



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 20, 2026 – 07:30 PM UTC

PDB ID : 4WSM / pdb_00004wsm
Title : Complex of 70S ribosome with tRNA-Leu and mRNA with G-U mismatch in the first position in the A- and P-sites
Authors : Rozov, A.; Demeshkina, N.; Yusupov, M.; Yusupova, G.
Deposited on : 2014-10-28
Resolution : 3.30 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

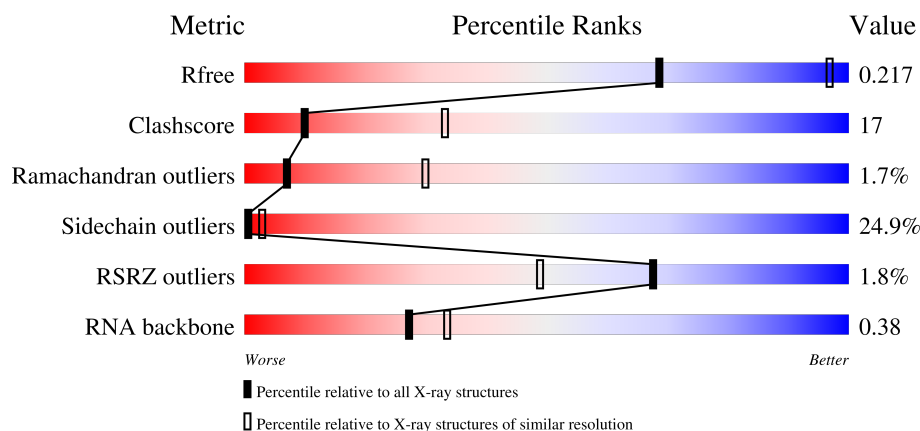
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.30 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1169 (3.32-3.28)
Clashscore	190562	1209 (3.32-3.28)
Ramachandran outliers	187476	1188 (3.32-3.28)
Sidechain outliers	187428	1187 (3.32-3.28)
RSRZ outliers	180081	1169 (3.32-3.28)
RNA backbone	3983	1048 (3.60-3.00)

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

Mol	Chain	Length	Quality of chain
1	13	1522	40% 46% 12% .
1	1G	1522	40% 44% 14% .
2	12	256	3% 38% 38% 17% 7%
2	1E	256	39% 42% 11% 7%

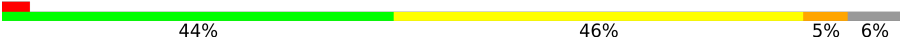
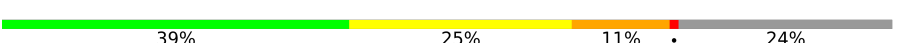
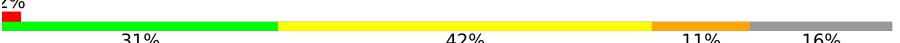
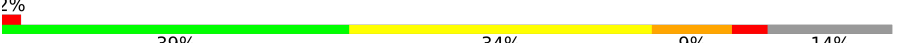
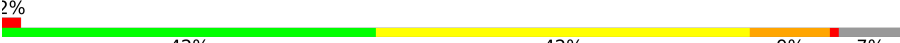
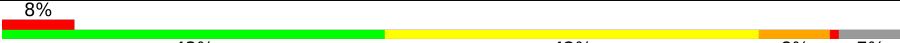
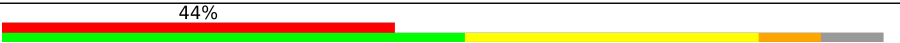
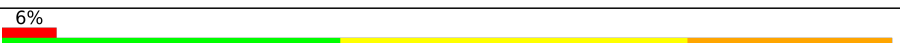
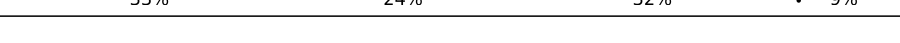
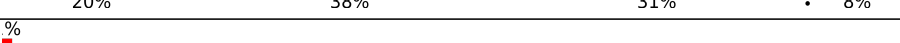
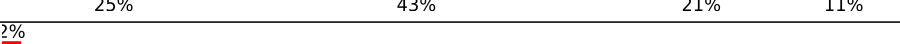
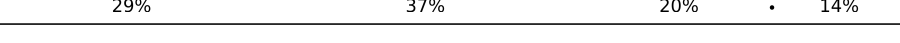
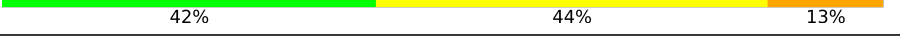
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Mol	Chain	Length	Quality of chain
3	22	239	
3	2E	239	
4	32	209	
4	3E	209	
5	42	162	
5	4E	162	
6	52	101	
6	5E	101	
7	62	156	
7	6E	156	
8	72	138	
8	7E	138	
9	82	128	
9	8E	128	
10	1A	105	
10	1I	105	
11	2A	129	
11	2I	129	
12	3A	132	
12	3I	132	
13	4A	126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

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Mol	Chain	Length	Quality of chain
15	6I	89	
16	7A	88	
16	7I	88	
17	8A	105	
17	8I	105	
18	9A	88	
18	9I	88	
19	AA	93	
19	AI	93	
20	BA	106	
20	BI	106	
21	1B	27	
21	1F	27	
22	1K	87	
22	1L	87	
23	2K	87	
23	2L	87	
24	3K	87	
24	3L	87	
25	4K	60	
25	4L	60	
26	14	2917	
26	1H	2917	
27	16	122	
27	1J	122	

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Mol	Chain	Length	Quality of chain
28	11	276	
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	15	140	
34	58	140	
35	25	122	
35	68	122	
36	35	150	
36	78	150	
37	45	141	
37	88	141	
38	55	118	
38	98	118	
39	65	112	
39	A8	112	
40	75	146	

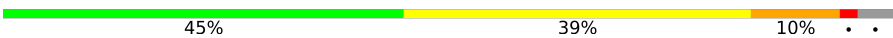
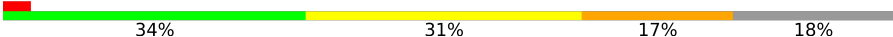
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Mol	Chain	Length	Quality of chain
40	B8	146	
41	85	118	
41	C8	118	
42	95	101	
42	D8	101	
43	A5	113	
43	E8	113	
44	B5	96	
44	F8	96	
45	C5	110	
45	G8	110	
46	D5	206	
46	H8	206	
47	E5	85	
47	I8	85	
48	F5	98	
48	J8	98	
49	G5	72	
49	K8	72	
50	H5	60	
50	L8	60	
51	I5	71	
51	M8	71	
52	J5	60	
52	N8	60	

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Mol	Chain	Length	Quality of chain
53	L5	49	
53	P8	49	
54	M5	65	
54	Q8	65	

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
55	MG	13	1715	-	-	-	X
55	MG	14	3270	-	-	-	X
55	MG	14	3290	-	-	-	X
55	MG	14	3335	-	-	-	X
55	MG	14	3350	-	-	-	X
55	MG	14	3360	-	-	-	X
55	MG	14	3387	-	-	-	X
55	MG	1G	1719	-	-	-	X
55	MG	1H	3126	-	-	-	X
55	MG	1H	3250	-	-	-	X
55	MG	1H	3356	-	-	-	X
55	MG	1H	3373	-	-	-	X

2 Entry composition

There are 57 unique types of molecules in this entry. The entry contains 299429 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a RNA chain called 16S ribosomal RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	13	1507	Total	C	N	O	P	0	0	0
			32389	14416	5999	10467	1507			
1	1G	1513	Total	C	N	O	P	0	0	0
			32511	14472	6018	10509	1512			

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

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

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

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

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

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

- Molecule 5 is a protein called 30S ribosomal protein S5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	4E	151	Total	C	N	O	S	0	0	0
			1155	729	218	204	4			
5	42	151	Total	C	N	O	S	0	0	0
			1155	729	218	204	4			

- Molecule 6 is a protein called 30S ribosomal protein S6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	5E	101	Total	C	N	O	S	0	0	0
			842	531	155	153	3			
6	52	101	Total	C	N	O	S	0	0	0
			842	531	155	153	3			

- Molecule 7 is a protein called 30S ribosomal protein S7.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	6E	144	Total	C	N	O	S	0	0	0
			1157	718	230	203	6			
7	62	147	Total	C	N	O	S	0	0	0
			1200	750	237	207	6			

- Molecule 8 is a protein called 30S ribosomal protein S8.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	7E	138	Total	C	N	O	S	0	0	0
			1115	705	215	192	3			
8	72	138	Total	C	N	O	S	0	0	0
			1115	705	215	192	3			

- Molecule 9 is a protein called 30S ribosomal protein S9.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	8E	127	Total	C	N	O		0	0	0
			1009	639	197	173				
9	82	124	Total	C	N	O		0	0	0
			983	624	190	169				

- Molecule 10 is a protein called 30S ribosomal protein S10.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	1I	99	Total	C	N	O	S	0	0	0
			801	504	157	139	1			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	1A	99	Total	C	N	O	S	0	0	0
			801	504	157	139	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	2I	116	Total	C	N	O	S	0	0	0
			864	537	164	160	3			
11	2A	116	Total	C	N	O	S	0	0	0
			864	537	164	160	3			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	3I	122	Total	C	N	O	S	0	0	0
			956	603	193	159	1			
12	3A	125	Total	C	N	O	S	0	0	0
			975	614	196	164	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	4I	116	Total	C	N	O	S	0	0	0
			928	574	191	161	2			
13	4A	116	Total	C	N	O	S	0	0	0
			928	574	191	161	2			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
14	5I	60	Total	C	N	O	S	0	0	0
			491	312	104	71	4			
14	5A	58	Total	C	N	O	S	0	0	0
			475	303	99	69	4			

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

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

- Molecule 16 is a protein called 30S ribosomal protein S16.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
16	7I	84	Total	C	N	O	S	0	0	0
			705	446	140	118	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
			823	528	151	142	2			

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
18	9I	67	Total	C	N	O	0	0	0
			550	352	107	91			
18	9A	69	Total	C	N	O	0	0	0
			564	361	110	93			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
19	AI	80	Total	C	N	O	S	0	0	0
			643	411	118	112	2			
19	AA	78	Total	C	N	O	S	0	0	0
			624	398	115	109	2			

- Molecule 20 is a protein called 30S ribosomal protein S20.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
20	BI	99	Total	C	N	O	S	0	0	0
			762	470	162	128	2			
20	BA	99	Total	C	N	O	S	0	0	0
			762	470	162	128	2			

- Molecule 21 is a protein called 30S ribosomal protein Thx.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
21	1F	23	Total	C	N	O	0	0	0
			199	122	48	29			
21	1B	25	Total	C	N	O	0	0	0
			217	134	52	31			

- Molecule 22 is a RNA chain called tRNA-Leu.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
22	1K	87	Total	C	N	O	P	0	0	0
			1863	831	333	612	87			
22	1L	87	Total	C	N	O	P	0	0	0
			1863	831	333	612	87			

- Molecule 23 is a RNA chain called tRNA-Leu.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
23	2K	79	Total	C	N	O	P	0	0	0
			1692	755	300	558	79			
23	2L	80	Total	C	N	O	P	0	0	0
			1712	764	303	565	80			

- Molecule 24 is a RNA chain called tRNA-Leu.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
24	3K	77	Total	C	N	O	P	0	0	0
			1646	733	292	544	77			
24	3L	75	Total	C	N	O	P	0	0	0
			1601	713	282	531	75			

- Molecule 25 is a RNA chain called mRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
25	4K	16	Total	C	N	O	P	0	0	0
			336	150	50	120	16			
25	4L	21	Total	C	N	O	P	0	0	0
			438	196	64	157	21			

- Molecule 26 is a RNA chain called 23S ribosomal RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
26	1H	2912	Total	C	N	O	P	0	0	0
			62707	27911	11722	20163	2911			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
26	14	2909	Total	C	N	O	P	0	0	0
			62647	27884	11716	20139	2908			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
1H	161	U	-	insertion	GB 48268
1H	493	G	-	insertion	GB 48268
1H	1228	G	-	insertion	GB 48268
14	161	U	-	insertion	GB 48268
14	493	G	-	insertion	GB 48268
14	1228	G	-	insertion	GB 48268

- Molecule 27 is a RNA chain called 5S ribosomal RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
27	16	122	Total	C	N	O	P	0	0	0
			2617	1166	486	844	121			
27	1J	122	Total	C	N	O	P	0	0	0
			2617	1166	486	844	121			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
28	11	273	Total	C	N	O	S	0	0	0
			2126	1341	424	358	3			
28	19	273	Total	C	N	O	S	0	0	0
			2120	1338	421	358	3			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
29	21	205	Total	C	N	O	S	0	0	0
			1568	991	300	271	6			
29	29	205	Total	C	N	O	S	0	0	0
			1568	991	300	271	6			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
30	31	202	Total	C	N	O	S	0	0	0
			1585	1011	297	275	2			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
30	39	208	Total	C	N	O	S	0	0	0
			1627	1037	304	283	3			

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
32	51	174	Total	C	N	O	S	0	0	0
			1336	848	251	236	1			
32	59	170	Total	C	N	O	S	0	0	0
			1307	829	245	232	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 L13.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
34	58	138	Total	C	N	O	S	0	0	0
			1104	712	206	182	4			
34	15	138	Total	C	N	O	S	0	0	0
			1104	712	206	182	4			

- Molecule 35 is a protein called 50S ribosomal protein L14.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
35	68	122	Total	C	N	O	S	0	0	0
			932	588	171	169	4			
35	25	122	Total	C	N	O	S	0	0	0
			932	588	171	169	4			

- Molecule 36 is a protein called 50S ribosomal protein L15.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
36	78	147	Total	C	N	O	S	0	0	0
			1122	698	229	192	3			
36	35	150	Total	C	N	O	S	0	0	0
			1144	712	232	197	3			

- Molecule 37 is a protein called 50S ribosomal protein L16.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
37	88	141	Total	C	N	O	S	0	0	0
			1121	715	212	187	7			
37	45	140	Total	C	N	O	S	0	0	0
			1113	710	211	186	6			

- Molecule 38 is a protein called 50S ribosomal protein L17.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
38	98	118	Total	C	N	O	S	0	0	0
			967	604	203	159	1			
38	55	117	Total	C	N	O		0	0	0
			959	599	202	158				

- Molecule 39 is a protein called 50S ribosomal protein L18.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
39	A8	111	Total	C	N	O	0	0	0
			881	556	176	149			
39	65	111	Total	C	N	O	0	0	0
			881	556	176	149			

- Molecule 40 is a protein called 50S ribosomal protein L19.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
40	B8	129	Total	C	N	O	S	0	0	0
			1081	674	223	183	1			
40	75	137	Total	C	N	O	S	0	0	0
			1141	710	234	196	1			

- Molecule 41 is a protein called 50S ribosomal protein L20.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
41	C8	117	Total	C	N	O	S	0	0	0
			963	610	202	150	1			
41	85	117	Total	C	N	O	S	0	0	0
			963	610	202	150	1			

- Molecule 42 is a protein called 50S ribosomal protein L21.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
42	D8	101	Total	C	N	O	S	0	0	0
			778	501	142	134	1			
42	95	101	Total	C	N	O	S	0	0	0
			778	501	142	134	1			

- Molecule 43 is a protein called 50S ribosomal protein L22.

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

- Molecule 44 is a protein called 50S ribosomal protein L23.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
44	F8	94	Total	C	N	O	S	0	0	0
			742	482	134	125	1			
44	B5	92	Total	C	N	O		0	0	0
			725	471	131	123				

- Molecule 45 is a protein called 50S ribosomal protein L24.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
45	G8	103	Total	C	N	O	S	0	0	0
			783	504	148	126	5			
45	C5	104	Total	C	N	O	S	0	0	0
			794	510	152	127	5			

- Molecule 46 is a protein called 50S ribosomal protein L25.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
46	H8	171	Total	C	N	O	S	0	0	0
			1373	876	247	247	3			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
46	D5	135	Total	C	N	O	S	0	0	0
			1120	720	202	195	3			

- Molecule 47 is a protein called 50S ribosomal protein L27.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
47	I8	83	Total	C	N	O	S	0	0	0
			656	407	139	109	1			
47	E5	80	Total	C	N	O	S	0	0	0
			627	388	132	106	1			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
I8	6	ALA	GLY	conflict	UNP P60493
I8	8	ALA	GLY	conflict	UNP P60493
E5	6	ALA	GLY	conflict	UNP P60493
E5	8	ALA	GLY	conflict	UNP P60493

- Molecule 48 is a protein called 50S ribosomal protein L28.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
48	J8	95	Total	C	N	O	S	0	0	0
			746	469	148	128	1			
48	F5	94	Total	C	N	O	S	0	0	0
			737	463	146	127	1			

- Molecule 49 is a protein called 50S ribosomal protein L29.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
49	K8	68	Total	C	N	O	S	0	0	0
			575	358	116	100	1			
49	G5	67	Total	C	N	O	S	0	0	0
			567	351	115	100	1			

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
50	L8	57	Total	C	N	O	0	0	0
			452	288	88	76			
50	H5	59	Total	C	N	O	0	0	0
			468	298	90	80			

- Molecule 51 is a protein called 50S ribosomal protein L31.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
51	M8	66	Total	C	N	O	S	0	0	0
			533	335	96	97	5			
51	I5	63	Total	C	N	O	S	0	0	0
			515	326	93	91	5			

- Molecule 52 is a protein called 50S ribosomal protein L32.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
52	N8	55	Total	C	N	O	S	0	0	0
			429	269	86	69	5			
52	J5	56	Total	C	N	O	S	0	0	0
			434	272	87	70	5			

- Molecule 53 is a protein called 50S ribosomal protein L34.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
53	P8	47	Total	C	N	O	S	0	0	0
			409	251	102	54	2			
53	L5	47	Total	C	N	O	S	0	0	0
			409	251	102	54	2			

- Molecule 54 is a protein called 50S ribosomal protein L35.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
54	Q8	60	Total	C	N	O	S	0	0	0
			480	306	98	74	2			
54	M5	53	Total	C	N	O	S	0	0	0
			422	270	87	63	2			

- Molecule 55 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
55	13	146	Total	Mg	0	0
			146	146		
55	3E	1	Total	Mg	0	0
			1	1		
55	5E	1	Total	Mg	0	0
			1	1		
55	3I	1	Total	Mg	0	0
			1	1		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
55	1K	1	Total 1	Mg 1	0	0
55	2K	3	Total 3	Mg 3	0	0
55	1H	512	Total 512	Mg 512	0	0
55	16	5	Total 5	Mg 5	0	0
55	11	1	Total 1	Mg 1	0	0
55	21	2	Total 2	Mg 2	0	0
55	31	1	Total 1	Mg 1	0	0
55	78	1	Total 1	Mg 1	0	0
55	88	4	Total 4	Mg 4	0	0
55	98	1	Total 1	Mg 1	0	0
55	G8	1	Total 1	Mg 1	0	0
55	I8	2	Total 2	Mg 2	0	0
55	J8	1	Total 1	Mg 1	0	0
55	P8	1	Total 1	Mg 1	0	0
55	1G	143	Total 143	Mg 143	0	0
55	32	1	Total 1	Mg 1	0	0
55	7A	1	Total 1	Mg 1	0	0
55	2L	2	Total 2	Mg 2	0	0
55	14	490	Total 490	Mg 490	0	0
55	1J	2	Total 2	Mg 2	0	0
55	29	3	Total 3	Mg 3	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
55	25	1	Total 1	Mg 1	0	0
55	45	2	Total 2	Mg 2	0	0
55	85	2	Total 2	Mg 2	0	0
55	E5	2	Total 2	Mg 2	0	0

- Molecule 56 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
56	3E	1	Total 1	Zn 1	0	0
56	5I	1	Total 1	Zn 1	0	0
56	G8	1	Total 1	Zn 1	0	0
56	32	1	Total 1	Zn 1	0	0
56	5A	1	Total 1	Zn 1	0	0
56	C5	1	Total 1	Zn 1	0	0

- Molecule 57 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
57	13	74	Total 74	O 74	0	0
57	3E	1	Total 1	O 1	0	0
57	6I	1	Total 1	O 1	0	0
57	BI	1	Total 1	O 1	0	0
57	1H	552	Total 552	O 552	0	0
57	11	1	Total 1	O 1	0	0
57	21	1	Total 1	O 1	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
57	31	4	Total 4	O 4	0	0
57	78	2	Total 2	O 2	0	0
57	B8	1	Total 1	O 1	0	0
57	C8	2	Total 2	O 2	0	0
57	D8	1	Total 1	O 1	0	0
57	E8	1	Total 1	O 1	0	0
57	I8	3	Total 3	O 3	0	0
57	J8	1	Total 1	O 1	0	0
57	P8	1	Total 1	O 1	0	0
57	1G	73	Total 73	O 73	0	0
57	6A	2	Total 2	O 2	0	0
57	7A	1	Total 1	O 1	0	0
57	4L	2	Total 2	O 2	0	0
57	14	520	Total 520	O 520	0	0
57	19	8	Total 8	O 8	0	0
57	29	2	Total 2	O 2	0	0
57	39	4	Total 4	O 4	0	0
57	35	1	Total 1	O 1	0	0
57	55	2	Total 2	O 2	0	0
57	85	1	Total 1	O 1	0	0
57	A5	1	Total 1	O 1	0	0

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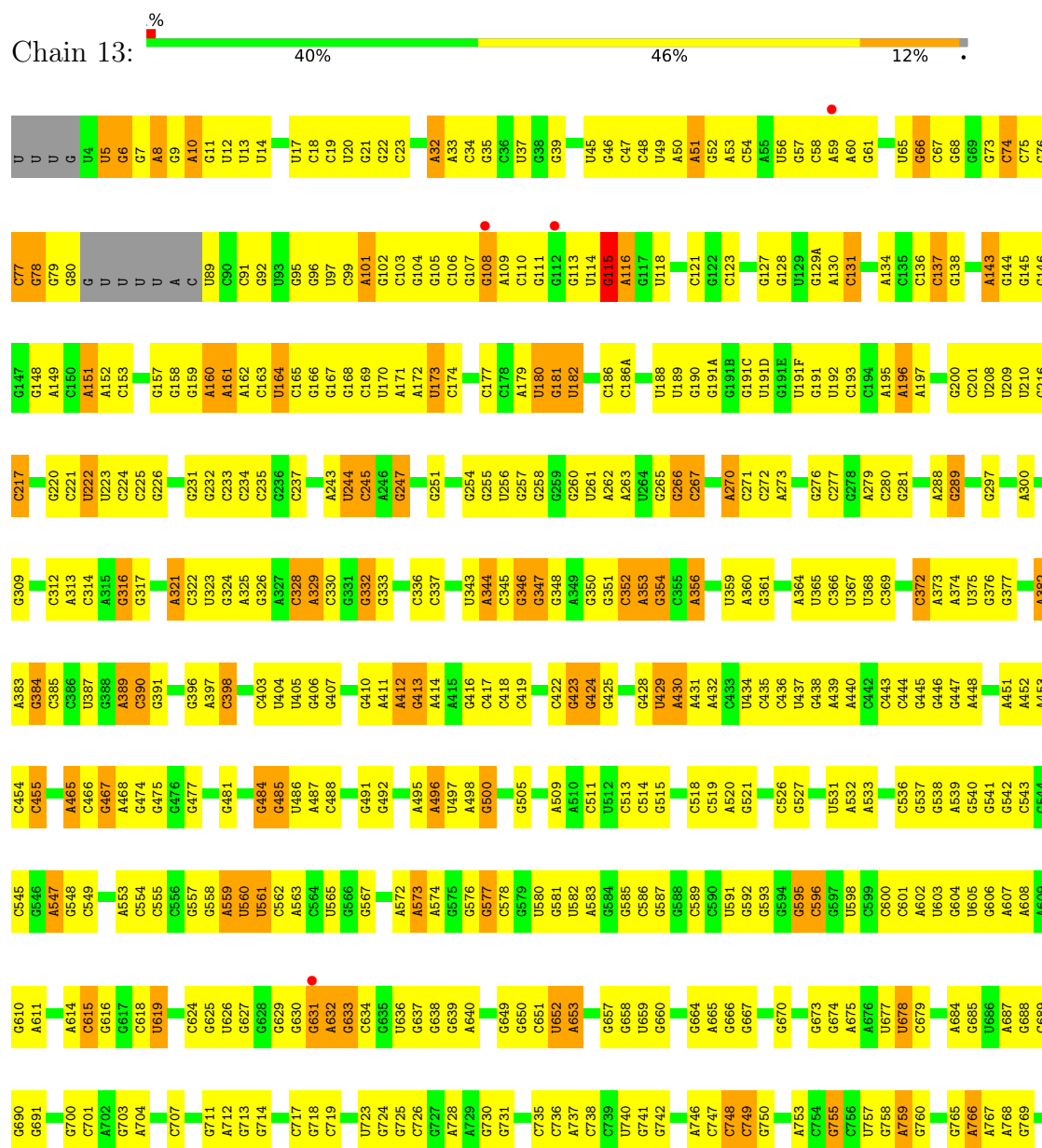
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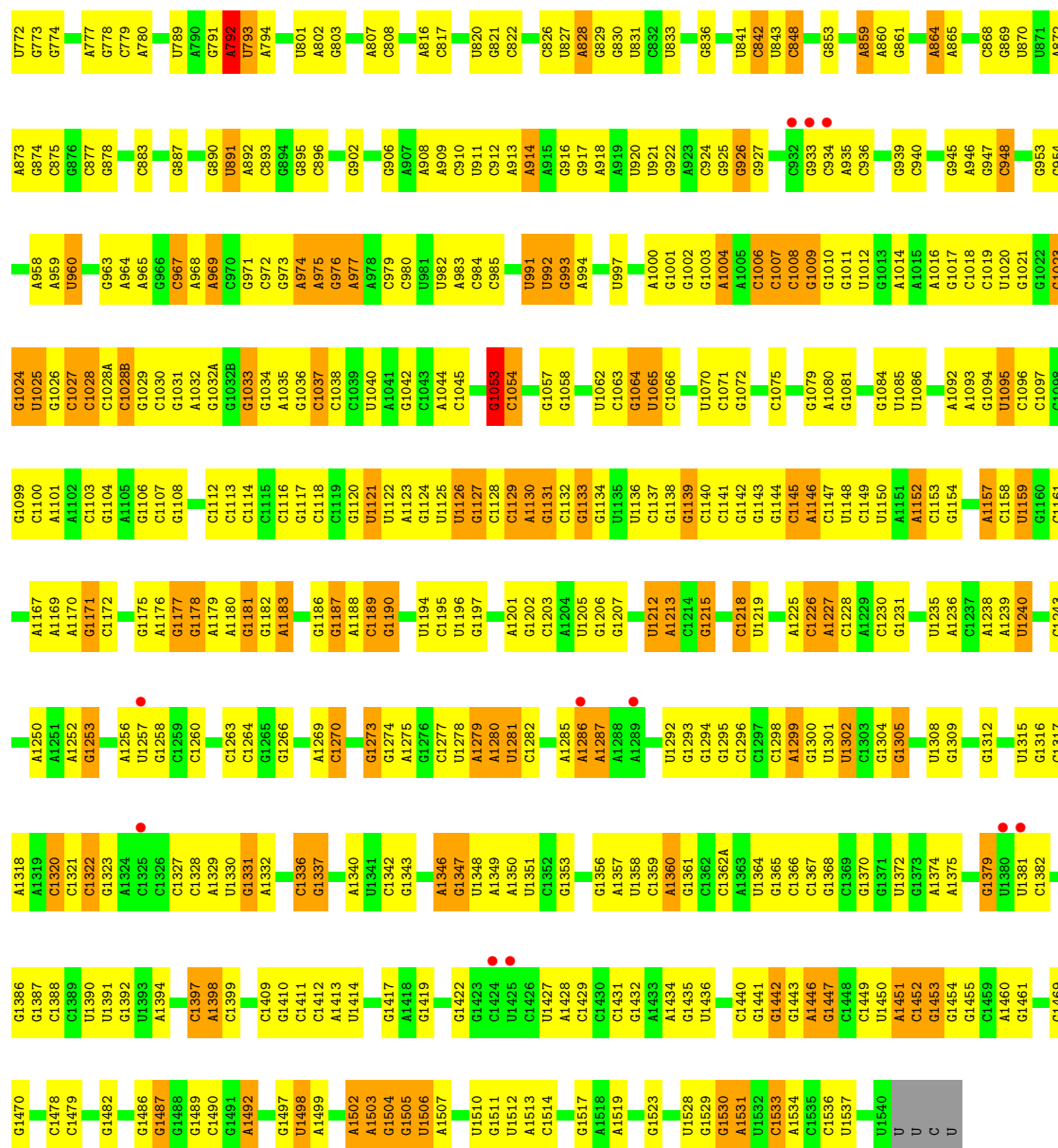
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
57	M5	3	Total	O	0	0
			3	3		

3 Residue-property plots [i](#)

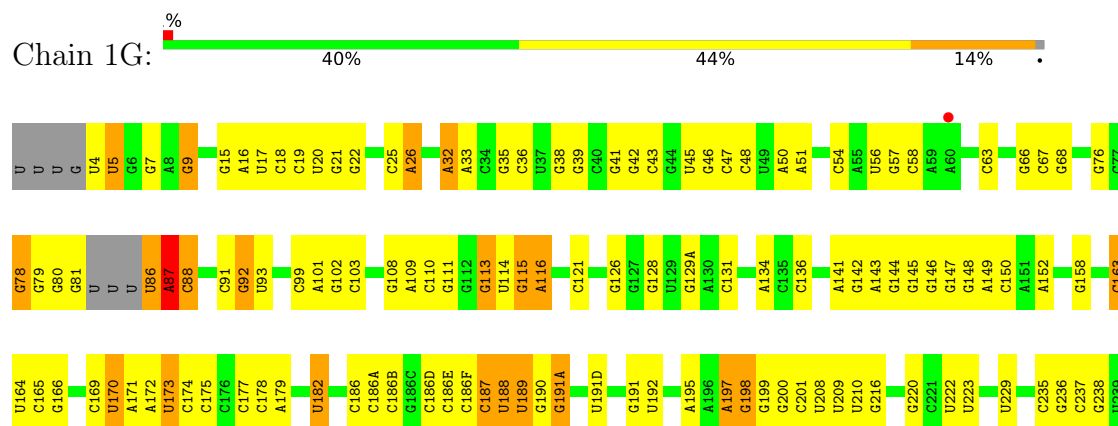
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

• Molecule 1: 16S ribosomal RNA

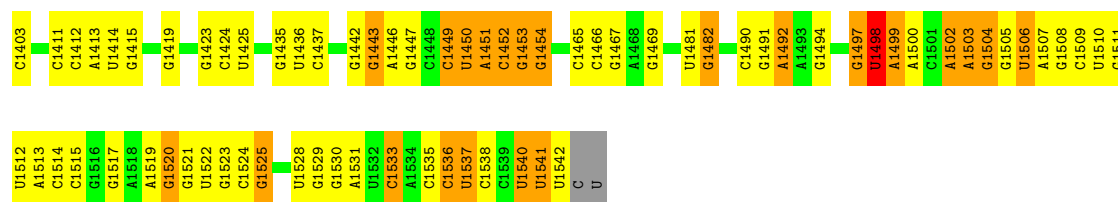




• Molecule 1: 16S ribosomal RNA

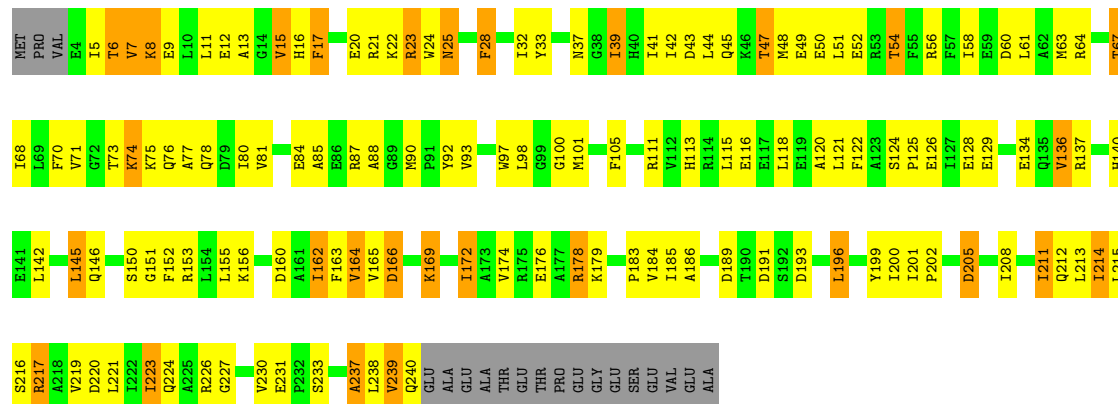


C1328	C1329	U1330	G1331	C1335	C1336	G1337	G1338	A1339	A1340	C1341	C1342	G1343	C1344	C1345	A1346	G1347	U1348	A1349	C1352	G1353	C1354	G1355	G1356	A1357	U1358	C1359	C1362A	A1363	U1364	G1365	G1370	G1371	U1372	G1373	A1374	A1375	G1379	C1384	G1385	G1386	G1387	C1388	G1389	U1390	U1391	G1392	C1397	A1398	C1399	G1400	C1402							
C1262	C1263	C1264	G1265	A1268	A1269	C1270	G1271	G1272	G1273	G1274	A1275	G1276	C1277	U1278	A1279	A1280	U1281	C1282	A1285	A1286	A1287	A1288	A1289	G1290	G1291	G1294	G1295	C1296	C1297	A1298	A1299	G1300	U1301	G1305	A1306	U1307	U1308	G1309	G1312	U1313	G1314	U1315	G1316	C1317	A1318	A1319	C1320	C1321	C1322	G1323	A1324	C1325	C1326	C1327				
A1191	C1192	G1193	U1194	C1195	U1196	G1197	G1198	U1199	G1200	A1201	G1202	C1203	A1204	U1205	G1206	G1207	C1208	G1209	C1210	U1211	U1212	A1213	C1214	G1215	G1216	C1217	U1218	G1219	G1222	G1223	G1224	A1225	C1226	U1227	U1235	A1236	C1237	A1238	U1239	U1240	G1241	C1245	A1246	G1247	A1250	A1251	A1252	G1253	G1254	G1255	G1256	U1257	G1258	C1259	A1261			
G1124	U1125	U1126	G1127	C1128	C1129	A1130	G1131	G1132	G1133	G1134	U1135	U1136	C1137	G1138	G1139	G1140	C1141	G1142	G1143	G1144	C1145	A1146	C1147	U1148	C1149	U1150	A1151	A1152	C1153	G1154	G1155	G1156	A1157	C1158	U1159	G1160	C1161	C1162	G1171	G1172	G1173	G1174	G1175	G1176	G1177	G1178	A1179	A1180	A1181	G1182	G1183	G1184	G1185	G1186	G1187	C1188	A1189	G1190
A1046	G1047	U1052	G1053	C1054	A1055	U1056	G1057	C1058	C1059	C1063	G1064	U1065	G1066	A1067	G1068	C1069	U1070	C1071	G1072	C1075	A1080	G1081	U1082	U1083	G1084	U1085	U1086	G1087	G1088	A1093	G1094	U1095	C1096	G1099	C1100	A1101	A1102	G1106	C1107	G1108	C1109	A1110	A1111	C1112	C1116	G1117	G1118	C1119	U1122	A1123								
G988	C989	C990	U991	G992	G993	A994	C995	G998	C998A	U999	A1000	G1001	G1002	G1003	A1004	A1005	C1006	G1009	G1010	G1011	G1012	A1014	A1015	A1016	G1017	G1018	G1019	U1020	G1021	G1022	G1023	U1024	U1025	G1026	C1027	U1028	C1028A	G1033	G1034	A1035	G1036	C1037	C1038	U1039	U1040	C1043	A1044	C1045										
A1046	G1047	U1052	G1053	C1054	A1055	U1056	G1057	C1058	C1059	C1063	G1064	U1065	G1066	A1067	G1068	C1069	U1070	C1071	G1072	C1075	A1080	G1081	U1082	U1083	G1084	U1085	U1086	G1087	G1088	A1093	G1094	U1095	C1096	G1099	C1102A	G1108	C1109	A1110	A1111	C1112	C1116	G1117	G1118	C1119	U1122	A1123												
G988	C989	C990	U991	G992	G993	A994	C995	G998	C998A	U999	A1000	G1001	G1002	G1003	A1004	A1005	C1006	G1009	G1010	G1011	G1012	A1014	A1015	A1016	G1017	G1018	G1019	U1020	G1021	G1022	G1023	U1024	U1025	G1026	C1027	U1028	C1028A	G1033	G1034	A1035	G1036	C1037	C1038	U1039	U1040	C1043	A1044	C1045										
A1046	G1047	U1052	G1053	C1054	A1055	U1056	G1057	C1058	C1059	C1063	G1064	U1065	G1066	A1067	G1068	C1069	U1070	C1071	G1072	C1075	A1080	G1081	U1082	U1083	G1084	U1085	U1086	G1087	G1088	A1093	G1094	U1095	C1096	G1099	C1100	A1101	A1102	G1106	C1107	G1108	C1109	A1110	A1111	C1112	C1116	G1117	G1118	C1119	U1122	A1123								
G1124	U1125	U1126	G1127	C1128	C1129	A1130	G1131	G1132	G1133	G1134	U1135	U1136	C1137	G1138	G1139	G1140	C1141	G1142	G1143	G1144	C1145	A1146	C1147	U1148	C1149	U1150	A1151	A1152	C1153	G1154	G1155	G1156	A1157	C1158	U1159	G1160	C1161	C1162	G1171	G1172	G1173	G1174	G1175	G1176	G1177	G1178	A1179	A1180	A1181	G1182	G1183	G1184	G1185	G1186	G1187	C1188	A1189	G1190
A1191	C1192	G1193	U1194	C1195	U1196	G1197	G1198	U1199	G1200	A1201	G1202	C1203	A1204	U1205	G1206	G1207	C1208	G1209	C1210	U1211	U1212	A1213	C1214	G1215	G1216	C1217	U1218	G1219	G1222	G1223	G1224	A1225	C1226	U1227	U1235	A1236	C1237	A1238	U1239	U1240	G1241	C1245	A1246	G1247	A1250	A1251	A1252	G1253	G1254	G1255	G1256	U1257	G1258	C1259	A1261			
C1262	C1263	C1264	G1265	A1268	A1269	C1270	G1271	G1272	G1273	G1274	A1275	G1276	C1277	U1278	A1279	A1280	U1281	C1282	A1285	A1286	A1287	A1288	A1289	G1290	G1291	G1294	G1295	C1296	C1297	A1298	A1299	G1300	U1301	G1305	A1306	U1307	U1308	G1309	G1312	U1313	G1314	U1315	G1316	C1317	A1318	A1319	C1320	C1321	C1322	G1323	A1324	C1325	C1326	C1327				
C1328	C1329	U1330	G1331	C1335	C1336	G1337	G1338	A1339	A1340	C1341	C1342	G1343	C1344	C1345	A1346	G1347	U1348	A1349	C1352	G1353	C1354	G1355	G1356	A1357	U1358	C1359	C1362A	A1363	U1364	G1365	G1370	G1371	U1372	G1373	A1374	A1375	G1379	C1384	G1385	G1386	G1387	C1388	G1389	U1390	U1391	G1392	C1397	A1398	C1399	G1400	C1402							



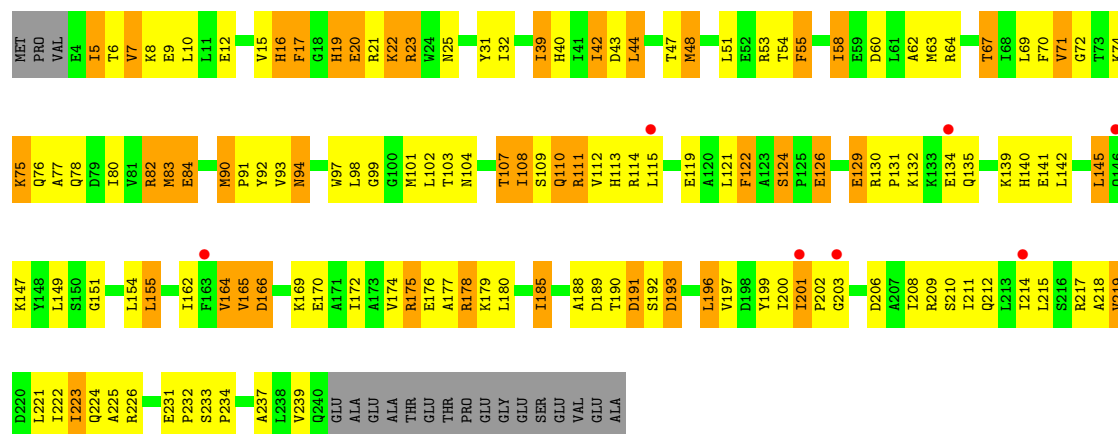
• Molecule 2: 30S ribosomal protein S2

Chain 1E: 39% 42% 11% 7%



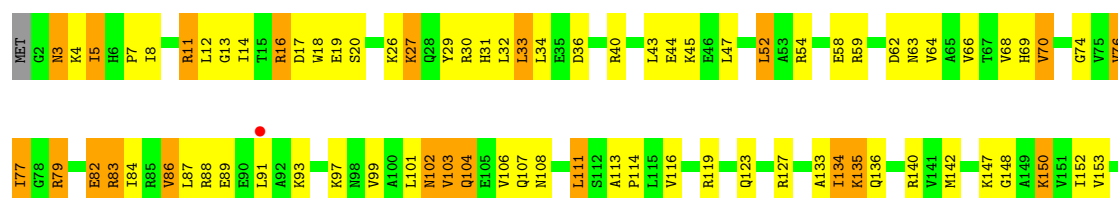
• Molecule 2: 30S ribosomal protein S2

Chain 12: 3% 38% 38% 17% 7%



• Molecule 3: 30S ribosomal protein S3

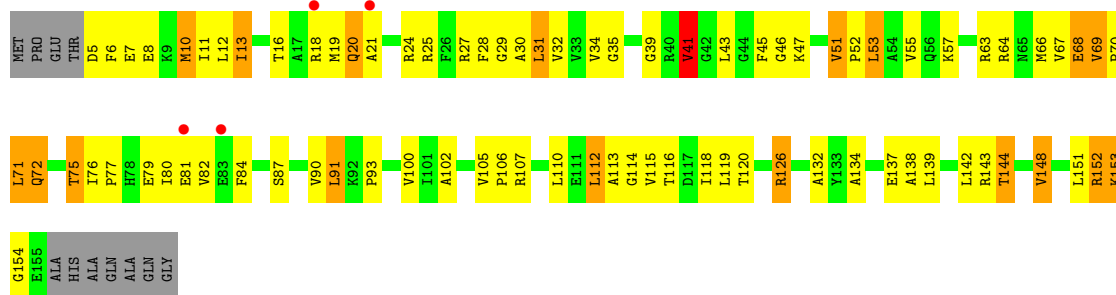
Chain 2E: 43% 31% 11% 14%





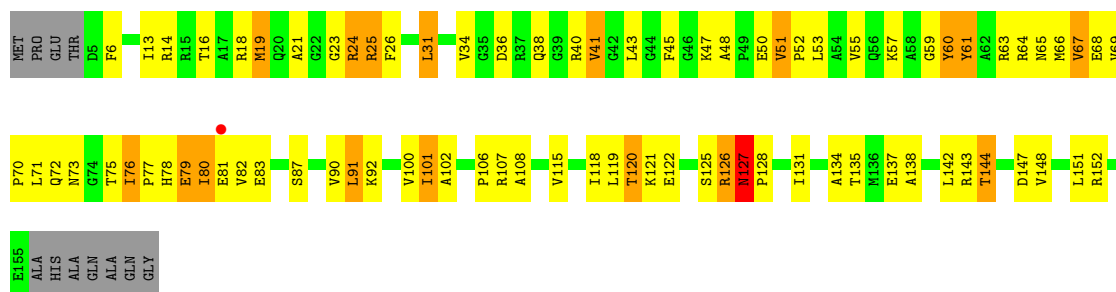
• Molecule 5: 30S ribosomal protein S5

Chain 4E: 2% 42% 40% 11% 7%



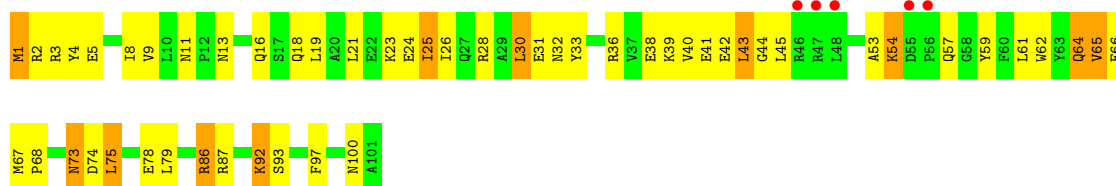
• Molecule 5: 30S ribosomal protein S5

Chain 42: 43% 40% 10% 7%



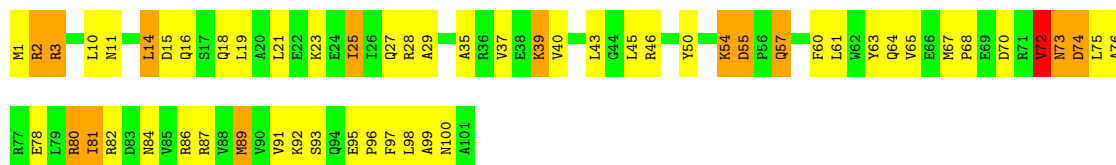
• Molecule 6: 30S ribosomal protein S6

Chain 5E: 5% 48% 42% 11%

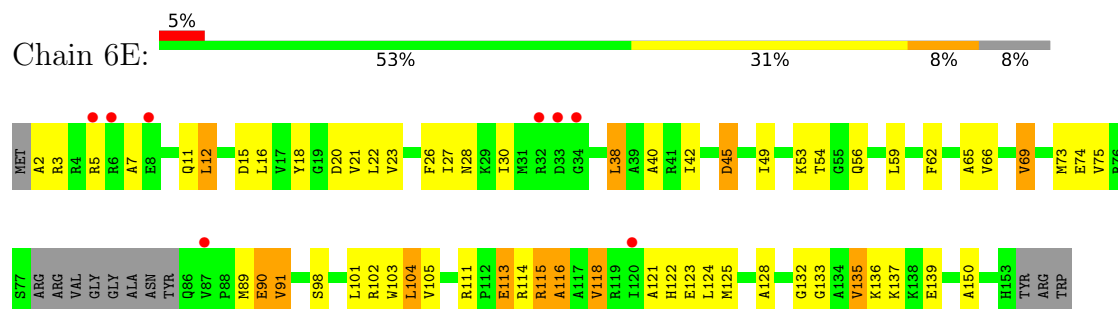


• Molecule 6: 30S ribosomal protein S6

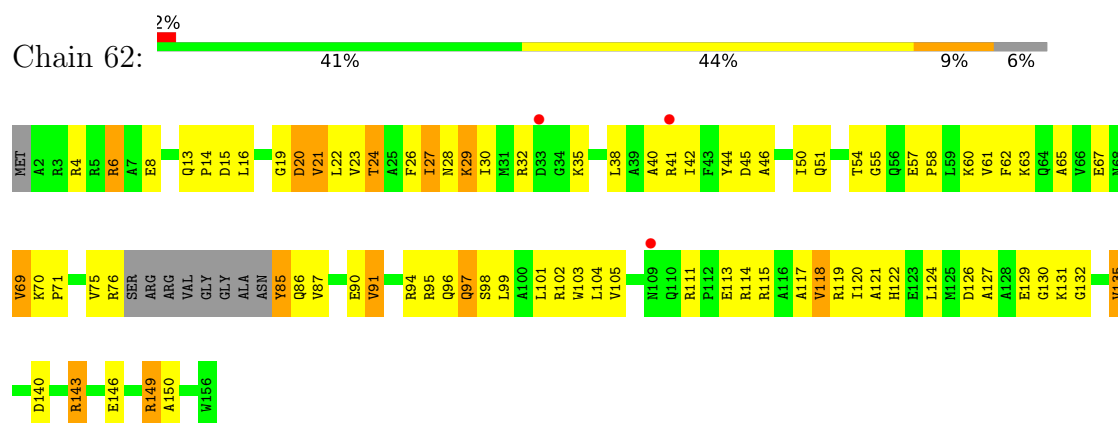
Chain 52: 44% 43% 13%



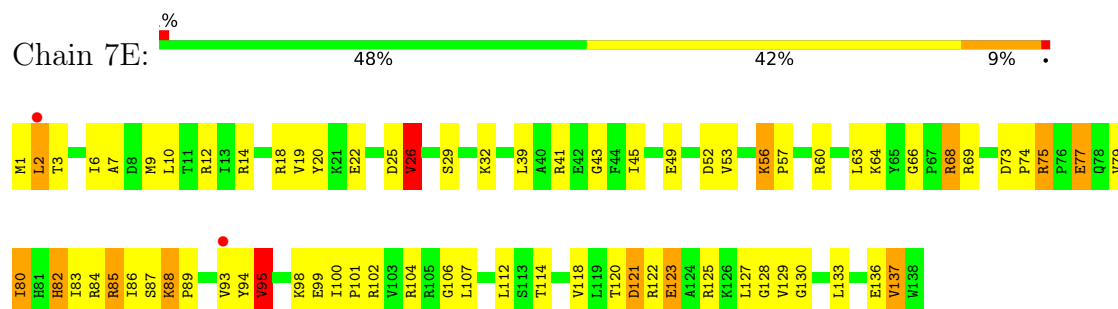
- Molecule 7: 30S ribosomal protein S7



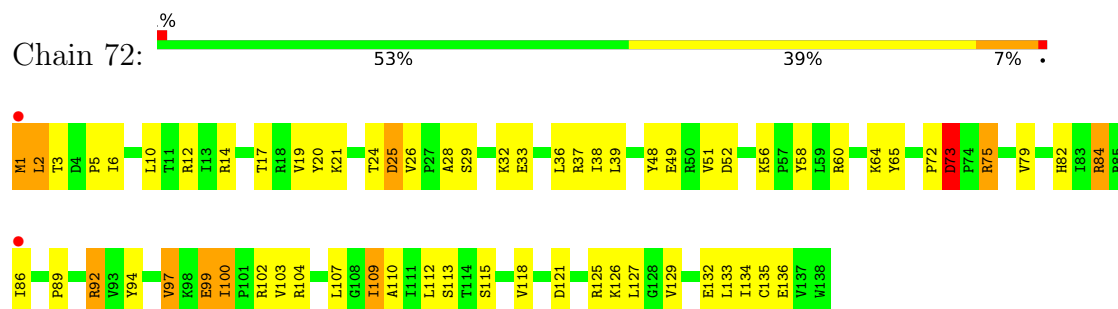
- Molecule 7: 30S ribosomal protein S7



- Molecule 8: 30S ribosomal protein S8



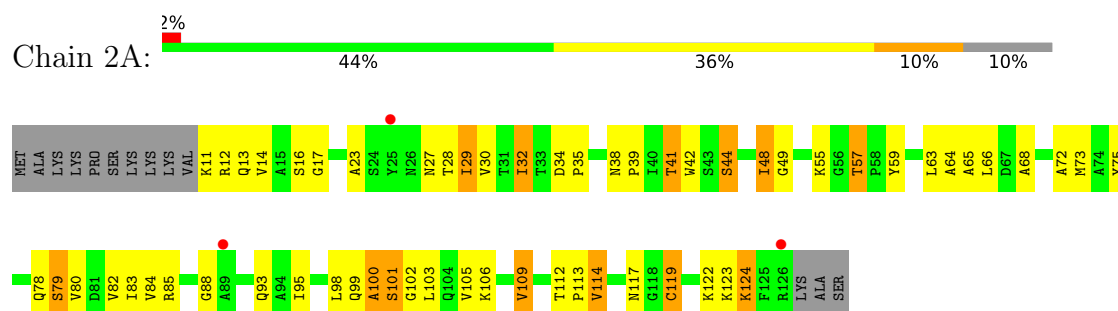
- Molecule 8: 30S ribosomal protein S8



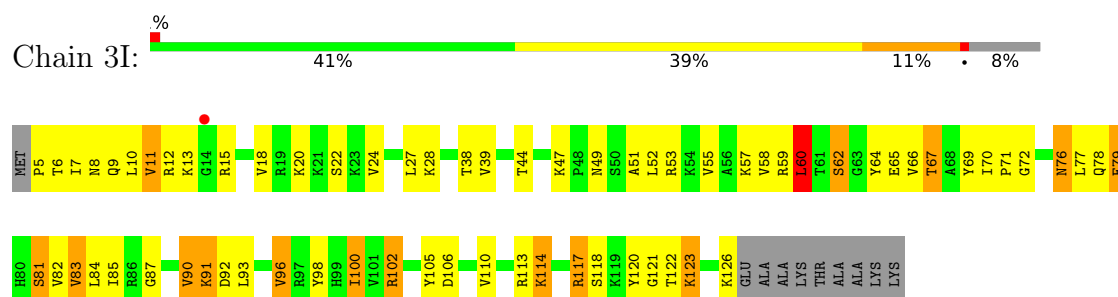
- Molecule 9: 30S ribosomal protein S9



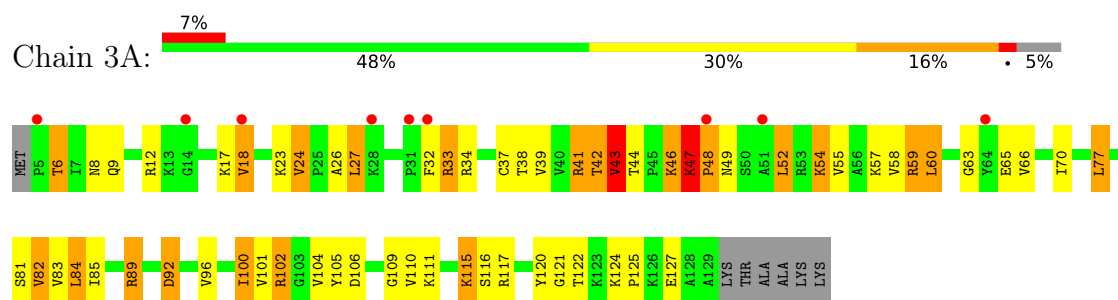
• Molecule 11: 30S ribosomal protein S11



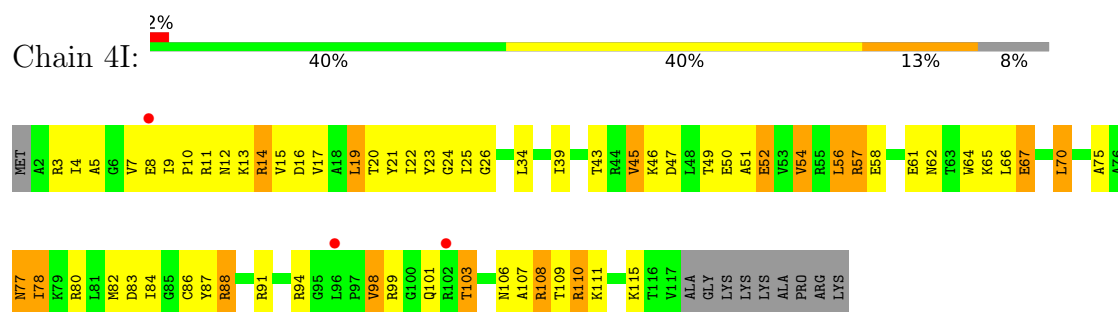
• Molecule 12: 30S ribosomal protein S12



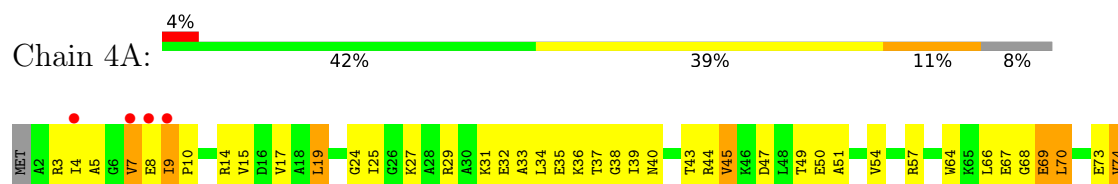
• Molecule 12: 30S ribosomal protein S12



• Molecule 13: 30S ribosomal protein S13

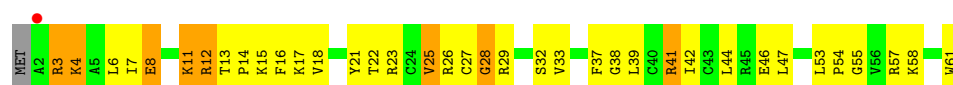


• Molecule 13: 30S ribosomal protein S13

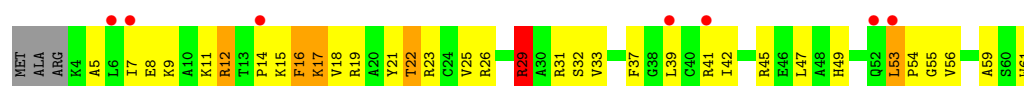




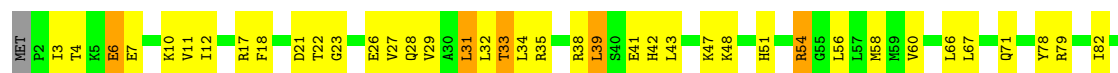
- Molecule 14: 30S ribosomal protein S14 type Z



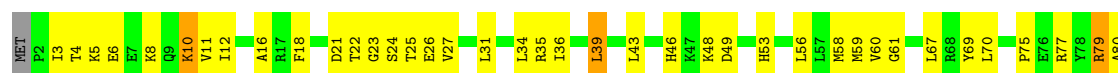
- Molecule 14: 30S ribosomal protein S14 type Z



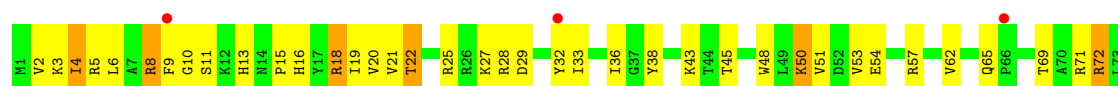
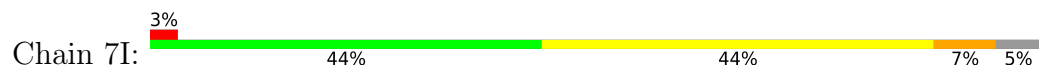
- Molecule 15: 30S ribosomal protein S15



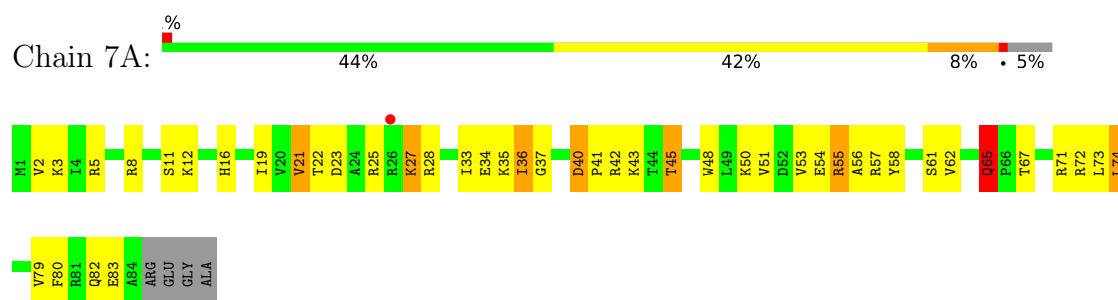
- Molecule 15: 30S ribosomal protein S15



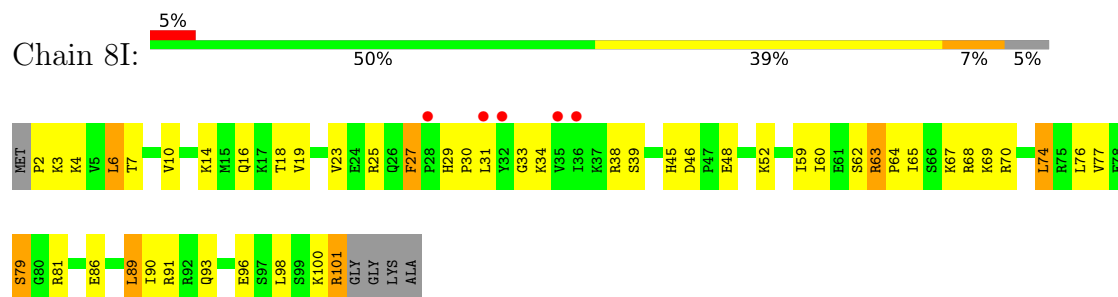
- Molecule 16: 30S ribosomal protein S16



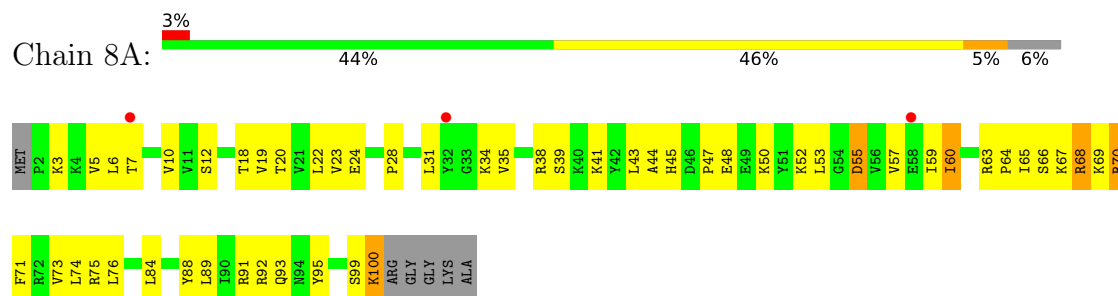
- Molecule 16: 30S ribosomal protein S16



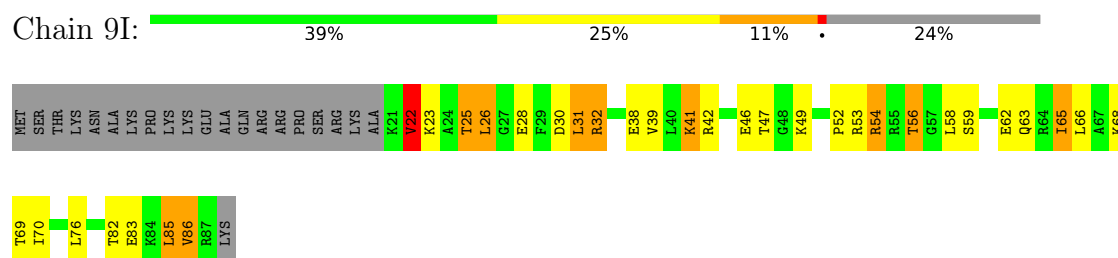
• Molecule 17: 30S ribosomal protein S17



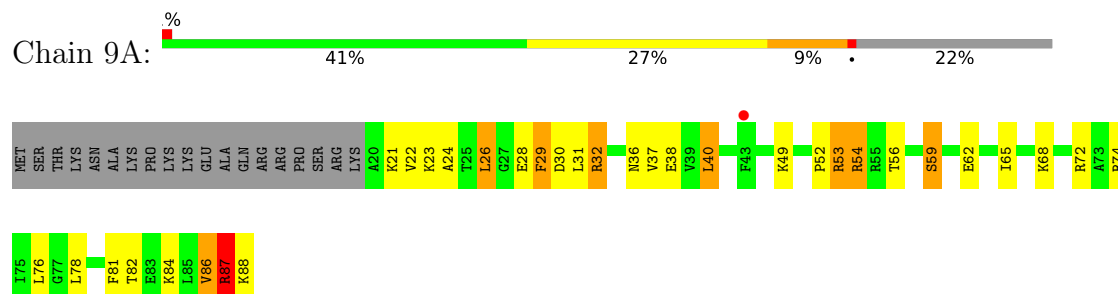
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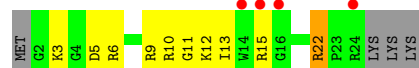
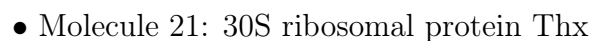
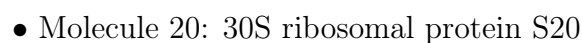
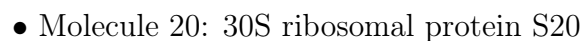
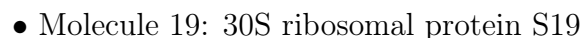
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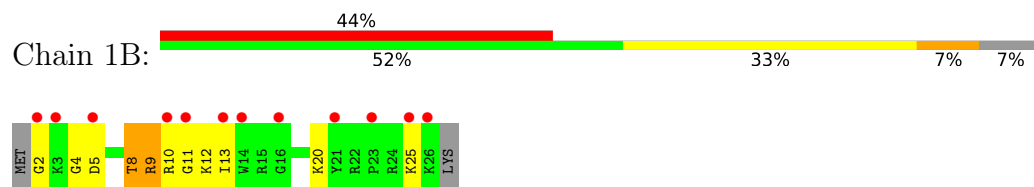
• Molecule 18: 30S ribosomal protein S18



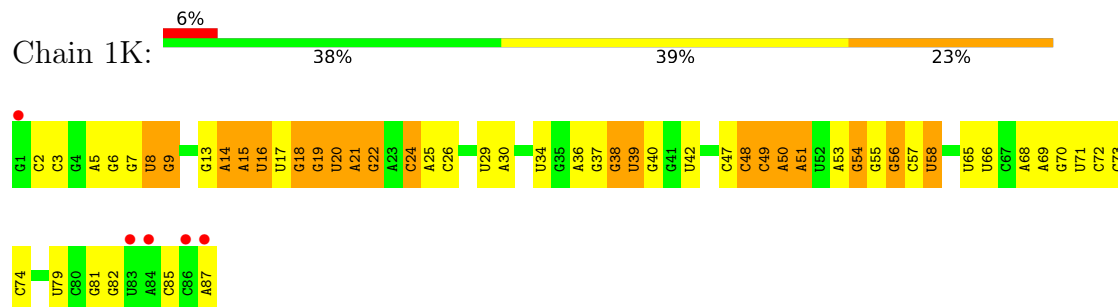
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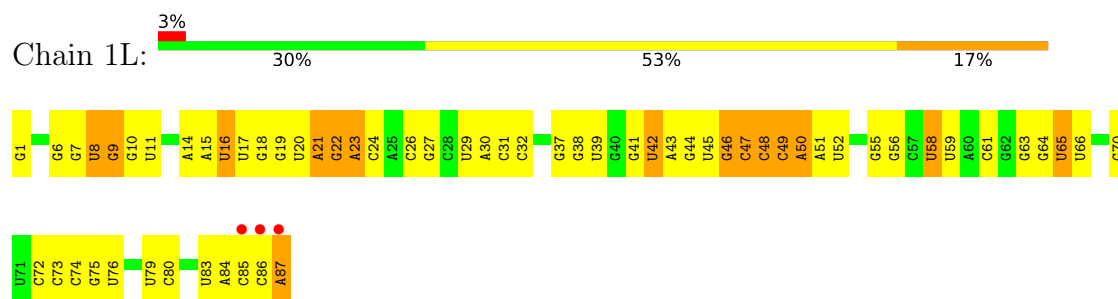
- Molecule 21: 30S ribosomal protein Thx



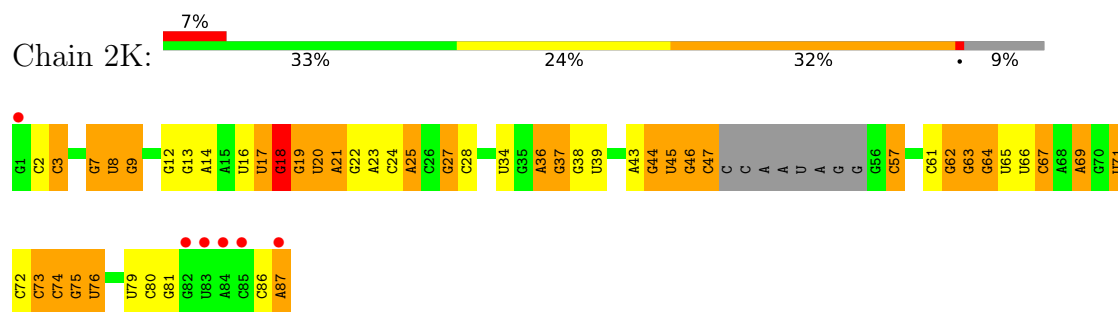
- Molecule 22: tRNA-Leu



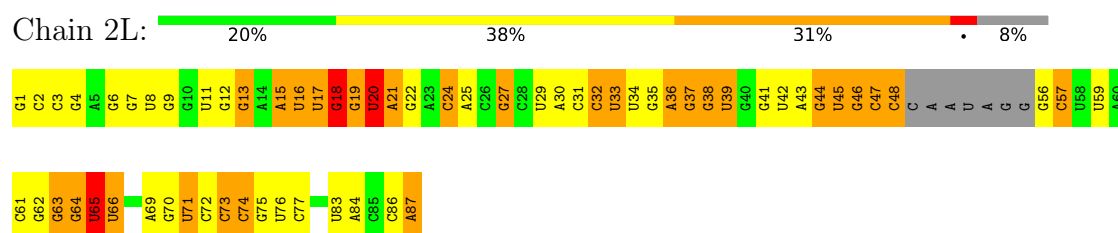
- Molecule 22: tRNA-Leu



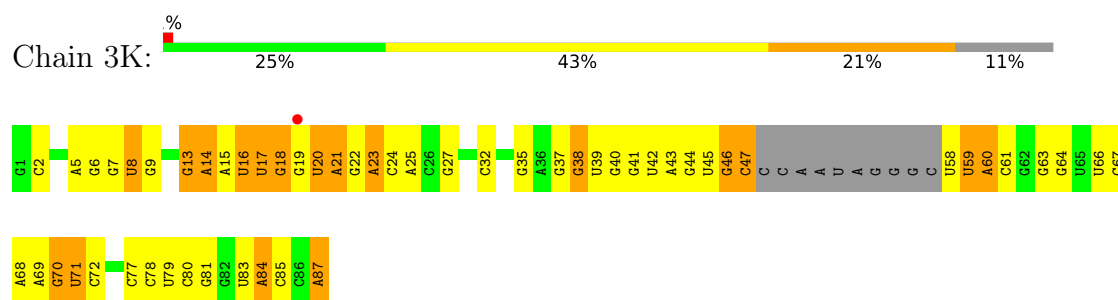
- Molecule 23: tRNA-Leu



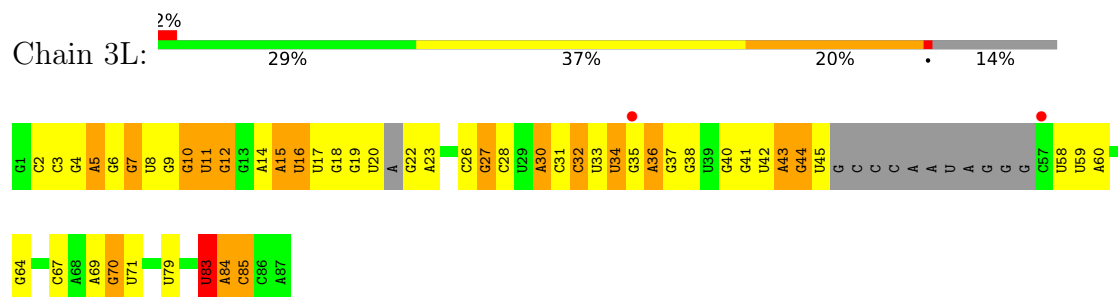
- Molecule 23: tRNA-Leu



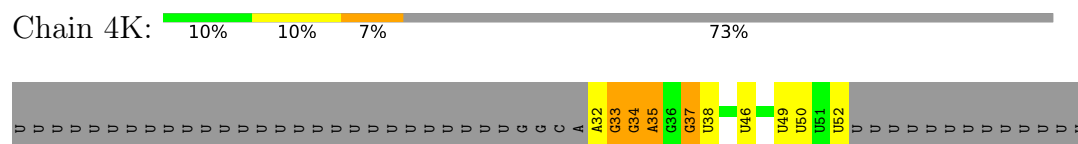
- Molecule 24: tRNA-Leu



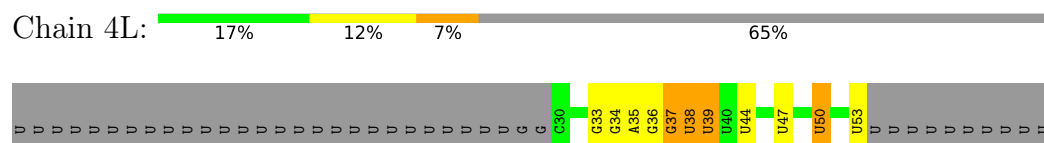
- Molecule 24: tRNA-Leu



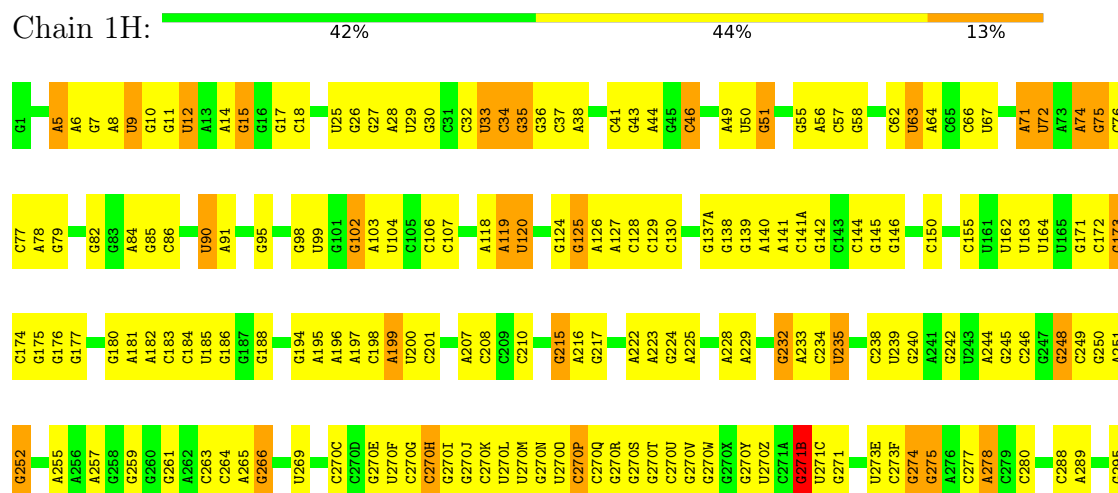
- Molecule 25: mRNA



- Molecule 25: mRNA

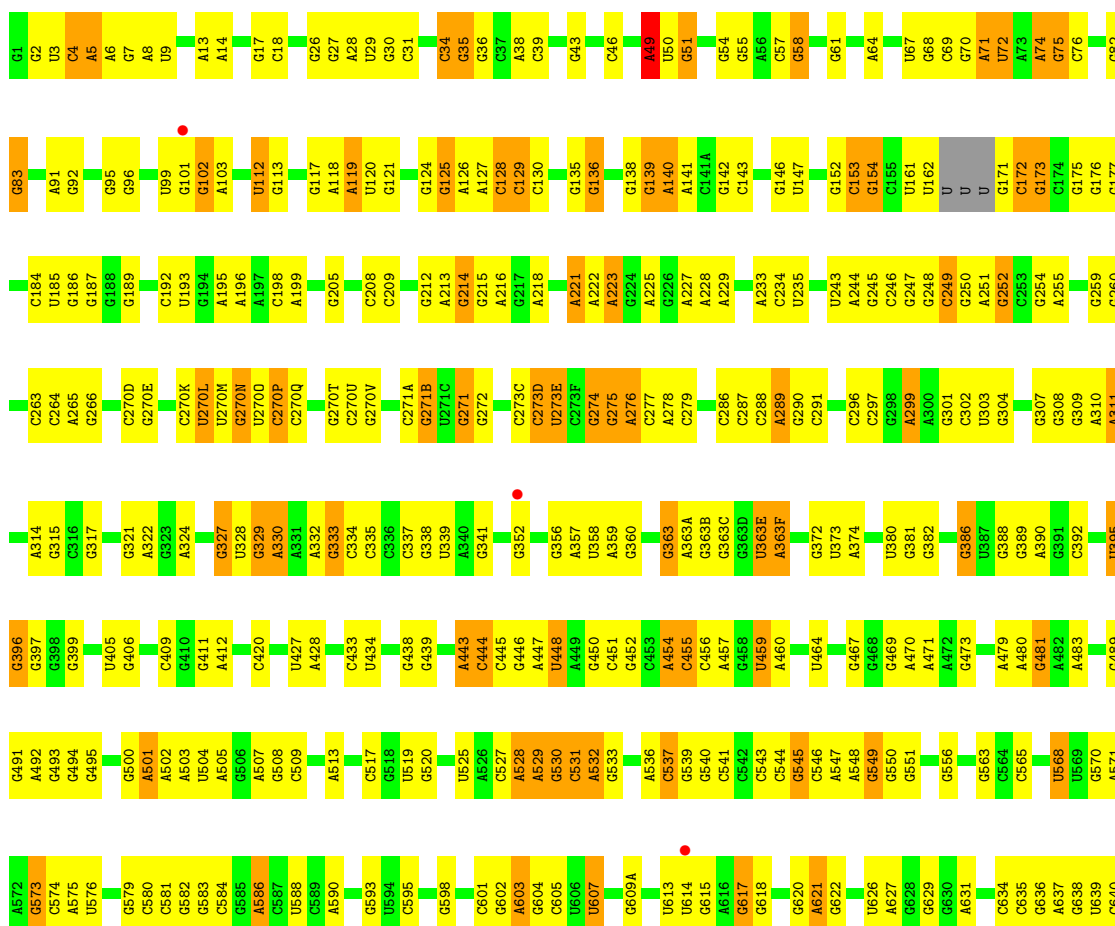


- Molecule 26: 23S ribosomal RNA



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G997	C998	U999	A1000	G1003	C1006	C1007	C1008	A1009	A1010	G1011	U1012	C1013	U1014	U1015	G1016	G1017	A1020	U1021	G1022	U1023	G1024	G1025	U1026	A1027	A1028	A1032	U1033	A1034	G1035	U1036	G1037	C1038	G1039	C1040	C1041	G1044	A1045	U1046	G1047	A1050	G1051	C1052	C1053	A1054	G1055	A1056	U1057	U1058	G1059	U1060	U1061	G1062	C1063				
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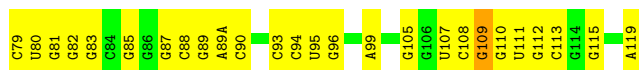
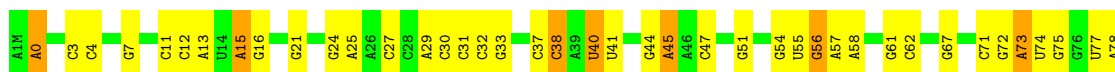
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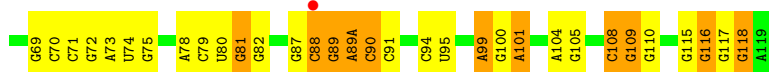
• Molecule 27: 5S ribosomal RNA

Chain 16: 45% 48% 7%



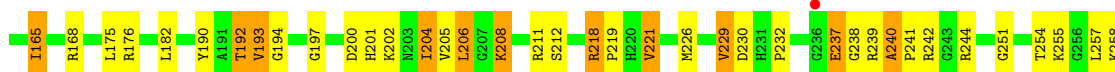
• Molecule 27: 5S ribosomal RNA

Chain 1J: 38% 40% 22%



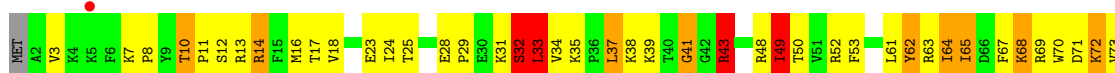
• Molecule 28: 50S ribosomal protein L2

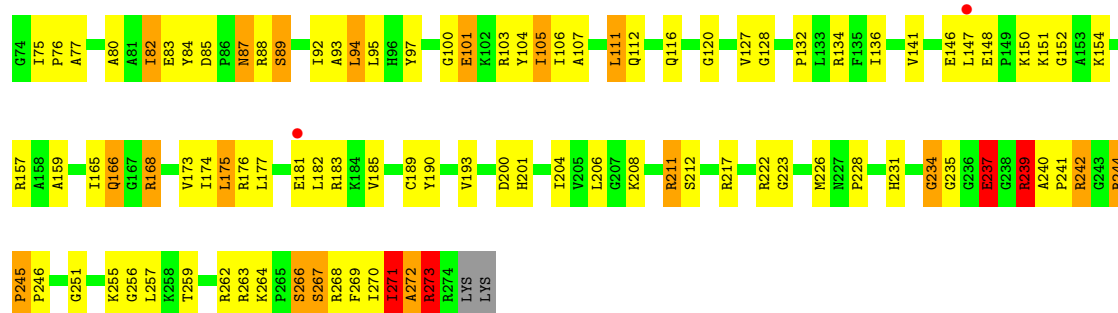
Chain 11: 54% 34% 10%



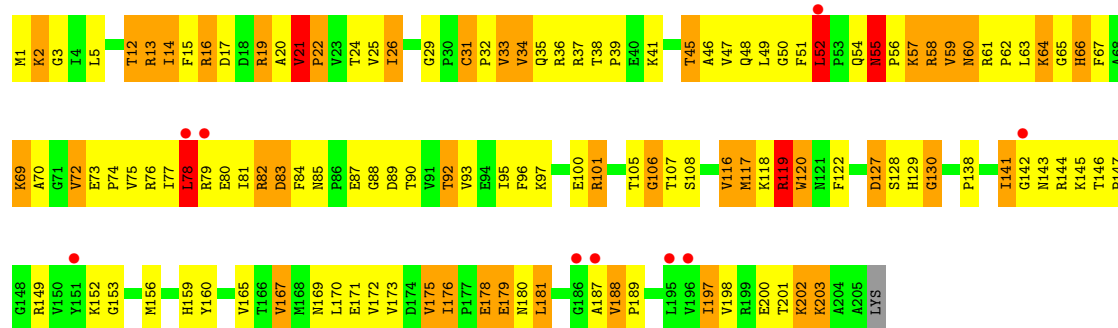
• Molecule 28: 50S ribosomal protein L2

Chain 19: 49% 38% 10%

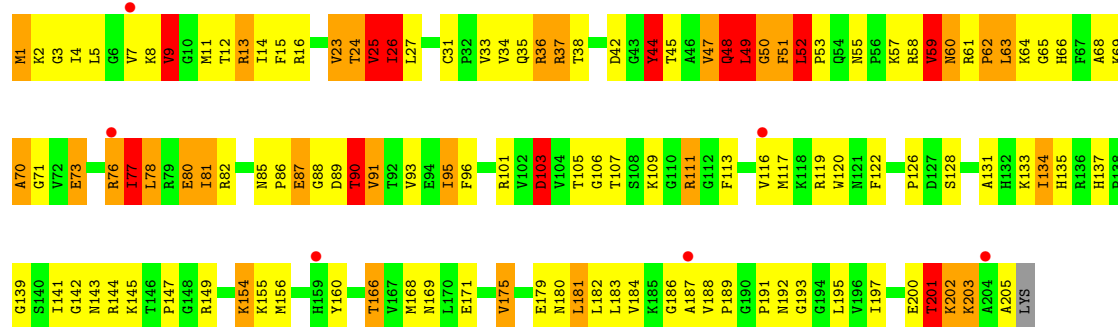




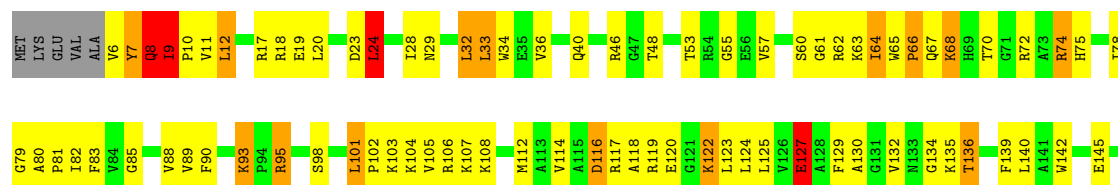
• Molecule 29: 50S ribosomal protein L3

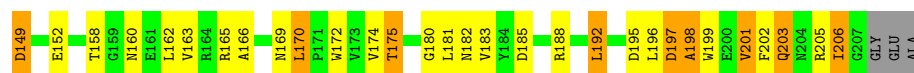


• Molecule 29: 50S ribosomal protein L3



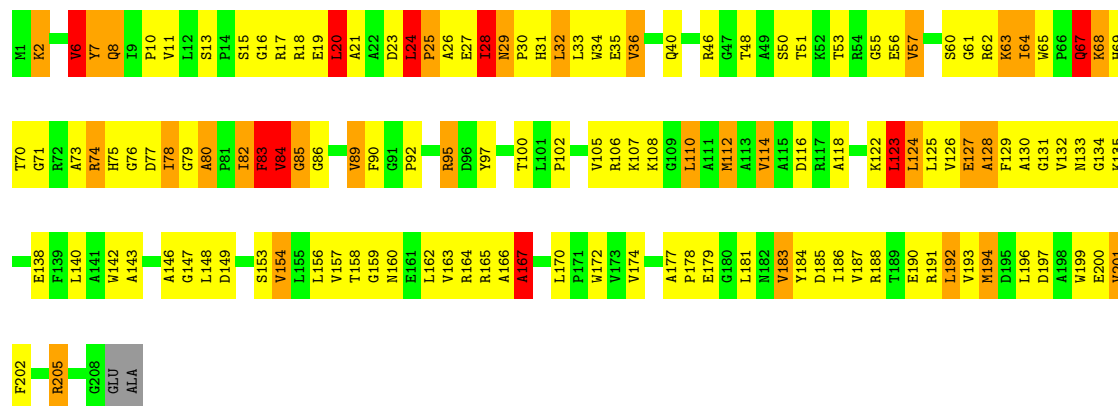
• Molecule 30: 50S ribosomal protein L4





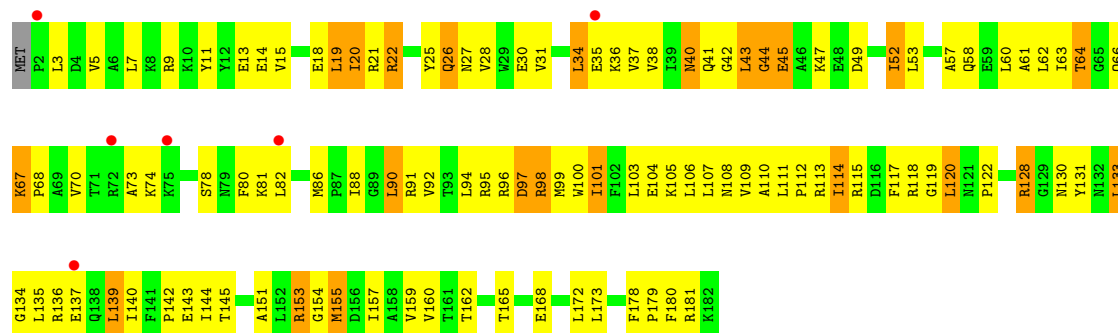
- Molecule 30: 50S ribosomal protein L4

Chain 39: 34% 47% 14% ..



- Molecule 31: 50S ribosomal protein L5

Chain 41: 3% 38% 49% 13% ..

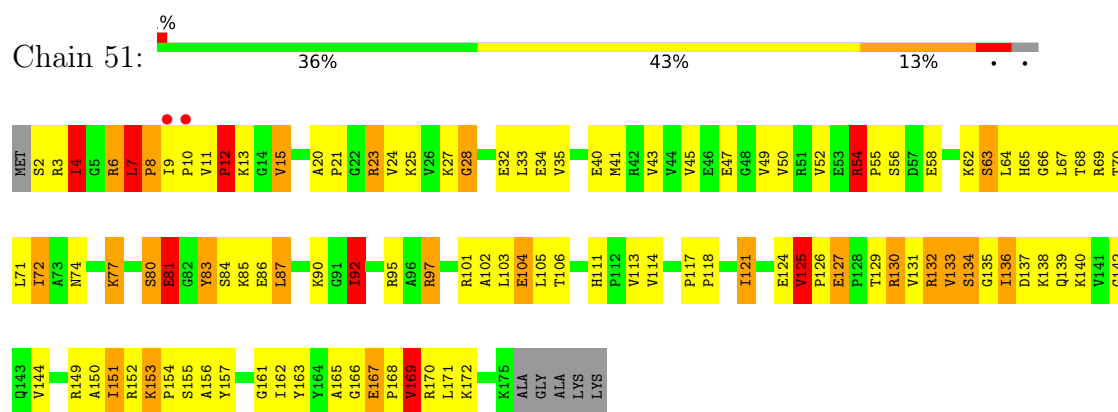


- Molecule 31: 50S ribosomal protein L5

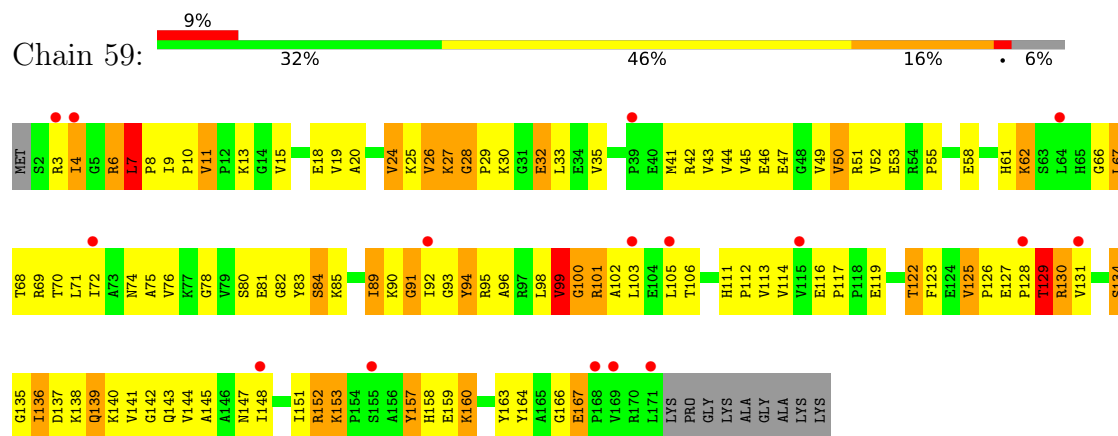
Chain 49: % 46% 42% 11% ..



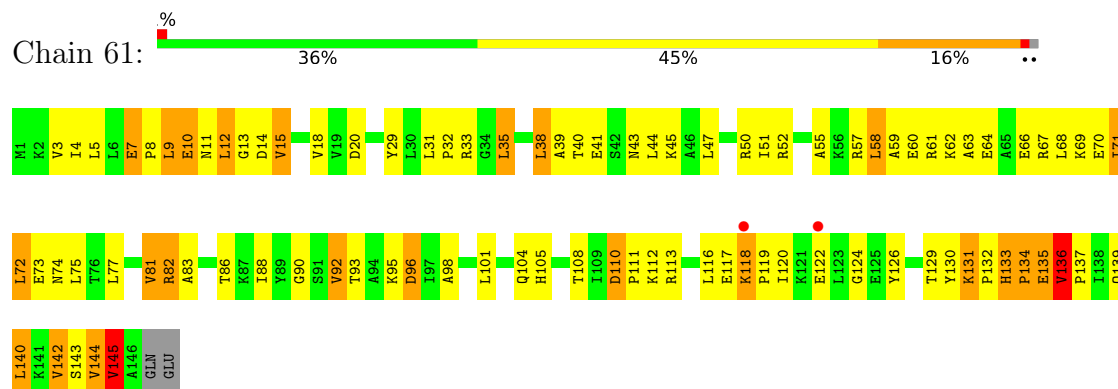
- Molecule 32: 50S ribosomal protein L6



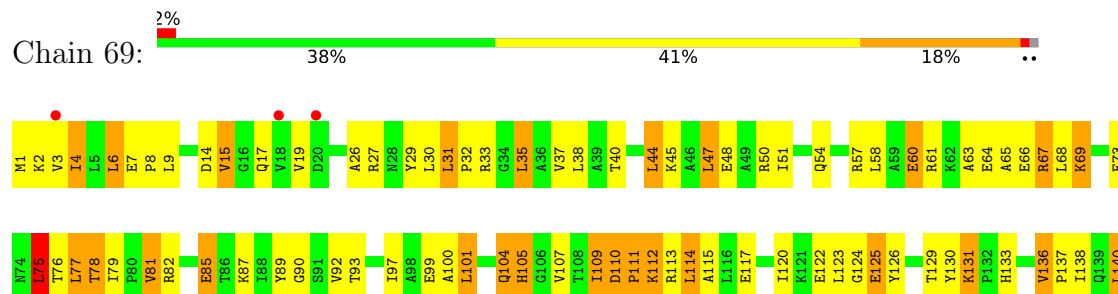
- Molecule 32: 50S ribosomal protein L6



- Molecule 33: 50S ribosomal protein L9

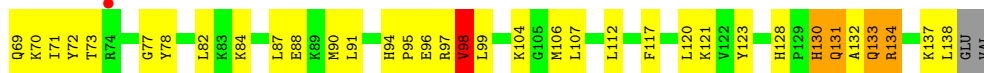
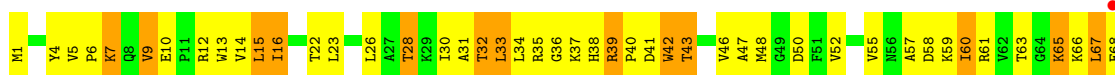


- Molecule 33: 50S ribosomal protein L9

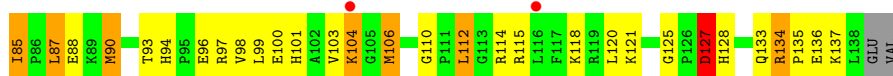
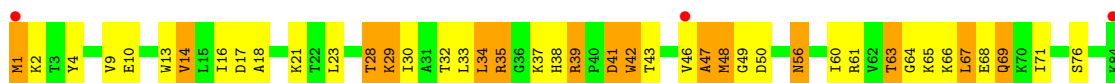




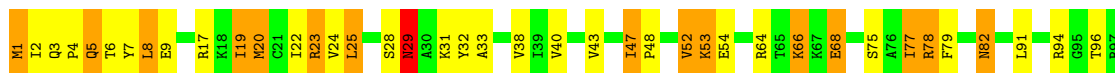
• Molecule 34: 50S ribosomal protein L13



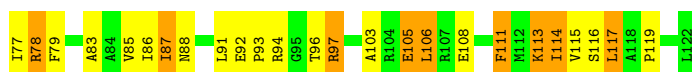
• Molecule 34: 50S ribosomal protein L13



• Molecule 35: 50S ribosomal protein L14

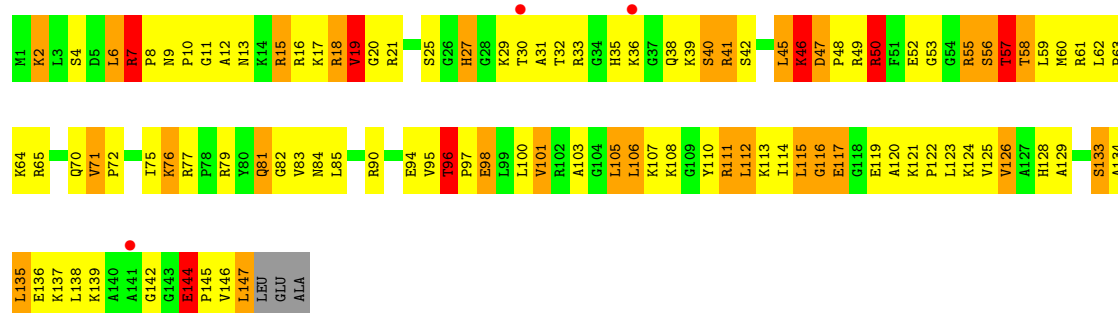


• Molecule 35: 50S ribosomal protein L14

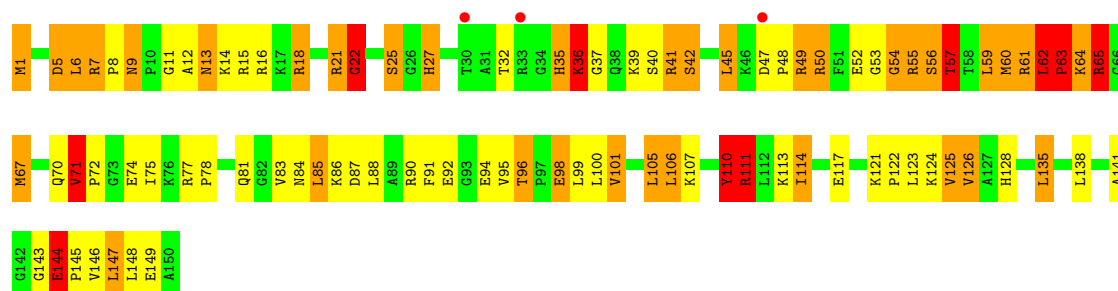


• Molecule 36: 50S ribosomal protein L15

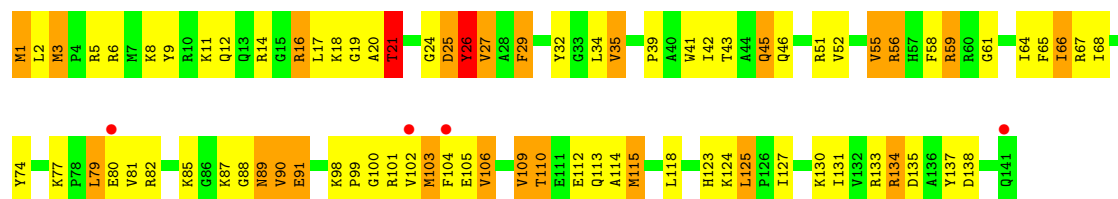
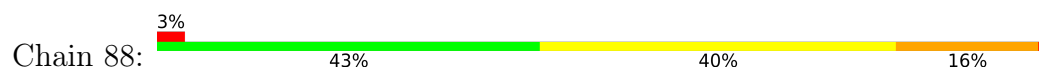




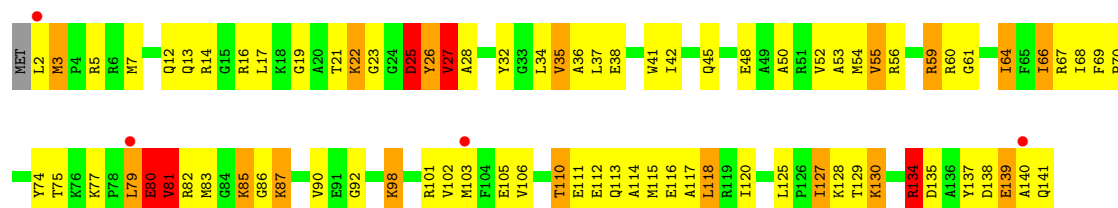
• Molecule 36: 50S ribosomal protein L15



• Molecule 37: 50S ribosomal protein L16



• Molecule 37: 50S ribosomal protein L16



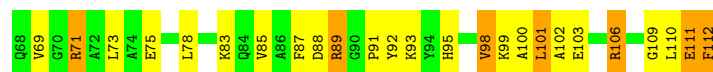
• Molecule 38: 50S ribosomal protein L17



- Molecule 38: 50S ribosomal protein L17



- Molecule 39: 50S ribosomal protein L18



- Molecule 39: 50S ribosomal protein L18



- Molecule 40: 50S ribosomal protein L19



LYS
ALA
GLN
GLU
PRO
LYS
LYS
ALA
SER
GLN
GLU

• Molecule 40: 50S ribosomal protein L19

Chain 75: 

M1 M2 M3 M4 M5 M6 M7 M8 M9 M10 M11 M12 M13 M14 M15 M16 M17 M18 M19 M20 M21 M22 M23 M24 M25 M26 M27 M28 M29 M30 M31 M32 M33 M34 M35 M36 M37 M38 M39 M40 M41 M42 M43 M44 M45 M46 M47 M48 M49 M50 M51 M52 M53 M54 M55 M56 M57 M58 M59 M60 M61 M62 M63 M64 M65 M66

S67 T68 G69 V70 G71 L72 E73 R74 L75 F76 F77 L78 L79 S80 S81 P81 L82 L83 Q84 Q85 R86 D87 T88 G92 T92 V93 R94 R95 R96 R97 R98 R99 Y100 F101 I102 N103 R104 L105 S106 D107 R108 E109 I110 R111 R112 K113 L114 R115 A116 K119 R120 I121 D124 R125 R126 R127 K137 ALA

GLN
GLU
PRO
LYS
ALA
SER
GLN
GLU

• Molecule 41: 50S ribosomal protein L20

Chain C8: 

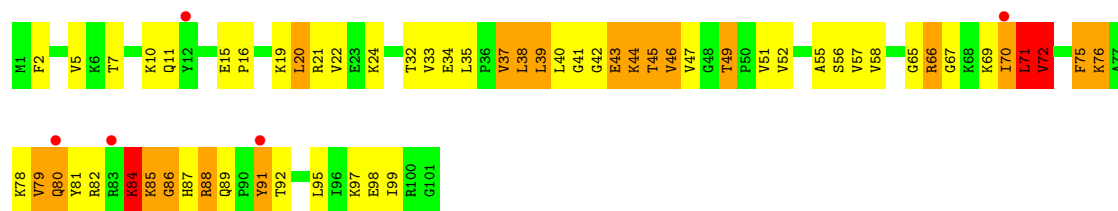
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L83 R84 R85 A86 G87 T88 E89 V90 D91 R92 R93 R94 R95 A96 A97 L98 L99 V100 V105 F106 E107 E108 L109 L110 V111 E111 R112 R113 K114 A115 G116

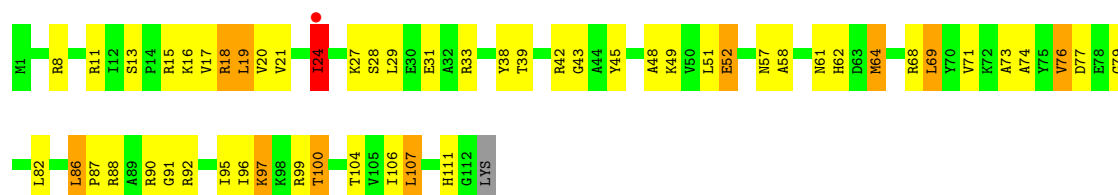
• Molecule 41: 50S ribosomal protein L20

Chain 85: 

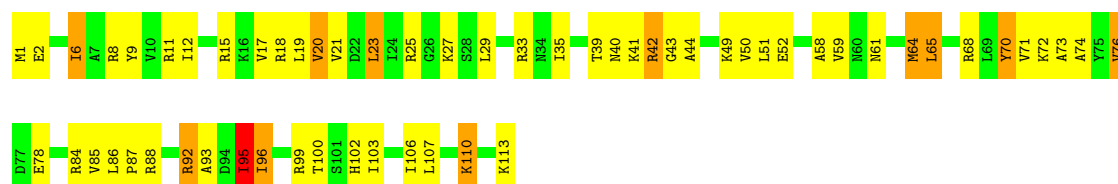
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R844 R845 R846 R847 R848 R849 R850 R851 R852 R853 R854 R855 R856 R857 R858 R859 R860 R861 R862 R863 R864 R865 R866 R867 R868 R869 R870 R871 R872 R873 R874 R875 R876 R877 R878 R879 R880 R881 R882 R883 R884 R885 R886 R887 R888 R889 R890 R891 R892 R893 R894 R895 R896 R897 R898 R899 R900 R901 R902 R903 R904 R905 R906 R907 R908 R909 R910 R911 R912 R913 R914 R915 R916 R917 R918 R919 R920 R921 R922 R923 R924 R925 R926 R927 R928 R929 R930 R931 R932 R933 R934 R935 R936 R937 R938 R939 R940 R941 R942 R943 R944 R945 R946 R947 R948 R949 R950 R951 R952 R953 R954 R955 R956 R957 R958 R959 R960 R961 R962 R963 R964 R965 R966 R967 R968 R969 R970 R971 R972 R973 R974 R975 R976 R977 R978 R979 R980 R981 R982 R983 R984 R985 R986 R987 R988 R989 R990 R991 R992 R993 R994 R995 R996 R997 R998 R999 R1000 R1001 R1002 R1003 R1004 R1005 R1006 R1007 R1008 R1009 R1010 R1011 R1012 R1013 R1014 R1015 R1016 R1017 R1018 R1019 R1020 R1021 R1022 R1023 R1024 R1025 R1026 R1027 R1028 R1029 R1030 R1031 R1032 R1033 R1034 R1035 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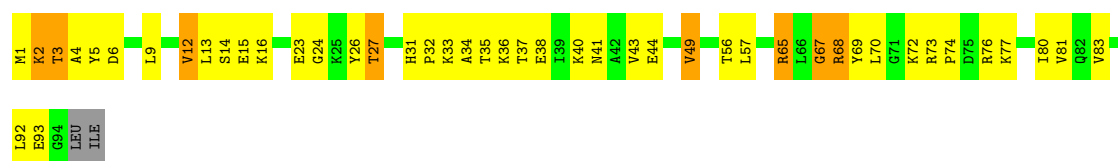
• Molecule 43: 50S ribosomal protein L22



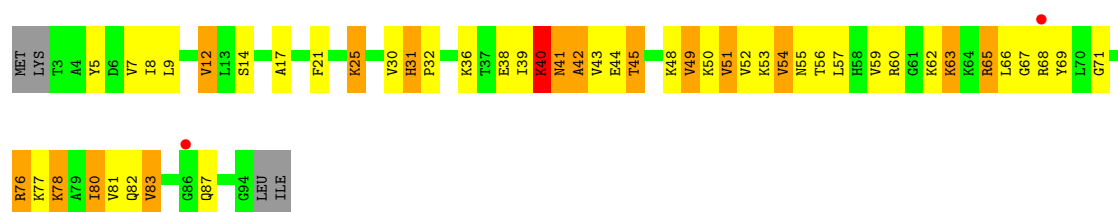
• Molecule 43: 50S ribosomal protein L22



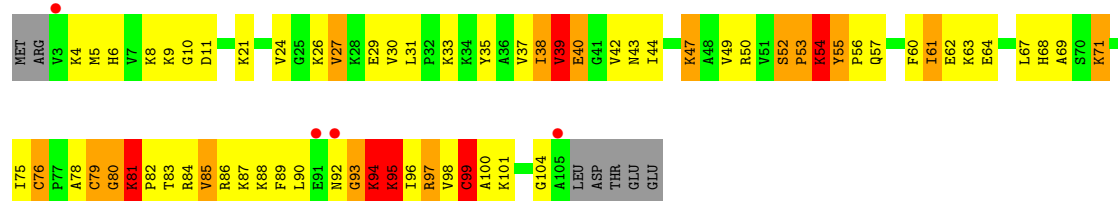
• Molecule 44: 50S ribosomal protein L23



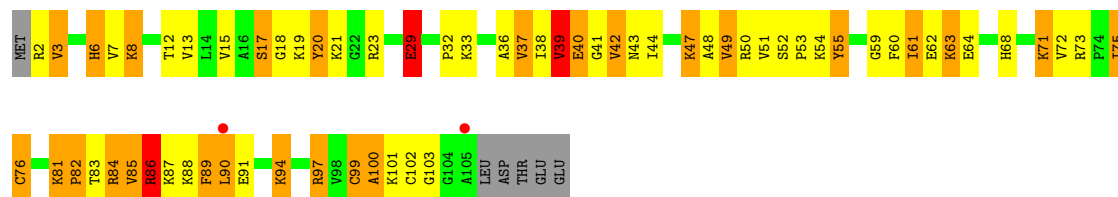
• Molecule 44: 50S ribosomal protein L23



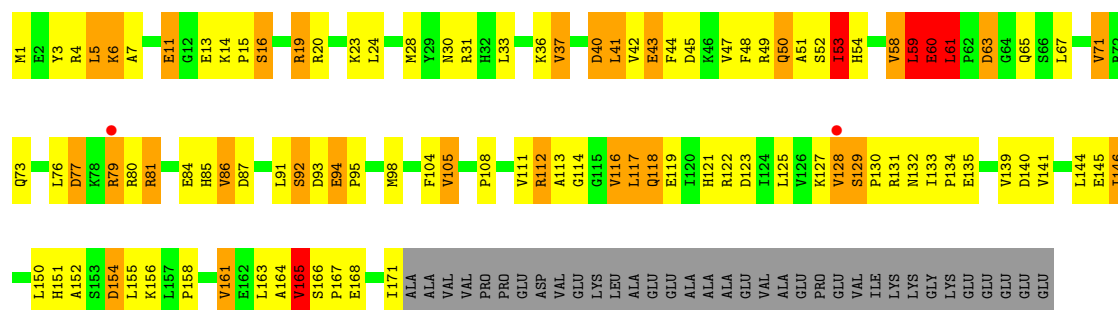
• Molecule 45: 50S ribosomal protein L24



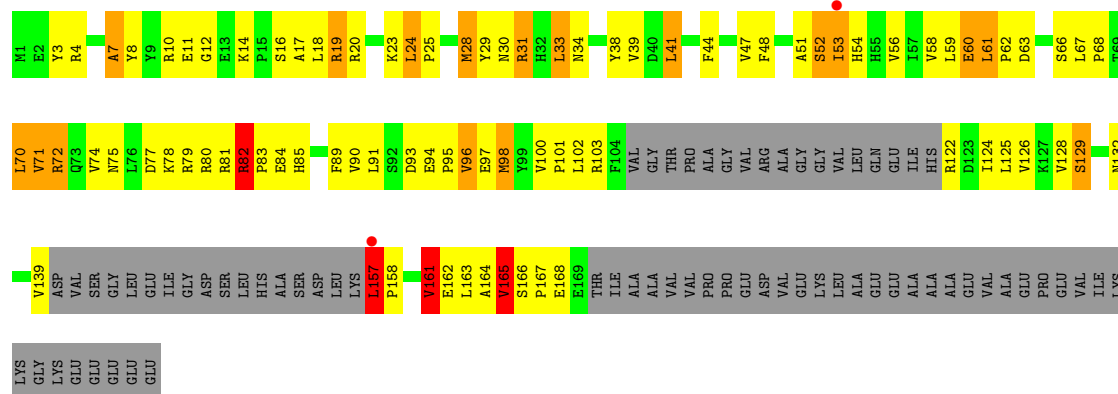
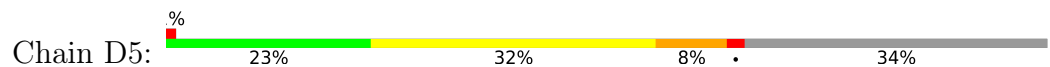
• Molecule 45: 50S ribosomal protein L24



• Molecule 46: 50S ribosomal protein L25



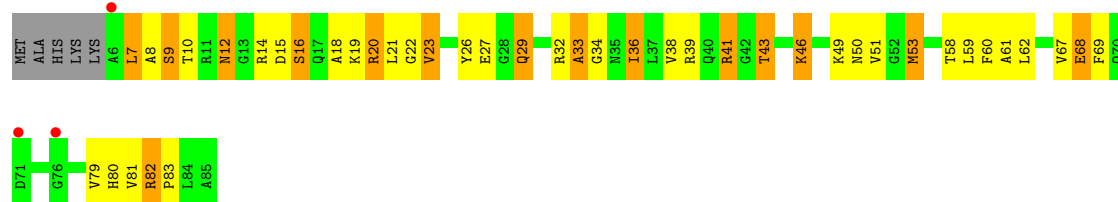
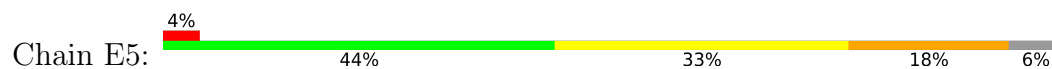
• Molecule 46: 50S ribosomal protein L25



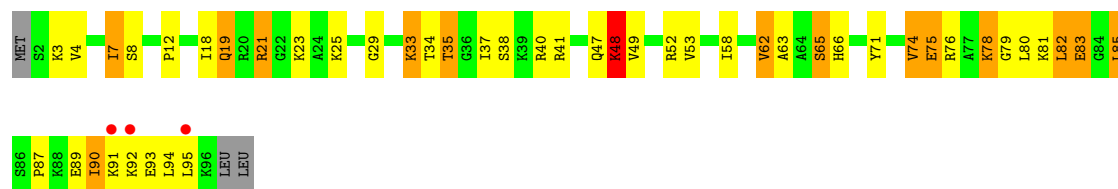
• Molecule 47: 50S ribosomal protein L27



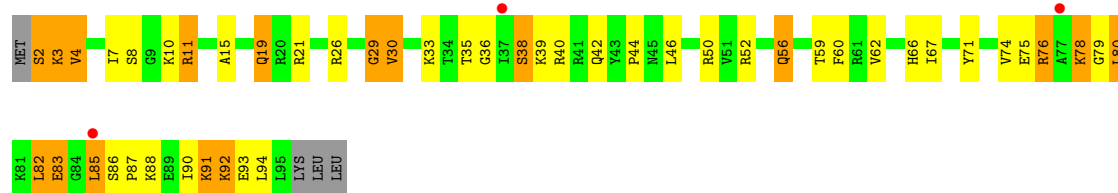
• Molecule 47: 50S ribosomal protein L27



• Molecule 48: 50S ribosomal protein L28



• Molecule 48: 50S ribosomal protein L28



• Molecule 49: 50S ribosomal protein L29



• Molecule 49: 50S ribosomal protein L29



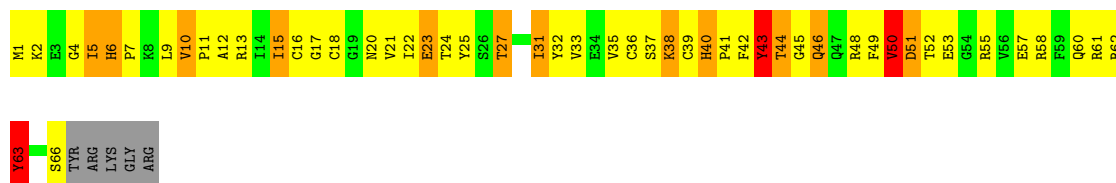
- Molecule 50: 50S ribosomal protein L30



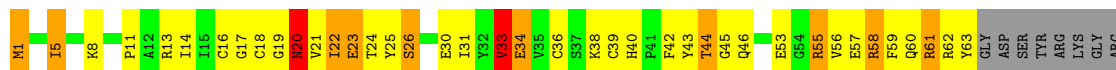
- Molecule 50: 50S ribosomal protein L30



- Molecule 51: 50S ribosomal protein L31



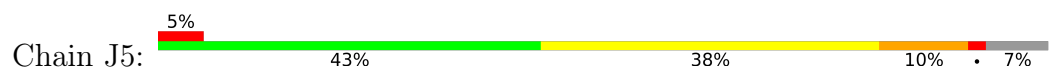
- Molecule 51: 50S ribosomal protein L31



- Molecule 52: 50S ribosomal protein L32



- Molecule 52: 50S ribosomal protein L32





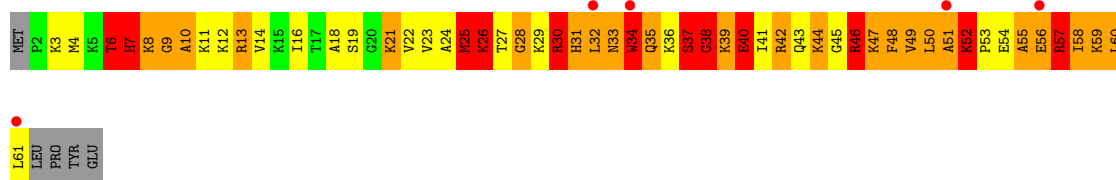
- Molecule 53: 50S ribosomal protein L34



- Molecule 53: 50S ribosomal protein L34



- Molecule 54: 50S ribosomal protein L35



- Molecule 54: 50S ribosomal protein L35



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	209.50Å 449.90Å 618.70Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	153.31 – 3.30 153.31 – 3.30	Depositor EDS
% Data completeness (in resolution range)	100.0 (153.31-3.30) 91.4 (153.31-3.30)	Depositor EDS
R_{merge}	0.54	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.47 (at 3.33Å)	Xtriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.185 , (Not available) (Not available) , 0.217	Depositor DCC
R_{free} test set	2000 reflections (0.23%)	wwPDB-VP
Wilson B-factor (Å ²)	96.6	Xtriage
Anisotropy	0.284	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.27 , 64.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.27$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	299429	wwPDB-VP
Average B, all atoms (Å ²)	116.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.55% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: OMG, PSU, 5MU, MG, 1MG, ZN, H2U

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	0.38	0/36254	0.62	7/56581 (0.0%)
1	1G	0.36	0/36390	0.60	8/56793 (0.0%)
2	12	0.54	0/1959	1.11	16/2642 (0.6%)
2	1E	0.55	0/1959	1.03	6/2642 (0.2%)
3	22	0.58	0/1636	1.02	8/2205 (0.4%)
3	2E	0.63	0/1629	0.98	1/2195 (0.0%)
4	32	0.63	0/1732	1.17	15/2318 (0.6%)
4	3E	0.67	0/1732	1.13	11/2318 (0.5%)
5	42	0.61	0/1171	1.10	7/1576 (0.4%)
5	4E	0.68	0/1171	1.06	5/1576 (0.3%)
6	52	0.63	0/855	1.09	7/1154 (0.6%)
6	5E	0.68	0/855	0.96	3/1154 (0.3%)
7	62	0.53	0/1218	0.99	2/1632 (0.1%)
7	6E	0.53	0/1171	0.93	1/1567 (0.1%)
8	72	0.55	0/1135	1.03	5/1527 (0.3%)
8	7E	0.63	0/1135	1.23	12/1527 (0.8%)
9	82	0.50	0/1002	1.00	1/1346 (0.1%)
9	8E	0.54	0/1028	0.99	1/1379 (0.1%)
10	1A	0.54	0/814	1.02	5/1095 (0.5%)
10	1I	0.68	0/814	1.10	5/1095 (0.5%)
11	2A	0.63	0/879	1.16	5/1187 (0.4%)
11	2I	0.64	0/879	1.17	6/1187 (0.5%)
12	3A	0.76	0/991	1.12	3/1327 (0.2%)
12	3I	0.80	0/972	1.31	8/1301 (0.6%)
13	4A	0.48	0/938	0.93	2/1258 (0.2%)
13	4I	0.54	0/938	1.02	2/1258 (0.2%)
14	5A	0.56	0/484	1.02	2/643 (0.3%)
14	5I	0.66	0/500	1.19	2/664 (0.3%)
15	6A	0.64	0/744	0.95	0/992
15	6I	0.63	0/744	1.04	0/992
16	7A	0.67	0/721	1.08	5/970 (0.5%)
16	7I	0.61	0/721	1.00	0/970

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
17	8A	0.60	0/836	1.03	0/1117
17	8I	0.61	0/847	1.11	5/1131 (0.4%)
18	9A	0.68	0/569	1.19	4/757 (0.5%)
18	9I	0.62	0/555	0.99	2/739 (0.3%)
19	AA	0.56	0/638	1.05	3/860 (0.3%)
19	AI	0.62	1/657 (0.2%)	1.10	3/885 (0.3%)
20	BA	0.63	0/764	1.17	5/1007 (0.5%)
20	BI	0.54	0/764	1.04	5/1007 (0.5%)
21	1B	0.58	0/221	0.99	0/288
21	1F	0.48	0/203	1.07	2/266 (0.8%)
22	1K	0.30	0/1988	0.48	0/3099
22	1L	0.25	0/1988	0.46	0/3099
23	2K	0.42	0/1746	0.71	0/2719
23	2L	0.41	0/1768	0.73	1/2753 (0.0%)
24	3K	0.29	0/1838	0.52	0/2862
24	3L	0.32	0/1786	0.59	1/2778 (0.0%)
25	4K	0.42	0/372	0.52	0/574
25	4L	0.36	0/485	0.45	0/749
26	14	0.45	0/70167	0.68	10/109541 (0.0%)
26	1H	0.48	0/70233	0.71	15/109643 (0.0%)
27	16	0.42	0/2928	0.67	0/4568
27	1J	0.39	0/2928	0.67	0/4568
28	11	0.85	1/2176 (0.0%)	1.32	12/2933 (0.4%)
28	19	0.85	1/2170 (0.0%)	1.36	34/2926 (1.2%)
29	21	0.79	0/1601	1.45	22/2160 (1.0%)
29	29	0.86	0/1601	1.43	20/2160 (0.9%)
30	31	0.84	0/1620	1.29	14/2194 (0.6%)
30	39	0.79	1/1662 (0.1%)	1.36	24/2249 (1.1%)
31	41	0.55	0/1498	1.03	3/2016 (0.1%)
31	49	0.47	0/1498	1.02	6/2016 (0.3%)
32	51	0.73	0/1362	1.37	22/1841 (1.2%)
32	59	0.59	0/1332	1.31	21/1802 (1.2%)
33	61	0.69	0/1151	1.14	10/1558 (0.6%)
33	69	0.64	1/1151 (0.1%)	1.10	6/1558 (0.4%)
34	15	0.67	0/1131	1.16	9/1525 (0.6%)
34	58	0.71	0/1131	1.21	9/1525 (0.6%)
35	25	0.77	0/942	1.19	7/1269 (0.6%)
35	68	0.74	0/942	1.15	5/1269 (0.4%)
36	35	0.75	0/1161	1.51	27/1544 (1.7%)
36	78	0.81	0/1139	1.46	24/1514 (1.6%)
37	45	0.80	1/1134 (0.1%)	1.22	9/1517 (0.6%)
37	88	0.84	1/1142 (0.1%)	1.32	10/1527 (0.7%)
38	55	0.77	0/973	1.16	6/1302 (0.5%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
38	98	0.68	0/981	1.15	6/1312 (0.5%)
39	65	0.72	1/891 (0.1%)	1.27	13/1187 (1.1%)
39	A8	0.70	0/891	1.12	2/1187 (0.2%)
40	75	0.74	0/1155	1.12	6/1542 (0.4%)
40	B8	0.76	0/1095	1.18	4/1463 (0.3%)
41	85	0.72	0/981	1.13	2/1306 (0.2%)
41	C8	0.81	0/981	1.16	6/1306 (0.5%)
42	95	0.83	1/789 (0.1%)	1.29	7/1057 (0.7%)
42	D8	0.74	0/789	1.20	6/1057 (0.6%)
43	A5	0.85	1/910 (0.1%)	1.18	3/1220 (0.2%)
43	E8	0.81	0/901	1.18	4/1209 (0.3%)
44	B5	0.85	0/739	1.20	7/993 (0.7%)
44	F8	0.82	0/756	1.19	6/1014 (0.6%)
45	C5	0.85	0/807	1.31	6/1076 (0.6%)
45	G8	0.96	1/796 (0.1%)	1.45	13/1062 (1.2%)
46	D5	0.61	0/1145	1.19	12/1547 (0.8%)
46	H8	0.62	1/1403 (0.1%)	1.18	10/1901 (0.5%)
47	E5	0.77	0/635	1.33	8/848 (0.9%)
47	I8	0.80	0/665	1.13	3/885 (0.3%)
48	F5	0.79	0/744	1.26	4/989 (0.4%)
48	J8	0.82	0/753	1.26	4/1000 (0.4%)
49	G5	0.67	0/569	1.26	6/753 (0.8%)
49	K8	0.78	0/577	1.32	6/763 (0.8%)
50	H5	0.64	0/473	1.20	3/635 (0.5%)
50	L8	0.79	0/457	1.28	5/613 (0.8%)
51	I5	0.64	0/527	1.19	2/709 (0.3%)
51	M8	0.57	0/545	1.13	2/733 (0.3%)
52	J5	0.82	1/448 (0.2%)	1.28	6/606 (1.0%)
52	N8	0.85	1/443 (0.2%)	1.55	8/599 (1.3%)
53	L5	0.80	0/417	1.18	1/550 (0.2%)
53	P8	0.92	0/417	1.13	1/550 (0.2%)
54	M5	0.86	0/426	1.26	3/556 (0.5%)
54	Q8	1.27	3/486 (0.6%)	1.91	16/638 (2.5%)
All	All	0.52	17/322561 (0.0%)	0.83	708/483352 (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	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
2	1E	0	3
4	32	0	3
4	3E	0	1
9	82	0	1
9	8E	0	1
10	1A	0	1
11	2A	0	1
12	3A	0	2
12	3I	0	1
13	4A	0	1
14	5A	0	1
19	AI	0	2
20	BA	0	2
28	11	0	1
28	19	0	3
29	21	0	4
29	29	0	8
30	31	0	1
30	39	0	6
31	49	0	1
33	61	0	3
33	69	0	3
34	15	0	1
36	35	0	7
36	78	0	2
37	45	0	5
37	88	0	3
38	55	0	2
38	98	0	1
40	75	0	2
40	B8	0	2
41	85	0	2
41	C8	0	1
42	95	0	1
43	A5	0	1
45	C5	0	4
45	G8	0	4
46	H8	0	3
47	E5	0	2
47	I8	0	2
48	F5	0	1
48	J8	0	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
49	G5	0	3
49	K8	0	5
51	I5	0	1
51	M8	0	3
52	J5	0	1
52	N8	0	2
53	P8	0	1
54	M5	0	2
54	Q8	0	12
All	All	0	128

The worst 5 of 17 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
45	G8	79	CYS	CA-C	10.46	1.57	1.52
39	65	88	ASP	CA-C	-6.92	1.49	1.53
42	95	72	VAL	CA-CB	6.58	1.63	1.54
54	Q8	6	THR	CA-CB	6.31	1.64	1.53
52	J5	6	VAL	CA-C	6.26	1.57	1.52

The worst 5 of 708 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	29	52	LEU	CA-C-N	14.73	136.12	119.32
29	29	52	LEU	C-N-CA	14.73	136.12	119.32
32	59	153	LYS	CA-C-N	-14.00	102.34	119.84
32	59	153	LYS	C-N-CA	-14.00	102.34	119.84
36	35	144	GLU	CA-C-N	13.41	133.79	120.52

There are no chirality outliers.

5 of 128 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	1E	15	VAL	Peptide
2	1E	169	LYS	Peptide
2	1E	237	ALA	Peptide
4	3E	31	CYS	Peptide
9	8E	47	LEU	Peptide

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	13	32389	0	16350	724	0
1	1G	32511	0	16414	718	0
2	12	1924	0	1975	101	0
2	1E	1924	0	1975	92	0
3	22	1612	0	1677	84	0
3	2E	1605	0	1668	71	0
4	32	1702	0	1763	106	0
4	3E	1702	0	1763	81	0
5	42	1155	0	1213	52	0
5	4E	1155	0	1213	55	0
6	52	842	0	857	35	0
6	5E	842	0	857	35	0
7	62	1200	0	1238	51	0
7	6E	1157	0	1202	45	0
8	72	1115	0	1177	47	0
8	7E	1115	0	1177	43	0
9	82	983	0	1006	79	0
9	8E	1009	0	1037	69	0
10	1A	801	0	849	58	0
10	1I	801	0	849	54	0
11	2A	864	0	881	38	0
11	2I	864	0	881	40	0
12	3A	975	0	1062	42	0
12	3I	956	0	1046	48	0
13	4A	928	0	987	53	0
13	4I	928	0	987	58	0
14	5A	475	0	511	36	0
14	5I	491	0	529	33	0
15	6A	733	0	771	34	0
15	6I	733	0	771	26	0
16	7A	705	0	725	27	0
16	7I	705	0	725	41	0
17	8A	823	0	891	32	0
17	8I	834	0	904	39	0
18	9A	564	0	631	26	0
18	9I	550	0	613	23	0
19	AA	624	0	636	42	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
19	AI	643	0	662	43	0
20	BA	762	0	861	42	0
20	BI	762	0	861	41	0
21	1B	217	0	234	11	0
21	1F	199	0	208	8	0
22	1K	1863	0	942	42	0
22	1L	1863	0	942	37	0
23	2K	1692	0	859	44	0
23	2L	1712	0	870	61	0
24	3K	1646	0	830	36	0
24	3L	1601	0	809	30	0
25	4K	336	0	168	8	0
25	4L	438	0	220	11	0
26	14	62647	0	31582	1260	0
26	1H	62707	0	31614	1355	1
27	16	2617	0	1328	60	0
27	1J	2617	0	1328	71	0
28	11	2126	0	2208	91	0
28	19	2120	0	2197	88	0
29	21	1568	0	1634	97	0
29	29	1568	0	1634	109	0
30	31	1585	0	1632	88	0
30	39	1627	0	1680	99	0
31	41	1473	0	1535	96	0
31	49	1473	0	1535	70	0
32	51	1336	0	1418	81	0
32	59	1307	0	1382	73	0
33	61	1136	0	1223	59	0
33	69	1136	0	1223	58	0
34	15	1104	0	1180	55	0
34	58	1104	0	1180	58	0
35	25	932	0	996	44	0
35	68	932	0	996	36	0
36	35	1144	0	1228	85	0
36	78	1122	0	1206	98	0
37	45	1113	0	1167	64	0
37	88	1121	0	1179	69	0
38	55	959	0	1021	53	0
38	98	967	0	1033	58	0
39	65	881	0	943	59	0
39	A8	881	0	943	57	0
40	75	1141	0	1202	55	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
40	B8	1081	0	1141	65	0
41	85	963	0	1022	65	0
41	C8	963	0	1022	64	0
42	95	778	0	852	64	0
42	D8	778	0	852	42	0
43	A5	899	0	964	34	0
43	E8	890	0	951	32	0
44	B5	725	0	778	41	0
44	F8	742	0	803	32	0
45	C5	794	0	884	52	0
45	G8	783	0	870	45	0
46	D5	1120	0	1146	55	0
46	H8	1373	0	1402	80	0
47	E5	627	0	645	41	0
47	I8	656	0	679	32	0
48	F5	737	0	813	40	0
48	J8	746	0	826	35	0
49	G5	567	0	618	21	0
49	K8	575	0	634	39	0
50	H5	468	0	518	15	1
50	L8	452	0	503	19	0
51	I5	515	0	514	33	0
51	M8	533	0	526	51	0
52	J5	434	0	454	21	0
52	N8	429	0	449	31	0
53	L5	409	0	454	22	0
53	P8	409	0	454	19	0
54	M5	422	0	484	30	0
54	Q8	480	0	549	96	0
55	11	1	0	0	0	0
55	13	146	0	0	0	0
55	14	490	0	0	0	0
55	16	5	0	0	0	0
55	1G	143	0	0	0	0
55	1H	512	0	0	0	0
55	1J	2	0	0	0	0
55	1K	1	0	0	0	0
55	21	2	0	0	0	0
55	25	1	0	0	0	0
55	29	3	0	0	0	0
55	2K	3	0	0	0	0
55	2L	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
55	31	1	0	0	0	0
55	32	1	0	0	0	0
55	3E	1	0	0	0	0
55	3I	1	0	0	0	0
55	45	2	0	0	0	0
55	5E	1	0	0	0	0
55	78	1	0	0	0	0
55	7A	1	0	0	0	0
55	85	2	0	0	0	0
55	88	4	0	0	0	0
55	98	1	0	0	0	0
55	E5	2	0	0	0	0
55	G8	1	0	0	0	0
55	I8	2	0	0	0	0
55	J8	1	0	0	0	0
55	P8	1	0	0	0	0
56	32	1	0	0	0	0
56	3E	1	0	0	0	0
56	5A	1	0	0	0	0
56	5I	1	0	0	0	0
56	C5	1	0	0	0	0
56	G8	1	0	0	0	0
57	11	1	0	0	0	0
57	13	74	0	0	11	0
57	14	520	0	0	102	0
57	19	8	0	0	2	0
57	1G	73	0	0	6	0
57	1H	552	0	0	122	0
57	21	1	0	0	1	0
57	29	2	0	0	0	0
57	31	4	0	0	2	0
57	35	1	0	0	0	0
57	39	4	0	0	0	0
57	3E	1	0	0	0	0
57	4L	2	0	0	0	0
57	55	2	0	0	0	0
57	6A	2	0	0	0	0
57	6I	1	0	0	0	0
57	78	2	0	0	0	0
57	7A	1	0	0	0	0
57	85	1	0	0	0	0
57	A5	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
57	B8	1	0	0	0	0
57	BI	1	0	0	0	0
57	C8	2	0	0	1	0
57	D8	1	0	0	0	0
57	E8	1	0	0	0	0
57	I8	3	0	0	0	0
57	J8	1	0	0	0	0
57	M5	3	0	0	0	0
57	P8	1	0	0	0	0
All	All	299429	0	199511	8330	1

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 17.

The worst 5 of 8330 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)
26:1H:2032:G:N7	57:1H:4116:HOH:O	1.81	1.11
2:12:185:ILE:HG22	2:12:199:TYR:HB2	1.39	1.04
26:1H:810:U:OP1	57:1H:4123:HOH:O	1.75	1.03
26:1H:2308:G:H1	26:1H:2311:A:H2	1.07	1.02
26:1H:763:G:OP1	57:1H:3623:HOH:O	1.80	1.00

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

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:1H:654(O):G:N2	50:H5:57:GLU:OE1[2_464]	2.18	0.02

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	12	235/256 (92%)	198 (84%)	35 (15%)	2 (1%)	14	43
2	1E	235/256 (92%)	200 (85%)	33 (14%)	2 (1%)	14	43
3	22	204/239 (85%)	181 (89%)	23 (11%)	0	100	100
3	2E	203/239 (85%)	185 (91%)	18 (9%)	0	100	100
4	32	206/209 (99%)	175 (85%)	30 (15%)	1 (0%)	24	55
4	3E	206/209 (99%)	194 (94%)	9 (4%)	3 (2%)	8	32
5	42	149/162 (92%)	139 (93%)	10 (7%)	0	100	100
5	4E	149/162 (92%)	142 (95%)	6 (4%)	1 (1%)	18	49
6	52	99/101 (98%)	97 (98%)	2 (2%)	0	100	100
6	5E	99/101 (98%)	94 (95%)	5 (5%)	0	100	100
7	62	143/156 (92%)	137 (96%)	6 (4%)	0	100	100
7	6E	140/156 (90%)	134 (96%)	6 (4%)	0	100	100
8	72	136/138 (99%)	125 (92%)	10 (7%)	1 (1%)	18	49
8	7E	136/138 (99%)	124 (91%)	11 (8%)	1 (1%)	18	49
9	82	122/128 (95%)	109 (89%)	12 (10%)	1 (1%)	16	45
9	8E	125/128 (98%)	106 (85%)	19 (15%)	0	100	100
10	1A	97/105 (92%)	90 (93%)	7 (7%)	0	100	100
10	1I	97/105 (92%)	90 (93%)	7 (7%)	0	100	100
11	2A	114/129 (88%)	103 (90%)	8 (7%)	3 (3%)	4	23
11	2I	114/129 (88%)	102 (90%)	10 (9%)	2 (2%)	6	29
12	3A	123/132 (93%)	99 (80%)	20 (16%)	4 (3%)	3	19
12	3I	120/132 (91%)	102 (85%)	18 (15%)	0	100	100
13	4A	114/126 (90%)	95 (83%)	18 (16%)	1 (1%)	14	43
13	4I	114/126 (90%)	95 (83%)	18 (16%)	1 (1%)	14	43
14	5A	56/61 (92%)	46 (82%)	9 (16%)	1 (2%)	6	29
14	5I	58/61 (95%)	49 (84%)	8 (14%)	1 (2%)	7	30
15	6A	86/89 (97%)	81 (94%)	5 (6%)	0	100	100
15	6I	86/89 (97%)	80 (93%)	6 (7%)	0	100	100
16	7A	82/88 (93%)	77 (94%)	5 (6%)	0	100	100
16	7I	82/88 (93%)	76 (93%)	6 (7%)	0	100	100
17	8A	97/105 (92%)	92 (95%)	5 (5%)	0	100	100
17	8I	98/105 (93%)	91 (93%)	7 (7%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
18	9A	67/88 (76%)	61 (91%)	6 (9%)	0	100	100
18	9I	65/88 (74%)	63 (97%)	1 (2%)	1 (2%)	8	32
19	AA	76/93 (82%)	62 (82%)	12 (16%)	2 (3%)	4	23
19	AI	78/93 (84%)	65 (83%)	11 (14%)	2 (3%)	4	23
20	BA	97/106 (92%)	87 (90%)	8 (8%)	2 (2%)	5	26
20	BI	97/106 (92%)	82 (84%)	15 (16%)	0	100	100
21	1B	23/27 (85%)	21 (91%)	2 (9%)	0	100	100
21	1F	21/27 (78%)	20 (95%)	1 (5%)	0	100	100
28	11	271/276 (98%)	257 (95%)	10 (4%)	4 (2%)	8	32
28	19	271/276 (98%)	247 (91%)	17 (6%)	7 (3%)	4	23
29	21	203/206 (98%)	162 (80%)	32 (16%)	9 (4%)	2	13
29	29	203/206 (98%)	154 (76%)	38 (19%)	11 (5%)	1	10
30	31	200/210 (95%)	183 (92%)	15 (8%)	2 (1%)	12	40
30	39	206/210 (98%)	165 (80%)	33 (16%)	8 (4%)	2	16
31	41	179/182 (98%)	156 (87%)	20 (11%)	3 (2%)	7	30
31	49	179/182 (98%)	153 (86%)	24 (13%)	2 (1%)	11	39
32	51	172/180 (96%)	148 (86%)	17 (10%)	7 (4%)	2	15
32	59	168/180 (93%)	131 (78%)	33 (20%)	4 (2%)	4	24
33	61	144/148 (97%)	117 (81%)	24 (17%)	3 (2%)	5	26
33	69	144/148 (97%)	116 (81%)	25 (17%)	3 (2%)	5	26
34	15	136/140 (97%)	119 (88%)	16 (12%)	1 (1%)	18	49
34	58	136/140 (97%)	118 (87%)	15 (11%)	3 (2%)	5	26
35	25	120/122 (98%)	115 (96%)	5 (4%)	0	100	100
35	68	120/122 (98%)	114 (95%)	6 (5%)	0	100	100
36	35	148/150 (99%)	115 (78%)	24 (16%)	9 (6%)	1	9
36	78	145/150 (97%)	117 (81%)	23 (16%)	5 (3%)	3	18
37	45	138/141 (98%)	109 (79%)	27 (20%)	2 (1%)	9	33
37	88	139/141 (99%)	115 (83%)	21 (15%)	3 (2%)	5	26
38	55	115/118 (98%)	101 (88%)	12 (10%)	2 (2%)	7	30
38	98	116/118 (98%)	101 (87%)	14 (12%)	1 (1%)	14	43
39	65	109/112 (97%)	87 (80%)	20 (18%)	2 (2%)	6	29

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
39	A8	109/112 (97%)	92 (84%)	16 (15%)	1 (1%)	14	43
40	75	135/146 (92%)	120 (89%)	14 (10%)	1 (1%)	18	49
40	B8	127/146 (87%)	113 (89%)	14 (11%)	0	100	100
41	85	115/118 (98%)	104 (90%)	10 (9%)	1 (1%)	14	43
41	C8	115/118 (98%)	104 (90%)	8 (7%)	3 (3%)	4	23
42	95	99/101 (98%)	77 (78%)	17 (17%)	5 (5%)	1	11
42	D8	99/101 (98%)	91 (92%)	6 (6%)	2 (2%)	6	27
43	A5	111/113 (98%)	104 (94%)	5 (4%)	2 (2%)	6	29
43	E8	110/113 (97%)	101 (92%)	9 (8%)	0	100	100
44	B5	90/96 (94%)	84 (93%)	4 (4%)	2 (2%)	5	26
44	F8	92/96 (96%)	83 (90%)	7 (8%)	2 (2%)	5	26
45	C5	102/110 (93%)	73 (72%)	24 (24%)	5 (5%)	1	12
45	G8	101/110 (92%)	78 (77%)	19 (19%)	4 (4%)	2	15
46	D5	129/206 (63%)	101 (78%)	24 (19%)	4 (3%)	3	20
46	H8	169/206 (82%)	137 (81%)	26 (15%)	6 (4%)	2	17
47	E5	78/85 (92%)	68 (87%)	9 (12%)	1 (1%)	9	35
47	I8	81/85 (95%)	74 (91%)	7 (9%)	0	100	100
48	F5	92/98 (94%)	82 (89%)	9 (10%)	1 (1%)	11	39
48	J8	93/98 (95%)	84 (90%)	7 (8%)	2 (2%)	5	26
49	G5	65/72 (90%)	61 (94%)	2 (3%)	2 (3%)	3	20
49	K8	66/72 (92%)	61 (92%)	2 (3%)	3 (4%)	2	13
50	H5	57/60 (95%)	55 (96%)	2 (4%)	0	100	100
50	L8	55/60 (92%)	53 (96%)	1 (2%)	1 (2%)	6	29
51	I5	61/71 (86%)	35 (57%)	23 (38%)	3 (5%)	1	12
51	M8	64/71 (90%)	41 (64%)	20 (31%)	3 (5%)	2	12
52	J5	54/60 (90%)	50 (93%)	4 (7%)	0	100	100
52	N8	53/60 (88%)	46 (87%)	5 (9%)	2 (4%)	2	16
53	L5	45/49 (92%)	44 (98%)	1 (2%)	0	100	100
53	P8	45/49 (92%)	41 (91%)	3 (7%)	1 (2%)	5	26
54	M5	49/65 (75%)	41 (84%)	7 (14%)	1 (2%)	6	27
54	Q8	58/65 (89%)	34 (59%)	18 (31%)	6 (10%)	0	2

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	11130/11946 (93%)	9701 (87%)	1242 (11%)	187 (2%)	7 30

5 of 187 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
29	21	83	ASP
32	51	169	VAL
36	78	57	THR
38	98	11	ASN
46	H8	165	VAL

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
2	12	205/220 (93%)	155 (76%)	50 (24%)	1 3
2	1E	205/220 (93%)	158 (77%)	47 (23%)	1 4
3	22	160/188 (85%)	119 (74%)	41 (26%)	0 2
3	2E	159/188 (85%)	116 (73%)	43 (27%)	0 2
4	32	180/181 (99%)	140 (78%)	40 (22%)	1 5
4	3E	180/181 (99%)	147 (82%)	33 (18%)	2 7
5	42	116/123 (94%)	81 (70%)	35 (30%)	0 1
5	4E	116/123 (94%)	87 (75%)	29 (25%)	0 3
6	52	90/90 (100%)	64 (71%)	26 (29%)	0 2
6	5E	90/90 (100%)	71 (79%)	19 (21%)	1 5
7	62	121/127 (95%)	91 (75%)	30 (25%)	1 3
7	6E	118/127 (93%)	99 (84%)	19 (16%)	2 12
8	72	119/119 (100%)	99 (83%)	20 (17%)	2 11
8	7E	119/119 (100%)	88 (74%)	31 (26%)	0 2
9	82	95/99 (96%)	81 (85%)	14 (15%)	3 14
9	8E	98/99 (99%)	71 (72%)	27 (28%)	0 2

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
10	1A	89/92 (97%)	72 (81%)	17 (19%)	1	7
10	1I	89/92 (97%)	71 (80%)	18 (20%)	1	6
11	2A	88/99 (89%)	71 (81%)	17 (19%)	1	6
11	2I	88/99 (89%)	71 (81%)	17 (19%)	1	6
12	3A	104/109 (95%)	72 (69%)	32 (31%)	0	1
12	3I	103/109 (94%)	82 (80%)	21 (20%)	1	6
13	4A	94/101 (93%)	76 (81%)	18 (19%)	1	7
13	4I	94/101 (93%)	71 (76%)	23 (24%)	1	3
14	5A	48/50 (96%)	41 (85%)	7 (15%)	3	14
14	5I	49/50 (98%)	36 (74%)	13 (26%)	0	2
15	6A	79/80 (99%)	68 (86%)	11 (14%)	3	15
15	6I	79/80 (99%)	66 (84%)	13 (16%)	2	11
16	7A	72/74 (97%)	54 (75%)	18 (25%)	0	3
16	7I	72/74 (97%)	58 (81%)	14 (19%)	1	6
17	8A	94/97 (97%)	76 (81%)	18 (19%)	1	7
17	8I	95/97 (98%)	77 (81%)	18 (19%)	1	7
18	9A	60/77 (78%)	46 (77%)	14 (23%)	1	4
18	9I	59/77 (77%)	44 (75%)	15 (25%)	0	3
19	AA	67/80 (84%)	56 (84%)	11 (16%)	2	11
19	AI	70/80 (88%)	50 (71%)	20 (29%)	0	2
20	BA	76/82 (93%)	63 (83%)	13 (17%)	2	10
20	BI	76/82 (93%)	58 (76%)	18 (24%)	1	4
21	1B	20/22 (91%)	18 (90%)	2 (10%)	7	27
21	1F	18/22 (82%)	17 (94%)	1 (6%)	19	47
28	11	215/218 (99%)	172 (80%)	43 (20%)	1	6
28	19	214/218 (98%)	163 (76%)	51 (24%)	1	4
29	21	165/166 (99%)	121 (73%)	44 (27%)	0	2
29	29	165/166 (99%)	121 (73%)	44 (27%)	0	2
30	31	161/166 (97%)	123 (76%)	38 (24%)	1	4
30	39	165/166 (99%)	122 (74%)	43 (26%)	0	2
31	41	155/156 (99%)	117 (76%)	38 (24%)	1	3

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
31	49	155/156 (99%)	126 (81%)	29 (19%)	1	7
32	51	145/148 (98%)	104 (72%)	41 (28%)	0	2
32	59	142/148 (96%)	106 (75%)	36 (25%)	0	3
33	61	122/124 (98%)	87 (71%)	35 (29%)	0	2
33	69	122/124 (98%)	84 (69%)	38 (31%)	0	1
34	15	117/119 (98%)	83 (71%)	34 (29%)	0	2
34	58	117/119 (98%)	88 (75%)	29 (25%)	1	3
35	25	100/100 (100%)	71 (71%)	29 (29%)	0	2
35	68	100/100 (100%)	74 (74%)	26 (26%)	0	2
36	35	116/116 (100%)	73 (63%)	43 (37%)	0	1
36	78	114/116 (98%)	80 (70%)	34 (30%)	0	1
37	45	110/111 (99%)	77 (70%)	33 (30%)	0	1
37	88	111/111 (100%)	81 (73%)	30 (27%)	0	2
38	55	100/101 (99%)	70 (70%)	30 (30%)	0	1
38	98	101/101 (100%)	72 (71%)	29 (29%)	0	2
39	65	87/88 (99%)	59 (68%)	28 (32%)	0	1
39	A8	87/88 (99%)	60 (69%)	27 (31%)	0	1
40	75	120/127 (94%)	84 (70%)	36 (30%)	0	1
40	B8	115/127 (91%)	79 (69%)	36 (31%)	0	1
41	85	93/94 (99%)	77 (83%)	16 (17%)	2	10
41	C8	93/94 (99%)	75 (81%)	18 (19%)	1	6
42	95	82/82 (100%)	58 (71%)	24 (29%)	0	2
42	D8	82/82 (100%)	55 (67%)	27 (33%)	0	1
43	A5	92/92 (100%)	68 (74%)	24 (26%)	0	2
43	E8	91/92 (99%)	67 (74%)	24 (26%)	0	2
44	B5	74/78 (95%)	54 (73%)	20 (27%)	0	2
44	F8	76/78 (97%)	60 (79%)	16 (21%)	1	5
45	C5	85/91 (93%)	55 (65%)	30 (35%)	0	1
45	G8	84/91 (92%)	56 (67%)	28 (33%)	0	1
46	D5	125/179 (70%)	92 (74%)	33 (26%)	0	2
46	H8	152/179 (85%)	116 (76%)	36 (24%)	1	4

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
47	E5	62/67 (92%)	46 (74%)	16 (26%)	0	2
47	I8	66/67 (98%)	52 (79%)	14 (21%)	1	5
48	F5	79/83 (95%)	56 (71%)	23 (29%)	0	2
48	J8	80/83 (96%)	58 (72%)	22 (28%)	0	2
49	G5	63/67 (94%)	45 (71%)	18 (29%)	0	2
49	K8	64/67 (96%)	43 (67%)	21 (33%)	0	1
50	H5	51/52 (98%)	38 (74%)	13 (26%)	0	3
50	L8	49/52 (94%)	38 (78%)	11 (22%)	1	5
51	I5	57/63 (90%)	41 (72%)	16 (28%)	0	2
51	M8	59/63 (94%)	43 (73%)	16 (27%)	0	2
52	J5	48/52 (92%)	38 (79%)	10 (21%)	1	6
52	N8	48/52 (92%)	36 (75%)	12 (25%)	0	3
53	L5	40/42 (95%)	27 (68%)	13 (32%)	0	1
53	P8	40/42 (95%)	31 (78%)	9 (22%)	1	5
54	M5	44/55 (80%)	30 (68%)	14 (32%)	0	1
54	Q8	50/55 (91%)	28 (56%)	22 (44%)	0	0
All	All	9404/9894 (95%)	7061 (75%)	2343 (25%)	0	3

5 of 2343 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
34	15	46	VAL
51	I5	20	ASN
36	35	18	ARG
34	15	37	LYS
41	85	74	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 57 such sidechains are listed below:

Mol	Chain	Res	Type
4	32	201	GLN
49	G5	38	GLN
9	82	58	HIS
48	F5	19	GLN
37	45	12	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	13	1505/1522 (98%)	330 (21%)	31 (2%)
1	1G	1512/1522 (99%)	371 (24%)	38 (2%)
22	1K	86/87 (98%)	23 (26%)	1 (1%)
22	1L	86/87 (98%)	31 (36%)	4 (4%)
23	2K	77/87 (88%)	32 (41%)	8 (10%)
23	2L	79/87 (90%)	32 (40%)	8 (10%)
24	3K	75/87 (86%)	35 (46%)	4 (5%)
24	3L	72/87 (82%)	34 (47%)	5 (6%)
25	4K	14/60 (23%)	6 (42%)	0
25	4L	19/60 (31%)	5 (26%)	0
26	14	2908/2917 (99%)	700 (24%)	40 (1%)
26	1H	2911/2917 (99%)	674 (23%)	52 (1%)
27	16	121/122 (99%)	21 (17%)	1 (0%)
27	1J	121/122 (99%)	36 (29%)	4 (3%)
All	All	9586/9764 (98%)	2330 (24%)	196 (2%)

5 of 2330 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	13	5	U
1	13	6	G
1	13	8	A
1	13	9	G
1	13	10	A

5 of 196 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	1G	723	U
23	2L	44	G
1	1G	992	U
1	1G	1300	G
24	3L	83	U

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

20 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
23	OMG	2K	18	23	23,26,27	5.23	11 (47%)	32,38,41	4.71	17 (53%)
23	H2U	2K	17	23	18,21,22	2.25	4 (22%)	19,30,33	1.93	4 (21%)
22	PSU	1L	66	22	18,21,22	1.03	1 (5%)	21,30,33	1.76	3 (14%)
23	1MG	2L	38	23	23,26,27	2.95	6 (26%)	33,39,42	1.82	9 (27%)
23	H2U	2L	17	23	18,21,22	1.98	4 (22%)	19,30,33	1.76	4 (21%)
22	1MG	1L	38	22	23,26,27	2.87	6 (26%)	33,39,42	1.74	9 (27%)
23	5MU	2K	65	23	19,22,23	3.95	5 (26%)	27,32,35	3.30	10 (37%)
22	PSU	1L	39	22	18,21,22	1.40	2 (11%)	21,30,33	1.53	3 (14%)
23	PSU	2K	39	23	18,21,22	1.10	1 (5%)	21,30,33	1.92	3 (14%)
23	PSU	2K	66	23	18,21,22	1.51	1 (5%)	21,30,33	1.94	4 (19%)
22	PSU	1K	39	22	18,21,22	1.31	1 (5%)	21,30,33	1.59	2 (9%)
23	PSU	2L	66	23	18,21,22	1.30	1 (5%)	21,30,33	1.72	3 (14%)
22	5MU	1K	65	22	19,22,23	3.91	5 (26%)	27,32,35	3.20	9 (33%)
23	5MU	2L	65	23	19,22,23	3.97	5 (26%)	27,32,35	3.25	9 (33%)
23	1MG	2K	38	23	23,26,27	2.60	6 (26%)	33,39,42	1.63	7 (21%)
23	PSU	2L	39	23	18,21,22	1.10	1 (5%)	21,30,33	1.88	3 (14%)
23	OMG	2L	18	23	23,26,27	5.22	10 (43%)	32,38,41	4.69	15 (46%)
22	PSU	1K	66	22	18,21,22	1.27	1 (5%)	21,30,33	1.86	4 (19%)
22	5MU	1L	65	22	19,22,23	3.89	5 (26%)	27,32,35	3.22	9 (33%)
22	1MG	1K	38	22	23,26,27	2.83	6 (26%)	33,39,42	1.92	11 (33%)

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
23	OMG	2K	18	23	-	0/9/27/28	0/3/3/3
23	H2U	2K	17	23	-	0/7/38/39	0/2/2/2
22	PSU	1L	66	22	-	2/7/25/26	0/2/2/2
23	1MG	2L	38	23	-	0/7/25/26	0/3/3/3
23	H2U	2L	17	23	-	1/7/38/39	0/2/2/2
22	1MG	1L	38	22	-	0/7/25/26	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
23	5MU	2K	65	23	-	0/7/25/26	0/2/2/2
22	PSU	1L	39	22	-	0/7/25/26	0/2/2/2
23	PSU	2K	39	23	-	0/7/25/26	0/2/2/2
23	PSU	2K	66	23	-	0/7/25/26	0/2/2/2
22	PSU	1K	39	22	-	0/7/25/26	0/2/2/2
23	PSU	2L	66	23	-	0/7/25/26	0/2/2/2
22	5MU	1K	65	22	-	0/7/25/26	0/2/2/2
23	5MU	2L	65	23	-	3/7/25/26	0/2/2/2
23	1MG	2K	38	23	-	0/7/25/26	0/3/3/3
23	PSU	2L	39	23	-	0/7/25/26	0/2/2/2
23	OMG	2L	18	23	-	3/9/27/28	0/3/3/3
22	PSU	1K	66	22	-	0/7/25/26	0/2/2/2
22	5MU	1L	65	22	-	0/7/25/26	0/2/2/2
22	1MG	1K	38	22	-	2/7/25/26	0/3/3/3

The worst 5 of 82 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	2L	65	5MU	C2-N1	13.07	1.58	1.38
22	1K	65	5MU	C2-N1	12.62	1.58	1.38
23	2K	65	5MU	C2-N1	12.60	1.58	1.38
23	2K	18	OMG	C4-N3	12.56	1.63	1.34
22	1L	65	5MU	C2-N1	12.48	1.58	1.38

The worst 5 of 138 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	2K	65	5MU	C5-C4-N3	11.27	125.12	115.32
23	2K	18	OMG	C6-C5-N7	10.86	150.06	130.29
22	1K	65	5MU	C5-C4-N3	10.42	124.38	115.32
23	2K	18	OMG	C8-N7-C5	10.40	122.79	104.26
23	2L	18	OMG	N9-C4-N3	10.33	146.61	125.95

There are no chirality outliers.

5 of 11 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
23	2L	18	OMG	C4'-C5'-O5'-P
23	2L	18	OMG	O4'-C4'-C5'-O5'
23	2L	65	5MU	C3'-C4'-C5'-O5'
23	2L	65	5MU	O4'-C4'-C5'-O5'

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Mol	Chain	Res	Type	Atoms
23	2L	18	OMG	C3'-C4'-C5'-O5'

There are no ring outliers.

9 monomers are involved in 10 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
23	2K	18	OMG	2	0
23	2L	38	1MG	2	0
22	1K	39	PSU	1	0
23	2L	66	PSU	1	0
23	2L	65	5MU	1	0
23	2L	39	PSU	2	0
23	2L	18	OMG	2	0
22	1L	65	5MU	1	0
22	1K	38	1MG	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 1340 ligands modelled in this entry, 1340 are monoatomic - leaving 0 for Mogul analysis.

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.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues

The following chains have linkage breaks:

Mol	Chain	Number of breaks
25	4K	1
25	4L	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	4K	38:U	O3'	44:U	P	28.59
1	4L	40:U	O3'	44:U	P	16.09

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	13	1507/1522 (99%)	-0.38	15 (0%) 79 63	70, 113, 194, 267	0
1	1G	1513/1522 (99%)	-0.41	10 (0%) 84 70	79, 120, 189, 288	0
2	12	237/256 (92%)	0.20	7 (2%) 52 35	133, 170, 199, 207	0
2	1E	237/256 (92%)	-0.01	0 100 100	116, 156, 187, 198	0
3	22	206/239 (86%)	0.20	7 (3%) 48 32	128, 150, 185, 189	0
3	2E	205/239 (85%)	-0.27	1 (0%) 87 76	94, 120, 157, 169	0
4	32	208/209 (99%)	0.31	12 (5%) 29 19	100, 121, 146, 158	0
4	3E	208/209 (99%)	0.21	9 (4%) 40 25	91, 113, 135, 145	0
5	42	151/162 (93%)	0.12	1 (0%) 84 70	105, 124, 142, 169	0
5	4E	151/162 (93%)	0.03	4 (2%) 57 38	89, 108, 128, 159	0
6	52	101/101 (100%)	-0.38	0 100 100	87, 107, 126, 138	0
6	5E	101/101 (100%)	-0.17	5 (4%) 34 23	87, 109, 129, 140	0
7	62	147/156 (94%)	-0.19	3 (2%) 65 46	123, 138, 159, 171	0
7	6E	144/156 (92%)	0.02	8 (5%) 30 20	118, 136, 154, 175	0
8	72	138/138 (100%)	0.10	2 (1%) 73 55	100, 125, 141, 147	0
8	7E	138/138 (100%)	-0.09	2 (1%) 73 55	97, 116, 130, 141	0
9	82	124/128 (96%)	0.36	7 (5%) 30 20	112, 154, 172, 181	0
9	8E	127/128 (99%)	0.40	7 (5%) 30 21	105, 145, 167, 173	0
10	1A	99/105 (94%)	0.43	7 (7%) 22 15	126, 158, 184, 196	0
10	1I	99/105 (94%)	0.16	1 (1%) 79 63	96, 144, 175, 179	0
11	2A	116/129 (89%)	-0.06	3 (2%) 57 38	92, 114, 138, 155	0
11	2I	116/129 (89%)	0.07	5 (4%) 40 25	86, 117, 142, 184	0
12	3A	125/132 (94%)	0.14	9 (7%) 21 15	91, 108, 136, 189	0
12	3I	122/132 (92%)	-0.21	1 (0%) 82 68	78, 86, 112, 144	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å ²)	Q<0.9
13	4A	116/126 (92%)	0.03	5 (4%)	40	25	128, 165, 190, 202	0
13	4I	116/126 (92%)	0.02	3 (2%)	57	38	106, 146, 164, 175	0
14	5A	58/61 (95%)	0.74	7 (12%)	8	7	131, 143, 165, 167	0
14	5I	60/61 (98%)	0.20	1 (1%)	69	50	98, 110, 131, 142	0
15	6A	88/89 (98%)	-0.09	0	100	100	90, 113, 134, 136	0
15	6I	88/89 (98%)	-0.12	0	100	100	87, 108, 130, 139	0
16	7A	84/88 (95%)	0.02	1 (1%)	76	58	93, 108, 135, 169	0
16	7I	84/88 (95%)	0.55	3 (3%)	46	31	108, 120, 155, 187	0
17	8A	99/105 (94%)	0.12	3 (3%)	52	35	98, 112, 126, 131	0
17	8I	100/105 (95%)	0.20	5 (5%)	34	23	95, 113, 129, 133	0
18	9A	69/88 (78%)	-0.28	1 (1%)	73	55	93, 115, 139, 172	0
18	9I	67/88 (76%)	-0.11	0	100	100	93, 111, 135, 144	0
19	AA	78/93 (83%)	0.02	2 (2%)	57	38	150, 182, 201, 206	0
19	AI	80/93 (86%)	0.07	2 (2%)	58	39	116, 149, 171, 175	0
20	BA	99/106 (93%)	0.00	2 (2%)	65	46	90, 115, 143, 158	0
20	BI	99/106 (93%)	0.54	9 (9%)	15	11	113, 132, 170, 175	0
21	1B	25/27 (92%)	1.85	12 (48%)	0	0	121, 142, 155, 172	0
21	1F	23/27 (85%)	0.87	4 (17%)	4	4	115, 129, 133, 136	0
22	1K	83/87 (95%)	-0.21	5 (6%)	27	19	95, 175, 257, 267	0
22	1L	83/87 (95%)	-0.08	3 (3%)	46	31	111, 193, 298, 318	0
23	2K	73/87 (83%)	0.11	6 (8%)	17	13	90, 130, 190, 235	0
23	2L	74/87 (85%)	-0.15	0	100	100	89, 140, 212, 243	0
24	3K	77/87 (88%)	0.26	1 (1%)	75	56	82, 248, 274, 282	0
24	3L	75/87 (86%)	-0.04	2 (2%)	56	37	82, 207, 221, 226	0
25	4K	16/60 (26%)	0.23	0	100	100	89, 147, 205, 218	0
25	4L	21/60 (35%)	0.16	0	100	100	105, 147, 219, 221	0
26	14	2909/2917 (99%)	-0.64	12 (0%)	88	79	61, 91, 244, 328	0
26	1H	2912/2917 (99%)	-0.68	4 (0%)	92	90	55, 86, 243, 301	0
27	16	122/122 (100%)	-0.61	0	100	100	87, 113, 138, 224	0
27	1J	122/122 (100%)	-0.43	2 (1%)	70	52	92, 126, 154, 207	0
28	11	273/276 (98%)	-0.03	4 (1%)	72	53	55, 76, 93, 103	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
28	19	273/276 (98%)	-0.12	3 (1%) 78 60	60, 80, 97, 113	0
29	21	205/206 (99%)	0.18	9 (4%) 39 25	63, 98, 141, 156	0
29	29	205/206 (99%)	0.13	6 (2%) 53 35	68, 96, 137, 158	0
30	31	202/210 (96%)	-0.26	0 100 100	59, 88, 127, 140	0
30	39	208/210 (99%)	-0.15	0 100 100	67, 106, 167, 200	0
31	41	181/182 (99%)	0.00	6 (3%) 49 33	113, 144, 175, 183	0
31	49	181/182 (99%)	0.02	1 (0%) 85 73	131, 162, 190, 207	0
32	51	174/180 (96%)	0.00	2 (1%) 78 60	93, 118, 133, 143	0
32	59	170/180 (94%)	0.52	16 (9%) 14 11	154, 211, 241, 256	0
33	61	146/148 (98%)	-0.11	2 (1%) 73 55	86, 134, 157, 167	0
33	69	146/148 (98%)	0.10	3 (2%) 63 44	90, 135, 158, 166	0
34	15	138/140 (98%)	0.17	5 (3%) 46 31	79, 105, 142, 157	0
34	58	138/140 (98%)	0.06	2 (1%) 73 55	78, 100, 136, 154	0
35	25	122/122 (100%)	-0.27	2 (1%) 70 52	77, 93, 110, 116	0
35	68	122/122 (100%)	-0.25	0 100 100	66, 89, 105, 114	0
36	35	150/150 (100%)	0.15	3 (2%) 65 46	68, 107, 146, 170	0
36	78	147/150 (98%)	0.07	3 (2%) 65 46	64, 92, 114, 126	0
37	45	140/141 (99%)	0.13	4 (2%) 53 35	77, 106, 132, 154	0
37	88	141/141 (100%)	-0.02	4 (2%) 55 36	73, 95, 118, 143	0
38	55	117/118 (99%)	-0.19	2 (1%) 69 50	68, 86, 107, 119	0
38	98	118/118 (100%)	0.00	2 (1%) 69 50	76, 94, 113, 126	0
39	65	111/112 (99%)	0.24	5 (4%) 38 25	91, 117, 141, 150	0
39	A8	111/112 (99%)	0.12	3 (2%) 56 37	90, 107, 127, 141	0
40	75	137/146 (93%)	0.01	7 (5%) 33 22	83, 101, 163, 193	0
40	B8	129/146 (88%)	0.15	4 (3%) 51 35	84, 103, 135, 159	0
41	85	117/118 (99%)	-0.00	0 100 100	69, 93, 134, 152	0
41	C8	117/118 (99%)	0.28	2 (1%) 69 50	65, 89, 124, 139	0
42	95	101/101 (100%)	0.11	5 (4%) 34 23	70, 121, 143, 174	0
42	D8	101/101 (100%)	0.19	4 (3%) 42 28	69, 110, 140, 150	0
43	A5	113/113 (100%)	0.01	0 100 100	68, 80, 112, 185	0
43	E8	112/113 (99%)	0.07	1 (0%) 81 65	72, 84, 120, 154	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
44	B5	92/96 (95%)	-0.14	2 (2%) 62 43	76, 92, 116, 127	0
44	F8	94/96 (97%)	-0.23	0 100 100	67, 81, 107, 132	0
45	C5	104/110 (94%)	0.27	2 (1%) 66 48	96, 121, 156, 170	0
45	G8	103/110 (93%)	0.22	4 (3%) 43 29	83, 103, 144, 153	0
46	D5	135/206 (65%)	-0.17	2 (1%) 72 53	110, 142, 177, 191	0
46	H8	171/206 (83%)	-0.06	2 (1%) 76 58	100, 140, 212, 221	0
47	E5	80/85 (94%)	0.43	3 (3%) 44 30	76, 92, 114, 143	0
47	I8	83/85 (97%)	-0.00	3 (3%) 46 31	75, 88, 104, 115	0
48	F5	94/98 (95%)	0.30	3 (3%) 50 34	70, 88, 127, 146	0
48	J8	95/98 (96%)	0.05	3 (3%) 50 34	67, 85, 135, 140	0
49	G5	67/72 (93%)	-0.05	1 (1%) 72 53	90, 112, 131, 146	0
49	K8	68/72 (94%)	-0.06	1 (1%) 72 53	71, 90, 105, 126	0
50	H5	59/60 (98%)	-0.04	2 (3%) 48 32	85, 101, 151, 166	0
50	L8	57/60 (95%)	-0.32	0 100 100	76, 94, 117, 137	0
51	I5	63/71 (88%)	-0.21	0 100 100	157, 205, 225, 231	0
51	M8	66/71 (92%)	0.00	0 100 100	142, 184, 199, 204	0
52	J5	56/60 (93%)	0.00	3 (5%) 31 21	63, 85, 141, 149	0
52	N8	55/60 (91%)	0.31	3 (5%) 30 21	60, 100, 170, 184	0
53	L5	47/49 (95%)	-0.29	0 100 100	64, 69, 88, 95	0
53	P8	47/49 (95%)	-0.37	0 100 100	57, 64, 82, 108	0
54	M5	53/65 (81%)	0.15	2 (3%) 44 30	68, 83, 101, 111	0
54	Q8	60/65 (92%)	0.60	5 (8%) 17 13	69, 84, 110, 124	0
All	All	20915/21710 (96%)	-0.22	372 (1%) 67 49	55, 108, 195, 328	0

The worst 5 of 372 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
9	82	115	GLY	8.3
40	B8	1	MET	6.6
27	1J	88	C	6.3
9	8E	126	SER	6.2
4	32	73	ARG	5.9

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

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
23	H2U	2K	17	20/21	0.73	0.10	125,135,173,181	0
23	H2U	2L	17	20/21	0.74	0.10	129,137,180,190	0
23	PSU	2K	66	20/21	0.83	0.08	117,125,133,135	0
22	PSU	1K	66	20/21	0.85	0.07	113,134,150,151	0
23	PSU	2L	66	20/21	0.85	0.07	120,131,136,140	0
23	OMG	2K	18	24/25	0.86	0.09	125,139,151,157	0
22	PSU	1L	66	20/21	0.88	0.06	123,141,157,157	0
23	5MU	2K	65	21/22	0.89	0.07	119,125,131,134	0
23	5MU	2L	65	21/22	0.89	0.08	116,128,142,149	0
23	OMG	2L	18	24/25	0.91	0.07	136,144,154,157	0
23	1MG	2L	38	24/25	0.91	0.08	103,110,121,121	0
22	5MU	1K	65	21/22	0.93	0.06	109,126,139,143	0
22	PSU	1K	39	20/21	0.93	0.09	97,105,110,111	0
22	5MU	1L	65	21/22	0.93	0.06	126,135,149,154	0
23	PSU	2L	39	20/21	0.93	0.07	95,108,114,117	0
22	PSU	1L	39	20/21	0.94	0.07	112,122,132,132	0
23	1MG	2K	38	24/25	0.94	0.08	87,96,107,111	0
23	PSU	2K	39	20/21	0.95	0.09	83,96,104,110	0
22	1MG	1L	38	24/25	0.96	0.09	106,120,124,127	0
22	1MG	1K	38	24/25	0.96	0.09	93,100,106,107	0

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
55	MG	1G	1719	1/1	0.43	0.51	118,118,118,118	0
55	MG	14	3276	1/1	0.46	0.28	86,86,86,86	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
55	MG	14	3124	1/1	0.50	0.27	77,77,77,77	0
55	MG	14	3223	1/1	0.51	0.30	118,118,118,118	0
55	MG	13	1676	1/1	0.52	0.36	103,103,103,103	0
55	MG	1H	3193	1/1	0.52	0.30	116,116,116,116	0
55	MG	14	3297	1/1	0.52	0.35	85,85,85,85	0
55	MG	1H	3248	1/1	0.53	0.24	106,106,106,106	0
55	MG	13	1673	1/1	0.53	0.38	145,145,145,145	0
55	MG	1H	3198	1/1	0.54	0.30	113,113,113,113	0
55	MG	1G	1649	1/1	0.54	0.31	109,109,109,109	0
55	MG	14	3130	1/1	0.54	0.32	102,102,102,102	0
55	MG	14	3304	1/1	0.54	0.37	109,109,109,109	0
55	MG	14	3119	1/1	0.57	0.23	90,90,90,90	0
55	MG	13	1717	1/1	0.58	0.35	100,100,100,100	0
55	MG	1H	3242	1/1	0.58	0.27	97,97,97,97	0
55	MG	1H	3211	1/1	0.59	0.30	104,104,104,104	0
55	MG	1H	3395	1/1	0.60	0.32	100,100,100,100	0
55	MG	1H	3272	1/1	0.61	0.28	85,85,85,85	0
55	MG	1G	1698	1/1	0.61	0.27	112,112,112,112	0
55	MG	14	3370	1/1	0.61	0.33	88,88,88,88	0
55	MG	13	1686	1/1	0.62	0.30	93,93,93,93	0
55	MG	13	1620	1/1	0.62	0.23	92,92,92,92	0
55	MG	14	3179	1/1	0.63	0.27	90,90,90,90	0
55	MG	1H	3203	1/1	0.63	0.22	110,110,110,110	0
55	MG	1H	3179	1/1	0.63	0.28	71,71,71,71	0
55	MG	13	1635	1/1	0.64	0.39	101,101,101,101	0
55	MG	13	1657	1/1	0.64	0.17	90,90,90,90	0
55	MG	1H	3033	1/1	0.64	0.18	92,92,92,92	0
55	MG	14	3139	1/1	0.64	0.22	98,98,98,98	0
55	MG	14	3321	1/1	0.64	0.25	110,110,110,110	0
55	MG	1H	3175	1/1	0.64	0.25	112,112,112,112	0
55	MG	14	3238	1/1	0.65	0.18	98,98,98,98	0
55	MG	3E	301	1/1	0.65	0.28	109,109,109,109	0
55	MG	1H	3354	1/1	0.65	0.23	107,107,107,107	0
55	MG	14	3283	1/1	0.66	0.32	101,101,101,101	0
55	MG	14	3140	1/1	0.66	0.23	108,108,108,108	0
55	MG	14	3159	1/1	0.66	0.34	102,102,102,102	0
55	MG	14	3270	1/1	0.66	0.48	87,87,87,87	0
55	MG	1G	1724	1/1	0.66	0.28	99,99,99,99	0
55	MG	1H	3086	1/1	0.67	0.30	84,84,84,84	0
55	MG	14	3280	1/1	0.67	0.20	87,87,87,87	0
55	MG	1G	1654	1/1	0.67	0.32	97,97,97,97	0
55	MG	1H	3335	1/1	0.67	0.23	101,101,101,101	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
55	MG	1H	3094	1/1	0.67	0.18	73,73,73,73	0
55	MG	1H	3250	1/1	0.67	0.49	97,97,97,97	0
55	MG	14	3272	1/1	0.67	0.20	90,90,90,90	0
55	MG	1G	1625	1/1	0.68	0.36	99,99,99,99	0
55	MG	1H	3314	1/1	0.68	0.19	92,92,92,92	0
55	MG	14	3332	1/1	0.68	0.29	80,80,80,80	0
55	MG	14	3162	1/1	0.68	0.30	94,94,94,94	0
55	MG	14	3231	1/1	0.69	0.23	79,79,79,79	0
55	MG	13	1624	1/1	0.69	0.30	92,92,92,92	0
55	MG	1H	3356	1/1	0.69	0.66	100,100,100,100	0
55	MG	1G	1664	1/1	0.69	0.34	95,95,95,95	0
55	MG	1H	3188	1/1	0.69	0.36	92,92,92,92	0
55	MG	1H	3241	1/1	0.69	0.33	92,92,92,92	0
55	MG	13	1715	1/1	0.70	0.41	88,88,88,88	0
55	MG	1H	3396	1/1	0.70	0.17	98,98,98,98	0
55	MG	14	3308	1/1	0.70	0.29	89,89,89,89	0
55	MG	2K	102	1/1	0.70	0.23	118,118,118,118	0
55	MG	13	1613	1/1	0.70	0.22	92,92,92,92	0
55	MG	14	3349	1/1	0.70	0.32	95,95,95,95	0
55	MG	14	3247	1/1	0.70	0.11	78,78,78,78	0
55	MG	1G	1686	1/1	0.71	0.25	108,108,108,108	0
55	MG	1H	3373	1/1	0.71	0.47	85,85,85,85	0
55	MG	13	1716	1/1	0.71	0.25	103,103,103,103	0
55	MG	1H	3208	1/1	0.71	0.26	96,96,96,96	0
55	MG	14	3145	1/1	0.71	0.30	79,79,79,79	0
55	MG	14	3350	1/1	0.71	0.41	84,84,84,84	0
55	MG	1G	1614	1/1	0.71	0.29	98,98,98,98	0
55	MG	29	303	1/1	0.71	0.20	79,79,79,79	0
55	MG	1G	1725	1/1	0.72	0.34	104,104,104,104	0
55	MG	14	3192	1/1	0.72	0.23	102,102,102,102	0
55	MG	14	3099	1/1	0.72	0.13	57,57,57,57	0
55	MG	13	1679	1/1	0.72	0.34	135,135,135,135	0
55	MG	14	3236	1/1	0.72	0.19	119,119,119,119	0
55	MG	14	3367	1/1	0.72	0.24	102,102,102,102	0
55	MG	1G	1677	1/1	0.72	0.31	105,105,105,105	0
55	MG	14	3395	1/1	0.72	0.20	98,98,98,98	0
55	MG	1G	1611	1/1	0.72	0.14	122,122,122,122	0
55	MG	14	3185	1/1	0.73	0.29	74,74,74,74	0
55	MG	16	203	1/1	0.73	0.26	102,102,102,102	0
55	MG	1G	1670	1/1	0.73	0.25	117,117,117,117	0
55	MG	14	3225	1/1	0.73	0.23	87,87,87,87	0
55	MG	88	302	1/1	0.73	0.25	95,95,95,95	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
55	MG	1H	3291	1/1	0.73	0.21	117,117,117,117	0
55	MG	1G	1690	1/1	0.73	0.19	97,97,97,97	0
55	MG	1H	3226	1/1	0.73	0.19	93,93,93,93	0
55	MG	14	3360	1/1	0.73	0.46	93,93,93,93	0
55	MG	13	1730	1/1	0.73	0.30	95,95,95,95	0
55	MG	13	1729	1/1	0.73	0.18	122,122,122,122	0
55	MG	1H	3398	1/1	0.73	0.18	109,109,109,109	0
55	MG	14	3096	1/1	0.73	0.23	62,62,62,62	0
55	MG	1H	3183	1/1	0.74	0.32	90,90,90,90	0
55	MG	14	3264	1/1	0.74	0.24	78,78,78,78	0
55	MG	1H	3290	1/1	0.74	0.23	71,71,71,71	0
55	MG	13	1670	1/1	0.74	0.28	99,99,99,99	0
55	MG	14	3002	1/1	0.74	0.31	61,61,61,61	0
55	MG	14	3027	1/1	0.74	0.25	85,85,85,85	0
55	MG	1G	1655	1/1	0.74	0.28	108,108,108,108	0
55	MG	14	3290	1/1	0.74	0.45	76,76,76,76	0
55	MG	14	3098	1/1	0.74	0.28	87,87,87,87	0
55	MG	1H	3294	1/1	0.74	0.19	96,96,96,96	0
55	MG	1G	1618	1/1	0.75	0.35	76,76,76,76	0
55	MG	14	3110	1/1	0.75	0.25	74,74,74,74	0
55	MG	1G	1693	1/1	0.75	0.24	109,109,109,109	0
55	MG	13	1698	1/1	0.75	0.35	89,89,89,89	0
55	MG	1G	1700	1/1	0.75	0.22	99,99,99,99	0
55	MG	13	1669	1/1	0.75	0.32	97,97,97,97	0
55	MG	14	3335	1/1	0.75	0.42	86,86,86,86	0
55	MG	13	1611	1/1	0.75	0.24	115,115,115,115	0
55	MG	13	1634	1/1	0.75	0.31	77,77,77,77	0
55	MG	14	3154	1/1	0.75	0.32	81,81,81,81	0
55	MG	1H	3044	1/1	0.75	0.29	63,63,63,63	0
55	MG	13	1722	1/1	0.75	0.31	106,106,106,106	0
55	MG	13	1696	1/1	0.75	0.27	73,73,73,73	0
55	MG	14	3488	1/1	0.75	0.33	64,64,64,64	0
55	MG	1H	3264	1/1	0.75	0.18	86,86,86,86	0
55	MG	1H	3144	1/1	0.76	0.13	93,93,93,93	0
55	MG	1G	1610	1/1	0.76	0.28	86,86,86,86	0
55	MG	13	1618	1/1	0.76	0.32	124,124,124,124	0
55	MG	1H	3204	1/1	0.76	0.27	83,83,83,83	0
55	MG	13	1643	1/1	0.76	0.22	104,104,104,104	0
55	MG	1H	3358	1/1	0.76	0.22	81,81,81,81	0
55	MG	1G	1629	1/1	0.76	0.26	89,89,89,89	0
55	MG	1H	3362	1/1	0.76	0.28	56,56,56,56	0
55	MG	14	3062	1/1	0.76	0.23	71,71,71,71	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
55	MG	14	3204	1/1	0.76	0.28	89,89,89,89	0
55	MG	13	1680	1/1	0.76	0.17	93,93,93,93	0
55	MG	1H	3276	1/1	0.76	0.23	100,100,100,100	0
55	MG	13	1711	1/1	0.76	0.15	107,107,107,107	0
55	MG	1H	3233	1/1	0.76	0.28	100,100,100,100	0
55	MG	1H	3408	1/1	0.76	0.19	82,82,82,82	0
55	MG	14	3242	1/1	0.76	0.25	98,98,98,98	0
55	MG	14	3369	1/1	0.76	0.28	105,105,105,105	0
55	MG	1H	3126	1/1	0.76	0.48	84,84,84,84	0
55	MG	14	3379	1/1	0.76	0.22	107,107,107,107	0
55	MG	14	3249	1/1	0.76	0.21	100,100,100,100	0
55	MG	14	3250	1/1	0.76	0.19	87,87,87,87	0
55	MG	16	204	1/1	0.76	0.14	103,103,103,103	0
55	MG	45	202	1/1	0.76	0.25	99,99,99,99	0
55	MG	1H	3145	1/1	0.77	0.31	83,83,83,83	0
55	MG	13	1709	1/1	0.77	0.29	99,99,99,99	0
55	MG	13	1663	1/1	0.77	0.32	93,93,93,93	0
55	MG	1G	1702	1/1	0.77	0.18	95,95,95,95	0
55	MG	1G	1703	1/1	0.77	0.27	106,106,106,106	0
55	MG	1G	1706	1/1	0.77	0.23	91,91,91,91	0
55	MG	14	3246	1/1	0.77	0.30	97,97,97,97	0
55	MG	1H	3313	1/1	0.77	0.34	98,98,98,98	0
55	MG	13	1619	1/1	0.77	0.21	111,111,111,111	0
55	MG	13	1703	1/1	0.77	0.27	85,85,85,85	0
55	MG	1G	1729	1/1	0.77	0.24	89,89,89,89	0
55	MG	14	3161	1/1	0.77	0.35	74,74,74,74	0
55	MG	1H	3337	1/1	0.77	0.24	82,82,82,82	0
55	MG	1G	1683	1/1	0.77	0.17	132,132,132,132	0
55	MG	1H	3344	1/1	0.77	0.22	85,85,85,85	0
55	MG	1G	1687	1/1	0.77	0.35	101,101,101,101	0
55	MG	1H	3407	1/1	0.77	0.33	102,102,102,102	0
56	ZN	C5	201	1/1	0.77	0.17	201,201,201,201	0
55	MG	13	1678	1/1	0.78	0.17	85,85,85,85	0
55	MG	1H	3150	1/1	0.78	0.21	84,84,84,84	0
55	MG	1H	3266	1/1	0.78	0.24	79,79,79,79	0
55	MG	14	3273	1/1	0.78	0.29	87,87,87,87	0
55	MG	1H	3167	1/1	0.78	0.22	75,75,75,75	0
55	MG	14	3237	1/1	0.78	0.14	65,65,65,65	0
55	MG	1H	3388	1/1	0.78	0.29	90,90,90,90	0
55	MG	14	3178	1/1	0.78	0.24	89,89,89,89	0
55	MG	14	3387	1/1	0.78	0.45	92,92,92,92	0
55	MG	1H	3063	1/1	0.78	0.38	90,90,90,90	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
55	MG	1H	3067	1/1	0.78	0.30	68,68,68,68	0
55	MG	1J	202	1/1	0.78	0.17	107,107,107,107	0
55	MG	1G	1665	1/1	0.78	0.23	108,108,108,108	0
55	MG	1H	3073	1/1	0.78	0.30	68,68,68,68	0
55	MG	14	3253	1/1	0.78	0.26	98,98,98,98	0
55	MG	14	3334	1/1	0.79	0.29	76,76,76,76	0
55	MG	1H	3039	1/1	0.79	0.34	66,66,66,66	0
55	MG	1H	3132	1/1	0.79	0.23	63,63,63,63	0
55	MG	13	1704	1/1	0.79	0.29	93,93,93,93	0
55	MG	14	3352	1/1	0.79	0.27	99,99,99,99	0
55	MG	14	3275	1/1	0.79	0.30	96,96,96,96	0
55	MG	1H	3056	1/1	0.79	0.27	75,75,75,75	0
55	MG	1H	3087	1/1	0.79	0.22	76,76,76,76	0
55	MG	1G	1673	1/1	0.79	0.09	97,97,97,97	0
55	MG	13	1648	1/1	0.79	0.28	96,96,96,96	0
55	MG	1H	3270	1/1	0.79	0.22	99,99,99,99	0
55	MG	14	3301	1/1	0.79	0.21	90,90,90,90	0
55	MG	14	3188	1/1	0.79	0.32	82,82,82,82	0
55	MG	1G	1638	1/1	0.79	0.27	95,95,95,95	0
55	MG	14	3314	1/1	0.79	0.28	90,90,90,90	0
55	MG	1G	1646	1/1	0.79	0.23	109,109,109,109	0
55	MG	1H	3319	1/1	0.79	0.24	102,102,102,102	0
55	MG	1H	3261	1/1	0.80	0.33	85,85,85,85	0
55	MG	14	3164	1/1	0.80	0.35	101,101,101,101	0
55	MG	1G	1713	1/1	0.80	0.33	100,100,100,100	0
55	MG	13	1695	1/1	0.80	0.37	92,92,92,92	0
55	MG	1H	3360	1/1	0.80	0.25	70,70,70,70	0
55	MG	13	1668	1/1	0.80	0.29	78,78,78,78	0
55	MG	1G	1653	1/1	0.80	0.16	97,97,97,97	0
55	MG	13	1601	1/1	0.80	0.26	63,63,63,63	0
55	MG	14	3317	1/1	0.80	0.15	88,88,88,88	0
55	MG	13	1682	1/1	0.80	0.21	108,108,108,108	0
55	MG	14	3036	1/1	0.80	0.27	71,71,71,71	0
55	MG	1H	3147	1/1	0.80	0.27	81,81,81,81	0
55	MG	14	3077	1/1	0.80	0.27	63,63,63,63	0
55	MG	1H	3031	1/1	0.80	0.25	57,57,57,57	0
55	MG	1H	3153	1/1	0.80	0.20	79,79,79,79	0
55	MG	1H	3154	1/1	0.80	0.24	81,81,81,81	0
55	MG	1H	3303	1/1	0.80	0.36	91,91,91,91	0
55	MG	14	3115	1/1	0.80	0.19	77,77,77,77	0
55	MG	1H	3161	1/1	0.80	0.24	80,80,80,80	0
55	MG	1H	3166	1/1	0.80	0.13	83,83,83,83	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
55	MG	14	3252	1/1	0.80	0.20	97,97,97,97	0
55	MG	13	1667	1/1	0.80	0.31	88,88,88,88	0
55	MG	1G	1602	1/1	0.80	0.28	80,80,80,80	0
55	MG	13	1707	1/1	0.80	0.23	92,92,92,92	0
55	MG	1H	3043	1/1	0.80	0.19	83,83,83,83	0
55	MG	1H	3181	1/1	0.80	0.32	92,92,92,92	0
55	MG	1H	3351	1/1	0.80	0.30	86,86,86,86	0
55	MG	1H	3259	1/1	0.80	0.39	98,98,98,98	0
55	MG	1G	1628	1/1	0.81	0.28	93,93,93,93	0
55	MG	1H	3135	1/1	0.81	0.41	61,61,61,61	0
55	MG	1G	1636	1/1	0.81	0.22	93,93,93,93	0
55	MG	1H	3369	1/1	0.81	0.24	86,86,86,86	0
55	MG	14	3284	1/1	0.81	0.24	79,79,79,79	0
55	MG	1H	3299	1/1	0.81	0.17	79,79,79,79	0
55	MG	1H	3302	1/1	0.81	0.19	86,86,86,86	0
55	MG	1H	3042	1/1	0.81	0.19	84,84,84,84	0
55	MG	13	1660	1/1	0.81	0.20	99,99,99,99	0
55	MG	14	3306	1/1	0.81	0.25	95,95,95,95	0
55	MG	14	3015	1/1	0.81	0.30	69,69,69,69	0
55	MG	14	3198	1/1	0.81	0.16	95,95,95,95	0
55	MG	14	3025	1/1	0.81	0.27	82,82,82,82	0
55	MG	14	3318	1/1	0.81	0.18	77,77,77,77	0
55	MG	14	3219	1/1	0.81	0.23	86,86,86,86	0
55	MG	13	1609	1/1	0.81	0.22	80,80,80,80	0
55	MG	13	1645	1/1	0.81	0.24	84,84,84,84	0
55	MG	1H	3232	1/1	0.81	0.18	90,90,90,90	0
55	MG	14	3338	1/1	0.81	0.24	66,66,66,66	0
55	MG	14	3235	1/1	0.81	0.29	91,91,91,91	0
55	MG	1G	1669	1/1	0.81	0.14	100,100,100,100	0
55	MG	1H	3152	1/1	0.81	0.34	54,54,54,54	0
55	MG	1H	3338	1/1	0.81	0.22	82,82,82,82	0
55	MG	1G	1674	1/1	0.81	0.17	113,113,113,113	0
55	MG	21	302	1/1	0.81	0.18	77,77,77,77	0
55	MG	1H	3125	1/1	0.81	0.41	73,73,73,73	0
55	MG	14	3374	1/1	0.81	0.23	102,102,102,102	0
55	MG	1H	3279	1/1	0.81	0.27	86,86,86,86	0
55	MG	14	3381	1/1	0.81	0.23	95,95,95,95	0
55	MG	1H	3352	1/1	0.81	0.27	87,87,87,87	0
55	MG	1H	3285	1/1	0.81	0.28	83,83,83,83	0
55	MG	13	1713	1/1	0.81	0.33	99,99,99,99	0
55	MG	13	1672	1/1	0.81	0.32	89,89,89,89	0
55	MG	1G	1624	1/1	0.81	0.18	103,103,103,103	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
55	MG	14	3152	1/1	0.81	0.25	99,99,99,99	0
56	ZN	G8	202	1/1	0.81	0.17	205,205,205,205	0
55	MG	1H	3292	1/1	0.81	0.27	90,90,90,90	0
55	MG	1G	1711	1/1	0.82	0.29	88,88,88,88	0
55	MG	14	3122	1/1	0.82	0.28	84,84,84,84	0
55	MG	1H	3383	1/1	0.82	0.28	90,90,90,90	0
55	MG	14	3309	1/1	0.82	0.09	95,95,95,95	0
55	MG	14	3129	1/1	0.82	0.21	86,86,86,86	0
55	MG	1H	3066	1/1	0.82	0.27	86,86,86,86	0
55	MG	1H	3389	1/1	0.82	0.45	99,99,99,99	0
55	MG	1H	3128	1/1	0.82	0.34	66,66,66,66	0
55	MG	14	3240	1/1	0.82	0.12	68,68,68,68	0
55	MG	13	1714	1/1	0.82	0.11	103,103,103,103	0
55	MG	14	3148	1/1	0.82	0.35	72,72,72,72	0
55	MG	14	3150	1/1	0.82	0.18	92,92,92,92	0
55	MG	14	3347	1/1	0.82	0.21	84,84,84,84	0
55	MG	13	1674	1/1	0.82	0.18	112,112,112,112	0
55	MG	1H	3400	1/1	0.82	0.35	94,94,94,94	0
55	MG	14	3016	1/1	0.82	0.26	74,74,74,74	0
55	MG	13	1617	1/1	0.82	0.34	83,83,83,83	0
55	MG	13	1684	1/1	0.82	0.27	98,98,98,98	0
55	MG	14	3032	1/1	0.82	0.31	71,71,71,71	0
55	MG	14	3171	1/1	0.82	0.31	103,103,103,103	0
55	MG	1H	3414	1/1	0.82	0.34	97,97,97,97	0
55	MG	1H	3331	1/1	0.82	0.15	68,68,68,68	0
55	MG	1G	1696	1/1	0.82	0.23	94,94,94,94	0
55	MG	14	3384	1/1	0.82	0.17	92,92,92,92	0
55	MG	1H	3092	1/1	0.82	0.31	73,73,73,73	0
55	MG	13	1720	1/1	0.82	0.27	94,94,94,94	0
55	MG	14	3196	1/1	0.82	0.25	65,65,65,65	0
55	MG	1J	201	1/1	0.82	0.20	115,115,115,115	0
55	MG	13	1705	1/1	0.82	0.29	102,102,102,102	0
55	MG	14	3292	1/1	0.82	0.28	79,79,79,79	0
55	MG	14	3296	1/1	0.82	0.27	94,94,94,94	0
55	MG	1G	1601	1/1	0.82	0.27	91,91,91,91	0
55	MG	1H	3380	1/1	0.82	0.19	100,100,100,100	0
55	MG	1H	3317	1/1	0.83	0.23	79,79,79,79	0
55	MG	1H	3035	1/1	0.83	0.28	82,82,82,82	0
55	MG	1H	3394	1/1	0.83	0.18	82,82,82,82	0
55	MG	1H	3324	1/1	0.83	0.23	89,89,89,89	0
55	MG	1H	3269	1/1	0.83	0.22	99,99,99,99	0
55	MG	7A	101	1/1	0.83	0.20	85,85,85,85	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
55	MG	14	3175	1/1	0.83	0.40	95,95,95,95	0
55	MG	14	3177	1/1	0.83	0.23	75,75,75,75	0
55	MG	1H	3332	1/1	0.83	0.25	78,78,78,78	0
55	MG	1H	3399	1/1	0.83	0.25	94,94,94,94	0
55	MG	14	3180	1/1	0.83	0.17	82,82,82,82	0
55	MG	13	1631	1/1	0.83	0.28	80,80,80,80	0
55	MG	14	3024	1/1	0.83	0.33	79,79,79,79	0
55	MG	14	3315	1/1	0.83	0.16	92,92,92,92	0
55	MG	13	1688	1/1	0.83	0.18	92,92,92,92	0
55	MG	1H	3158	1/1	0.83	0.37	88,88,88,88	0
55	MG	13	1689	1/1	0.83	0.34	92,92,92,92	0
55	MG	14	3322	1/1	0.83	0.22	93,93,93,93	0
55	MG	14	3035	1/1	0.83	0.28	91,91,91,91	0
55	MG	1H	3510	1/1	0.83	0.38	65,65,65,65	0
55	MG	14	3043	1/1	0.83	0.27	83,83,83,83	0
55	MG	1H	3346	1/1	0.83	0.25	105,105,105,105	0
55	MG	14	3229	1/1	0.83	0.22	77,77,77,77	0
55	MG	13	1694	1/1	0.83	0.25	88,88,88,88	0
55	MG	14	3233	1/1	0.83	0.27	91,91,91,91	0
55	MG	14	3087	1/1	0.83	0.21	84,84,84,84	0
55	MG	1G	1675	1/1	0.83	0.18	102,102,102,102	0
55	MG	16	205	1/1	0.83	0.23	87,87,87,87	0
55	MG	1H	3286	1/1	0.83	0.16	94,94,94,94	0
55	MG	14	3103	1/1	0.83	0.15	73,73,73,73	0
55	MG	1H	3353	1/1	0.83	0.27	75,75,75,75	0
55	MG	13	1662	1/1	0.83	0.06	98,98,98,98	0
55	MG	1H	3130	1/1	0.83	0.24	70,70,70,70	0
55	MG	13	1607	1/1	0.83	0.27	77,77,77,77	0
55	MG	13	1644	1/1	0.83	0.41	91,91,91,91	0
55	MG	1H	3249	1/1	0.83	0.31	80,80,80,80	0
55	MG	1H	3017	1/1	0.83	0.36	56,56,56,56	0
55	MG	1G	1622	1/1	0.83	0.28	95,95,95,95	0
55	MG	13	1702	1/1	0.83	0.20	96,96,96,96	0
55	MG	1H	3079	1/1	0.83	0.20	79,79,79,79	0
55	MG	1G	1709	1/1	0.83	0.31	81,81,81,81	0
55	MG	1G	1710	1/1	0.83	0.23	87,87,87,87	0
55	MG	13	1685	1/1	0.83	0.18	103,103,103,103	0
55	MG	14	3311	1/1	0.84	0.30	103,103,103,103	0
55	MG	13	1622	1/1	0.84	0.12	85,85,85,85	0
55	MG	1G	1708	1/1	0.84	0.25	66,66,66,66	0
55	MG	1G	1667	1/1	0.84	0.16	84,84,84,84	0
55	MG	1H	3184	1/1	0.84	0.29	75,75,75,75	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
55	MG	1G	1623	1/1	0.84	0.22	89,89,89,89	0
55	MG	1H	3304	1/1	0.84	0.20	82,82,82,82	0
55	MG	1G	1717	1/1	0.84	0.29	99,99,99,99	0
55	MG	16	201	1/1	0.84	0.23	97,97,97,97	0
55	MG	1G	1722	1/1	0.84	0.26	84,84,84,84	0
55	MG	14	3182	1/1	0.84	0.18	78,78,78,78	0
55	MG	14	3254	1/1	0.84	0.12	117,117,117,117	0
55	MG	14	3348	1/1	0.84	0.24	86,86,86,86	0
55	MG	1H	3283	1/1	0.84	0.39	85,85,85,85	0
55	MG	14	3265	1/1	0.84	0.22	88,88,88,88	0
55	MG	13	1701	1/1	0.84	0.34	83,83,83,83	0
55	MG	14	3189	1/1	0.84	0.17	91,91,91,91	0
55	MG	1G	1678	1/1	0.84	0.21	97,97,97,97	0
55	MG	1G	1630	1/1	0.84	0.28	91,91,91,91	0
55	MG	1H	3189	1/1	0.84	0.24	85,85,85,85	0
55	MG	14	3008	1/1	0.84	0.28	61,61,61,61	0
55	MG	14	3282	1/1	0.84	0.19	89,89,89,89	0
55	MG	14	3205	1/1	0.84	0.25	83,83,83,83	0
55	MG	14	3207	1/1	0.84	0.28	92,92,92,92	0
55	MG	14	3215	1/1	0.84	0.21	77,77,77,77	0
55	MG	1H	3104	1/1	0.84	0.32	77,77,77,77	0
55	MG	1G	1645	1/1	0.84	0.27	80,80,80,80	0
55	MG	1H	3112	1/1	0.84	0.21	69,69,69,69	0
55	MG	13	1649	1/1	0.84	0.29	91,91,91,91	0
55	MG	1H	3244	1/1	0.84	0.17	92,92,92,92	0
55	MG	1H	3295	1/1	0.84	0.25	87,87,87,87	0
55	MG	1H	3405	1/1	0.84	0.21	89,89,89,89	0
55	MG	1H	3038	1/1	0.84	0.13	96,96,96,96	0
55	MG	1H	3172	1/1	0.85	0.33	103,103,103,103	0
55	MG	1H	3230	1/1	0.85	0.27	84,84,84,84	0
55	MG	14	3300	1/1	0.85	0.23	64,64,64,64	0
55	MG	1H	3280	1/1	0.85	0.17	92,92,92,92	0
55	MG	14	3108	1/1	0.85	0.16	61,61,61,61	0
55	MG	1H	3107	1/1	0.85	0.40	76,76,76,76	0
55	MG	13	1665	1/1	0.85	0.11	103,103,103,103	0
55	MG	1H	3404	1/1	0.85	0.35	83,83,83,83	0
55	MG	1H	3342	1/1	0.85	0.10	73,73,73,73	0
55	MG	14	3312	1/1	0.85	0.24	96,96,96,96	0
55	MG	1H	3234	1/1	0.85	0.12	78,78,78,78	0
55	MG	14	3128	1/1	0.85	0.30	89,89,89,89	0
55	MG	1H	3117	1/1	0.85	0.23	74,74,74,74	0
55	MG	1H	3123	1/1	0.85	0.17	64,64,64,64	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
55	MG	1G	1650	1/1	0.85	0.29	92,92,92,92	0
55	MG	1H	3499	1/1	0.85	0.17	103,103,103,103	0
55	MG	14	3328	1/1	0.85	0.33	38,38,38,38	0
55	MG	14	3329	1/1	0.85	0.34	58,58,58,58	0
55	MG	13	1666	1/1	0.85	0.30	78,78,78,78	0
55	MG	14	3146	1/1	0.85	0.16	73,73,73,73	0
55	MG	1H	3245	1/1	0.85	0.32	81,81,81,81	0
55	MG	14	3336	1/1	0.85	0.21	70,70,70,70	0
55	MG	13	1658	1/1	0.85	0.12	82,82,82,82	0
55	MG	14	3243	1/1	0.85	0.24	75,75,75,75	0
55	MG	13	1606	1/1	0.85	0.25	89,89,89,89	0
55	MG	14	3153	1/1	0.85	0.36	71,71,71,71	0
55	MG	1H	3300	1/1	0.85	0.34	91,91,91,91	0
55	MG	1G	1668	1/1	0.85	0.32	96,96,96,96	0
55	MG	1H	3155	1/1	0.85	0.15	67,67,67,67	0
55	MG	14	3364	1/1	0.85	0.16	89,89,89,89	0
55	MG	1H	3037	1/1	0.85	0.21	94,94,94,94	0
55	MG	13	1602	1/1	0.85	0.20	85,85,85,85	0
55	MG	14	3263	1/1	0.85	0.25	92,92,92,92	0
55	MG	14	3167	1/1	0.85	0.16	50,50,50,50	0
55	MG	1H	3133	1/1	0.85	0.20	79,79,79,79	0
55	MG	1G	1608	1/1	0.85	0.18	99,99,99,99	0
55	MG	14	3382	1/1	0.85	0.21	91,91,91,91	0
55	MG	1G	1609	1/1	0.85	0.26	101,101,101,101	0
55	MG	1H	3376	1/1	0.85	0.23	71,71,71,71	0
55	MG	1H	3206	1/1	0.85	0.31	69,69,69,69	0
55	MG	13	1608	1/1	0.85	0.35	64,64,64,64	0
55	MG	14	3181	1/1	0.85	0.22	78,78,78,78	0
55	MG	1H	3171	1/1	0.85	0.20	80,80,80,80	0
55	MG	1G	1619	1/1	0.85	0.16	105,105,105,105	0
55	MG	25	201	1/1	0.85	0.28	107,107,107,107	0
55	MG	1G	1692	1/1	0.85	0.15	100,100,100,100	0
55	MG	1H	3225	1/1	0.85	0.22	80,80,80,80	0
55	MG	1H	3325	1/1	0.85	0.25	92,92,92,92	0
55	MG	13	1646	1/1	0.86	0.41	76,76,76,76	0
55	MG	1G	1707	1/1	0.86	0.34	92,92,92,92	0
55	MG	1H	3322	1/1	0.86	0.17	109,109,109,109	0
55	MG	14	3214	1/1	0.86	0.18	78,78,78,78	0
55	MG	1H	3374	1/1	0.86	0.33	89,89,89,89	0
55	MG	1H	3239	1/1	0.86	0.20	93,93,93,93	0
55	MG	13	1650	1/1	0.86	0.38	88,88,88,88	0
55	MG	1G	1659	1/1	0.86	0.17	83,83,83,83	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
55	MG	14	3127	1/1	0.86	0.22	76,76,76,76	0
55	MG	14	3230	1/1	0.86	0.24	85,85,85,85	0
55	MG	14	3319	1/1	0.86	0.22	89,89,89,89	0
55	MG	1H	3080	1/1	0.86	0.23	89,89,89,89	0
55	MG	1H	3384	1/1	0.86	0.11	79,79,79,79	0
55	MG	13	1731	1/1	0.86	0.23	82,82,82,82	0
55	MG	1H	3333	1/1	0.86	0.16	85,85,85,85	0
55	MG	13	1737	1/1	0.86	0.13	114,114,114,114	0
55	MG	1G	1727	1/1	0.86	0.27	98,98,98,98	0
55	MG	13	1652	1/1	0.86	0.22	94,94,94,94	0
55	MG	13	1700	1/1	0.86	0.23	87,87,87,87	0
55	MG	14	3149	1/1	0.86	0.21	77,77,77,77	0
55	MG	14	3339	1/1	0.86	0.21	71,71,71,71	0
55	MG	1H	3009	1/1	0.86	0.21	56,56,56,56	0
55	MG	1H	3210	1/1	0.86	0.30	82,82,82,82	0
55	MG	13	1708	1/1	0.86	0.30	81,81,81,81	0
55	MG	1H	3401	1/1	0.86	0.21	80,80,80,80	0
55	MG	14	3155	1/1	0.86	0.23	72,72,72,72	0
55	MG	14	3156	1/1	0.86	0.27	82,82,82,82	0
55	MG	1H	3402	1/1	0.86	0.26	86,86,86,86	0
55	MG	13	1690	1/1	0.86	0.28	90,90,90,90	0
55	MG	14	3368	1/1	0.86	0.27	91,91,91,91	0
55	MG	1H	3180	1/1	0.86	0.17	79,79,79,79	0
55	MG	14	3028	1/1	0.86	0.28	46,46,46,46	0
55	MG	1H	3268	1/1	0.86	0.25	66,66,66,66	0
55	MG	14	3378	1/1	0.86	0.21	83,83,83,83	0
55	MG	1H	3228	1/1	0.86	0.18	68,68,68,68	0
55	MG	1G	1635	1/1	0.86	0.26	82,82,82,82	0
55	MG	1H	3312	1/1	0.86	0.19	88,88,88,88	0
55	MG	14	3044	1/1	0.86	0.24	79,79,79,79	0
55	MG	14	3060	1/1	0.86	0.47	80,80,80,80	0
55	MG	14	3388	1/1	0.86	0.33	94,94,94,94	0
55	MG	14	3393	1/1	0.86	0.12	79,79,79,79	0
55	MG	1H	3032	1/1	0.86	0.21	79,79,79,79	0
55	MG	14	3066	1/1	0.86	0.26	62,62,62,62	0
55	MG	1G	1699	1/1	0.86	0.21	100,100,100,100	0
55	MG	13	1616	1/1	0.86	0.20	102,102,102,102	0
55	MG	1G	1701	1/1	0.86	0.10	119,119,119,119	0
55	MG	14	3097	1/1	0.86	0.37	91,91,91,91	0
55	MG	1H	3124	1/1	0.86	0.22	68,68,68,68	0
55	MG	1G	1647	1/1	0.86	0.19	92,92,92,92	0
55	MG	14	3101	1/1	0.86	0.24	89,89,89,89	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
55	MG	1H	3348	1/1	0.87	0.18	88,88,88,88	0
55	MG	14	3014	1/1	0.87	0.23	77,77,77,77	0
55	MG	1G	1634	1/1	0.87	0.26	77,77,77,77	0
55	MG	1H	3387	1/1	0.87	0.13	73,73,73,73	0
55	MG	14	3022	1/1	0.87	0.16	81,81,81,81	0
55	MG	1H	3174	1/1	0.87	0.25	74,74,74,74	0
55	MG	1G	1637	1/1	0.87	0.31	84,84,84,84	0
55	MG	1H	3224	1/1	0.87	0.12	80,80,80,80	0
55	MG	1G	1644	1/1	0.87	0.23	96,96,96,96	0
55	MG	1H	3391	1/1	0.87	0.15	78,78,78,78	0
55	MG	21	301	1/1	0.87	0.28	64,64,64,64	0
55	MG	13	1723	1/1	0.87	0.29	88,88,88,88	0
55	MG	13	1610	1/1	0.87	0.16	90,90,90,90	0
55	MG	1H	3355	1/1	0.87	0.19	62,62,62,62	0
55	MG	14	3049	1/1	0.87	0.18	80,80,80,80	0
55	MG	14	3160	1/1	0.87	0.20	98,98,98,98	0
55	MG	14	3340	1/1	0.87	0.30	66,66,66,66	0
55	MG	1G	1651	1/1	0.87	0.14	93,93,93,93	0
55	MG	14	3061	1/1	0.87	0.15	62,62,62,62	0
55	MG	1H	3200	1/1	0.87	0.23	68,68,68,68	0
55	MG	1H	3274	1/1	0.87	0.40	83,83,83,83	0
55	MG	14	3069	1/1	0.87	0.18	65,65,65,65	0
55	MG	14	3356	1/1	0.87	0.28	77,77,77,77	0
55	MG	14	3173	1/1	0.87	0.27	76,76,76,76	0
55	MG	1H	3275	1/1	0.87	0.16	89,89,89,89	0
55	MG	14	3080	1/1	0.87	0.21	65,65,65,65	0
55	MG	1G	1658	1/1	0.87	0.12	78,78,78,78	0
55	MG	14	3089	1/1	0.87	0.20	89,89,89,89	0
55	MG	13	1659	1/1	0.87	0.21	91,91,91,91	0
55	MG	14	3372	1/1	0.87	0.18	77,77,77,77	0
55	MG	14	3373	1/1	0.87	0.29	74,74,74,74	0
55	MG	1H	3367	1/1	0.87	0.19	77,77,77,77	0
55	MG	13	1687	1/1	0.87	0.39	90,90,90,90	0
55	MG	14	3281	1/1	0.87	0.11	79,79,79,79	0
55	MG	1H	3102	1/1	0.87	0.21	64,64,64,64	0
55	MG	1H	3406	1/1	0.87	0.33	87,87,87,87	0
55	MG	1G	1720	1/1	0.87	0.15	102,102,102,102	0
55	MG	14	3289	1/1	0.87	0.13	98,98,98,98	0
55	MG	1H	3305	1/1	0.87	0.22	96,96,96,96	0
55	MG	1H	3041	1/1	0.87	0.21	72,72,72,72	0
55	MG	1H	3412	1/1	0.87	0.19	103,103,103,103	0
55	MG	1H	3262	1/1	0.87	0.22	93,93,93,93	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
55	MG	1G	1626	1/1	0.87	0.19	80,80,80,80	0
55	MG	1H	3136	1/1	0.87	0.27	72,72,72,72	0
55	MG	14	3126	1/1	0.87	0.18	83,83,83,83	0
55	MG	1H	3508	1/1	0.87	0.26	103,103,103,103	0
55	MG	14	3217	1/1	0.87	0.23	98,98,98,98	0
55	MG	85	201	1/1	0.87	0.27	83,83,83,83	0
55	MG	14	3007	1/1	0.87	0.23	68,68,68,68	0
55	MG	14	3220	1/1	0.87	0.22	80,80,80,80	0
55	MG	1H	3339	1/1	0.88	0.25	88,88,88,88	0
55	MG	1H	3023	1/1	0.88	0.30	48,48,48,48	0
55	MG	14	3184	1/1	0.88	0.21	59,59,59,59	0
55	MG	1H	3029	1/1	0.88	0.19	56,56,56,56	0
55	MG	14	3187	1/1	0.88	0.10	81,81,81,81	0
55	MG	1H	3057	1/1	0.88	0.29	73,73,73,73	0
55	MG	13	1647	1/1	0.88	0.18	93,93,93,93	0
55	MG	1H	3192	1/1	0.88	0.27	88,88,88,88	0
55	MG	1H	3064	1/1	0.88	0.17	95,95,95,95	0
55	MG	1G	1640	1/1	0.88	0.19	90,90,90,90	0
55	MG	14	3200	1/1	0.88	0.15	77,77,77,77	0
55	MG	1H	3119	1/1	0.88	0.23	75,75,75,75	0
55	MG	1H	3413	1/1	0.88	0.25	89,89,89,89	0
55	MG	14	3206	1/1	0.88	0.25	92,92,92,92	0
55	MG	1H	3246	1/1	0.88	0.16	90,90,90,90	0
55	MG	14	3212	1/1	0.88	0.20	88,88,88,88	0
55	MG	1H	3297	1/1	0.88	0.18	87,87,87,87	0
55	MG	14	3109	1/1	0.88	0.27	66,66,66,66	0
55	MG	1H	3122	1/1	0.88	0.12	68,68,68,68	0
55	MG	13	1726	1/1	0.88	0.27	93,93,93,93	0
55	MG	14	3116	1/1	0.88	0.15	65,65,65,65	0
55	MG	14	3118	1/1	0.88	0.08	69,69,69,69	0
55	MG	13	1712	1/1	0.88	0.34	86,86,86,86	0
55	MG	14	3228	1/1	0.88	0.06	78,78,78,78	0
55	MG	1H	3361	1/1	0.88	0.28	78,78,78,78	0
55	MG	1H	3254	1/1	0.88	0.20	56,56,56,56	0
55	MG	1H	3366	1/1	0.88	0.10	76,76,76,76	0
55	MG	1H	3165	1/1	0.88	0.25	76,76,76,76	0
55	MG	1G	1728	1/1	0.88	0.15	92,92,92,92	0
55	MG	1H	3260	1/1	0.88	0.32	85,85,85,85	0
55	MG	1G	1662	1/1	0.88	0.17	98,98,98,98	0
55	MG	14	3001	1/1	0.88	0.28	81,81,81,81	0
55	MG	1H	3207	1/1	0.88	0.22	86,86,86,86	0
55	MG	13	1642	1/1	0.88	0.25	85,85,85,85	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
55	MG	13	1623	1/1	0.88	0.22	94,94,94,94	0
55	MG	14	3009	1/1	0.88	0.29	62,62,62,62	0
55	MG	14	3365	1/1	0.88	0.36	89,89,89,89	0
55	MG	1G	1603	1/1	0.88	0.33	65,65,65,65	0
55	MG	13	1661	1/1	0.88	0.23	89,89,89,89	0
55	MG	1H	3267	1/1	0.88	0.22	85,85,85,85	0
55	MG	1H	3320	1/1	0.88	0.24	82,82,82,82	0
55	MG	1H	3213	1/1	0.88	0.15	55,55,55,55	0
55	MG	1G	1613	1/1	0.88	0.32	92,92,92,92	0
55	MG	14	3261	1/1	0.88	0.34	91,91,91,91	0
55	MG	14	3375	1/1	0.88	0.30	81,81,81,81	0
55	MG	14	3262	1/1	0.88	0.26	89,89,89,89	0
55	MG	1H	3214	1/1	0.88	0.20	56,56,56,56	0
55	MG	1G	1615	1/1	0.88	0.15	84,84,84,84	0
55	MG	14	3031	1/1	0.88	0.36	66,66,66,66	0
55	MG	1H	3223	1/1	0.88	0.14	68,68,68,68	0
55	MG	14	3271	1/1	0.88	0.31	75,75,75,75	0
55	MG	1H	3330	1/1	0.88	0.25	75,75,75,75	0
55	MG	1H	3084	1/1	0.88	0.20	65,65,65,65	0
55	MG	14	3394	1/1	0.88	0.12	90,90,90,90	0
55	MG	14	3038	1/1	0.88	0.35	57,57,57,57	0
55	MG	14	3465	1/1	0.88	0.14	115,115,115,115	0
55	MG	1G	1689	1/1	0.88	0.26	103,103,103,103	0
55	MG	14	3279	1/1	0.88	0.16	80,80,80,80	0
55	MG	13	1626	1/1	0.88	0.30	68,68,68,68	0
55	MG	29	301	1/1	0.88	0.19	88,88,88,88	0
55	MG	13	1651	1/1	0.88	0.20	91,91,91,91	0
55	MG	13	1628	1/1	0.88	0.24	64,64,64,64	0
55	MG	13	1637	1/1	0.88	0.35	72,72,72,72	0
55	MG	1G	1697	1/1	0.88	0.16	88,88,88,88	0
55	MG	14	3286	1/1	0.88	0.44	91,91,91,91	0
55	MG	1H	3096	1/1	0.88	0.16	62,62,62,62	0
55	MG	14	3307	1/1	0.89	0.26	91,91,91,91	0
55	MG	1H	3347	1/1	0.89	0.16	80,80,80,80	0
55	MG	13	1691	1/1	0.89	0.22	89,89,89,89	0
55	MG	14	3310	1/1	0.89	0.17	84,84,84,84	0
55	MG	1G	1672	1/1	0.89	0.15	95,95,95,95	0
55	MG	1H	3349	1/1	0.89	0.08	66,66,66,66	0
55	MG	14	3313	1/1	0.89	0.24	82,82,82,82	0
55	MG	14	3125	1/1	0.89	0.36	75,75,75,75	0
55	MG	13	1641	1/1	0.89	0.18	75,75,75,75	0
55	MG	1H	3020	1/1	0.89	0.24	68,68,68,68	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
55	MG	14	3226	1/1	0.89	0.27	92,92,92,92	0
55	MG	13	1615	1/1	0.89	0.20	88,88,88,88	0
55	MG	1H	3212	1/1	0.89	0.22	71,71,71,71	0
55	MG	1H	3129	1/1	0.89	0.22	61,61,61,61	0
55	MG	14	3327	1/1	0.89	0.21	98,98,98,98	0
55	MG	14	3138	1/1	0.89	0.46	83,83,83,83	0
55	MG	14	3232	1/1	0.89	0.09	82,82,82,82	0
55	MG	14	3020	1/1	0.89	0.26	80,80,80,80	0
55	MG	13	1603	1/1	0.89	0.15	73,73,73,73	0
55	MG	1H	3053	1/1	0.89	0.14	72,72,72,72	0
55	MG	1H	3410	1/1	0.89	0.26	85,85,85,85	0
55	MG	14	3026	1/1	0.89	0.15	83,83,83,83	0
55	MG	1H	3177	1/1	0.89	0.24	93,93,93,93	0
55	MG	1H	3030	1/1	0.89	0.21	63,63,63,63	0
55	MG	14	3341	1/1	0.89	0.56	77,77,77,77	0
55	MG	14	3030	1/1	0.89	0.26	70,70,70,70	0
55	MG	1H	3095	1/1	0.89	0.17	58,58,58,58	0
55	MG	1G	1694	1/1	0.89	0.12	80,80,80,80	0
55	MG	14	3033	1/1	0.89	0.17	77,77,77,77	0
55	MG	1H	3447	1/1	0.89	0.15	77,77,77,77	0
55	MG	1H	3460	1/1	0.89	0.11	72,72,72,72	0
55	MG	14	3359	1/1	0.89	0.40	90,90,90,90	0
55	MG	13	1721	1/1	0.89	0.14	84,84,84,84	0
55	MG	1H	3142	1/1	0.89	0.22	68,68,68,68	0
55	MG	1G	1641	1/1	0.89	0.19	91,91,91,91	0
55	MG	14	3163	1/1	0.89	0.23	81,81,81,81	0
55	MG	1G	1642	1/1	0.89	0.15	89,89,89,89	0
55	MG	1H	3231	1/1	0.89	0.13	90,90,90,90	0
55	MG	1H	3370	1/1	0.89	0.27	75,75,75,75	0
55	MG	14	3269	1/1	0.89	0.16	93,93,93,93	0
55	MG	16	202	1/1	0.89	0.17	90,90,90,90	0
55	MG	14	3065	1/1	0.89	0.33	47,47,47,47	0
55	MG	1H	3100	1/1	0.89	0.17	65,65,65,65	0
55	MG	1G	1648	1/1	0.89	0.21	82,82,82,82	0
55	MG	14	3075	1/1	0.89	0.11	70,70,70,70	0
55	MG	1H	3329	1/1	0.89	0.21	62,62,62,62	0
55	MG	1H	3186	1/1	0.89	0.17	76,76,76,76	0
55	MG	1H	3060	1/1	0.89	0.35	59,59,59,59	0
55	MG	14	3385	1/1	0.89	0.23	97,97,97,97	0
55	MG	13	1743	1/1	0.89	0.06	142,142,142,142	0
55	MG	13	1745	1/1	0.89	0.18	88,88,88,88	0
55	MG	14	3391	1/1	0.89	0.17	90,90,90,90	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
55	MG	1H	3065	1/1	0.89	0.21	80,80,80,80	0
55	MG	13	1632	1/1	0.89	0.29	74,74,74,74	0
55	MG	13	1639	1/1	0.89	0.15	85,85,85,85	0
55	MG	14	3396	1/1	0.89	0.16	79,79,79,79	0
55	MG	14	3288	1/1	0.89	0.14	89,89,89,89	0
55	MG	1G	1723	1/1	0.89	0.20	87,87,87,87	0
55	MG	1H	3201	1/1	0.89	0.15	62,62,62,62	0
55	MG	14	3291	1/1	0.89	0.23	91,91,91,91	0
55	MG	14	3106	1/1	0.89	0.31	80,80,80,80	0
55	MG	1H	3392	1/1	0.89	0.19	86,86,86,86	0
55	MG	1G	1726	1/1	0.89	0.30	90,90,90,90	0
55	MG	1H	3121	1/1	0.89	0.34	54,54,54,54	0
55	MG	14	3113	1/1	0.89	0.27	76,76,76,76	0
55	MG	1H	3071	1/1	0.89	0.26	74,74,74,74	0
55	MG	1H	3005	1/1	0.89	0.26	45,45,45,45	0
55	MG	14	3079	1/1	0.90	0.24	46,46,46,46	0
55	MG	1G	1738	1/1	0.90	0.12	137,137,137,137	0
55	MG	14	3158	1/1	0.90	0.31	68,68,68,68	0
55	MG	14	3081	1/1	0.90	0.26	72,72,72,72	0
55	MG	1G	1739	1/1	0.90	0.16	107,107,107,107	0
55	MG	14	3324	1/1	0.90	0.12	80,80,80,80	0
55	MG	1H	3315	1/1	0.90	0.26	92,92,92,92	0
55	MG	1H	3048	1/1	0.90	0.13	87,87,87,87	0
55	MG	31	400	1/1	0.90	0.11	65,65,65,65	0
55	MG	1H	3019	1/1	0.90	0.32	51,51,51,51	0
55	MG	14	3165	1/1	0.90	0.19	61,61,61,61	0
55	MG	14	3248	1/1	0.90	0.28	74,74,74,74	0
55	MG	1H	3054	1/1	0.90	0.29	51,51,51,51	0
55	MG	14	3170	1/1	0.90	0.19	67,67,67,67	0
55	MG	14	3100	1/1	0.90	0.22	77,77,77,77	0
55	MG	1H	3321	1/1	0.90	0.23	80,80,80,80	0
55	MG	1H	3148	1/1	0.90	0.20	75,75,75,75	0
55	MG	14	3257	1/1	0.90	0.17	78,78,78,78	0
55	MG	14	3104	1/1	0.90	0.20	87,87,87,87	0
55	MG	1G	1606	1/1	0.90	0.20	89,89,89,89	0
55	MG	1H	3323	1/1	0.90	0.20	83,83,83,83	0
55	MG	1H	3251	1/1	0.90	0.15	85,85,85,85	0
55	MG	1H	3253	1/1	0.90	0.27	90,90,90,90	0
55	MG	1G	1652	1/1	0.90	0.28	99,99,99,99	0
55	MG	1H	3227	1/1	0.90	0.11	61,61,61,61	0
55	MG	1H	3256	1/1	0.90	0.22	82,82,82,82	0
55	MG	1G	1705	1/1	0.90	0.14	105,105,105,105	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
55	MG	1H	3258	1/1	0.90	0.14	92,92,92,92	0
55	MG	14	3120	1/1	0.90	0.10	69,69,69,69	0
55	MG	14	3190	1/1	0.90	0.37	75,75,75,75	0
55	MG	14	3191	1/1	0.90	0.10	62,62,62,62	0
55	MG	14	3371	1/1	0.90	0.19	91,91,91,91	0
55	MG	13	1655	1/1	0.90	0.21	77,77,77,77	0
55	MG	1H	3411	1/1	0.90	0.13	87,87,87,87	0
55	MG	1H	3371	1/1	0.90	0.15	84,84,84,84	0
55	MG	1G	1621	1/1	0.90	0.21	80,80,80,80	0
55	MG	14	3201	1/1	0.90	0.12	68,68,68,68	0
55	MG	14	3202	1/1	0.90	0.27	85,85,85,85	0
55	MG	14	3380	1/1	0.90	0.29	93,93,93,93	0
55	MG	1H	3151	1/1	0.90	0.25	81,81,81,81	0
55	MG	1H	3178	1/1	0.90	0.20	69,69,69,69	0
55	MG	13	1727	1/1	0.90	0.14	90,90,90,90	0
55	MG	1H	3083	1/1	0.90	0.27	55,55,55,55	0
55	MG	14	3386	1/1	0.90	0.29	79,79,79,79	0
55	MG	14	3131	1/1	0.90	0.31	93,93,93,93	0
55	MG	14	3133	1/1	0.90	0.28	76,76,76,76	0
55	MG	14	3134	1/1	0.90	0.17	76,76,76,76	0
55	MG	14	3392	1/1	0.90	0.14	88,88,88,88	0
55	MG	14	3298	1/1	0.90	0.29	54,54,54,54	0
55	MG	1H	3003	1/1	0.90	0.19	58,58,58,58	0
55	MG	1G	1721	1/1	0.90	0.16	102,102,102,102	0
55	MG	14	3051	1/1	0.90	0.24	55,55,55,55	0
55	MG	14	3305	1/1	0.90	0.32	89,89,89,89	0
55	MG	14	3470	1/1	0.90	0.09	119,119,119,119	0
55	MG	14	3221	1/1	0.90	0.28	92,92,92,92	0
55	MG	1H	3503	1/1	0.90	0.18	76,76,76,76	0
55	MG	14	3224	1/1	0.90	0.34	73,73,73,73	0
55	MG	1H	3236	1/1	0.90	0.12	72,72,72,72	0
55	MG	1H	3114	1/1	0.90	0.32	69,69,69,69	0
55	MG	13	1625	1/1	0.90	0.33	78,78,78,78	0
55	MG	13	1653	1/1	0.90	0.26	79,79,79,79	0
55	MG	1H	3013	1/1	0.90	0.28	54,54,54,54	0
55	MG	E5	202	1/1	0.90	0.24	92,92,92,92	0
55	MG	1H	3273	1/1	0.90	0.12	93,93,93,93	0
55	MG	13	1746	1/1	0.90	0.26	100,100,100,100	0
55	MG	14	3323	1/1	0.91	0.28	79,79,79,79	0
55	MG	14	3074	1/1	0.91	0.24	53,53,53,53	0
55	MG	14	3326	1/1	0.91	0.36	88,88,88,88	0
55	MG	13	1693	1/1	0.91	0.34	62,62,62,62	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
55	MG	1H	3307	1/1	0.91	0.32	83,83,83,83	0
55	MG	1H	3101	1/1	0.91	0.31	60,60,60,60	0
55	MG	14	3331	1/1	0.91	0.28	63,63,63,63	0
55	MG	1H	3194	1/1	0.91	0.08	86,86,86,86	0
55	MG	13	1640	1/1	0.91	0.22	73,73,73,73	0
55	MG	14	3082	1/1	0.91	0.25	76,76,76,76	0
55	MG	1G	1620	1/1	0.91	0.24	88,88,88,88	0
55	MG	14	3166	1/1	0.91	0.16	61,61,61,61	0
55	MG	1H	3357	1/1	0.91	0.21	78,78,78,78	0
55	MG	1H	3074	1/1	0.91	0.15	59,59,59,59	0
55	MG	1H	3235	1/1	0.91	0.26	88,88,88,88	0
55	MG	14	3344	1/1	0.91	0.23	73,73,73,73	0
55	MG	14	3345	1/1	0.91	0.30	89,89,89,89	0
55	MG	1H	3024	1/1	0.91	0.25	58,58,58,58	0
55	MG	14	3259	1/1	0.91	0.27	88,88,88,88	0
55	MG	1H	3108	1/1	0.91	0.32	58,58,58,58	0
55	MG	1H	3169	1/1	0.91	0.22	90,90,90,90	0
55	MG	2L	101	1/1	0.91	0.16	82,82,82,82	0
55	MG	14	3355	1/1	0.91	0.25	71,71,71,71	0
55	MG	1G	1627	1/1	0.91	0.25	88,88,88,88	0
55	MG	14	3357	1/1	0.91	0.26	93,93,93,93	0
55	MG	1G	1679	1/1	0.91	0.17	88,88,88,88	0
55	MG	1H	3205	1/1	0.91	0.34	75,75,75,75	0
55	MG	1H	3110	1/1	0.91	0.17	54,54,54,54	0
55	MG	14	3183	1/1	0.91	0.23	64,64,64,64	0
55	MG	1H	3025	1/1	0.91	0.17	55,55,55,55	0
55	MG	1G	1631	1/1	0.91	0.30	88,88,88,88	0
55	MG	14	3111	1/1	0.91	0.29	56,56,56,56	0
55	MG	1H	3281	1/1	0.91	0.19	65,65,65,65	0
55	MG	14	3114	1/1	0.91	0.30	81,81,81,81	0
55	MG	1H	3141	1/1	0.91	0.18	50,50,50,50	0
55	MG	14	3018	1/1	0.91	0.27	52,52,52,52	0
55	MG	1H	3509	1/1	0.91	0.35	47,47,47,47	0
55	MG	1H	3059	1/1	0.91	0.21	69,69,69,69	0
55	MG	14	3377	1/1	0.91	0.17	82,82,82,82	0
55	MG	1G	1695	1/1	0.91	0.21	95,95,95,95	0
55	MG	1H	3143	1/1	0.91	0.23	96,96,96,96	0
55	MG	14	3123	1/1	0.91	0.20	63,63,63,63	0
55	MG	1H	3377	1/1	0.91	0.28	87,87,87,87	0
55	MG	14	3203	1/1	0.91	0.20	84,84,84,84	0
55	MG	1H	3116	1/1	0.91	0.22	56,56,56,56	0
55	MG	1H	3006	1/1	0.91	0.20	53,53,53,53	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
55	MG	1G	1643	1/1	0.91	0.27	78,78,78,78	0
55	MG	13	1699	1/1	0.91	0.31	72,72,72,72	0
55	MG	1H	3218	1/1	0.91	0.18	52,52,52,52	0
55	MG	14	3390	1/1	0.91	0.14	70,70,70,70	0
55	MG	1H	3222	1/1	0.91	0.17	91,91,91,91	0
55	MG	1H	3296	1/1	0.91	0.20	84,84,84,84	0
55	MG	1H	3120	1/1	0.91	0.20	53,53,53,53	0
55	MG	88	304	1/1	0.91	0.10	77,77,77,77	0
55	MG	14	3042	1/1	0.91	0.22	47,47,47,47	0
55	MG	1H	3343	1/1	0.91	0.37	90,90,90,90	0
55	MG	14	3432	1/1	0.91	0.09	93,93,93,93	0
55	MG	14	3454	1/1	0.91	0.07	111,111,111,111	0
55	MG	1H	3298	1/1	0.91	0.11	68,68,68,68	0
55	MG	14	3141	1/1	0.91	0.33	78,78,78,78	0
55	MG	13	1725	1/1	0.91	0.30	71,71,71,71	0
55	MG	14	3050	1/1	0.91	0.20	72,72,72,72	0
55	MG	14	3147	1/1	0.91	0.26	80,80,80,80	0
55	MG	13	1627	1/1	0.91	0.18	85,85,85,85	0
55	MG	29	302	1/1	0.91	0.24	65,65,65,65	0
55	MG	14	3056	1/1	0.91	0.28	71,71,71,71	0
55	MG	1H	3047	1/1	0.91	0.17	96,96,96,96	0
55	MG	1G	1716	1/1	0.91	0.19	98,98,98,98	0
55	MG	2K	103	1/1	0.91	0.11	143,143,143,143	0
55	MG	1G	1718	1/1	0.91	0.20	76,76,76,76	0
55	MG	1H	3350	1/1	0.91	0.20	79,79,79,79	0
55	MG	1H	3070	1/1	0.91	0.35	73,73,73,73	0
55	MG	14	3241	1/1	0.92	0.15	83,83,83,83	0
55	MG	1H	3512	1/1	0.92	0.22	72,72,72,72	0
55	MG	32	301	1/1	0.92	0.21	86,86,86,86	0
55	MG	14	3245	1/1	0.92	0.28	81,81,81,81	0
55	MG	1G	1681	1/1	0.92	0.08	86,86,86,86	0
55	MG	1G	1632	1/1	0.92	0.21	81,81,81,81	0
55	MG	1G	1684	1/1	0.92	0.13	109,109,109,109	0
55	MG	14	3168	1/1	0.92	0.17	66,66,66,66	0
55	MG	13	1629	1/1	0.92	0.24	65,65,65,65	0
55	MG	14	3006	1/1	0.92	0.21	54,54,54,54	0
55	MG	1H	3240	1/1	0.92	0.26	74,74,74,74	0
55	MG	14	3174	1/1	0.92	0.13	61,61,61,61	0
55	MG	13	1681	1/1	0.92	0.16	91,91,91,91	0
55	MG	1H	3118	1/1	0.92	0.18	74,74,74,74	0
55	MG	14	3010	1/1	0.92	0.18	54,54,54,54	0
55	MG	5E	201	1/1	0.92	0.10	92,92,92,92	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
55	MG	1H	3146	1/1	0.92	0.23	64,64,64,64	0
55	MG	1H	3397	1/1	0.92	0.26	76,76,76,76	0
55	MG	1H	3090	1/1	0.92	0.33	77,77,77,77	0
55	MG	1K	101	1/1	0.92	0.19	90,90,90,90	0
55	MG	14	3354	1/1	0.92	0.23	76,76,76,76	0
55	MG	88	303	1/1	0.92	0.15	71,71,71,71	0
55	MG	1H	3215	1/1	0.92	0.12	45,45,45,45	0
55	MG	1H	3282	1/1	0.92	0.24	89,89,89,89	0
55	MG	2K	101	1/1	0.92	0.17	85,85,85,85	0
55	MG	13	1604	1/1	0.92	0.15	71,71,71,71	0
55	MG	13	1683	1/1	0.92	0.18	83,83,83,83	0
55	MG	14	3277	1/1	0.92	0.26	74,74,74,74	0
55	MG	1H	3002	1/1	0.92	0.20	53,53,53,53	0
55	MG	1H	3255	1/1	0.92	0.12	72,72,72,72	0
55	MG	1H	3027	1/1	0.92	0.18	51,51,51,51	0
55	MG	1H	3409	1/1	0.92	0.09	75,75,75,75	0
55	MG	1H	3045	1/1	0.92	0.19	64,64,64,64	0
55	MG	1H	3156	1/1	0.92	0.22	76,76,76,76	0
55	MG	14	3285	1/1	0.92	0.22	72,72,72,72	0
55	MG	14	3037	1/1	0.92	0.19	58,58,58,58	0
55	MG	14	3287	1/1	0.92	0.17	98,98,98,98	0
55	MG	13	1740	1/1	0.92	0.06	106,106,106,106	0
55	MG	14	3040	1/1	0.92	0.37	59,59,59,59	0
55	MG	1G	1617	1/1	0.92	0.25	72,72,72,72	0
55	MG	1G	1712	1/1	0.92	0.13	87,87,87,87	0
55	MG	1G	1660	1/1	0.92	0.16	82,82,82,82	0
55	MG	14	3293	1/1	0.92	0.13	72,72,72,72	0
55	MG	14	3383	1/1	0.92	0.17	95,95,95,95	0
55	MG	14	3294	1/1	0.92	0.27	69,69,69,69	0
55	MG	14	3295	1/1	0.92	0.18	84,84,84,84	0
55	MG	1G	1714	1/1	0.92	0.34	94,94,94,94	0
55	MG	1G	1661	1/1	0.92	0.19	65,65,65,65	0
55	MG	13	1718	1/1	0.92	0.25	78,78,78,78	0
55	MG	14	3299	1/1	0.92	0.25	64,64,64,64	0
55	MG	14	3216	1/1	0.92	0.11	77,77,77,77	0
55	MG	14	3054	1/1	0.92	0.31	72,72,72,72	0
55	MG	1G	1663	1/1	0.92	0.18	75,75,75,75	0
55	MG	14	3142	1/1	0.92	0.21	77,77,77,77	0
55	MG	14	3059	1/1	0.92	0.19	54,54,54,54	0
55	MG	1H	3131	1/1	0.92	0.30	65,65,65,65	0
55	MG	1H	3263	1/1	0.92	0.11	67,67,67,67	0
55	MG	1H	3449	1/1	0.92	0.09	110,110,110,110	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
55	MG	14	3459	1/1	0.92	0.06	122,122,122,122	0
55	MG	14	3464	1/1	0.92	0.14	116,116,116,116	0
55	MG	14	3063	1/1	0.92	0.21	69,69,69,69	0
55	MG	14	3227	1/1	0.92	0.12	90,90,90,90	0
55	MG	1H	3340	1/1	0.92	0.13	75,75,75,75	0
55	MG	1H	3484	1/1	0.92	0.18	104,104,104,104	0
55	MG	1H	3490	1/1	0.92	0.08	128,128,128,128	0
55	MG	14	3070	1/1	0.92	0.15	57,57,57,57	0
55	MG	14	3072	1/1	0.92	0.43	52,52,52,52	0
55	MG	1H	3494	1/1	0.92	0.08	125,125,125,125	0
55	MG	1H	3049	1/1	0.92	0.14	89,89,89,89	0
55	MG	1H	3051	1/1	0.92	0.26	74,74,74,74	0
55	MG	13	1675	1/1	0.92	0.26	87,87,87,87	0
55	MG	E5	201	1/1	0.92	0.12	62,62,62,62	0
55	MG	1H	3113	1/1	0.92	0.15	78,78,78,78	0
55	MG	1H	3008	1/1	0.92	0.17	64,64,64,64	0
55	MG	14	3325	1/1	0.92	0.08	72,72,72,72	0
55	MG	1H	3163	1/1	0.93	0.29	83,83,83,83	0
55	MG	1H	3390	1/1	0.93	0.28	86,86,86,86	0
55	MG	14	3278	1/1	0.93	0.21	69,69,69,69	0
55	MG	1H	3164	1/1	0.93	0.27	66,66,66,66	0
55	MG	1G	1685	1/1	0.93	0.23	92,92,92,92	0
55	MG	1H	3137	1/1	0.93	0.11	72,72,72,72	0
55	MG	1H	3138	1/1	0.93	0.25	74,74,74,74	0
55	MG	1H	3265	1/1	0.93	0.24	65,65,65,65	0
55	MG	14	3211	1/1	0.93	0.14	74,74,74,74	0
55	MG	1H	3078	1/1	0.93	0.31	54,54,54,54	0
55	MG	14	3144	1/1	0.93	0.29	61,61,61,61	0
55	MG	1G	1691	1/1	0.93	0.13	98,98,98,98	0
55	MG	1H	3046	1/1	0.93	0.15	56,56,56,56	0
55	MG	1H	3306	1/1	0.93	0.32	84,84,84,84	0
55	MG	1H	3170	1/1	0.93	0.23	75,75,75,75	0
55	MG	14	3078	1/1	0.93	0.23	68,68,68,68	0
55	MG	J8	101	1/1	0.93	0.30	65,65,65,65	0
55	MG	1H	3308	1/1	0.93	0.14	77,77,77,77	0
55	MG	1H	3309	1/1	0.93	0.27	78,78,78,78	0
55	MG	1H	3238	1/1	0.93	0.36	77,77,77,77	0
55	MG	14	3084	1/1	0.93	0.27	86,86,86,86	0
55	MG	1H	3097	1/1	0.93	0.29	48,48,48,48	0
55	MG	14	3157	1/1	0.93	0.31	83,83,83,83	0
55	MG	14	3088	1/1	0.93	0.16	73,73,73,73	0
55	MG	1H	3099	1/1	0.93	0.25	59,59,59,59	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
55	MG	14	3094	1/1	0.93	0.13	60,60,60,60	0
55	MG	14	3303	1/1	0.93	0.11	71,71,71,71	0
55	MG	1H	3173	1/1	0.93	0.32	70,70,70,70	0
55	MG	13	1728	1/1	0.93	0.15	80,80,80,80	0
55	MG	1H	3081	1/1	0.93	0.29	85,85,85,85	0
55	MG	1G	1704	1/1	0.93	0.23	78,78,78,78	0
55	MG	13	1614	1/1	0.93	0.24	92,92,92,92	0
55	MG	1H	3068	1/1	0.93	0.25	83,83,83,83	0
55	MG	1H	3149	1/1	0.93	0.33	74,74,74,74	0
55	MG	1H	3085	1/1	0.93	0.20	75,75,75,75	0
55	MG	14	3169	1/1	0.93	0.11	55,55,55,55	0
55	MG	1H	3069	1/1	0.93	0.13	69,69,69,69	0
55	MG	1H	3219	1/1	0.93	0.08	64,64,64,64	0
55	MG	1H	3284	1/1	0.93	0.13	69,69,69,69	0
55	MG	1H	3372	1/1	0.93	0.25	75,75,75,75	0
55	MG	14	3034	1/1	0.93	0.27	60,60,60,60	0
55	MG	14	3112	1/1	0.93	0.15	77,77,77,77	0
55	MG	1H	3252	1/1	0.93	0.27	79,79,79,79	0
55	MG	13	1612	1/1	0.93	0.20	74,74,74,74	0
55	MG	14	3452	1/1	0.93	0.11	94,94,94,94	0
55	MG	1G	1715	1/1	0.93	0.21	83,83,83,83	0
55	MG	1H	3375	1/1	0.93	0.16	70,70,70,70	0
55	MG	1H	3089	1/1	0.93	0.26	71,71,71,71	0
55	MG	1H	3004	1/1	0.93	0.19	60,60,60,60	0
55	MG	1H	3501	1/1	0.93	0.11	105,105,105,105	0
55	MG	14	3487	1/1	0.93	0.15	103,103,103,103	0
55	MG	14	3121	1/1	0.93	0.20	69,69,69,69	0
55	MG	1H	3091	1/1	0.93	0.24	58,58,58,58	0
55	MG	14	3046	1/1	0.93	0.17	67,67,67,67	0
55	MG	14	3047	1/1	0.93	0.16	67,67,67,67	0
55	MG	14	3333	1/1	0.93	0.25	58,58,58,58	0
55	MG	14	3267	1/1	0.93	0.13	74,74,74,74	0
55	MG	1H	3257	1/1	0.93	0.19	82,82,82,82	0
55	MG	45	201	1/1	0.93	0.27	76,76,76,76	0
55	MG	1H	3115	1/1	0.93	0.18	73,73,73,73	0
55	MG	1H	3385	1/1	0.93	0.12	106,106,106,106	0
55	MG	1H	3052	1/1	0.93	0.30	67,67,67,67	0
55	MG	13	1742	1/1	0.93	0.10	111,111,111,111	0
55	MG	1G	1680	1/1	0.93	0.21	88,88,88,88	0
55	MG	14	3343	1/1	0.93	0.26	75,75,75,75	0
55	MG	1H	3001	1/1	0.94	0.24	51,51,51,51	0
55	MG	14	3172	1/1	0.94	0.28	69,69,69,69	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
55	MG	14	3019	1/1	0.94	0.16	80,80,80,80	0
55	MG	14	3255	1/1	0.94	0.08	90,90,90,90	0
55	MG	13	1638	1/1	0.94	0.19	74,74,74,74	0
55	MG	14	3258	1/1	0.94	0.10	101,101,101,101	0
55	MG	1H	3287	1/1	0.94	0.14	75,75,75,75	0
55	MG	14	3260	1/1	0.94	0.04	95,95,95,95	0
55	MG	1H	3289	1/1	0.94	0.06	80,80,80,80	0
55	MG	1H	3382	1/1	0.94	0.23	73,73,73,73	0
55	MG	1H	3220	1/1	0.94	0.12	55,55,55,55	0
55	MG	13	1741	1/1	0.94	0.09	128,128,128,128	0
55	MG	13	1633	1/1	0.94	0.26	59,59,59,59	0
55	MG	14	3266	1/1	0.94	0.09	69,69,69,69	0
55	MG	13	1724	1/1	0.94	0.30	63,63,63,63	0
55	MG	1H	3160	1/1	0.94	0.23	88,88,88,88	0
55	MG	1H	3190	1/1	0.94	0.19	71,71,71,71	0
55	MG	1H	3341	1/1	0.94	0.15	83,83,83,83	0
55	MG	13	1636	1/1	0.94	0.14	73,73,73,73	0
55	MG	1H	3162	1/1	0.94	0.27	89,89,89,89	0
55	MG	13	1706	1/1	0.94	0.14	95,95,95,95	0
55	MG	1H	3196	1/1	0.94	0.24	77,77,77,77	0
55	MG	13	1621	1/1	0.94	0.17	75,75,75,75	0
55	MG	14	3362	1/1	0.94	0.21	77,77,77,77	0
55	MG	14	3363	1/1	0.94	0.17	67,67,67,67	0
55	MG	98	201	1/1	0.94	0.41	71,71,71,71	0
55	MG	I8	101	1/1	0.94	0.19	55,55,55,55	0
55	MG	14	3366	1/1	0.94	0.16	89,89,89,89	0
55	MG	14	3197	1/1	0.94	0.13	82,82,82,82	0
55	MG	1H	3055	1/1	0.94	0.15	66,66,66,66	0
55	MG	1H	3034	1/1	0.94	0.13	54,54,54,54	0
55	MG	14	3045	1/1	0.94	0.18	55,55,55,55	0
55	MG	1H	3202	1/1	0.94	0.27	71,71,71,71	0
55	MG	13	1677	1/1	0.94	0.34	77,77,77,77	0
55	MG	1G	1604	1/1	0.94	0.12	79,79,79,79	0
55	MG	1H	3058	1/1	0.94	0.15	67,67,67,67	0
55	MG	1H	3014	1/1	0.94	0.24	40,40,40,40	0
55	MG	14	3376	1/1	0.94	0.15	59,59,59,59	0
55	MG	14	3052	1/1	0.94	0.13	62,62,62,62	0
55	MG	14	3210	1/1	0.94	0.23	86,86,86,86	0
55	MG	1H	3403	1/1	0.94	0.32	79,79,79,79	0
55	MG	14	3136	1/1	0.94	0.24	71,71,71,71	0
55	MG	1H	3015	1/1	0.94	0.22	53,53,53,53	0
55	MG	1H	3310	1/1	0.94	0.27	52,52,52,52	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
55	MG	1H	3061	1/1	0.94	0.17	75,75,75,75	0
55	MG	1H	3016	1/1	0.94	0.16	70,70,70,70	0
55	MG	1H	3209	1/1	0.94	0.21	63,63,63,63	0
55	MG	1H	3040	1/1	0.94	0.11	69,69,69,69	0
55	MG	1H	3316	1/1	0.94	0.15	87,87,87,87	0
55	MG	1H	3277	1/1	0.94	0.24	74,74,74,74	0
55	MG	14	3067	1/1	0.94	0.24	54,54,54,54	0
55	MG	1H	3363	1/1	0.94	0.36	54,54,54,54	0
55	MG	1H	3278	1/1	0.94	0.20	84,84,84,84	0
55	MG	14	3071	1/1	0.94	0.28	48,48,48,48	0
55	MG	14	3151	1/1	0.94	0.21	68,68,68,68	0
55	MG	13	1671	1/1	0.94	0.09	106,106,106,106	0
55	MG	1H	3368	1/1	0.94	0.23	88,88,88,88	0
55	MG	14	3400	1/1	0.94	0.08	91,91,91,91	0
55	MG	14	3401	1/1	0.94	0.09	78,78,78,78	0
55	MG	14	3420	1/1	0.94	0.09	91,91,91,91	0
55	MG	1H	3247	1/1	0.94	0.42	77,77,77,77	0
55	MG	14	3438	1/1	0.94	0.18	117,117,117,117	0
55	MG	1G	1682	1/1	0.94	0.11	80,80,80,80	0
55	MG	2L	102	1/1	0.94	0.17	71,71,71,71	0
55	MG	14	3234	1/1	0.94	0.15	76,76,76,76	0
55	MG	1H	3451	1/1	0.94	0.09	105,105,105,105	0
55	MG	1H	3456	1/1	0.94	0.14	88,88,88,88	0
55	MG	14	3468	1/1	0.94	0.22	107,107,107,107	0
55	MG	14	3003	1/1	0.94	0.12	63,63,63,63	0
55	MG	14	3316	1/1	0.94	0.29	78,78,78,78	0
55	MG	14	3005	1/1	0.94	0.18	62,62,62,62	0
55	MG	14	3239	1/1	0.94	0.08	90,90,90,90	0
55	MG	13	1719	1/1	0.94	0.23	89,89,89,89	0
55	MG	14	3320	1/1	0.94	0.15	81,81,81,81	0
55	MG	1H	3468	1/1	0.94	0.07	106,106,106,106	0
55	MG	1H	3476	1/1	0.94	0.06	119,119,119,119	0
55	MG	13	1710	1/1	0.94	0.34	80,80,80,80	0
55	MG	1H	3022	1/1	0.94	0.17	57,57,57,57	0
55	MG	14	3095	1/1	0.94	0.18	54,54,54,54	0
55	MG	14	3011	1/1	0.94	0.20	48,48,48,48	0
55	MG	13	1654	1/1	0.94	0.20	78,78,78,78	0
55	MG	1H	3496	1/1	0.94	0.12	99,99,99,99	0
55	MG	1H	3326	1/1	0.94	0.22	51,51,51,51	0
55	MG	14	3251	1/1	0.94	0.23	74,74,74,74	0
55	MG	1H	3134	1/1	0.95	0.22	67,67,67,67	0
55	MG	14	3023	1/1	0.95	0.18	56,56,56,56	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
55	MG	11	301	1/1	0.95	0.09	53,53,53,53	0
55	MG	14	3083	1/1	0.95	0.25	68,68,68,68	0
55	MG	1H	3082	1/1	0.95	0.14	70,70,70,70	0
55	MG	14	3361	1/1	0.95	0.12	88,88,88,88	0
55	MG	14	3085	1/1	0.95	0.26	58,58,58,58	0
55	MG	14	3086	1/1	0.95	0.17	77,77,77,77	0
55	MG	1H	3010	1/1	0.95	0.30	48,48,48,48	0
55	MG	1G	1671	1/1	0.95	0.29	84,84,84,84	0
55	MG	13	1697	1/1	0.95	0.37	67,67,67,67	0
55	MG	14	3090	1/1	0.95	0.21	58,58,58,58	0
55	MG	14	3091	1/1	0.95	0.34	53,53,53,53	0
55	MG	78	201	1/1	0.95	0.10	74,74,74,74	0
55	MG	1H	3021	1/1	0.95	0.23	43,43,43,43	0
55	MG	1H	3195	1/1	0.95	0.23	84,84,84,84	0
55	MG	1G	1676	1/1	0.95	0.29	93,93,93,93	0
55	MG	1H	3140	1/1	0.95	0.35	82,82,82,82	0
55	MG	1H	3075	1/1	0.95	0.15	69,69,69,69	0
55	MG	1H	3157	1/1	0.95	0.31	60,60,60,60	0
55	MG	1H	3221	1/1	0.95	0.26	57,57,57,57	0
55	MG	1G	1639	1/1	0.95	0.25	79,79,79,79	0
55	MG	1H	3465	1/1	0.95	0.07	108,108,108,108	0
55	MG	14	3105	1/1	0.95	0.10	90,90,90,90	0
55	MG	1H	3334	1/1	0.95	0.19	75,75,75,75	0
55	MG	1H	3474	1/1	0.95	0.10	102,102,102,102	0
55	MG	1H	3243	1/1	0.95	0.27	69,69,69,69	0
55	MG	1H	3336	1/1	0.95	0.15	70,70,70,70	0
55	MG	1G	1607	1/1	0.95	0.13	86,86,86,86	0
55	MG	1H	3365	1/1	0.95	0.12	46,46,46,46	0
55	MG	14	3048	1/1	0.95	0.14	66,66,66,66	0
55	MG	1G	1742	1/1	0.95	0.05	131,131,131,131	0
55	MG	1G	1743	1/1	0.95	0.12	98,98,98,98	0
55	MG	1H	3026	1/1	0.95	0.15	53,53,53,53	0
55	MG	14	3117	1/1	0.95	0.07	73,73,73,73	0
55	MG	1H	3495	1/1	0.95	0.05	112,112,112,112	0
55	MG	14	3053	1/1	0.95	0.32	69,69,69,69	0
55	MG	1H	3159	1/1	0.95	0.17	76,76,76,76	0
55	MG	1G	1612	1/1	0.95	0.08	88,88,88,88	0
55	MG	14	3058	1/1	0.95	0.27	53,53,53,53	0
55	MG	1H	3127	1/1	0.95	0.16	58,58,58,58	0
55	MG	1H	3088	1/1	0.95	0.24	44,44,44,44	0
55	MG	14	3404	1/1	0.95	0.13	105,105,105,105	0
55	MG	13	1656	1/1	0.95	0.23	63,63,63,63	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
55	MG	14	3422	1/1	0.95	0.07	68,68,68,68	0
55	MG	14	3423	1/1	0.95	0.06	99,99,99,99	0
55	MG	1G	1616	1/1	0.95	0.31	62,62,62,62	0
55	MG	1H	3062	1/1	0.95	0.21	70,70,70,70	0
55	MG	14	3442	1/1	0.95	0.07	109,109,109,109	0
55	MG	1G	1656	1/1	0.95	0.24	74,74,74,74	0
55	MG	14	3193	1/1	0.95	0.09	83,83,83,83	0
55	MG	14	3457	1/1	0.95	0.06	103,103,103,103	0
55	MG	1G	1657	1/1	0.95	0.28	92,92,92,92	0
55	MG	14	3460	1/1	0.95	0.15	114,114,114,114	0
55	MG	1H	3103	1/1	0.95	0.23	48,48,48,48	0
55	MG	14	3068	1/1	0.95	0.24	57,57,57,57	0
55	MG	14	3467	1/1	0.95	0.12	97,97,97,97	0
55	MG	14	3132	1/1	0.95	0.09	78,78,78,78	0
55	MG	1H	3293	1/1	0.95	0.19	78,78,78,78	0
55	MG	14	3485	1/1	0.95	0.11	101,101,101,101	0
55	MG	14	3337	1/1	0.95	0.21	64,64,64,64	0
55	MG	1H	3511	1/1	0.95	0.05	75,75,75,75	0
55	MG	14	3013	1/1	0.95	0.12	66,66,66,66	0
55	MG	14	3137	1/1	0.95	0.21	77,77,77,77	0
55	MG	14	3274	1/1	0.95	0.24	83,83,83,83	0
55	MG	14	3342	1/1	0.95	0.16	99,99,99,99	0
55	MG	1H	3318	1/1	0.95	0.08	50,50,50,50	0
55	MG	14	3073	1/1	0.95	0.20	70,70,70,70	0
55	MG	1H	3271	1/1	0.95	0.21	77,77,77,77	0
55	MG	14	3208	1/1	0.95	0.24	74,74,74,74	0
55	MG	1H	3050	1/1	0.95	0.17	65,65,65,65	0
55	MG	1H	3105	1/1	0.95	0.24	50,50,50,50	0
55	MG	1H	3378	1/1	0.95	0.12	84,84,84,84	0
55	MG	14	3213	1/1	0.95	0.23	59,59,59,59	0
55	MG	1G	1666	1/1	0.95	0.29	71,71,71,71	0
55	MG	1H	3418	1/1	0.96	0.08	71,71,71,71	0
55	MG	1H	3423	1/1	0.96	0.09	110,110,110,110	0
55	MG	1H	3428	1/1	0.96	0.09	85,85,85,85	0
55	MG	1H	3441	1/1	0.96	0.09	103,103,103,103	0
55	MG	14	3017	1/1	0.96	0.15	70,70,70,70	0
55	MG	1H	3393	1/1	0.96	0.07	58,58,58,58	0
55	MG	1H	3288	1/1	0.96	0.30	68,68,68,68	0
55	MG	1G	1688	1/1	0.96	0.13	103,103,103,103	0
55	MG	14	3194	1/1	0.96	0.07	66,66,66,66	0
55	MG	13	1733	1/1	0.96	0.06	95,95,95,95	0
55	MG	14	3244	1/1	0.96	0.25	75,75,75,75	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
55	MG	14	3064	1/1	0.96	0.23	54,54,54,54	0
55	MG	1H	3185	1/1	0.96	0.23	66,66,66,66	0
55	MG	14	3199	1/1	0.96	0.24	75,75,75,75	0
55	MG	1H	3011	1/1	0.96	0.20	49,49,49,49	0
55	MG	1H	3187	1/1	0.96	0.11	66,66,66,66	0
55	MG	14	3403	1/1	0.96	0.07	96,96,96,96	0
55	MG	13	1630	1/1	0.96	0.09	65,65,65,65	0
55	MG	14	3408	1/1	0.96	0.07	63,63,63,63	0
55	MG	14	3413	1/1	0.96	0.06	100,100,100,100	0
55	MG	1H	3470	1/1	0.96	0.13	79,79,79,79	0
55	MG	1H	3473	1/1	0.96	0.06	100,100,100,100	0
55	MG	14	3351	1/1	0.96	0.20	104,104,104,104	0
55	MG	14	3029	1/1	0.96	0.15	63,63,63,63	0
55	MG	1H	3139	1/1	0.96	0.12	63,63,63,63	0
55	MG	1G	1732	1/1	0.96	0.05	123,123,123,123	0
55	MG	14	3446	1/1	0.96	0.05	122,122,122,122	0
55	MG	G8	201	1/1	0.96	0.23	65,65,65,65	0
55	MG	14	3209	1/1	0.96	0.13	91,91,91,91	0
55	MG	14	3358	1/1	0.96	0.38	89,89,89,89	0
55	MG	1H	3359	1/1	0.96	0.23	45,45,45,45	0
55	MG	14	3076	1/1	0.96	0.24	45,45,45,45	0
55	MG	14	3461	1/1	0.96	0.04	117,117,117,117	0
55	MG	14	3462	1/1	0.96	0.09	103,103,103,103	0
55	MG	14	3463	1/1	0.96	0.06	119,119,119,119	0
55	MG	3I	201	1/1	0.96	0.12	68,68,68,68	0
55	MG	1H	3485	1/1	0.96	0.08	84,84,84,84	0
55	MG	1H	3381	1/1	0.96	0.38	79,79,79,79	0
55	MG	1H	3491	1/1	0.96	0.04	122,122,122,122	0
55	MG	1H	3311	1/1	0.96	0.05	65,65,65,65	0
55	MG	14	3482	1/1	0.96	0.06	81,81,81,81	0
55	MG	1H	3328	1/1	0.96	0.10	70,70,70,70	0
55	MG	14	3486	1/1	0.96	0.06	138,138,138,138	0
55	MG	14	3041	1/1	0.96	0.17	53,53,53,53	0
55	MG	14	3268	1/1	0.96	0.32	69,69,69,69	0
55	MG	1H	3345	1/1	0.96	0.12	70,70,70,70	0
55	MG	1H	3497	1/1	0.96	0.08	113,113,113,113	0
55	MG	1H	3364	1/1	0.96	0.27	75,75,75,75	0
55	MG	1H	3386	1/1	0.96	0.21	87,87,87,87	0
55	MG	1H	3229	1/1	0.96	0.37	82,82,82,82	0
55	MG	1H	3216	1/1	0.96	0.17	65,65,65,65	0
55	MG	13	1664	1/1	0.96	0.20	76,76,76,76	0
55	MG	14	3135	1/1	0.96	0.14	75,75,75,75	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
55	MG	1H	3109	1/1	0.96	0.27	39,39,39,39	0
55	MG	85	202	1/1	0.96	0.09	79,79,79,79	0
55	MG	14	3093	1/1	0.96	0.18	60,60,60,60	0
55	MG	13	1732	1/1	0.96	0.10	113,113,113,113	0
55	MG	1H	3111	1/1	0.96	0.21	51,51,51,51	0
55	MG	14	3012	1/1	0.96	0.16	48,48,48,48	0
55	MG	1H	3007	1/1	0.97	0.21	50,50,50,50	0
55	MG	14	3330	1/1	0.97	0.21	43,43,43,43	0
55	MG	1H	3427	1/1	0.97	0.04	91,91,91,91	0
55	MG	1H	3498	1/1	0.97	0.13	100,100,100,100	0
55	MG	14	3389	1/1	0.97	0.10	77,77,77,77	0
55	MG	1H	3301	1/1	0.97	0.21	73,73,73,73	0
55	MG	1H	3500	1/1	0.97	0.06	105,105,105,105	0
55	MG	14	3176	1/1	0.97	0.30	63,63,63,63	0
55	MG	1G	1740	1/1	0.97	0.05	112,112,112,112	0
55	MG	1H	3429	1/1	0.97	0.11	91,91,91,91	0
55	MG	14	3039	1/1	0.97	0.23	63,63,63,63	0
55	MG	1H	3430	1/1	0.97	0.09	87,87,87,87	0
55	MG	1H	3504	1/1	0.97	0.12	95,95,95,95	0
55	MG	1H	3507	1/1	0.97	0.09	100,100,100,100	0
55	MG	1H	3431	1/1	0.97	0.10	74,74,74,74	0
55	MG	1H	3434	1/1	0.97	0.08	72,72,72,72	0
55	MG	13	1605	1/1	0.97	0.10	86,86,86,86	0
55	MG	14	3409	1/1	0.97	0.06	83,83,83,83	0
55	MG	14	3410	1/1	0.97	0.08	68,68,68,68	0
55	MG	14	3186	1/1	0.97	0.13	69,69,69,69	0
55	MG	14	3414	1/1	0.97	0.05	85,85,85,85	0
55	MG	14	3416	1/1	0.97	0.10	96,96,96,96	0
55	MG	14	3346	1/1	0.97	0.04	62,62,62,62	0
55	MG	13	1736	1/1	0.97	0.09	111,111,111,111	0
55	MG	14	3092	1/1	0.97	0.27	64,64,64,64	0
55	MG	14	3427	1/1	0.97	0.06	97,97,97,97	0
55	MG	14	3431	1/1	0.97	0.06	86,86,86,86	0
55	MG	13	1692	1/1	0.97	0.18	52,52,52,52	0
55	MG	14	3433	1/1	0.97	0.06	91,91,91,91	0
55	MG	1H	3197	1/1	0.97	0.27	48,48,48,48	0
55	MG	1H	3454	1/1	0.97	0.06	94,94,94,94	0
55	MG	14	3143	1/1	0.97	0.31	64,64,64,64	0
55	MG	14	3451	1/1	0.97	0.05	91,91,91,91	0
55	MG	14	3353	1/1	0.97	0.34	84,84,84,84	0
55	MG	1H	3182	1/1	0.97	0.23	59,59,59,59	0
55	MG	14	3455	1/1	0.97	0.07	121,121,121,121	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
55	MG	1H	3199	1/1	0.97	0.13	74,74,74,74	0
55	MG	14	3195	1/1	0.97	0.26	69,69,69,69	0
55	MG	1H	3462	1/1	0.97	0.10	91,91,91,91	0
55	MG	14	3302	1/1	0.97	0.12	85,85,85,85	0
55	MG	1H	3168	1/1	0.97	0.17	72,72,72,72	0
55	MG	1H	3018	1/1	0.97	0.28	46,46,46,46	0
55	MG	14	3055	1/1	0.97	0.26	68,68,68,68	0
55	MG	1H	3237	1/1	0.97	0.16	74,74,74,74	0
55	MG	1H	3472	1/1	0.97	0.07	86,86,86,86	0
55	MG	1H	3036	1/1	0.97	0.31	77,77,77,77	0
55	MG	88	301	1/1	0.97	0.12	82,82,82,82	0
55	MG	14	3471	1/1	0.97	0.17	113,113,113,113	0
55	MG	14	3475	1/1	0.97	0.12	104,104,104,104	0
55	MG	14	3479	1/1	0.97	0.09	78,78,78,78	0
55	MG	14	3107	1/1	0.97	0.26	50,50,50,50	0
55	MG	14	3483	1/1	0.97	0.09	104,104,104,104	0
55	MG	1G	1633	1/1	0.97	0.26	73,73,73,73	0
55	MG	13	1739	1/1	0.97	0.07	111,111,111,111	0
55	MG	1H	3098	1/1	0.97	0.19	40,40,40,40	0
55	MG	1H	3479	1/1	0.97	0.05	103,103,103,103	0
55	MG	14	3490	1/1	0.97	0.11	81,81,81,81	0
55	MG	1H	3481	1/1	0.97	0.05	116,116,116,116	0
55	MG	14	3021	1/1	0.97	0.13	60,60,60,60	0
55	MG	1H	3482	1/1	0.97	0.06	83,83,83,83	0
55	MG	1H	3012	1/1	0.97	0.11	52,52,52,52	0
55	MG	1H	3076	1/1	0.97	0.12	67,67,67,67	0
55	MG	1H	3486	1/1	0.97	0.06	129,129,129,129	0
55	MG	1H	3077	1/1	0.97	0.10	65,65,65,65	0
55	MG	1H	3191	1/1	0.97	0.10	75,75,75,75	0
55	MG	1H	3493	1/1	0.97	0.06	122,122,122,122	0
55	MG	14	3218	1/1	0.97	0.18	57,57,57,57	0
55	MG	1G	1605	1/1	0.97	0.11	85,85,85,85	0
55	MG	1H	3415	1/1	0.97	0.08	59,59,59,59	0
55	MG	13	1744	1/1	0.97	0.05	117,117,117,117	0
55	MG	14	3222	1/1	0.97	0.11	73,73,73,73	0
55	MG	14	3440	1/1	0.98	0.04	105,105,105,105	0
55	MG	14	3441	1/1	0.98	0.05	102,102,102,102	0
55	MG	1H	3379	1/1	0.98	0.29	69,69,69,69	0
55	MG	14	3445	1/1	0.98	0.04	97,97,97,97	0
55	MG	1H	3464	1/1	0.98	0.05	92,92,92,92	0
55	MG	14	3447	1/1	0.98	0.04	95,95,95,95	0
55	MG	14	3448	1/1	0.98	0.06	109,109,109,109	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
55	MG	1H	3028	1/1	0.98	0.17	52,52,52,52	0
55	MG	1H	3466	1/1	0.98	0.04	77,77,77,77	0
55	MG	14	3453	1/1	0.98	0.15	91,91,91,91	0
55	MG	1H	3093	1/1	0.98	0.09	60,60,60,60	0
55	MG	1H	3469	1/1	0.98	0.04	107,107,107,107	0
55	MG	1H	3217	1/1	0.98	0.04	56,56,56,56	0
55	MG	14	3057	1/1	0.98	0.21	45,45,45,45	0
55	MG	1H	3106	1/1	0.98	0.08	47,47,47,47	0
55	MG	1H	3435	1/1	0.98	0.04	80,80,80,80	0
55	MG	1H	3416	1/1	0.98	0.06	60,60,60,60	0
55	MG	1H	3445	1/1	0.98	0.05	86,86,86,86	0
55	MG	I8	102	1/1	0.98	0.07	108,108,108,108	0
55	MG	1H	3478	1/1	0.98	0.05	118,118,118,118	0
55	MG	1H	3327	1/1	0.98	0.21	83,83,83,83	0
55	MG	14	3402	1/1	0.98	0.06	63,63,63,63	0
55	MG	14	3469	1/1	0.98	0.05	96,96,96,96	0
55	MG	1H	3419	1/1	0.98	0.04	88,88,88,88	0
55	MG	1H	3420	1/1	0.98	0.04	99,99,99,99	0
55	MG	14	3474	1/1	0.98	0.08	107,107,107,107	0
55	MG	14	3406	1/1	0.98	0.05	62,62,62,62	0
55	MG	14	3476	1/1	0.98	0.06	65,65,65,65	0
55	MG	14	3478	1/1	0.98	0.04	109,109,109,109	0
55	MG	1H	3453	1/1	0.98	0.07	89,89,89,89	0
55	MG	13	1735	1/1	0.98	0.04	111,111,111,111	0
55	MG	1H	3455	1/1	0.98	0.05	62,62,62,62	0
55	MG	14	3411	1/1	0.98	0.04	88,88,88,88	0
55	MG	1H	3487	1/1	0.98	0.04	102,102,102,102	0
55	MG	1H	3489	1/1	0.98	0.04	97,97,97,97	0
55	MG	1H	3425	1/1	0.98	0.05	62,62,62,62	0
55	MG	14	3489	1/1	0.98	0.05	99,99,99,99	0
55	MG	14	3417	1/1	0.98	0.05	72,72,72,72	0
55	MG	14	3418	1/1	0.98	0.04	72,72,72,72	0
55	MG	14	3102	1/1	0.98	0.13	62,62,62,62	0
55	MG	1G	1731	1/1	0.98	0.11	113,113,113,113	0
55	MG	13	1738	1/1	0.98	0.04	100,100,100,100	0
55	MG	14	3424	1/1	0.98	0.04	72,72,72,72	0
55	MG	1G	1733	1/1	0.98	0.04	93,93,93,93	0
55	MG	14	3430	1/1	0.98	0.06	69,69,69,69	0
55	MG	14	3256	1/1	0.98	0.06	95,95,95,95	0
55	MG	1G	1735	1/1	0.98	0.05	97,97,97,97	0
55	MG	1G	1737	1/1	0.98	0.05	93,93,93,93	0
55	MG	14	3434	1/1	0.98	0.11	89,89,89,89	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
55	MG	14	3435	1/1	0.98	0.05	117,117,117,117	0
55	MG	1H	3492	1/1	0.98	0.12	101,101,101,101	0
55	MG	14	3439	1/1	0.98	0.04	105,105,105,105	0
55	MG	14	3437	1/1	0.99	0.04	88,88,88,88	0
55	MG	13	1734	1/1	0.99	0.04	93,93,93,93	0
55	MG	1H	3446	1/1	0.99	0.05	83,83,83,83	0
55	MG	1H	3176	1/1	0.99	0.25	59,59,59,59	0
55	MG	1H	3475	1/1	0.99	0.03	92,92,92,92	0
55	MG	1H	3448	1/1	0.99	0.06	86,86,86,86	0
55	MG	14	3443	1/1	0.99	0.09	74,74,74,74	0
55	MG	14	3444	1/1	0.99	0.04	106,106,106,106	0
55	MG	1H	3477	1/1	0.99	0.07	92,92,92,92	0
55	MG	1H	3421	1/1	0.99	0.06	66,66,66,66	0
55	MG	1H	3450	1/1	0.99	0.04	74,74,74,74	0
55	MG	1H	3480	1/1	0.99	0.06	118,118,118,118	0
55	MG	14	3449	1/1	0.99	0.05	82,82,82,82	0
55	MG	14	3450	1/1	0.99	0.04	65,65,65,65	0
55	MG	1H	3422	1/1	0.99	0.03	85,85,85,85	0
55	MG	1H	3452	1/1	0.99	0.04	91,91,91,91	0
55	MG	1G	1730	1/1	0.99	0.04	77,77,77,77	0
55	MG	1H	3483	1/1	0.99	0.04	86,86,86,86	0
55	MG	1H	3417	1/1	0.99	0.05	70,70,70,70	0
55	MG	14	3456	1/1	0.99	0.06	82,82,82,82	0
55	MG	1H	3432	1/1	0.99	0.04	58,58,58,58	0
55	MG	14	3458	1/1	0.99	0.03	91,91,91,91	0
55	MG	14	3397	1/1	0.99	0.03	64,64,64,64	0
55	MG	14	3398	1/1	0.99	0.04	66,66,66,66	0
55	MG	14	3399	1/1	0.99	0.06	75,75,75,75	0
55	MG	1G	1734	1/1	0.99	0.03	108,108,108,108	0
55	MG	1H	3433	1/1	0.99	0.05	67,67,67,67	0
55	MG	1G	1736	1/1	0.99	0.03	114,114,114,114	0
55	MG	1H	3424	1/1	0.99	0.04	72,72,72,72	0
55	MG	14	3466	1/1	0.99	0.10	103,103,103,103	0
55	MG	1H	3488	1/1	0.99	0.04	66,66,66,66	0
55	MG	14	3405	1/1	0.99	0.05	70,70,70,70	0
55	MG	1H	3457	1/1	0.99	0.04	79,79,79,79	0
55	MG	14	3407	1/1	0.99	0.04	66,66,66,66	0
55	MG	1H	3458	1/1	0.99	0.05	67,67,67,67	0
55	MG	14	3472	1/1	0.99	0.05	103,103,103,103	0
55	MG	14	3473	1/1	0.99	0.06	61,61,61,61	0
55	MG	1G	1741	1/1	0.99	0.03	105,105,105,105	0
55	MG	1H	3459	1/1	0.99	0.05	75,75,75,75	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
55	MG	1H	3072	1/1	0.99	0.20	33,33,33,33	0
55	MG	14	3477	1/1	0.99	0.05	63,63,63,63	0
55	MG	14	3412	1/1	0.99	0.04	77,77,77,77	0
55	MG	1H	3461	1/1	0.99	0.03	67,67,67,67	0
55	MG	14	3480	1/1	0.99	0.04	92,92,92,92	0
55	MG	14	3481	1/1	0.99	0.03	78,78,78,78	0
55	MG	1H	3436	1/1	0.99	0.03	77,77,77,77	0
55	MG	14	3415	1/1	0.99	0.03	71,71,71,71	0
55	MG	14	3484	1/1	0.99	0.07	95,95,95,95	0
55	MG	1H	3463	1/1	0.99	0.10	91,91,91,91	0
55	MG	1H	3438	1/1	0.99	0.03	75,75,75,75	0
55	MG	P8	101	1/1	0.99	0.18	72,72,72,72	0
55	MG	14	3419	1/1	0.99	0.04	56,56,56,56	0
55	MG	1H	3440	1/1	0.99	0.02	66,66,66,66	0
55	MG	14	3421	1/1	0.99	0.07	55,55,55,55	0
55	MG	1H	3426	1/1	0.99	0.04	62,62,62,62	0
55	MG	14	3004	1/1	0.99	0.15	59,59,59,59	0
55	MG	1H	3467	1/1	0.99	0.04	67,67,67,67	0
55	MG	14	3425	1/1	0.99	0.05	66,66,66,66	0
55	MG	1H	3442	1/1	0.99	0.05	77,77,77,77	0
55	MG	14	3428	1/1	0.99	0.06	95,95,95,95	0
55	MG	14	3429	1/1	0.99	0.03	72,72,72,72	0
55	MG	1H	3443	1/1	0.99	0.04	90,90,90,90	0
55	MG	1H	3502	1/1	0.99	0.04	60,60,60,60	0
55	MG	1H	3444	1/1	0.99	0.04	94,94,94,94	0
55	MG	1H	3471	1/1	0.99	0.04	90,90,90,90	0
55	MG	1H	3505	1/1	0.99	0.03	64,64,64,64	0
56	ZN	3E	302	1/1	0.99	0.24	86,86,86,86	0
56	ZN	5I	101	1/1	0.99	0.03	109,109,109,109	0
55	MG	1H	3506	1/1	0.99	0.04	81,81,81,81	0
56	ZN	32	302	1/1	0.99	0.22	100,100,100,100	0
56	ZN	5A	101	1/1	0.99	0.03	125,125,125,125	0
55	MG	14	3436	1/1	0.99	0.04	69,69,69,69	0
55	MG	1H	3437	1/1	1.00	0.03	60,60,60,60	0
55	MG	14	3426	1/1	1.00	0.04	84,84,84,84	0
55	MG	1H	3439	1/1	1.00	0.03	59,59,59,59	0

6.5 Other polymers

There are no such residues in this entry.