



wwPDB X-ray Structure Validation Summary Report ⓘ

Nov 11, 2020 – 06:31 AM GMT

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 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 : 2.14.6
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) : 2.14.6

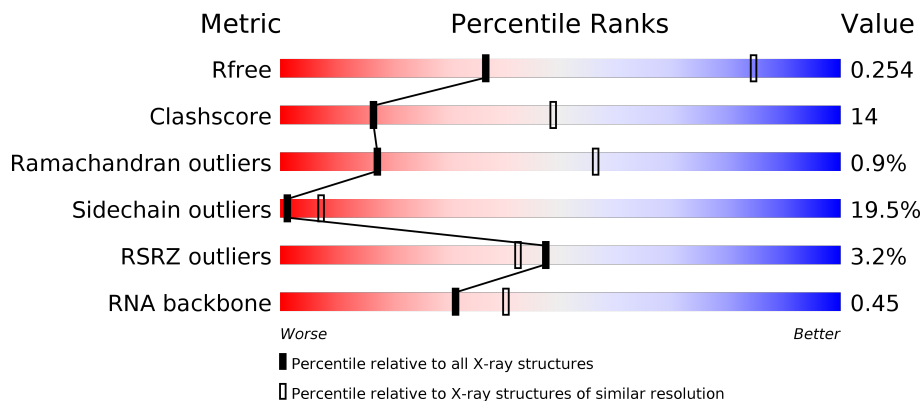
1 Overall quality at a glance

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.



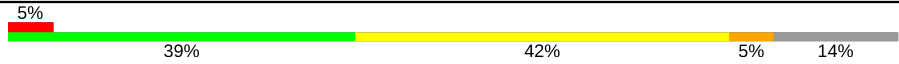



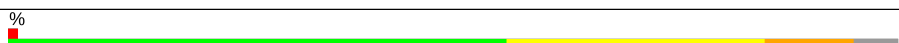
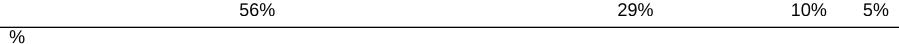






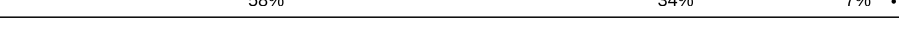


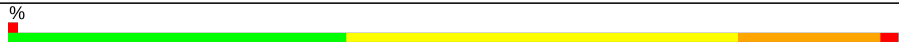




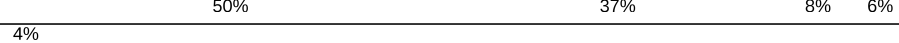




Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1659 (3.60-3.40)
Clashscore	141614	1036 (3.58-3.42)
Ramachandran outliers	138981	1005 (3.58-3.42)
Sidechain outliers	138945	1006 (3.58-3.42)
RSRZ outliers	127900	1559 (3.60-3.40)
RNA backbone	3102	1002 (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 on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	13	1522	 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%






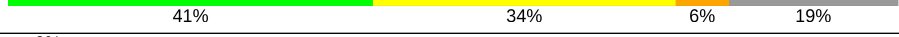
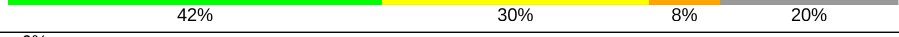

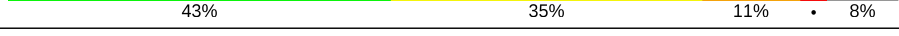


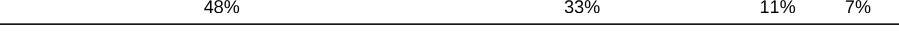

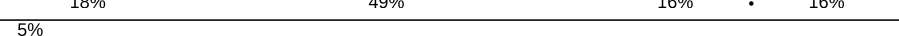


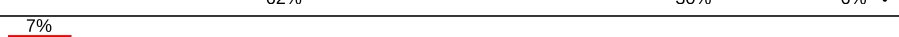
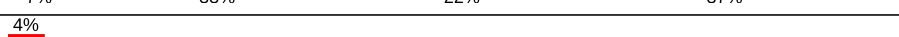
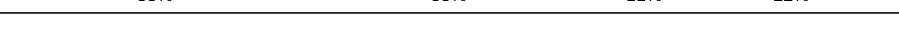
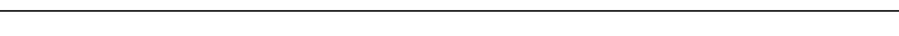

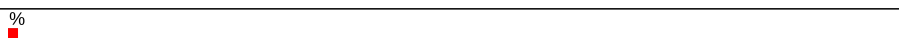
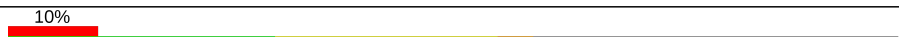


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Mol	Chain	Length	Quality of chain
3	22	239	
3	2E	239	
4	32	209	
4	3E	209	
5	42	162	
5	4E	162	
6	52	101	
6	5E	101	
7	62	156	
7	6E	156	
8	72	138	
8	7E	138	
9	82	128	
9	8E	128	
10	1A	105	
10	1I	105	
11	2A	129	
11	2I	129	
12	3A	132	
12	3I	132	
13	4A	126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




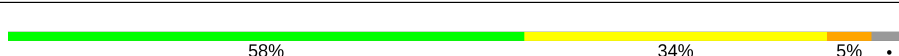
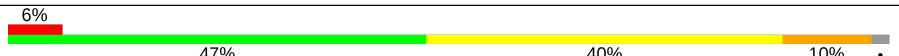

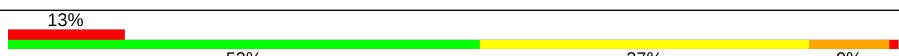


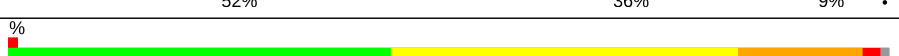

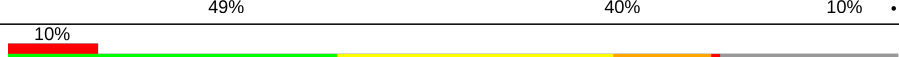
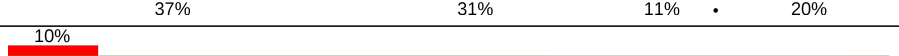
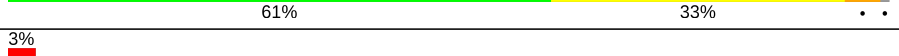
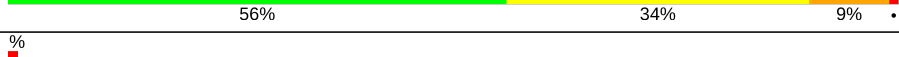






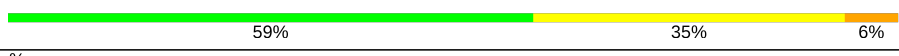



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Mol	Chain	Length	Quality of chain
15	6I	89	 % 62% 30% 7%
16	7A	88	 61% 25% 9% 5%
16	7I	88	 53% 33% 8% 6%
17	8A	105	 53% 35% 6% 6%
17	8I	105	 59% 30% 6% 5%
18	9A	88	 7% 41% 34% 6% 19%
18	9I	88	 9% 42% 30% 8% 20%
19	AA	93	 6% 32% 45% 11% 11%
19	AI	93	 43% 35% 11% 8%
20	BA	106	 51% 39% 8%
20	BI	106	 53% 39% 5%
21	1B	27	 48% 33% 11% 7%
21	1F	27	 41% 52% 7%
22	1K	77	 39% 18% 49% 16% 16%
22	3K	77	 5% 32% 53% 14%
22	3L	77	 3% 30% 48% 21%
23	2K	77	 62% 30% 6%
24	4K	27	 7% 7% 33% 22% 37%
24	4L	27	 4% 33% 33% 11% 22%
25	14	2917	 43% 41% 14%
25	1H	2917	 47% 38% 12%
26	16	122	 49% 36% 13%
26	1J	122	 % 24% 53% 23%
27	7I	229	 10% 30% 25% 41%
28	11	276	 64% 29% 7%

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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
			Total	C	N	O	P			
1	13	1506	Total 32387	C 14423	N 5999	O 10459	P 1506	0	0	0
1	1G	1510	Total 32470	C 14460	N 6012	O 10488	P 1510	0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	1E	237	Total 1924	C 1228	N 344	O 347	S 5	0	0	0
2	12	236	Total 1915	C 1223	N 343	O 344	S 5	0	0	0

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

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

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

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

- 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
			Total	C	N	O	S			
10	1A	99	801	504	157	139	1	0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
11	2I	117	864	537	162	162	3	0	0	0
11	2A	119	889	554	169	163	3	0	0	0

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
13	4I	119	946	585	195	164	2	0	0	0
13	4A	118	937	579	193	163	2	0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
14	5I	60	491	312	104	71	4	0	0	0
14	5A	60	485	309	101	71	4	0	0	0

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

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

- 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
			Total	C	N	O	P			
26	1J	122	2617	1166	486	844	121	0	0	0

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

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

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

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

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

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

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

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

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

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

- 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
			Total	C	N	O	S			
38	88	141	Total 1121	C 715	N 212	O 187	S 7	0	0	0
38	45	140	Total 1112	C 710	N 210	O 185	S 7	0	0	0

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

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

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

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

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

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

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

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

- 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
			Total	C	N	O	S			
48	E5	79	623	386	131	105	1	0	0	0

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

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

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

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

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

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

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

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

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

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

- 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	0
			1643	735	297	534	76	1			

- Molecule 58 is POTASSIUM ION (three-letter code: K) (formula: K) (labeled as "Ligand of Interest" by author).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
58	14	94	Total	K	0	0
			94	94		
58	21	1	Total	K	0	0
			1	1		
58	31	2	Total	K	0	0
			2	2		
58	52	1	Total	K	0	0
			1	1		
58	32	1	Total	K	0	0
			1	1		

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
58	8I	1	Total K 1 1	0	0
58	19	1	Total K 1 1	0	0
58	13	37	Total K 38 38	0	1
58	39	1	Total K 1 1	0	0
58	1G	25	Total K 25 25	0	0
58	11	1	Total K 1 1	0	0
58	3A	1	Total K 1 1	0	0
58	41	2	Total K 2 2	0	0
58	5I	1	Total K 1 1	0	0
58	1H	121	Total K 122 122	0	1
58	BA	1	Total K 1 1	0	0
58	5E	1	Total K 1 1	0	0
58	29	2	Total K 2 2	0	0
58	16	2	Total K 2 2	0	0

- Molecule 59 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

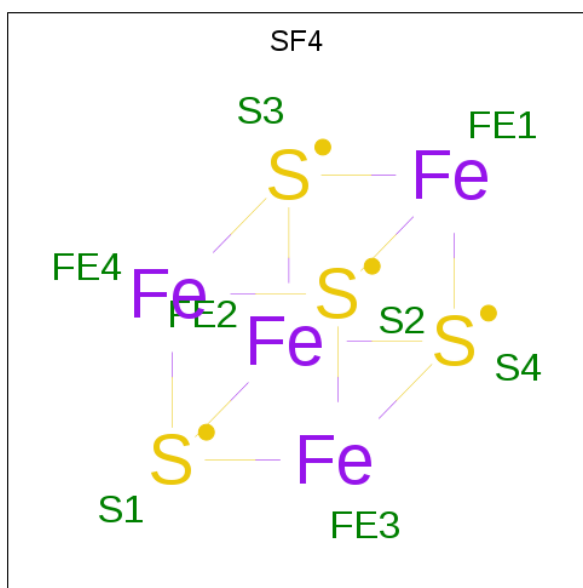
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
59	32	1	Total Mg 1 1	0	0
59	13	111	Total Mg 111 111	0	0
59	1J	5	Total Mg 5 5	0	0
59	BI	2	Total Mg 2 2	0	0
59	16	8	Total Mg 8 8	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
59	21	2	Total 2	Mg 2	0	0
59	78	1	Total 1	Mg 1	0	0
59	Q8	1	Total 1	Mg 1	0	0
59	4I	1	Total 1	Mg 1	0	0
59	I8	2	Total 2	Mg 2	0	0
59	D8	3	Total 3	Mg 3	0	0
59	8E	1	Total 1	Mg 1	0	0
59	29	2	Total 2	Mg 2	0	0
59	41	1	Total 1	Mg 1	0	0
59	2K	1	Total 1	Mg 1	0	0
59	J8	1	Total 1	Mg 1	0	0
59	1G	102	Total 102	Mg 102	0	0
59	1H	404	Total 405	Mg 405	0	1
59	7I	1	Total 1	Mg 1	0	0
59	E5	1	Total 1	Mg 1	0	0
59	N8	1	Total 1	Mg 1	0	0
59	14	312	Total 312	Mg 312	0	0
59	3E	1	Total 1	Mg 1	0	0
59	55	1	Total 1	Mg 1	0	0
59	G8	1	Total 1	Mg 1	0	0
59	2L	2	Total 2	Mg 2	0	0

- Molecule 60 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe₄S₄).



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	5A	1	Total	Zn	0	0
			1	1		
61	5I	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 O 4 4	0	0
62	42	1	Total O 1 1	0	0
62	3A	1	Total O 1 1	0	0
62	7A	5	Total O 5 5	0	0
62	BA	1	Total O 1 1	0	0
62	2L	6	Total O 6 6	0	0
62	4L	4	Total O 4 4	0	0
62	14	681	Total O 681 681	0	0
62	1J	16	Total O 16 16	0	0
62	19	12	Total O 12 12	0	0
62	29	3	Total O 3 3	0	0
62	39	3	Total O 3 3	0	0
62	35	3	Total O 3 3	0	0
62	55	2	Total O 2 2	0	0
62	75	1	Total O 1 1	0	0
62	85	1	Total O 1 1	0	0
62	B5	2	Total O 2 2	0	0
62	C5	2	Total O 2 2	0	0
62	F5	1	Total O 1 1	0	0
62	G5	1	Total O 1 1	0	0
62	L5	1	Total O 1 1	0	0

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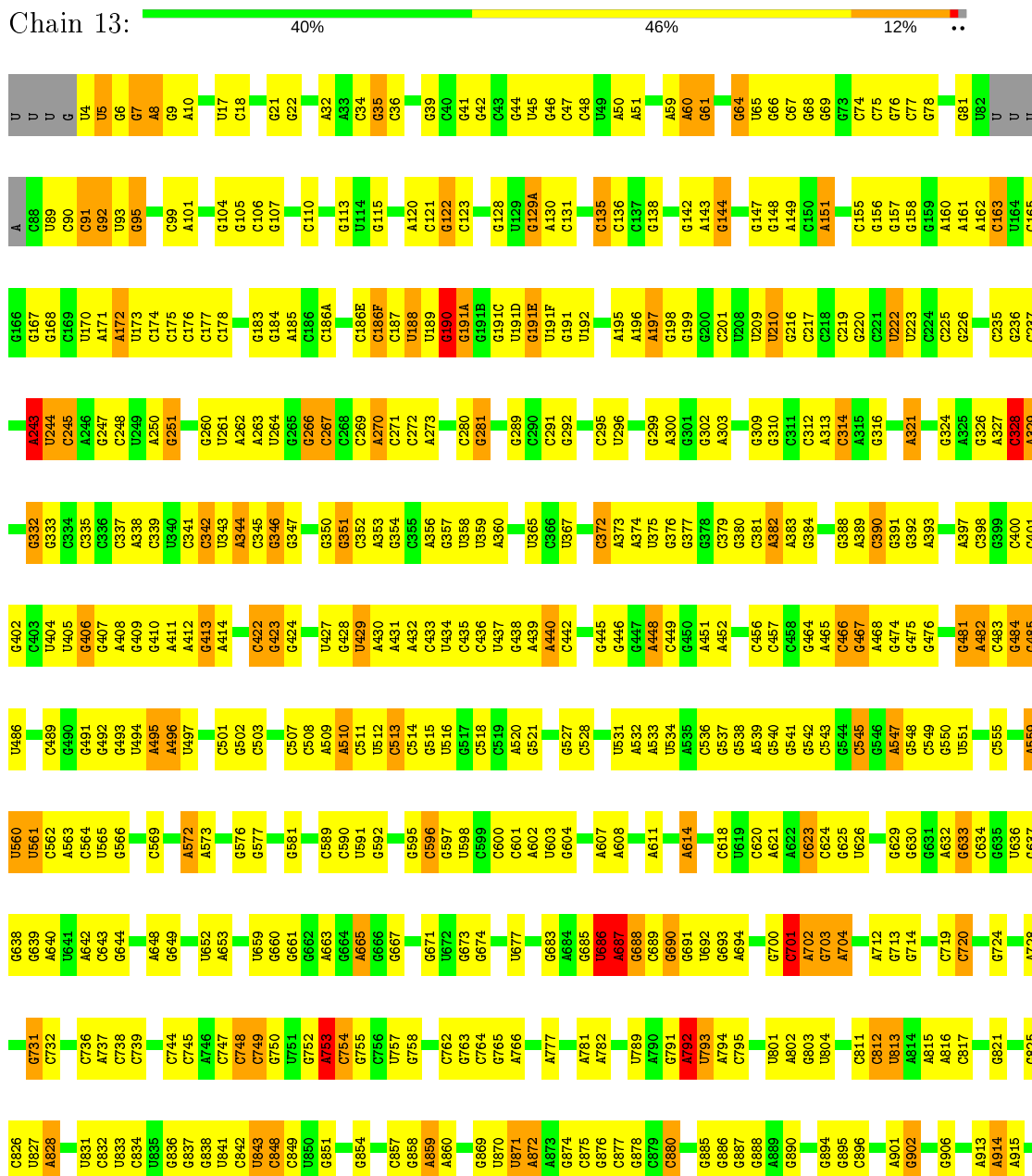
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
62	M5	1	Total	O	0	0
			1	1		

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



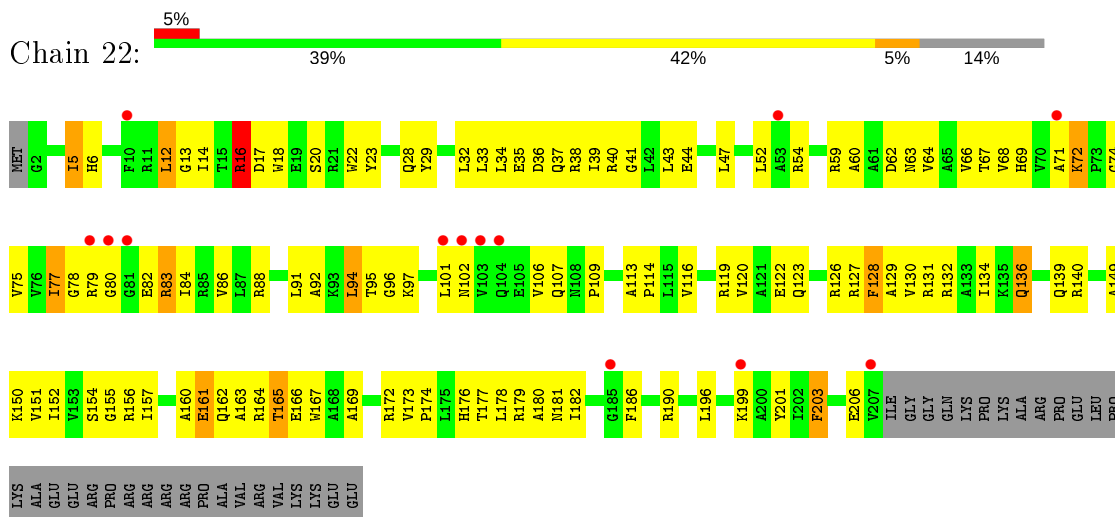
A919	G993	G1131	G1206	G1276	A1339	C1400	G1487	G181	C267	G346
G922	A994	C1132	G1207	C1277	A1340	G1401	A1492	U	G347	G347
G926	U997	G1133	C1210	U1278	A1341	C1402	A1493	U	A270	G351
G927	G998	G1134	U1211	A1279	C1342	C1403	G1494	U	C271	G352
G933	C998A	U1135	U1212	U1280	G1343	C1404	U1495	U	G276	A353
C934	U999	U1065	A1213	U1281	G1344	G1405	U1496	U	C277	G354
A935	A1000	C1066	G1216	G1282	U1345	U1406	A1497	U	G278	C355
C936	G1001	U1070	G1217	G1283	A1346	A1407	A1498	U	A279	A356
A937	G1002	C1071	C1218	C1284	G1347	C1408	A1502	A	C186F	U359
A938	G1003	G1072	U1219	A1285	A1348	C1409	A1503	U89	C187	C280
G939	A1004	U1073	U1219	A1286	A1349	G1410	G1504	U	U188	C281
C940	A1005	G1074	G1222	A1287	A1350	C1411	G1505	U	U189	G284
G944	C1006	U1075	G1223	A1288	U1351	U1414	U1506	U	G285	G285
G947	C1007	C1076	C1224	A1289	C1352	G1415	A1507	U	G286	G286
C948	C1008	G1077	C1225	G1290	G1353	G1416	U1510	G	A279	U365
A949	G1009	U1078	C1226	G1291	C1354	G1419	G1511	U	C186G	C366
U950	G1010	A1080	A1227	G1292	G1355	G1422	U1512	U	G191E	U367
G951	G1011	U1083	G1231	C1296	A1356	G1423	A1513	U	U191F	U368
G951	U1012	G1083	G1232	C1297	G1357	G1424	A1514	U	G191	C369
G951	A1014	U1084	U1232	C1298	A1360	U1425	G1515	U	U192	C295
U952	A1015	G1085	G1233	C1299	G1361	C1426	G1516	U	C296	G371
U952	A1016	U1086	U1234	A1299	G1362	U1427	G1517	U	C297	C372
G953	G1017	U1086	U1235	G1300	C1362A	U1428	A1518	U	A298	A373
G954	U1020	G1087	A1236	U1301	A1363	C1429	A1519	U	A196	A374
U955	G1021	U1090	C1237	U1302	A1364	C1430	G1529	U	C201	U375
U956	C1022	U1090	A1238	G1303	G1365	C1431	G1530	U	G115	G376
U957	G1023	U1094	A1239	G1304	G1366	G1432	G1531	U	A116	G377
A958	G1024	U1095	U1240	G1305	C1367	G1433	A1531	U	A117	U209
U959	U1025	U1095	G1241	G1306	C1368	A1434	U1532	U	A119	U210
U960	U1026	A1101	C1242	G1309	C1369	G1435	C1533	U	A120	G216
U961	G1028	G1104	C1243	U1310	G1370	U1436	A1534	U	C121	C217
G962	C1027	G1104	C1246	U1311	G1371	C1437	C1535	U	G122	U222
G963	C1028	A1105	U1247	G1312	G1372	G1438	C1536	U	C123	U223
A964	C1028A	G1106	U1247	C1313	G1373	U1442	U	U	G127	U224
A965	C1028B	G1107	A1250	C1314	A1374	G1443	U	U	G127	C224
G966	G1029	G1107	A1251	C1315	A1375	G1444	U	U	G127	C225
C967	G1032A	G1108	A1252	C1316	U1376	G1445	U	U	G127	G226
A968	G1033	C1109	A1253	C1317	A1446	A1447	U	U	C137	G232
A969	G1033B	A1110	G1254	C1318	A1447	G1448	U	U	G138	C233
G971	G1034	A1111	G1255	C1319	C1378	C1449	U	U	G142	U239
G972	A1035	C1112	A1256	C1320	U1380	U1450	U	U	G143	U239
G973	G1036	C1113	U1257	C1321	U1381	A1451	U	U	G144	C245
A974	C1037	C1114	U1258	C1322	U1382	C1452	U	U	G145	A246
A975	A1038	G1117	G1258	C1323	C1383	G1453	U	U	G146	G247
G976	C1038	C1118	C1259	C1324	C1384	U1454	U	U	G147	U256
A977	U1039	C1119	G1260	C1325	G1385	G1455	U	U	G148	U256
A978	U1040	C1119	A1261	C1326	G1386	C1459	U	U	A250	G260
C979	G1044	G1120	C1262	C1327	G1387	A1460	U	U	G251	U261
C980	U1044	U1121	C1263	C1328	C1388	G1461	U	U	G254	A262
C981	U1049	U1122	C1267	C1329	C1389	U1462	U	U	G255	C266
U982	U1081	A1123	G1267	C1330	U1390	C1463	U	U	G256	C266
U983	C1054	G1124	G1270	C1331	U1391	G1463	U	U	U256	C266
C984	U1055	U1195	G1271	C1332	U1392	C1463	U	U	G256	C266
C985	G1056	U1196	G1272	C1333	G1392	G1463	U	U	G256	C266
U991	G1057	G1197	G1272	C1334	A1396	C1463	U	U	G256	C266
U992	C1059	A1200	G1273	C1335	A1397	G1463	U	U	G256	C266
		C1129	G1274	C1336	A1398	G1463	U	U	G256	C266
		A1130	A1275	C1337	A1399	G1463	U	U	G256	C266
				G1338	C1399	G1463	U	U	G256	C266

• Molecule 1: 16S ribosomal RNA

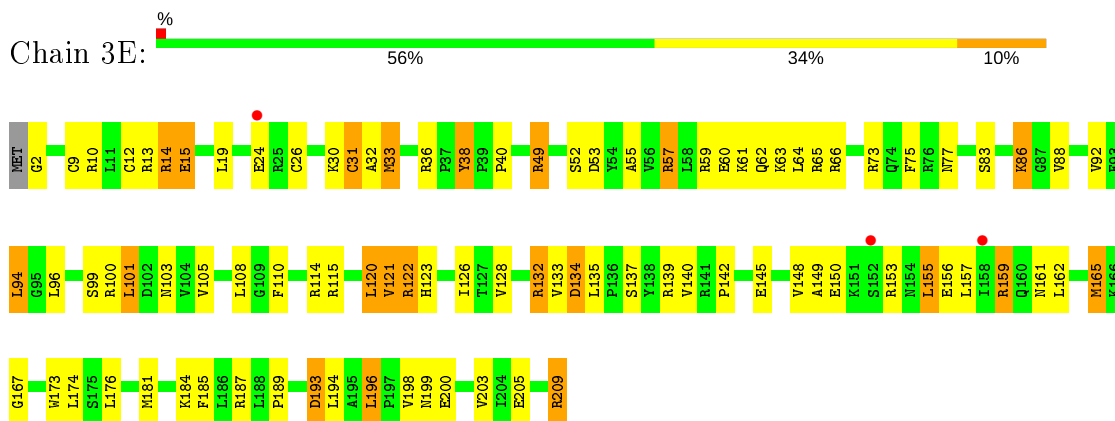
Chain 1G: 

U	U	U	G3	U4	U5	G6	A8	G9	A10	U13	U14	G15	A16	U17	C18	G22	G28	G29	U30	G31	A32	A33	C34	G35	U36	U37	U38	G39	C40	G44	U45	G46	C47	C48	A51	C54	A55	U56	G57	C58	A59	A60	U65	G66	C67	G68	C69	G69	G73	C74	C75	G76	C77
G78	G79	G80	G81	U	U	U	A	C88	U89	C90	C91	G92	U93	G95	U97	C99	A101	G108	A109	C110	G111	G115	A116	U119	A120	C121	G122	C123	G127	G129A	C137	G138	G142	A143	G144	G145	G146	G147	G148	A151	C163	U164	C165	C175	C176	C177	G266						
G181	U182	G183	G184	A185	C186	C186A	C186B	C186F	C187	U188	U189	G190	G191A	U191D	G191E	U191F	U192	C193	C194	A195	A196	C201	U208	U209	U210	G216	C217	U222	U223	C224	C225	G226	G232	C233	U239	C245	A246	G247	A250	G251	G254	G255	U256	C333	C334	C335	C341	A344	U420	U421			
C267	A270	C271	G276	C277	G278	A279	C280	C281	G284	G285	G286	U294	C295	U296	G297	A298	G299	A300	G301	G302	U303	U304	U305	G306	G310	C311	C312	A313	C314	A315	G316	A321	C322	U323	G324	A325	U326	A327	C328	A329	G332	A411	C412	G413	A414	C419	U420	U421					

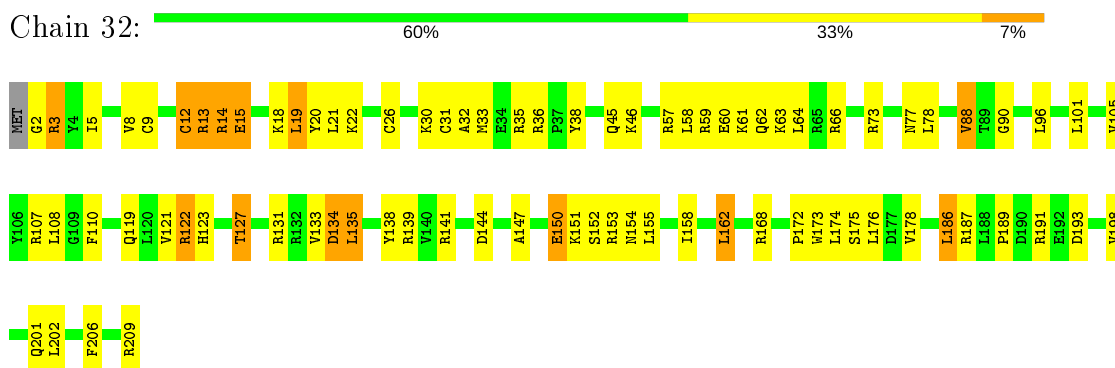
- Molecule 3: 30S ribosomal protein S3



- Molecule 4: 30S ribosomal protein S4

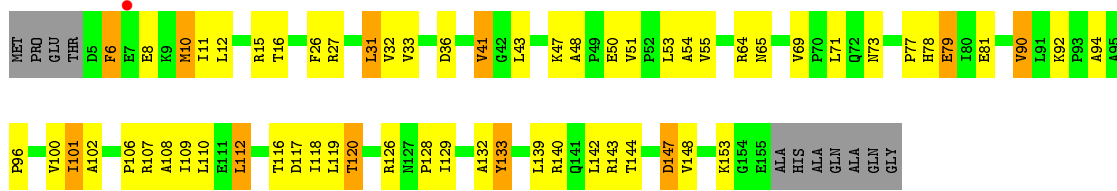


- Molecule 4: 30S ribosomal protein S4

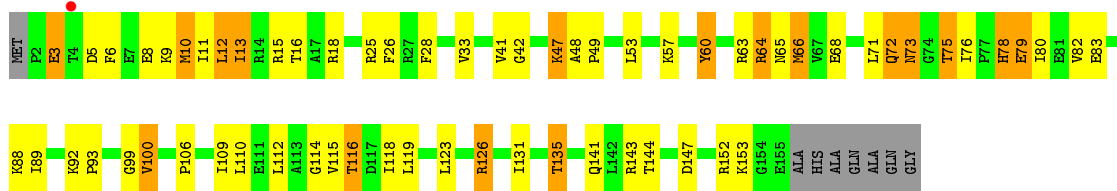


- Molecule 5: 30S ribosomal protein S5

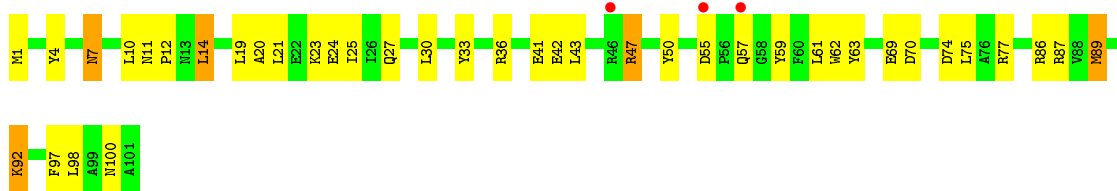




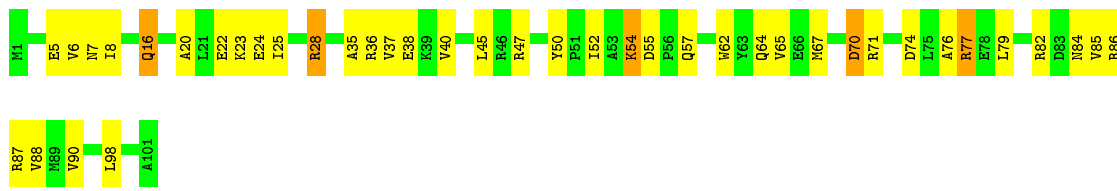
• Molecule 5: 30S ribosomal protein S5



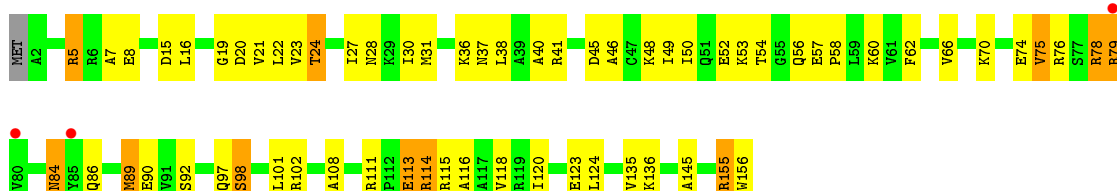
• Molecule 6: 30S ribosomal protein S6



• Molecule 6: 30S ribosomal protein S6

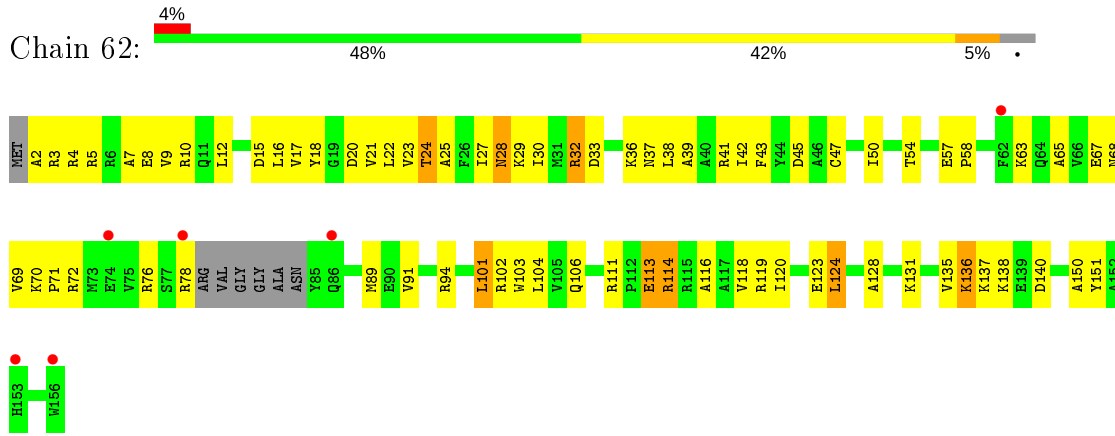


• Molecule 7: 30S ribosomal protein S7

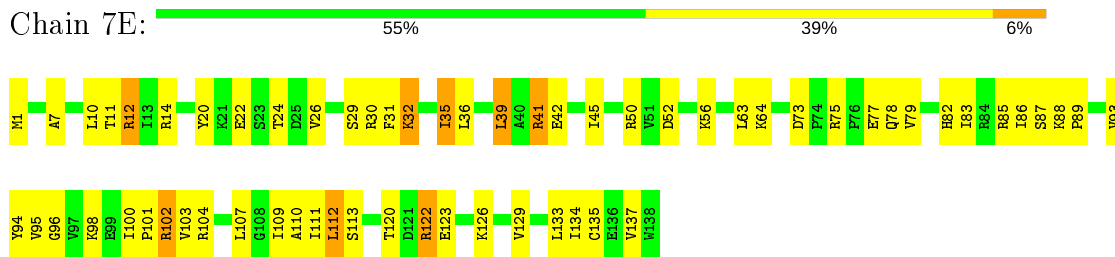


• Molecule 7: 30S ribosomal protein S7

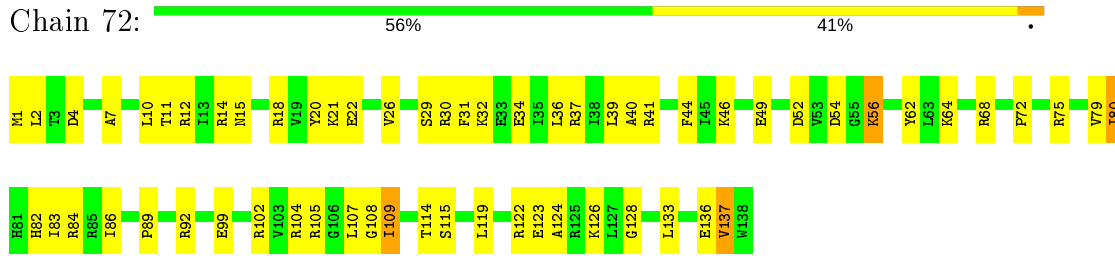




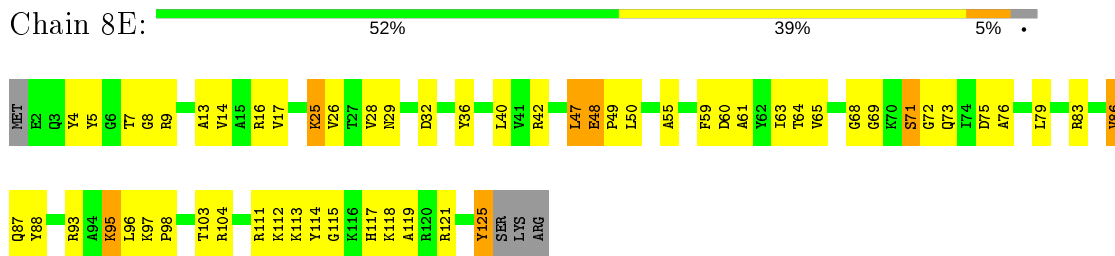
• Molecule 8: 30S ribosomal protein S8



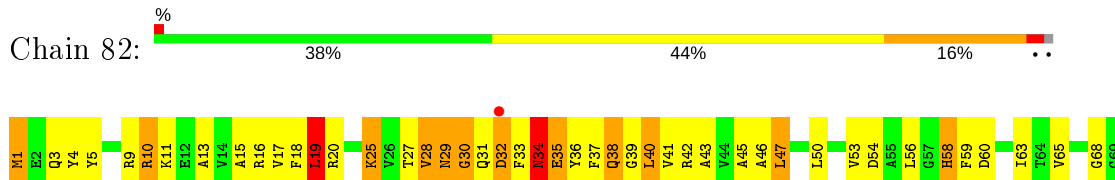
• Molecule 8: 30S ribosomal protein S8



• Molecule 9: 30S ribosomal protein S9

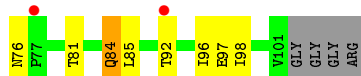
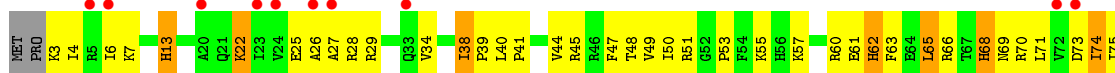


• Molecule 9: 30S ribosomal protein S9

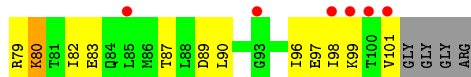
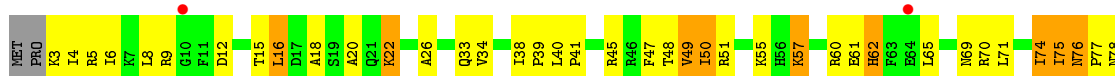




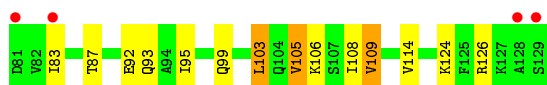
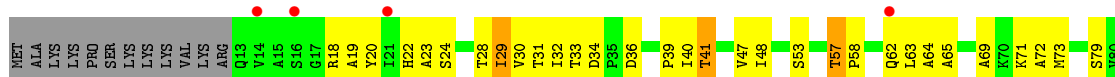
- Molecule 10: 30S ribosomal protein S10



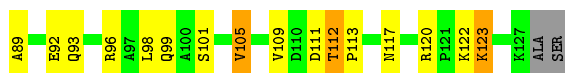
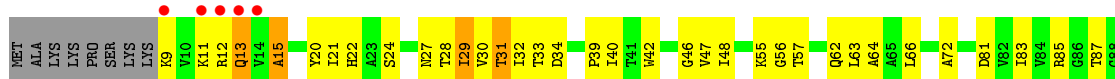
- Molecule 10: 30S ribosomal protein S10



- Molecule 11: 30S ribosomal protein S11



- Molecule 11: 30S ribosomal protein S11

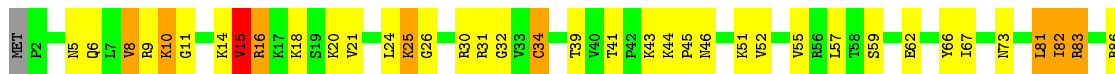


- Molecule 12: 30S ribosomal protein S12





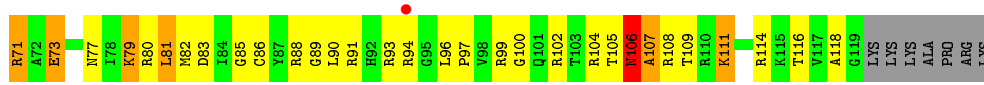
• Molecule 12: 30S ribosomal protein S12



• Molecule 13: 30S ribosomal protein S13



• Molecule 13: 30S ribosomal protein S13



• Molecule 14: 30S ribosomal protein S14 type Z



• Molecule 14: 30S ribosomal protein S14 type Z

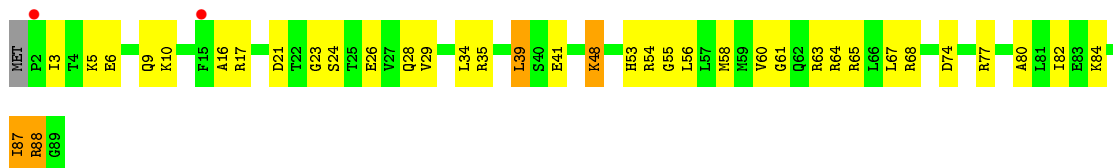




- Molecule 15: 30S ribosomal protein S15



- Molecule 15: 30S ribosomal protein S15



- Molecule 16: 30S ribosomal protein S16



- Molecule 16: 30S ribosomal protein S16

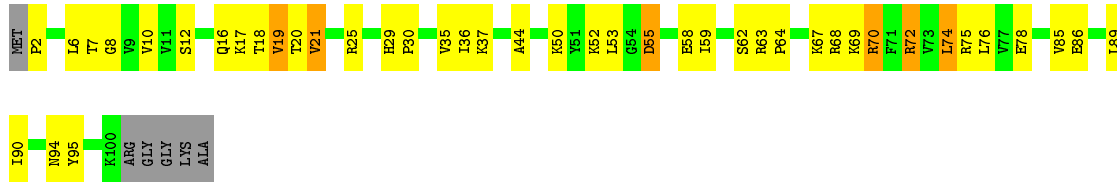


- Molecule 17: 30S ribosomal protein S17

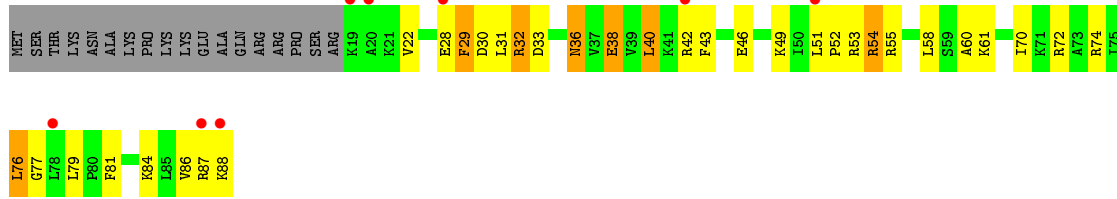


- Molecule 17: 30S ribosomal protein S17

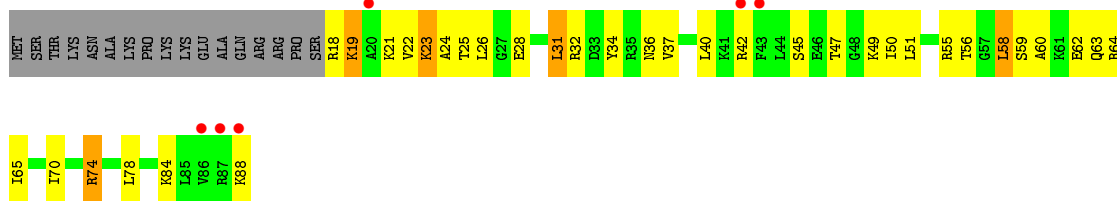




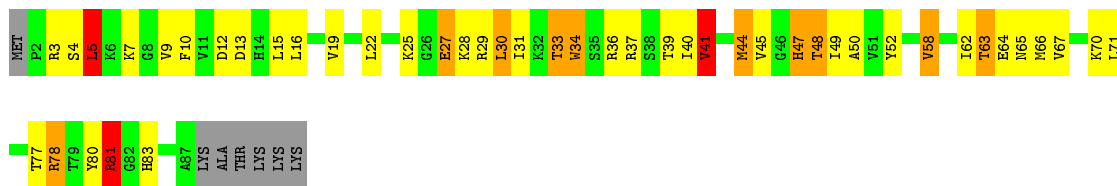
• Molecule 18: 30S ribosomal protein S18



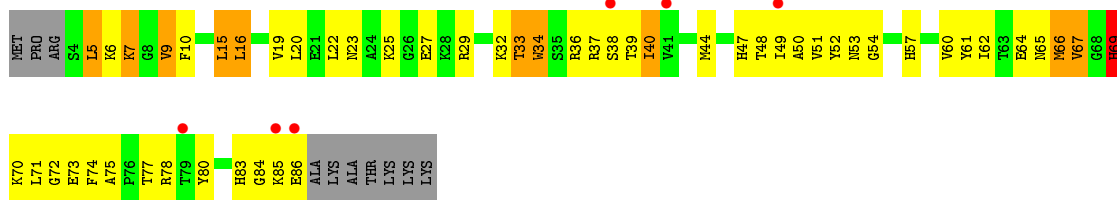
• Molecule 18: 30S ribosomal protein S18



• Molecule 19: 30S ribosomal protein S19

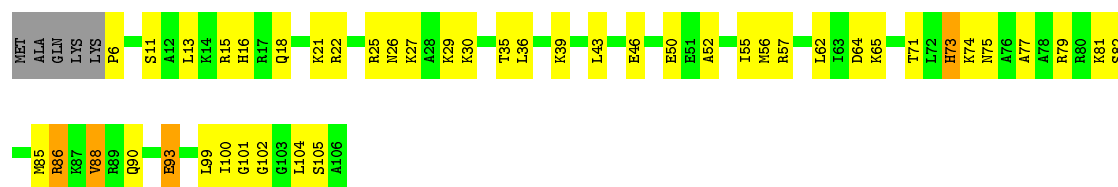


• Molecule 19: 30S ribosomal protein S19



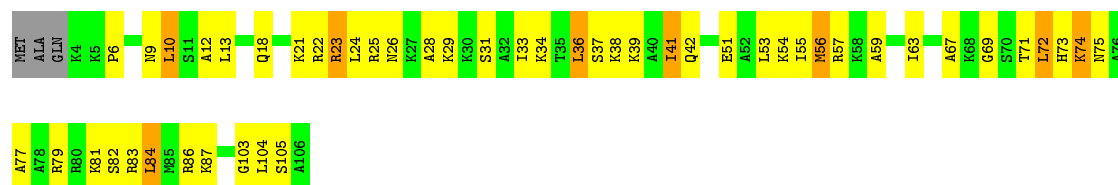
• Molecule 20: 30S ribosomal protein S20

Chain BI: 



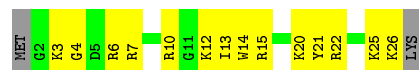
- Molecule 20: 30S ribosomal protein S20

Chain BA: 



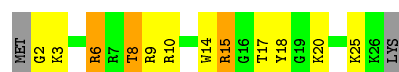
- Molecule 21: 30S ribosomal protein Thx

Chain 1F: 




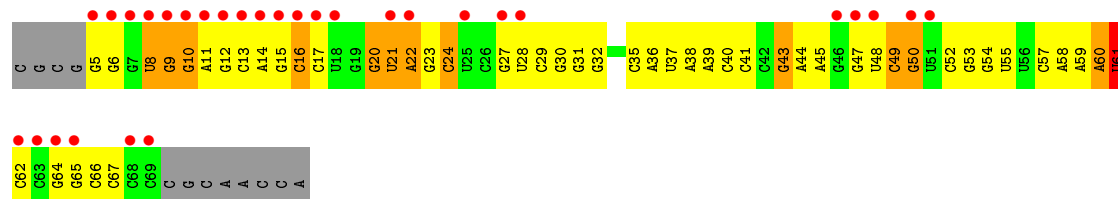
- Molecule 21: 30S ribosomal protein Thx

Chain 1B: 



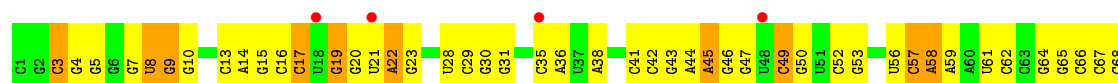
- Molecule 22: E. coli tRNA^{fMet}

Chain 1K: 



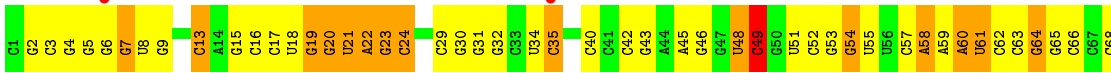
- Molecule 22: E. coli tRNA^{fMet}

Chain 3K: 

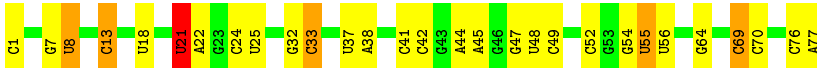




● Molecule 22: E. coli tRNAfMet



● Molecule 23: E. coli tRNAfMet



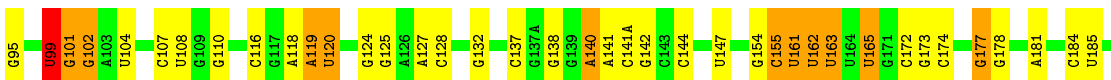
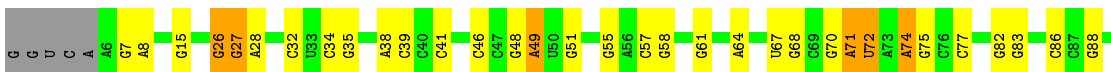
● Molecule 24: mRNA



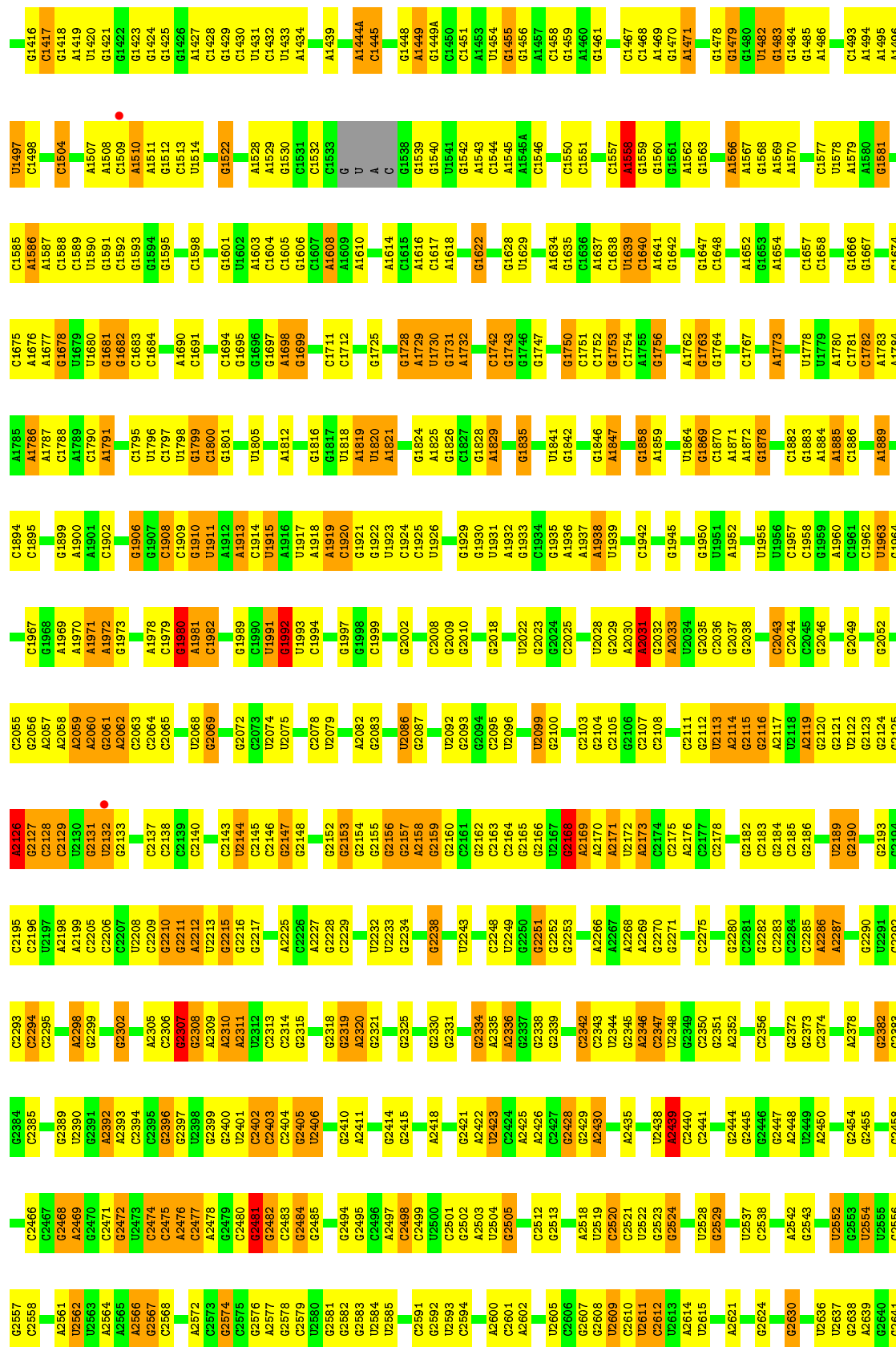
● Molecule 24: mRNA

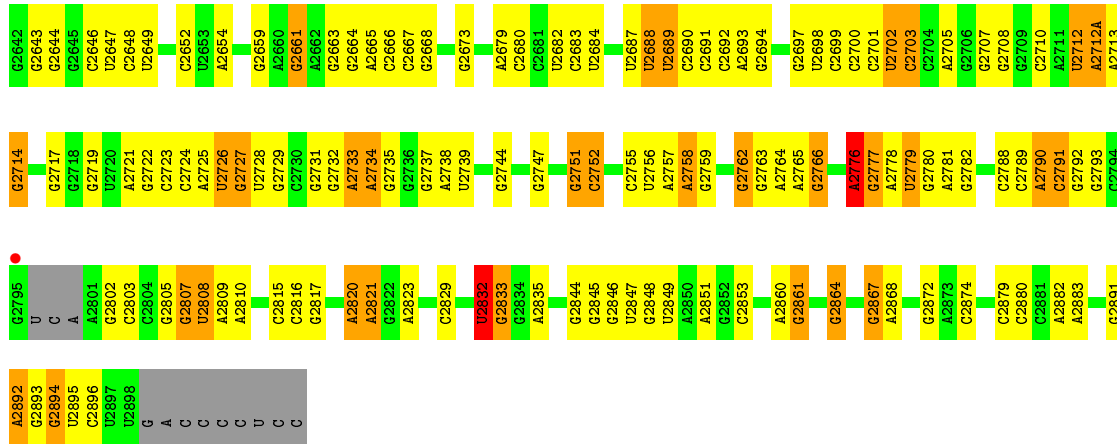


● Molecule 25: 23S ribosomal RNA

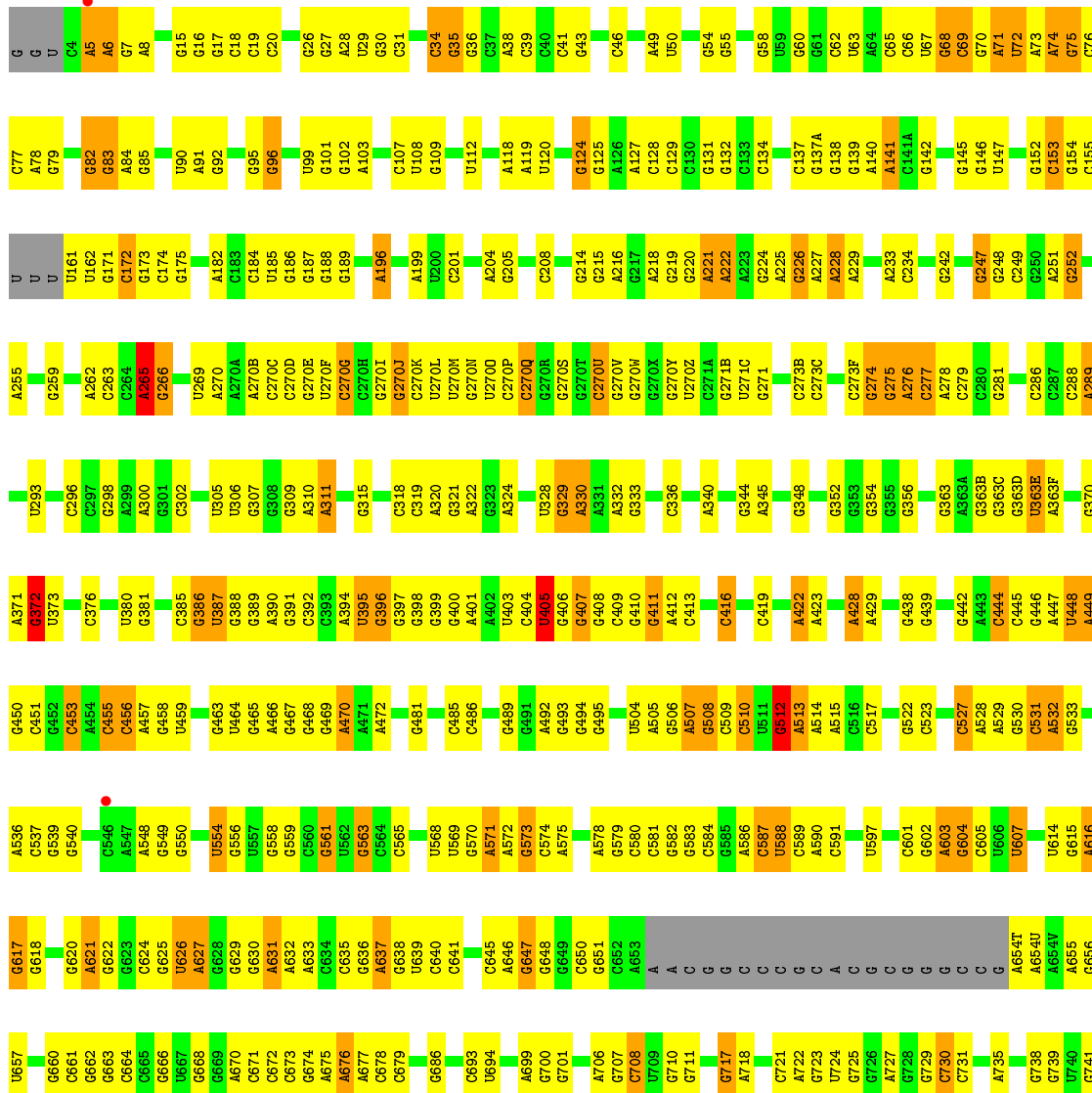


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G1325	U1240	C1150	U1065	A1001	G994	U779	C683	G636	U566	C484	A402	G317	A270
G1326	A1241	G1151	U1066	G1002	C935	A781	G686	A637	A567	C485	U403	G318	C270C
G1327	G1242	A1067	A1068	G1003	G936	A782	G687	G638	U569	C486	C404	C319	C270D
G1328	G1243	G1069	G1069	C1004	U937	A783	G704	U639	U569	C487	U405	C320	G40E
G1329	A1244	A1070	A1070	C1005	G938	A784	G705	C640	G406	C488	C640	G321	U270F
G1330	G1248	G1071	G1071	C1006	G939	A785	G706	C641	G407	C489	G407	A322	C270G
G1331	C1251	U1165	G1074	C1007	G940	G786	G707	G642	G408	C490	G408	A323	C270H
G1332	G1252	C1166	C1075	C1008	A941	G787	G708	A643	G411	C411	G411	A324	G270I
G1333	A1253	U1167	A1076	A1009	G942	A787	U709	A644	A412	C412	A412	G329	U270L
G1334	G1254	G1168	A1077	A1010	U943	A788	G710	C645	A575	C413	A413	A330	U270M
G1335	U1255	G1169	U1078	C1011	G944	G789	G711	A646	U576	C414	C414	A331	G270N
G1336	C1256	G1170	C1079	A1012	G945	G790	U714	A653	G573	C415	C415	A332	U270O
G1337	G1257	G1171	A1080	A1013	A953	A791	G715	A654	C580	C416	C416	A333	U270P
G1338	A1258	U1172	U1081	G1014	G954	G792	A716	G654A	C581	C417	C417	A334	C270Q
G1339	G1259	G1173	U1082	G1015	G955	G793	A717	G654B	G582	C418	C418	A335	G270R
G1340	A1260	A1074	U1083	G1016	C955	G794	A718	G	U421	C419	C419	A336	C270S
G1341	U1261	U1075	U1084	U1019	G956	G801	C719	C	A423	C420	C420	A337	G270T
G1342	G1262	G1176	A1084	A1020	A957	A802	C720	C	G424	C421	C421	A338	G270U
G1343	U1263	A1177	A1085	A1021	U958	A803	G723	C	U427	C422	C422	A339	G270V
G1344	A1264	C1178	A1086	G1022	A959	G805	U724	C	A428	C423	C423	A340	G270W
G1345	G1265	G1179	G1087	U1023	A960	U810	G725	C	G431	C424	C424	A341	G270X
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G1348	A1268	U1187	U1090	U1026	C893	C813	G	C	G438	C427	C427	A344	G270A
G1349	U1269	U1188	C1091	A1027	C894	C814	G	C	G439	C428	C428	A345	G270B
G1350	G1270	G1189	C1092	U1032	U985	C815	G	C	G440	C429	C429	A346	G270C
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G1354	U1274	G1194	A1097	U1035	A899	A821	G	C	G444	C433	C433	A350	G270G
G1355	A1275	U1195	A1098	G1036	A900	U822	G	C	G445	C434	C434	A351	G270H
G1356	G1276	G1196	U1099	G1037	A901	U823	G	C	G446	C435	C435	A352	G270I
G1357	U1277	U1187	C1093	U1038	A902	U824	G	C	G447	C436	C436	A353	G270J
G1358	A1278	G1198	U1094	G1039	A903	U825	G	C	G448	C437	C437	A354	G270K
G1359	G1279	G1199	A1095	C1040	C904	U826	G	C	G449	C438	C438	A355	G270L
G1360	U1280	U1203	U1101	C1041	G977	A829	G	C	G450	C439	C439	A356	G270M
G1361	A1281	A1204	A1102	G1042	G978	A830	G	C	G451	C440	C440	A357	G270N
G1362	G1282	U1205	A1103	C1043	G979	G831	G	C	G452	C441	C441	A358	G270O
G1363	U1283	U1206	U1104	G1044	A980	G832	G	C	G453	C442	C442	A359	G270P
G1364	A1284	G1207	U1105	C1045	A981	U833	G	C	G454	C443	C443	A360	G270Q
G1365	G1285	U1210	G1106	G1046	A982	U834	G	C	G455	C444	C444	A361	G270R
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G1367	A1287	G1212	G1108	A1048	A984	U836	G	C	G457	C446	C446	A363	G270T
G1368	G1288	U1213	U1109	C1049	A985	U837	G	C	G458	C447	C447	A364	G270U
G1369	U1289	G1214	U1110	G1050	C986	U838	G	C	G459	C448	C448	A365	G270V
G1370	A1290	U1215	G1111	G1051	C987	U839	G	C	G460	C449	C449	A366	G270W
G1371	G1291	G1216	U1112	G1052	A988	U840	G	C	G461	C450	C450	A367	G270X
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G1374	G1294	G1219	G1115	A1055	U907	U843	G	C	G464	C453	C453	A370	G270A
G1375	U1295	C1221	U1116	C1056	C908	U844	G	C	G465	C454	C454	A371	G270B
G1376	A1296	G1222	G1117	G1057	C909	U845	G	C	G466	C455	C455	A372	G270C
G1377	G1297	C1223	U1118	A1058	C910	U846	G	C	G467	C456	C456	A373	G270D
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G1379	A1299	G1225	U1120	U1060	A991	U848	G	C	G469	C458	C458	A375	G270F
G1380	G1299	U1226	G1121	C1061	U908	U849	G	C	G470	C459	C459	A376	G270G
G1381	U1300	G1227	U1122	U1062	C909	U850	G	C	G471	C460	C460	A377	G270H
G1382	A1301	U1228	U1123	G1063	C910	U851	G	C	G472	C461	C461	A378	G270I
G1383	G1299	G1229	G1124	A1064	C911	U852	G	C	G473	C462	C462	A379	G270J
G1384	U1301	U1230	U1125	U1065	C912	U853	G	C	G474	C463	C463	A380	G270K
G1385	A1302	G1231	G1126	G1066	C913	U854	G	C	G475	C464	C464	A381	G270L
G1386	G1303	U1232	U1127	C1067	C914	U855	G	C	G476	C465	C465	A382	G270M
G1387	U1304	G1233	G1128	U1068	C915	U856	G	C	G477	C466	C466	A383	G270N
G1388	A1305	U1234	U1129	C1069	C916	U857	G	C	G478	C467	C467	A384	G270O
G1389	G1306	G1235	G1130	U1070	C917	U858	G	C	G479	C468	C468	A385	G270P
G1390	U1307	U1236	U1131	U1071	C918	U859	G	C	G480	C469	C469	A386	G270Q
G1391	A1308	G1237	G1132	C1070	C919	U860	G	C	G481	C470	C470	A387	G270R
G1392	G1309	U1238	U1133	U1072	C920	U861	G	C	G482	C471	C471	A388	G270S
G1393	U1310	G1239	G1134	G1073	C921	U862	G	C	G483	C472	C472	A389	G270T
G1394	A1309	U1240	U1135	U1074	C922	U863	G	C	G484	C473	C473	A390	G270U
G1395	G1310	G1241	G1136	C1074	C923	U864	G	C	G485	C474	C474	A391	G270V
G1396	U1311	U1242	U1137	U1075	C924	U865	G	C	G486	C475	C475	A392	G270W
G1397	A1312	G1243	G1138	U1076	C925	U866	G	C	G487	C476	C476	A393	G270X
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• Molecule 25: 23S ribosomal RNA

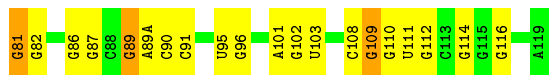
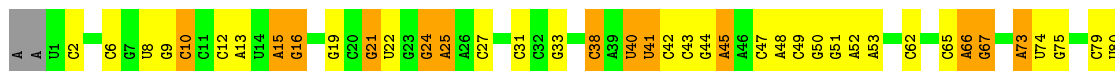


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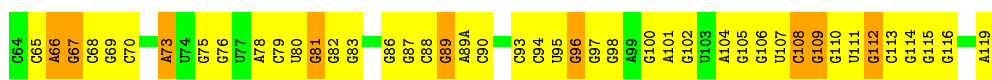
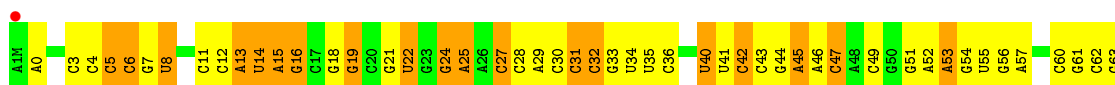
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• Molecule 26: 5S ribosomal RNA

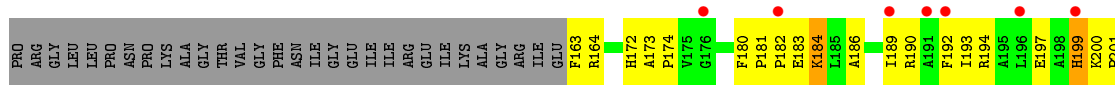
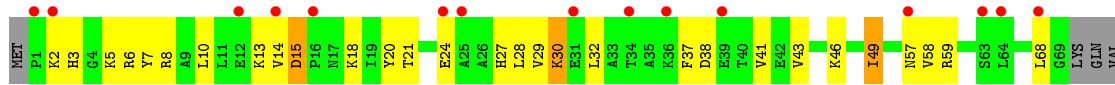
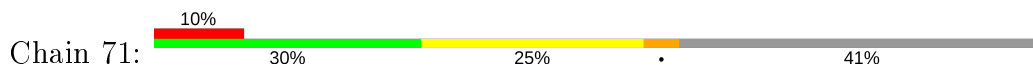




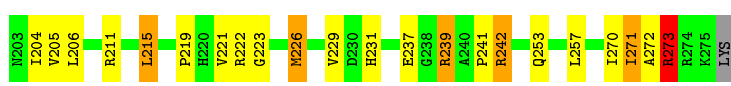
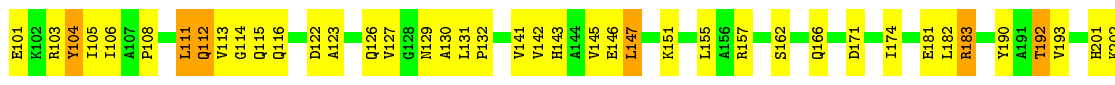
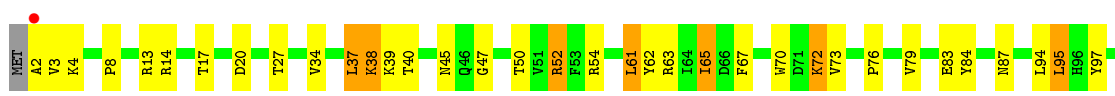
• Molecule 26: 5S ribosomal RNA



• Molecule 27: 50S ribosomal protein L1

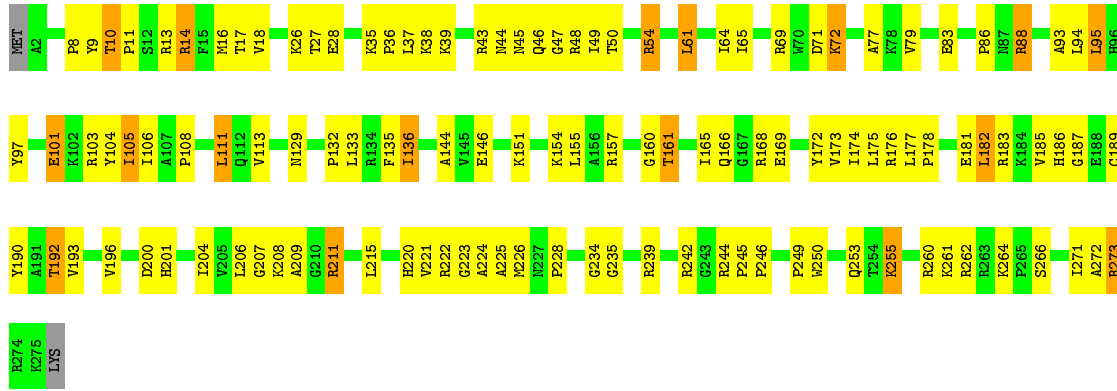


• Molecule 28: 50S ribosomal protein L2

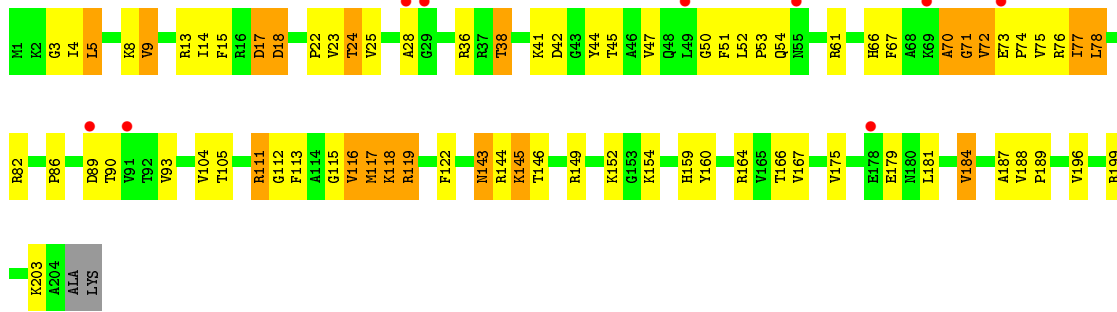


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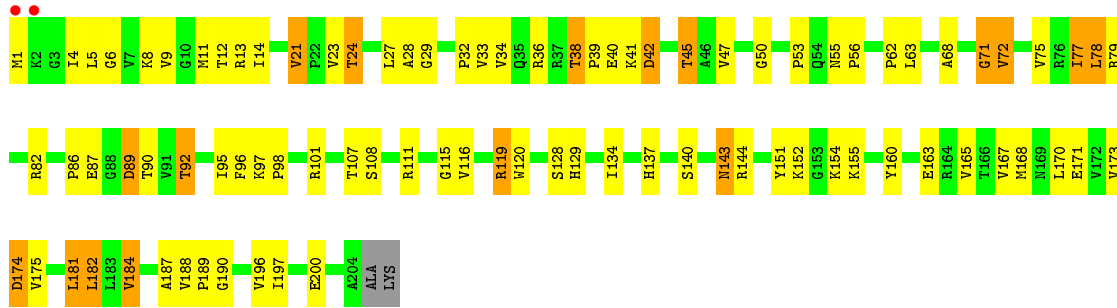




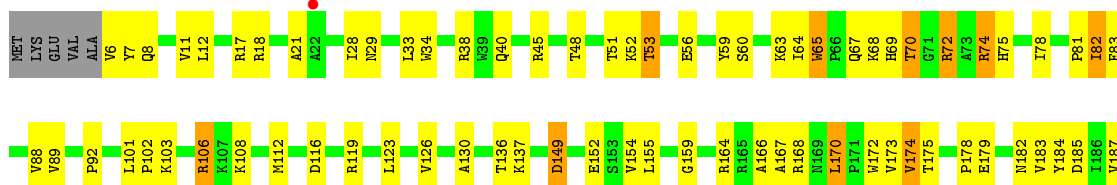
• Molecule 29: 50S ribosomal protein L3



• Molecule 29: 50S ribosomal protein L3

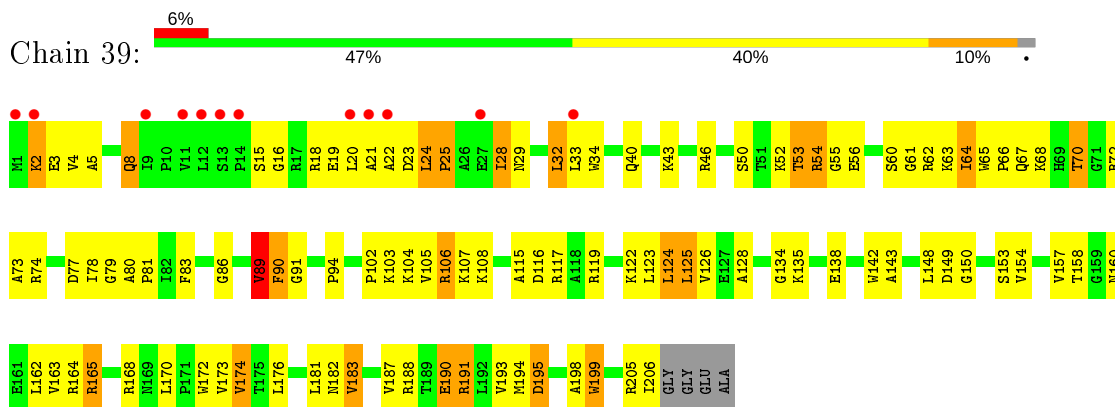


• Molecule 30: 50S ribosomal protein L4

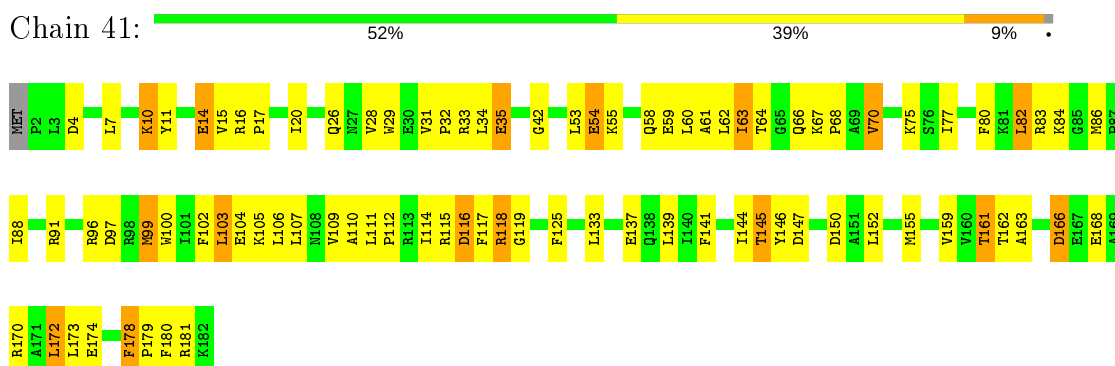




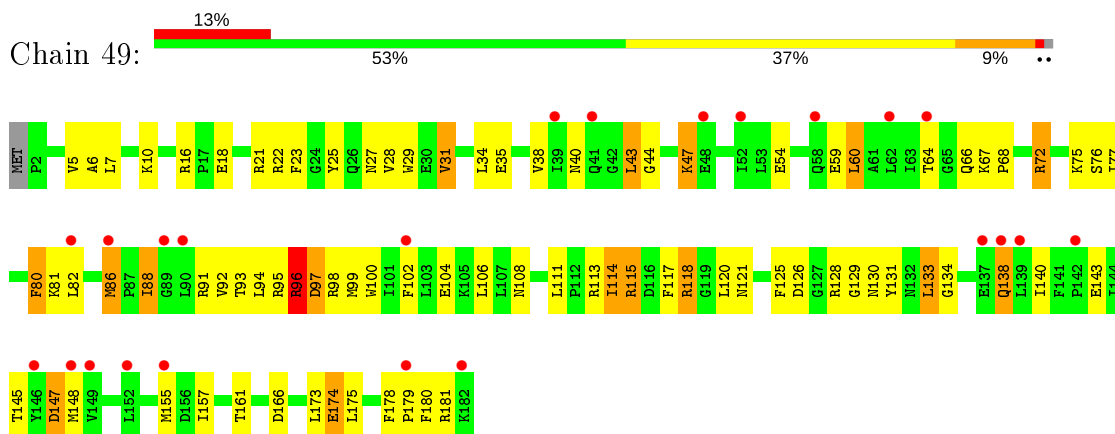
- Molecule 30: 50S ribosomal protein L4



- Molecule 31: 50S ribosomal protein L5



- Molecule 31: 50S ribosomal protein L5

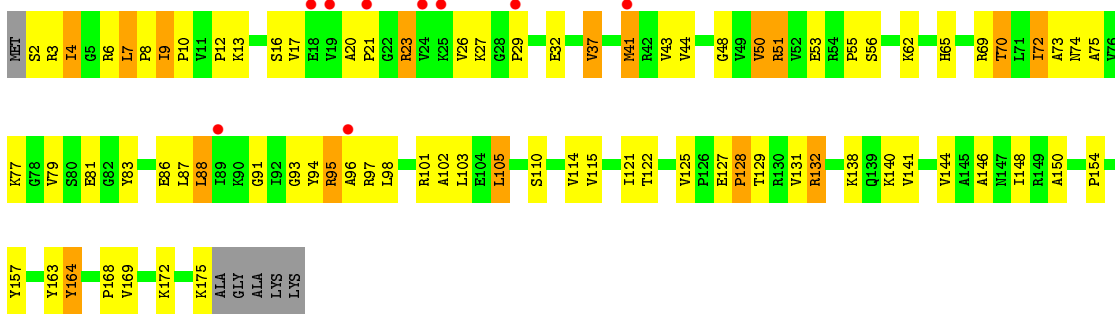


- Molecule 32: 50S ribosomal protein L6

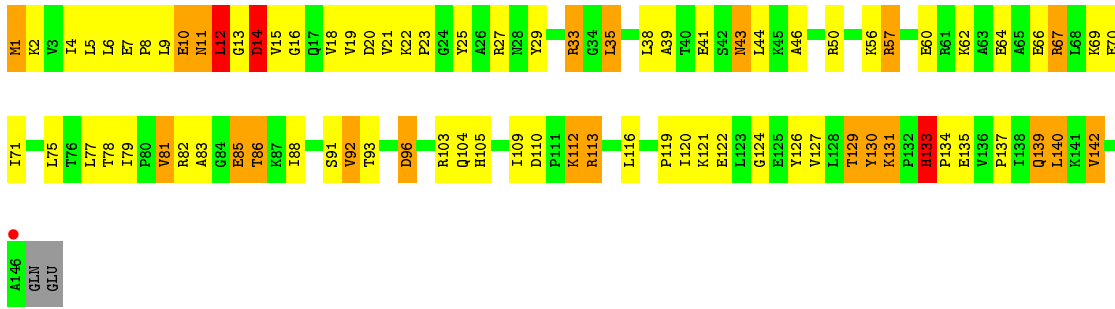




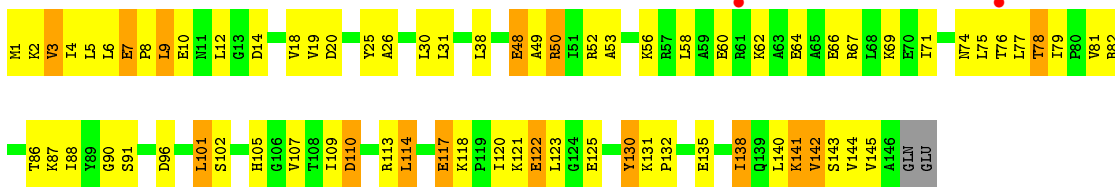
• Molecule 32: 50S ribosomal protein L6



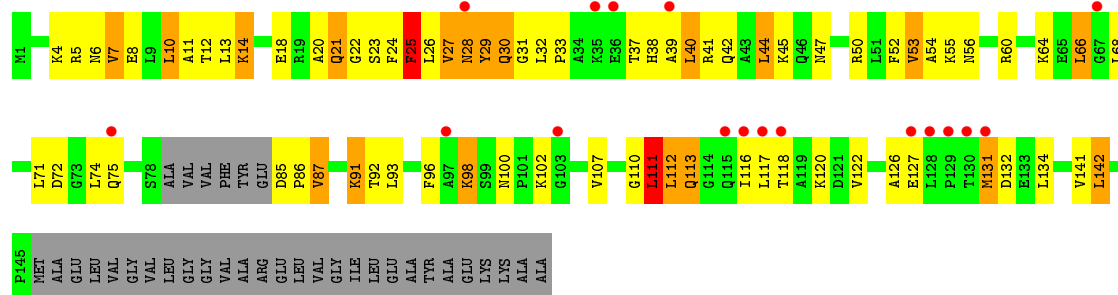
• Molecule 33: 50S ribosomal protein L9



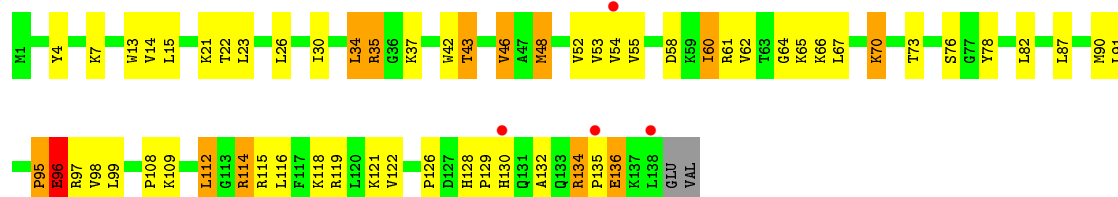
• Molecule 33: 50S ribosomal protein L9



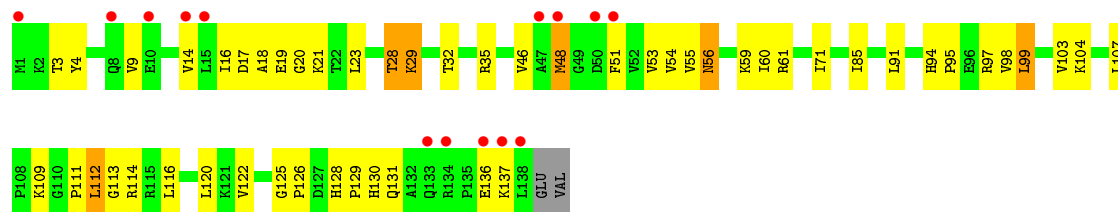
• Molecule 34: 50S ribosomal protein L10



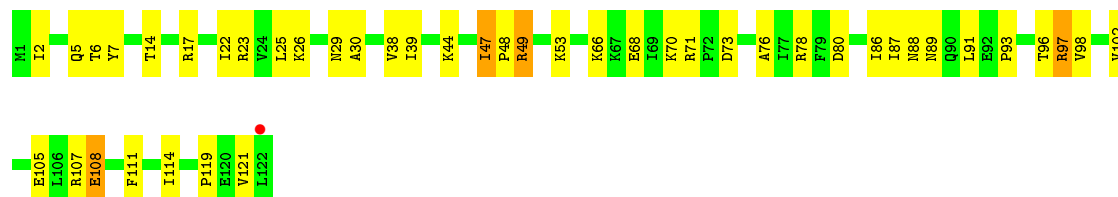
- Molecule 35: 50S ribosomal protein L13



- Molecule 35: 50S ribosomal protein L13

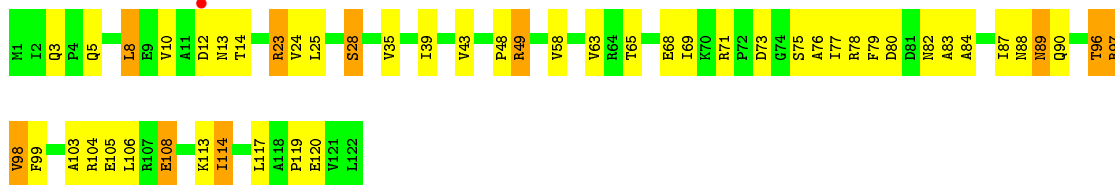


- Molecule 36: 50S ribosomal protein L14

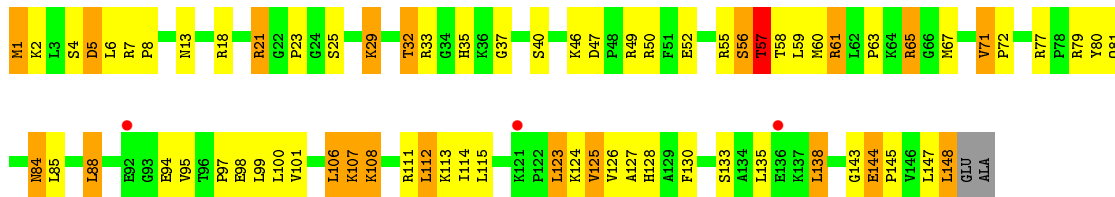


- Molecule 36: 50S ribosomal protein L14

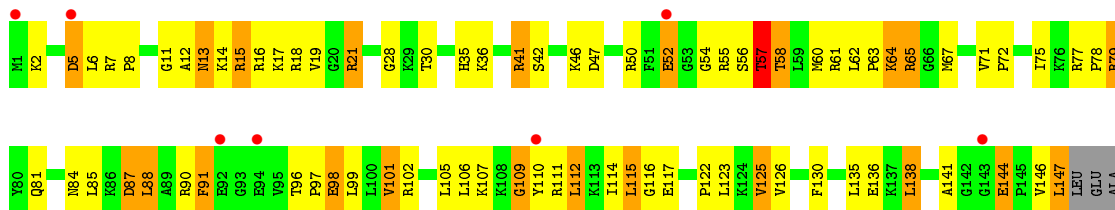




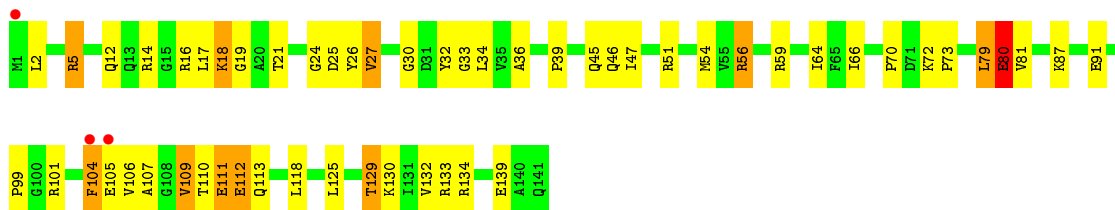
• Molecule 37: 50S ribosomal protein L15



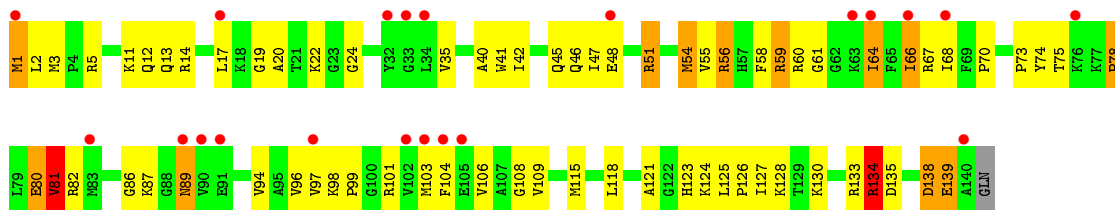
• Molecule 37: 50S ribosomal protein L15



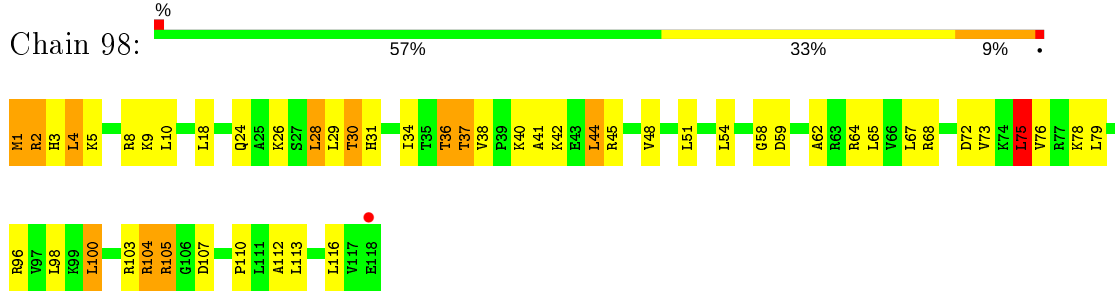
• Molecule 38: 50S ribosomal protein L16



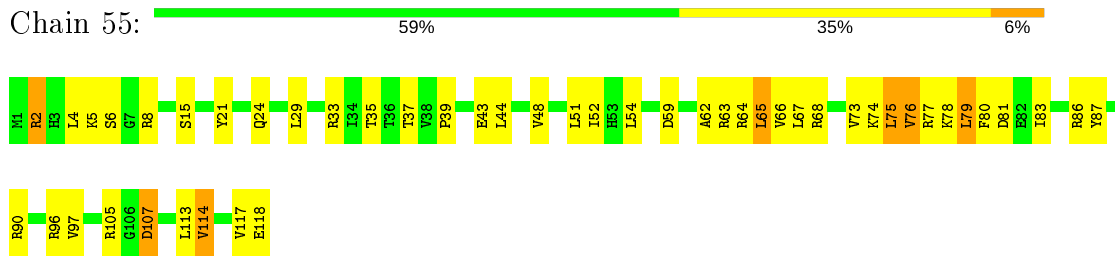
• Molecule 38: 50S ribosomal protein L16



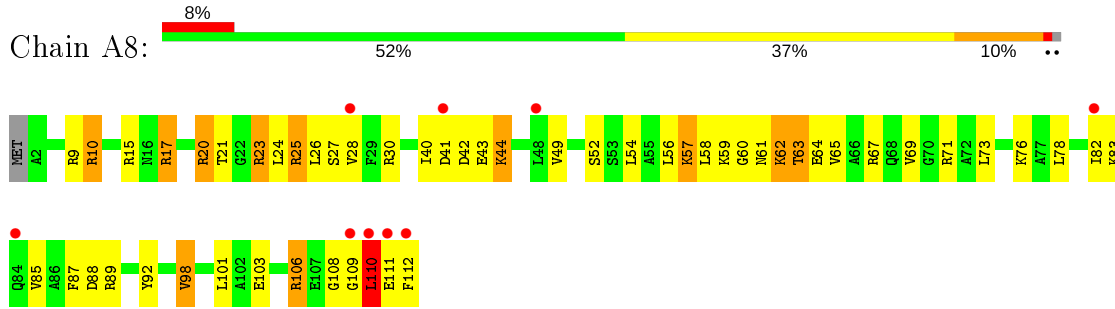
• Molecule 39: 50S ribosomal protein L17



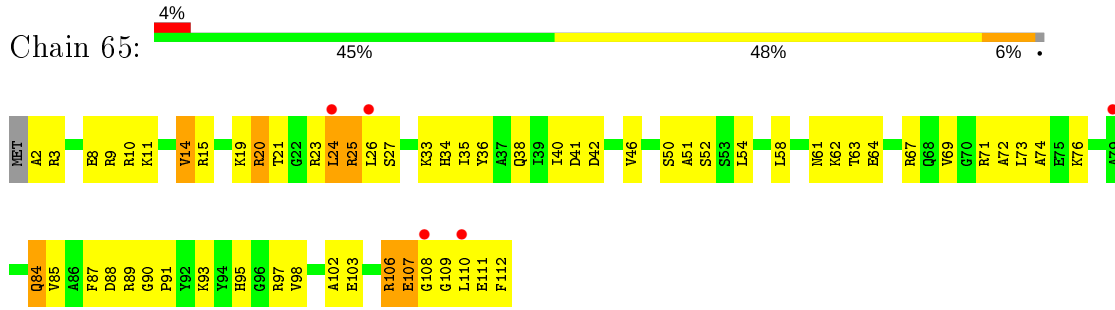
• Molecule 39: 50S ribosomal protein L17



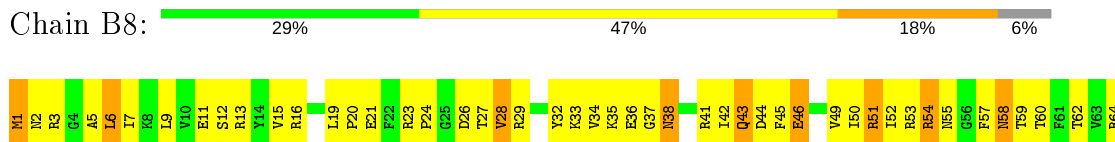
• Molecule 40: 50S ribosomal protein L18

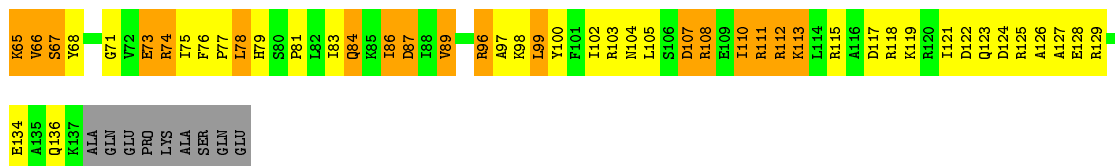


• Molecule 40: 50S ribosomal protein L18

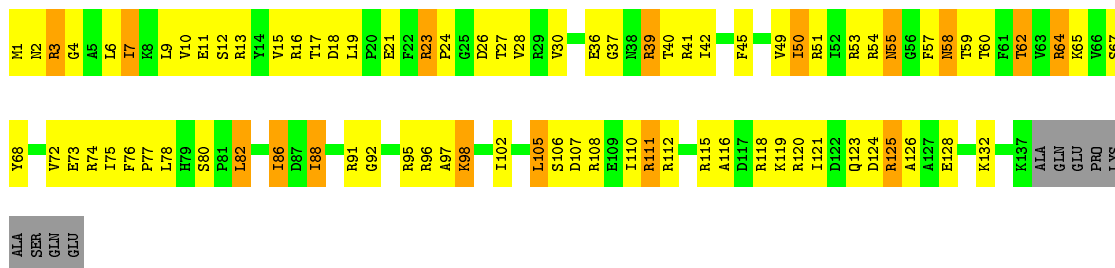


• Molecule 41: 50S ribosomal protein L19

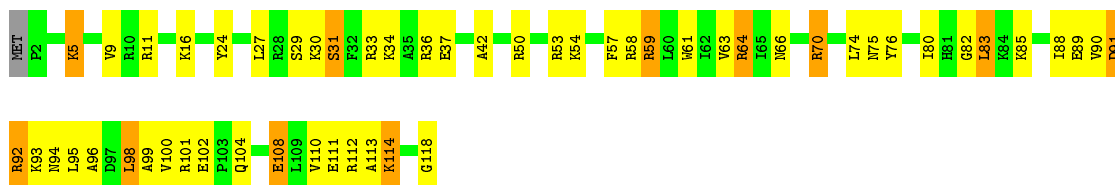




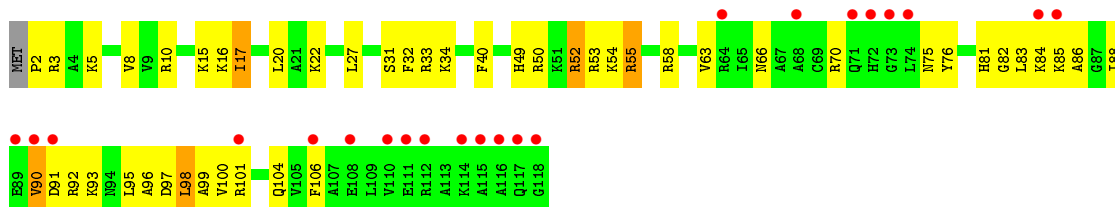
● Molecule 41: 50S ribosomal protein L19



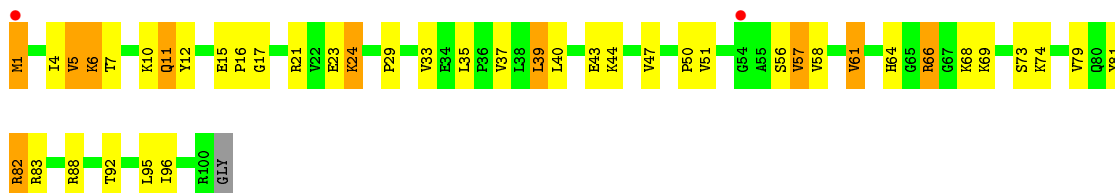
● Molecule 42: 50S ribosomal protein L20



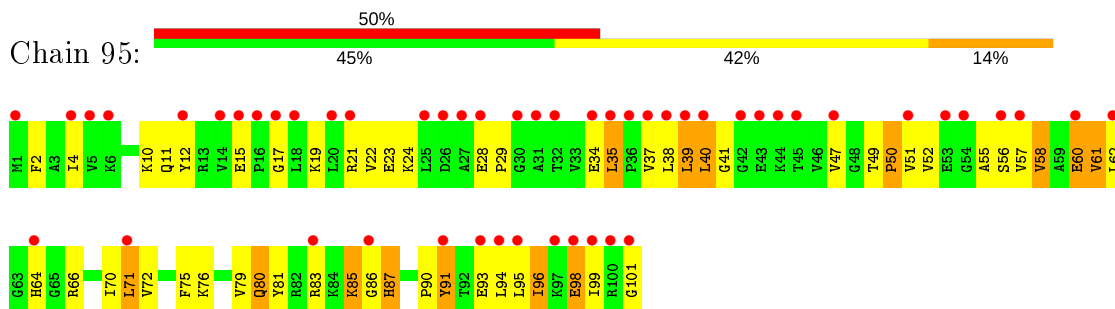
● Molecule 42: 50S ribosomal protein L20



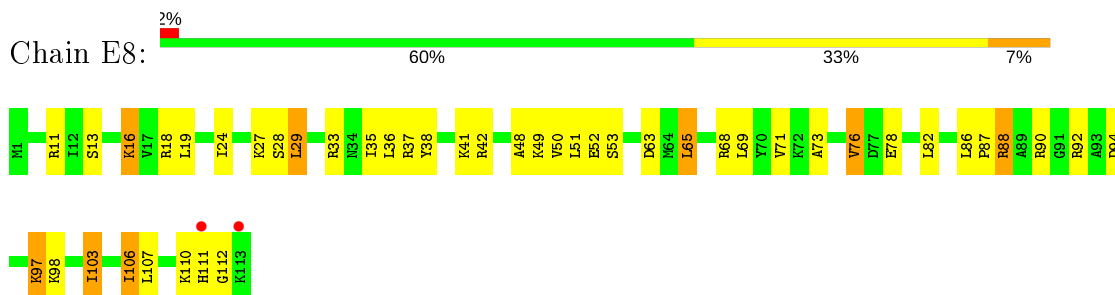
● Molecule 43: 50S ribosomal protein L21



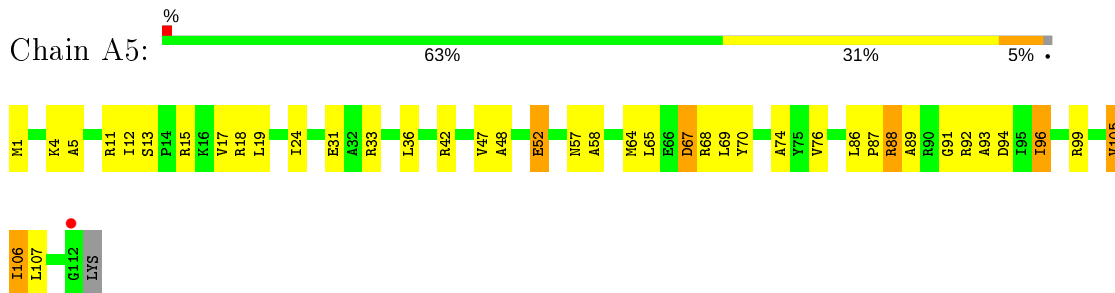
- Molecule 43: 50S ribosomal protein L21



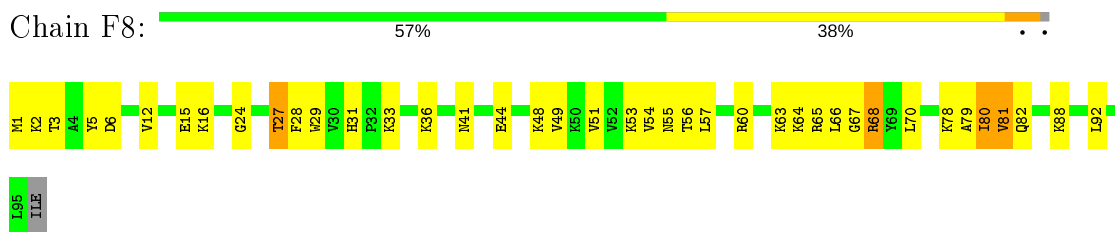
- Molecule 44: 50S ribosomal protein L22



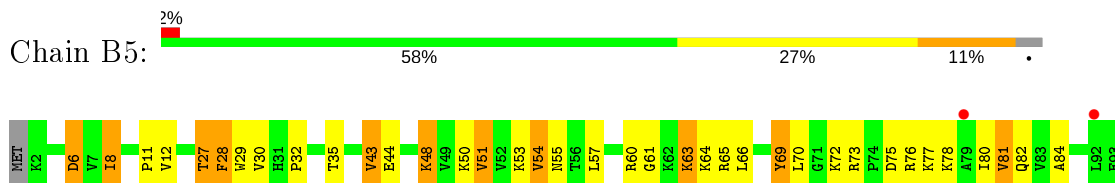
- Molecule 44: 50S ribosomal protein L22



- Molecule 45: 50S ribosomal protein L23



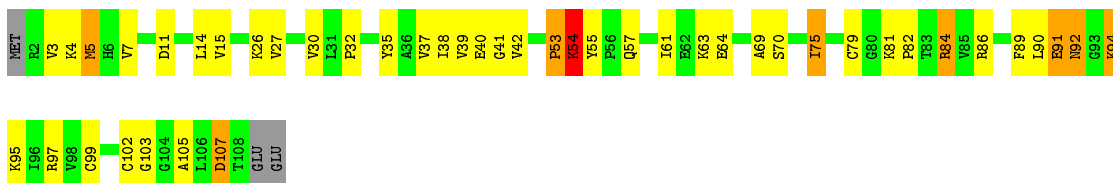
- Molecule 45: 50S ribosomal protein L23



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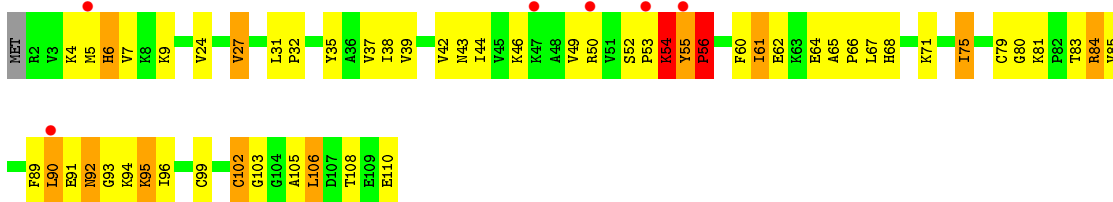
- Molecule 46: 50S ribosomal protein L24

Chain G8:  56% 33% 7% ..



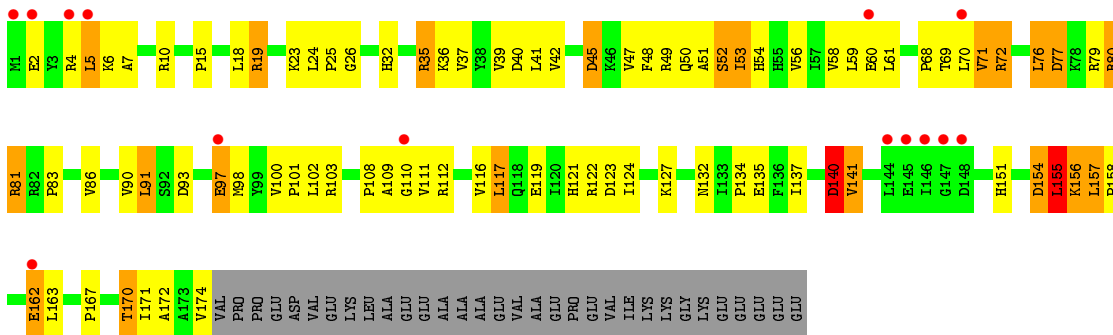
- Molecule 46: 50S ribosomal protein L24

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



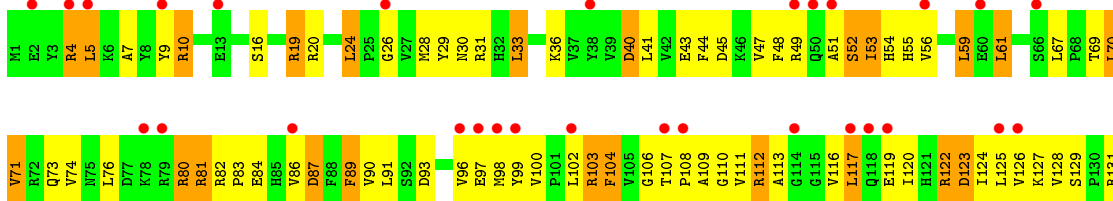
- Molecule 47: 50S ribosomal protein L25

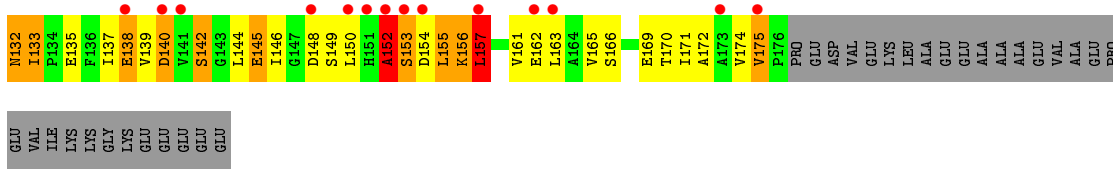
Chain H8:  7% 42% 32% 10% 16%



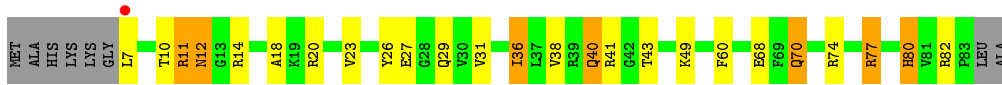
- Molecule 47: 50S ribosomal protein L25

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

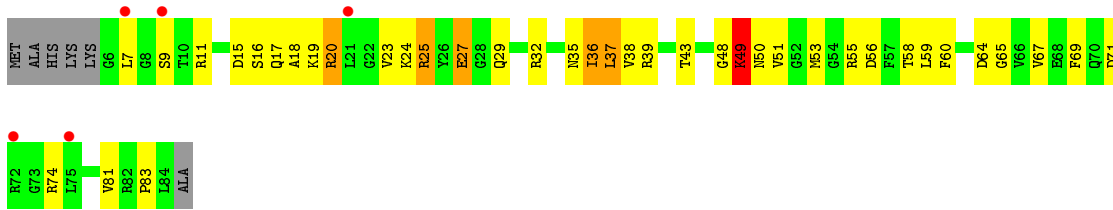




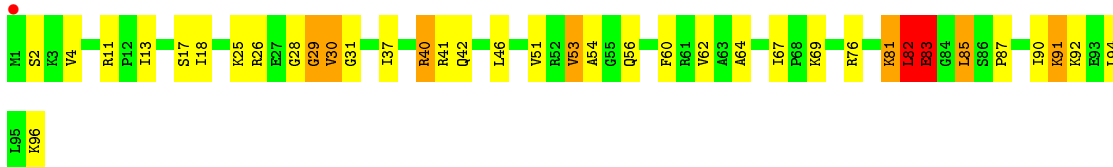
- Molecule 48: 50S ribosomal protein L27



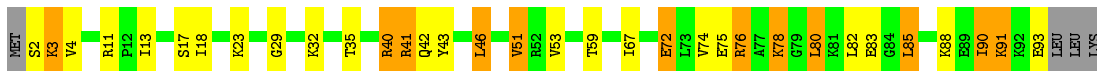
- Molecule 48: 50S ribosomal protein L27



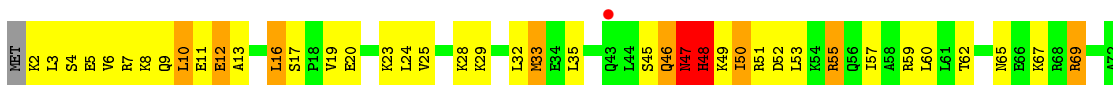
- Molecule 49: 50S ribosomal protein L28



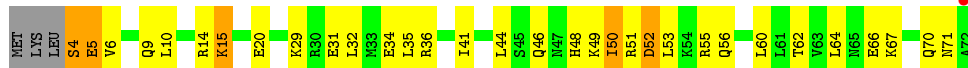
- Molecule 49: 50S ribosomal protein L28



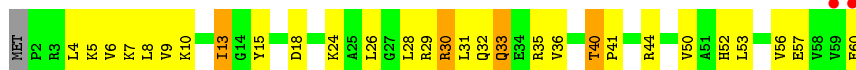
- Molecule 50: 50S ribosomal protein L29



- Molecule 50: 50S ribosomal protein L29



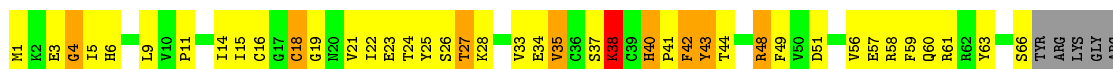
- Molecule 51: 50S ribosomal protein L30



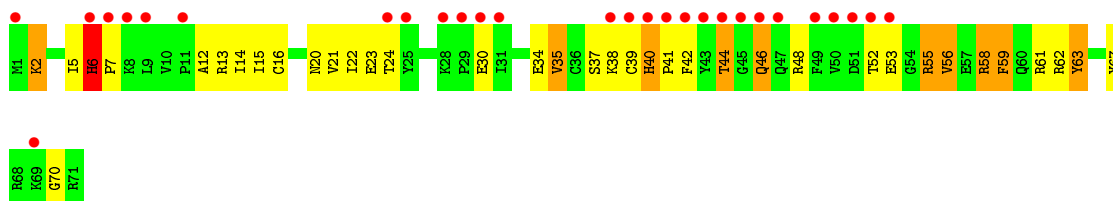
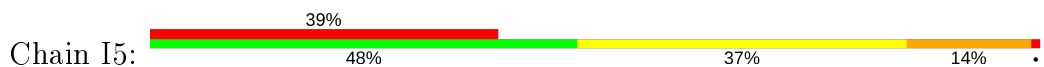
- Molecule 51: 50S ribosomal protein L30



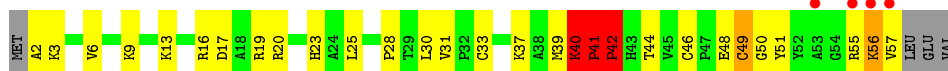
- Molecule 52: 50S ribosomal protein L31



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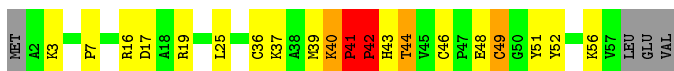


- Molecule 53: 50S ribosomal protein L32

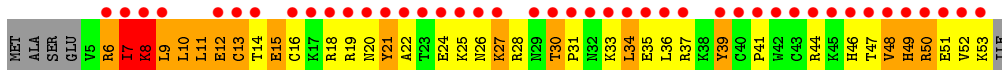
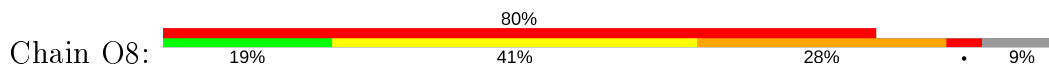


- Molecule 53: 50S ribosomal protein L32

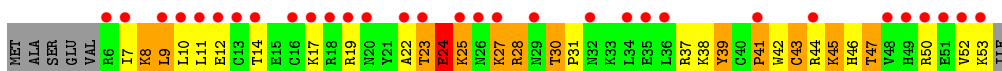




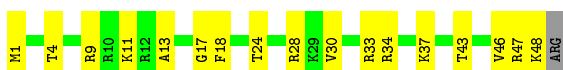
- Molecule 54: 50S ribosomal protein L33



- Molecule 54: 50S ribosomal protein L33



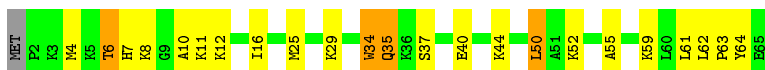
- Molecule 55: 50S ribosomal protein L34



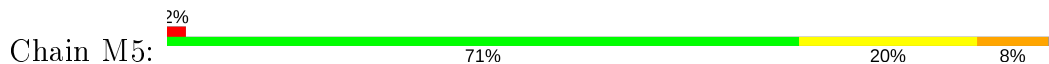
- Molecule 55: 50S ribosomal protein L34



- Molecule 56: 50S ribosomal protein L35

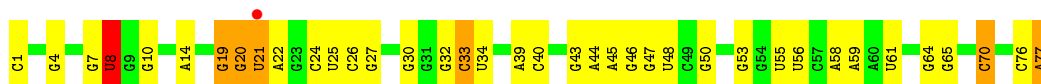


- Molecule 56: 50S ribosomal protein L35



- 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)	Xtrriage
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	Xtrriage
Anisotropy	0.113	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.23 , 62.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.40$, $\langle L^2 \rangle = 0.22$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
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

Xtrriage'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 [i](#)

5.1 Standard geometry [i](#)

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	13	0.28	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(^o)	Ideal(^o)
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	7I	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 [i](#)

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
47	H8	157	LEU
4	32	14	ARG
47	D5	9	TYR
50	K8	3	LEU
56	Q8	37	SER

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

Mol	Chain	Res	Type
2	12	146	GLN
4	32	77	ASN
30	39	40	GLN
43	D8	11	GLN
31	49	66	GLN

5.3.3 RNA [i](#)

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
25	1H	2351	G
1	1G	353	A
25	14	1992	G
25	1H	2481	G
25	1H	2832	U

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	PSU	14	1911	25	17,21,22	1.07	2 (11%)	20,30,33	3.24	6 (30%)
25	5MC	14	1942	25	15,22,23	3.32	5 (33%)	19,32,35	1.28	3 (15%)
1	M2G	1G	966	1	20,27,28	4.20	6 (30%)	22,40,43	1.69	6 (27%)
25	5MC	1H	1962	25,58	15,22,23	3.32	5 (33%)	19,32,35	1.35	4 (21%)
23	4SU	2K	8	23	14,21,22	3.18	2 (14%)	15,30,33	1.26	2 (13%)
25	5MU	1H	1915	25	15,22,23	2.17	3 (20%)	16,32,35	1.63	2 (12%)
25	PSU	1H	1911	25	17,21,22	1.04	2 (11%)	20,30,33	3.12	5 (25%)
23	7MG	2K	47	23	22,26,27	3.51	6 (27%)	28,39,42	2.42	10 (35%)
1	2MG	13	1207	1	19,26,27	5.00	7 (36%)	21,38,41	2.21	8 (38%)
57	OMC	2L	33	57	15,22,23	2.34	4 (26%)	17,31,34	1.36	2 (11%)
25	PSU	14	1917	25	17,21,22	1.03	1 (5%)	20,30,33	3.13	7 (35%)
25	5MC	14	1962	25	15,22,23	3.34	5 (33%)	19,32,35	1.34	2 (10%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	UR3	1G	1498	1	14,22,23	2.92	4 (28%)	15,32,35	1.04	1 (6%)
1	M2G	13	966	1	20,27,28	4.30	6 (30%)	22,40,43	1.65	5 (22%)
1	UR3	13	1498	1	14,22,23	2.89	4 (28%)	15,32,35	1.01	1 (6%)
1	MA6	1G	1518	1	19,26,27	0.99	2 (10%)	18,38,41	2.51	2 (11%)
25	5MU	14	1915	25	15,22,23	2.15	3 (20%)	16,32,35	1.72	2 (12%)
1	MA6	13	1519	1	19,26,27	1.06	2 (10%)	18,38,41	2.53	2 (11%)
1	5MC	13	967	1	15,22,23	3.34	5 (33%)	19,32,35	1.26	2 (10%)
1	5MC	1G	1407	1	15,22,23	3.25	5 (33%)	19,32,35	1.40	4 (21%)
25	2MA	1H	2503	25,59,58	17,25,26	3.44	5 (29%)	19,37,40	1.92	4 (21%)
25	OMG	14	2251	25,57,58	18,26,27	5.70	6 (33%)	20,38,41	5.40	7 (35%)
1	7MG	1G	527	1,58	22,26,27	3.48	6 (27%)	28,39,42	2.49	10 (35%)
25	2MA	14	2503	25,59,58	17,25,26	3.54	6 (35%)	19,37,40	2.24	6 (31%)
25	OMC	14	1920	25	15,22,23	2.31	4 (26%)	17,31,34	1.28	2 (11%)
1	5MC	13	1400	1	15,22,23	3.48	5 (33%)	19,32,35	1.27	3 (15%)
25	5MC	1H	1942	25	15,22,23	3.11	5 (33%)	19,32,35	1.32	4 (21%)
25	OMU	1H	2552	25,59	14,22,23	3.49	5 (35%)	14,31,34	0.69	0
23	OMC	2K	33	23	15,22,23	2.29	4 (26%)	17,31,34	1.45	2 (11%)
25	PSU	1H	1917	25	17,21,22	1.02	2 (11%)	20,30,33	3.02	6 (30%)
1	5MC	13	1407	1	15,22,23	3.26	5 (33%)	19,32,35	1.35	3 (15%)
57	4SU	2L	8	57	14,21,22	3.36	2 (14%)	15,30,33	1.56	2 (13%)
57	PSU	2L	56	57	17,21,22	1.08	1 (5%)	20,30,33	3.18	6 (30%)
1	2MG	1G	1207	1	19,26,27	5.09	7 (36%)	21,38,41	2.11	7 (33%)
25	5MU	14	1939	25,58	15,22,23	2.09	3 (20%)	16,32,35	1.89	2 (12%)
1	5MC	1G	1404	1	15,22,23	3.35	5 (33%)	19,32,35	1.19	2 (10%)
25	OMC	1H	1920	25	15,22,23	2.30	4 (26%)	17,31,34	1.51	2 (11%)
1	5MC	1G	967	1	15,22,23	3.35	5 (33%)	19,32,35	1.31	2 (10%)
23	H2U	2K	21	23	18,21,22	2.11	4 (22%)	21,30,33	1.96	4 (19%)
1	5MC	1G	1400	1	15,22,23	3.31	5 (33%)	19,32,35	1.28	3 (15%)
57	5MU	2L	55	57	15,22,23	2.16	3 (20%)	16,32,35	1.68	2 (12%)
25	PSU	1H	2605	25	17,21,22	1.21	3 (17%)	20,30,33	3.04	6 (30%)
25	OMG	1H	2251	25,58,23	18,26,27	5.61	7 (38%)	20,38,41	5.40	7 (35%)
1	MA6	1G	1519	1	19,26,27	0.98	2 (10%)	18,38,41	2.75	2 (11%)
1	4OC	1G	1402	1	16,23,24	3.15	6 (37%)	17,32,35	2.15	1 (5%)
1	MA6	13	1518	1	19,26,27	0.98	1 (5%)	18,38,41	2.64	2 (11%)
25	OMU	14	2552	25,59	14,22,23	3.49	5 (35%)	14,31,34	0.72	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
12	0TD	3A	89	12	4,9,10	1.13	0	3,11,13	2.55	1 (33%)
1	PSU	1G	516	1,59	17,21,22	1.03	2 (11%)	20,30,33	3.08	6 (30%)
57	7MG	2L	47	57	22,26,27	3.46	6 (27%)	28,39,42	2.45	10 (35%)
23	PSU	2K	56	23	17,21,22	1.05	1 (5%)	20,30,33	3.07	5 (25%)
1	4OC	13	1402	1	16,23,24	3.35	6 (37%)	17,32,35	1.24	1 (5%)
1	PSU	13	516	1,59	17,21,22	1.04	2 (11%)	20,30,33	3.25	6 (30%)
12	0TD	3I	89	12	4,9,10	1.16	0	3,11,13	2.78	1 (33%)
1	5MC	13	1404	1	15,22,23	3.32	5 (33%)	19,32,35	1.16	2 (10%)
25	5MU	1H	1939	25,58	15,22,23	2.13	3 (20%)	16,32,35	1.99	2 (12%)
1	7MG	13	527	1,58	22,26,27	3.45	6 (27%)	28,39,42	2.45	10 (35%)
23	5MU	2K	55	23	15,22,23	2.17	3 (20%)	16,32,35	1.71	2 (12%)
25	PSU	14	2605	25	17,21,22	1.10	1 (5%)	20,30,33	3.33	6 (30%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
25	PSU	14	1911	25	-	1/7/25/26	0/2/2/2
25	5MC	14	1942	25	-	0/5/25/26	0/2/2/2
1	M2G	1G	966	1	-	0/7/29/30	0/3/3/3
25	5MC	1H	1962	25,58	-	4/5/25/26	0/2/2/2
23	4SU	2K	8	23	-	0/5/25/26	0/2/2/2
25	5MU	1H	1915	25	-	0/5/25/26	0/2/2/2
25	PSU	1H	1911	25	-	0/7/25/26	0/2/2/2
23	7MG	2K	47	23	-	2/7/37/38	0/3/3/3
1	2MG	13	1207	1	-	1/5/27/28	0/3/3/3
57	OMC	2L	33	57	-	2/7/27/28	0/2/2/2
25	PSU	14	1917	25	-	0/7/25/26	0/2/2/2
25	5MC	14	1962	25	-	2/5/25/26	0/2/2/2
1	UR3	1G	1498	1	-	0/5/25/26	0/2/2/2
1	M2G	13	966	1	-	1/7/29/30	0/3/3/3
1	UR3	13	1498	1	-	0/5/25/26	0/2/2/2
1	MA6	1G	1518	1	-	3/7/29/30	0/3/3/3
25	5MU	14	1915	25	-	2/5/25/26	0/2/2/2
1	MA6	13	1519	1	-	5/7/29/30	0/3/3/3
1	5MC	13	967	1	-	2/5/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	5MC	1G	1407	1	-	0/5/25/26	0/2/2/2
25	2MA	1H	2503	25,59,58	-	3/3/25/26	0/3/3/3
25	OMG	14	2251	25,57,58	-	0/5/27/28	0/3/3/3
1	7MG	1G	527	1,58	-	3/7/37/38	0/3/3/3
25	2MA	14	2503	25,59,58	-	1/3/25/26	0/3/3/3
25	OMC	14	1920	25	-	2/7/27/28	0/2/2/2
1	5MC	13	1400	1	-	4/5/25/26	0/2/2/2
25	5MC	1H	1942	25	-	0/5/25/26	0/2/2/2
25	OMU	1H	2552	25,59	-	0/7/27/28	0/2/2/2
23	OMC	2K	33	23	-	1/7/27/28	0/2/2/2
25	PSU	1H	1917	25	-	0/7/25/26	0/2/2/2
1	5MC	13	1407	1	-	0/5/25/26	0/2/2/2
57	4SU	2L	8	57	-	3/5/25/26	0/2/2/2
57	PSU	2L	56	57	-	0/7/25/26	0/2/2/2
1	2MG	1G	1207	1	-	0/5/27/28	0/3/3/3
25	5MU	14	1939	25,58	-	2/5/25/26	0/2/2/2
1	5MC	1G	1404	1	-	0/5/25/26	0/2/2/2
25	OMC	1H	1920	25	-	1/7/27/28	0/2/2/2
1	5MC	1G	967	1	-	0/5/25/26	0/2/2/2
23	H2U	2K	21	23	-	4/7/38/39	0/2/2/2
1	5MC	1G	1400	1	-	2/5/25/26	0/2/2/2
57	5MU	2L	55	57	-	0/5/25/26	0/2/2/2
25	PSU	1H	2605	25	-	0/7/25/26	0/2/2/2
25	OMG	1H	2251	25,58,23	-	1/5/27/28	0/3/3/3
1	MA6	1G	1519	1	-	3/7/29/30	0/3/3/3
1	4OC	1G	1402	1	-	2/9/29/30	0/2/2/2
1	MA6	13	1518	1	-	0/7/29/30	0/3/3/3
25	OMU	14	2552	25,59	-	0/7/27/28	0/2/2/2
12	0TD	3A	89	12	-	2/3/12/14	-
1	PSU	1G	516	1,59	-	0/7/25/26	0/2/2/2
57	7MG	2L	47	57	-	3/7/37/38	0/3/3/3
23	PSU	2K	56	23	-	0/7/25/26	0/2/2/2
1	4OC	13	1402	1	-	2/9/29/30	0/2/2/2
1	PSU	13	516	1,59	-	0/7/25/26	0/2/2/2
12	0TD	3I	89	12	-	1/3/12/14	-
1	5MC	13	1404	1	-	0/5/25/26	0/2/2/2
25	5MU	1H	1939	25,58	-	0/5/25/26	0/2/2/2
1	7MG	13	527	1,58	-	2/7/37/38	0/3/3/3
23	5MU	2K	55	23	-	0/5/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
25	PSU	14	2605	25	-	0/7/25/26	0/2/2/2

The worst 5 of 230 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	1G	1207	2MG	C2-N2	16.75	1.48	1.34
1	13	1207	2MG	C2-N2	16.25	1.47	1.34
25	14	2251	OMG	C4-N3	16.20	1.61	1.35
25	1H	2251	OMG	C4-N3	15.79	1.60	1.35
25	14	2251	OMG	C8-N7	-14.56	1.08	1.34

The worst 5 of 225 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	1H	2251	OMG	C1'-N9-C4	14.08	151.39	126.64
25	14	2251	OMG	C6-C5-C4	-13.88	107.55	120.80
25	1H	2251	OMG	C6-C5-C4	-13.77	107.65	120.80
25	14	2251	OMG	C1'-N9-C4	13.59	150.52	126.64
1	13	516	PSU	N1-C2-N3	-11.18	119.54	128.43

There are no chirality outliers.

5 of 67 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
25	1H	1962	5MC	O4'-C1'-N1-C6
25	1H	1962	5MC	C2'-C1'-N1-C6
57	2L	33	OMC	C2'-C1'-N1-C6
1	1G	1518	MA6	C5-C6-N6-C10
25	14	1915	5MU	C2'-C1'-N1-C6

There are no ring outliers.

29 monomers are involved in 50 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
25	14	1911	PSU	1	0
25	14	1942	5MC	2	0
25	1H	1915	5MU	1	0
25	1H	1911	PSU	1	0
57	2L	33	OMC	1	0
25	14	1962	5MC	1	0
1	1G	1498	UR3	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	13	966	M2G	1	0
1	13	1498	UR3	1	0
1	1G	1518	MA6	2	0
1	13	1519	MA6	1	0
25	14	2251	OMG	3	0
25	14	2503	2MA	4	0
25	14	1920	OMC	2	0
25	1H	2552	OMU	1	0
23	2K	33	OMC	2	0
1	13	1407	5MC	1	0
57	2L	8	4SU	3	0
1	1G	1207	2MG	3	0
1	1G	1404	5MC	1	0
25	1H	1920	OMC	3	0
23	2K	21	H2U	2	0
1	1G	1400	5MC	1	0
25	1H	2251	OMG	3	0
1	1G	1519	MA6	1	0
1	1G	1402	4OC	2	0
12	3A	89	0TD	1	0
1	13	1402	4OC	1	0
23	2K	55	5MU	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	0.00	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
60	SF4	32	303	-	0,12,12	0.00	-	-		

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
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 i

6.1 Protein, DNA and RNA chains i

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	115, 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	115, 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
57	4SU	2L	8	20/21	0.88	0.12	120,131,140,141	0
23	H2U	2K	21	20/21	0.88	0.22	117,140,147,150	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	PSU	2K	56	20/21	0.91	0.11	92,104,120,124	0
23	5MU	2K	55	21/22	0.91	0.12	103,113,125,145	0
1	PSU	1G	516	20/21	0.92	0.12	98,102,108,110	0
57	7MG	2L	47	24/25	0.92	0.15	114,141,151,162	0
23	7MG	2K	47	24/25	0.93	0.13	96,105,114,126	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
1	7MG	1G	527	24/25	0.94	0.13	88,99,101,102	0
1	5MC	1G	967	21/22	0.94	0.09	92,107,118,120	0
1	M2G	1G	966	25/26	0.94	0.12	87,107,115,124	0
25	PSU	14	1911	20/21	0.94	0.10	86,94,118,121	0
1	MA6	1G	1519	24/25	0.94	0.16	64,79,84,86	0
1	4OC	1G	1402	22/23	0.94	0.14	71,84,91,99	0
1	5MC	13	967	21/22	0.95	0.16	71,82,94,99	0
25	2MA	1H	2503	23/24	0.95	0.17	30,38,48,59	0
25	5MU	1H	1915	21/22	0.95	0.12	75,91,102,116	0
25	OMC	14	1920	21/22	0.95	0.17	73,91,99,102	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	5MC	14	1962	21/22	0.95	0.13	59,67,76,83	0
1	M2G	13	966	25/26	0.95	0.15	68,77,90,94	0
1	2MG	1G	1207	24/25	0.95	0.12	115,120,125,127	0
1	7MG	13	527	24/25	0.95	0.14	71,80,86,92	0
23	4SU	2K	8	20/21	0.95	0.12	85,91,97,101	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
25	OMC	1H	1920	21/22	0.96	0.12	60,66,70,72	0
25	5MC	1H	1962	21/22	0.96	0.14	50,57,61,66	0
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	5MC	1H	1942	21/22	0.96	0.14	39,50,56,61	0
25	PSU	1H	2605	20/21	0.96	0.15	35,40,48,53	0
25	OMU	1H	2552	21/22	0.96	0.18	37,45,51,53	0
23	OMC	2K	33	21/22	0.96	0.13	77,82,89,101	0
1	MA6	13	1518	24/25	0.96	0.15	50,57,61,62	0
1	UR3	1G	1498	21/22	0.96	0.14	65,76,83,86	0
1	5MC	1G	1407	21/22	0.96	0.11	75,80,85,98	0
1	5MC	13	1407	21/22	0.96	0.13	53,59,65,67	0
25	5MC	14	1942	21/22	0.96	0.18	62,71,82,90	0
25	OMG	14	2251	24/25	0.96	0.12	51,57,64,69	0
1	PSU	13	516	20/21	0.96	0.09	84,95,98,98	0
1	UR3	13	1498	21/22	0.96	0.16	44,62,69,73	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
1	5MC	1G	1404	21/22	0.96	0.11	77,85,89,91	0
25	PSU	14	2605	20/21	0.96	0.12	42,52,74,77	0
1	4OC	13	1402	22/23	0.97	0.15	61,71,79,84	0
25	PSU	1H	1911	20/21	0.97	0.12	50,63,72,74	0
1	MA6	1G	1518	24/25	0.97	0.13	68,78,82,84	0
1	5MC	13	1404	21/22	0.97	0.12	54,59,69,79	0
57	OMC	2L	33	21/22	0.97	0.12	91,100,107,111	0
25	OMG	1H	2251	24/25	0.97	0.12	36,43,49,53	0
1	MA6	13	1519	24/25	0.97	0.14	51,56,62,64	0
25	OMU	14	2552	21/22	0.97	0.14	48,55,62,67	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(Å 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	2L	102	1/1	0.44	0.12	132,132,132,132	0
59	MG	1G	1696	1/1	0.44	0.11	129,129,129,129	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	1G	1716	1/1	0.57	0.10	107,107,107,107	0
59	MG	13	1741	1/1	0.57	0.08	106,106,106,106	0
59	MG	13	1733	1/1	0.57	0.15	117,117,117,117	0
59	MG	14	3243	1/1	0.58	0.23	74,74,74,74	0
59	MG	14	3389	1/1	0.60	0.14	69,69,69,69	0
59	MG	1H	3430	1/1	0.60	0.08	79,79,79,79	0
59	MG	1G	1704	1/1	0.61	0.07	110,110,110,110	0
59	MG	1G	1648	1/1	0.62	0.42	83,83,83,83	0
58	K	1G	1604	1/1	0.62	0.19	111,111,111,111	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
59	MG	1G	1691	1/1	0.63	0.11	84,84,84,84	0
58	K	1G	1606	1/1	0.63	0.11	102,102,102,102	0
59	MG	14	3378	1/1	0.64	0.13	71,71,71,71	0
59	MG	1H	3435	1/1	0.65	0.10	72,72,72,72	0
58	K	14	3091	1/1	0.65	0.11	103,103,103,103	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	1G	1725	1/1	0.66	0.08	97,97,97,97	0
59	MG	1H	3514	1/1	0.67	0.08	88,88,88,88	0
59	MG	1H	3446	1/1	0.67	0.07	92,92,92,92	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	14	3293	1/1	0.69	0.05	91,91,91,91	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	1G	1661	1/1	0.70	0.24	114,114,114,114	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
59	MG	1H	3498	1/1	0.70	0.18	37,37,37,37	0
59	MG	14	3350	1/1	0.70	0.18	69,69,69,69	0
59	MG	1H	3487	1/1	0.70	0.09	85,85,85,85	0
58	K	13	1634	1/1	0.70	0.12	111,111,111,111	0
59	MG	14	3356	1/1	0.70	0.14	84,84,84,84	0
59	MG	1H	3522	1/1	0.70	0.12	102,102,102,102	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
58	K	1H	3099	1/1	0.71	0.21	81,81,81,81	0
59	MG	1H	3509	1/1	0.71	0.08	101,101,101,101	0
59	MG	14	3172	1/1	0.71	0.13	72,72,72,72	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	14	3277	1/1	0.71	0.14	53,53,53,53	0
59	MG	1H	3363	1/1	0.72	0.13	32,32,32,32	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
58	K	5I	101	1/1	0.72	0.09	129,129,129,129	0
59	MG	14	3275	1/1	0.73	0.07	58,58,58,58	0
58	K	1G	1613	1/1	0.73	0.09	96,96,96,96	0
59	MG	14	3370	1/1	0.73	0.12	56,56,56,56	0
59	MG	14	3274	1/1	0.73	0.12	30,30,30,30	0
59	MG	1H	3492	1/1	0.73	0.09	67,67,67,67	0
59	MG	14	3174	1/1	0.73	0.21	78,78,78,78	0
59	MG	1H	3450	1/1	0.74	0.05	91,91,91,91	0
59	MG	1J	202	1/1	0.74	0.16	69,69,69,69	0
59	MG	1H	3424	1/1	0.74	0.14	84,84,84,84	0
59	MG	1G	1709	1/1	0.74	0.12	102,102,102,102	0
59	MG	1H	3457	1/1	0.74	0.12	35,35,35,35	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	1G	1693	1/1	0.74	0.06	89,89,89,89	0
59	MG	1H	3474	1/1	0.74	0.09	47,47,47,47	0
59	MG	1H	3327	1/1	0.75	0.33	72,72,72,72	0
58	K	13	1605	1/1	0.75	0.17	94,94,94,94	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	3419	1/1	0.75	0.13	43,43,43,43	0
58	K	16	202	1/1	0.75	0.11	116,116,116,116	0
58	K	14	3036	1/1	0.75	0.10	85,85,85,85	0
59	MG	1G	1695	1/1	0.75	0.05	97,97,97,97	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
59	MG	1H	3337	1/1	0.75	0.09	37,37,37,37	0
59	MG	1H	3515	1/1	0.75	0.10	90,90,90,90	0
59	MG	3E	301	1/1	0.75	0.15	84,84,84,84	0
58	K	39	301	1/1	0.75	0.07	107,107,107,107	0
59	MG	1H	3244	1/1	0.76	0.17	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	1H	3472	1/1	0.76	0.09	71,71,71,71	0
59	MG	14	3250	1/1	0.76	0.27	84,84,84,84	0
59	MG	1G	1703	1/1	0.76	0.06	93,93,93,93	0
58	K	1H	3030	1/1	0.76	0.26	86,86,86,86	0
59	MG	1H	3476	1/1	0.76	0.17	42,42,42,42	0
59	MG	1H	3215	1/1	0.76	0.27	65,65,65,65	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	13	1740	1/1	0.76	0.09	105,105,105,105	0
59	MG	14	3300	1/1	0.77	0.11	41,41,41,41	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
58	K	1H	3034	1/1	0.77	0.11	83,83,83,83	0
59	MG	1H	3511	1/1	0.77	0.06	93,93,93,93	0
59	MG	13	1734	1/1	0.78	0.07	61,61,61,61	0
59	MG	1G	1690	1/1	0.78	0.11	109,109,109,109	0
59	MG	14	3288	1/1	0.78	0.13	79,79,79,79	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
59	MG	13	1710	1/1	0.78	0.37	97,97,97,97	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	1H	3486	1/1	0.78	0.10	54,54,54,54	0
59	MG	1H	3301	1/1	0.78	0.18	59,59,59,59	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	3374	1/1	0.78	0.13	96,96,96,96	0
59	MG	1H	3347	1/1	0.79	0.20	50,50,50,50	0
58	K	13	1606	1/1	0.79	0.08	87,87,87,87	0
59	MG	1H	3211	1/1	0.79	0.21	47,47,47,47	0
58	K	1H	3117	1/1	0.79	0.21	85,85,85,85	0
59	MG	14	3386	1/1	0.79	0.10	82,82,82,82	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	1H	3504	1/1	0.79	0.18	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	1H	3242	1/1	0.79	0.13	57,57,57,57	0
58	K	14	3067	1/1	0.79	0.09	90,90,90,90	0
59	MG	14	3361	1/1	0.79	0.06	71,71,71,71	0
59	MG	1H	3461	1/1	0.79	0.16	33,33,33,33	0
59	MG	1H	3161	1/1	0.79	0.15	32,32,32,32	0
59	MG	1H	3402	1/1	0.79	0.13	63,63,63,63	0
58	K	1H	3094	1/1	0.79	0.14	65,65,65,65	0
58	K	1H	3013	1/1	0.79	0.11	83,83,83,83	0
58	K	1G	1619	1/1	0.79	0.06	79,79,79,79	0
59	MG	1G	1722	1/1	0.79	0.07	97,97,97,97	0
58	K	14	3055	1/1	0.79	0.14	116,116,116,116	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	3489	1/1	0.80	0.06	76,76,76,76	0
59	MG	1H	3480	1/1	0.80	0.10	58,58,58,58	0
58	K	13	1635	1/1	0.80	0.55	104,104,104,104	0
59	MG	1H	3284	1/1	0.80	0.20	66,66,66,66	0
59	MG	29	304	1/1	0.80	0.14	62,62,62,62	0
59	MG	14	3186	1/1	0.80	0.17	48,48,48,48	0
58	K	1H	3088	1/1	0.80	0.13	74,74,74,74	0
59	MG	13	1700	1/1	0.80	0.19	63,63,63,63	0
59	MG	1H	3311	1/1	0.80	0.29	57,57,57,57	0
59	MG	14	3251	1/1	0.80	0.17	52,52,52,52	0
59	MG	14	3102	1/1	0.80	0.10	57,57,57,57	0
59	MG	1H	3222	1/1	0.80	0.28	67,67,67,67	0
59	MG	1H	3389	1/1	0.80	0.14	38,38,38,38	0
59	MG	1H	3380	1/1	0.80	0.11	61,61,61,61	0
59	MG	14	3234	1/1	0.80	0.23	67,67,67,67	0
59	MG	1H	3288	1/1	0.80	0.12	51,51,51,51	0
58	K	1G	1605	1/1	0.80	0.10	92,92,92,92	0
58	K	1G	1622	1/1	0.80	0.08	118,118,118,118	0
59	MG	1G	1641	1/1	0.80	0.16	53,53,53,53	0
59	MG	1H	3426	1/1	0.80	0.15	68,68,68,68	0
59	MG	1H	3423	1/1	0.80	0.12	33,33,33,33	0
59	MG	1H	3465	1/1	0.80	0.14	39,39,39,39	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
59	MG	1H	3170	1/1	0.81	0.16	47,47,47,47	0
59	MG	1H	3322	1/1	0.81	0.16	60,60,60,60	0
58	K	13	1608	1/1	0.81	0.15	96,96,96,96	0
58	K	1H	3061	1/1	0.81	0.17	47,47,47,47	0
58	K	1H	3072	1/1	0.81	0.16	100,100,100,100	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
59	MG	1H	3471	1/1	0.81	0.13	30,30,30,30	0
59	MG	1H	3318	1/1	0.81	0.35	85,85,85,85	0
59	MG	1H	3296	1/1	0.81	0.08	50,50,50,50	0
59	MG	1H	3477	1/1	0.81	0.11	43,43,43,43	0
59	MG	1H	3265	1/1	0.81	0.26	63,63,63,63	0
59	MG	1H	3292	1/1	0.81	0.14	54,54,54,54	0
59	MG	14	3321	1/1	0.81	0.11	51,51,51,51	0
59	MG	1H	3404	1/1	0.81	0.14	65,65,65,65	0
59	MG	1H	3434	1/1	0.81	0.13	68,68,68,68	0
59	MG	14	3387	1/1	0.81	0.18	45,45,45,45	0
59	MG	1H	3503	1/1	0.81	0.08	63,63,63,63	0
59	MG	14	3347	1/1	0.81	0.15	57,57,57,57	0
58	K	14	3052	1/1	0.81	0.13	105,105,105,105	0
58	K	1G	1601	1/1	0.81	0.09	102,102,102,102	0
59	MG	1H	3414	1/1	0.81	0.05	89,89,89,89	0
59	MG	14	3351	1/1	0.81	0.10	61,61,61,61	0
59	MG	1H	3326[B]	1/1	0.81	0.46	55,55,55,55	1
59	MG	1H	3427	1/1	0.81	0.21	41,41,41,41	0
58	K	14	3027	1/1	0.81	0.10	97,97,97,97	0
59	MG	1H	3326[A]	1/1	0.81	0.46	58,58,58,58	1
59	MG	1H	3282	1/1	0.81	0.16	48,48,48,48	0
58	K	16	201	1/1	0.81	0.08	102,102,102,102	0
58	K	14	3075	1/1	0.82	0.28	116,116,116,116	0
59	MG	1J	201	1/1	0.82	0.11	131,131,131,131	0
59	MG	14	3327	1/1	0.82	0.09	66,66,66,66	0
58	K	1H	3113[A]	1/1	0.82	0.16	45,45,45,45	1
59	MG	1H	3177	1/1	0.82	0.15	54,54,54,54	0
59	MG	14	3379	1/1	0.82	0.19	42,42,42,42	0
59	MG	1H	3180	1/1	0.82	0.28	72,72,72,72	0
59	MG	1H	3325	1/1	0.82	0.20	65,65,65,65	0
59	MG	13	1691	1/1	0.82	0.22	88,88,88,88	0
59	MG	14	3103	1/1	0.82	0.12	82,82,82,82	0
59	MG	BI	202	1/1	0.82	0.10	94,94,94,94	0
59	MG	1G	1628	1/1	0.82	0.36	92,92,92,92	0
59	MG	14	3252	1/1	0.82	0.24	75,75,75,75	0
58	K	14	3094	1/1	0.82	0.10	111,111,111,111	0
58	K	1H	3113[B]	1/1	0.82	0.16	39,39,39,39	1
59	MG	1H	3385	1/1	0.82	0.08	69,69,69,69	0
59	MG	D8	201	1/1	0.82	0.14	71,71,71,71	0
58	K	14	3026	1/1	0.82	0.08	109,109,109,109	0
59	MG	14	3155	1/1	0.82	0.11	57,57,57,57	0
59	MG	1H	3373	1/1	0.83	0.12	39,39,39,39	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
59	MG	1H	3203	1/1	0.83	0.21	52,52,52,52	0
58	K	14	3088	1/1	0.83	0.16	101,101,101,101	0
59	MG	1H	3520	1/1	0.83	0.14	70,70,70,70	0
59	MG	1H	3285	1/1	0.83	0.28	66,66,66,66	0
59	MG	1H	3355	1/1	0.83	0.10	32,32,32,32	0
58	K	1G	1609	1/1	0.83	0.12	113,113,113,113	0
59	MG	13	1732	1/1	0.83	0.18	81,81,81,81	0
59	MG	14	3291	1/1	0.83	0.12	64,64,64,64	0
59	MG	1H	3348	1/1	0.83	0.11	34,34,34,34	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	3328	1/1	0.83	0.14	61,61,61,61	0
59	MG	1G	1727	1/1	0.83	0.05	93,93,93,93	0
59	MG	14	3323	1/1	0.83	0.09	47,47,47,47	0
59	MG	1H	3207	1/1	0.83	0.17	56,56,56,56	0
58	K	1H	3089	1/1	0.83	0.08	50,50,50,50	0
59	MG	14	3289	1/1	0.83	0.10	53,53,53,53	0
59	MG	13	1730	1/1	0.83	0.09	79,79,79,79	0
59	MG	13	1707	1/1	0.83	0.22	65,65,65,65	0
59	MG	1H	3278	1/1	0.83	0.29	68,68,68,68	0
58	K	14	3089	1/1	0.83	0.09	97,97,97,97	0
58	K	1H	3003	1/1	0.83	0.09	76,76,76,76	0
58	K	14	3079	1/1	0.83	0.08	112,112,112,112	0
59	MG	14	3233	1/1	0.83	0.14	80,80,80,80	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	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	3275	1/1	0.84	0.20	60,60,60,60	0
59	MG	1H	3200	1/1	0.84	0.14	67,67,67,67	0
59	MG	1G	1711	1/1	0.84	0.10	104,104,104,104	0
59	MG	13	1739	1/1	0.84	0.06	97,97,97,97	0
58	K	1H	3039	1/1	0.84	0.10	81,81,81,81	0
58	K	31	301	1/1	0.84	0.11	60,60,60,60	0
59	MG	13	1662	1/1	0.84	0.19	67,67,67,67	0
58	K	1H	3008	1/1	0.84	0.15	61,61,61,61	0
59	MG	BI	201	1/1	0.84	0.13	108,108,108,108	0
59	MG	1H	3416	1/1	0.84	0.20	59,59,59,59	0
59	MG	1H	3350	1/1	0.84	0.12	26,26,26,26	0
59	MG	14	3384	1/1	0.84	0.06	108,108,108,108	0
58	K	13	1601	1/1	0.84	0.09	87,87,87,87	0
59	MG	1H	3523	1/1	0.84	0.10	34,34,34,34	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
59	MG	1H	3392	1/1	0.84	0.12	32,32,32,32	0
59	MG	14	3295	1/1	0.84	0.15	51,51,51,51	0
58	K	1H	3112	1/1	0.84	0.15	87,87,87,87	0
59	MG	13	1671	1/1	0.84	0.14	65,65,65,65	0
59	MG	13	1718	1/1	0.84	0.06	89,89,89,89	0
59	MG	1H	3178	1/1	0.84	0.17	34,34,34,34	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	3270	1/1	0.84	0.10	57,57,57,57	0
59	MG	1H	3231	1/1	0.84	0.40	67,67,67,67	0
58	K	1H	3090	1/1	0.84	0.08	65,65,65,65	0
59	MG	1H	3375	1/1	0.84	0.08	69,69,69,69	0
58	K	1G	1607	1/1	0.84	0.07	93,93,93,93	0
59	MG	1G	1686	1/1	0.84	0.07	94,94,94,94	0
59	MG	1H	3449	1/1	0.84	0.08	57,57,57,57	0
59	MG	14	3332	1/1	0.84	0.06	110,110,110,110	0
58	K	1H	3041	1/1	0.85	0.10	66,66,66,66	0
59	MG	13	1670	1/1	0.85	0.25	72,72,72,72	0
59	MG	13	1736	1/1	0.85	0.08	100,100,100,100	0
59	MG	1H	3352	1/1	0.85	0.15	59,59,59,59	0
59	MG	14	3173	1/1	0.85	0.27	64,64,64,64	0
58	K	14	3012	1/1	0.85	0.07	91,91,91,91	0
59	MG	14	3368	1/1	0.85	0.15	40,40,40,40	0
59	MG	14	3310	1/1	0.85	0.11	27,27,27,27	0
58	K	14	3001	1/1	0.85	0.13	87,87,87,87	0
58	K	1G	1615	1/1	0.85	0.18	106,106,106,106	0
59	MG	14	3377	1/1	0.85	0.11	70,70,70,70	0
59	MG	1H	3429	1/1	0.85	0.08	63,63,63,63	0
59	MG	1H	3431	1/1	0.85	0.07	85,85,85,85	0
59	MG	21	301	1/1	0.85	0.08	34,34,34,34	0
59	MG	1H	3235	1/1	0.85	0.18	62,62,62,62	0
59	MG	1H	3335	1/1	0.85	0.18	50,50,50,50	0
59	MG	1H	3470	1/1	0.85	0.09	45,45,45,45	0
59	MG	1H	3315	1/1	0.85	0.20	70,70,70,70	0
59	MG	14	3297	1/1	0.85	0.05	44,44,44,44	0
59	MG	14	3290	1/1	0.85	0.09	48,48,48,48	0
58	K	1H	3069	1/1	0.85	0.10	74,74,74,74	0
59	MG	13	1695	1/1	0.85	0.22	76,76,76,76	0
59	MG	1G	1710	1/1	0.85	0.05	70,70,70,70	0
59	MG	1G	1712	1/1	0.85	0.07	106,106,106,106	0
59	MG	1H	3369	1/1	0.85	0.11	52,52,52,52	0
58	K	1H	3121	1/1	0.85	0.14	66,66,66,66	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
58	K	13	1636	1/1	0.85	0.16	136,136,136,136	0
59	MG	14	3181	1/1	0.86	0.17	46,46,46,46	0
59	MG	1H	3133	1/1	0.86	0.18	55,55,55,55	0
59	MG	14	3394	1/1	0.86	0.10	82,82,82,82	0
59	MG	14	3145	1/1	0.86	0.20	86,86,86,86	0
59	MG	1H	3312	1/1	0.86	0.13	70,70,70,70	0
59	MG	14	3141	1/1	0.86	0.22	60,60,60,60	0
59	MG	13	1701	1/1	0.86	0.16	72,72,72,72	0
58	K	14	3050	1/1	0.86	0.15	81,81,81,81	0
59	MG	14	3154	1/1	0.86	0.25	72,72,72,72	0
59	MG	1G	1681	1/1	0.86	0.09	49,49,49,49	0
59	MG	1H	3221	1/1	0.86	0.28	77,77,77,77	0
59	MG	1H	3201	1/1	0.86	0.15	48,48,48,48	0
59	MG	1H	3151	1/1	0.86	0.26	54,54,54,54	0
59	MG	14	3302	1/1	0.86	0.07	52,52,52,52	0
59	MG	1G	1630	1/1	0.86	0.20	64,64,64,64	0
58	K	1H	3086	1/1	0.86	0.18	79,79,79,79	0
59	MG	14	3140	1/1	0.86	0.20	45,45,45,45	0
59	MG	1H	3290	1/1	0.86	0.26	51,51,51,51	0
59	MG	1H	3484	1/1	0.86	0.14	47,47,47,47	0
59	MG	1H	3496	1/1	0.86	0.08	64,64,64,64	0
59	MG	1H	3239	1/1	0.86	0.41	83,83,83,83	0
59	MG	14	3357	1/1	0.86	0.21	95,95,95,95	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	13	1665	1/1	0.86	0.19	50,50,50,50	0
59	MG	13	1669	1/1	0.86	0.13	53,53,53,53	0
59	MG	14	3382	1/1	0.86	0.07	77,77,77,77	0
58	K	1H	3103	1/1	0.86	0.13	65,65,65,65	0
59	MG	14	3395	1/1	0.86	0.12	50,50,50,50	0
58	K	14	3031	1/1	0.86	0.05	78,78,78,78	0
58	K	1H	3084	1/1	0.86	0.11	77,77,77,77	0
59	MG	14	3359	1/1	0.86	0.16	94,94,94,94	0
59	MG	14	3267	1/1	0.86	0.20	92,92,92,92	0
59	MG	1G	1651	1/1	0.86	0.20	63,63,63,63	0
58	K	1G	1624	1/1	0.86	0.12	116,116,116,116	0
59	MG	1H	3167	1/1	0.86	0.17	33,33,33,33	0
58	K	14	3082	1/1	0.86	0.20	76,76,76,76	0
59	MG	13	1658	1/1	0.86	0.13	35,35,35,35	0
59	MG	14	3190	1/1	0.86	0.13	81,81,81,81	0
58	K	14	3013	1/1	0.86	0.08	98,98,98,98	0
59	MG	1H	3319	1/1	0.86	0.11	55,55,55,55	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
59	MG	14	3375	1/1	0.86	0.17	57,57,57,57	0
59	MG	14	3185	1/1	0.86	0.27	76,76,76,76	0
59	MG	1G	1697	1/1	0.86	0.09	81,81,81,81	0
59	MG	14	3256	1/1	0.86	0.18	64,64,64,64	0
59	MG	14	3344	1/1	0.87	0.13	89,89,89,89	0
58	K	14	3037	1/1	0.87	0.08	60,60,60,60	0
59	MG	13	1688	1/1	0.87	0.25	83,83,83,83	0
59	MG	1H	3360	1/1	0.87	0.12	39,39,39,39	0
58	K	1H	3010	1/1	0.87	0.12	93,93,93,93	0
58	K	1H	3031	1/1	0.87	0.11	96,96,96,96	0
59	MG	1H	3391	1/1	0.87	0.11	31,31,31,31	0
59	MG	1H	3374	1/1	0.87	0.06	70,70,70,70	0
59	MG	13	1664	1/1	0.87	0.10	53,53,53,53	0
59	MG	13	1690	1/1	0.87	0.22	77,77,77,77	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	1H	3323	1/1	0.87	0.34	73,73,73,73	0
59	MG	13	1666	1/1	0.87	0.16	83,83,83,83	0
59	MG	1H	3518	1/1	0.87	0.11	40,40,40,40	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	3371	1/1	0.87	0.10	35,35,35,35	0
58	K	13	1610	1/1	0.87	0.10	114,114,114,114	0
59	MG	1G	1684	1/1	0.87	0.14	75,75,75,75	0
59	MG	1H	3159	1/1	0.87	0.17	68,68,68,68	0
58	K	13	1623	1/1	0.87	0.10	121,121,121,121	0
59	MG	1G	1700	1/1	0.87	0.11	108,108,108,108	0
59	MG	1H	3324	1/1	0.87	0.34	59,59,59,59	0
59	MG	1H	3341	1/1	0.87	0.20	31,31,31,31	0
59	MG	14	3376	1/1	0.87	0.21	61,61,61,61	0
59	MG	1H	3173	1/1	0.87	0.14	57,57,57,57	0
59	MG	1H	3506	1/1	0.87	0.08	65,65,65,65	0
59	MG	1H	3466	1/1	0.88	0.14	34,34,34,34	0
58	K	1H	3002	1/1	0.88	0.06	71,71,71,71	0
59	MG	14	3262	1/1	0.88	0.13	45,45,45,45	0
59	MG	1H	3525	1/1	0.88	0.07	46,46,46,46	0
58	K	14	3014	1/1	0.88	0.09	82,82,82,82	0
59	MG	1H	3439	1/1	0.88	0.08	55,55,55,55	0
59	MG	1G	1639	1/1	0.88	0.29	55,55,55,55	0
59	MG	13	1726	1/1	0.88	0.04	122,122,122,122	0
58	K	14	3057	1/1	0.88	0.08	68,68,68,68	0
59	MG	1J	203	1/1	0.88	0.05	105,105,105,105	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
59	MG	1H	3212	1/1	0.88	0.14	57,57,57,57	0
59	MG	1H	3455	1/1	0.88	0.19	55,55,55,55	0
59	MG	14	3246	1/1	0.88	0.07	76,76,76,76	0
58	K	1G	1625	1/1	0.88	0.12	106,106,106,106	0
59	MG	1H	3500	1/1	0.88	0.18	45,45,45,45	0
59	MG	1H	3276	1/1	0.88	0.22	63,63,63,63	0
59	MG	14	3124	1/1	0.88	0.08	63,63,63,63	0
59	MG	14	3353	1/1	0.88	0.05	65,65,65,65	0
58	K	14	3029	1/1	0.88	0.10	68,68,68,68	0
59	MG	1H	3198	1/1	0.88	0.21	82,82,82,82	0
59	MG	1H	3340	1/1	0.88	0.12	29,29,29,29	0
58	K	13	1614	1/1	0.88	0.18	103,103,103,103	0
59	MG	55	201	1/1	0.88	0.19	59,59,59,59	0
59	MG	1H	3238	1/1	0.88	0.33	82,82,82,82	0
59	MG	1H	3139	1/1	0.88	0.31	76,76,76,76	0
59	MG	1H	3493	1/1	0.88	0.12	63,63,63,63	0
59	MG	1H	3279	1/1	0.88	0.21	74,74,74,74	0
59	MG	14	3325	1/1	0.88	0.08	81,81,81,81	0
59	MG	1H	3122	1/1	0.88	0.22	29,29,29,29	0
59	MG	1H	3271	1/1	0.88	0.14	45,45,45,45	0
59	MG	14	3385	1/1	0.88	0.13	63,63,63,63	0
58	K	14	3054	1/1	0.88	0.06	77,77,77,77	0
59	MG	1H	3359	1/1	0.88	0.12	55,55,55,55	0
59	MG	14	3261	1/1	0.88	0.12	75,75,75,75	0
59	MG	1H	3377	1/1	0.88	0.09	44,44,44,44	0
59	MG	1H	3309	1/1	0.88	0.15	56,56,56,56	0
59	MG	16	207	1/1	0.88	0.27	88,88,88,88	0
58	K	14	3063	1/1	0.88	0.11	84,84,84,84	0
59	MG	14	3203	1/1	0.88	0.13	85,85,85,85	0
59	MG	14	3396	1/1	0.88	0.10	51,51,51,51	0
59	MG	14	3157	1/1	0.88	0.14	57,57,57,57	0
59	MG	14	3188	1/1	0.88	0.13	54,54,54,54	0
59	MG	1G	1659	1/1	0.88	0.10	72,72,72,72	0
58	K	13	1630	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	3406	1/1	0.88	0.08	95,95,95,95	0
59	MG	1H	3283	1/1	0.88	0.10	58,58,58,58	0
59	MG	13	1653	1/1	0.88	0.23	74,74,74,74	0
59	MG	1H	3257	1/1	0.88	0.11	49,49,49,49	0
58	K	1H	3044	1/1	0.88	0.10	82,82,82,82	0
59	MG	14	3209	1/1	0.88	0.16	72,72,72,72	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
59	MG	1H	3236	1/1	0.88	0.09	54,54,54,54	0
58	K	1H	3038	1/1	0.89	0.11	86,86,86,86	0
59	MG	1G	1688	1/1	0.89	0.06	82,82,82,82	0
59	MG	14	3225	1/1	0.89	0.12	62,62,62,62	0
58	K	14	3017	1/1	0.89	0.18	107,107,107,107	0
58	K	14	3035	1/1	0.89	0.09	62,62,62,62	0
59	MG	14	3322	1/1	0.89	0.06	93,93,93,93	0
59	MG	14	3263	1/1	0.89	0.26	66,66,66,66	0
59	MG	14	3358	1/1	0.89	0.07	35,35,35,35	0
59	MG	1H	3240	1/1	0.89	0.19	52,52,52,52	0
58	K	13	1632	1/1	0.89	0.10	83,83,83,83	0
58	K	13	1627	1/1	0.89	0.12	91,91,91,91	0
59	MG	1H	3252	1/1	0.89	0.18	72,72,72,72	0
58	K	1H	3104	1/1	0.89	0.08	53,53,53,53	0
59	MG	1G	1635	1/1	0.89	0.26	80,80,80,80	0
59	MG	1H	3490	1/1	0.89	0.06	53,53,53,53	0
58	K	1H	3066	1/1	0.89	0.09	80,80,80,80	0
58	K	14	3015	1/1	0.89	0.16	52,52,52,52	0
59	MG	1G	1702	1/1	0.89	0.08	87,87,87,87	0
59	MG	1J	204	1/1	0.89	0.07	115,115,115,115	0
58	K	14	3002	1/1	0.89	0.07	90,90,90,90	0
59	MG	N8	101	1/1	0.89	0.14	56,56,56,56	0
58	K	14	3076	1/1	0.89	0.13	89,89,89,89	0
59	MG	14	3195	1/1	0.89	0.16	64,64,64,64	0
59	MG	13	1696	1/1	0.89	0.18	80,80,80,80	0
59	MG	1H	3246	1/1	0.89	0.20	58,58,58,58	0
58	K	13	1607	1/1	0.89	0.08	90,90,90,90	0
59	MG	14	3369	1/1	0.89	0.17	43,43,43,43	0
59	MG	1H	3524	1/1	0.89	0.11	35,35,35,35	0
59	MG	1H	3512	1/1	0.89	0.14	61,61,61,61	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
59	MG	1H	3258	1/1	0.89	0.15	48,48,48,48	0
59	MG	1H	3230	1/1	0.89	0.15	38,38,38,38	0
59	MG	14	3200	1/1	0.89	0.22	102,102,102,102	0
59	MG	14	3371	1/1	0.89	0.06	61,61,61,61	0
59	MG	1H	3456	1/1	0.89	0.13	38,38,38,38	0
59	MG	1H	3219	1/1	0.89	0.15	50,50,50,50	0
59	MG	14	3239	1/1	0.89	0.15	66,66,66,66	0
59	MG	1G	1676	1/1	0.89	0.24	81,81,81,81	0
59	MG	1H	3390	1/1	0.89	0.16	39,39,39,39	0
59	MG	13	1715	1/1	0.89	0.09	75,75,75,75	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
59	MG	14	3100	1/1	0.89	0.12	47,47,47,47	0
59	MG	1H	3475	1/1	0.89	0.08	91,91,91,91	0
59	MG	1G	1723	1/1	0.89	0.06	85,85,85,85	0
59	MG	14	3315	1/1	0.89	0.06	84,84,84,84	0
58	K	1G	1610	1/1	0.89	0.10	95,95,95,95	0
59	MG	13	1680	1/1	0.89	0.21	71,71,71,71	0
59	MG	1H	3505	1/1	0.89	0.13	34,34,34,34	0
58	K	1H	3016	1/1	0.89	0.14	114,114,114,114	0
59	MG	1H	3329	1/1	0.89	0.17	73,73,73,73	0
59	MG	1H	3225	1/1	0.89	0.18	58,58,58,58	0
59	MG	1H	3463	1/1	0.89	0.12	40,40,40,40	0
59	MG	13	1737	1/1	0.89	0.05	90,90,90,90	0
58	K	13	1629	1/1	0.89	0.07	92,92,92,92	0
59	MG	13	1742	1/1	0.89	0.07	94,94,94,94	0
59	MG	13	1706	1/1	0.89	0.22	63,63,63,63	0
58	K	14	3069	1/1	0.89	0.12	89,89,89,89	0
59	MG	14	3148	1/1	0.89	0.13	58,58,58,58	0
59	MG	1H	3153	1/1	0.90	0.18	44,44,44,44	0
59	MG	1H	3196	1/1	0.90	0.15	42,42,42,42	0
59	MG	14	3273	1/1	0.90	0.10	46,46,46,46	0
59	MG	14	3309	1/1	0.90	0.09	85,85,85,85	0
59	MG	1H	3227	1/1	0.90	0.20	58,58,58,58	0
59	MG	1H	3372	1/1	0.90	0.15	77,77,77,77	0
59	MG	13	1685	1/1	0.90	0.31	85,85,85,85	0
59	MG	1H	3417	1/1	0.90	0.12	44,44,44,44	0
58	K	14	3065	1/1	0.90	0.06	92,92,92,92	0
59	MG	1H	3502	1/1	0.90	0.05	94,94,94,94	0
59	MG	13	1676	1/1	0.90	0.11	53,53,53,53	0
59	MG	14	3391	1/1	0.90	0.09	62,62,62,62	0
59	MG	1H	3345	1/1	0.90	0.10	24,24,24,24	0
58	K	1H	3102	1/1	0.90	0.09	94,94,94,94	0
59	MG	1H	3331	1/1	0.90	0.20	55,55,55,55	0
58	K	1H	3018	1/1	0.90	0.09	93,93,93,93	0
59	MG	1H	3183	1/1	0.90	0.14	49,49,49,49	0
59	MG	1H	3362	1/1	0.90	0.10	33,33,33,33	0
59	MG	13	1689	1/1	0.90	0.11	80,80,80,80	0
59	MG	1H	3226	1/1	0.90	0.10	42,42,42,42	0
59	MG	14	3222	1/1	0.90	0.07	57,57,57,57	0
59	MG	14	3399	1/1	0.90	0.10	55,55,55,55	0
59	MG	1G	1668	1/1	0.90	0.25	55,55,55,55	0
59	MG	1H	3403	1/1	0.90	0.07	59,59,59,59	0
58	K	1G	1616	1/1	0.90	0.06	89,89,89,89	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
58	K	1H	3033	1/1	0.90	0.08	94,94,94,94	0
59	MG	1H	3436	1/1	0.90	0.07	33,33,33,33	0
59	MG	1G	1717	1/1	0.90	0.06	88,88,88,88	0
59	MG	1G	1714	1/1	0.90	0.13	82,82,82,82	0
58	K	14	3049	1/1	0.90	0.12	103,103,103,103	0
58	K	1G	1608	1/1	0.90	0.17	113,113,113,113	0
59	MG	1H	3241	1/1	0.90	0.15	39,39,39,39	0
58	K	13	1637	1/1	0.90	0.09	123,123,123,123	0
59	MG	14	3231	1/1	0.90	0.09	48,48,48,48	0
59	MG	14	3279	1/1	0.90	0.06	46,46,46,46	0
59	MG	1H	3304	1/1	0.90	0.29	69,69,69,69	0
59	MG	14	3214	1/1	0.90	0.21	57,57,57,57	0
59	MG	1H	3379	1/1	0.90	0.07	67,67,67,67	0
59	MG	14	3156	1/1	0.90	0.10	55,55,55,55	0
58	K	14	3008	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	3183	1/1	0.90	0.11	63,63,63,63	0
59	MG	1H	3192	1/1	0.90	0.14	49,49,49,49	0
59	MG	14	3208	1/1	0.90	0.09	61,61,61,61	0
58	K	14	3028	1/1	0.90	0.07	56,56,56,56	0
58	K	1H	3001	1/1	0.90	0.07	88,88,88,88	0
59	MG	14	3151	1/1	0.90	0.19	57,57,57,57	0
59	MG	14	3197	1/1	0.90	0.14	60,60,60,60	0
59	MG	1H	3366	1/1	0.91	0.09	44,44,44,44	0
59	MG	1H	3438	1/1	0.91	0.10	36,36,36,36	0
58	K	1H	3024	1/1	0.91	0.08	56,56,56,56	0
59	MG	1H	3386	1/1	0.91	0.11	67,67,67,67	0
59	MG	14	3143	1/1	0.91	0.15	72,72,72,72	0
59	MG	14	3341	1/1	0.91	0.13	52,52,52,52	0
59	MG	14	3348	1/1	0.91	0.17	102,102,102,102	0
58	K	1H	3035	1/1	0.91	0.10	98,98,98,98	0
58	K	1H	3040	1/1	0.91	0.33	111,111,111,111	0
59	MG	1H	3415	1/1	0.91	0.09	94,94,94,94	0
59	MG	1H	3291	1/1	0.91	0.17	62,62,62,62	0
59	MG	1H	3479	1/1	0.91	0.12	47,47,47,47	0
58	K	14	3093	1/1	0.91	0.10	72,72,72,72	0
59	MG	1H	3495	1/1	0.91	0.10	80,80,80,80	0
59	MG	1H	3382	1/1	0.91	0.16	36,36,36,36	0
59	MG	14	3129	1/1	0.91	0.11	44,44,44,44	0
59	MG	13	1713	1/1	0.91	0.05	83,83,83,83	0
59	MG	1H	3519	1/1	0.91	0.06	56,56,56,56	0
58	K	14	3022	1/1	0.91	0.05	92,92,92,92	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
59	MG	1G	1706	1/1	0.91	0.05	96,96,96,96	0
59	MG	14	3360	1/1	0.91	0.09	64,64,64,64	0
59	MG	1H	3184	1/1	0.91	0.26	65,65,65,65	0
59	MG	1H	3134	1/1	0.91	0.20	59,59,59,59	0
59	MG	1H	3204	1/1	0.91	0.24	51,51,51,51	0
59	MG	14	3280	1/1	0.91	0.08	48,48,48,48	0
59	MG	1H	3181	1/1	0.91	0.17	41,41,41,41	0
58	K	1H	3118	1/1	0.91	0.38	89,89,89,89	0
59	MG	1G	1649	1/1	0.91	0.14	85,85,85,85	0
59	MG	1H	3223	1/1	0.91	0.10	64,64,64,64	0
58	K	14	3003	1/1	0.91	0.10	86,86,86,86	0
59	MG	14	3249	1/1	0.91	0.11	54,54,54,54	0
59	MG	13	1735	1/1	0.91	0.04	57,57,57,57	0
59	MG	1H	3440	1/1	0.91	0.11	63,63,63,63	0
58	K	14	3040	1/1	0.91	0.12	72,72,72,72	0
58	K	1H	3005	1/1	0.91	0.11	67,67,67,67	0
59	MG	14	3196	1/1	0.91	0.14	90,90,90,90	0
59	MG	1G	1724	1/1	0.91	0.10	109,109,109,109	0
59	MG	1G	1652	1/1	0.91	0.12	94,94,94,94	0
59	MG	1H	3273	1/1	0.91	0.11	49,49,49,49	0
59	MG	1H	3442	1/1	0.91	0.08	80,80,80,80	0
58	K	14	3085	1/1	0.91	0.08	94,94,94,94	0
59	MG	1H	3501	1/1	0.91	0.05	78,78,78,78	0
59	MG	1H	3468	1/1	0.91	0.09	50,50,50,50	0
58	K	13	1628	1/1	0.91	0.14	103,103,103,103	0
59	MG	14	3340	1/1	0.91	0.13	74,74,74,74	0
59	MG	16	204	1/1	0.91	0.25	80,80,80,80	0
59	MG	1H	3447	1/1	0.91	0.05	98,98,98,98	0
59	MG	14	3169	1/1	0.91	0.08	57,57,57,57	0
59	MG	1H	3339	1/1	0.91	0.11	33,33,33,33	0
59	MG	1H	3370	1/1	0.91	0.13	38,38,38,38	0
58	K	1H	3063	1/1	0.91	0.10	55,55,55,55	0
59	MG	1H	3507	1/1	0.91	0.06	45,45,45,45	0
59	MG	1G	1687	1/1	0.91	0.08	93,93,93,93	0
59	MG	14	3206	1/1	0.91	0.11	67,67,67,67	0
59	MG	14	3201	1/1	0.91	0.11	68,68,68,68	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	3138	1/1	0.91	0.29	66,66,66,66	0
59	MG	14	3193	1/1	0.91	0.08	63,63,63,63	0
59	MG	1H	3394	1/1	0.91	0.09	38,38,38,38	0
59	MG	1G	1705	1/1	0.92	0.03	105,105,105,105	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
59	MG	1H	3190	1/1	0.92	0.17	49,49,49,49	0
59	MG	1H	3316	1/1	0.92	0.20	59,59,59,59	0
58	K	1H	3004	1/1	0.92	0.24	66,66,66,66	0
58	K	13	1615	1/1	0.92	0.08	91,91,91,91	0
58	K	1H	3106	1/1	0.92	0.13	92,92,92,92	0
59	MG	1H	3289	1/1	0.92	0.21	75,75,75,75	0
59	MG	1H	3302	1/1	0.92	0.19	41,41,41,41	0
59	MG	1H	3248	1/1	0.92	0.12	47,47,47,47	0
59	MG	1H	3332	1/1	0.92	0.20	59,59,59,59	0
59	MG	1H	3516	1/1	0.92	0.07	60,60,60,60	0
58	K	14	3048	1/1	0.92	0.11	101,101,101,101	0
59	MG	14	3235	1/1	0.92	0.16	61,61,61,61	0
58	K	14	3062	1/1	0.92	0.06	65,65,65,65	0
58	K	1H	3120	1/1	0.92	0.13	79,79,79,79	0
59	MG	13	1684	1/1	0.92	0.14	56,56,56,56	0
59	MG	1H	3478	1/1	0.92	0.08	38,38,38,38	0
59	MG	14	3406	1/1	0.92	0.07	55,55,55,55	0
59	MG	E5	101	1/1	0.92	0.17	36,36,36,36	0
59	MG	1H	3307	1/1	0.92	0.09	39,39,39,39	0
58	K	13	1624	1/1	0.92	0.18	83,83,83,83	0
58	K	1H	3011	1/1	0.92	0.08	61,61,61,61	0
59	MG	14	3269	1/1	0.92	0.10	79,79,79,79	0
59	MG	1H	3454	1/1	0.92	0.12	42,42,42,42	0
59	MG	1H	3194	1/1	0.92	0.21	45,45,45,45	0
59	MG	14	3373	1/1	0.92	0.06	84,84,84,84	0
59	MG	1H	3313	1/1	0.92	0.14	52,52,52,52	0
59	MG	1H	3338	1/1	0.92	0.13	35,35,35,35	0
59	MG	14	3226	1/1	0.92	0.08	49,49,49,49	0
59	MG	14	3242	1/1	0.92	0.16	44,44,44,44	0
59	MG	1H	3388	1/1	0.92	0.14	38,38,38,38	0
59	MG	1H	3259	1/1	0.92	0.12	59,59,59,59	0
59	MG	14	3307	1/1	0.92	0.07	51,51,51,51	0
58	K	1H	3119	1/1	0.92	0.11	92,92,92,92	0
58	K	14	3043	1/1	0.92	0.05	71,71,71,71	0
59	MG	14	3346	1/1	0.92	0.05	76,76,76,76	0
59	MG	13	1679	1/1	0.92	0.13	89,89,89,89	0
59	MG	1H	3237	1/1	0.92	0.29	51,51,51,51	0
59	MG	14	3366	1/1	0.92	0.08	77,77,77,77	0
58	K	1H	3026	1/1	0.92	0.31	62,62,62,62	0
59	MG	14	3272	1/1	0.92	0.13	26,26,26,26	0
59	MG	1G	1634	1/1	0.92	0.33	110,110,110,110	0
59	MG	14	3244	1/1	0.92	0.25	46,46,46,46	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
59	MG	14	3303	1/1	0.92	0.06	73,73,73,73	0
59	MG	14	3393	1/1	0.92	0.25	81,81,81,81	0
59	MG	13	1746	1/1	0.92	0.06	93,93,93,93	0
59	MG	1G	1673	1/1	0.92	0.29	73,73,73,73	0
59	MG	1H	3186	1/1	0.92	0.20	50,50,50,50	0
59	MG	14	3176	1/1	0.92	0.21	67,67,67,67	0
59	MG	1H	3174	1/1	0.92	0.08	71,71,71,71	0
58	K	1H	3085	1/1	0.92	0.12	64,64,64,64	0
58	K	13	1609	1/1	0.92	0.20	91,91,91,91	0
58	K	14	3005	1/1	0.92	0.21	91,91,91,91	0
58	K	52	201	1/1	0.92	0.27	116,116,116,116	0
58	K	14	3047	1/1	0.92	0.16	97,97,97,97	0
59	MG	1H	3191	1/1	0.92	0.41	72,72,72,72	0
59	MG	14	3365	1/1	0.92	0.08	80,80,80,80	0
58	K	14	3041	1/1	0.92	0.12	54,54,54,54	0
58	K	13	1603	1/1	0.92	0.11	117,117,117,117	0
59	MG	13	1721	1/1	0.92	0.06	68,68,68,68	0
59	MG	13	1709	1/1	0.92	0.21	85,85,85,85	0
58	K	13	1613	1/1	0.92	0.09	100,100,100,100	0
59	MG	14	3314	1/1	0.92	0.04	91,91,91,91	0
59	MG	1H	3182	1/1	0.92	0.16	47,47,47,47	0
58	K	1H	3071	1/1	0.92	0.13	65,65,65,65	0
59	MG	14	3312	1/1	0.92	0.09	87,87,87,87	0
59	MG	1H	3228	1/1	0.92	0.11	48,48,48,48	0
59	MG	1G	1654	1/1	0.92	0.17	58,58,58,58	0
59	MG	1H	3483	1/1	0.92	0.14	75,75,75,75	0
59	MG	14	3390	1/1	0.92	0.07	78,78,78,78	0
59	MG	1H	3293	1/1	0.92	0.11	55,55,55,55	0
58	K	1H	3020	1/1	0.92	0.19	105,105,105,105	0
59	MG	1H	3305	1/1	0.92	0.25	57,57,57,57	0
58	K	14	3092	1/1	0.92	0.08	83,83,83,83	0
58	K	1H	3076	1/1	0.92	0.14	86,86,86,86	0
58	K	41	201	1/1	0.92	0.20	114,114,114,114	0
59	MG	14	3213	1/1	0.92	0.19	58,58,58,58	0
59	MG	1H	3452	1/1	0.92	0.10	48,48,48,48	0
59	MG	14	3283	1/1	0.92	0.14	36,36,36,36	0
59	MG	1H	3199	1/1	0.92	0.16	60,60,60,60	0
59	MG	13	1683	1/1	0.92	0.09	55,55,55,55	0
58	K	14	3058	1/1	0.92	0.22	84,84,84,84	0
59	MG	13	1712	1/1	0.92	0.11	50,50,50,50	0
59	MG	13	1714	1/1	0.92	0.05	106,106,106,106	0
59	MG	1G	1694	1/1	0.92	0.10	62,62,62,62	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
59	MG	1G	1633	1/1	0.92	0.21	65,65,65,65	0
59	MG	1H	3396	1/1	0.92	0.11	35,35,35,35	0
58	K	1H	3012	1/1	0.92	0.11	80,80,80,80	0
58	K	1G	1614	1/1	0.92	0.12	100,100,100,100	0
59	MG	1H	3208	1/1	0.92	0.18	52,52,52,52	0
59	MG	1H	3409	1/1	0.93	0.07	64,64,64,64	0
58	K	1G	1617	1/1	0.93	0.09	94,94,94,94	0
58	K	1G	1612	1/1	0.93	0.06	101,101,101,101	0
59	MG	1H	3274	1/1	0.93	0.10	56,56,56,56	0
59	MG	14	3139	1/1	0.93	0.15	46,46,46,46	0
58	K	14	3074	1/1	0.93	0.14	94,94,94,94	0
59	MG	14	3335	1/1	0.93	0.12	50,50,50,50	0
59	MG	1H	3521	1/1	0.93	0.07	113,113,113,113	0
59	MG	1G	1665	1/1	0.93	0.27	84,84,84,84	0
59	MG	13	1728	1/1	0.93	0.07	106,106,106,106	0
59	MG	14	3401	1/1	0.93	0.20	89,89,89,89	0
59	MG	13	1687	1/1	0.93	0.19	75,75,75,75	0
59	MG	13	1663	1/1	0.93	0.26	68,68,68,68	0
59	MG	1H	3488	1/1	0.93	0.04	83,83,83,83	0
58	K	1H	3064	1/1	0.93	0.09	49,49,49,49	0
59	MG	1H	3354	1/1	0.93	0.06	70,70,70,70	0
59	MG	13	1697	1/1	0.93	0.15	70,70,70,70	0
59	MG	14	3131	1/1	0.93	0.21	66,66,66,66	0
58	K	1H	3091	1/1	0.93	0.12	62,62,62,62	0
58	K	14	3084	1/1	0.93	0.07	75,75,75,75	0
59	MG	1H	3481	1/1	0.93	0.16	43,43,43,43	0
59	MG	14	3260	1/1	0.93	0.18	56,56,56,56	0
59	MG	13	1642	1/1	0.93	0.27	59,59,59,59	0
59	MG	1G	1644	1/1	0.93	0.23	55,55,55,55	0
59	MG	14	3355	1/1	0.93	0.12	64,64,64,64	0
59	MG	1G	1698	1/1	0.93	0.12	103,103,103,103	0
58	K	1H	3021	1/1	0.93	0.09	78,78,78,78	0
59	MG	1H	3444	1/1	0.93	0.13	94,94,94,94	0
59	MG	1H	3168	1/1	0.93	0.25	46,46,46,46	0
58	K	14	3039	1/1	0.93	0.10	94,94,94,94	0
59	MG	16	203	1/1	0.93	0.13	57,57,57,57	0
59	MG	1G	1656	1/1	0.93	0.30	100,100,100,100	0
59	MG	14	3383	1/1	0.93	0.08	71,71,71,71	0
59	MG	1H	3262	1/1	0.93	0.09	49,49,49,49	0
59	MG	1G	1658	1/1	0.93	0.27	76,76,76,76	0
59	MG	14	3130	1/1	0.93	0.14	45,45,45,45	0
59	MG	1H	3408	1/1	0.93	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	1H	3233	1/1	0.93	0.22	59,59,59,59	0
59	MG	14	3304	1/1	0.93	0.08	38,38,38,38	0
59	MG	14	3113	1/1	0.93	0.18	51,51,51,51	0
58	K	14	3087	1/1	0.93	0.07	84,84,84,84	0
58	K	1G	1602	1/1	0.93	0.21	70,70,70,70	0
58	K	14	3077	1/1	0.93	0.17	72,72,72,72	0
58	K	14	3034	1/1	0.93	0.07	49,49,49,49	0
58	K	1H	3025	1/1	0.93	0.06	100,100,100,100	0
58	K	1G	1611	1/1	0.93	0.11	94,94,94,94	0
59	MG	1H	3320	1/1	0.93	0.22	43,43,43,43	0
59	MG	14	3198	1/1	0.93	0.17	63,63,63,63	0
59	MG	1H	3400	1/1	0.93	0.07	46,46,46,46	0
58	K	1H	3075	1/1	0.93	0.11	81,81,81,81	0
59	MG	1G	1672	1/1	0.93	0.18	63,63,63,63	0
59	MG	1H	3499	1/1	0.93	0.10	68,68,68,68	0
58	K	14	3030	1/1	0.93	0.07	56,56,56,56	0
59	MG	1H	3441	1/1	0.93	0.06	51,51,51,51	0
59	MG	14	3191	1/1	0.93	0.20	45,45,45,45	0
58	K	1H	3042	1/1	0.93	0.21	62,62,62,62	0
59	MG	14	3305	1/1	0.93	0.05	69,69,69,69	0
59	MG	1H	3393	1/1	0.93	0.16	44,44,44,44	0
58	K	1H	3109	1/1	0.93	0.12	54,54,54,54	0
58	K	13	1620	1/1	0.93	0.08	115,115,115,115	0
59	MG	1G	1646	1/1	0.93	0.27	107,107,107,107	0
58	K	1H	3017	1/1	0.93	0.10	94,94,94,94	0
58	K	1H	3050	1/1	0.93	0.15	70,70,70,70	0
59	MG	1H	3280	1/1	0.93	0.27	64,64,64,64	0
58	K	1H	3060	1/1	0.93	0.18	55,55,55,55	0
59	MG	13	1655	1/1	0.93	0.14	80,80,80,80	0
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	1H	3093	1/1	0.93	0.11	79,79,79,79	0
59	MG	1H	3260	1/1	0.93	0.09	43,43,43,43	0
59	MG	29	303	1/1	0.93	0.12	37,37,37,37	0
59	MG	13	1682	1/1	0.93	0.43	101,101,101,101	0
58	K	1H	3114	1/1	0.93	0.07	58,58,58,58	0
59	MG	14	3112	1/1	0.93	0.07	55,55,55,55	0
59	MG	1H	3179	1/1	0.93	0.13	51,51,51,51	0
59	MG	13	1678	1/1	0.93	0.26	79,79,79,79	0
59	MG	14	3221	1/1	0.94	0.19	52,52,52,52	0
59	MG	1H	3425	1/1	0.94	0.13	42,42,42,42	0
59	MG	14	3171	1/1	0.94	0.11	71,71,71,71	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
58	K	14	3059	1/1	0.94	0.12	73,73,73,73	0
59	MG	14	3362	1/1	0.94	0.05	69,69,69,69	0
59	MG	1H	3195	1/1	0.94	0.19	51,51,51,51	0
59	MG	14	3115	1/1	0.94	0.10	46,46,46,46	0
59	MG	1H	3306	1/1	0.94	0.18	44,44,44,44	0
58	K	1H	3065	1/1	0.94	0.10	43,43,43,43	0
58	K	1H	3096	1/1	0.94	0.16	75,75,75,75	0
58	K	1H	3032	1/1	0.94	0.20	58,58,58,58	0
59	MG	16	209	1/1	0.94	0.07	75,75,75,75	0
59	MG	1G	1643	1/1	0.94	0.10	56,56,56,56	0
59	MG	16	205	1/1	0.94	0.21	84,84,84,84	0
59	MG	1H	3216	1/1	0.94	0.11	45,45,45,45	0
58	K	13	1633	1/1	0.94	0.06	108,108,108,108	0
59	MG	1H	3448	1/1	0.94	0.07	61,61,61,61	0
59	MG	14	3178	1/1	0.94	0.11	36,36,36,36	0
59	MG	14	3296	1/1	0.94	0.07	44,44,44,44	0
59	MG	1H	3232	1/1	0.94	0.13	40,40,40,40	0
59	MG	1H	3464	1/1	0.94	0.14	19,19,19,19	0
59	MG	13	1745	1/1	0.94	0.07	78,78,78,78	0
59	MG	1H	3130	1/1	0.94	0.19	28,28,28,28	0
58	K	14	3009	1/1	0.94	0.09	69,69,69,69	0
58	K	1H	3037	1/1	0.94	0.09	77,77,77,77	0
59	MG	14	3101	1/1	0.94	0.09	61,61,61,61	0
59	MG	1H	3156	1/1	0.94	0.20	55,55,55,55	0
59	MG	1G	1692	1/1	0.94	0.09	97,97,97,97	0
59	MG	1G	1647	1/1	0.94	0.21	80,80,80,80	0
58	K	13	1621	1/1	0.94	0.05	59,59,59,59	0
58	K	3A	201	1/1	0.94	0.13	93,93,93,93	0
59	MG	Q8	101	1/1	0.94	0.14	32,32,32,32	0
59	MG	1G	1718	1/1	0.94	0.10	91,91,91,91	0
58	K	1H	3105	1/1	0.94	0.07	60,60,60,60	0
58	K	1H	3015	1/1	0.94	0.09	80,80,80,80	0
58	K	14	3080	1/1	0.94	0.07	94,94,94,94	0
59	MG	1H	3157	1/1	0.94	0.23	62,62,62,62	0
58	K	14	3061	1/1	0.94	0.06	103,103,103,103	0
58	K	1H	3019	1/1	0.94	0.07	78,78,78,78	0
59	MG	1G	1670	1/1	0.94	0.10	60,60,60,60	0
59	MG	1H	3136	1/1	0.94	0.25	37,37,37,37	0
59	MG	14	3343	1/1	0.94	0.08	76,76,76,76	0
59	MG	1H	3317	1/1	0.94	0.35	63,63,63,63	0
59	MG	14	3334	1/1	0.94	0.07	48,48,48,48	0
59	MG	13	1692	1/1	0.94	0.16	70,70,70,70	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
59	MG	1H	3412	1/1	0.94	0.15	85,85,85,85	0
59	MG	1H	3155	1/1	0.94	0.12	35,35,35,35	0
59	MG	1H	3358	1/1	0.94	0.05	43,43,43,43	0
59	MG	1H	3432	1/1	0.94	0.11	73,73,73,73	0
58	K	1H	3043	1/1	0.94	0.10	82,82,82,82	0
58	K	1H	3007	1/1	0.94	0.09	54,54,54,54	0
59	MG	14	3162	1/1	0.94	0.20	58,58,58,58	0
59	MG	1H	3437	1/1	0.94	0.13	49,49,49,49	0
59	MG	14	3345	1/1	0.94	0.09	89,89,89,89	0
58	K	1H	3055	1/1	0.94	0.09	40,40,40,40	0
59	MG	1G	1642	1/1	0.94	0.23	59,59,59,59	0
59	MG	14	3318	1/1	0.94	0.09	68,68,68,68	0
59	MG	13	1640	1/1	0.94	0.19	72,72,72,72	0
59	MG	14	3210	1/1	0.94	0.16	45,45,45,45	0
58	K	BA	201	1/1	0.94	0.26	96,96,96,96	0
59	MG	1H	3462	1/1	0.94	0.08	46,46,46,46	0
59	MG	78	201	1/1	0.94	0.30	32,32,32,32	0
59	MG	14	3132	1/1	0.94	0.05	47,47,47,47	0
59	MG	1H	3254	1/1	0.94	0.16	50,50,50,50	0
59	MG	1H	3267	1/1	0.94	0.14	60,60,60,60	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
59	MG	13	1641	1/1	0.94	0.15	90,90,90,90	0
59	MG	1G	1660	1/1	0.94	0.18	79,79,79,79	0
59	MG	1G	1627	1/1	0.94	0.25	88,88,88,88	0
58	K	13	1604	1/1	0.94	0.11	90,90,90,90	0
58	K	14	3018	1/1	0.94	0.09	71,71,71,71	0
58	K	1H	3059	1/1	0.94	0.06	38,38,38,38	0
59	MG	I8	102	1/1	0.94	0.07	72,72,72,72	0
59	MG	1H	3399	1/1	0.94	0.15	54,54,54,54	0
59	MG	14	3149	1/1	0.94	0.16	46,46,46,46	0
59	MG	16	206	1/1	0.94	0.23	62,62,62,62	0
59	MG	1H	3142	1/1	0.94	0.17	71,71,71,71	0
59	MG	13	1743	1/1	0.94	0.04	105,105,105,105	0
59	MG	14	3400	1/1	0.94	0.07	92,92,92,92	0
58	K	14	3045	1/1	0.94	0.09	71,71,71,71	0
59	MG	1H	3149	1/1	0.94	0.16	29,29,29,29	0
59	MG	14	3299	1/1	0.94	0.05	57,57,57,57	0
59	MG	1H	3147	1/1	0.94	0.12	19,19,19,19	0
59	MG	13	1703	1/1	0.94	0.35	69,69,69,69	0
59	MG	14	3177	1/1	0.94	0.15	64,64,64,64	0
58	K	1H	3047	1/1	0.94	0.19	37,37,37,37	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
59	MG	1H	3224	1/1	0.94	0.13	51,51,51,51	0
59	MG	14	3313	1/1	0.94	0.05	89,89,89,89	0
59	MG	1H	3193	1/1	0.94	0.23	43,43,43,43	0
58	K	1G	1623	1/1	0.94	0.10	126,126,126,126	0
58	K	13	1619	1/1	0.94	0.05	77,77,77,77	0
58	K	8I	201	1/1	0.94	0.10	104,104,104,104	0
59	MG	14	3205	1/1	0.94	0.10	37,37,37,37	0
58	K	13	1626	1/1	0.94	0.22	99,99,99,99	0
58	K	1H	3116	1/1	0.94	0.06	80,80,80,80	0
59	MG	13	1727	1/1	0.94	0.08	47,47,47,47	0
58	K	14	3023	1/1	0.94	0.16	93,93,93,93	0
58	K	1H	3101	1/1	0.94	0.08	60,60,60,60	0
59	MG	14	3142	1/1	0.94	0.23	62,62,62,62	0
59	MG	14	3287	1/1	0.94	0.06	50,50,50,50	0
59	MG	1G	1726	1/1	0.94	0.05	98,98,98,98	0
59	MG	14	3364	1/1	0.94	0.14	71,71,71,71	0
59	MG	14	3179	1/1	0.94	0.15	66,66,66,66	0
59	MG	14	3166	1/1	0.94	0.12	37,37,37,37	0
59	MG	1H	3367	1/1	0.94	0.10	61,61,61,61	0
59	MG	1H	3247	1/1	0.94	0.20	44,44,44,44	0
59	MG	1H	3517	1/1	0.94	0.07	55,55,55,55	0
59	MG	13	1639	1/1	0.94	0.13	62,62,62,62	0
59	MG	1H	3143	1/1	0.94	0.15	63,63,63,63	0
59	MG	14	3147	1/1	0.94	0.12	54,54,54,54	0
59	MG	1H	3132	1/1	0.94	0.28	58,58,58,58	0
58	K	13	1631	1/1	0.94	0.12	93,93,93,93	0
59	MG	14	3199	1/1	0.94	0.19	105,105,105,105	0
58	K	1G	1620	1/1	0.94	0.10	101,101,101,101	0
59	MG	1H	3349	1/1	0.94	0.08	28,28,28,28	0
59	MG	D8	202	1/1	0.94	0.10	52,52,52,52	0
58	K	1H	3100	1/1	0.94	0.19	78,78,78,78	0
58	K	1H	3023	1/1	0.94	0.10	68,68,68,68	0
59	MG	13	1704	1/1	0.94	0.15	53,53,53,53	0
59	MG	1G	1719	1/1	0.94	0.11	101,101,101,101	0
59	MG	1H	3378	1/1	0.95	0.08	30,30,30,30	0
59	MG	1H	3342	1/1	0.95	0.10	50,50,50,50	0
59	MG	1G	1715	1/1	0.95	0.04	92,92,92,92	0
59	MG	13	1649	1/1	0.95	0.22	101,101,101,101	0
59	MG	14	3258	1/1	0.95	0.07	37,37,37,37	0
59	MG	1G	1689	1/1	0.95	0.06	90,90,90,90	0
59	MG	14	3204	1/1	0.95	0.09	44,44,44,44	0
59	MG	13	1677	1/1	0.95	0.07	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	14	3064	1/1	0.95	0.17	70,70,70,70	0
59	MG	1H	3197	1/1	0.95	0.08	50,50,50,50	0
59	MG	14	3182	1/1	0.95	0.09	42,42,42,42	0
59	MG	1H	3129	1/1	0.95	0.21	34,34,34,34	0
59	MG	1G	1713	1/1	0.95	0.12	80,80,80,80	0
59	MG	1G	1699	1/1	0.95	0.11	101,101,101,101	0
59	MG	14	3127	1/1	0.95	0.12	41,41,41,41	0
59	MG	13	1711	1/1	0.95	0.25	48,48,48,48	0
58	K	14	3086	1/1	0.95	0.25	97,97,97,97	0
58	K	1H	3036	1/1	0.95	0.07	55,55,55,55	0
58	K	1H	3056	1/1	0.95	0.09	43,43,43,43	0
59	MG	14	3349	1/1	0.95	0.04	77,77,77,77	0
59	MG	14	3167	1/1	0.95	0.29	60,60,60,60	0
58	K	14	3033	1/1	0.95	0.23	84,84,84,84	0
58	K	14	3078	1/1	0.95	0.15	98,98,98,98	0
59	MG	14	3136	1/1	0.95	0.22	77,77,77,77	0
59	MG	14	3121	1/1	0.95	0.12	43,43,43,43	0
59	MG	2K	101	1/1	0.95	0.23	42,42,42,42	0
59	MG	1G	1657	1/1	0.95	0.17	74,74,74,74	0
59	MG	1H	3269	1/1	0.95	0.13	54,54,54,54	0
59	MG	14	3184	1/1	0.95	0.14	73,73,73,73	0
59	MG	1H	3154	1/1	0.95	0.14	31,31,31,31	0
59	MG	14	3339	1/1	0.95	0.03	77,77,77,77	0
58	K	14	3066	1/1	0.95	0.18	80,80,80,80	0
59	MG	1H	3250	1/1	0.95	0.19	47,47,47,47	0
59	MG	1G	1645	1/1	0.95	0.12	40,40,40,40	0
59	MG	1H	3264	1/1	0.95	0.25	47,47,47,47	0
59	MG	14	3317	1/1	0.95	0.08	94,94,94,94	0
59	MG	1H	3176	1/1	0.95	0.19	32,32,32,32	0
58	K	1H	3029	1/1	0.95	0.07	104,104,104,104	0
59	MG	14	3286	1/1	0.95	0.09	47,47,47,47	0
59	MG	13	1654	1/1	0.95	0.15	36,36,36,36	0
58	K	14	3016	1/1	0.95	0.10	72,72,72,72	0
59	MG	14	3150	1/1	0.95	0.25	63,63,63,63	0
59	MG	1H	3308	1/1	0.95	0.19	55,55,55,55	0
59	MG	14	3255	1/1	0.95	0.18	52,52,52,52	0
59	MG	1G	1682	1/1	0.95	0.08	60,60,60,60	0
59	MG	1G	1701	1/1	0.95	0.08	108,108,108,108	0
59	MG	1H	3473	1/1	0.95	0.11	27,27,27,27	0
59	MG	41	203	1/1	0.95	0.12	40,40,40,40	0
59	MG	13	1725	1/1	0.95	0.05	116,116,116,116	0
59	MG	14	3298	1/1	0.95	0.05	54,54,54,54	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
59	MG	14	3216	1/1	0.95	0.09	42,42,42,42	0
58	K	14	3090	1/1	0.95	0.07	65,65,65,65	0
59	MG	14	3133	1/1	0.95	0.19	50,50,50,50	0
59	MG	1H	3494	1/1	0.95	0.07	78,78,78,78	0
59	MG	1H	3214	1/1	0.95	0.17	26,26,26,26	0
59	MG	13	1648	1/1	0.95	0.17	61,61,61,61	0
59	MG	14	3192	1/1	0.95	0.20	63,63,63,63	0
59	MG	14	3125	1/1	0.95	0.10	45,45,45,45	0
58	K	14	3004	1/1	0.95	0.12	55,55,55,55	0
59	MG	14	3119	1/1	0.95	0.15	51,51,51,51	0
58	K	14	3020	1/1	0.95	0.05	72,72,72,72	0
58	K	1H	3045	1/1	0.95	0.07	72,72,72,72	0
59	MG	13	1675	1/1	0.95	0.16	91,91,91,91	0
59	MG	1H	3469	1/1	0.95	0.09	87,87,87,87	0
59	MG	1H	3150	1/1	0.95	0.32	76,76,76,76	0
58	K	1H	3108	1/1	0.95	0.17	86,86,86,86	0
58	K	13	1612[A]	1/1	0.95	0.24	35,35,35,35	1
59	MG	16	208	1/1	0.95	0.11	63,63,63,63	0
59	MG	14	3218	1/1	0.95	0.11	66,66,66,66	0
58	K	13	1612[B]	1/1	0.95	0.24	23,23,23,23	1
59	MG	1G	1629	1/1	0.95	0.12	69,69,69,69	0
59	MG	13	1645	1/1	0.95	0.14	71,71,71,71	0
59	MG	1H	3294	1/1	0.95	0.14	35,35,35,35	0
59	MG	14	3397	1/1	0.95	0.08	46,46,46,46	0
59	MG	8E	201	1/1	0.95	0.26	49,49,49,49	0
58	K	13	1617	1/1	0.95	0.16	72,72,72,72	0
59	MG	14	3278	1/1	0.95	0.10	43,43,43,43	0
59	MG	1G	1677	1/1	0.95	0.08	76,76,76,76	0
59	MG	13	1693	1/1	0.95	0.16	78,78,78,78	0
58	K	1H	3097	1/1	0.95	0.12	69,69,69,69	0
59	MG	14	3232	1/1	0.95	0.07	69,69,69,69	0
59	MG	14	3212	1/1	0.95	0.12	34,34,34,34	0
59	MG	1H	3321	1/1	0.95	0.15	55,55,55,55	0
59	MG	14	3120	1/1	0.95	0.08	44,44,44,44	0
59	MG	13	1722	1/1	0.95	0.15	77,77,77,77	0
59	MG	1H	3261	1/1	0.95	0.34	49,49,49,49	0
59	MG	1H	3451	1/1	0.95	0.05	63,63,63,63	0
59	MG	1H	3343	1/1	0.95	0.12	35,35,35,35	0
59	MG	1H	3405	1/1	0.95	0.06	50,50,50,50	0
59	MG	1H	3460	1/1	0.95	0.06	62,62,62,62	0
59	MG	1H	3256	1/1	0.95	0.15	47,47,47,47	0
59	MG	1H	3249	1/1	0.95	0.23	53,53,53,53	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
59	MG	13	1747	1/1	0.95	0.07	91,91,91,91	0
59	MG	13	1694	1/1	0.95	0.09	43,43,43,43	0
59	MG	1H	3421	1/1	0.95	0.06	80,80,80,80	0
59	MG	13	1674	1/1	0.95	0.19	92,92,92,92	0
59	MG	13	1686	1/1	0.95	0.22	95,95,95,95	0
58	K	13	1622	1/1	0.95	0.10	73,73,73,73	0
59	MG	14	3257	1/1	0.95	0.13	48,48,48,48	0
59	MG	14	3219	1/1	0.95	0.07	45,45,45,45	0
59	MG	14	3337	1/1	0.95	0.08	66,66,66,66	0
59	MG	14	3229	1/1	0.95	0.19	65,65,65,65	0
59	MG	13	1724	1/1	0.95	0.09	80,80,80,80	0
59	MG	1H	3281	1/1	0.95	0.12	93,93,93,93	0
59	MG	1H	3445	1/1	0.95	0.06	42,42,42,42	0
59	MG	14	3292	1/1	0.95	0.07	49,49,49,49	0
58	K	1H	3078	1/1	0.95	0.14	61,61,61,61	0
58	K	14	3044	1/1	0.96	0.11	95,95,95,95	0
59	MG	1H	3125	1/1	0.96	0.20	41,41,41,41	0
59	MG	1H	3263	1/1	0.96	0.22	33,33,33,33	0
59	MG	14	3098	1/1	0.96	0.15	38,38,38,38	0
58	K	13	1618	1/1	0.96	0.14	90,90,90,90	0
59	MG	1H	3229	1/1	0.96	0.08	51,51,51,51	0
59	MG	14	3268	1/1	0.96	0.07	79,79,79,79	0
59	MG	1H	3401	1/1	0.96	0.03	73,73,73,73	0
59	MG	1G	1678	1/1	0.96	0.15	71,71,71,71	0
58	K	21	302	1/1	0.96	0.07	66,66,66,66	0
59	MG	14	3163	1/1	0.96	0.08	48,48,48,48	0
59	MG	13	1681	1/1	0.96	0.13	76,76,76,76	0
59	MG	14	3095	1/1	0.96	0.22	57,57,57,57	0
59	MG	14	3118	1/1	0.96	0.23	53,53,53,53	0
59	MG	14	3342	1/1	0.96	0.11	54,54,54,54	0
59	MG	14	3284	1/1	0.96	0.08	39,39,39,39	0
59	MG	14	3238	1/1	0.96	0.10	42,42,42,42	0
59	MG	14	3220	1/1	0.96	0.09	53,53,53,53	0
59	MG	13	1660	1/1	0.96	0.14	60,60,60,60	0
59	MG	1H	3297	1/1	0.96	0.27	52,52,52,52	0
59	MG	14	3253	1/1	0.96	0.20	52,52,52,52	0
58	K	1H	3022	1/1	0.96	0.06	51,51,51,51	0
59	MG	14	3294	1/1	0.96	0.06	77,77,77,77	0
58	K	1H	3054	1/1	0.96	0.20	68,68,68,68	0
59	MG	13	1716	1/1	0.96	0.05	66,66,66,66	0
59	MG	1H	3334	1/1	0.96	0.27	55,55,55,55	0
58	K	1H	3028	1/1	0.96	0.13	50,50,50,50	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
58	K	1H	3027	1/1	0.96	0.16	91,91,91,91	0
59	MG	1H	3453	1/1	0.96	0.05	67,67,67,67	0
59	MG	1H	3210	1/1	0.96	0.12	50,50,50,50	0
59	MG	1H	3314	1/1	0.96	0.10	49,49,49,49	0
58	K	14	3051	1/1	0.96	0.11	93,93,93,93	0
59	MG	14	3282	1/1	0.96	0.09	50,50,50,50	0
59	MG	1H	3187	1/1	0.96	0.09	37,37,37,37	0
59	MG	1H	3255	1/1	0.96	0.19	36,36,36,36	0
59	MG	14	3099	1/1	0.96	0.14	32,32,32,32	0
58	K	14	3010	1/1	0.96	0.12	53,53,53,53	0
59	MG	1H	3172	1/1	0.96	0.16	48,48,48,48	0
59	MG	1H	3164	1/1	0.96	0.08	45,45,45,45	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	1H	3148	1/1	0.96	0.18	39,39,39,39	0
59	MG	1G	1721	1/1	0.96	0.06	88,88,88,88	0
59	MG	1H	3298	1/1	0.96	0.13	23,23,23,23	0
59	MG	14	3107	1/1	0.96	0.14	40,40,40,40	0
58	K	1H	3080	1/1	0.96	0.10	51,51,51,51	0
59	MG	1G	1667	1/1	0.96	0.22	60,60,60,60	0
58	K	14	3068	1/1	0.96	0.13	48,48,48,48	0
59	MG	1H	3383	1/1	0.96	0.07	54,54,54,54	0
59	MG	14	3137	1/1	0.96	0.10	83,83,83,83	0
59	MG	14	3329	1/1	0.96	0.10	70,70,70,70	0
59	MG	1H	3433	1/1	0.96	0.11	44,44,44,44	0
59	MG	1H	3510	1/1	0.96	0.05	80,80,80,80	0
59	MG	32	302	1/1	0.96	0.10	92,92,92,92	0
58	K	1H	3006	1/1	0.96	0.07	59,59,59,59	0
58	K	14	3025	1/1	0.96	0.09	97,97,97,97	0
58	K	1G	1618	1/1	0.96	0.11	102,102,102,102	0
59	MG	G8	201	1/1	0.96	0.08	89,89,89,89	0
59	MG	14	3215	1/1	0.96	0.15	45,45,45,45	0
59	MG	1H	3135	1/1	0.96	0.08	50,50,50,50	0
58	K	14	3070	1/1	0.96	0.13	95,95,95,95	0
59	MG	1G	1720	1/1	0.96	0.07	106,106,106,106	0
59	MG	14	3109	1/1	0.96	0.07	36,36,36,36	0
59	MG	14	3330	1/1	0.96	0.06	48,48,48,48	0
59	MG	1H	3413	1/1	0.96	0.06	42,42,42,42	0
59	MG	13	1643	1/1	0.96	0.18	76,76,76,76	0
58	K	1G	1603	1/1	0.96	0.17	79,79,79,79	0
59	MG	14	3165	1/1	0.96	0.16	70,70,70,70	0
59	MG	1G	1666	1/1	0.96	0.22	77,77,77,77	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
59	MG	14	3153	1/1	0.96	0.15	68,68,68,68	0
59	MG	14	3363	1/1	0.96	0.07	85,85,85,85	0
59	MG	13	1708	1/1	0.96	0.21	59,59,59,59	0
59	MG	14	3331	1/1	0.96	0.07	58,58,58,58	0
59	MG	1H	3213	1/1	0.96	0.12	73,73,73,73	0
59	MG	14	3311	1/1	0.96	0.07	56,56,56,56	0
59	MG	1H	3295	1/1	0.96	0.17	46,46,46,46	0
59	MG	14	3320	1/1	0.96	0.12	90,90,90,90	0
58	K	1H	3081	1/1	0.96	0.17	66,66,66,66	0
61	ZN	5A	101	1/1	0.96	0.11	115,115,115,115	0
59	MG	1H	3491	1/1	0.96	0.07	51,51,51,51	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	13	1650	1/1	0.96	0.14	73,73,73,73	0
58	K	14	3032	1/1	0.96	0.07	61,61,61,61	0
58	K	1H	3095	1/1	0.96	0.06	44,44,44,44	0
59	MG	1H	3287	1/1	0.96	0.13	43,43,43,43	0
59	MG	14	3160	1/1	0.96	0.19	73,73,73,73	0
59	MG	1H	3407	1/1	0.96	0.04	65,65,65,65	0
58	K	1G	1621	1/1	0.96	0.08	74,74,74,74	0
59	MG	14	3164	1/1	0.96	0.15	70,70,70,70	0
59	MG	1H	3458	1/1	0.96	0.04	89,89,89,89	0
58	K	31	302	1/1	0.96	0.12	90,90,90,90	0
59	MG	14	3161	1/1	0.96	0.14	44,44,44,44	0
58	K	29	302	1/1	0.96	0.07	89,89,89,89	0
59	MG	14	3259	1/1	0.96	0.07	45,45,45,45	0
59	MG	14	3333	1/1	0.96	0.08	39,39,39,39	0
59	MG	1H	3270	1/1	0.96	0.10	37,37,37,37	0
59	MG	13	1668	1/1	0.96	0.10	41,41,41,41	0
59	MG	1G	1662	1/1	0.96	0.17	74,74,74,74	0
59	MG	1H	3205	1/1	0.96	0.06	34,34,34,34	0
59	MG	14	3096	1/1	0.96	0.15	59,59,59,59	0
58	K	14	3038	1/1	0.97	0.16	63,63,63,63	0
59	MG	1G	1669	1/1	0.97	0.09	72,72,72,72	0
59	MG	1G	1708	1/1	0.97	0.07	69,69,69,69	0
59	MG	14	3138	1/1	0.97	0.14	40,40,40,40	0
58	K	14	3071	1/1	0.97	0.30	75,75,75,75	0
59	MG	14	3266	1/1	0.97	0.18	74,74,74,74	0
59	MG	14	3144	1/1	0.97	0.10	50,50,50,50	0
59	MG	1H	3202	1/1	0.97	0.17	46,46,46,46	0
59	MG	14	3170	1/1	0.97	0.18	52,52,52,52	0
59	MG	13	1720	1/1	0.97	0.04	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	3285	1/1	0.97	0.08	43,43,43,43	0
59	MG	1G	1680	1/1	0.97	0.05	90,90,90,90	0
59	MG	1H	3124	1/1	0.97	0.22	28,28,28,28	0
58	K	14	3072	1/1	0.97	0.05	89,89,89,89	0
59	MG	1H	3220	1/1	0.97	0.14	45,45,45,45	0
59	MG	14	3211	1/1	0.97	0.21	64,64,64,64	0
58	K	14	3060	1/1	0.97	0.03	67,67,67,67	0
59	MG	14	3159	1/1	0.97	0.21	53,53,53,53	0
59	MG	13	1705	1/1	0.97	0.21	60,60,60,60	0
59	MG	1H	3300	1/1	0.97	0.21	31,31,31,31	0
58	K	1H	3049	1/1	0.97	0.11	66,66,66,66	0
59	MG	13	1647	1/1	0.97	0.20	59,59,59,59	0
58	K	14	3081	1/1	0.97	0.14	89,89,89,89	0
59	MG	1G	1638	1/1	0.97	0.10	43,43,43,43	0
59	MG	1H	3381	1/1	0.97	0.11	59,59,59,59	0
59	MG	14	3168	1/1	0.97	0.04	37,37,37,37	0
58	K	1H	3074	1/1	0.97	0.10	53,53,53,53	0
59	MG	1H	3443	1/1	0.97	0.02	61,61,61,61	0
59	MG	13	1661	1/1	0.97	0.07	42,42,42,42	0
58	K	1H	3098	1/1	0.97	0.08	67,67,67,67	0
59	MG	14	3237	1/1	0.97	0.12	58,58,58,58	0
59	MG	1H	3141	1/1	0.97	0.17	37,37,37,37	0
59	MG	1H	3218	1/1	0.97	0.20	53,53,53,53	0
59	MG	14	3228	1/1	0.97	0.23	88,88,88,88	0
59	MG	14	3319	1/1	0.97	0.07	59,59,59,59	0
59	MG	14	3326	1/1	0.97	0.07	45,45,45,45	0
58	K	1H	3083	1/1	0.97	0.08	43,43,43,43	0
58	K	1H	3107	1/1	0.97	0.09	82,82,82,82	0
59	MG	14	3223	1/1	0.97	0.06	53,53,53,53	0
59	MG	14	3367	1/1	0.97	0.06	52,52,52,52	0
59	MG	1G	1679	1/1	0.97	0.07	64,64,64,64	0
59	MG	1H	3497	1/1	0.97	0.07	83,83,83,83	0
59	MG	14	3146	1/1	0.97	0.09	30,30,30,30	0
59	MG	1H	3420	1/1	0.97	0.02	95,95,95,95	0
59	MG	1H	3376	1/1	0.97	0.12	29,29,29,29	0
59	MG	1H	3485	1/1	0.97	0.12	27,27,27,27	0
59	MG	14	3264	1/1	0.97	0.21	55,55,55,55	0
58	K	14	3011	1/1	0.97	0.07	56,56,56,56	0
59	MG	14	3236	1/1	0.97	0.14	41,41,41,41	0
59	MG	14	3241	1/1	0.97	0.10	34,34,34,34	0
59	MG	14	3316	1/1	0.97	0.07	53,53,53,53	0
59	MG	1H	3206	1/1	0.97	0.08	35,35,35,35	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
59	MG	1G	1636	1/1	0.97	0.22	89,89,89,89	0
58	K	1H	3111	1/1	0.97	0.15	75,75,75,75	0
59	MG	1H	3189	1/1	0.97	0.17	46,46,46,46	0
59	MG	14	3158	1/1	0.97	0.08	35,35,35,35	0
59	MG	1H	3217	1/1	0.97	0.27	52,52,52,52	0
59	MG	J8	101	1/1	0.97	0.05	49,49,49,49	0
59	MG	1H	3171	1/1	0.97	0.19	28,28,28,28	0
58	K	1H	3077	1/1	0.97	0.08	49,49,49,49	0
58	K	1H	3051	1/1	0.97	0.06	58,58,58,58	0
59	MG	14	3405	1/1	0.97	0.06	45,45,45,45	0
59	MG	14	3388	1/1	0.97	0.05	53,53,53,53	0
59	MG	1G	1637	1/1	0.97	0.21	77,77,77,77	0
58	K	1H	3046	1/1	0.97	0.10	50,50,50,50	0
58	K	19	301	1/1	0.97	0.18	61,61,61,61	0
59	MG	14	3122	1/1	0.97	0.13	49,49,49,49	0
59	MG	1H	3245	1/1	0.97	0.16	41,41,41,41	0
58	K	14	3006	1/1	0.97	0.14	62,62,62,62	0
59	MG	14	3126	1/1	0.97	0.22	69,69,69,69	0
59	MG	13	1646	1/1	0.97	0.19	59,59,59,59	0
59	MG	1G	1675	1/1	0.97	0.07	54,54,54,54	0
59	MG	14	3180	1/1	0.97	0.16	40,40,40,40	0
59	MG	1H	3422	1/1	0.97	0.05	43,43,43,43	0
59	MG	13	1719	1/1	0.97	0.05	112,112,112,112	0
59	MG	14	3105	1/1	0.97	0.25	36,36,36,36	0
59	MG	14	3403	1/1	0.97	0.07	75,75,75,75	0
58	K	14	3046	1/1	0.97	0.10	68,68,68,68	0
59	MG	1H	3152	1/1	0.97	0.15	37,37,37,37	0
58	K	13	1611	1/1	0.97	0.05	79,79,79,79	0
59	MG	1H	3410	1/1	0.97	0.05	86,86,86,86	0
59	MG	13	1638	1/1	0.97	0.15	58,58,58,58	0
59	MG	1H	3127	1/1	0.97	0.19	54,54,54,54	0
59	MG	14	3324	1/1	0.97	0.05	62,62,62,62	0
59	MG	1H	3128	1/1	0.97	0.18	40,40,40,40	0
58	K	13	1616	1/1	0.97	0.08	96,96,96,96	0
58	K	14	3007	1/1	0.97	0.20	52,52,52,52	0
59	MG	1H	3253	1/1	0.98	0.09	53,53,53,53	0
59	MG	13	1667	1/1	0.98	0.23	39,39,39,39	0
58	K	1H	3073	1/1	0.98	0.09	47,47,47,47	0
59	MG	1H	3346	1/1	0.98	0.16	27,27,27,27	0
58	K	1H	3115	1/1	0.98	0.04	50,50,50,50	0
59	MG	14	3097	1/1	0.98	0.13	38,38,38,38	0
59	MG	1H	3185	1/1	0.98	0.10	41,41,41,41	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
59	MG	14	3271	1/1	0.98	0.07	52,52,52,52	0
59	MG	14	3114	1/1	0.98	0.17	57,57,57,57	0
58	K	1H	3058	1/1	0.98	0.06	56,56,56,56	0
59	MG	13	1651	1/1	0.98	0.19	51,51,51,51	0
59	MG	13	1657	1/1	0.98	0.13	26,26,26,26	0
58	K	14	3073	1/1	0.98	0.18	81,81,81,81	0
59	MG	14	3227	1/1	0.98	0.06	41,41,41,41	0
58	K	1H	3070	1/1	0.98	0.08	54,54,54,54	0
59	MG	14	3135	1/1	0.98	0.12	42,42,42,42	0
59	MG	1H	3162	1/1	0.98	0.23	21,21,21,21	0
59	MG	1H	3158	1/1	0.98	0.26	89,89,89,89	0
59	MG	1G	1655	1/1	0.98	0.27	67,67,67,67	0
58	K	11	301	1/1	0.98	0.05	47,47,47,47	0
59	MG	1H	3131	1/1	0.98	0.21	42,42,42,42	0
59	MG	13	1717	1/1	0.98	0.07	66,66,66,66	0
59	MG	13	1748	1/1	0.98	0.08	104,104,104,104	0
59	MG	1G	1640	1/1	0.98	0.16	53,53,53,53	0
58	K	14	3053	1/1	0.98	0.08	63,63,63,63	0
58	K	14	3021	1/1	0.98	0.06	47,47,47,47	0
59	MG	1H	3384	1/1	0.98	0.05	60,60,60,60	0
58	K	1H	3053	1/1	0.98	0.13	63,63,63,63	0
59	MG	14	3207	1/1	0.98	0.16	58,58,58,58	0
59	MG	1H	3251	1/1	0.98	0.07	52,52,52,52	0
59	MG	1H	3166	1/1	0.98	0.15	17,17,17,17	0
59	MG	1H	3145	1/1	0.98	0.18	32,32,32,32	0
59	MG	1G	1653	1/1	0.98	0.17	52,52,52,52	0
61	ZN	5I	102	1/1	0.98	0.11	110,110,110,110	0
59	MG	1H	3356	1/1	0.98	0.07	31,31,31,31	0
59	MG	21	303	1/1	0.98	0.15	30,30,30,30	0
59	MG	1H	3272	1/1	0.98	0.17	60,60,60,60	0
59	MG	14	3336	1/1	0.98	0.07	47,47,47,47	0
59	MG	14	3354	1/1	0.98	0.06	70,70,70,70	0
59	MG	2L	101	1/1	0.98	0.14	55,55,55,55	0
59	MG	14	3328	1/1	0.98	0.06	66,66,66,66	0
58	K	1H	3062	1/1	0.98	0.07	42,42,42,42	0
59	MG	14	3116	1/1	0.98	0.15	41,41,41,41	0
59	MG	14	3194	1/1	0.98	0.12	64,64,64,64	0
59	MG	1H	3330	1/1	0.98	0.06	45,45,45,45	0
59	MG	14	3106	1/1	0.98	0.28	34,34,34,34	0
59	MG	1H	3144	1/1	0.98	0.10	38,38,38,38	0
59	MG	13	1672	1/1	0.98	0.15	24,24,24,24	0
59	MG	13	1652	1/1	0.98	0.33	95,95,95,95	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
59	MG	1H	3299	1/1	0.98	0.12	34,34,34,34	0
59	MG	1H	3353	1/1	0.98	0.03	53,53,53,53	0
59	MG	1H	3387	1/1	0.98	0.07	37,37,37,37	0
59	MG	1H	3268	1/1	0.98	0.13	50,50,50,50	0
59	MG	13	1673	1/1	0.98	0.20	56,56,56,56	0
59	MG	1H	3169	1/1	0.98	0.18	43,43,43,43	0
59	MG	14	3352	1/1	0.98	0.05	64,64,64,64	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
58	K	1H	3067	1/1	0.98	0.13	49,49,49,49	0
59	MG	1H	3303	1/1	0.98	0.12	41,41,41,41	0
59	MG	14	3108	1/1	0.98	0.15	62,62,62,62	0
59	MG	1H	3123	1/1	0.98	0.15	20,20,20,20	0
59	MG	1H	3411	1/1	0.98	0.07	28,28,28,28	0
59	MG	I8	101	1/1	0.98	0.13	48,48,48,48	0
59	MG	14	3247	1/1	0.98	0.20	60,60,60,60	0
59	MG	1H	3365	1/1	0.98	0.09	40,40,40,40	0
58	K	14	3019	1/1	0.98	0.09	81,81,81,81	0
59	MG	14	3187	1/1	0.98	0.12	41,41,41,41	0
58	K	1H	3068	1/1	0.98	0.05	37,37,37,37	0
59	MG	1G	1674	1/1	0.98	0.20	50,50,50,50	0
59	MG	1H	3165	1/1	0.98	0.20	30,30,30,30	0
59	MG	14	3104	1/1	0.98	0.18	29,29,29,29	0
58	K	14	3024	1/1	0.99	0.07	57,57,57,57	0
59	MG	1H	3266	1/1	0.99	0.31	40,40,40,40	0
59	MG	13	1644	1/1	0.99	0.08	49,49,49,49	0
59	MG	14	3224	1/1	0.99	0.05	53,53,53,53	0
59	MG	14	3110	1/1	0.99	0.15	48,48,48,48	0
59	MG	1H	3234	1/1	0.99	0.24	33,33,33,33	0
59	MG	1H	3364	1/1	0.99	0.08	28,28,28,28	0
59	MG	14	3189	1/1	0.99	0.24	26,26,26,26	0
60	SF4	32	303	8/8	0.99	0.19	73,95,102,116	0
59	MG	1H	3137	1/1	0.99	0.22	42,42,42,42	0
59	MG	1H	3209	1/1	0.99	0.16	33,33,33,33	0
59	MG	1H	3368	1/1	0.99	0.05	20,20,20,20	0
59	MG	1H	3146	1/1	0.99	0.18	24,24,24,24	0
59	MG	14	3128	1/1	0.99	0.14	35,35,35,35	0
59	MG	1H	3277	1/1	0.99	0.13	18,18,18,18	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
59	MG	1H	3163	1/1	0.99	0.23	40,40,40,40	0
59	MG	14	3117	1/1	0.99	0.15	42,42,42,42	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
59	MG	14	3111	1/1	0.99	0.06	44,44,44,44	0
59	MG	1H	3160	1/1	0.99	0.26	29,29,29,29	0
59	MG	1G	1632	1/1	0.99	0.21	109,109,109,109	0
59	MG	1H	3126	1/1	0.99	0.19	53,53,53,53	0
59	MG	13	1702	1/1	0.99	0.26	62,62,62,62	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	3357	1/1	0.99	0.05	34,34,34,34	0
59	MG	14	3301	1/1	0.99	0.04	53,53,53,53	0
59	MG	1G	1631	1/1	0.99	0.17	49,49,49,49	0
59	MG	13	1659	1/1	0.99	0.22	54,54,54,54	0

6.5 Other polymers [\(i\)](#)

There are no such residues in this entry.