0.92	0.09	100,100,100,100	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
59	MG	14	3269	1/1	0.92	0.10	79,79,79,79	0
59	MG	13	1709	1/1	0.92	0.21	85,85,85,85	0
59	MG	14	3272	1/1	0.92	0.13	26,26,26,26	0
58	K	14	3043	1/1	0.92	0.05	71,71,71,71	0
59	MG	E5	101	1/1	0.92	0.17	36,36,36,36	0
59	MG	1H	3233	1/1	0.93	0.22	59,59,59,59	0
59	MG	1G	1672	1/1	0.93	0.18	63,63,63,63	0
58	K	1H	3075	1/1	0.93	0.11	81,81,81,81	0
59	MG	1H	3179	1/1	0.93	0.13	51,51,51,51	0
59	MG	1H	3499	1/1	0.93	0.10	68,68,68,68	0
59	MG	13	1682	1/1	0.93	0.43	101,101,101,101	0
59	MG	14	3191	1/1	0.93	0.20	45,45,45,45	0
58	K	1H	3093	1/1	0.93	0.11	79,79,79,79	0
58	K	14	3084	1/1	0.93	0.07	75,75,75,75	0
58	K	1H	3021	1/1	0.93	0.09	78,78,78,78	0
59	MG	13	1687	1/1	0.93	0.19	75,75,75,75	0
59	MG	14	3198	1/1	0.93	0.17	63,63,63,63	0
58	K	14	3087	1/1	0.93	0.07	84,84,84,84	0
59	MG	14	3335	1/1	0.93	0.12	50,50,50,50	0
58	K	1H	3060	1/1	0.93	0.18	55,55,55,55	0
58	K	1G	1611	1/1	0.93	0.11	94,94,94,94	0
59	MG	1H	3441	1/1	0.93	0.06	51,51,51,51	0
58	K	1G	1612	1/1	0.93	0.06	101,101,101,101	0
59	MG	1H	3444	1/1	0.93	0.13	94,94,94,94	0
58	K	1H	3017	1/1	0.93	0.10	94,94,94,94	0
58	K	1H	3025	1/1	0.93	0.06	100,100,100,100	0
59	MG	1G	1698	1/1	0.93	0.12	103,103,103,103	0
59	MG	1H	3320	1/1	0.93	0.22	43,43,43,43	0
59	MG	13	1697	1/1	0.93	0.15	70,70,70,70	0
59	MG	14	3355	1/1	0.93	0.12	64,64,64,64	0
58	K	1H	3064	1/1	0.93	0.09	49,49,49,49	0
58	K	1H	3042	1/1	0.93	0.21	62,62,62,62	0
59	MG	1H	3260	1/1	0.93	0.09	43,43,43,43	0
59	MG	1H	3262	1/1	0.93	0.09	49,49,49,49	0
59	MG	1H	3521	1/1	0.93	0.07	113,113,113,113	0
58	K	1G	1617	1/1	0.93	0.09	94,94,94,94	0
59	MG	13	1642	1/1	0.93	0.27	59,59,59,59	0
58	K	1H	3109	1/1	0.93	0.12	54,54,54,54	0
59	MG	1H	3274	1/1	0.93	0.10	56,56,56,56	0
59	MG	16	203	1/1	0.93	0.13	57,57,57,57	0
59	MG	13	1655	1/1	0.93	0.14	80,80,80,80	0
59	MG	1H	3393	1/1	0.93	0.16	44,44,44,44	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
58	K	1H	3014	1/1	0.93	0.41	84,84,84,84	0
59	MG	1H	3395	1/1	0.93	0.12	56,56,56,56	0
58	K	13	1620	1/1	0.93	0.08	115,115,115,115	0
58	K	14	3030	1/1	0.93	0.07	56,56,56,56	0
59	MG	1H	3280	1/1	0.93	0.27	64,64,64,64	0
59	MG	14	3260	1/1	0.93	0.18	56,56,56,56	0
59	MG	1H	3400	1/1	0.93	0.07	46,46,46,46	0
59	MG	13	1663	1/1	0.93	0.26	68,68,68,68	0
58	K	1G	1602	1/1	0.93	0.21	70,70,70,70	0
58	K	14	3034	1/1	0.93	0.07	49,49,49,49	0
59	MG	14	3112	1/1	0.93	0.07	55,55,55,55	0
59	MG	14	3383	1/1	0.93	0.08	71,71,71,71	0
59	MG	14	3113	1/1	0.93	0.18	51,51,51,51	0
58	K	1H	3050	1/1	0.93	0.15	70,70,70,70	0
59	MG	1H	3408	1/1	0.93	0.05	60,60,60,60	0
59	MG	14	3130	1/1	0.93	0.14	45,45,45,45	0
59	MG	14	3131	1/1	0.93	0.21	66,66,66,66	0
59	MG	1H	3409	1/1	0.93	0.07	64,64,64,64	0
59	MG	14	3139	1/1	0.93	0.15	46,46,46,46	0
59	MG	1G	1644	1/1	0.93	0.23	55,55,55,55	0
59	MG	1G	1646	1/1	0.93	0.27	107,107,107,107	0
59	MG	1H	3481	1/1	0.93	0.16	43,43,43,43	0
58	K	14	3074	1/1	0.93	0.14	94,94,94,94	0
58	K	1H	3091	1/1	0.93	0.12	62,62,62,62	0
58	K	1H	3114	1/1	0.93	0.07	58,58,58,58	0
59	MG	1H	3168	1/1	0.93	0.25	46,46,46,46	0
59	MG	14	3401	1/1	0.93	0.20	89,89,89,89	0
59	MG	13	1728	1/1	0.93	0.07	106,106,106,106	0
59	MG	1G	1656	1/1	0.93	0.30	100,100,100,100	0
59	MG	1G	1658	1/1	0.93	0.27	76,76,76,76	0
59	MG	1H	3488	1/1	0.93	0.04	83,83,83,83	0
58	K	14	3077	1/1	0.93	0.17	72,72,72,72	0
59	MG	13	1678	1/1	0.93	0.26	79,79,79,79	0
58	K	14	3039	1/1	0.93	0.10	94,94,94,94	0
59	MG	1G	1665	1/1	0.93	0.27	84,84,84,84	0
59	MG	29	303	1/1	0.93	0.12	37,37,37,37	0
59	MG	14	3304	1/1	0.93	0.08	38,38,38,38	0
59	MG	14	3305	1/1	0.93	0.05	69,69,69,69	0
59	MG	1H	3354	1/1	0.93	0.06	70,70,70,70	0
59	MG	13	1692	1/1	0.94	0.16	70,70,70,70	0
58	K	1H	3059	1/1	0.94	0.06	38,38,38,38	0
58	K	1G	1620	1/1	0.94	0.10	101,101,101,101	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
59	MG	1H	3399	1/1	0.94	0.15	54,54,54,54	0
58	K	13	1633	1/1	0.94	0.06	108,108,108,108	0
59	MG	1H	3224	1/1	0.94	0.13	51,51,51,51	0
59	MG	1H	3317	1/1	0.94	0.35	63,63,63,63	0
59	MG	1H	3130	1/1	0.94	0.19	28,28,28,28	0
59	MG	1H	3132	1/1	0.94	0.28	58,58,58,58	0
58	K	1G	1623	1/1	0.94	0.10	126,126,126,126	0
58	K	8I	201	1/1	0.94	0.10	104,104,104,104	0
59	MG	1H	3412	1/1	0.94	0.15	85,85,85,85	0
59	MG	1H	3136	1/1	0.94	0.25	37,37,37,37	0
58	K	1H	3019	1/1	0.94	0.07	78,78,78,78	0
59	MG	1H	3232	1/1	0.94	0.13	40,40,40,40	0
58	K	1H	3037	1/1	0.94	0.09	77,77,77,77	0
59	MG	13	1703	1/1	0.94	0.35	69,69,69,69	0
59	MG	1H	3142	1/1	0.94	0.17	71,71,71,71	0
59	MG	1H	3143	1/1	0.94	0.15	63,63,63,63	0
59	MG	1H	3147	1/1	0.94	0.12	19,19,19,19	0
59	MG	1G	1718	1/1	0.94	0.10	91,91,91,91	0
59	MG	14	3287	1/1	0.94	0.06	50,50,50,50	0
59	MG	1G	1719	1/1	0.94	0.11	101,101,101,101	0
59	MG	1H	3425	1/1	0.94	0.13	42,42,42,42	0
59	MG	1H	3149	1/1	0.94	0.16	29,29,29,29	0
59	MG	13	1704	1/1	0.94	0.15	53,53,53,53	0
59	MG	1H	3517	1/1	0.94	0.07	55,55,55,55	0
59	MG	1G	1726	1/1	0.94	0.05	98,98,98,98	0
59	MG	14	3296	1/1	0.94	0.07	44,44,44,44	0
58	K	1H	3065	1/1	0.94	0.10	43,43,43,43	0
59	MG	14	3299	1/1	0.94	0.05	57,57,57,57	0
59	MG	1H	3155	1/1	0.94	0.12	35,35,35,35	0
59	MG	1H	3156	1/1	0.94	0.20	55,55,55,55	0
59	MG	14	3101	1/1	0.94	0.09	61,61,61,61	0
59	MG	1H	3157	1/1	0.94	0.23	62,62,62,62	0
59	MG	1H	3432	1/1	0.94	0.11	73,73,73,73	0
58	K	14	3045	1/1	0.94	0.09	71,71,71,71	0
59	MG	1H	3247	1/1	0.94	0.20	44,44,44,44	0
59	MG	14	3115	1/1	0.94	0.10	46,46,46,46	0
59	MG	13	1639	1/1	0.94	0.13	62,62,62,62	0
59	MG	1H	3437	1/1	0.94	0.13	49,49,49,49	0
59	MG	13	1640	1/1	0.94	0.19	72,72,72,72	0
59	MG	14	3313	1/1	0.94	0.05	89,89,89,89	0
59	MG	16	205	1/1	0.94	0.21	84,84,84,84	0
59	MG	14	3132	1/1	0.94	0.05	47,47,47,47	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
59	MG	14	3318	1/1	0.94	0.09	68,68,68,68	0
59	MG	16	206	1/1	0.94	0.23	62,62,62,62	0
59	MG	1H	3254	1/1	0.94	0.16	50,50,50,50	0
59	MG	16	209	1/1	0.94	0.07	75,75,75,75	0
59	MG	13	1641	1/1	0.94	0.15	90,90,90,90	0
59	MG	14	3142	1/1	0.94	0.23	62,62,62,62	0
58	K	3A	201	1/1	0.94	0.13	93,93,93,93	0
59	MG	14	3334	1/1	0.94	0.07	48,48,48,48	0
59	MG	78	201	1/1	0.94	0.30	32,32,32,32	0
59	MG	14	3147	1/1	0.94	0.12	54,54,54,54	0
58	K	BA	201	1/1	0.94	0.26	96,96,96,96	0
59	MG	14	3149	1/1	0.94	0.16	46,46,46,46	0
59	MG	14	3343	1/1	0.94	0.08	76,76,76,76	0
59	MG	D8	202	1/1	0.94	0.10	52,52,52,52	0
59	MG	14	3345	1/1	0.94	0.09	89,89,89,89	0
59	MG	1H	3349	1/1	0.94	0.08	28,28,28,28	0
59	MG	I8	102	1/1	0.94	0.07	72,72,72,72	0
58	K	1H	3096	1/1	0.94	0.16	75,75,75,75	0
59	MG	Q8	101	1/1	0.94	0.14	32,32,32,32	0
59	MG	14	3162	1/1	0.94	0.20	58,58,58,58	0
59	MG	14	3166	1/1	0.94	0.12	37,37,37,37	0
59	MG	1G	1627	1/1	0.94	0.25	88,88,88,88	0
59	MG	14	3171	1/1	0.94	0.11	71,71,71,71	0
58	K	13	1604	1/1	0.94	0.11	90,90,90,90	0
59	MG	1H	3448	1/1	0.94	0.07	61,61,61,61	0
58	K	1H	3100	1/1	0.94	0.19	78,78,78,78	0
59	MG	1H	3267	1/1	0.94	0.14	60,60,60,60	0
58	K	1H	3101	1/1	0.94	0.08	60,60,60,60	0
59	MG	14	3362	1/1	0.94	0.05	69,69,69,69	0
59	MG	14	3364	1/1	0.94	0.14	71,71,71,71	0
59	MG	14	3177	1/1	0.94	0.15	64,64,64,64	0
59	MG	14	3178	1/1	0.94	0.11	36,36,36,36	0
59	MG	14	3179	1/1	0.94	0.15	66,66,66,66	0
59	MG	1H	3358	1/1	0.94	0.05	43,43,43,43	0
58	K	13	1621	1/1	0.94	0.05	59,59,59,59	0
59	MG	1G	1642	1/1	0.94	0.23	59,59,59,59	0
59	MG	1G	1643	1/1	0.94	0.10	56,56,56,56	0
59	MG	13	1727	1/1	0.94	0.08	47,47,47,47	0
58	K	14	3009	1/1	0.94	0.09	69,69,69,69	0
59	MG	1G	1647	1/1	0.94	0.21	80,80,80,80	0
58	K	1H	3023	1/1	0.94	0.10	68,68,68,68	0
58	K	14	3059	1/1	0.94	0.12	73,73,73,73	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
59	MG	1H	3462	1/1	0.94	0.08	46,46,46,46	0
58	K	14	3061	1/1	0.94	0.06	103,103,103,103	0
59	MG	1H	3464	1/1	0.94	0.14	19,19,19,19	0
59	MG	14	3199	1/1	0.94	0.19	105,105,105,105	0
59	MG	1H	3367	1/1	0.94	0.10	61,61,61,61	0
58	K	13	1626	1/1	0.94	0.22	99,99,99,99	0
58	K	1H	3105	1/1	0.94	0.07	60,60,60,60	0
58	K	13	1631	1/1	0.94	0.12	93,93,93,93	0
59	MG	14	3205	1/1	0.94	0.10	37,37,37,37	0
59	MG	1G	1660	1/1	0.94	0.18	79,79,79,79	0
58	K	1H	3043	1/1	0.94	0.10	82,82,82,82	0
59	MG	1H	3193	1/1	0.94	0.23	43,43,43,43	0
59	MG	14	3210	1/1	0.94	0.16	45,45,45,45	0
58	K	14	3018	1/1	0.94	0.09	71,71,71,71	0
59	MG	1H	3195	1/1	0.94	0.19	51,51,51,51	0
59	MG	14	3221	1/1	0.94	0.19	52,52,52,52	0
58	K	13	1619	1/1	0.94	0.05	77,77,77,77	0
59	MG	1G	1670	1/1	0.94	0.10	60,60,60,60	0
58	K	14	3023	1/1	0.94	0.16	93,93,93,93	0
58	K	1H	3047	1/1	0.94	0.19	37,37,37,37	0
59	MG	14	3400	1/1	0.94	0.07	92,92,92,92	0
58	K	1H	3015	1/1	0.94	0.09	80,80,80,80	0
58	K	1H	3007	1/1	0.94	0.09	54,54,54,54	0
58	K	14	3080	1/1	0.94	0.07	94,94,94,94	0
59	MG	13	1743	1/1	0.94	0.04	105,105,105,105	0
58	K	1H	3032	1/1	0.94	0.20	58,58,58,58	0
59	MG	13	1745	1/1	0.94	0.07	78,78,78,78	0
58	K	1H	3116	1/1	0.94	0.06	80,80,80,80	0
59	MG	1H	3306	1/1	0.94	0.18	44,44,44,44	0
59	MG	14	3245	1/1	0.94	0.23	64,64,64,64	0
58	K	1H	3087	1/1	0.94	0.09	76,76,76,76	0
58	K	1H	3055	1/1	0.94	0.09	40,40,40,40	0
59	MG	1H	3216	1/1	0.94	0.11	45,45,45,45	0
59	MG	1G	1692	1/1	0.94	0.09	97,97,97,97	0
58	K	1H	3056	1/1	0.95	0.09	43,43,43,43	0
58	K	1H	3108	1/1	0.95	0.17	86,86,86,86	0
58	K	14	3020	1/1	0.95	0.05	72,72,72,72	0
59	MG	14	3150	1/1	0.95	0.25	63,63,63,63	0
58	K	14	3086	1/1	0.95	0.25	97,97,97,97	0
59	MG	14	3292	1/1	0.95	0.07	49,49,49,49	0
58	K	13	1612[B]	1/1	0.95	0.24	23,23,23,23	1
58	K	1H	3097	1/1	0.95	0.12	69,69,69,69	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
58	K	14	3064	1/1	0.95	0.17	70,70,70,70	0
59	MG	1H	3294	1/1	0.95	0.14	35,35,35,35	0
59	MG	14	3298	1/1	0.95	0.05	54,54,54,54	0
59	MG	1H	3176	1/1	0.95	0.19	32,32,32,32	0
58	K	14	3090	1/1	0.95	0.07	65,65,65,65	0
59	MG	14	3167	1/1	0.95	0.29	60,60,60,60	0
58	K	14	3004	1/1	0.95	0.12	55,55,55,55	0
59	MG	1G	1677	1/1	0.95	0.08	76,76,76,76	0
58	K	14	3066	1/1	0.95	0.18	80,80,80,80	0
59	MG	1G	1682	1/1	0.95	0.08	60,60,60,60	0
59	MG	13	1674	1/1	0.95	0.19	92,92,92,92	0
59	MG	13	1747	1/1	0.95	0.07	91,91,91,91	0
59	MG	13	1675	1/1	0.95	0.16	91,91,91,91	0
59	MG	1H	3308	1/1	0.95	0.19	55,55,55,55	0
59	MG	1H	3445	1/1	0.95	0.06	42,42,42,42	0
59	MG	8E	201	1/1	0.95	0.26	49,49,49,49	0
59	MG	1G	1689	1/1	0.95	0.06	90,90,90,90	0
59	MG	14	3182	1/1	0.95	0.09	42,42,42,42	0
59	MG	14	3317	1/1	0.95	0.08	94,94,94,94	0
58	K	1H	3045	1/1	0.95	0.07	72,72,72,72	0
59	MG	14	3184	1/1	0.95	0.14	73,73,73,73	0
59	MG	13	1711	1/1	0.95	0.25	48,48,48,48	0
59	MG	13	1677	1/1	0.95	0.07	63,63,63,63	0
59	MG	1H	3378	1/1	0.95	0.08	30,30,30,30	0
59	MG	1H	3451	1/1	0.95	0.05	63,63,63,63	0
58	K	13	1612[A]	1/1	0.95	0.24	35,35,35,35	1
59	MG	14	3192	1/1	0.95	0.20	63,63,63,63	0
59	MG	2K	101	1/1	0.95	0.23	42,42,42,42	0
59	MG	14	3337	1/1	0.95	0.08	66,66,66,66	0
58	K	1H	3029	1/1	0.95	0.07	104,104,104,104	0
59	MG	14	3339	1/1	0.95	0.03	77,77,77,77	0
59	MG	1H	3129	1/1	0.95	0.21	34,34,34,34	0
59	MG	1G	1699	1/1	0.95	0.11	101,101,101,101	0
59	MG	1H	3249	1/1	0.95	0.23	53,53,53,53	0
59	MG	1G	1701	1/1	0.95	0.08	108,108,108,108	0
59	MG	1H	3250	1/1	0.95	0.19	47,47,47,47	0
59	MG	1H	3460	1/1	0.95	0.06	62,62,62,62	0
58	K	1H	3078	1/1	0.95	0.14	61,61,61,61	0
59	MG	1H	3321	1/1	0.95	0.15	55,55,55,55	0
59	MG	14	3349	1/1	0.95	0.04	77,77,77,77	0
59	MG	14	3204	1/1	0.95	0.09	44,44,44,44	0
59	MG	16	208	1/1	0.95	0.11	63,63,63,63	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
58	K	13	1617	1/1	0.95	0.16	72,72,72,72	0
59	MG	1H	3256	1/1	0.95	0.15	47,47,47,47	0
58	K	14	3033	1/1	0.95	0.23	84,84,84,84	0
59	MG	41	203	1/1	0.95	0.12	40,40,40,40	0
59	MG	14	3212	1/1	0.95	0.12	34,34,34,34	0
59	MG	1H	3197	1/1	0.95	0.08	50,50,50,50	0
59	MG	1G	1713	1/1	0.95	0.12	80,80,80,80	0
59	MG	14	3216	1/1	0.95	0.09	42,42,42,42	0
59	MG	14	3218	1/1	0.95	0.11	66,66,66,66	0
59	MG	14	3219	1/1	0.95	0.07	45,45,45,45	0
59	MG	13	1722	1/1	0.95	0.15	77,77,77,77	0
59	MG	1G	1715	1/1	0.95	0.04	92,92,92,92	0
58	K	14	3078	1/1	0.95	0.15	98,98,98,98	0
59	MG	1H	3469	1/1	0.95	0.09	87,87,87,87	0
59	MG	14	3229	1/1	0.95	0.19	65,65,65,65	0
59	MG	1H	3261	1/1	0.95	0.34	49,49,49,49	0
59	MG	14	3232	1/1	0.95	0.07	69,69,69,69	0
59	MG	13	1724	1/1	0.95	0.09	80,80,80,80	0
59	MG	1H	3264	1/1	0.95	0.25	47,47,47,47	0
59	MG	1H	3473	1/1	0.95	0.11	27,27,27,27	0
59	MG	13	1725	1/1	0.95	0.05	116,116,116,116	0
59	MG	1G	1629	1/1	0.95	0.12	69,69,69,69	0
58	K	1H	3036	1/1	0.95	0.07	55,55,55,55	0
59	MG	1H	3269	1/1	0.95	0.13	54,54,54,54	0
59	MG	13	1686	1/1	0.95	0.22	95,95,95,95	0
59	MG	1H	3405	1/1	0.95	0.06	50,50,50,50	0
59	MG	13	1645	1/1	0.95	0.14	71,71,71,71	0
59	MG	13	1648	1/1	0.95	0.17	61,61,61,61	0
59	MG	13	1649	1/1	0.95	0.22	101,101,101,101	0
59	MG	1H	3150	1/1	0.95	0.32	76,76,76,76	0
59	MG	1H	3214	1/1	0.95	0.17	26,26,26,26	0
59	MG	1G	1645	1/1	0.95	0.12	40,40,40,40	0
59	MG	14	3255	1/1	0.95	0.18	52,52,52,52	0
59	MG	14	3119	1/1	0.95	0.15	51,51,51,51	0
59	MG	14	3257	1/1	0.95	0.13	48,48,48,48	0
59	MG	14	3258	1/1	0.95	0.07	37,37,37,37	0
59	MG	14	3120	1/1	0.95	0.08	44,44,44,44	0
59	MG	14	3121	1/1	0.95	0.12	43,43,43,43	0
58	K	13	1622	1/1	0.95	0.10	73,73,73,73	0
59	MG	14	3125	1/1	0.95	0.10	45,45,45,45	0
59	MG	14	3397	1/1	0.95	0.08	46,46,46,46	0
59	MG	14	3127	1/1	0.95	0.12	41,41,41,41	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
59	MG	1H	3342	1/1	0.95	0.10	50,50,50,50	0
59	MG	1H	3343	1/1	0.95	0.12	35,35,35,35	0
59	MG	13	1654	1/1	0.95	0.15	36,36,36,36	0
59	MG	1H	3281	1/1	0.95	0.12	93,93,93,93	0
59	MG	14	3133	1/1	0.95	0.19	50,50,50,50	0
59	MG	1H	3421	1/1	0.95	0.06	80,80,80,80	0
59	MG	14	3136	1/1	0.95	0.22	77,77,77,77	0
59	MG	1H	3154	1/1	0.95	0.14	31,31,31,31	0
58	K	14	3016	1/1	0.95	0.10	72,72,72,72	0
59	MG	14	3278	1/1	0.95	0.10	43,43,43,43	0
59	MG	1H	3494	1/1	0.95	0.07	78,78,78,78	0
59	MG	1G	1657	1/1	0.95	0.17	74,74,74,74	0
59	MG	13	1693	1/1	0.95	0.16	78,78,78,78	0
59	MG	13	1694	1/1	0.95	0.09	43,43,43,43	0
59	MG	14	3286	1/1	0.95	0.09	47,47,47,47	0
59	MG	1H	3213	1/1	0.96	0.12	73,73,73,73	0
59	MG	1H	3263	1/1	0.96	0.22	33,33,33,33	0
59	MG	1H	3164	1/1	0.96	0.08	45,45,45,45	0
59	MG	13	1681	1/1	0.96	0.13	76,76,76,76	0
58	K	1G	1618	1/1	0.96	0.11	102,102,102,102	0
59	MG	13	1643	1/1	0.96	0.18	76,76,76,76	0
59	MG	32	302	1/1	0.96	0.10	92,92,92,92	0
59	MG	14	3311	1/1	0.96	0.07	56,56,56,56	0
59	MG	1H	3383	1/1	0.96	0.07	54,54,54,54	0
59	MG	14	3095	1/1	0.96	0.22	57,57,57,57	0
59	MG	14	3096	1/1	0.96	0.15	59,59,59,59	0
59	MG	14	3098	1/1	0.96	0.15	38,38,38,38	0
59	MG	14	3099	1/1	0.96	0.14	32,32,32,32	0
59	MG	1H	3270	1/1	0.96	0.10	37,37,37,37	0
59	MG	14	3320	1/1	0.96	0.12	90,90,90,90	0
59	MG	1H	3172	1/1	0.96	0.16	48,48,48,48	0
59	MG	13	1716	1/1	0.96	0.05	66,66,66,66	0
58	K	1H	3022	1/1	0.96	0.06	51,51,51,51	0
59	MG	14	3107	1/1	0.96	0.14	40,40,40,40	0
59	MG	14	3109	1/1	0.96	0.07	36,36,36,36	0
59	MG	14	3329	1/1	0.96	0.10	70,70,70,70	0
59	MG	14	3330	1/1	0.96	0.06	48,48,48,48	0
59	MG	14	3331	1/1	0.96	0.07	58,58,58,58	0
59	MG	14	3215	1/1	0.96	0.15	45,45,45,45	0
59	MG	14	3333	1/1	0.96	0.08	39,39,39,39	0
59	MG	1H	3510	1/1	0.96	0.05	80,80,80,80	0
59	MG	1G	1662	1/1	0.96	0.17	74,74,74,74	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
58	K	1H	3006	1/1	0.96	0.07	59,59,59,59	0
59	MG	14	3220	1/1	0.96	0.09	53,53,53,53	0
59	MG	14	3118	1/1	0.96	0.23	53,53,53,53	0
58	K	14	3051	1/1	0.96	0.11	93,93,93,93	0
59	MG	13	1650	1/1	0.96	0.14	73,73,73,73	0
59	MG	14	3342	1/1	0.96	0.11	54,54,54,54	0
59	MG	1G	1666	1/1	0.96	0.22	77,77,77,77	0
59	MG	14	3123	1/1	0.96	0.11	47,47,47,47	0
59	MG	14	3230	1/1	0.96	0.05	44,44,44,44	0
59	MG	1G	1667	1/1	0.96	0.22	60,60,60,60	0
59	MG	1H	3453	1/1	0.96	0.05	67,67,67,67	0
58	K	1G	1621	1/1	0.96	0.08	74,74,74,74	0
59	MG	1H	3125	1/1	0.96	0.20	41,41,41,41	0
59	MG	1H	3229	1/1	0.96	0.08	51,51,51,51	0
59	MG	14	3238	1/1	0.96	0.10	42,42,42,42	0
59	MG	1H	3334	1/1	0.96	0.27	55,55,55,55	0
59	MG	1H	3458	1/1	0.96	0.04	89,89,89,89	0
58	K	14	3010	1/1	0.96	0.12	53,53,53,53	0
59	MG	1G	1678	1/1	0.96	0.15	71,71,71,71	0
58	K	14	3032	1/1	0.96	0.07	61,61,61,61	0
59	MG	14	3137	1/1	0.96	0.10	83,83,83,83	0
58	K	14	3056	1/1	0.96	0.08	57,57,57,57	0
58	K	1H	3057	1/1	0.96	0.06	43,43,43,43	0
59	MG	1H	3401	1/1	0.96	0.03	73,73,73,73	0
59	MG	14	3363	1/1	0.96	0.07	85,85,85,85	0
59	MG	13	1660	1/1	0.96	0.14	60,60,60,60	0
59	MG	1H	3287	1/1	0.96	0.13	43,43,43,43	0
59	MG	14	3253	1/1	0.96	0.20	52,52,52,52	0
59	MG	1H	3187	1/1	0.96	0.09	37,37,37,37	0
59	MG	1H	3135	1/1	0.96	0.08	50,50,50,50	0
58	K	1H	3080	1/1	0.96	0.10	51,51,51,51	0
59	MG	1H	3407	1/1	0.96	0.04	65,65,65,65	0
58	K	21	302	1/1	0.96	0.07	66,66,66,66	0
59	MG	14	3259	1/1	0.96	0.07	45,45,45,45	0
58	K	1H	3081	1/1	0.96	0.17	66,66,66,66	0
59	MG	14	3153	1/1	0.96	0.15	68,68,68,68	0
58	K	31	302	1/1	0.96	0.12	90,90,90,90	0
59	MG	1H	3413	1/1	0.96	0.06	42,42,42,42	0
58	K	1H	3027	1/1	0.96	0.16	91,91,91,91	0
59	MG	1H	3295	1/1	0.96	0.17	46,46,46,46	0
59	MG	14	3268	1/1	0.96	0.07	79,79,79,79	0
59	MG	14	3160	1/1	0.96	0.19	73,73,73,73	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
59	MG	14	3161	1/1	0.96	0.14	44,44,44,44	0
59	MG	13	1668	1/1	0.96	0.10	41,41,41,41	0
59	MG	14	3163	1/1	0.96	0.08	48,48,48,48	0
59	MG	14	3164	1/1	0.96	0.15	70,70,70,70	0
59	MG	14	3165	1/1	0.96	0.16	70,70,70,70	0
59	MG	1H	3297	1/1	0.96	0.27	52,52,52,52	0
59	MG	1H	3298	1/1	0.96	0.13	23,23,23,23	0
59	MG	G8	201	1/1	0.96	0.08	89,89,89,89	0
58	K	1H	3028	1/1	0.96	0.13	50,50,50,50	0
59	MG	1H	3148	1/1	0.96	0.18	39,39,39,39	0
58	K	13	1618	1/1	0.96	0.14	90,90,90,90	0
59	MG	14	3282	1/1	0.96	0.09	50,50,50,50	0
58	K	1H	3095	1/1	0.96	0.06	44,44,44,44	0
59	MG	14	3284	1/1	0.96	0.08	39,39,39,39	0
58	K	1G	1603	1/1	0.96	0.17	79,79,79,79	0
58	K	14	3068	1/1	0.96	0.13	48,48,48,48	0
58	K	29	302	1/1	0.96	0.07	89,89,89,89	0
59	MG	13	1708	1/1	0.96	0.21	59,59,59,59	0
59	MG	1H	3255	1/1	0.96	0.19	36,36,36,36	0
59	MG	1H	3205	1/1	0.96	0.06	34,34,34,34	0
58	K	14	3044	1/1	0.96	0.11	95,95,95,95	0
59	MG	1H	3491	1/1	0.96	0.07	51,51,51,51	0
59	MG	14	3294	1/1	0.96	0.06	77,77,77,77	0
58	K	14	3070	1/1	0.96	0.13	95,95,95,95	0
59	MG	1H	3433	1/1	0.96	0.11	44,44,44,44	0
59	MG	1H	3314	1/1	0.96	0.10	49,49,49,49	0
59	MG	1H	3210	1/1	0.96	0.12	50,50,50,50	0
58	K	14	3025	1/1	0.96	0.09	97,97,97,97	0
58	K	1H	3054	1/1	0.96	0.20	68,68,68,68	0
59	MG	1G	1720	1/1	0.96	0.07	106,106,106,106	0
59	MG	1G	1721	1/1	0.96	0.06	88,88,88,88	0
61	ZN	5A	101	1/1	0.96	0.11	115,115,115,115	0
59	MG	14	3326	1/1	0.97	0.07	45,45,45,45	0
59	MG	14	3158	1/1	0.97	0.08	35,35,35,35	0
59	MG	14	3241	1/1	0.97	0.10	34,34,34,34	0
59	MG	14	3159	1/1	0.97	0.21	53,53,53,53	0
59	MG	1H	3141	1/1	0.97	0.17	37,37,37,37	0
58	K	1H	3049	1/1	0.97	0.11	66,66,66,66	0
59	MG	1H	3189	1/1	0.97	0.17	46,46,46,46	0
59	MG	1H	3420	1/1	0.97	0.02	95,95,95,95	0
58	K	1H	3046	1/1	0.97	0.10	50,50,50,50	0
59	MG	1H	3422	1/1	0.97	0.05	43,43,43,43	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
58	K	1H	3051	1/1	0.97	0.06	58,58,58,58	0
58	K	1H	3074	1/1	0.97	0.10	53,53,53,53	0
59	MG	14	3168	1/1	0.97	0.04	37,37,37,37	0
58	K	1H	3107	1/1	0.97	0.09	82,82,82,82	0
59	MG	14	3170	1/1	0.97	0.18	52,52,52,52	0
59	MG	1H	3376	1/1	0.97	0.12	29,29,29,29	0
58	K	14	3071	1/1	0.97	0.30	75,75,75,75	0
59	MG	13	1661	1/1	0.97	0.07	42,42,42,42	0
59	MG	1H	3152	1/1	0.97	0.15	37,37,37,37	0
59	MG	1G	1669	1/1	0.97	0.09	72,72,72,72	0
58	K	14	3072	1/1	0.97	0.05	89,89,89,89	0
59	MG	1H	3381	1/1	0.97	0.11	59,59,59,59	0
59	MG	13	1719	1/1	0.97	0.05	112,112,112,112	0
59	MG	14	3264	1/1	0.97	0.21	55,55,55,55	0
59	MG	13	1720	1/1	0.97	0.04	73,73,73,73	0
59	MG	14	3266	1/1	0.97	0.18	74,74,74,74	0
59	MG	14	3180	1/1	0.97	0.16	40,40,40,40	0
59	MG	1G	1675	1/1	0.97	0.07	54,54,54,54	0
58	K	14	3006	1/1	0.97	0.14	62,62,62,62	0
58	K	19	301	1/1	0.97	0.18	61,61,61,61	0
59	MG	1H	3202	1/1	0.97	0.17	46,46,46,46	0
59	MG	14	3105	1/1	0.97	0.25	36,36,36,36	0
59	MG	1G	1679	1/1	0.97	0.07	64,64,64,64	0
59	MG	1G	1680	1/1	0.97	0.05	90,90,90,90	0
59	MG	1H	3485	1/1	0.97	0.12	27,27,27,27	0
59	MG	1H	3245	1/1	0.97	0.16	41,41,41,41	0
58	K	14	3038	1/1	0.97	0.16	63,63,63,63	0
59	MG	14	3367	1/1	0.97	0.06	52,52,52,52	0
58	K	14	3007	1/1	0.97	0.20	52,52,52,52	0
58	K	1H	3098	1/1	0.97	0.08	67,67,67,67	0
59	MG	1H	3206	1/1	0.97	0.08	35,35,35,35	0
59	MG	13	1638	1/1	0.97	0.15	58,58,58,58	0
59	MG	14	3122	1/1	0.97	0.13	49,49,49,49	0
59	MG	J8	101	1/1	0.97	0.05	49,49,49,49	0
59	MG	14	3285	1/1	0.97	0.08	43,43,43,43	0
59	MG	1H	3443	1/1	0.97	0.02	61,61,61,61	0
58	K	13	1616	1/1	0.97	0.08	96,96,96,96	0
59	MG	14	3126	1/1	0.97	0.22	69,69,69,69	0
59	MG	1H	3300	1/1	0.97	0.21	31,31,31,31	0
59	MG	1H	3124	1/1	0.97	0.22	28,28,28,28	0
59	MG	1H	3171	1/1	0.97	0.19	28,28,28,28	0
59	MG	1H	3497	1/1	0.97	0.07	83,83,83,83	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
58	K	1H	3083	1/1	0.97	0.08	43,43,43,43	0
59	MG	1H	3127	1/1	0.97	0.19	54,54,54,54	0
59	MG	1H	3128	1/1	0.97	0.18	40,40,40,40	0
59	MG	14	3211	1/1	0.97	0.21	64,64,64,64	0
59	MG	1G	1636	1/1	0.97	0.22	89,89,89,89	0
59	MG	1G	1637	1/1	0.97	0.21	77,77,77,77	0
59	MG	14	3388	1/1	0.97	0.05	53,53,53,53	0
59	MG	14	3138	1/1	0.97	0.14	40,40,40,40	0
59	MG	1G	1638	1/1	0.97	0.10	43,43,43,43	0
58	K	14	3060	1/1	0.97	0.03	67,67,67,67	0
58	K	14	3081	1/1	0.97	0.14	89,89,89,89	0
59	MG	1H	3217	1/1	0.97	0.27	52,52,52,52	0
59	MG	1H	3218	1/1	0.97	0.20	53,53,53,53	0
59	MG	14	3144	1/1	0.97	0.10	50,50,50,50	0
58	K	14	3011	1/1	0.97	0.07	56,56,56,56	0
59	MG	14	3223	1/1	0.97	0.06	53,53,53,53	0
59	MG	14	3146	1/1	0.97	0.09	30,30,30,30	0
59	MG	1H	3220	1/1	0.97	0.14	45,45,45,45	0
59	MG	14	3228	1/1	0.97	0.23	88,88,88,88	0
58	K	1H	3111	1/1	0.97	0.15	75,75,75,75	0
59	MG	1G	1708	1/1	0.97	0.07	69,69,69,69	0
59	MG	14	3403	1/1	0.97	0.07	75,75,75,75	0
59	MG	13	1646	1/1	0.97	0.19	59,59,59,59	0
59	MG	14	3405	1/1	0.97	0.06	45,45,45,45	0
59	MG	1H	3410	1/1	0.97	0.05	86,86,86,86	0
59	MG	14	3316	1/1	0.97	0.07	53,53,53,53	0
59	MG	13	1705	1/1	0.97	0.21	60,60,60,60	0
59	MG	13	1647	1/1	0.97	0.20	59,59,59,59	0
59	MG	14	3319	1/1	0.97	0.07	59,59,59,59	0
58	K	13	1611	1/1	0.97	0.05	79,79,79,79	0
59	MG	14	3236	1/1	0.97	0.14	41,41,41,41	0
59	MG	14	3237	1/1	0.97	0.12	58,58,58,58	0
58	K	14	3046	1/1	0.97	0.10	68,68,68,68	0
59	MG	14	3324	1/1	0.97	0.05	62,62,62,62	0
58	K	1H	3077	1/1	0.97	0.08	49,49,49,49	0
59	MG	14	3207	1/1	0.98	0.16	58,58,58,58	0
58	K	1H	3053	1/1	0.98	0.13	63,63,63,63	0
59	MG	21	303	1/1	0.98	0.15	30,30,30,30	0
59	MG	1H	3353	1/1	0.98	0.03	53,53,53,53	0
59	MG	13	1672	1/1	0.98	0.15	24,24,24,24	0
59	MG	1H	3144	1/1	0.98	0.10	38,38,38,38	0
59	MG	14	3352	1/1	0.98	0.05	64,64,64,64	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
59	MG	1H	3356	1/1	0.98	0.07	31,31,31,31	0
59	MG	14	3354	1/1	0.98	0.06	70,70,70,70	0
59	MG	1H	3145	1/1	0.98	0.18	32,32,32,32	0
59	MG	13	1673	1/1	0.98	0.20	56,56,56,56	0
59	MG	14	3152	1/1	0.98	0.09	69,69,69,69	0
59	MG	14	3217	1/1	0.98	0.21	59,59,59,59	0
59	MG	1G	1674	1/1	0.98	0.20	50,50,50,50	0
59	MG	I8	101	1/1	0.98	0.13	48,48,48,48	0
58	K	14	3073	1/1	0.98	0.18	81,81,81,81	0
58	K	1H	3070	1/1	0.98	0.08	54,54,54,54	0
59	MG	2L	101	1/1	0.98	0.14	55,55,55,55	0
58	K	1H	3062	1/1	0.98	0.07	42,42,42,42	0
59	MG	1H	3123	1/1	0.98	0.15	20,20,20,20	0
59	MG	1H	3365	1/1	0.98	0.09	40,40,40,40	0
59	MG	14	3227	1/1	0.98	0.06	41,41,41,41	0
59	MG	14	3097	1/1	0.98	0.13	38,38,38,38	0
59	MG	1H	3411	1/1	0.98	0.07	28,28,28,28	0
59	MG	1H	3185	1/1	0.98	0.10	41,41,41,41	0
59	MG	13	1657	1/1	0.98	0.13	26,26,26,26	0
59	MG	1H	3251	1/1	0.98	0.07	52,52,52,52	0
59	MG	13	1717	1/1	0.98	0.07	66,66,66,66	0
59	MG	1H	3253	1/1	0.98	0.09	53,53,53,53	0
59	MG	14	3104	1/1	0.98	0.18	29,29,29,29	0
58	K	1H	3058	1/1	0.98	0.06	56,56,56,56	0
59	MG	14	3106	1/1	0.98	0.28	34,34,34,34	0
58	K	1H	3073	1/1	0.98	0.09	47,47,47,47	0
59	MG	14	3108	1/1	0.98	0.15	62,62,62,62	0
58	K	14	3053	1/1	0.98	0.08	63,63,63,63	0
59	MG	1H	3330	1/1	0.98	0.06	45,45,45,45	0
59	MG	1G	1640	1/1	0.98	0.16	53,53,53,53	0
59	MG	14	3114	1/1	0.98	0.17	57,57,57,57	0
58	K	14	3019	1/1	0.98	0.09	81,81,81,81	0
59	MG	14	3116	1/1	0.98	0.15	41,41,41,41	0
59	MG	1H	3158	1/1	0.98	0.26	89,89,89,89	0
59	MG	14	3247	1/1	0.98	0.20	60,60,60,60	0
59	MG	1H	3131	1/1	0.98	0.21	42,42,42,42	0
58	K	1H	3115	1/1	0.98	0.04	50,50,50,50	0
59	MG	1H	3162	1/1	0.98	0.23	21,21,21,21	0
59	MG	1H	3299	1/1	0.98	0.12	34,34,34,34	0
58	K	14	3021	1/1	0.98	0.06	47,47,47,47	0
59	MG	1H	3165	1/1	0.98	0.20	30,30,30,30	0
59	MG	1H	3384	1/1	0.98	0.05	60,60,60,60	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
59	MG	14	3187	1/1	0.98	0.12	41,41,41,41	0
59	MG	1H	3166	1/1	0.98	0.15	17,17,17,17	0
59	MG	1H	3303	1/1	0.98	0.12	41,41,41,41	0
59	MG	1H	3387	1/1	0.98	0.07	37,37,37,37	0
59	MG	14	3328	1/1	0.98	0.06	66,66,66,66	0
59	MG	1G	1653	1/1	0.98	0.17	52,52,52,52	0
58	K	11	301	1/1	0.98	0.05	47,47,47,47	0
59	MG	14	3194	1/1	0.98	0.12	64,64,64,64	0
59	MG	1G	1655	1/1	0.98	0.27	67,67,67,67	0
58	K	1H	3067	1/1	0.98	0.13	49,49,49,49	0
59	MG	1H	3268	1/1	0.98	0.13	50,50,50,50	0
59	MG	14	3135	1/1	0.98	0.12	42,42,42,42	0
59	MG	14	3336	1/1	0.98	0.07	47,47,47,47	0
59	MG	1H	3169	1/1	0.98	0.18	43,43,43,43	0
59	MG	13	1667	1/1	0.98	0.23	39,39,39,39	0
59	MG	1H	3346	1/1	0.98	0.16	27,27,27,27	0
58	K	1H	3068	1/1	0.98	0.05	37,37,37,37	0
59	MG	14	3271	1/1	0.98	0.07	52,52,52,52	0
59	MG	1H	3272	1/1	0.98	0.17	60,60,60,60	0
59	MG	13	1748	1/1	0.98	0.08	104,104,104,104	0
59	MG	13	1651	1/1	0.98	0.19	51,51,51,51	0
61	ZN	5I	102	1/1	0.98	0.11	110,110,110,110	0
59	MG	13	1652	1/1	0.98	0.33	95,95,95,95	0
59	MG	14	3224	1/1	0.99	0.05	53,53,53,53	0
59	MG	1H	3146	1/1	0.99	0.18	24,24,24,24	0
59	MG	1H	3234	1/1	0.99	0.24	33,33,33,33	0
59	MG	14	3128	1/1	0.99	0.14	35,35,35,35	0
59	MG	13	1702	1/1	0.99	0.26	62,62,62,62	0
59	MG	1H	3163	1/1	0.99	0.23	40,40,40,40	0
59	MG	1H	3357	1/1	0.99	0.05	34,34,34,34	0
58	K	14	3024	1/1	0.99	0.07	57,57,57,57	0
59	MG	1H	3126	1/1	0.99	0.19	53,53,53,53	0
59	MG	14	3110	1/1	0.99	0.15	48,48,48,48	0
59	MG	14	3111	1/1	0.99	0.06	44,44,44,44	0
59	MG	1G	1626	1/1	0.99	0.17	72,72,72,72	0
59	MG	1H	3175	1/1	0.99	0.20	34,34,34,34	0
59	MG	1H	3277	1/1	0.99	0.13	18,18,18,18	0
59	MG	1H	3137	1/1	0.99	0.22	42,42,42,42	0
59	MG	13	1644	1/1	0.99	0.08	49,49,49,49	0
59	MG	14	3189	1/1	0.99	0.24	26,26,26,26	0
59	MG	14	3117	1/1	0.99	0.15	42,42,42,42	0
59	MG	1G	1631	1/1	0.99	0.17	49,49,49,49	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
59	MG	1G	1632	1/1	0.99	0.21	109,109,109,109	0
59	MG	1H	3364	1/1	0.99	0.08	28,28,28,28	0
59	MG	1H	3266	1/1	0.99	0.31	40,40,40,40	0
59	MG	13	1659	1/1	0.99	0.22	54,54,54,54	0
59	MG	14	3301	1/1	0.99	0.04	53,53,53,53	0
59	MG	1H	3209	1/1	0.99	0.16	33,33,33,33	0
59	MG	14	3248	1/1	0.99	0.04	41,41,41,41	0
60	SF4	3E	302	8/8	0.99	0.18	78,87,103,104	0
60	SF4	32	303	8/8	0.99	0.19	73,95,102,116	0
59	MG	1H	3368	1/1	0.99	0.05	20,20,20,20	0
59	MG	1H	3160	1/1	0.99	0.26	29,29,29,29	0

6.5 Other polymers [i](#)

There are no such residues in this entry.