



# wwPDB X-ray Structure Validation Summary Report ⓘ

Jun 16, 2019 – 05:50 AM EDT

PDB ID : 4WZD  
Title : Complex of 70S ribosome with cognate tRNA-Tyr in the P-site  
Authors : Rozov, A.; Demeshkina, N.; Yusupov, M.; Yusupova, G.  
Deposited on : 2014-11-19  
Resolution : 3.10 Å(reported)

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

We welcome your comments at [validation@mail.wwpdb.org](mailto: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.

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

MolProbity : 4.02b-467  
Mogul : 1.8.0 (224370), CSD as540be (2019)  
Xtriage (Phenix) : 1.13  
EDS : 2.3.2  
Percentile statistics : 20171227.v01 (using entries in the PDB archive December 27th 2017)  
Refmac : 5.8.0158  
CCP4 : 7.0 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.3.2

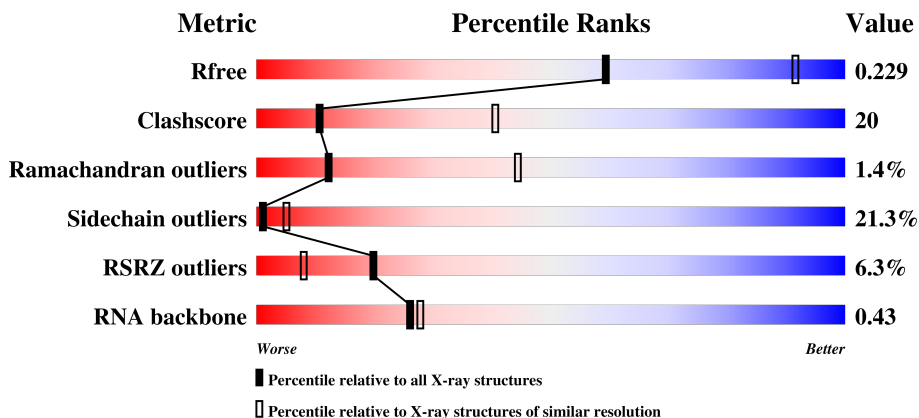
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.10 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	111664	1115 (3.12-3.08)
Clashscore	122126	1042 (3.10-3.10)
Ramachandran outliers	120053	1010 (3.10-3.10)
Sidechain outliers	120020	1010 (3.10-3.10)
RSRZ outliers	108989	1089 (3.12-3.08)
RNA backbone	2636	1015 (3.44-2.76)

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

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




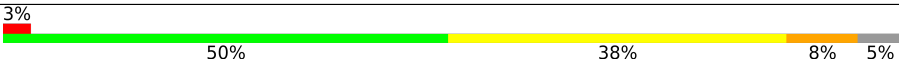
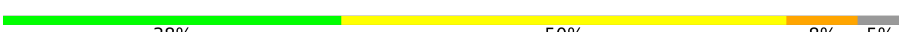
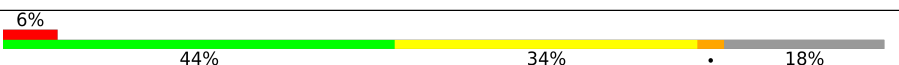

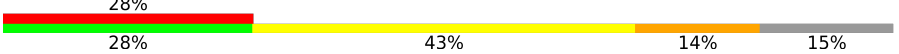
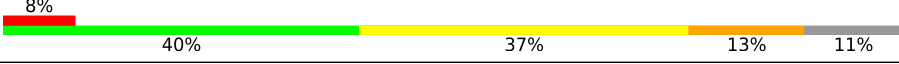
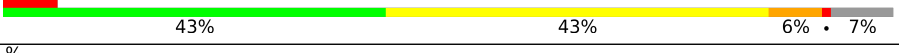
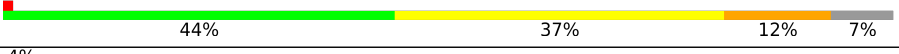
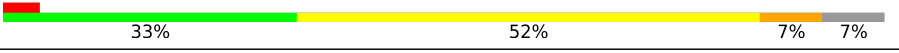
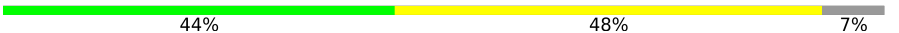

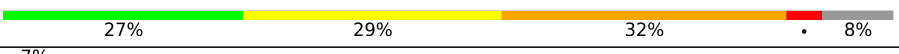
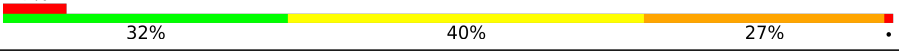
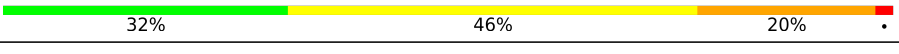
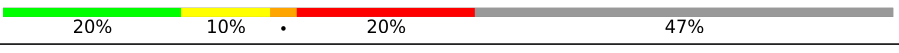

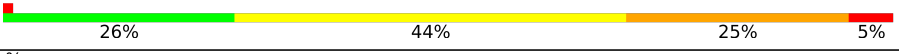



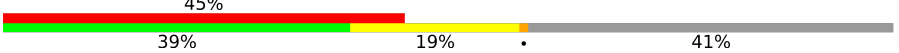
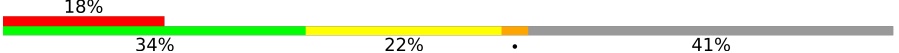
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Mol	Chain	Length	Quality of chain
3	22	239	
3	2E	239	
4	32	209	
4	3E	209	
5	42	162	
5	4E	162	
6	52	101	
6	5E	101	
7	62	156	
7	6E	156	
8	72	138	
8	7E	138	
9	82	128	
9	8E	128	
10	1A	105	
10	1I	105	
11	2A	129	
11	2I	129	
12	3A	132	
12	3I	132	
13	4A	126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




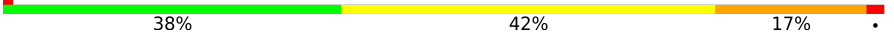

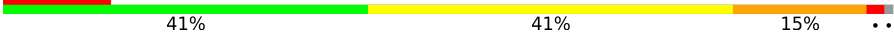

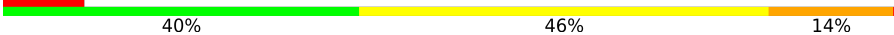
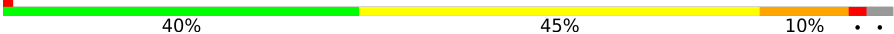
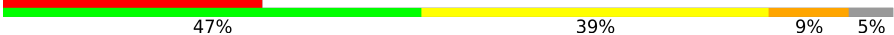
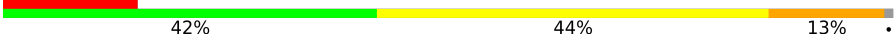
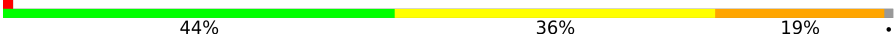

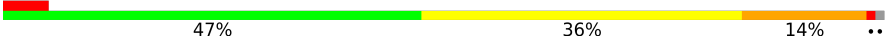











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Mol	Chain	Length	Quality of chain
15	6I	89	
16	7A	88	
16	7I	88	
17	8A	105	
17	8I	105	
18	9A	88	
18	9I	88	
19	AA	93	
19	AI	93	
20	BA	106	
20	BI	106	
21	1B	27	
21	1F	27	
22	2K	85	
22	2L	85	
22	3K	85	
22	3L	85	
23	4K	30	
23	4L	30	
24	14	2917	
24	1H	2917	
25	16	122	
25	1J	122	
26	71	229	
26	79	229	

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Mol	Chain	Length	Quality of chain
27	11	276	
27	19	276	
28	21	206	
28	29	206	
29	31	210	
29	39	210	
30	41	182	
30	49	182	
31	51	180	
31	59	180	
32	61	148	
32	69	148	
33	15	140	
33	58	140	
34	25	122	
34	68	122	
35	35	150	
35	78	150	
36	45	141	
36	88	141	
37	55	118	
37	98	118	
38	65	112	
38	A8	112	
39	75	146	

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

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Mol	Chain	Length	Quality of chain
52	K5	54	
52	O8	54	
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	1643	-	-	-	X
55	MG	13	1644	-	-	-	X
55	MG	13	1645	-	-	-	X
55	MG	13	1649	-	-	-	X
55	MG	13	1666	-	-	-	X
55	MG	13	1668	-	-	-	X
55	MG	13	1688	-	-	-	X
55	MG	13	1689	-	-	-	X
55	MG	13	1699	-	-	-	X
55	MG	13	1706	-	-	-	X
55	MG	13	1708	-	-	-	X
55	MG	13	1711	-	-	-	X
55	MG	14	3128	-	-	-	X
55	MG	14	3261	-	-	-	X
55	MG	1G	1620	-	-	-	X
55	MG	1G	1638	-	-	-	X
55	MG	1G	1639	-	-	-	X
55	MG	1G	1699	-	-	-	X
55	MG	1G	1721	-	-	-	X
55	MG	1G	1726	-	-	-	X
55	MG	1H	3058	-	-	-	X
55	MG	1H	3096	-	-	-	X
55	MG	1H	3106	-	-	-	X
55	MG	1H	3116	-	-	-	X
55	MG	1H	3149	-	-	-	X
55	MG	1H	3152	-	-	-	X
55	MG	1H	3185	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
55	MG	1H	3190	-	-	-	X
55	MG	1H	3196	-	-	-	X
55	MG	1H	3203	-	-	-	X
55	MG	1H	3209	-	-	-	X
55	MG	1H	3215	-	-	-	X
55	MG	1H	3216	-	-	-	X
55	MG	1H	3218	-	-	-	X
55	MG	1H	3231	-	-	-	X
55	MG	1H	3282	-	-	-	X
55	MG	1H	3283	-	-	-	X
55	MG	1H	3292	-	-	-	X
55	MG	1H	3294	-	-	-	X
55	MG	1H	3311	-	-	-	X
55	MG	1H	3330	-	-	-	X
55	MG	1H	3336	-	-	-	X
55	MG	1H	3339	-	-	-	X
55	MG	1H	3342	-	-	-	X
55	MG	1H	3350	-	-	-	X
55	MG	1H	3355	-	-	-	X
55	MG	1H	3356	-	-	-	X
55	MG	1H	3406	-	-	-	X
55	MG	29	304	-	-	-	X
55	MG	2K	104	-	-	-	X
55	MG	32	301	-	-	-	X



## 2 Entry composition [i](#)

There are 57 unique types of molecules in this entry. The entry contains 299705 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	1499	Total	C	N	O	P	0	5	0
			32337	14392	5999	10442	1504			
1	1G	1503	Total	C	N	O	P	0	0	0
			32309	14381	5990	10436	1502			

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

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

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

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	6E	155	Total	C	N	O	S	0	0	0
			1256	781	252	217	6			
7	62	155	Total	C	N	O	S	0	0	0
			1256	781	252	217	6			

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	2I	116	Total	C	N	O	S	0	0	0
			864	537	164	160	3			
11	2A	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	125	Total	C	N	O	S	0	0	0
			975	614	196	164	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	117	Total	C	N	O	S	0	0	0
			933	577	192	162	2			

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
16	7I	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	100	Total	C	N	O	S	0	0	0
			834	534	155	143	2			

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
18	9I	72	Total	C	N	O	0	0	0
			590	376	117	97			
18	9A	72	Total	C	N	O	0	0	0
			590	376	117	97			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
19	AI	83	Total	C	N	O	S	0	0	0
			665	424	124	115	2			
19	AA	79	Total	C	N	O	S	0	0	0
			633	404	117	110	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	25	Total	C	N	O	0	0	0
			217	134	52	31			
21	1B	25	Total	C	N	O	0	0	0
			217	134	52	31			

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

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
22	2K	82	Total	C	N	O	P	S	0	0	0
			1765	795	315	571	82	2			
22	3K	85	Total	C	N	O	P	S	0	0	0
			1824	822	323	592	85	2			
22	2L	78	Total	C	N	O	P	S	0	0	0
			1678	756	297	545	78	2			
22	3L	85	Total	C	N	O	P	S	0	0	0
			1825	822	323	593	85	2			

- Molecule 23 is a RNA chain called mRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
23	4K	16	Total	C	N	O	P	0	0	0
			348	157	72	103	16			
23	4L	8	Total	C	N	O	P	0	0	0
			170	77	32	53	8			

- Molecule 24 is a RNA chain called 23S ribosomal RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
24	1H	2912	Total	C	N	O	P	0	0	0
			62707	27911	11722	20163	2911			
24	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 25 is a RNA chain called 5S ribosomal RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
25	16	122	Total	C	N	O	P	0	0	0
			2617	1166	486	844	121			
25	1J	122	Total	C	N	O	P	0	0	0
			2617	1166	486	844	121			

- Molecule 26 is a protein called 50S ribosomal protein L1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
26	71	135	Total	C	N	O	S	0	0	0
			1049	662	197	189	1			
26	79	135	Total	C	N	O	S	0	0	0
			1049	662	197	189	1			

- Molecule 27 is a protein called 50S ribosomal protein L2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
27	11	272	Total	C	N	O	S	0	0	0
			2115	1335	420	357	3			
27	19	273	Total	C	N	O	S	0	0	0
			2120	1338	421	358	3			

- Molecule 28 is a protein called 50S ribosomal protein L3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
28	21	205	Total	C	N	O	S	0	0	0
			1568	991	300	271	6			
28	29	205	Total	C	N	O	S	0	0	0
			1568	991	300	271	6			

- Molecule 29 is a protein called 50S ribosomal protein L4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
29	31	202	Total	C	N	O	S	0	0	0
			1585	1011	297	275	2			
29	39	208	Total	C	N	O	S	0	0	0
			1627	1037	304	283	3			

- Molecule 30 is a protein called 50S ribosomal protein L5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
30	41	181	Total	C	N	O	S	0	0	0
			1473	942	268	259	4			
30	49	181	Total	C	N	O	S	0	0	0
			1473	942	268	259	4			

- Molecule 31 is a protein called 50S ribosomal protein L6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
31	51	174	Total	C	N	O	S	0	0	0
			1336	848	251	236	1			
31	59	171	Total	C	N	O	S	0	0	0
			1312	832	246	233	1			

- Molecule 32 is a protein called 50S ribosomal protein L9.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
32	61	146	Total	C	N	O	S	0	0	0
			1136	726	201	208	1			
32	69	146	Total	C	N	O	S	0	0	0
			1136	726	201	208	1			

- Molecule 33 is a protein called 50S ribosomal protein L13.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
33	58	138	Total	C	N	O	S	0	0	0
			1104	712	206	182	4			
33	15	138	Total	C	N	O	S	0	0	0
			1104	712	206	182	4			

- Molecule 34 is a protein called 50S ribosomal protein L14.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
34	68	122	Total	C	N	O	S	0	0	0
			932	588	171	169	4			
34	25	122	Total	C	N	O	S	0	0	0
			932	588	171	169	4			

- Molecule 35 is a protein called 50S ribosomal protein L15.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
35	78	150	Total	C	N	O	S	0	0	0
			1144	712	232	197	3			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
35	35	150	Total	C	N	O	S	0	0	0
			1144	712	232	197	3			

- Molecule 36 is a protein called 50S ribosomal protein L16.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
36	88	141	Total	C	N	O	S	0	0	0
			1121	715	212	187	7			
36	45	141	Total	C	N	O	S	0	0	0
			1121	715	212	187	7			

- Molecule 37 is a protein called 50S ribosomal protein L17.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
37	98	118	Total	C	N	O	S	0	0	0
			967	604	203	159	1			
37	55	117	Total	C	N	O		0	0	0
			959	599	202	158				

- Molecule 38 is a protein called 50S ribosomal protein L18.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
38	A8	111	Total	C	N	O	0	0	0
			881	556	176	149			
38	65	111	Total	C	N	O	0	0	0
			881	556	176	149			

- Molecule 39 is a protein called 50S ribosomal protein L19.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
39	B8	137	Total	C	N	O	S	0	0	0
			1141	710	234	196	1			
39	75	137	Total	C	N	O		0	0	0
			1131	704	232	195				

- Molecule 40 is a protein called 50S ribosomal protein L20.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
40	C8	117	Total	C	N	O	S	0	0	0
			963	610	202	150	1			
40	85	117	Total	C	N	O	S	0	0	0
			963	610	202	150	1			



- Molecule 41 is a protein called 50S ribosomal protein L21.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
41	D8	101	Total	C	N	O	S	0	0	0
			778	501	142	134	1			
41	95	101	Total	C	N	O	S	0	0	0
			778	501	142	134	1			

- Molecule 42 is a protein called 50S ribosomal protein L22.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
42	E8	113	Total	C	N	O	S	0	0	0
			899	566	177	154	2			
42	A5	113	Total	C	N	O	S	0	0	0
			899	566	177	154	2			

- Molecule 43 is a protein called 50S ribosomal protein L23.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
43	F8	92	Total	C	N	O	0	0	0
			725	471	131	123			
43	B5	93	Total	C	N	O	0	0	0
			730	474	132	124			

- Molecule 44 is a protein called 50S ribosomal protein L24.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
44	G8	104	Total	C	N	O	S	0	0	0
			791	510	149	127	5			
44	C5	104	Total	C	N	O	S	0	0	0
			794	510	152	127	5			

- Molecule 45 is a protein called 50S ribosomal protein L25.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
45	H8	175	Total	C	N	O	S	0	0	0
			1397	892	251	251	3			
45	D5	179	Total	C	N	O	S	0	0	0
			1428	911	255	259	3			

- Molecule 46 is a protein called 50S ribosomal protein L27.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
46	I8	83	Total	C	N	O	S	0	0	0
			656	407	139	109	1			
46	E5	77	Total	C	N	O	S	0	0	0
			612	379	129	103	1			

- Molecule 47 is a protein called 50S ribosomal protein L28.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
47	J8	97	Total	C	N	O	S	0	0	0
			762	481	150	130	1			
47	F5	97	Total	C	N	O	S	0	0	0
			762	481	150	130	1			

- Molecule 48 is a protein called 50S ribosomal protein L29.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
48	K8	66	Total	C	N	O	S	0	0	0
			558	346	113	98	1			
48	G5	69	Total	C	N	O	S	0	0	0
			580	358	118	103	1			

- Molecule 49 is a protein called 50S ribosomal protein L30.

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

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

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

- Molecule 51 is a protein called 50S ribosomal protein L32.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
51	N8	59	Total	C	N	O	S	0	0	0
			458	288	90	75	5			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
51	J5	59	Total	C	N	O	S	0	0	0
			458	288	90	75	5			

- Molecule 52 is a protein called 50S ribosomal protein L33.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
52	O8	45	Total	C	N	O	S	0	0	0
			389	241	79	65	4			
52	K5	45	Total	C	N	O	S	0	0	0
			389	241	79	65	4			

- 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	49	Total	C	N	O	S	0	0	0
			429	263	108	56	2			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
54	Q8	62	Total	C	N	O	S	0	0	0
			483	308	98	75	2			
54	M5	62	Total	C	N	O	S	0	0	0
			495	317	100	76	2			

- Molecule 55 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
55	98	1	Total	Mg	0	0
			1	1		
55	45	1	Total	Mg	0	0
			1	1		
55	55	1	Total	Mg	0	0
			1	1		
55	32	1	Total	Mg	0	0
			1	1		
55	C5	1	Total	Mg	0	0
			1	1		
55	13	139	Total	Mg	0	0
			139	139		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
55	1J	10	Total 10	Mg 10	0	0
55	16	15	Total 15	Mg 15	0	0
55	42	1	Total 1	Mg 1	0	0
55	25	1	Total 1	Mg 1	0	0
55	21	2	Total 2	Mg 2	0	0
55	4A	1	Total 1	Mg 1	0	0
55	Q8	2	Total 2	Mg 2	0	0
55	3I	1	Total 1	Mg 1	0	0
55	I8	3	Total 3	Mg 3	0	0
55	52	1	Total 1	Mg 1	0	0
55	5E	1	Total 1	Mg 1	0	0
55	29	4	Total 4	Mg 4	0	0
55	2K	5	Total 5	Mg 5	0	0
55	15	1	Total 1	Mg 1	0	0
55	7E	1	Total 1	Mg 1	0	0
55	39	1	Total 1	Mg 1	0	0
55	1G	148	Total 148	Mg 148	0	0
55	11	2	Total 2	Mg 2	0	0
55	1H	523	Total 523	Mg 523	0	0
55	F5	1	Total 1	Mg 1	0	0
55	E5	1	Total 1	Mg 1	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
55	88	1	Total 1	Mg 1	0	0
55	14	465	Total 465	Mg 465	0	0
55	3E	1	Total 1	Mg 1	0	0
55	19	1	Total 1	Mg 1	0	0
55	3L	1	Total 1	Mg 1	0	0
55	4K	1	Total 1	Mg 1	0	0
55	3A	1	Total 1	Mg 1	0	0
55	G8	1	Total 1	Mg 1	0	0
55	2L	4	Total 4	Mg 4	0	0

- Molecule 56 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
56	32	1	Total 1	Zn 1	0	0
56	3E	1	Total 1	Zn 1	0	0
56	5I	1	Total 1	Zn 1	0	0
56	5A	1	Total 1	Zn 1	0	0
56	G8	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	125	Total 125	O 125	0	0
57	5I	1	Total 1	O 1	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
57	AI	3	Total 3	O 3	0	0
57	2K	2	Total 2	O 2	0	0
57	4K	3	Total 3	O 3	0	0
57	1H	652	Total 652	O 652	0	0
57	16	12	Total 12	O 12	0	0
57	11	8	Total 8	O 8	0	0
57	21	2	Total 2	O 2	0	0
57	31	5	Total 5	O 5	0	0
57	78	4	Total 4	O 4	0	0
57	98	1	Total 1	O 1	0	0
57	C8	2	Total 2	O 2	0	0
57	E8	1	Total 1	O 1	0	0
57	F8	2	Total 2	O 2	0	0
57	G8	2	Total 2	O 2	0	0
57	1G	96	Total 96	O 96	0	0
57	32	1	Total 1	O 1	0	0
57	5A	1	Total 1	O 1	0	0
57	7A	2	Total 2	O 2	0	0
57	BA	1	Total 1	O 1	0	0
57	2L	6	Total 6	O 6	0	0
57	14	523	Total 523	O 523	0	0

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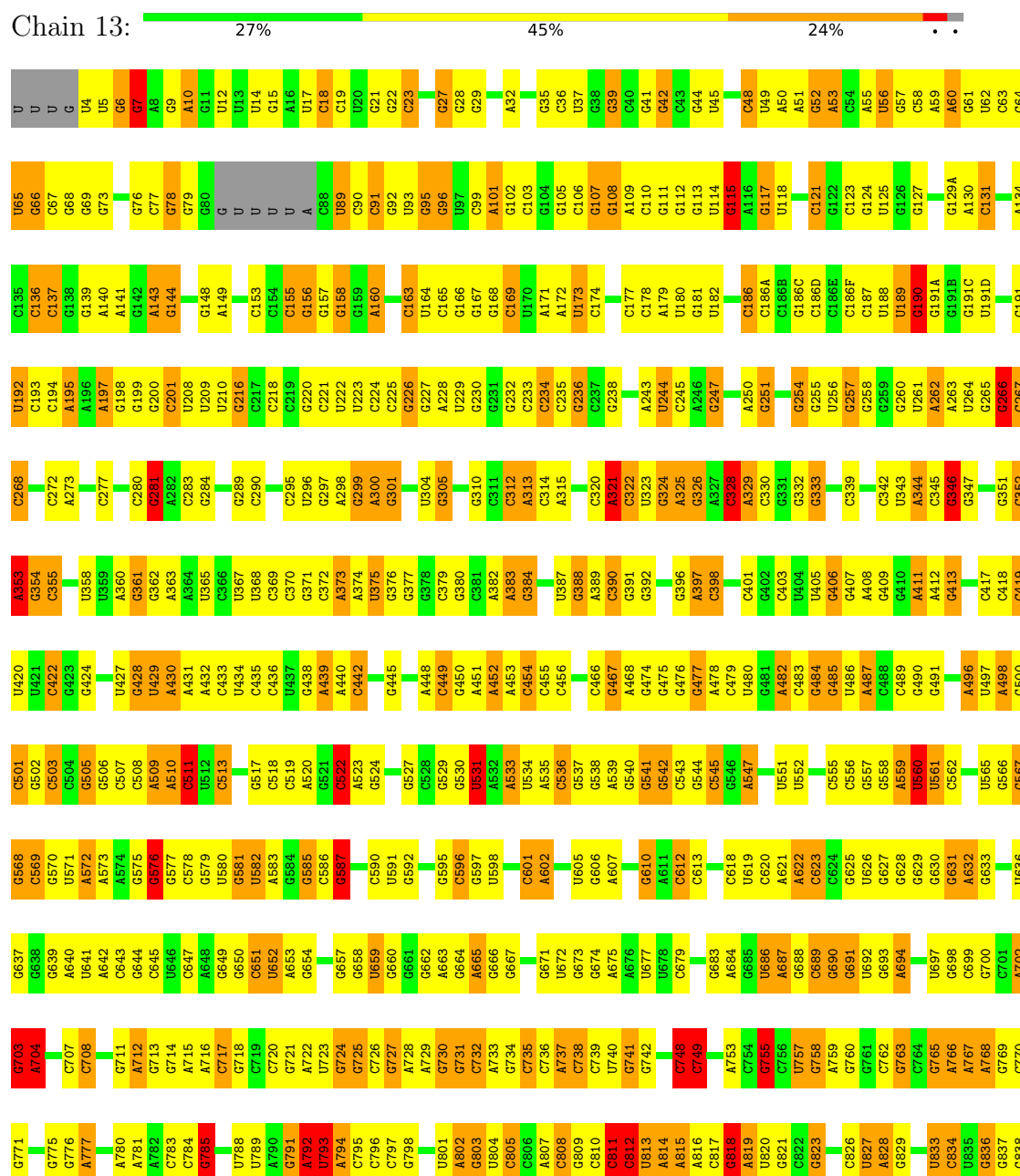
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
57	1J	22	Total 22	O 22	0	0
57	19	11	Total 11	O 11	0	0
57	39	3	Total 3	O 3	0	0
57	25	6	Total 6	O 6	0	0
57	35	1	Total 1	O 1	0	0
57	75	1	Total 1	O 1	0	0
57	85	4	Total 4	O 4	0	0
57	F5	1	Total 1	O 1	0	0
57	H5	2	Total 2	O 2	0	0

### 3 Residue-property plots

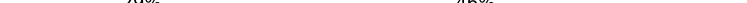
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are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

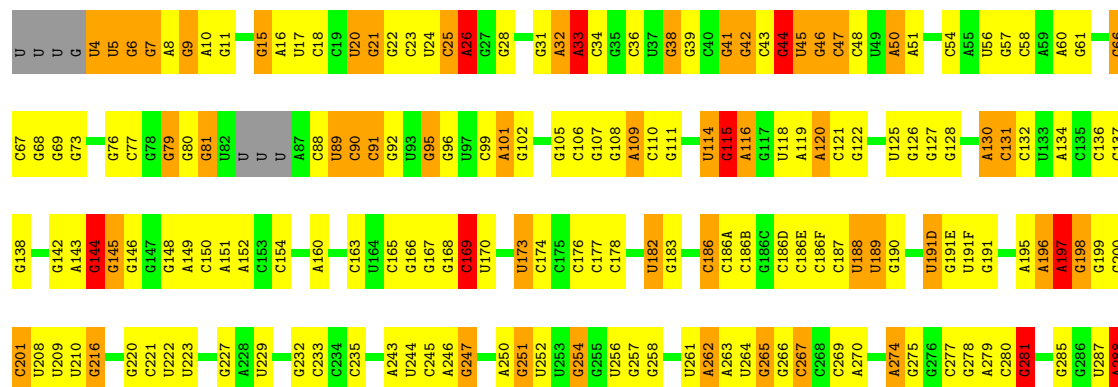
- Molecule 1: 16S ribosomal RNA



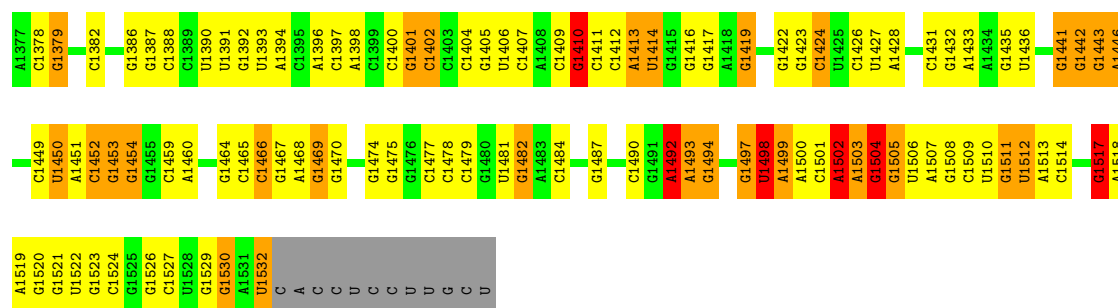


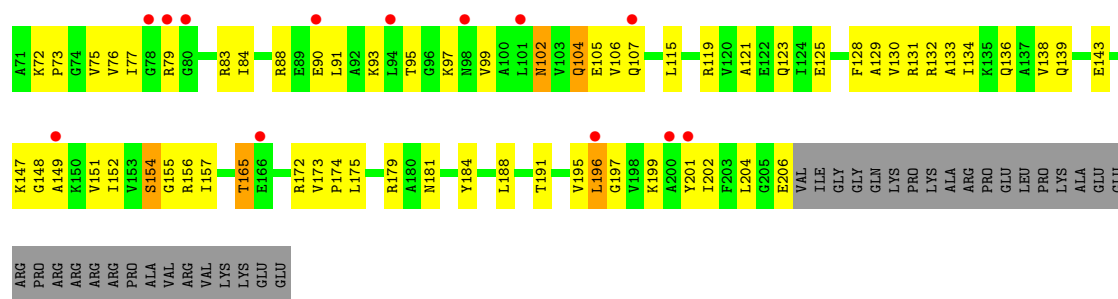


Chain 1G: 

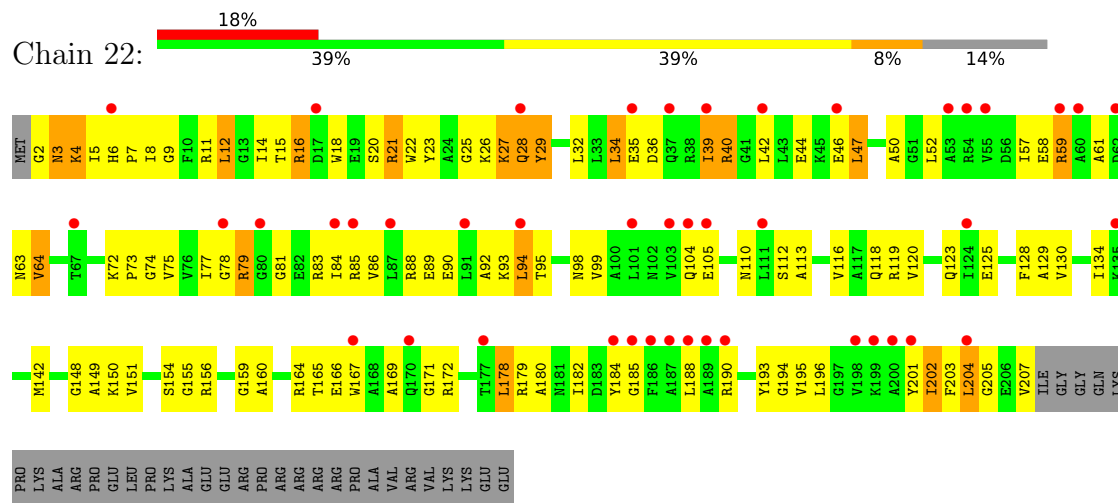




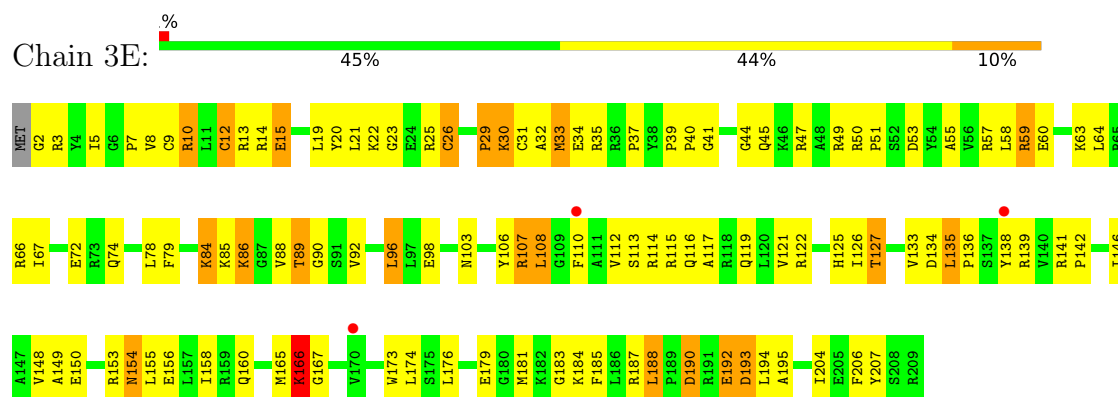




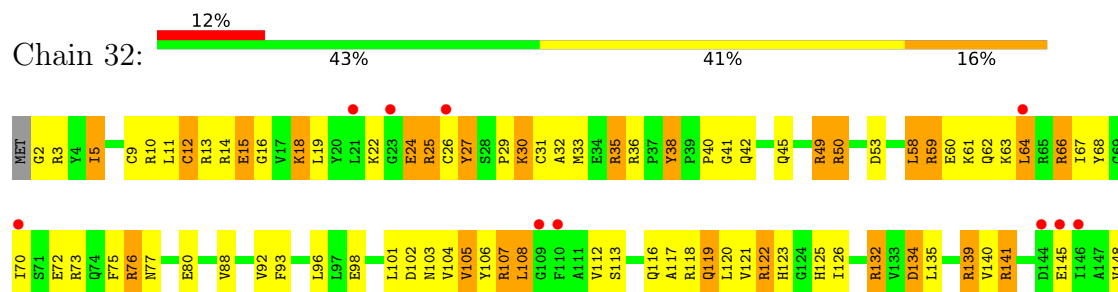
• Molecule 3: 30S ribosomal protein S3

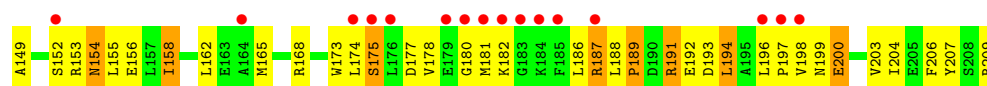


• Molecule 4: 30S ribosomal protein S4



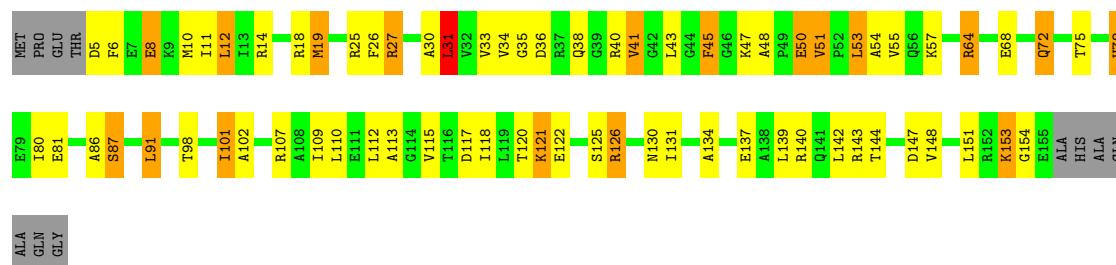
• Molecule 4: 30S ribosomal protein S4





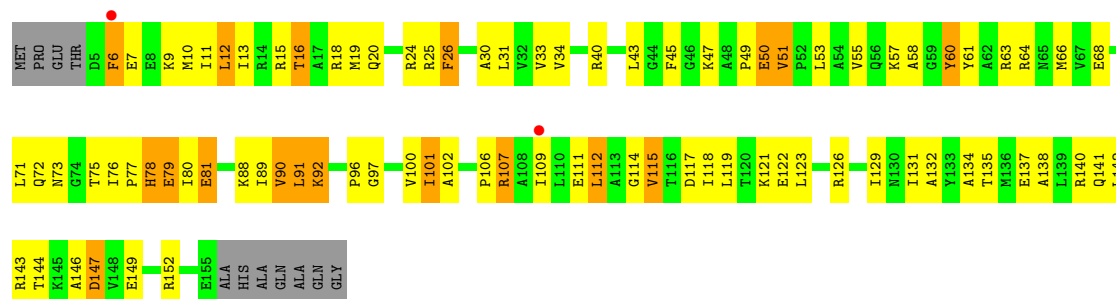
- Molecule 5: 30S ribosomal protein S5

Chain 4E: 49% 32% 11% 7%



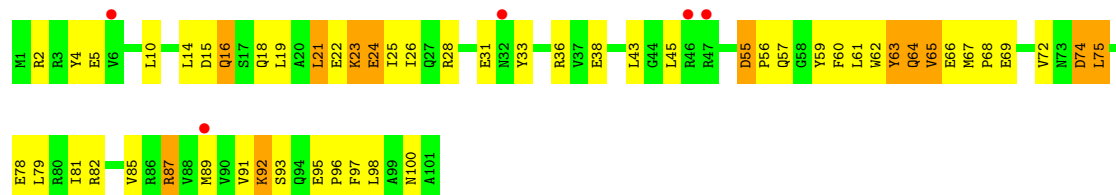
- Molecule 5: 30S ribosomal protein S5

Chain 42: 40% 42% 11% 7%



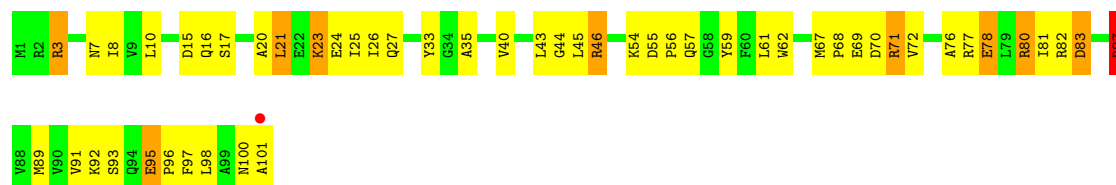
- Molecule 6: 30S ribosomal protein S6

Chain 5E: 5% 47% 42% 12%

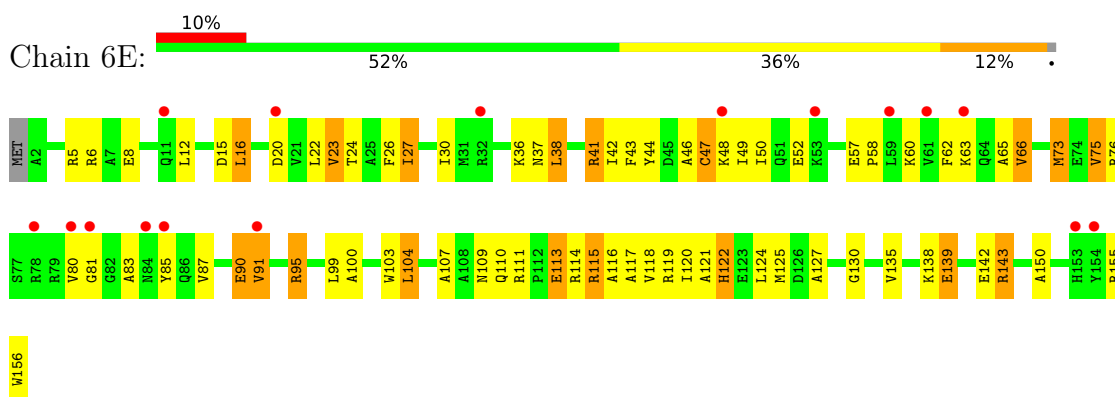


- Molecule 6: 30S ribosomal protein S6

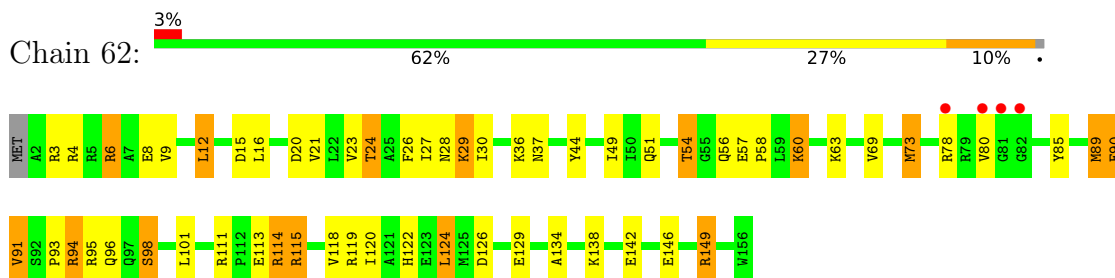
Chain 52: 49% 42% 9%



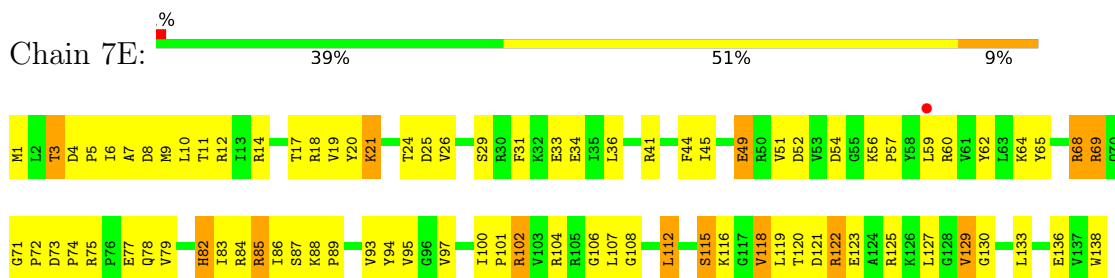
- Molecule 7: 30S ribosomal protein S7



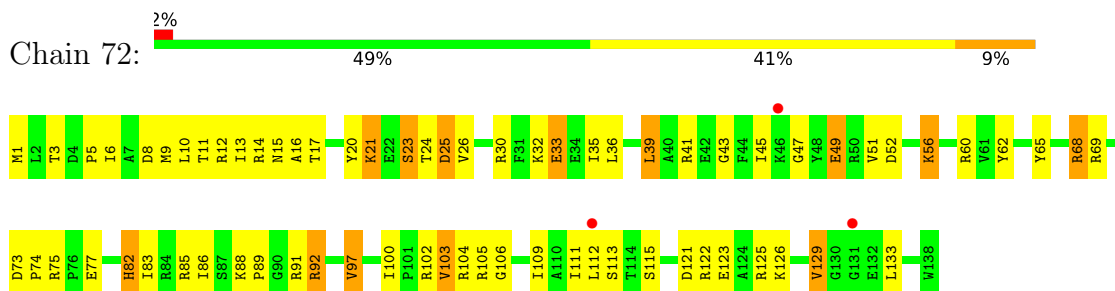
- Molecule 7: 30S ribosomal protein S7



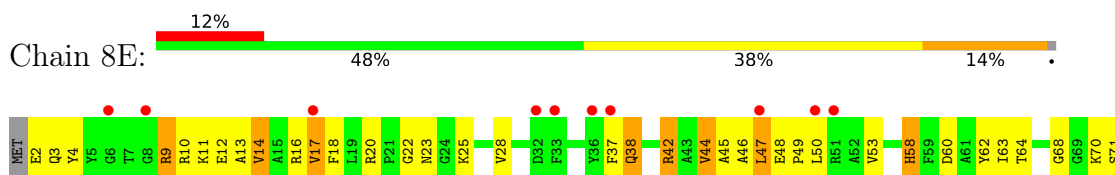
- Molecule 8: 30S ribosomal protein S8

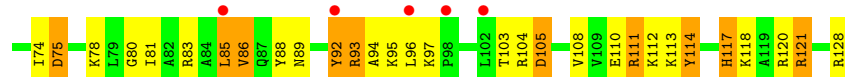


- Molecule 8: 30S ribosomal protein S8

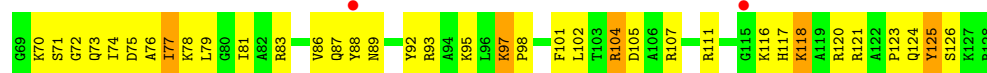
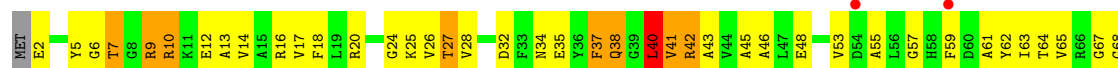


- Molecule 9: 30S ribosomal protein S9

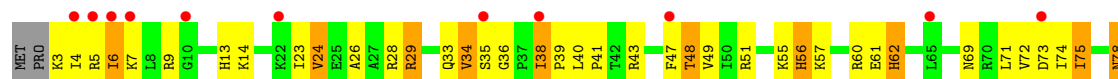




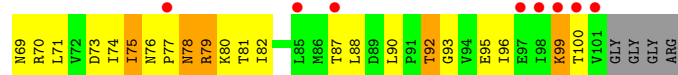
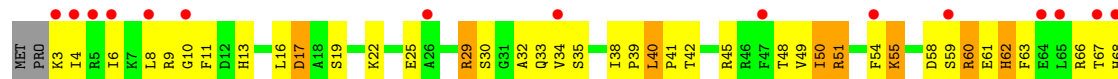
- Molecule 9: 30S ribosomal protein S9



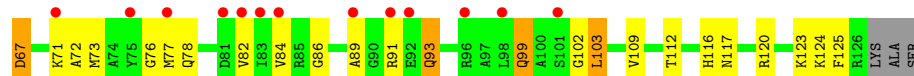
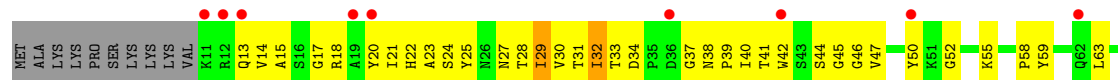
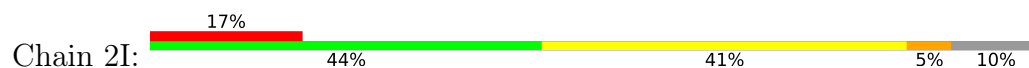
- Molecule 10: 30S ribosomal protein S10



- Molecule 10: 30S ribosomal protein S10

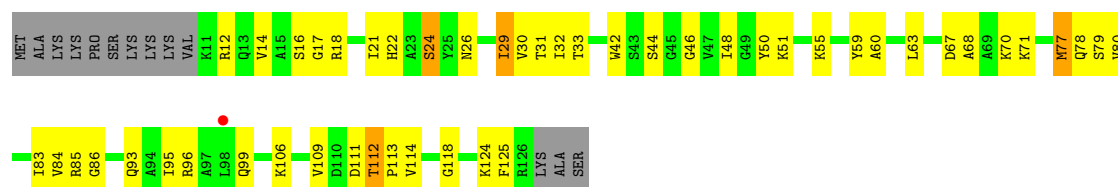


- Molecule 11: 30S ribosomal protein S11

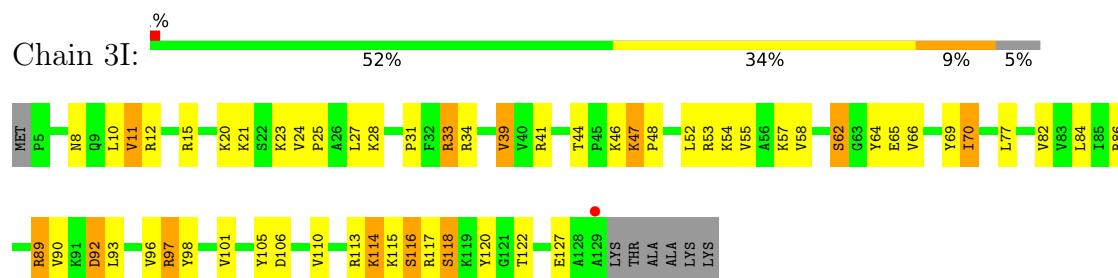


- Molecule 11: 30S ribosomal protein S11

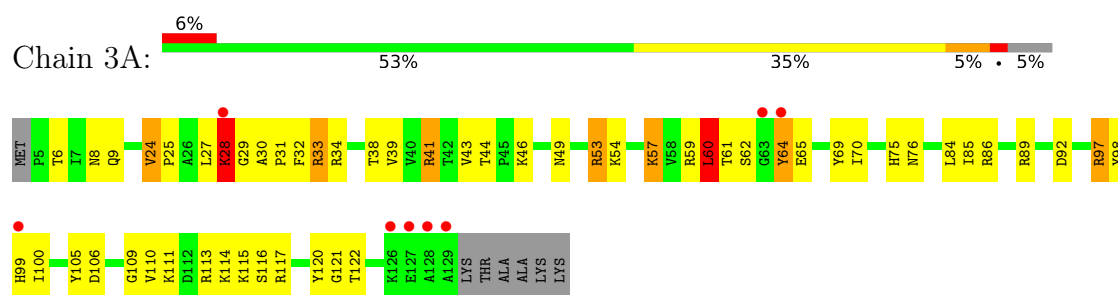




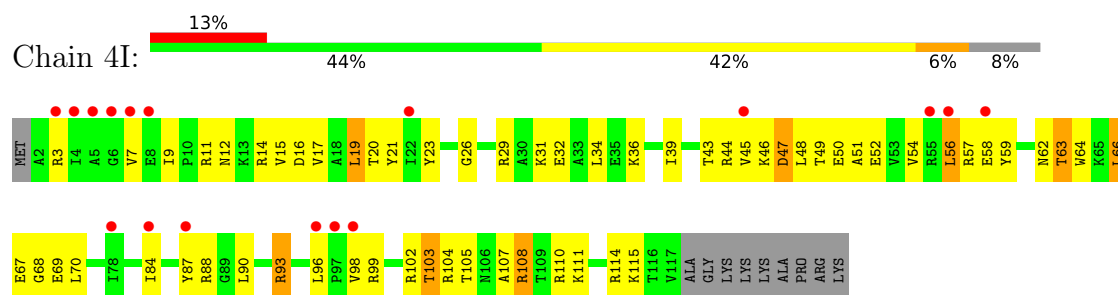
• Molecule 12: 30S ribosomal protein S12



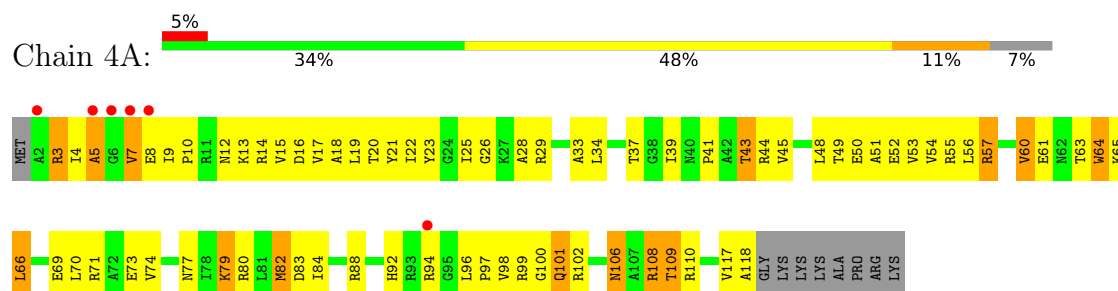
• Molecule 12: 30S ribosomal protein S12



• Molecule 13: 30S ribosomal protein S13

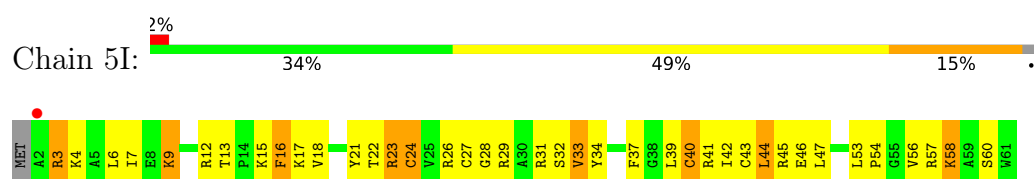


• Molecule 13: 30S ribosomal protein S13

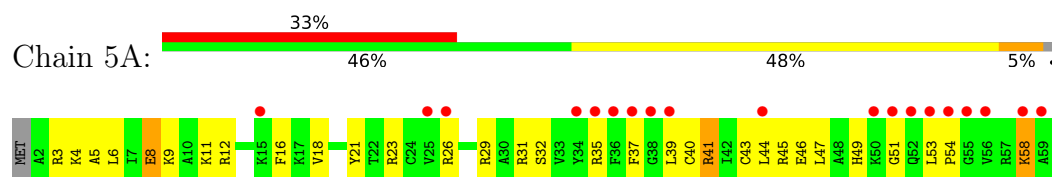


• Molecule 14: 30S ribosomal protein S14 type Z

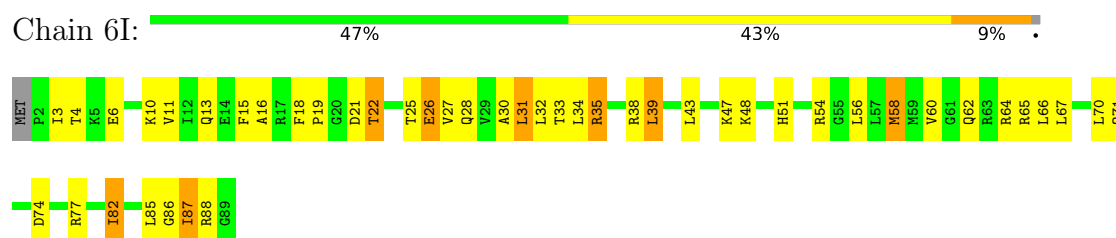




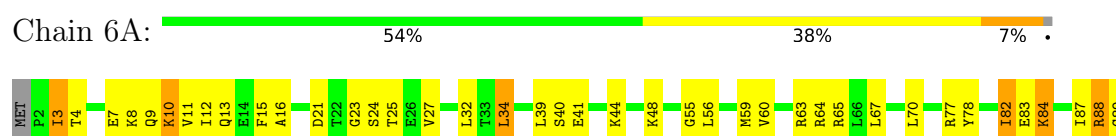
- Molecule 14: 30S ribosomal protein S14 type Z



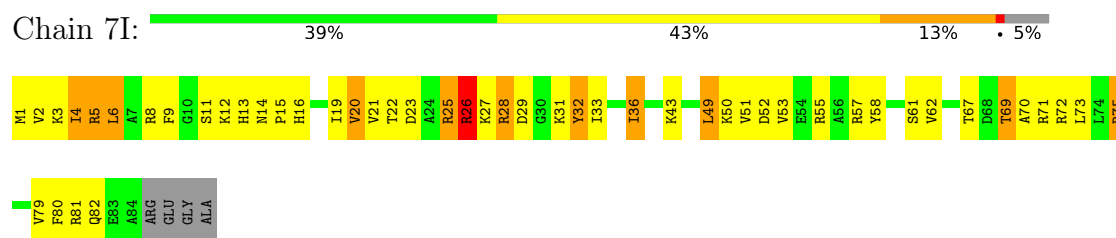
- Molecule 15: 30S ribosomal protein S15



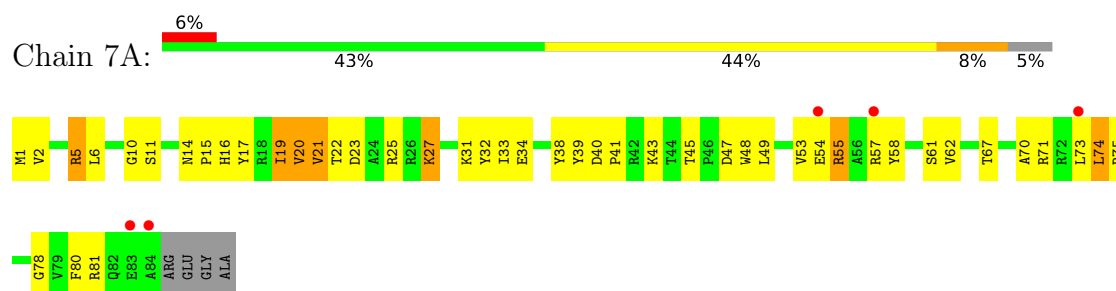
- Molecule 15: 30S ribosomal protein S15



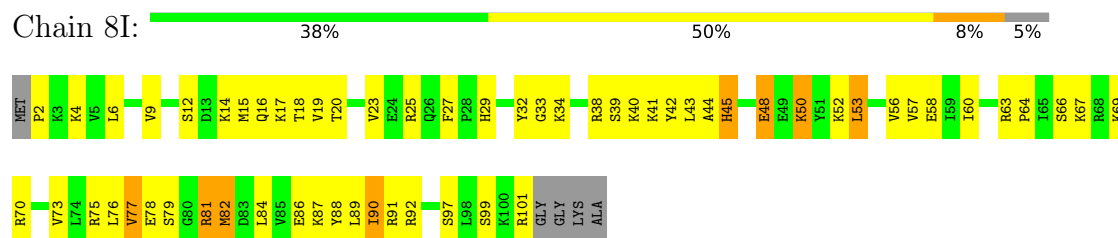
- Molecule 16: 30S ribosomal protein S16



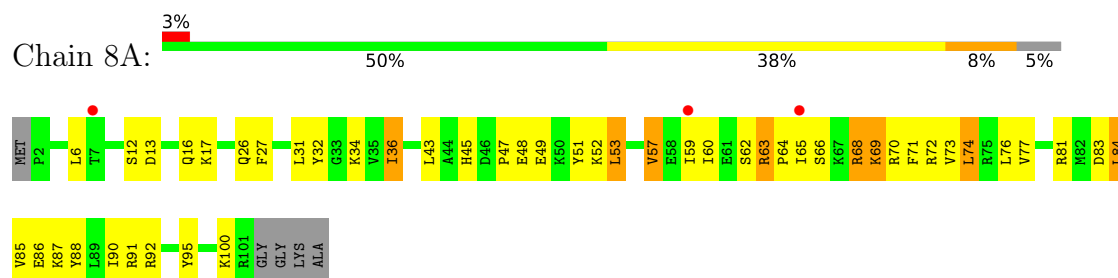
- Molecule 16: 30S ribosomal protein S16



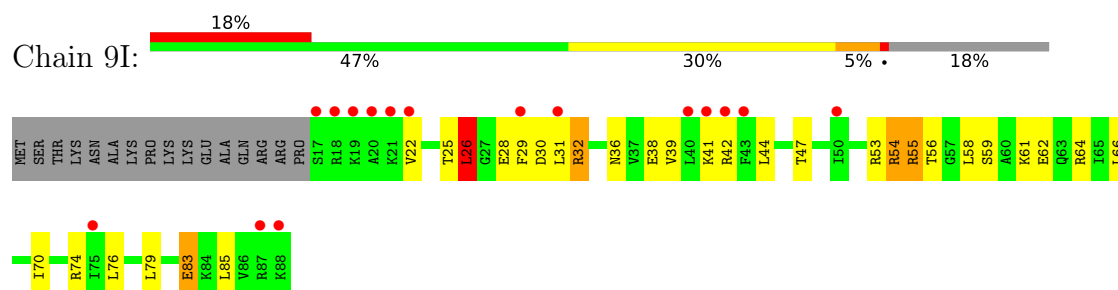
- Molecule 17: 30S ribosomal protein S17



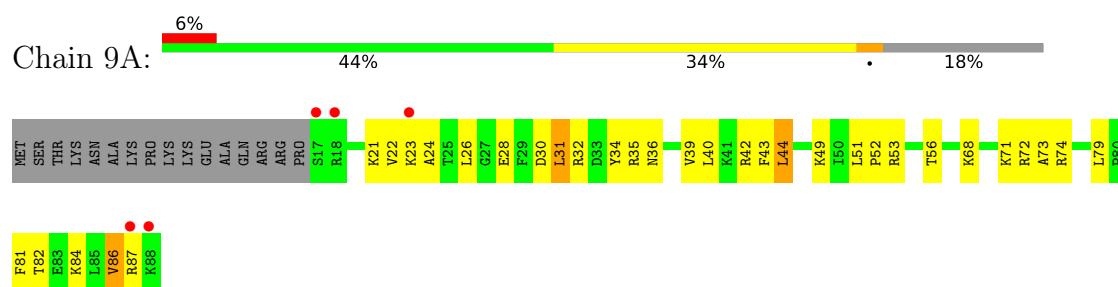
- Molecule 17: 30S ribosomal protein S17



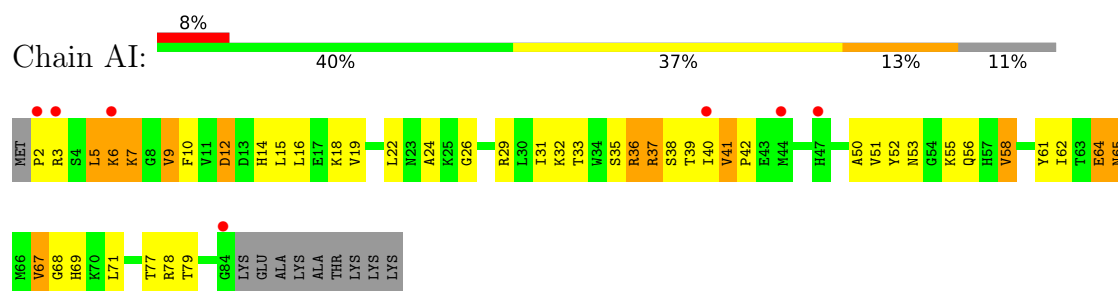
- Molecule 18: 30S ribosomal protein S18



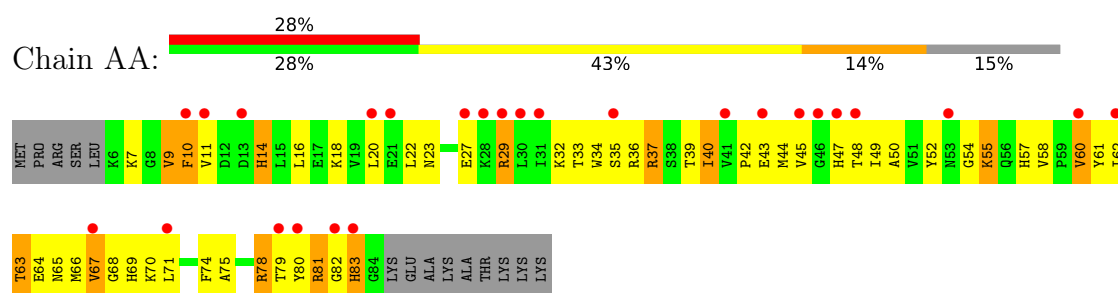
- Molecule 18: 30S ribosomal protein S18



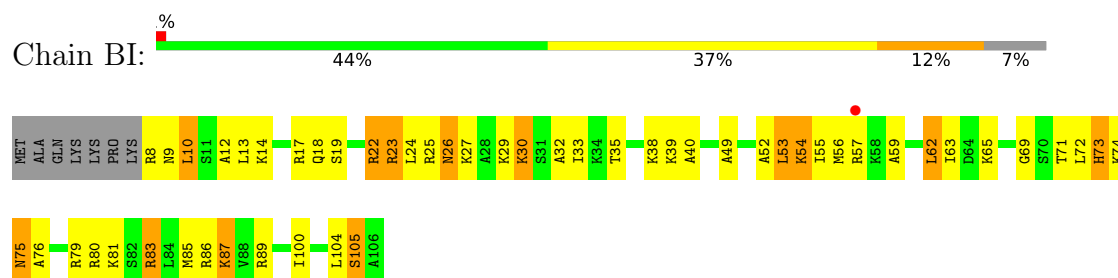
- Molecule 19: 30S ribosomal protein S19



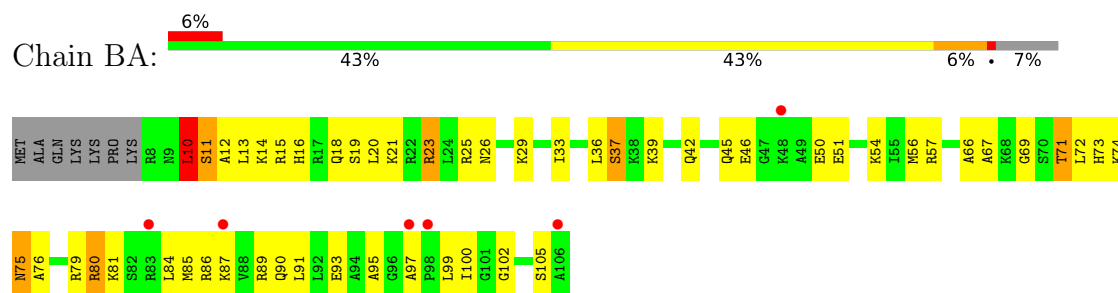
- Molecule 19: 30S ribosomal protein S19



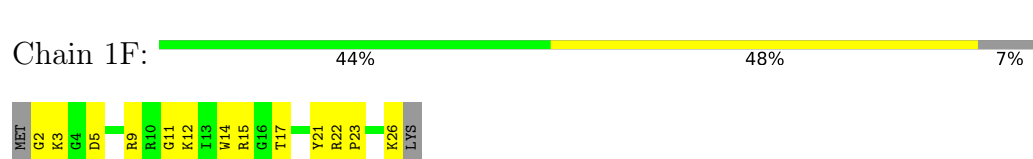
• Molecule 20: 30S ribosomal protein S20



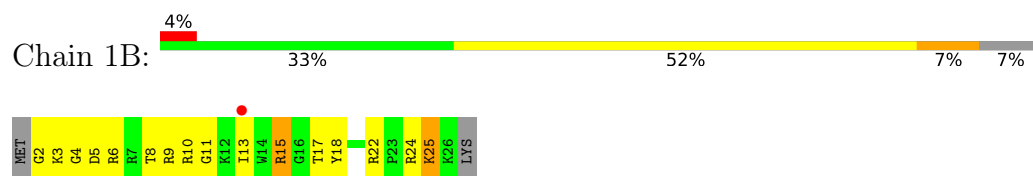
• Molecule 20: 30S ribosomal protein S20



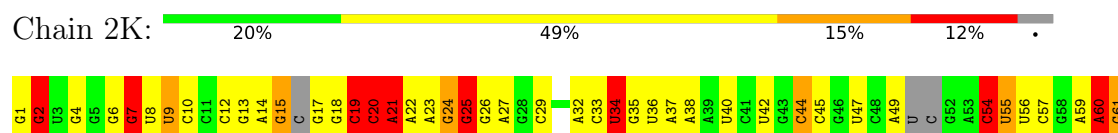
• Molecule 21: 30S ribosomal protein Thx



• Molecule 21: 30S ribosomal protein Thx



• Molecule 22: tRNA-Tyr







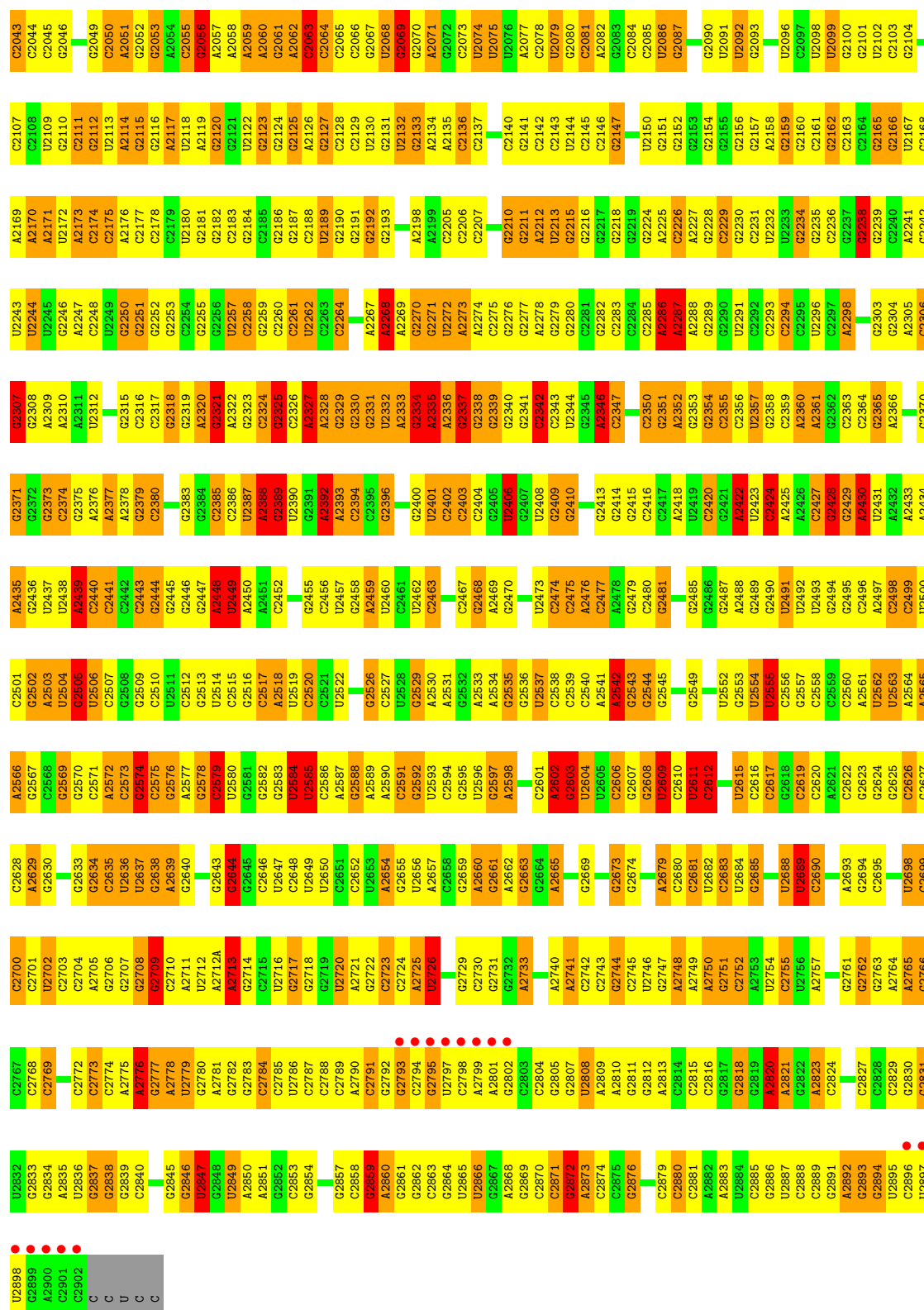
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A1936	A1852	A1787	G1696	C1636	A1569	C1505	G1435	G1374	G1309	G1245	G1185	G1053	C987
A1938	A1853	C1788	G1696	A1570	A1570	C1506	C1436	C1375	G1310	G1186	G1123	A1054	A988
U1939	A1854	A1789	G1697	A1637	A1571	A1507	C1437	C1376	G1311	U1249	G1187	G1055	G989
U1940	G1855	C1790	G1698	C1638	A1572	A1508	G1441	G1377	U1312	G1250	G1188	G1056	A950
C1941	G1856	A1791	U1699	U1639	G1573	C1509	G1442	A1378	U1313	C1251	A1126	C991	C991
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U1943	G1858	C1793	G1701	A1641	C1575	A1511	G1444	G1380	C1315	A1254	A1128	U1058	G993
U1944	A1859	C1794	G1703	G1642	U1576	G1512	A1444A	G1381	G1316	U1255	G1129	G1059	C994
G1945	G1860	C1795	G1703	G1643	C1577	A1513	G1445	G1382	A1317	G1256	U1130	U1060	C995
U1946	G1863	U1709	U1709	C1644	U1578	G1516	G1446	G1383	C1318	G1257	G1131	U1061	A956
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A1952	G1878	A1803	G1730	G1651	A1587	G1521	C1450	G1389	G1324	A1262	C1201	A1067	G1004
A1953	G1882	A1804	G1731	A1652	C1588	U1522	C1451	U1390	G1325	U1263	G1139	G1068	C1004
G1954	C1882	U1805	G1732	G1653	C1589	U1523	A1453	U1391	U1326	G1264	G1203	A1069	C1005
U1955	A1883	C1806	G1733	A1654	U1590	G1525	U1454	A1392	C1327	A1265	A1204	A1070	C1006
U1956	A1884	G1807	G1733	A1655	U1591	G1526	G1455	A1393	G1328	U1267	U1142	G1071	C1007
C1957	A1885	U1808	G1742	C1656	G1592	G1527	G1456	A1394	U1329	C1267	A1142A	C1072	C1008
C1958	C1886	A1809	G1743	C1657	G1593	U1528	A1459	A1395	C1330	A1268	G1143	G1073	A1009
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C1962	A1891	G1813	C1751	C1660	A1596	C1531	G1467	C1399	G1334	A1272	A1148	C1077	U1013
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C1967	A1900	U1818	G1759	C1666	U1602	G1537	A1471	U1406	U1340	A1278	G1154	A1086	A1020
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A1971	G1904	A1825	G1763	U1671	C1607	U1541	G1479	G1410	G1347	U1284	G1223	U1090	G1024
A1972	C1905	G1826	G1764	C1672	A1608	A1543	G1483	A1411	G1348	G1285	C1224	G1091	G1025
C1973	G1906	C1827	U1766	G1674	A1610	A1545	G1484	G1412	A1349	A1286	G1225	C1092	A1027
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U1976	A1913	A1829	U1768	A1676	C1612	C1546	G1486	G1416	A1354	U1288	G1164	A1096	A1029
A1977	C1914	C1830	G1769	A1677	G1613	C1547	G1487	C1417	G1355	C1289	U1165	U1097	G1031
C1978	U1915	G1831	G1770	G1678	U1614	C1548	U1488	G1418	G1356	C1290	G1168	C1100	A1032
G1979	A1916	C1832	C1771	U1679	A1615	C1549	U1489	A1419	U1357	C1291	G1169	U1101	A1033
A1981	U1917	U1833	G1772	U1680	A1616	G1554	A1490	U1420	G1358	U1292	C1230	G1102	G1036
C1982	A1918	G1834	A1773	G1681	C1617	A1554	G1491	G1421	A1359	G1293	G1231	A1103	G1037
G1983	A1919	C1836	C1774	G1682	A1618	G1557	G1492	G1422	A1360	U1294	G1232	C1104	C1038
C1984	C1920	C1837	U1775	C1683	G1619	A1558	C1493	G1423	C1362	G1296	C1233	U1105	C1040
G1985	U1926	C1838	G1776	C1684	G1620	G1559	A1495	G1424	G1361	G1297	U1175	G1106	G1039
A1986	U1927	G1839	U1777	C1685	U1621	G1560	A1496	G1425	A1365	C1298	G1176	C1097	G1036
G1987	A1928	C1843	U1779	G1686	G1622	U1561	U1497	A1426	A1367	U1299	A1177	G1110	G1043
C1989	G1929	A1844	A1780	U1687	G1626	G1563	G1498	A1428	A1367	U1300	C1178	A1111	G1044
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- Molecule 24: 23S ribosomal RNA

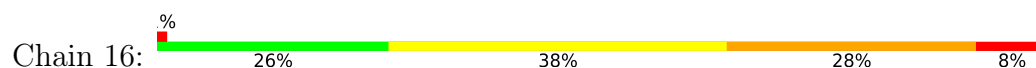


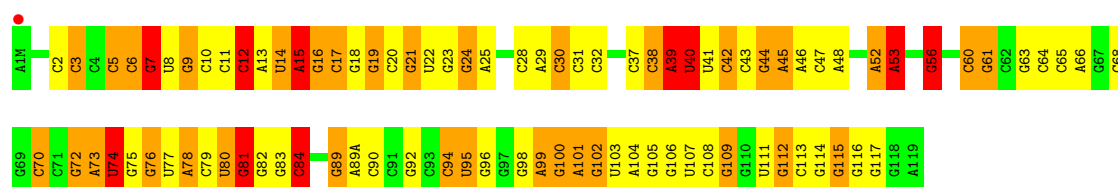


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G1983	A1912	G1836	G1776	G1892		C1564	A1494	G1428	A1365	C1298	U1237	U1165	U1105	C1041
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	A1916	G1839	A1780	G1695	G1632	A1567	U1497	C1431	G1368	A1301	U1240	G1171	U1109	C1044
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	U1940	G1863	G1800		G1653	G1591	U1520	A1453	G1389	A1322	G1260	G1192	A1129	C1064
A2013	G1870	A1871	G1801	G1728	A1854	C1592	G1521	U1454	U1390	U1323	C1261	G1193	U1130	U1065
A2014	U1943	A1872	A1802	A1729	A1655		G1522		A1392	G1325	A1262		G1131	U1066
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U2017	U1946	C1875	U1805	A1732	C1658	A1597	G1525	A1460	G1395	G1328	U1267	G1135	G1136	A1069
G2018	C1947	C1880	C1806	G1733	U1659	C1598	G1526	G1461	A1395	U1329	A1268	C1201	G1137	A1070
A2019	G1948	G1881	G1807		C1660	C1599	G1527	C1462	U1396	C1302	A1269	G1202	G1138	G1071
G2023	G1949	C1882	U1808	C1742	G1661	G1600	A1528	C1463	U1397	C1303	G1270	G1203	G1139	C1072
G2024	A1889	G1883	A1809	G1743	C1662	G1601	A1529	C1464	C1399	G1332	G1271	A1204	C1140	A1073
G2025	U1951	A1884	A1810	G1746	A1663	A1602	C1530	G1465	C1399	G1332	A1272	U1141	C1075	G1074
G2026	A1952	A1885	G1812	C1751	A1664	A1603	C1531	G1466	G1400	C1333				C1076
G2027	C1954	C1887	G1813	C1752	G1665	C1604	C1532	C1467	G1401		U1273	U1142		
	U1955	G1888	G1814	G1753	G1667	G1605	C1533		G1402	A1336	A1274	G1209	A1142A	
U2028	C1961	A1889	A1815	C1754	A1668	G1606	G1534	G1470	C1403	G1337	A1275	A1210	A1143	C1079
G2029	A1890	G1889	G1816	A1755	C1669	C1607	U1535	A1471	C1404	G1338	A1276	U1211	G1144	A1080
A2030	G1962	A1891	G1817	A1756	A1669	A1608	A1536	A1472	U1405	G1212	G1277	C1145	C1145	U1081
A2031	U1963	C1890	U1818	G1756	U1671	A1609	G1537	G1473	U1406	A1213	A1278	A1213	C1146	U1082
G2032	G1964	G1891	G1819	A1759	C1672	A1610	G1538	C1474	C1407		G1279	G1147	C1147	U1083
A2033	C1965	C1892	U1820	A1760	C1673	C1612	G1540	G1475	G1408		G1280	G1216	A1148	A1084
U2034	G1966	G1893	A1821	C1761	G1674	G1613	U1541	C1476	G1409	C1345	G1281	C1217	G1149	A1085
G2035	C1967	G1894	G1822	A1762	C1675	A1614	G1542	A1477	G1410	G1346	U1282		G1150	A1086
G2036	G1968	U1897	G1823	G1763	A1676	A1615	A1543	G1478	C1411	G1347	G1283	A1220	G1151	G1087
A1969	G1969	G1898	G1824	G1764	A1677	C1616	A1543	G1479	G1348	A1284	A1284		C1152	A1088
G2037	A1969	G1899	G1825	G1765	A1678	C1617	G1547	G1480	A1349	G1285	G1285	G1224	G1153	G1089
G2038	A1970	A1900	A1826	C1765	A1678	C1617	U1482	G1480	G1416	A1286	G1286	G1225	G1154	C1092
G2039	A1971	A1901	G1826	U1766	U1679	A1618	G1548	G1483	G1418	A1287	A1287	G1226	G1155	A1155
U2040	A1972	G1902	C1827	C1767	U1680	G1619	G1484	G1484	A1419	U1288	A1227	G1226	A1156	G1093
G1973	G1973	G1903	G1828	U1768	G1681	G1620	G1485	G1485	A1363	C1289	C1289	G1157	G1157	U1094
A2042	C1974		A1829	G1769		U1621	G1555	A1486	G1421	G1355	C1290	G1229	C1158	A1095



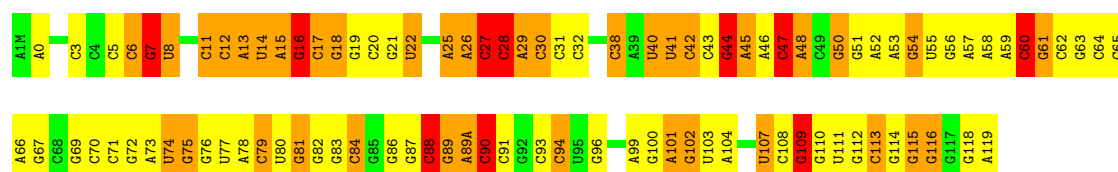
• Molecule 25: 5S ribosomal RNA





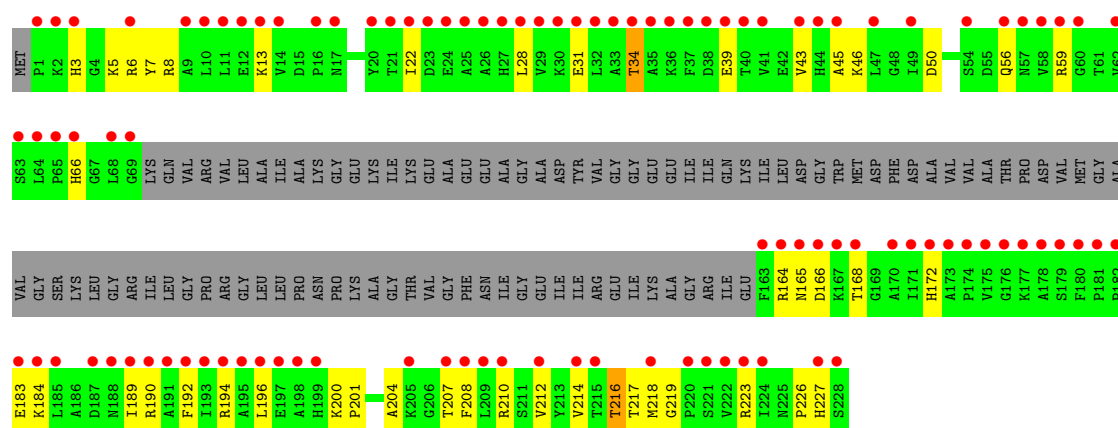
• Molecule 25: 5S ribosomal RNA

Chain 1J: 20% 42% 30% 8%



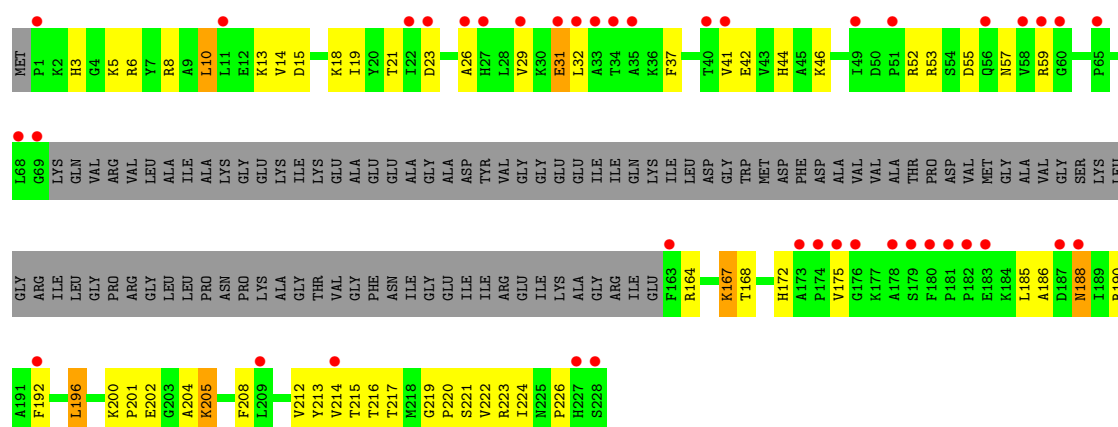
• Molecule 26: 50S ribosomal protein L1

Chain 71: 45% 39% 19% 41%

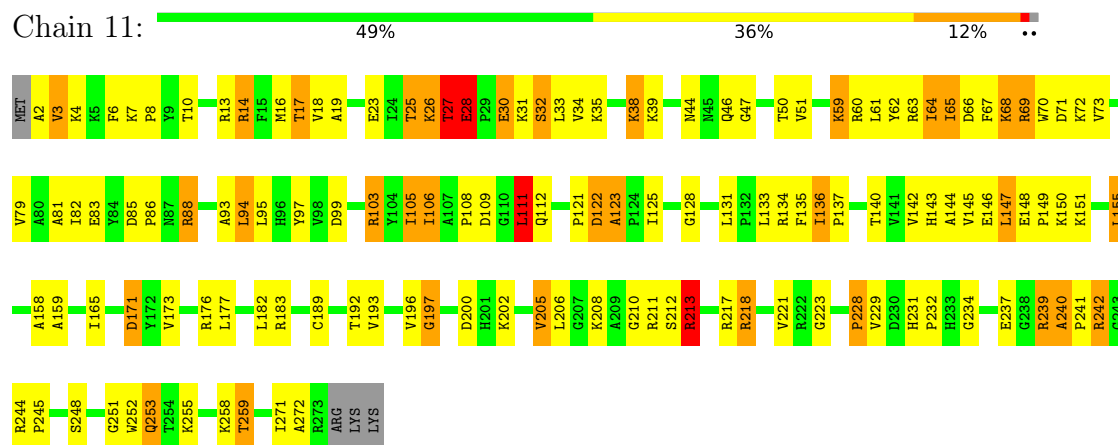


• Molecule 26: 50S ribosomal protein L1

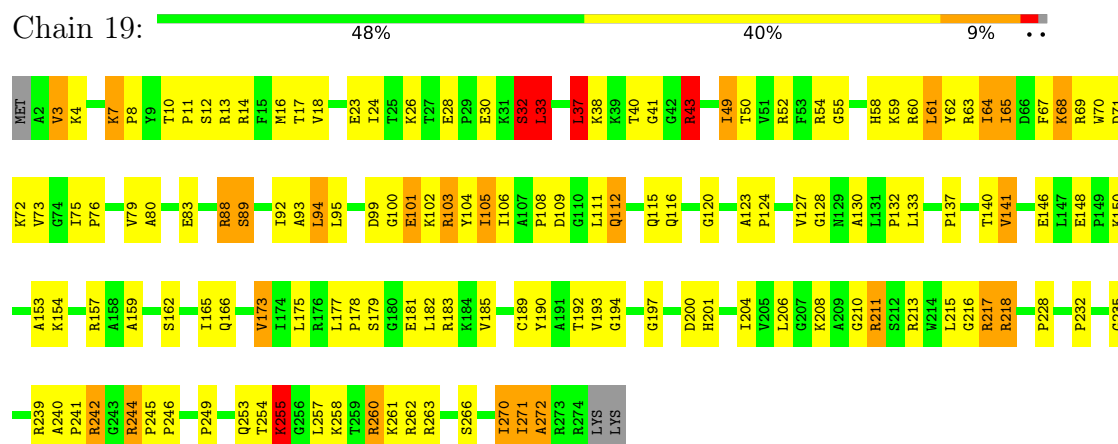
Chain 79: 18% 34% 22% 41%



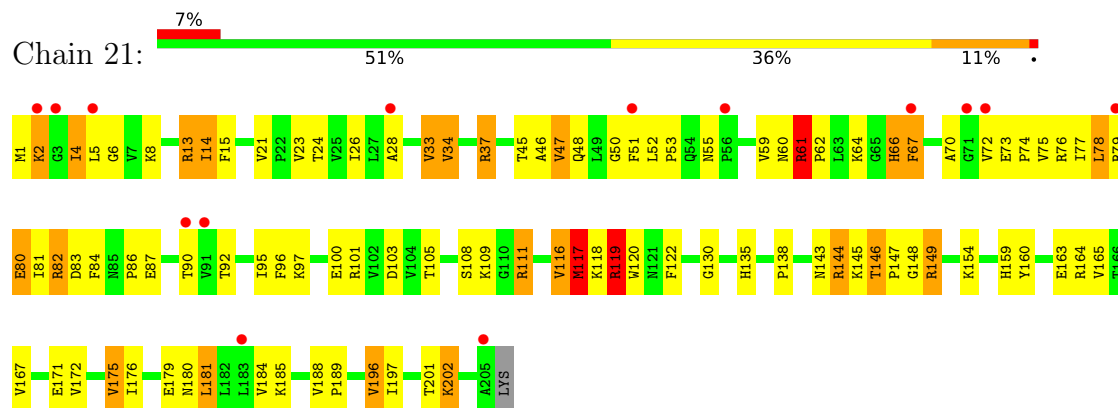
• Molecule 27: 50S ribosomal protein L2



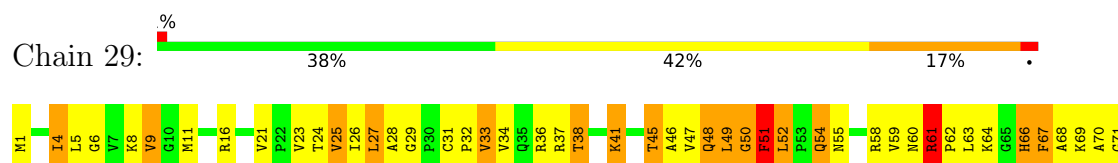
- Molecule 27: 50S ribosomal protein L2

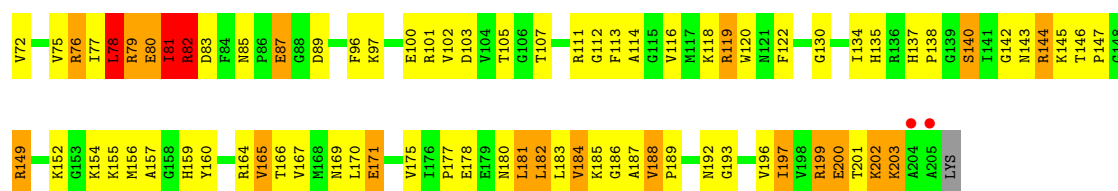


- Molecule 28: 50S ribosomal protein L3

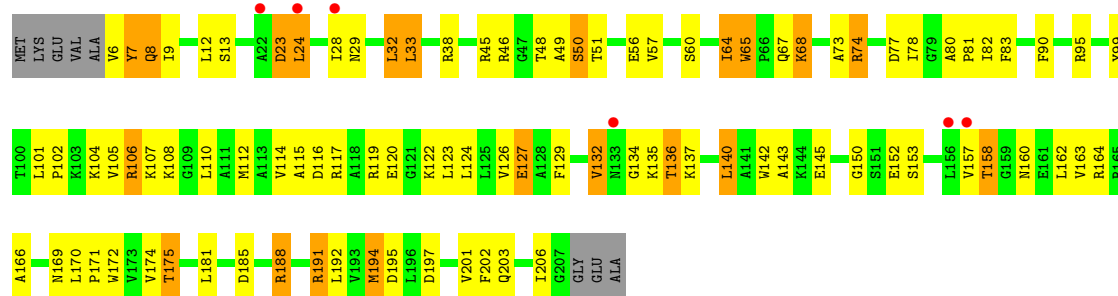


- Molecule 28: 50S ribosomal protein L3

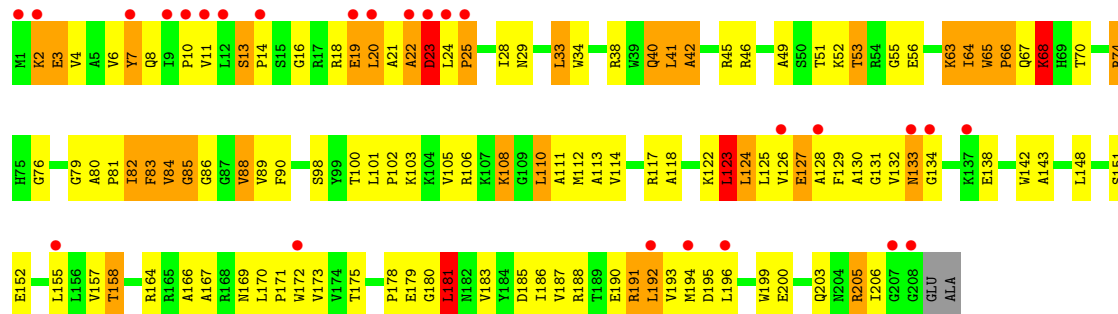




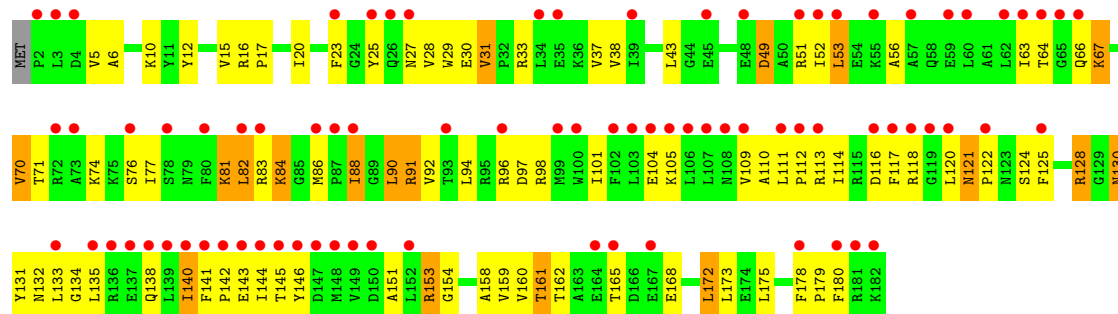
• Molecule 29: 50S ribosomal protein L4



• Molecule 29: 50S ribosomal protein L4

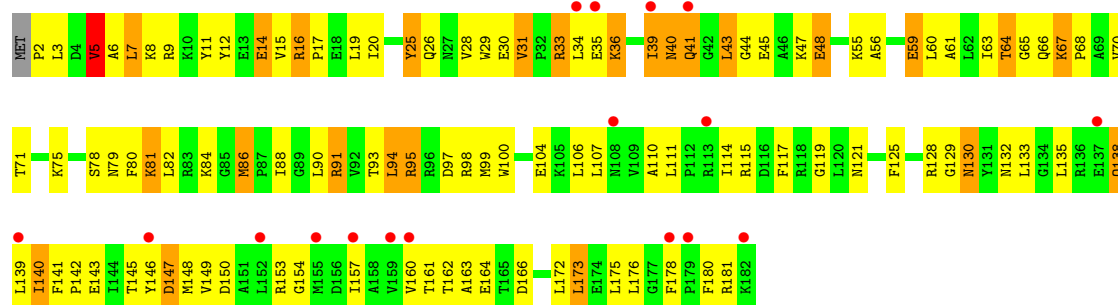


• Molecule 30: 50S ribosomal protein L5

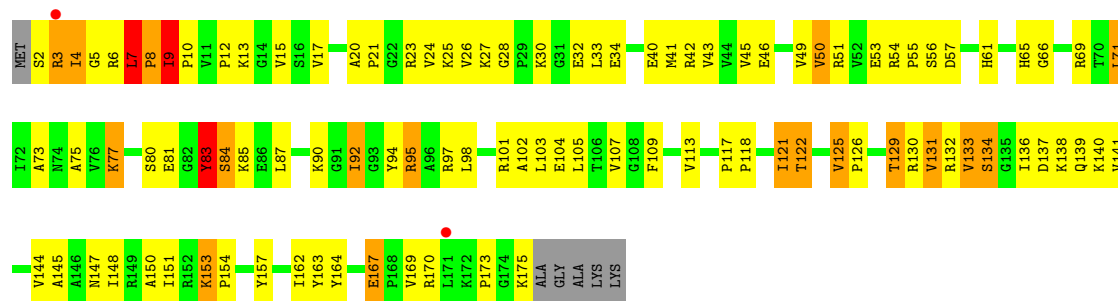


• Molecule 30: 50S ribosomal protein L5

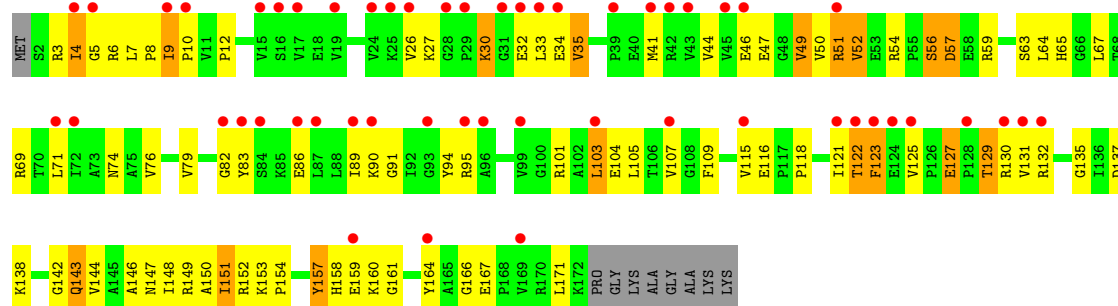




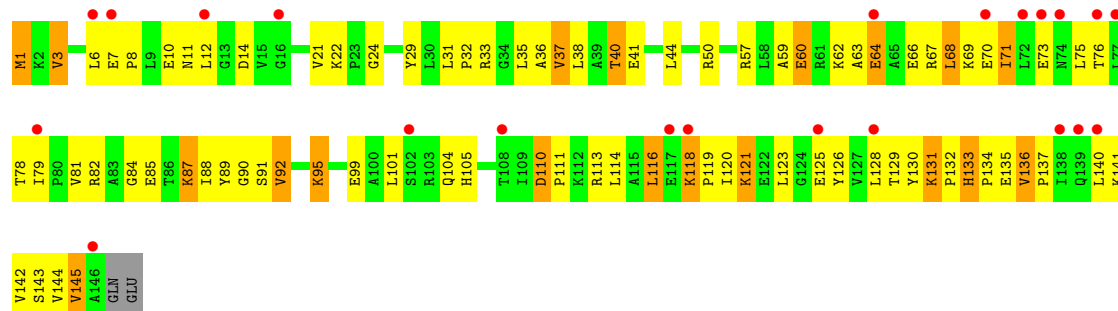
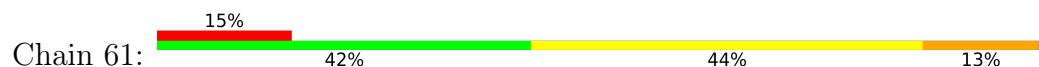
• Molecule 31: 50S ribosomal protein L6



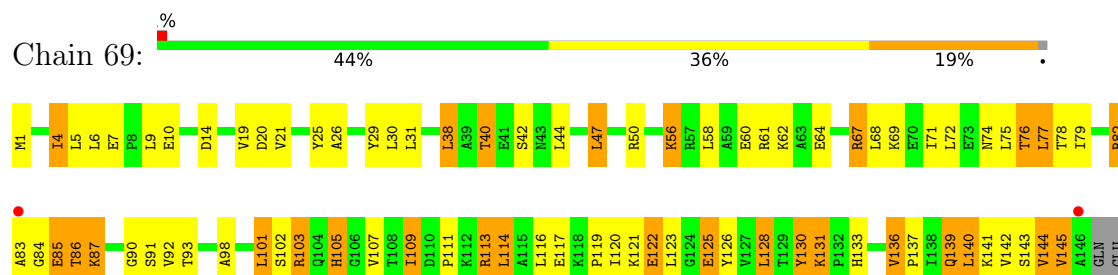
• Molecule 31: 50S ribosomal protein L6



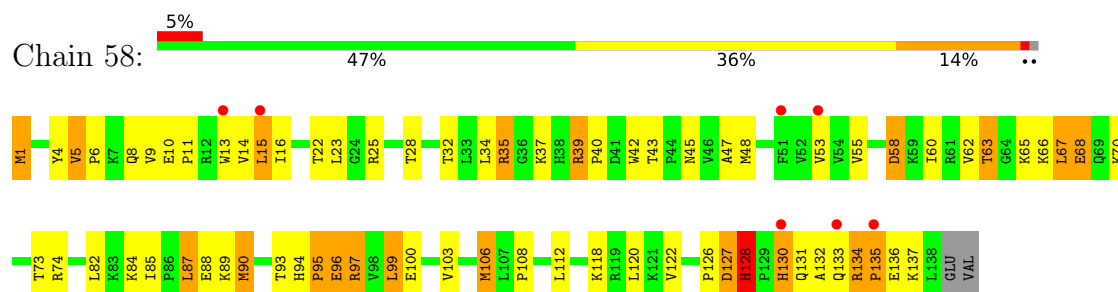
• Molecule 32: 50S ribosomal protein L9



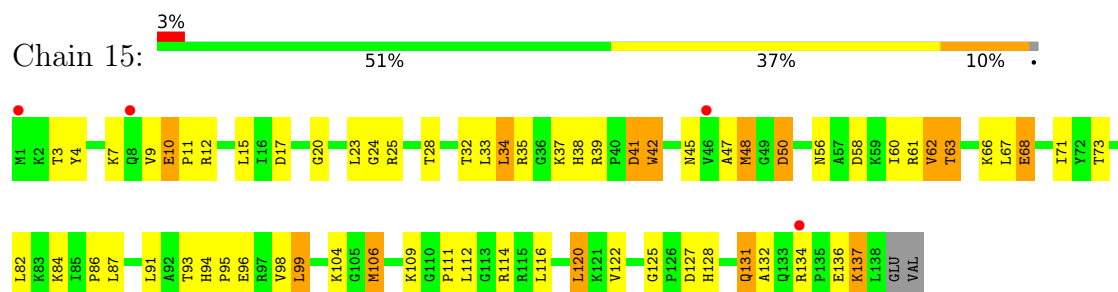
- Molecule 32: 50S ribosomal protein L9



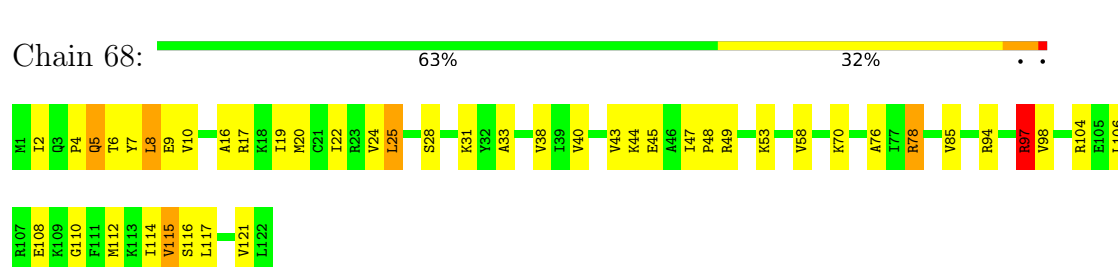
- Molecule 33: 50S ribosomal protein L13



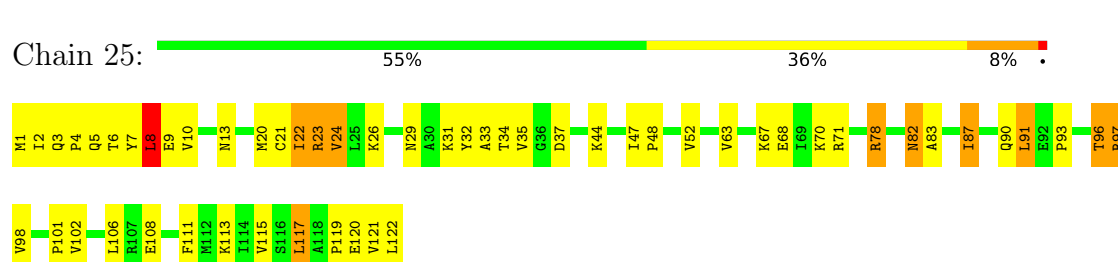
- Molecule 33: 50S ribosomal protein L13



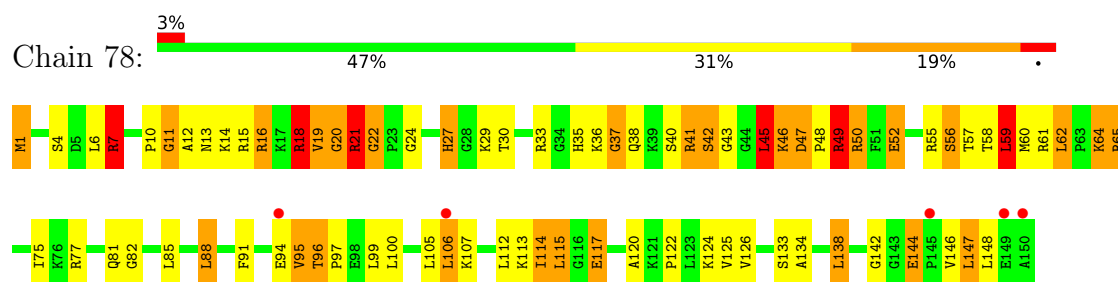
- Molecule 34: 50S ribosomal protein L14



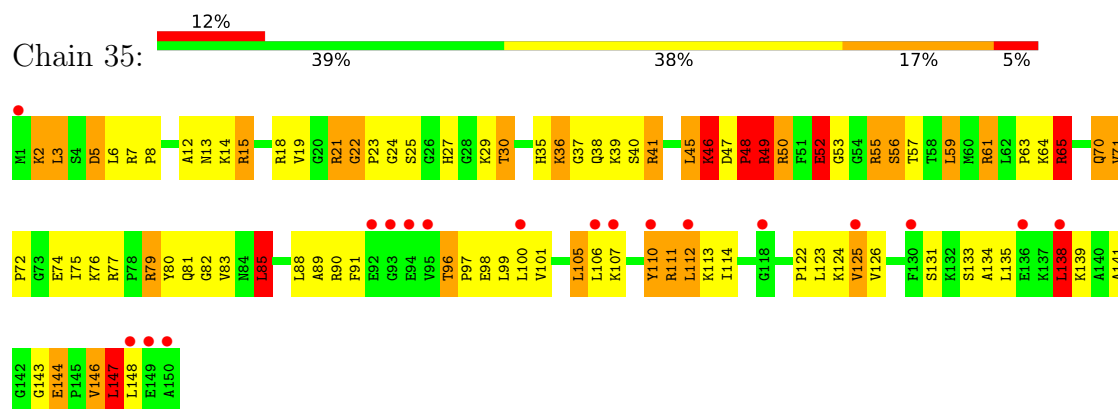
- Molecule 34: 50S ribosomal protein L14



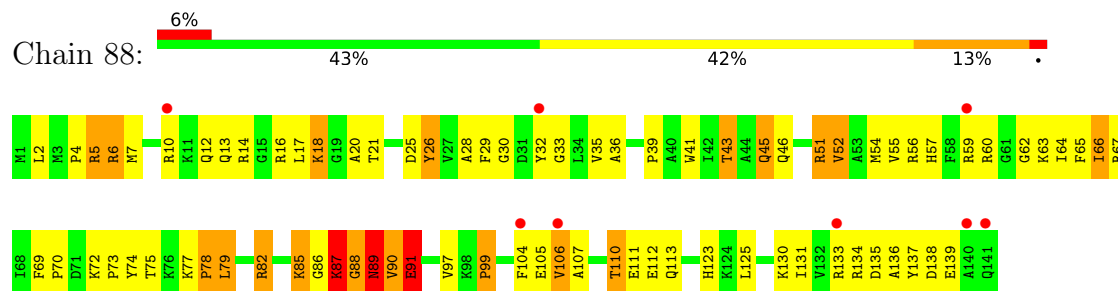
- Molecule 35: 50S ribosomal protein L15



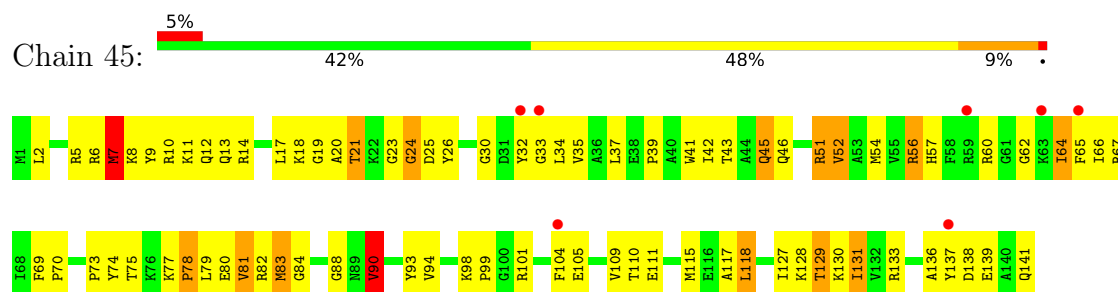
- Molecule 35: 50S ribosomal protein L15



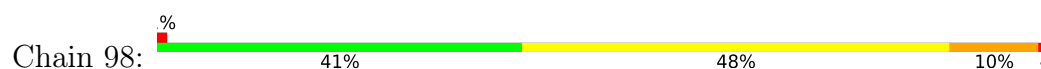
- Molecule 36: 50S ribosomal protein L16



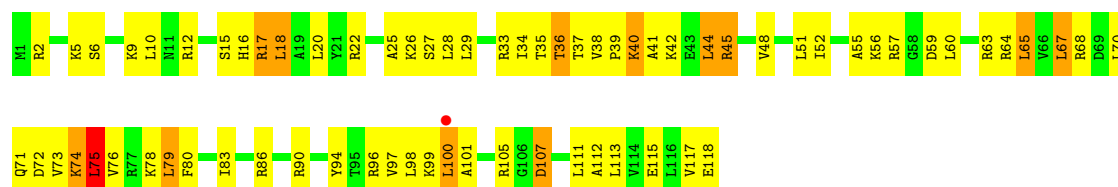
- Molecule 36: 50S ribosomal protein L16



- Molecule 37: 50S ribosomal protein L17

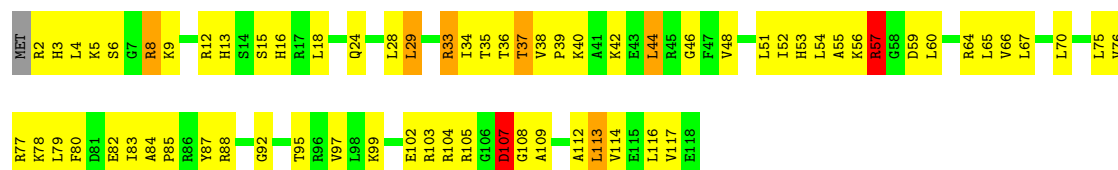






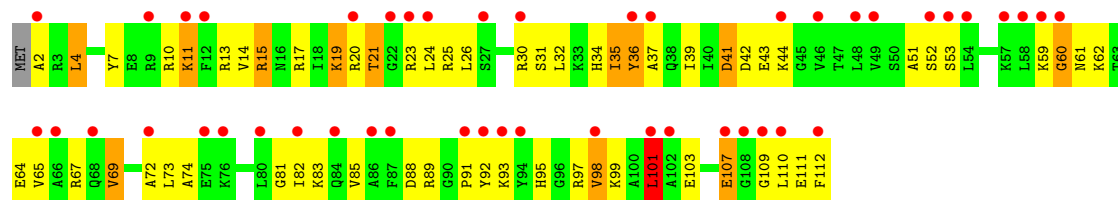
• Molecule 37: 50S ribosomal protein L17

Chain 55: 41% 52% 5% ..



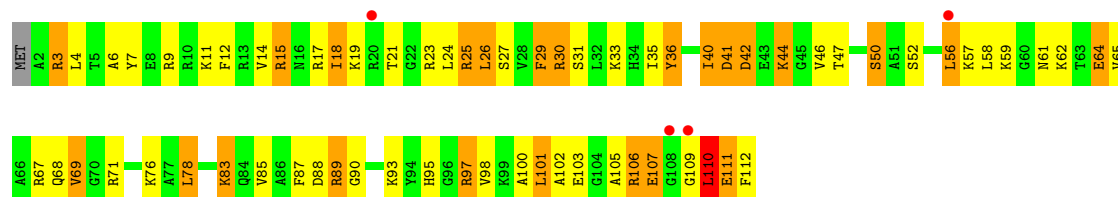
• Molecule 38: 50S ribosomal protein L18

Chain A8: 41% 44% 44% 11% ..



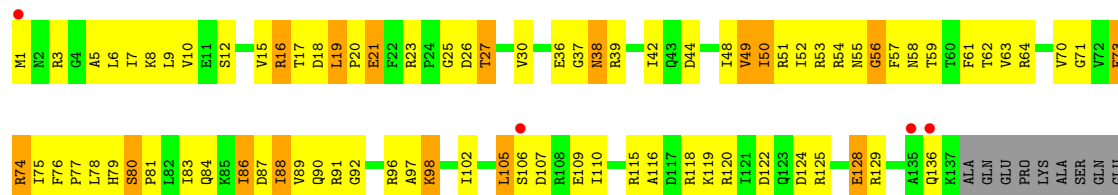
• Molecule 38: 50S ribosomal protein L18

Chain 65: 4% 39% 38% 21% ..



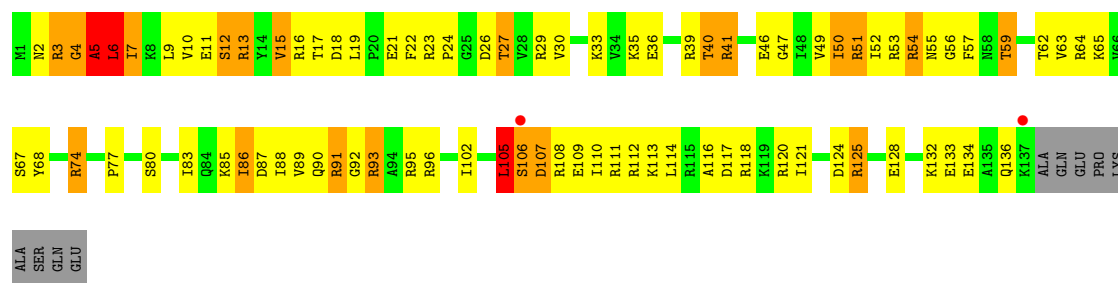
• Molecule 39: 50S ribosomal protein L19

Chain B8: 3% 37% 46% 11% 6%

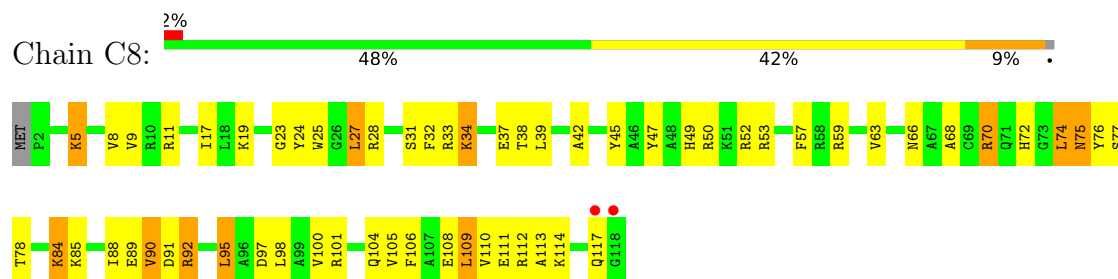


• Molecule 39: 50S ribosomal protein L19

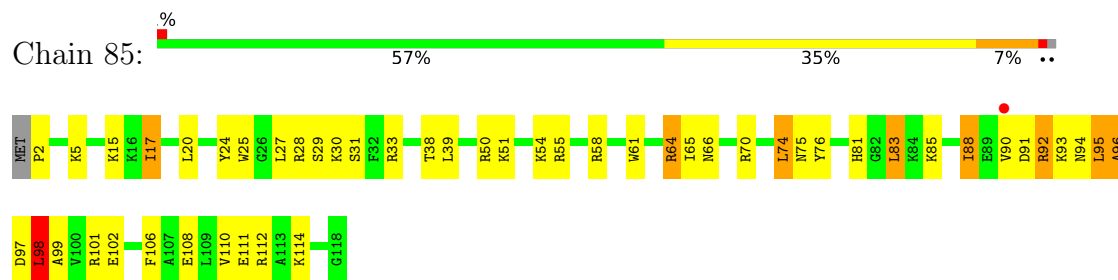
Chain 75: % 35% 43% 14% 6%



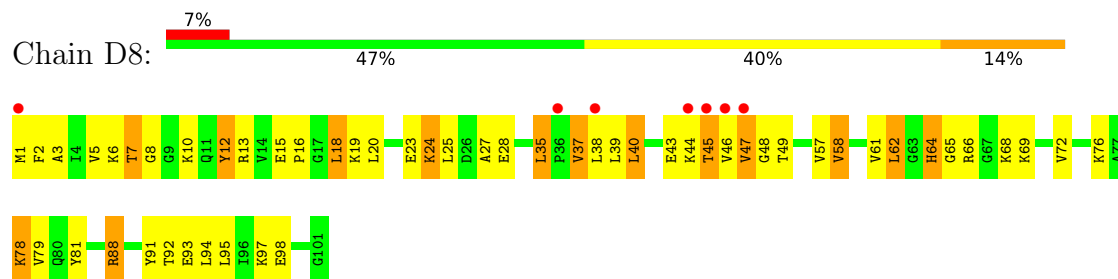
• Molecule 40: 50S ribosomal protein L20



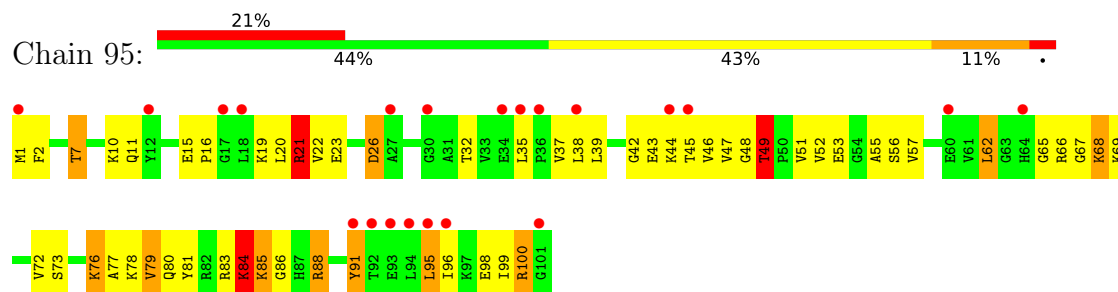
• Molecule 40: 50S ribosomal protein L20



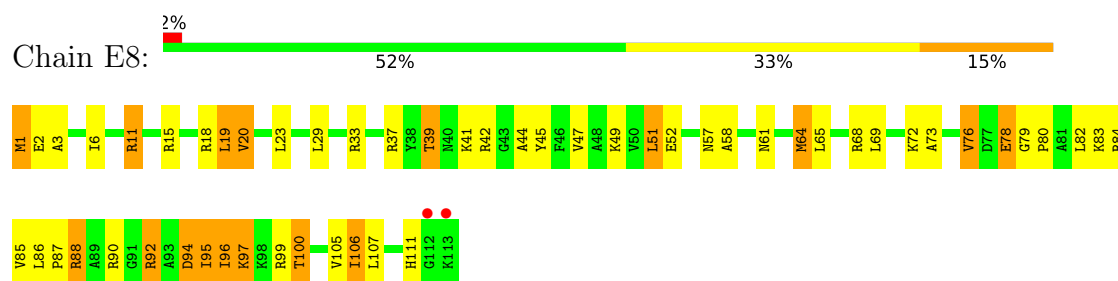
• Molecule 41: 50S ribosomal protein L21



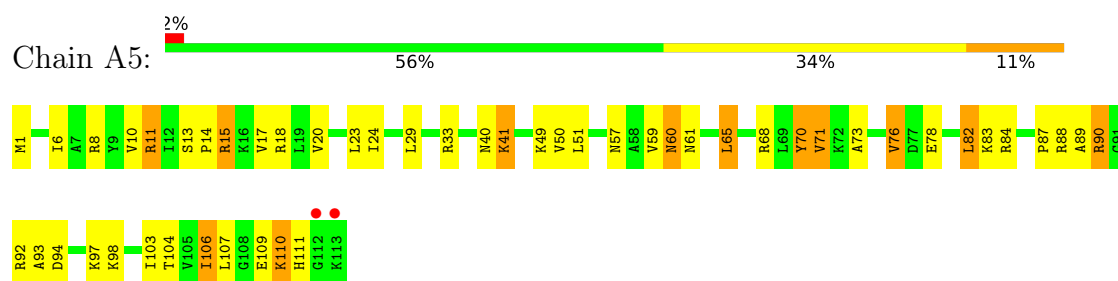
• Molecule 41: 50S ribosomal protein L21



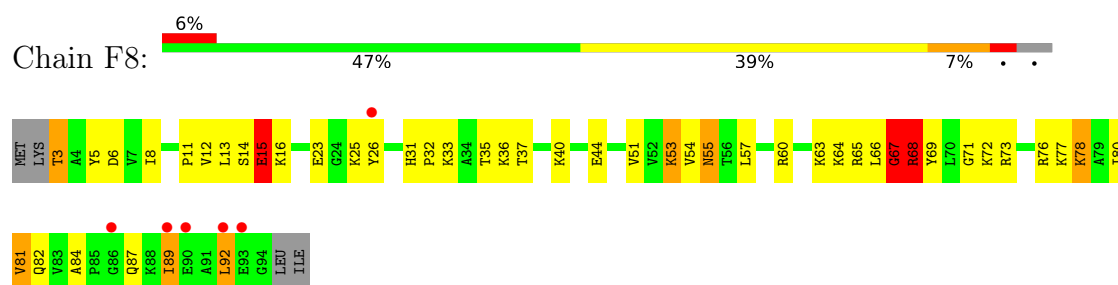
• Molecule 42: 50S ribosomal protein L22



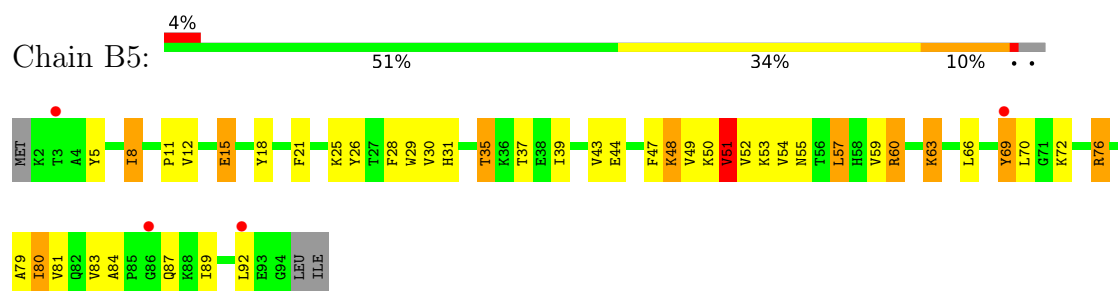
- Molecule 42: 50S ribosomal protein L22



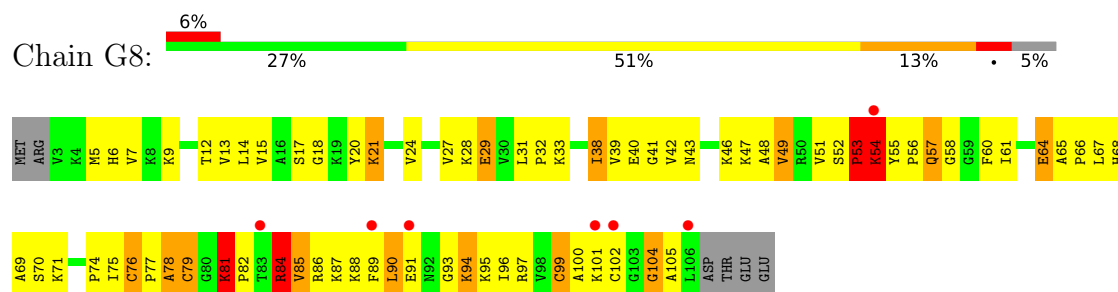
- Molecule 43: 50S ribosomal protein L23



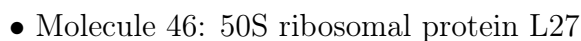
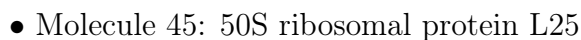
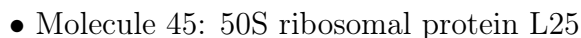
- Molecule 43: 50S ribosomal protein L23

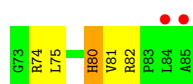


- Molecule 44: 50S ribosomal protein L24

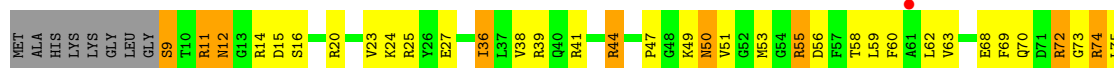


- Molecule 44: 50S ribosomal protein L24

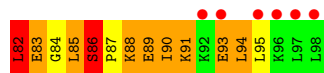
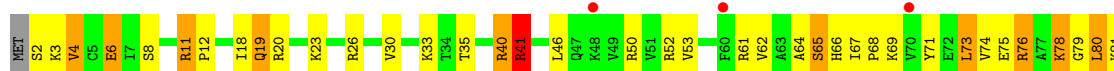




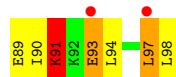
- Molecule 46: 50S ribosomal protein L27



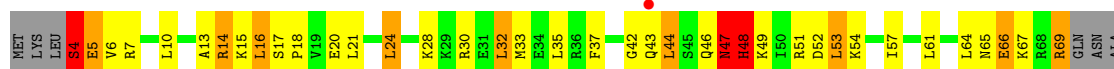
- Molecule 47: 50S ribosomal protein L28



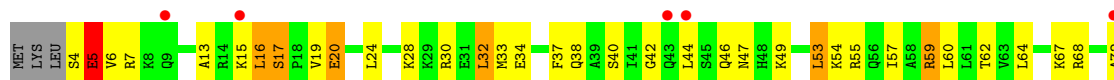
- Molecule 47: 50S ribosomal protein L28



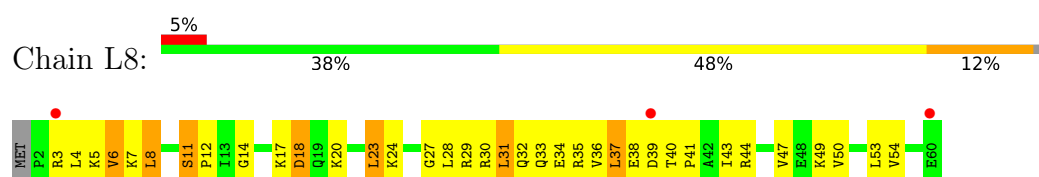
- Molecule 48: 50S ribosomal protein L29



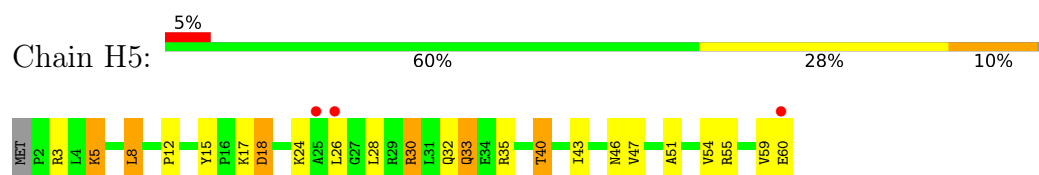
- Molecule 48: 50S ribosomal protein L29



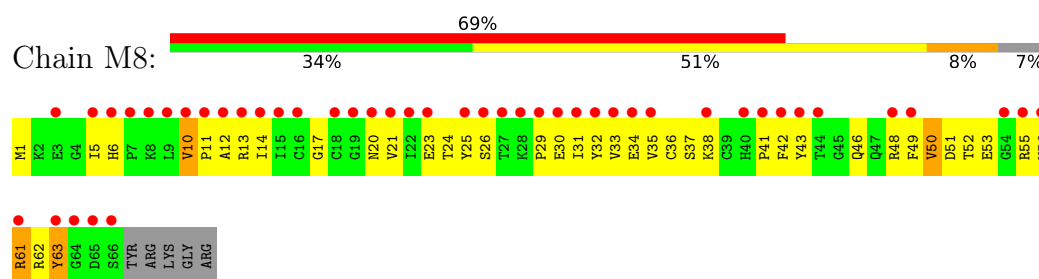
- Molecule 49: 50S ribosomal protein L30



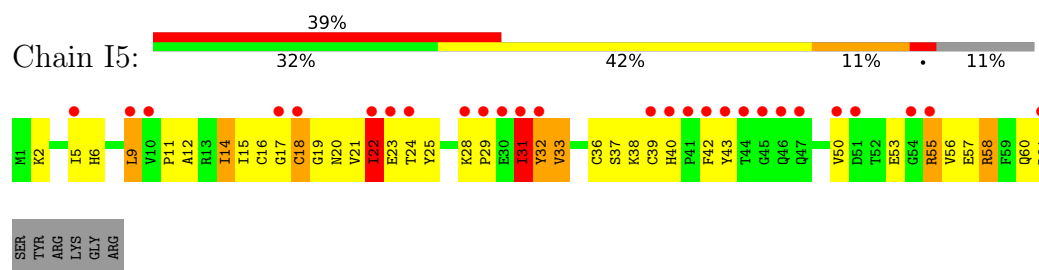
- Molecule 49: 50S ribosomal protein L30



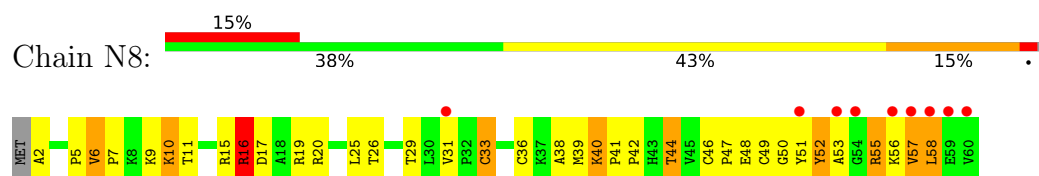
- Molecule 50: 50S ribosomal protein L31



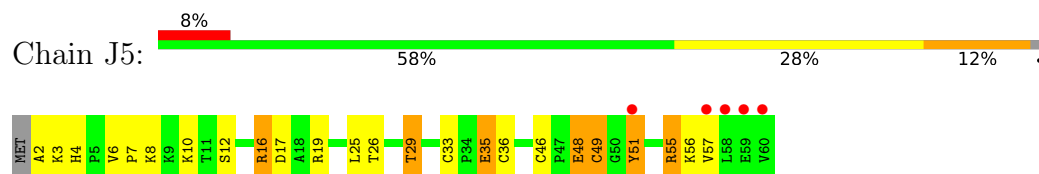
- Molecule 50: 50S ribosomal protein L31



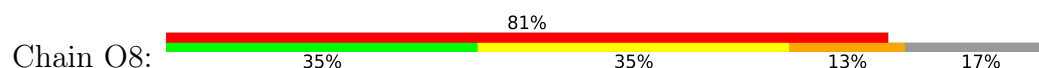
- Molecule 51: 50S ribosomal protein L32

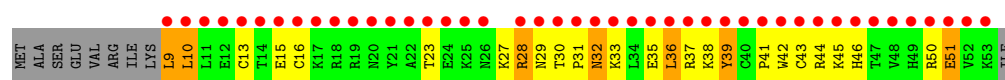


- Molecule 51: 50S ribosomal protein L32

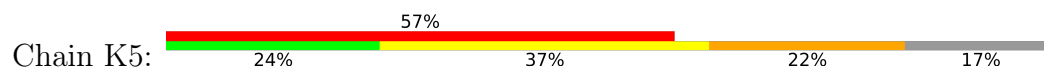


- Molecule 52: 50S ribosomal protein L33





- Molecule 52: 50S ribosomal protein L33



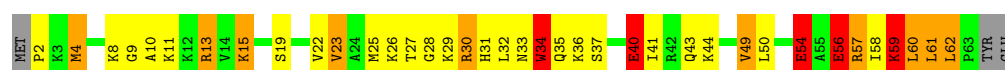
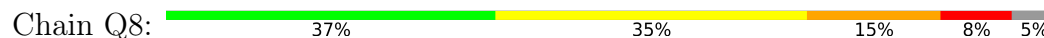
- Molecule 53: 50S ribosomal protein L34



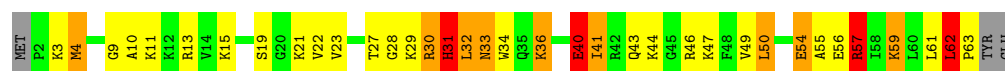
- Molecule 53: 50S ribosomal protein L34



- 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, $\alpha$ , $\beta$ , $\gamma$	210.70Å 448.40Å 616.30Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	153.54 – 3.10 253.96 – 3.10	Depositor EDS
% Data completeness (in resolution range)	99.8 (153.54-3.10) 91.1 (253.96-3.10)	Depositor EDS
$R_{merge}$	0.22	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	0.83 (at 3.07Å)	Xtriage
Refinement program	PHENIX	Depositor
R, $R_{free}$	0.227 , 0.193 0.193 , 0.229	Depositor DCC
$R_{free}$ test set	2000 reflections (0.19%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	84.3	Xtriage
Anisotropy	0.119	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.28 , 81.2	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	299705	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	114.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.48% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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: 5MU, ZN, OMG, MIA, MG, 4SU, QUO, PSU

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z  > 5$	RMSZ	$\# Z  > 5$
1	13	0.81	9/36199 (0.0%)	1.50	567/56498 (1.0%)
1	1G	0.81	7/36167 (0.0%)	1.49	517/56448 (0.9%)
2	12	0.39	0/1959	0.65	0/2642
2	1E	0.43	0/1959	0.67	1/2642 (0.0%)
3	22	0.47	0/1636	0.68	0/2205
3	2E	0.47	0/1629	0.63	0/2195
4	32	0.57	0/1732	0.80	1/2318 (0.0%)
4	3E	0.65	2/1732 (0.1%)	0.78	4/2318 (0.2%)
5	42	0.60	0/1171	0.78	0/1576
5	4E	0.59	0/1171	0.77	1/1576 (0.1%)
6	52	0.61	0/855	0.76	2/1154 (0.2%)
6	5E	0.57	0/855	0.72	0/1154
7	62	0.48	0/1275	0.65	0/1709
7	6E	0.47	0/1275	0.62	0/1709
8	72	0.52	0/1135	0.70	0/1527
8	7E	0.52	0/1135	0.78	1/1527 (0.1%)
9	82	0.46	0/1028	0.67	0/1379
9	8E	0.45	0/1028	0.65	1/1379 (0.1%)
10	1A	0.43	0/814	0.66	0/1095
10	1I	0.44	0/814	0.62	0/1095
11	2A	0.57	0/879	0.75	0/1187
11	2I	0.57	0/879	0.74	0/1187
12	3A	0.65	0/991	0.82	0/1327
12	3I	0.68	0/991	0.87	1/1327 (0.1%)
13	4A	0.40	0/943	0.62	0/1265
13	4I	0.40	0/938	0.70	0/1258
14	5A	0.53	0/500	0.74	0/664
14	5I	0.56	0/500	0.77	1/664 (0.2%)
15	6A	0.61	0/744	0.72	0/992
15	6I	0.59	0/744	0.78	0/992
16	7A	0.59	0/721	0.76	0/970
16	7I	0.51	0/721	0.80	1/970 (0.1%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
17	8A	0.62	0/847	0.76	0/1131
17	8I	0.55	0/847	0.74	0/1131
18	9A	0.58	0/595	0.79	2/790 (0.3%)
18	9I	0.52	0/595	0.73	1/790 (0.1%)
19	AA	0.43	0/647	0.71	0/871
19	AI	0.41	0/680	0.70	0/915
20	BA	0.57	0/764	0.80	1/1007 (0.1%)
20	BI	0.44	0/764	0.72	0/1007
21	1B	0.44	0/221	0.69	0/288
21	1F	0.43	0/221	0.65	0/288
22	2K	0.82	0/1784	1.60	34/2771 (1.2%)
22	2L	0.83	0/1686	1.53	26/2618 (1.0%)
22	3K	0.45	0/1850	1.08	5/2875 (0.2%)
22	3L	0.50	0/1851	1.15	10/2877 (0.3%)
23	4K	1.22	0/392	1.69	14/609 (2.3%)
23	4L	0.96	0/190	1.70	5/293 (1.7%)
24	14	1.10	158/70167 (0.2%)	1.83	2510/109541 (2.3%)
24	1H	1.18	231/70233 (0.3%)	1.95	3196/109643 (2.9%)
25	16	0.89	0/2928	1.59	63/4568 (1.4%)
25	1J	0.85	0/2928	1.68	64/4568 (1.4%)
26	71	0.29	0/1072	0.51	0/1447
26	79	0.29	0/1072	0.48	0/1447
27	11	0.97	2/2165 (0.1%)	1.12	8/2919 (0.3%)
27	19	0.88	1/2170 (0.0%)	1.05	8/2926 (0.3%)
28	21	0.73	0/1601	0.97	4/2160 (0.2%)
28	29	0.80	0/1601	1.01	5/2160 (0.2%)
29	31	0.86	0/1620	0.99	2/2194 (0.1%)
29	39	0.73	1/1662 (0.1%)	0.94	3/2249 (0.1%)
30	41	0.44	0/1498	0.65	0/2016
30	49	0.45	0/1498	0.67	0/2016
31	51	0.63	0/1362	0.89	1/1841 (0.1%)
31	59	0.37	0/1337	0.69	0/1809
32	61	0.56	0/1151	0.83	3/1558 (0.2%)
32	69	0.54	0/1151	0.76	1/1558 (0.1%)
33	15	0.61	0/1131	0.81	0/1525
33	58	0.67	0/1131	0.83	0/1525
34	25	0.82	0/942	0.89	1/1269 (0.1%)
34	68	0.76	0/942	0.84	0/1269
35	35	0.76	1/1161 (0.1%)	1.10	5/1544 (0.3%)
35	78	0.83	0/1161	1.19	8/1544 (0.5%)
36	45	0.71	0/1142	0.97	3/1527 (0.2%)
36	88	0.82	2/1142 (0.2%)	0.99	3/1527 (0.2%)
37	55	0.77	0/973	1.03	3/1302 (0.2%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
37	98	0.70	0/981	0.96	1/1312 (0.1%)
38	65	0.61	0/891	0.88	1/1187 (0.1%)
38	A8	0.62	0/891	0.88	2/1187 (0.2%)
39	75	0.76	0/1145	0.95	2/1531 (0.1%)
39	B8	0.71	0/1155	0.88	1/1542 (0.1%)
40	85	0.69	0/981	0.84	2/1306 (0.2%)
40	C8	0.78	0/981	0.84	0/1306
41	95	4.12	8/789 (1.0%)	1.45	6/1057 (0.6%)
41	D8	0.73	0/789	0.89	2/1057 (0.2%)
42	A5	0.75	0/910	0.89	1/1220 (0.1%)
42	E8	0.79	0/910	0.93	3/1220 (0.2%)
43	B5	0.88	1/744 (0.1%)	0.85	0/1000
43	F8	0.95	1/739 (0.1%)	0.89	0/993
44	C5	0.69	0/807	0.93	1/1076 (0.1%)
44	G8	0.90	1/804 (0.1%)	1.06	3/1073 (0.3%)
45	D5	0.47	0/1460	0.71	0/1982
45	H8	0.45	0/1427	0.73	2/1935 (0.1%)
46	E5	0.72	0/620	0.93	0/827
46	I8	0.83	0/665	1.01	3/885 (0.3%)
47	F5	0.74	0/769	0.92	1/1022 (0.1%)
47	J8	0.78	0/769	1.09	6/1022 (0.6%)
48	G5	0.68	2/582 (0.3%)	0.89	1/771 (0.1%)
48	K8	1.01	2/560 (0.4%)	0.97	0/741
49	H5	0.61	0/473	0.81	0/635
49	L8	0.70	0/473	0.91	0/635
50	I5	0.44	0/527	0.68	0/709
50	M8	0.36	0/545	0.59	0/733
51	J5	0.65	0/472	0.84	0/639
51	N8	0.80	0/472	0.98	2/639 (0.3%)
52	K5	0.57	0/396	0.77	0/529
52	O8	0.51	0/396	0.72	0/529
53	L5	0.84	0/437	1.05	3/575 (0.5%)
53	P8	1.01	0/417	1.18	3/550 (0.5%)
54	M5	0.97	1/502 (0.2%)	1.27	5/661 (0.8%)
54	Q8	1.08	1/488 (0.2%)	1.19	2/641 (0.3%)
All	All	0.95	431/321962 (0.1%)	1.56	7140/481589 (1.5%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
2	12	0	2
2	1E	0	1
3	22	0	1
4	3E	0	3
9	82	0	2
12	3A	0	4
14	5I	0	1
19	AA	0	1
19	AI	0	3
20	BA	0	2
27	11	0	4
27	19	0	5
28	29	0	7
29	31	0	1
29	39	0	1
30	49	0	1
31	59	0	1
32	61	0	1
33	15	0	1
34	25	0	1
35	35	0	7
35	78	0	7
36	45	0	1
36	88	0	3
38	65	0	1
38	A8	0	2
39	75	0	3
39	B8	0	1
40	85	0	1
41	95	0	2
43	F8	0	1
44	C5	0	3
44	G8	0	5
45	D5	0	3
47	F5	0	2
47	J8	0	2
48	K8	0	2
49	L8	0	1
51	J5	0	1
52	K5	0	1
53	P8	0	2
54	M5	0	2
54	Q8	0	4

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Mol	Chain	#Chirality outliers	#Planarity outliers
All	All	0	100

The worst 5 of 431 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
41	95	91	TYR	CD1-CE1	59.58	2.28	1.39
41	95	91	TYR	CD2-CE2	57.56	2.25	1.39
41	95	91	TYR	CE2-CZ	41.48	1.92	1.38
41	95	91	TYR	CE1-CZ	39.94	1.90	1.38
41	95	91	TYR	CG-CD2	31.31	1.79	1.39

The worst 5 of 7140 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	1H	1332	G	N3-C4-N9	-24.58	111.25	126.00
24	1H	1332	G	N3-C4-C5	23.29	140.25	128.60
41	95	21	ARG	CD-NE-CZ	23.04	155.86	123.60
24	1H	1899	G	N3-C4-N9	-22.45	112.53	126.00
41	95	21	ARG	NE-CZ-NH1	22.42	131.51	120.30

There are no chirality outliers.

5 of 100 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	1E	71	VAL	Peptide
4	3E	166	LYS	Peptide
4	3E	193	ASP	Peptide
4	3E	29	PRO	Peptide
14	5I	13	THR	Peptide

## 5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	13	32337	0	16321	890	0
1	1G	32309	0	16307	834	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	12	1924	0	1975	95	0
2	1E	1924	0	1975	120	0
3	22	1612	0	1677	92	0
3	2E	1605	0	1668	72	0
4	32	1702	0	1763	112	1
4	3E	1702	0	1763	83	0
5	42	1155	0	1213	70	0
5	4E	1155	0	1213	52	0
6	52	842	0	857	38	0
6	5E	842	0	857	43	1
7	62	1256	0	1296	41	0
7	6E	1256	0	1296	55	0
8	72	1115	0	1177	50	0
8	7E	1115	0	1177	71	0
9	82	1009	0	1037	72	0
9	8E	1009	0	1037	67	0
10	1A	801	0	849	55	0
10	1I	801	0	849	44	0
11	2A	864	0	881	27	0
11	2I	864	0	881	39	0
12	3A	975	0	1062	39	0
12	3I	975	0	1062	43	0
13	4A	933	0	992	57	0
13	4I	928	0	987	50	0
14	5A	491	0	529	36	0
14	5I	491	0	529	45	0
15	6A	733	0	771	28	0
15	6I	733	0	771	36	0
16	7A	705	0	725	34	0
16	7I	705	0	725	47	0
17	8A	834	0	904	44	0
17	8I	834	0	904	47	0
18	9A	590	0	662	26	0
18	9I	590	0	662	20	0
19	AA	633	0	649	46	0
19	AI	665	0	686	36	0
20	BA	762	0	861	37	0
20	BI	762	0	861	54	0
21	1B	217	0	234	17	0
21	1F	217	0	234	12	0
22	2K	1765	0	916	65	0
22	2L	1678	0	872	64	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
22	3K	1824	0	945	58	0
22	3L	1825	0	946	52	0
23	4K	348	0	175	9	0
23	4L	170	0	87	3	0
24	14	62647	0	31572	1458	0
24	1H	62707	0	31606	1603	0
25	16	2617	0	1328	87	0
25	1J	2617	0	1328	93	0
26	71	1049	0	1071	31	0
26	79	1049	0	1071	42	0
27	11	2115	0	2195	134	0
27	19	2120	0	2197	114	0
28	21	1568	0	1634	95	0
28	29	1568	0	1634	121	0
29	31	1585	0	1632	79	0
29	39	1627	0	1680	103	0
30	41	1473	0	1535	72	0
30	49	1473	0	1535	89	0
31	51	1336	0	1418	89	0
31	59	1312	0	1384	64	0
32	61	1136	0	1223	55	0
32	69	1136	0	1223	65	0
33	15	1104	0	1180	47	0
33	58	1104	0	1180	51	0
34	25	932	0	996	39	0
34	68	932	0	996	32	0
35	35	1144	0	1228	81	0
35	78	1144	0	1228	90	0
36	45	1121	0	1179	71	0
36	88	1121	0	1179	84	0
37	55	959	0	1021	54	0
37	98	967	0	1033	68	0
38	65	881	0	943	77	0
38	A8	881	0	943	49	0
39	75	1131	0	1180	86	0
39	B8	1141	0	1202	58	0
40	85	963	0	1022	54	0
40	C8	963	0	1022	60	0
41	95	778	0	852	86	0
41	D8	778	0	852	32	0
42	A5	899	0	964	34	0
42	E8	899	0	964	40	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
43	B5	730	0	780	39	0
43	F8	725	0	778	46	0
44	C5	794	0	884	58	0
44	G8	791	0	880	67	0
45	D5	1428	0	1454	89	0
45	H8	1397	0	1430	86	0
46	E5	612	0	633	39	0
46	I8	656	0	683	55	0
47	F5	762	0	848	35	0
47	J8	762	0	848	47	0
48	G5	580	0	629	29	0
48	K8	558	0	610	30	0
49	H5	468	0	518	14	0
49	L8	468	0	518	36	0
50	I5	515	0	514	43	0
50	M8	533	0	526	40	0
51	J5	458	0	480	20	0
51	N8	458	0	480	36	0
52	K5	389	0	404	24	0
52	O8	389	0	404	27	0
53	L5	429	0	480	33	0
53	P8	409	0	454	20	0
54	M5	495	0	567	37	0
54	Q8	483	0	555	42	0
55	11	2	0	0	0	0
55	13	139	0	0	0	0
55	14	465	0	0	0	0
55	15	1	0	0	0	0
55	16	15	0	0	0	0
55	19	1	0	0	0	0
55	1G	148	0	0	0	0
55	1H	523	0	0	0	0
55	1J	10	0	0	0	0
55	21	2	0	0	0	0
55	25	1	0	0	0	0
55	29	4	0	0	0	0
55	2K	5	0	0	0	0
55	2L	4	0	0	0	0
55	32	1	0	0	0	0
55	39	1	0	0	0	0
55	3A	1	0	0	0	0
55	3E	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
55	3I	1	0	0	0	0
55	3L	1	0	0	0	0
55	42	1	0	0	0	0
55	45	1	0	0	0	0
55	4A	1	0	0	0	0
55	4K	1	0	0	0	0
55	52	1	0	0	0	0
55	55	1	0	0	0	0
55	5E	1	0	0	0	0
55	7E	1	0	0	0	0
55	88	1	0	0	0	0
55	98	1	0	0	0	0
55	C5	1	0	0	0	0
55	E5	1	0	0	0	0
55	F5	1	0	0	0	0
55	G8	1	0	0	0	0
55	I8	3	0	0	0	0
55	Q8	2	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	8	0	0	2	0
57	13	125	0	0	23	0
57	14	523	0	0	116	0
57	16	12	0	0	3	0
57	19	11	0	0	3	0
57	1G	96	0	0	18	0
57	1H	652	0	0	172	0
57	1J	22	0	0	2	0
57	21	2	0	0	2	0
57	25	6	0	0	0	0
57	2K	2	0	0	0	0
57	2L	6	0	0	0	0
57	31	5	0	0	0	0
57	32	1	0	0	0	0
57	35	1	0	0	0	0
57	39	3	0	0	0	0
57	4K	3	0	0	0	0
57	5A	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
57	5I	1	0	0	0	0
57	75	1	0	0	0	0
57	78	4	0	0	2	0
57	7A	2	0	0	0	0
57	85	4	0	0	0	0
57	98	1	0	0	2	0
57	AI	3	0	0	0	0
57	BA	1	0	0	0	0
57	C8	2	0	0	0	0
57	E8	1	0	0	0	0
57	F5	1	0	0	0	0
57	F8	2	0	0	0	0
57	G8	2	0	0	1	0
57	H5	2	0	0	0	0
All	All	299705	0	201607	9341	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 20.

The worst 5 of 9341 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)
41:95:91:TYR:CD1	41:95:91:TYR:CG	1.79	1.67
41:95:91:TYR:CD2	41:95:91:TYR:CG	1.79	1.65
41:95:91:TYR:CZ	41:95:91:TYR:CE1	1.90	1.56
41:95:91:TYR:CZ	41:95:91:TYR:CE2	1.92	1.55
22:2K:35:QUO:N3	22:2K:35:QUO:C4	1.68	1.55

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)
6:5E:15:ASP:OD1	4:32:27:TYR:OH[4_555]	2.04	0.16

## 5.3 Torsion angles ⓘ

### 5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	12	235/256 (92%)	196 (83%)	35 (15%)	4 (2%)	10	40
2	1E	235/256 (92%)	199 (85%)	32 (14%)	4 (2%)	10	40
3	22	204/239 (85%)	175 (86%)	29 (14%)	0	100	100
3	2E	203/239 (85%)	185 (91%)	18 (9%)	0	100	100
4	32	206/209 (99%)	176 (85%)	26 (13%)	4 (2%)	9	36
4	3E	206/209 (99%)	191 (93%)	15 (7%)	0	100	100
5	42	149/162 (92%)	142 (95%)	7 (5%)	0	100	100
5	4E	149/162 (92%)	141 (95%)	7 (5%)	1 (1%)	24	61
6	52	99/101 (98%)	95 (96%)	4 (4%)	0	100	100
6	5E	99/101 (98%)	93 (94%)	6 (6%)	0	100	100
7	62	153/156 (98%)	145 (95%)	8 (5%)	0	100	100
7	6E	153/156 (98%)	142 (93%)	11 (7%)	0	100	100
8	72	136/138 (99%)	127 (93%)	7 (5%)	2 (2%)	11	43
8	7E	136/138 (99%)	125 (92%)	11 (8%)	0	100	100
9	82	125/128 (98%)	112 (90%)	12 (10%)	1 (1%)	21	59
9	8E	125/128 (98%)	114 (91%)	11 (9%)	0	100	100
10	1A	97/105 (92%)	85 (88%)	12 (12%)	0	100	100
10	1I	97/105 (92%)	84 (87%)	13 (13%)	0	100	100
11	2A	114/129 (88%)	102 (90%)	12 (10%)	0	100	100
11	2I	114/129 (88%)	102 (90%)	11 (10%)	1 (1%)	19	56
12	3A	123/132 (93%)	111 (90%)	12 (10%)	0	100	100
12	3I	123/132 (93%)	112 (91%)	11 (9%)	0	100	100
13	4A	115/126 (91%)	98 (85%)	12 (10%)	5 (4%)	3	17
13	4I	114/126 (90%)	98 (86%)	16 (14%)	0	100	100
14	5A	58/61 (95%)	48 (83%)	10 (17%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
14	5I	58/61 (95%)	52 (90%)	5 (9%)	1 (2%)	10	40
15	6A	86/89 (97%)	80 (93%)	6 (7%)	0	100	100
15	6I	86/89 (97%)	77 (90%)	9 (10%)	0	100	100
16	7A	82/88 (93%)	76 (93%)	5 (6%)	1 (1%)	14	48
16	7I	82/88 (93%)	79 (96%)	3 (4%)	0	100	100
17	8A	98/105 (93%)	92 (94%)	6 (6%)	0	100	100
17	8I	98/105 (93%)	90 (92%)	7 (7%)	1 (1%)	17	53
18	9A	70/88 (80%)	65 (93%)	5 (7%)	0	100	100
18	9I	70/88 (80%)	63 (90%)	6 (9%)	1 (1%)	12	44
19	AA	77/93 (83%)	57 (74%)	17 (22%)	3 (4%)	3	20
19	AI	81/93 (87%)	66 (82%)	13 (16%)	2 (2%)	6	30
20	BA	97/106 (92%)	83 (86%)	14 (14%)	0	100	100
20	BI	97/106 (92%)	84 (87%)	13 (13%)	0	100	100
21	1B	23/27 (85%)	22 (96%)	1 (4%)	0	100	100
21	1F	23/27 (85%)	21 (91%)	2 (9%)	0	100	100
26	7I	131/229 (57%)	130 (99%)	1 (1%)	0	100	100
26	79	131/229 (57%)	129 (98%)	2 (2%)	0	100	100
27	11	270/276 (98%)	254 (94%)	12 (4%)	4 (2%)	11	43
27	19	271/276 (98%)	253 (93%)	15 (6%)	3 (1%)	16	50
28	21	203/206 (98%)	174 (86%)	28 (14%)	1 (0%)	31	68
28	29	203/206 (98%)	160 (79%)	34 (17%)	9 (4%)	3	17
29	31	200/210 (95%)	189 (94%)	10 (5%)	1 (0%)	31	68
29	39	206/210 (98%)	176 (85%)	21 (10%)	9 (4%)	3	17
30	41	179/182 (98%)	154 (86%)	24 (13%)	1 (1%)	27	64
30	49	179/182 (98%)	151 (84%)	25 (14%)	3 (2%)	10	40
31	51	172/180 (96%)	146 (85%)	20 (12%)	6 (4%)	4	23
31	59	169/180 (94%)	133 (79%)	35 (21%)	1 (1%)	27	64
32	61	144/148 (97%)	120 (83%)	21 (15%)	3 (2%)	8	34
32	69	144/148 (97%)	122 (85%)	19 (13%)	3 (2%)	8	34
33	15	136/140 (97%)	128 (94%)	7 (5%)	1 (1%)	24	61
33	58	136/140 (97%)	116 (85%)	13 (10%)	7 (5%)	2	14

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
34	25	120/122 (98%)	111 (92%)	9 (8%)	0	100	100
34	68	120/122 (98%)	115 (96%)	4 (3%)	1 (1%)	21	59
35	35	148/150 (99%)	118 (80%)	24 (16%)	6 (4%)	3	18
35	78	148/150 (99%)	117 (79%)	28 (19%)	3 (2%)	8	35
36	45	139/141 (99%)	114 (82%)	20 (14%)	5 (4%)	4	22
36	88	139/141 (99%)	111 (80%)	23 (16%)	5 (4%)	4	22
37	55	115/118 (98%)	103 (90%)	11 (10%)	1 (1%)	19	56
37	98	116/118 (98%)	104 (90%)	10 (9%)	2 (2%)	10	40
38	65	109/112 (97%)	93 (85%)	14 (13%)	2 (2%)	9	38
38	A8	109/112 (97%)	94 (86%)	13 (12%)	2 (2%)	9	38
39	75	135/146 (92%)	113 (84%)	19 (14%)	3 (2%)	7	33
39	B8	135/146 (92%)	117 (87%)	18 (13%)	0	100	100
40	85	115/118 (98%)	106 (92%)	9 (8%)	0	100	100
40	C8	115/118 (98%)	109 (95%)	6 (5%)	0	100	100
41	95	99/101 (98%)	82 (83%)	12 (12%)	5 (5%)	2	14
41	D8	99/101 (98%)	89 (90%)	9 (9%)	1 (1%)	17	53
42	A5	111/113 (98%)	104 (94%)	7 (6%)	0	100	100
42	E8	111/113 (98%)	103 (93%)	8 (7%)	0	100	100
43	B5	91/96 (95%)	86 (94%)	4 (4%)	1 (1%)	16	50
43	F8	90/96 (94%)	84 (93%)	4 (4%)	2 (2%)	7	33
44	C5	102/110 (93%)	72 (71%)	27 (26%)	3 (3%)	5	27
44	G8	102/110 (93%)	84 (82%)	12 (12%)	6 (6%)	2	11
45	D5	177/206 (86%)	145 (82%)	25 (14%)	7 (4%)	3	19
45	H8	173/206 (84%)	134 (78%)	32 (18%)	7 (4%)	3	19
46	E5	75/85 (88%)	73 (97%)	2 (3%)	0	100	100
46	I8	81/85 (95%)	70 (86%)	11 (14%)	0	100	100
47	F5	95/98 (97%)	87 (92%)	7 (7%)	1 (1%)	16	50
47	J8	95/98 (97%)	83 (87%)	10 (10%)	2 (2%)	8	34
48	G5	67/72 (93%)	56 (84%)	11 (16%)	0	100	100
48	K8	64/72 (89%)	61 (95%)	0	3 (5%)	2	16
49	H5	57/60 (95%)	55 (96%)	2 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
49	L8	57/60 (95%)	54 (95%)	3 (5%)	0	100	100
50	I5	61/71 (86%)	33 (54%)	24 (39%)	4 (7%)	1	8
50	M8	64/71 (90%)	45 (70%)	17 (27%)	2 (3%)	4	25
51	J5	57/60 (95%)	48 (84%)	8 (14%)	1 (2%)	9	38
51	N8	57/60 (95%)	49 (86%)	6 (10%)	2 (4%)	4	23
52	K5	43/54 (80%)	28 (65%)	15 (35%)	0	100	100
52	O8	43/54 (80%)	32 (74%)	11 (26%)	0	100	100
53	L5	47/49 (96%)	47 (100%)	0	0	100	100
53	P8	45/49 (92%)	39 (87%)	4 (9%)	2 (4%)	3	17
54	M5	60/65 (92%)	51 (85%)	6 (10%)	3 (5%)	2	15
54	Q8	60/65 (92%)	51 (85%)	7 (12%)	2 (3%)	4	24
All	All	11616/12512 (93%)	10210 (88%)	1239 (11%)	167 (1%)	12	44

5 of 167 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
18	9I	22	VAL
27	11	240	ALA
36	88	87	LYS
43	F8	68	ARG
44	G8	53	PRO

### 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%)	165 (80%)	40 (20%)	1	6
2	1E	205/220 (93%)	150 (73%)	55 (27%)	0	1
3	22	160/188 (85%)	123 (77%)	37 (23%)	1	3
3	2E	159/188 (85%)	135 (85%)	24 (15%)	3	13
4	32	180/181 (99%)	142 (79%)	38 (21%)	1	5

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	3E	180/181 (99%)	146 (81%)	34 (19%)	1	7
5	42	116/123 (94%)	89 (77%)	27 (23%)	1	3
5	4E	116/123 (94%)	89 (77%)	27 (23%)	1	3
6	52	90/90 (100%)	75 (83%)	15 (17%)	2	10
6	5E	90/90 (100%)	75 (83%)	15 (17%)	2	10
7	62	126/127 (99%)	100 (79%)	26 (21%)	1	6
7	6E	126/127 (99%)	98 (78%)	28 (22%)	1	4
8	72	119/119 (100%)	99 (83%)	20 (17%)	2	10
8	7E	119/119 (100%)	97 (82%)	22 (18%)	2	8
9	82	98/99 (99%)	77 (79%)	21 (21%)	1	5
9	8E	98/99 (99%)	78 (80%)	20 (20%)	1	6
10	1A	89/92 (97%)	68 (76%)	21 (24%)	1	3
10	1I	89/92 (97%)	74 (83%)	15 (17%)	2	10
11	2A	88/99 (89%)	73 (83%)	15 (17%)	2	10
11	2I	88/99 (89%)	74 (84%)	14 (16%)	3	12
12	3A	104/109 (95%)	89 (86%)	15 (14%)	3	15
12	3I	104/109 (95%)	87 (84%)	17 (16%)	2	11
13	4A	94/101 (93%)	75 (80%)	19 (20%)	1	6
13	4I	94/101 (93%)	76 (81%)	18 (19%)	1	7
14	5A	49/50 (98%)	42 (86%)	7 (14%)	3	15
14	5I	49/50 (98%)	36 (74%)	13 (26%)	0	1
15	6A	79/80 (99%)	68 (86%)	11 (14%)	4	17
15	6I	79/80 (99%)	66 (84%)	13 (16%)	2	11
16	7A	72/74 (97%)	58 (81%)	14 (19%)	1	6
16	7I	72/74 (97%)	53 (74%)	19 (26%)	0	1
17	8A	95/97 (98%)	79 (83%)	16 (17%)	2	10
17	8I	95/97 (98%)	77 (81%)	18 (19%)	1	7
18	9A	63/77 (82%)	54 (86%)	9 (14%)	3	15
18	9I	63/77 (82%)	54 (86%)	9 (14%)	3	15
19	AA	68/80 (85%)	53 (78%)	15 (22%)	1	4
19	AI	72/80 (90%)	59 (82%)	13 (18%)	2	8

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
20	BA	76/82 (93%)	64 (84%)	12 (16%)	3	12
20	BI	76/82 (93%)	60 (79%)	16 (21%)	1	5
21	1B	20/22 (91%)	16 (80%)	4 (20%)	1	6
21	1F	20/22 (91%)	19 (95%)	1 (5%)	27	61
26	71	111/181 (61%)	103 (93%)	8 (7%)	16	48
26	79	111/181 (61%)	99 (89%)	12 (11%)	7	28
27	11	214/218 (98%)	172 (80%)	42 (20%)	1	6
27	19	214/218 (98%)	176 (82%)	38 (18%)	2	9
28	21	165/166 (99%)	130 (79%)	35 (21%)	1	5
28	29	165/166 (99%)	132 (80%)	33 (20%)	1	6
29	31	161/166 (97%)	123 (76%)	38 (24%)	1	3
29	39	165/166 (99%)	126 (76%)	39 (24%)	1	3
30	41	155/156 (99%)	128 (83%)	27 (17%)	2	9
30	49	155/156 (99%)	116 (75%)	39 (25%)	0	2
31	51	145/148 (98%)	112 (77%)	33 (23%)	1	3
31	59	142/148 (96%)	112 (79%)	30 (21%)	1	5
32	61	122/124 (98%)	97 (80%)	25 (20%)	1	6
32	69	122/124 (98%)	85 (70%)	37 (30%)	0	1
33	15	117/119 (98%)	88 (75%)	29 (25%)	0	2
33	58	117/119 (98%)	84 (72%)	33 (28%)	0	1
34	25	100/100 (100%)	82 (82%)	18 (18%)	2	8
34	68	100/100 (100%)	85 (85%)	15 (15%)	3	14
35	35	116/116 (100%)	78 (67%)	38 (33%)	0	0
35	78	116/116 (100%)	75 (65%)	41 (35%)	0	0
36	45	111/111 (100%)	92 (83%)	19 (17%)	2	10
36	88	111/111 (100%)	88 (79%)	23 (21%)	1	5
37	55	100/101 (99%)	81 (81%)	19 (19%)	1	7
37	98	101/101 (100%)	84 (83%)	17 (17%)	2	10
38	65	87/88 (99%)	57 (66%)	30 (34%)	0	0
38	A8	87/88 (99%)	71 (82%)	16 (18%)	2	8
39	75	117/127 (92%)	89 (76%)	28 (24%)	1	2

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
39	B8	120/127 (94%)	83 (69%)	37 (31%)	0	1
40	85	93/94 (99%)	76 (82%)	17 (18%)	2	8
40	C8	93/94 (99%)	75 (81%)	18 (19%)	1	6
41	95	82/82 (100%)	65 (79%)	17 (21%)	1	5
41	D8	82/82 (100%)	57 (70%)	25 (30%)	0	1
42	A5	92/92 (100%)	71 (77%)	21 (23%)	1	3
42	E8	92/92 (100%)	68 (74%)	24 (26%)	0	1
43	B5	74/78 (95%)	59 (80%)	15 (20%)	1	6
43	F8	74/78 (95%)	57 (77%)	17 (23%)	1	3
44	C5	85/91 (93%)	64 (75%)	21 (25%)	0	2
44	G8	85/91 (93%)	66 (78%)	19 (22%)	1	4
45	D5	158/179 (88%)	122 (77%)	36 (23%)	1	3
45	H8	154/179 (86%)	116 (75%)	38 (25%)	0	2
46	E5	62/67 (92%)	51 (82%)	11 (18%)	2	9
46	I8	66/67 (98%)	52 (79%)	14 (21%)	1	5
47	F5	82/83 (99%)	62 (76%)	20 (24%)	1	2
47	J8	82/83 (99%)	58 (71%)	24 (29%)	0	1
48	G5	64/67 (96%)	51 (80%)	13 (20%)	1	6
48	K8	62/67 (92%)	47 (76%)	15 (24%)	1	2
49	H5	51/52 (98%)	42 (82%)	9 (18%)	2	9
49	L8	51/52 (98%)	41 (80%)	10 (20%)	1	6
50	I5	57/63 (90%)	44 (77%)	13 (23%)	1	3
50	M8	59/63 (94%)	51 (86%)	8 (14%)	4	17
51	J5	51/52 (98%)	39 (76%)	12 (24%)	1	3
51	N8	51/52 (98%)	35 (69%)	16 (31%)	0	0
52	K5	44/52 (85%)	27 (61%)	17 (39%)	0	0
52	O8	44/52 (85%)	33 (75%)	11 (25%)	0	2
53	L5	42/42 (100%)	32 (76%)	10 (24%)	1	2
53	P8	40/42 (95%)	32 (80%)	8 (20%)	1	6
54	M5	52/55 (94%)	39 (75%)	13 (25%)	0	2
54	Q8	50/55 (91%)	30 (60%)	20 (40%)	0	0

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	9806/10360 (95%)	7722 (79%)	2084 (21%)	<b>1</b> <b>5</b>

5 of 2084 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
47	J8	46	LEU
5	42	24	ARG
44	C5	89	PHE
48	K8	53	LEU
2	12	48	MET

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

Mol	Chain	Res	Type
50	M8	60	GLN
4	32	119	GLN
29	39	203	GLN
45	H8	54	HIS
40	85	81	HIS

### 5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	13	1492/1522 (98%)	352 (23%)	26 (1%)
1	1G	1502/1522 (98%)	370 (24%)	39 (2%)
22	2K	77/85 (90%)	33 (42%)	5 (6%)
22	2L	74/85 (87%)	25 (33%)	8 (10%)
22	3K	81/85 (95%)	23 (28%)	3 (3%)
22	3L	82/85 (96%)	21 (25%)	3 (3%)
23	4K	16/30 (53%)	7 (43%)	3 (18%)
23	4L	7/30 (23%)	4 (57%)	1 (14%)
24	14	2908/2917 (99%)	685 (23%)	48 (1%)
24	1H	2911/2917 (99%)	698 (23%)	56 (1%)
25	16	121/122 (99%)	38 (31%)	0
25	1J	121/122 (99%)	34 (28%)	0
All	All	9392/9522 (98%)	2290 (24%)	192 (2%)

5 of 2290 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	13	5	U
1	13	6	G
1	13	7	G
1	13	9	G
1	13	32	A

5 of 192 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
24	1H	2422	A
1	1G	632	A
24	14	2166	G
24	1H	2566	A
1	1G	115	G

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

28 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$
22	OMG	2K	17	22	18,26,27	5.79	6 (33%)	22,38,41	5.19	8 (36%)
22	QUO	2K	35	22,23	27,35,36	5.54	11 (40%)	31,52,55	5.30	11 (35%)
22	MIA	2K	38	22	22,31,32	2.17	3 (13%)	26,44,47	3.81	9 (34%)
22	PSU	2K	40	22	16,21,22	0.95	1 (6%)	20,30,33	3.09	5 (25%)
22	5MU	2K	63	22	13,22,23	1.89	3 (23%)	14,32,35	1.81	2 (14%)
22	PSU	2K	64	55,22	16,21,22	1.02	1 (6%)	20,30,33	3.14	8 (40%)
22	4SU	2K	8	22	13,21,22	3.58	2 (15%)	14,30,33	0.85	0
22	OMG	2L	17	22	18,26,27	5.64	6 (33%)	22,38,41	5.34	7 (31%)
22	QUO	2L	35	22,23	27,35,36	5.73	9 (33%)	31,52,55	5.53	16 (51%)
22	MIA	2L	38	22	22,31,32	2.09	2 (9%)	26,44,47	2.38	8 (30%)
22	PSU	2L	40	22	16,21,22	1.29	2 (12%)	20,30,33	3.42	5 (25%)
22	5MU	2L	63	22	13,22,23	1.86	2 (15%)	14,32,35	1.78	2 (14%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
22	PSU	2L	64	22	16,21,22	1.31	2 (12%)	20,30,33	3.68	7 (35%)
22	4SU	2L	8	22	13,21,22	3.11	3 (23%)	14,30,33	1.90	3 (21%)
22	OMG	3K	17	22	18,26,27	5.95	6 (33%)	22,38,41	5.49	7 (31%)
22	QUO	3K	35	22	27,35,36	5.79	9 (33%)	31,52,55	5.85	13 (41%)
22	MIA	3K	38	22	22,31,32	2.22	3 (13%)	26,44,47	3.03	11 (42%)
22	PSU	3K	40	22	16,21,22	1.07	1 (6%)	20,30,33	3.35	5 (25%)
22	5MU	3K	63	22	13,22,23	1.80	2 (15%)	14,32,35	1.90	2 (14%)
22	PSU	3K	64	22	16,21,22	1.09	1 (6%)	20,30,33	3.31	8 (40%)
22	4SU	3K	8	22	13,21,22	3.23	2 (15%)	14,30,33	0.97	1 (7%)
22	OMG	3L	17	22	18,26,27	5.88	7 (38%)	22,38,41	5.20	7 (31%)
22	QUO	3L	35	22	27,35,36	5.66	10 (37%)	31,52,55	5.29	15 (48%)
22	MIA	3L	38	22	22,31,32	2.19	3 (13%)	26,44,47	3.06	11 (42%)
22	PSU	3L	40	22	16,21,22	1.20	1 (6%)	20,30,33	3.26	7 (35%)
22	5MU	3L	63	22	13,22,23	1.85	2 (15%)	14,32,35	1.87	2 (14%)
22	PSU	3L	64	22	16,21,22	1.19	2 (12%)	20,30,33	3.56	7 (35%)
22	4SU	3L	8	55,22	13,21,22	3.49	2 (15%)	14,30,33	1.44	2 (14%)

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
22	OMG	2K	17	22	-	3/5/27/28	0/3/3/3
22	QUO	2K	35	22,23	-	2/6/43/44	0/4/4/4
22	MIA	2K	38	22	-	5/11/33/34	0/3/3/3
22	PSU	2K	40	22	-	0/7/25/26	0/2/2/2
22	5MU	2K	63	22	-	3/3/25/26	0/2/2/2
22	PSU	2K	64	55,22	-	5/7/25/26	0/2/2/2
22	4SU	2K	8	22	-	0/3/25/26	0/2/2/2
22	OMG	2L	17	22	-	2/5/27/28	0/3/3/3
22	QUO	2L	35	22,23	-	0/6/43/44	0/4/4/4
22	MIA	2L	38	22	-	3/11/33/34	0/3/3/3
22	PSU	2L	40	22	-	0/7/25/26	0/2/2/2
22	5MU	2L	63	22	-	3/3/25/26	0/2/2/2
22	PSU	2L	64	22	-	0/7/25/26	0/2/2/2
22	4SU	2L	8	22	-	0/3/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	OMG	3K	17	22	-	2/5/27/28	0/3/3/3
22	QUO	3K	35	22	-	3/6/43/44	0/4/4/4
22	MIA	3K	38	22	-	8/11/33/34	0/3/3/3
22	PSU	3K	40	22	-	0/7/25/26	0/2/2/2
22	5MU	3K	63	22	-	0/3/25/26	0/2/2/2
22	PSU	3K	64	22	-	0/7/25/26	0/2/2/2
22	4SU	3K	8	22	-	0/3/25/26	0/2/2/2
22	OMG	3L	17	22	-	3/5/27/28	0/3/3/3
22	QUO	3L	35	22	-	3/6/43/44	0/4/4/4
22	MIA	3L	38	22	-	8/11/33/34	0/3/3/3
22	PSU	3L	40	22	-	0/7/25/26	0/2/2/2
22	5MU	3L	63	22	-	0/3/25/26	0/2/2/2
22	PSU	3L	64	22	-	2/7/25/26	0/2/2/2
22	4SU	3L	8	55,22	-	0/3/25/26	0/2/2/2

The worst 5 of 104 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	2L	35	QUO	C4-N3	22.81	1.71	1.35
22	3L	35	QUO	C4-N3	22.74	1.71	1.35
22	3K	35	QUO	C4-N3	22.69	1.71	1.35
22	2K	35	QUO	C4-N3	21.04	1.68	1.35
22	3K	17	OMG	C4-N3	16.35	1.61	1.35

The worst 5 of 189 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	3K	35	QUO	C6-C5-C4	24.05	128.44	115.04
22	3L	35	QUO	C6-C5-C4	23.56	128.16	115.04
22	2K	35	QUO	C6-C5-C4	23.00	127.85	115.04
22	2L	35	QUO	C6-C5-C4	22.88	127.79	115.04
22	3K	17	OMG	C1'-N9-C4	16.10	154.44	126.64

There are no chirality outliers.

5 of 55 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
22	2L	17	OMG	C4'-C5'-O5'-P
22	2L	38	MIA	N1-C2-S10-C11
22	2L	38	MIA	N3-C2-S10-C11

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Mol	Chain	Res	Type	Atoms
22	2L	38	MIA	C12-C13-C14-C15
22	3K	35	QUO	O4'-C4'-C5'-O5'

There are no ring outliers.

22 monomers are involved in 45 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
22	2K	17	OMG	6	0
22	2K	35	QUO	2	0
22	2K	38	MIA	1	0
22	2K	64	PSU	4	0
22	2L	17	OMG	2	0
22	2L	35	QUO	5	0
22	2L	38	MIA	1	0
22	2L	63	5MU	4	0
22	2L	64	PSU	1	0
22	2L	8	4SU	3	0
22	3K	17	OMG	1	0
22	3K	35	QUO	2	0
22	3K	38	MIA	5	0
22	3K	63	5MU	1	0
22	3K	64	PSU	1	0
22	3K	8	4SU	2	0
22	3L	17	OMG	2	0
22	3L	35	QUO	3	0
22	3L	38	MIA	1	0
22	3L	63	5MU	1	0
22	3L	64	PSU	1	0
22	3L	8	4SU	1	0

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 1351 ligands modelled in this entry, 1351 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

There are no such residues in this entry.

## 5.8 Polymer linkage issues

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	13	1499/1522 (98%)	-0.56	1 (0%) 95 91	63, 117, 206, 445	0
1	1G	1503/1522 (98%)	-0.53	5 (0%) 93 88	68, 115, 190, 453	0
2	12	237/256 (92%)	0.90	41 (17%) 1 1	127, 170, 220, 245	0
2	1E	237/256 (92%)	0.72	29 (12%) 4 2	120, 163, 212, 246	0
3	22	206/239 (86%)	1.18	44 (21%) 1 0	120, 147, 179, 189	0
3	2E	205/239 (85%)	0.50	16 (7%) 13 5	111, 138, 196, 212	0
4	32	208/209 (99%)	0.84	26 (12%) 4 2	94, 119, 152, 172	0
4	3E	208/209 (99%)	-0.09	3 (1%) 75 56	87, 119, 147, 176	0
5	42	151/162 (93%)	0.21	2 (1%) 77 59	94, 113, 140, 210	0
5	4E	151/162 (93%)	0.02	0 100 100	87, 114, 139, 206	0
6	52	101/101 (100%)	-0.22	1 (0%) 82 67	85, 106, 127, 146	0
6	5E	101/101 (100%)	0.73	5 (4%) 29 13	95, 122, 138, 154	0
7	62	155/156 (99%)	-0.07	4 (2%) 56 32	111, 129, 145, 152	0
7	6E	155/156 (99%)	0.61	16 (10%) 6 2	106, 137, 161, 172	0
8	72	138/138 (100%)	0.32	3 (2%) 62 40	98, 117, 133, 158	0
8	7E	138/138 (100%)	0.07	1 (0%) 87 75	101, 121, 136, 150	0
9	82	127/128 (99%)	0.15	4 (3%) 49 26	111, 160, 187, 206	0
9	8E	127/128 (99%)	0.59	15 (11%) 4 2	104, 155, 177, 185	0
10	1A	99/105 (94%)	1.21	23 (23%) 0 0	121, 161, 193, 210	0
10	1I	99/105 (94%)	0.90	15 (15%) 2 1	105, 164, 206, 215	0
11	2A	116/129 (89%)	-0.05	1 (0%) 84 70	81, 110, 134, 164	0
11	2I	116/129 (89%)	1.12	22 (18%) 1 0	79, 114, 153, 224	0
12	3A	125/132 (94%)	0.45	8 (6%) 19 7	86, 102, 141, 189	0
12	3I	125/132 (94%)	-0.29	1 (0%) 86 72	79, 92, 125, 247	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
13	4A	117/126 (92%)	0.09	6 (5%) 28 12	122, 164, 193, 228	0
13	4I	116/126 (92%)	0.81	17 (14%) 2 1	117, 165, 186, 205	0
14	5A	60/61 (98%)	1.29	20 (33%) 0 0	131, 150, 178, 185	0
14	5I	60/61 (98%)	-0.07	1 (1%) 70 48	112, 128, 149, 170	0
15	6A	88/89 (98%)	0.11	0 100 100	84, 115, 134, 141	0
15	6I	88/89 (98%)	-0.11	0 100 100	92, 112, 133, 151	0
16	7A	84/88 (95%)	0.44	5 (5%) 22 9	94, 108, 132, 195	0
16	7I	84/88 (95%)	-0.43	0 100 100	107, 127, 154, 194	0
17	8A	100/105 (95%)	0.13	3 (3%) 50 26	91, 108, 126, 176	0
17	8I	100/105 (95%)	-0.46	0 100 100	97, 119, 133, 142	0
18	9A	72/88 (81%)	0.45	5 (6%) 17 6	91, 112, 166, 208	0
18	9I	72/88 (81%)	1.46	16 (22%) 0 0	100, 121, 150, 227	0
19	AA	79/93 (84%)	1.43	26 (32%) 0 0	144, 187, 220, 228	0
19	AI	83/93 (89%)	0.28	7 (8%) 11 4	142, 168, 204, 221	0
20	BA	99/106 (93%)	0.54	6 (6%) 21 9	86, 114, 153, 193	0
20	BI	99/106 (93%)	-0.23	1 (1%) 82 67	112, 138, 188, 193	0
21	1B	25/27 (92%)	0.20	1 (4%) 38 18	117, 140, 171, 190	0
21	1F	25/27 (92%)	0.37	0 100 100	125, 139, 170, 187	0
22	2K	75/85 (88%)	-0.39	0 100 100	74, 113, 195, 247	0
22	2L	71/85 (83%)	-0.59	0 100 100	73, 115, 176, 193	0
22	3K	78/85 (91%)	-0.03	6 (7%) 13 5	85, 189, 296, 344	0
22	3L	78/85 (91%)	-0.80	0 100 100	79, 195, 286, 321	0
23	4K	16/30 (53%)	-0.18	0 100 100	82, 126, 168, 170	0
23	4L	8/30 (26%)	-0.37	0 100 100	93, 107, 190, 231	0
24	14	2909/2917 (99%)	-0.38	39 (1%) 77 59	53, 84, 260, 407	0
24	1H	2912/2917 (99%)	-0.24	32 (1%) 80 64	48, 80, 247, 440	0
25	16	122/122 (100%)	-0.32	1 (0%) 86 72	85, 118, 144, 247	0
25	1J	122/122 (100%)	-0.70	0 100 100	86, 123, 143, 217	0
26	71	135/229 (58%)	3.72	103 (76%) 0 0	156, 219, 251, 258	0
26	79	135/229 (58%)	1.35	41 (30%) 0 0	152, 228, 253, 265	0
27	11	272/276 (98%)	0.06	0 100 100	48, 69, 90, 122	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
27	19	273/276 (98%)	-0.40	0 100 100	50, 73, 91, 122	0
28	21	205/206 (99%)	0.32	14 (6%) 17 7	54, 94, 152, 211	0
28	29	205/206 (99%)	-0.16	2 (0%) 82 67	57, 88, 164, 238	0
29	31	202/210 (96%)	0.23	6 (2%) 50 26	47, 81, 123, 148	0
29	39	208/210 (99%)	0.84	26 (12%) 4 2	60, 98, 174, 203	0
30	41	181/182 (99%)	2.25	81 (44%) 0 0	123, 154, 197, 210	0
30	49	181/182 (99%)	0.44	17 (9%) 8 3	120, 146, 190, 208	0
31	51	174/180 (96%)	0.09	2 (1%) 80 64	90, 117, 139, 161	0
31	59	171/180 (95%)	1.55	52 (30%) 0 0	141, 208, 248, 354	0
32	61	146/148 (98%)	1.05	22 (15%) 2 1	84, 128, 153, 169	0
32	69	146/148 (98%)	-0.23	2 (1%) 75 56	81, 137, 164, 177	0
33	15	138/140 (98%)	0.21	4 (2%) 51 28	72, 101, 143, 174	0
33	58	138/140 (98%)	0.36	7 (5%) 28 12	73, 98, 154, 181	0
34	25	122/122 (100%)	0.04	0 100 100	64, 82, 100, 110	0
34	68	122/122 (100%)	-0.18	0 100 100	58, 85, 103, 114	0
35	35	150/150 (100%)	0.68	18 (12%) 4 2	61, 105, 144, 203	0
35	78	150/150 (100%)	0.33	5 (3%) 46 24	55, 91, 117, 251	0
36	45	141/141 (100%)	0.13	7 (4%) 29 13	67, 104, 131, 154	0
36	88	141/141 (100%)	0.36	8 (5%) 24 10	64, 99, 134, 181	0
37	55	117/118 (99%)	-0.21	0 100 100	62, 82, 99, 121	0
37	98	118/118 (100%)	0.01	1 (0%) 86 72	68, 88, 107, 125	0
38	65	111/112 (99%)	0.17	4 (3%) 42 21	93, 119, 148, 171	0
38	A8	111/112 (99%)	1.79	46 (41%) 0 0	97, 119, 163, 218	0
39	75	137/146 (93%)	-0.22	2 (1%) 73 54	75, 91, 161, 227	0
39	B8	137/146 (93%)	-0.24	4 (2%) 51 28	84, 102, 165, 218	0
40	85	117/118 (99%)	0.08	1 (0%) 84 70	65, 95, 135, 167	0
40	C8	117/118 (99%)	0.10	2 (1%) 70 48	57, 83, 130, 183	0
41	95	101/101 (100%)	1.18	21 (20%) 1 0	67, 124, 148, 194	0
41	D8	101/101 (100%)	0.58	7 (6%) 17 6	58, 106, 160, 237	0
42	A5	113/113 (100%)	0.15	2 (1%) 68 46	63, 77, 110, 206	0
42	E8	113/113 (100%)	0.14	2 (1%) 68 46	61, 77, 109, 231	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
43	B5	93/96 (96%)	0.28	4 (4%) 35 17	73, 86, 119, 127	0
43	F8	92/96 (95%)	0.47	6 (6%) 19 7	64, 74, 98, 112	0
44	C5	104/110 (94%)	1.56	27 (25%) 0 0	89, 130, 221, 252	0
44	G8	104/110 (94%)	0.46	7 (6%) 18 7	71, 96, 149, 186	0
45	D5	179/206 (86%)	1.68	57 (31%) 0 0	111, 160, 262, 335	0
45	H8	175/206 (84%)	1.47	52 (29%) 0 0	105, 160, 274, 301	0
46	E5	77/85 (90%)	0.15	2 (2%) 56 32	74, 89, 109, 178	0
46	I8	83/85 (97%)	0.52	5 (6%) 22 9	70, 90, 112, 158	0
47	F5	97/98 (98%)	-0.19	2 (2%) 63 42	60, 83, 157, 204	0
47	J8	97/98 (98%)	0.82	9 (9%) 8 3	57, 82, 168, 218	0
48	G5	69/72 (95%)	0.68	5 (7%) 15 6	84, 109, 145, 187	0
48	K8	66/72 (91%)	0.32	1 (1%) 73 54	63, 82, 115, 177	0
49	H5	59/60 (98%)	0.49	3 (5%) 28 12	79, 97, 156, 188	0
49	L8	59/60 (98%)	0.35	3 (5%) 28 12	73, 91, 138, 151	0
50	I5	63/71 (88%)	2.56	28 (44%) 0 0	161, 233, 263, 283	0
50	M8	66/71 (92%)	4.31	49 (74%) 0 0	152, 233, 267, 285	0
51	J5	59/60 (98%)	0.14	5 (8%) 11 4	58, 87, 207, 244	0
51	N8	59/60 (98%)	0.84	9 (15%) 2 1	52, 92, 216, 240	0
52	K5	45/54 (83%)	3.25	31 (68%) 0 0	161, 210, 253, 272	0
52	O8	45/54 (83%)	6.27	44 (97%) 0 0	164, 213, 245, 256	0
53	L5	49/49 (100%)	-0.30	0 100 100	56, 61, 106, 147	0
53	P8	47/49 (95%)	-0.32	0 100 100	48, 54, 72, 121	0
54	M5	62/65 (95%)	-0.09	0 100 100	67, 77, 100, 127	0
54	Q8	62/65 (95%)	-0.06	0 100 100	62, 80, 108, 129	0
All	All	21209/22034 (96%)	0.13	1336 (6%) 20 8	47, 108, 216, 453	0

The worst 5 of 1336 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
31	59	96	ALA	26.6
26	71	1	PRO	21.7
24	14	654(K)	C	21.5
50	I5	42	PHE	18.1
24	14	654(L)	G	14.6

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

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
22	PSU	3L	64	20/21	0.67	0.15	180,200,211,213	0
22	PSU	3K	64	20/21	0.72	0.26	182,190,202,202	0
22	4SU	3L	8	20/21	0.73	0.14	184,194,207,207	0
22	PSU	2L	64	20/21	0.74	0.13	138,148,163,166	0
22	OMG	3K	17	24/25	0.75	0.18	194,212,234,239	0
22	4SU	3K	8	20/21	0.83	0.12	186,202,212,214	0
22	OMG	2L	17	24/25	0.84	0.15	136,152,154,155	0
22	OMG	3L	17	24/25	0.85	0.12	200,216,227,230	0
22	PSU	2K	64	20/21	0.85	0.15	133,144,150,155	0
22	5MU	3L	63	21/22	0.85	0.13	174,186,190,192	0
22	5MU	3K	63	21/22	0.86	0.19	176,183,187,190	0
22	OMG	2K	17	24/25	0.87	0.14	142,148,151,151	0
22	4SU	2K	8	20/21	0.91	0.13	106,112,119,121	0
22	PSU	3K	40	20/21	0.91	0.13	118,124,129,130	0
22	5MU	2K	63	21/22	0.91	0.12	135,139,149,156	0
22	5MU	2L	63	21/22	0.92	0.10	141,149,156,167	0
22	4SU	2L	8	20/21	0.92	0.11	112,122,128,139	0
22	QUO	3L	35	32/33	0.93	0.15	105,114,128,132	0
22	QUO	2L	35	32/33	0.94	0.18	91,112,118,124	0
22	QUO	3K	35	32/33	0.94	0.18	108,114,124,127	0
22	PSU	2L	40	20/21	0.94	0.15	89,100,105,105	0
22	MIA	3K	38	29/30	0.94	0.18	114,122,132,135	0
22	PSU	3L	40	20/21	0.94	0.12	107,122,124,127	0
22	MIA	3L	38	29/30	0.95	0.17	118,123,131,133	0
22	QUO	2K	35	32/33	0.95	0.18	84,96,115,117	6
22	MIA	2L	38	29/30	0.95	0.18	92,101,113,119	0
22	PSU	2K	40	20/21	0.96	0.17	83,91,99,105	0
22	MIA	2K	38	29/30	0.96	0.19	82,94,106,112	0

## 6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 6.4 Ligands ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
55	MG	16	208	1/1	0.20	0.34	113,113,113,113	0
55	MG	1H	3220	1/1	0.20	0.27	92,92,92,92	0
55	MG	1H	3240	1/1	0.21	0.32	92,92,92,92	0
55	MG	1H	3301	1/1	0.24	0.37	79,79,79,79	0
55	MG	1H	3364	1/1	0.28	0.34	103,103,103,103	0
55	MG	1G	1685	1/1	0.30	0.26	116,116,116,116	0
55	MG	1H	3360	1/1	0.30	0.34	167,167,167,167	0
55	MG	1H	3379	1/1	0.33	0.13	245,245,245,245	0
55	MG	42	201	1/1	0.34	0.35	101,101,101,101	0
55	MG	14	3335	1/1	0.34	0.24	90,90,90,90	0
56	ZN	G8	202	1/1	0.36	0.32	203,203,203,203	0
55	MG	13	1689	1/1	0.37	0.45	116,116,116,116	0
55	MG	14	3329	1/1	0.39	0.27	101,101,101,101	0
55	MG	13	1700	1/1	0.40	0.34	97,97,97,97	0
55	MG	14	3287	1/1	0.41	0.32	98,98,98,98	0
55	MG	14	3258	1/1	0.41	0.32	70,70,70,70	0
55	MG	14	3331	1/1	0.42	0.33	138,138,138,138	0
55	MG	14	3132	1/1	0.42	0.29	120,120,120,120	0
55	MG	14	3367	1/1	0.44	0.17	72,72,72,72	0
55	MG	13	1656	1/1	0.44	0.25	120,120,120,120	0
55	MG	1H	3346	1/1	0.45	0.24	113,113,113,113	0
55	MG	1G	1702	1/1	0.47	0.21	95,95,95,95	0
55	MG	14	3159	1/1	0.47	0.38	85,85,85,85	0
55	MG	13	1699	1/1	0.49	0.46	109,109,109,109	0
55	MG	1H	3186	1/1	0.49	0.23	70,70,70,70	0
55	MG	1H	3312	1/1	0.50	0.28	81,81,81,81	0
55	MG	1G	1613	1/1	0.50	0.08	92,92,92,92	0
55	MG	1H	3396	1/1	0.51	0.25	104,104,104,104	0
55	MG	13	1684	1/1	0.51	0.30	94,94,94,94	0
55	MG	1H	3405	1/1	0.52	0.14	74,74,74,74	0
55	MG	1H	3209	1/1	0.54	0.49	99,99,99,99	0
55	MG	14	3301	1/1	0.54	0.40	82,82,82,82	0
55	MG	1G	1721	1/1	0.54	0.55	129,129,129,129	0
55	MG	14	3113	1/1	0.54	0.35	97,97,97,97	0
55	MG	14	3190	1/1	0.54	0.36	95,95,95,95	0
55	MG	14	3300	1/1	0.55	0.17	83,83,83,83	0
55	MG	1H	3190	1/1	0.55	0.58	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	3407	1/1	0.55	0.37	89,89,89,89	0
55	MG	13	1621	1/1	0.55	0.27	87,87,87,87	0
55	MG	1H	3377	1/1	0.56	0.35	81,81,81,81	0
55	MG	14	3318	1/1	0.56	0.13	80,80,80,80	0
55	MG	1H	3386	1/1	0.57	0.30	66,66,66,66	0
55	MG	14	3373	1/1	0.57	0.23	98,98,98,98	0
55	MG	1H	3286	1/1	0.57	0.33	82,82,82,82	0
55	MG	13	1688	1/1	0.58	0.49	91,91,91,91	0
55	MG	1G	1669	1/1	0.58	0.25	86,86,86,86	0
55	MG	13	1706	1/1	0.58	0.44	93,93,93,93	0
55	MG	14	3127	1/1	0.58	0.39	84,84,84,84	0
55	MG	14	3082	1/1	0.58	0.15	64,64,64,64	0
55	MG	16	204	1/1	0.58	0.19	99,99,99,99	0
55	MG	16	203	1/1	0.59	0.24	92,92,92,92	0
55	MG	1G	1691	1/1	0.60	0.27	132,132,132,132	0
55	MG	1H	3162	1/1	0.60	0.21	94,94,94,94	0
55	MG	3E	301	1/1	0.60	0.11	156,156,156,156	0
55	MG	14	3174	1/1	0.60	0.36	107,107,107,107	0
55	MG	1H	3282	1/1	0.60	0.44	90,90,90,90	0
55	MG	1G	1701	1/1	0.60	0.13	93,93,93,93	0
55	MG	1G	1620	1/1	0.60	0.41	96,96,96,96	0
55	MG	4K	101	1/1	0.61	0.29	111,111,111,111	0
55	MG	1H	3121	1/1	0.61	0.25	98,98,98,98	0
55	MG	14	3038	1/1	0.61	0.25	86,86,86,86	0
55	MG	1G	1739	1/1	0.61	0.09	154,154,154,154	0
55	MG	13	1738	1/1	0.62	0.08	138,138,138,138	0
55	MG	1H	3518	1/1	0.62	0.17	135,135,135,135	0
55	MG	1H	3387	1/1	0.62	0.31	75,75,75,75	0
55	MG	1H	3398	1/1	0.63	0.17	106,106,106,106	0
55	MG	1H	3315	1/1	0.63	0.24	88,88,88,88	0
55	MG	16	211	1/1	0.63	0.23	98,98,98,98	0
55	MG	1H	3218	1/1	0.64	0.51	82,82,82,82	0
55	MG	14	3292	1/1	0.64	0.27	90,90,90,90	0
55	MG	1H	3511	1/1	0.64	0.07	119,119,119,119	0
55	MG	1G	1703	1/1	0.64	0.28	99,99,99,99	0
55	MG	1G	1718	1/1	0.64	0.34	118,118,118,118	0
55	MG	14	3368	1/1	0.64	0.23	76,76,76,76	0
55	MG	13	1693	1/1	0.64	0.38	100,100,100,100	0
55	MG	13	1610	1/1	0.64	0.33	115,115,115,115	0
55	MG	1H	3203	1/1	0.64	0.46	99,99,99,99	0
55	MG	1G	1726	1/1	0.64	0.44	124,124,124,124	0
55	MG	1G	1653	1/1	0.65	0.36	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	29	303	1/1	0.65	0.15	74,74,74,74	0
55	MG	1H	3370	1/1	0.65	0.33	73,73,73,73	0
55	MG	1H	3234	1/1	0.65	0.31	88,88,88,88	0
55	MG	14	3291	1/1	0.65	0.21	82,82,82,82	0
55	MG	1H	3027	1/1	0.66	0.34	86,86,86,86	0
55	MG	1H	3342	1/1	0.66	0.40	89,89,89,89	0
55	MG	14	3303	1/1	0.66	0.39	99,99,99,99	0
55	MG	1H	3375	1/1	0.67	0.36	85,85,85,85	0
55	MG	1H	3307	1/1	0.67	0.24	83,83,83,83	0
55	MG	2K	104	1/1	0.67	0.47	101,101,101,101	0
55	MG	13	1695	1/1	0.67	0.26	90,90,90,90	0
55	MG	1G	1699	1/1	0.67	0.46	101,101,101,101	0
55	MG	1G	1719	1/1	0.67	0.20	104,104,104,104	0
55	MG	1H	3043	1/1	0.67	0.26	92,92,92,92	0
55	MG	1H	3355	1/1	0.68	0.58	107,107,107,107	0
55	MG	1H	3336	1/1	0.68	0.43	83,83,83,83	0
55	MG	14	3282	1/1	0.68	0.23	87,87,87,87	0
55	MG	14	3309	1/1	0.68	0.34	84,84,84,84	0
55	MG	13	1644	1/1	0.68	0.44	116,116,116,116	0
55	MG	14	3128	1/1	0.69	0.43	76,76,76,76	0
55	MG	1H	3168	1/1	0.69	0.35	85,85,85,85	0
55	MG	1H	3330	1/1	0.69	0.51	90,90,90,90	0
55	MG	14	3286	1/1	0.69	0.20	100,100,100,100	0
55	MG	14	3255	1/1	0.69	0.36	92,92,92,92	0
55	MG	1H	3350	1/1	0.69	0.51	89,89,89,89	0
55	MG	13	1647	1/1	0.69	0.15	110,110,110,110	0
55	MG	14	3281	1/1	0.70	0.38	82,82,82,82	0
55	MG	14	3345	1/1	0.70	0.28	78,78,78,78	0
55	MG	14	3289	1/1	0.70	0.16	175,175,175,175	0
55	MG	1H	3185	1/1	0.70	0.53	91,91,91,91	0
55	MG	1G	1663	1/1	0.70	0.29	81,81,81,81	0
55	MG	13	1668	1/1	0.70	0.42	102,102,102,102	0
55	MG	13	1608	1/1	0.70	0.32	101,101,101,101	0
55	MG	13	1712	1/1	0.70	0.35	123,123,123,123	0
55	MG	1H	3283	1/1	0.70	0.41	104,104,104,104	0
56	ZN	C5	202	1/1	0.70	0.31	219,219,219,219	0
55	MG	13	1635	1/1	0.71	0.31	95,95,95,95	0
55	MG	1H	3352	1/1	0.71	0.35	97,97,97,97	0
55	MG	1H	3215	1/1	0.71	0.52	91,91,91,91	0
55	MG	1G	1639	1/1	0.71	0.46	97,97,97,97	0
55	MG	1H	3259	1/1	0.71	0.33	93,93,93,93	0
55	MG	3L	101	1/1	0.71	0.18	180,180,180,180	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	0.71	0.21	81,81,81,81	0
55	MG	1G	1638	1/1	0.71	0.43	88,88,88,88	0
55	MG	13	1611	1/1	0.71	0.26	83,83,83,83	0
55	MG	1H	3178	1/1	0.71	0.25	77,77,77,77	0
55	MG	1H	3120	1/1	0.71	0.23	69,69,69,69	0
55	MG	1G	1692	1/1	0.71	0.33	120,120,120,120	0
55	MG	1H	3232	1/1	0.72	0.24	103,103,103,103	0
55	MG	5E	201	1/1	0.72	0.20	106,106,106,106	0
55	MG	1H	3385	1/1	0.72	0.21	97,97,97,97	0
55	MG	1G	1741	1/1	0.72	0.09	112,112,112,112	0
55	MG	1H	3180	1/1	0.72	0.19	86,86,86,86	0
55	MG	1H	3039	1/1	0.72	0.22	68,68,68,68	0
55	MG	1G	1722	1/1	0.72	0.15	91,91,91,91	0
55	MG	14	3169	1/1	0.72	0.31	100,100,100,100	0
55	MG	14	3191	1/1	0.72	0.33	92,92,92,92	0
55	MG	14	3161	1/1	0.72	0.37	89,89,89,89	0
55	MG	13	1698	1/1	0.72	0.35	78,78,78,78	0
55	MG	14	3261	1/1	0.72	0.54	105,105,105,105	0
55	MG	14	3154	1/1	0.72	0.33	87,87,87,87	0
55	MG	1H	3167	1/1	0.72	0.25	66,66,66,66	0
55	MG	1G	1705	1/1	0.73	0.15	96,96,96,96	0
55	MG	2L	102	1/1	0.73	0.32	102,102,102,102	0
55	MG	14	3269	1/1	0.73	0.20	68,68,68,68	0
55	MG	14	3312	1/1	0.73	0.35	81,81,81,81	0
55	MG	1G	1686	1/1	0.73	0.11	95,95,95,95	0
55	MG	1H	3465	1/1	0.73	0.08	87,87,87,87	0
55	MG	29	304	1/1	0.73	0.45	89,89,89,89	0
55	MG	39	301	1/1	0.73	0.17	83,83,83,83	0
55	MG	1G	1636	1/1	0.73	0.32	80,80,80,80	0
55	MG	1H	3221	1/1	0.73	0.27	108,108,108,108	0
55	MG	14	3311	1/1	0.74	0.27	87,87,87,87	0
55	MG	13	1737	1/1	0.74	0.07	111,111,111,111	0
55	MG	14	3306	1/1	0.74	0.14	74,74,74,74	0
55	MG	14	3353	1/1	0.74	0.28	84,84,84,84	0
55	MG	14	3436	1/1	0.74	0.14	107,107,107,107	0
55	MG	1H	3366	1/1	0.74	0.29	84,84,84,84	0
55	MG	1H	3196	1/1	0.74	0.41	80,80,80,80	0
55	MG	16	209	1/1	0.74	0.25	80,80,80,80	0
55	MG	14	3283	1/1	0.74	0.32	87,87,87,87	0
55	MG	1H	3231	1/1	0.74	0.53	88,88,88,88	0
55	MG	13	1643	1/1	0.74	0.51	86,86,86,86	0
55	MG	14	3263	1/1	0.74	0.13	72,72,72,72	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
55	MG	13	1645	1/1	0.74	0.49	98,98,98,98	0
55	MG	52	201	1/1	0.74	0.17	84,84,84,84	0
55	MG	1H	3340	1/1	0.75	0.34	77,77,77,77	0
55	MG	4A	201	1/1	0.75	0.34	115,115,115,115	0
55	MG	14	3277	1/1	0.75	0.31	78,78,78,78	0
55	MG	1H	3253	1/1	0.75	0.30	71,71,71,71	0
55	MG	1H	3119	1/1	0.75	0.35	77,77,77,77	0
55	MG	13	1617	1/1	0.75	0.32	122,122,122,122	0
55	MG	14	3325	1/1	0.75	0.36	78,78,78,78	0
55	MG	1G	1683	1/1	0.75	0.31	103,103,103,103	0
55	MG	14	3119	1/1	0.75	0.33	70,70,70,70	0
55	MG	14	3186	1/1	0.75	0.33	113,113,113,113	0
55	MG	11	302	1/1	0.76	0.23	85,85,85,85	0
55	MG	14	3166	1/1	0.76	0.15	71,71,71,71	0
55	MG	1H	3193	1/1	0.76	0.39	77,77,77,77	0
55	MG	1G	1679	1/1	0.76	0.30	97,97,97,97	0
55	MG	14	3354	1/1	0.76	0.31	134,134,134,134	0
55	MG	14	3096	1/1	0.76	0.36	94,94,94,94	0
55	MG	1G	1694	1/1	0.76	0.18	118,118,118,118	0
55	MG	1G	1629	1/1	0.76	0.36	86,86,86,86	0
55	MG	14	3235	1/1	0.76	0.14	63,63,63,63	0
55	MG	14	3182	1/1	0.76	0.17	77,77,77,77	0
55	MG	1G	1708	1/1	0.76	0.22	133,133,133,133	0
55	MG	1H	3298	1/1	0.76	0.37	87,87,87,87	0
55	MG	14	3239	1/1	0.76	0.36	87,87,87,87	0
55	MG	14	3307	1/1	0.76	0.27	89,89,89,89	0
55	MG	13	1671	1/1	0.76	0.15	70,70,70,70	0
55	MG	1H	3351	1/1	0.76	0.25	90,90,90,90	0
55	MG	14	3330	1/1	0.76	0.24	81,81,81,81	0
55	MG	1H	3394	1/1	0.76	0.16	69,69,69,69	0
55	MG	13	1711	1/1	0.76	0.62	90,90,90,90	0
55	MG	1H	3353	1/1	0.76	0.32	83,83,83,83	0
55	MG	1H	3327	1/1	0.76	0.31	63,63,63,63	0
55	MG	14	3273	1/1	0.76	0.18	87,87,87,87	0
55	MG	14	3135	1/1	0.77	0.23	64,64,64,64	0
55	MG	1H	3096	1/1	0.77	0.43	71,71,71,71	0
55	MG	14	3357	1/1	0.77	0.19	76,76,76,76	0
55	MG	13	1731	1/1	0.77	0.14	153,153,153,153	0
55	MG	1H	3469	1/1	0.77	0.15	115,115,115,115	0
55	MG	1G	1709	1/1	0.77	0.21	96,96,96,96	0
55	MG	1H	3140	1/1	0.77	0.20	52,52,52,52	0
55	MG	13	1638	1/1	0.77	0.23	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	1G	1740	1/1	0.77	0.05	140,140,140,140	0
55	MG	1G	1688	1/1	0.77	0.23	102,102,102,102	0
55	MG	1G	1610	1/1	0.77	0.32	99,99,99,99	0
55	MG	14	3079	1/1	0.77	0.30	82,82,82,82	0
55	MG	14	3218	1/1	0.77	0.39	88,88,88,88	0
55	MG	13	1734	1/1	0.77	0.06	178,178,178,178	0
55	MG	13	1640	1/1	0.77	0.23	89,89,89,89	0
55	MG	1G	1677	1/1	0.77	0.29	89,89,89,89	0
55	MG	14	3262	1/1	0.77	0.37	86,86,86,86	0
55	MG	1H	3406	1/1	0.77	0.53	91,91,91,91	0
55	MG	1H	3265	1/1	0.77	0.17	83,83,83,83	0
55	MG	14	3336	1/1	0.77	0.20	73,73,73,73	0
55	MG	14	3314	1/1	0.78	0.28	105,105,105,105	0
55	MG	13	1624	1/1	0.78	0.36	107,107,107,107	0
55	MG	1H	3356	1/1	0.78	0.53	91,91,91,91	0
55	MG	2K	103	1/1	0.78	0.32	94,94,94,94	0
55	MG	32	301	1/1	0.78	0.42	113,113,113,113	0
55	MG	1H	3105	1/1	0.78	0.36	90,90,90,90	0
55	MG	1H	3106	1/1	0.78	0.40	85,85,85,85	0
55	MG	13	1666	1/1	0.78	0.47	104,104,104,104	0
55	MG	1H	3116	1/1	0.78	0.50	74,74,74,74	0
55	MG	13	1649	1/1	0.78	0.45	84,84,84,84	0
55	MG	14	3206	1/1	0.78	0.23	76,76,76,76	0
55	MG	14	3272	1/1	0.78	0.39	94,94,94,94	0
55	MG	13	1657	1/1	0.78	0.31	74,74,74,74	0
55	MG	14	3228	1/1	0.78	0.25	84,84,84,84	0
55	MG	1H	3349	1/1	0.78	0.15	77,77,77,77	0
55	MG	1H	3297	1/1	0.78	0.33	81,81,81,81	0
55	MG	1J	206	1/1	0.78	0.36	96,96,96,96	0
55	MG	14	3168	1/1	0.78	0.35	76,76,76,76	0
55	MG	1H	3294	1/1	0.78	0.54	85,85,85,85	0
55	MG	1H	3293	1/1	0.78	0.34	95,95,95,95	0
55	MG	1H	3501	1/1	0.78	0.09	99,99,99,99	0
55	MG	1H	3152	1/1	0.78	0.48	80,80,80,80	0
55	MG	13	1709	1/1	0.78	0.27	78,78,78,78	0
55	MG	1H	3311	1/1	0.78	0.55	83,83,83,83	0
55	MG	1H	3134	1/1	0.79	0.33	65,65,65,65	0
55	MG	1H	3058	1/1	0.79	0.47	60,60,60,60	0
55	MG	1H	3149	1/1	0.79	0.46	82,82,82,82	0
55	MG	1H	3388	1/1	0.79	0.34	74,74,74,74	0
55	MG	1H	3088	1/1	0.79	0.21	52,52,52,52	0
55	MG	1H	3357	1/1	0.79	0.35	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	14	3175	1/1	0.79	0.39	85,85,85,85	0
55	MG	1H	3292	1/1	0.79	0.44	82,82,82,82	0
55	MG	1H	3172	1/1	0.79	0.20	69,69,69,69	0
55	MG	13	1680	1/1	0.79	0.40	77,77,77,77	0
55	MG	1H	3495	1/1	0.79	0.11	79,79,79,79	0
55	MG	14	3449	1/1	0.79	0.08	108,108,108,108	0
55	MG	1H	3339	1/1	0.79	0.45	91,91,91,91	0
55	MG	13	1708	1/1	0.79	0.54	127,127,127,127	0
55	MG	1J	210	1/1	0.79	0.12	144,144,144,144	0
55	MG	1H	3363	1/1	0.79	0.39	104,104,104,104	0
55	MG	1G	1654	1/1	0.79	0.38	91,91,91,91	0
55	MG	14	3321	1/1	0.79	0.37	89,89,89,89	0
55	MG	1H	3033	1/1	0.79	0.20	83,83,83,83	0
55	MG	14	3150	1/1	0.79	0.38	107,107,107,107	0
55	MG	14	3143	1/1	0.80	0.42	87,87,87,87	0
55	MG	14	3230	1/1	0.80	0.28	75,75,75,75	0
55	MG	E5	101	1/1	0.80	0.39	88,88,88,88	0
55	MG	1H	3207	1/1	0.80	0.18	67,67,67,67	0
55	MG	1H	3135	1/1	0.80	0.19	72,72,72,72	0
55	MG	14	3156	1/1	0.80	0.17	75,75,75,75	0
55	MG	1H	3397	1/1	0.80	0.12	94,94,94,94	0
55	MG	1H	3076	1/1	0.80	0.23	77,77,77,77	0
55	MG	14	3147	1/1	0.80	0.39	83,83,83,83	0
55	MG	1H	3146	1/1	0.80	0.23	48,48,48,48	0
55	MG	14	3349	1/1	0.80	0.20	100,100,100,100	0
55	MG	1G	1748	1/1	0.80	0.25	90,90,90,90	0
55	MG	1H	3216	1/1	0.80	0.48	90,90,90,90	0
55	MG	1H	3276	1/1	0.80	0.23	88,88,88,88	0
55	MG	1H	3497	1/1	0.80	0.16	105,105,105,105	0
55	MG	1H	3303	1/1	0.80	0.24	63,63,63,63	0
55	MG	1G	1693	1/1	0.80	0.35	95,95,95,95	0
55	MG	1H	3523	1/1	0.80	0.10	78,78,78,78	0
55	MG	1H	3323	1/1	0.80	0.41	80,80,80,80	0
55	MG	14	3123	1/1	0.80	0.23	50,50,50,50	0
55	MG	1H	3205	1/1	0.80	0.59	103,103,103,103	0
55	MG	1G	1656	1/1	0.80	0.31	94,94,94,94	0
55	MG	14	3361	1/1	0.80	0.30	90,90,90,90	0
55	MG	14	3220	1/1	0.80	0.17	89,89,89,89	0
55	MG	I8	101	1/1	0.80	0.32	83,83,83,83	0
55	MG	1H	3244	1/1	0.80	0.28	55,55,55,55	0
55	MG	1H	3173	1/1	0.81	0.49	90,90,90,90	0
55	MG	13	1715	1/1	0.81	0.23	70,70,70,70	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
55	MG	14	3200	1/1	0.81	0.42	100,100,100,100	0
55	MG	1H	3159	1/1	0.81	0.34	66,66,66,66	0
55	MG	14	3219	1/1	0.81	0.20	67,67,67,67	0
55	MG	1H	3044	1/1	0.81	0.29	98,98,98,98	0
55	MG	13	1697	1/1	0.81	0.41	84,84,84,84	0
55	MG	13	1694	1/1	0.81	0.30	92,92,92,92	0
55	MG	14	3148	1/1	0.81	0.46	86,86,86,86	0
55	MG	14	3431	1/1	0.81	0.10	102,102,102,102	0
55	MG	1H	3325	1/1	0.81	0.39	97,97,97,97	0
55	MG	1G	1618	1/1	0.81	0.26	79,79,79,79	0
55	MG	14	3155	1/1	0.81	0.33	77,77,77,77	0
55	MG	1H	3488	1/1	0.81	0.11	66,66,66,66	0
55	MG	1H	3086	1/1	0.81	0.19	59,59,59,59	0
55	MG	1H	3452	1/1	0.81	0.13	58,58,58,58	0
55	MG	1G	1738	1/1	0.81	0.10	140,140,140,140	0
55	MG	14	3171	1/1	0.81	0.37	86,86,86,86	0
55	MG	1H	3313	1/1	0.81	0.22	91,91,91,91	0
55	MG	14	3459	1/1	0.81	0.05	130,130,130,130	0
55	MG	14	3134	1/1	0.81	0.30	80,80,80,80	0
55	MG	13	1733	1/1	0.81	0.08	141,141,141,141	0
55	MG	45	201	1/1	0.81	0.33	76,76,76,76	0
55	MG	1H	3457	1/1	0.81	0.07	102,102,102,102	0
55	MG	14	3141	1/1	0.81	0.41	85,85,85,85	0
55	MG	1H	3197	1/1	0.81	0.62	85,85,85,85	0
55	MG	1H	3333	1/1	0.82	0.34	81,81,81,81	0
55	MG	1H	3174	1/1	0.82	0.27	89,89,89,89	0
55	MG	1H	3188	1/1	0.82	0.42	81,81,81,81	0
55	MG	14	3142	1/1	0.82	0.30	72,72,72,72	0
55	MG	14	3244	1/1	0.82	0.33	86,86,86,86	0
55	MG	14	3158	1/1	0.82	0.27	97,97,97,97	0
55	MG	14	3297	1/1	0.82	0.26	78,78,78,78	0
55	MG	1G	1646	1/1	0.82	0.23	93,93,93,93	0
55	MG	14	3296	1/1	0.82	0.28	97,97,97,97	0
55	MG	1H	3519	1/1	0.82	0.09	103,103,103,103	0
55	MG	14	3236	1/1	0.82	0.44	94,94,94,94	0
55	MG	1H	3150	1/1	0.82	0.39	78,78,78,78	0
55	MG	1H	3322	1/1	0.82	0.26	92,92,92,92	0
55	MG	14	3157	1/1	0.82	0.40	80,80,80,80	0
55	MG	1J	208	1/1	0.82	0.07	97,97,97,97	0
55	MG	1G	1725	1/1	0.82	0.20	93,93,93,93	0
55	MG	1J	204	1/1	0.82	0.23	101,101,101,101	0
55	MG	14	3087	1/1	0.82	0.27	65,65,65,65	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
55	MG	1H	3514	1/1	0.82	0.10	109,109,109,109	0
55	MG	1H	3030	1/1	0.82	0.29	91,91,91,91	0
55	MG	14	3305	1/1	0.82	0.36	89,89,89,89	0
55	MG	1H	3139	1/1	0.82	0.58	69,69,69,69	0
55	MG	1H	3341	1/1	0.82	0.30	76,76,76,76	0
55	MG	14	3034	1/1	0.82	0.31	73,73,73,73	0
55	MG	14	3308	1/1	0.83	0.20	80,80,80,80	0
55	MG	13	1660	1/1	0.83	0.38	80,80,80,80	0
55	MG	1G	1676	1/1	0.83	0.39	98,98,98,98	0
55	MG	1H	3132	1/1	0.83	0.36	76,76,76,76	0
55	MG	13	1677	1/1	0.83	0.16	83,83,83,83	0
55	MG	13	1713	1/1	0.83	0.33	100,100,100,100	0
55	MG	1H	3263	1/1	0.83	0.46	84,84,84,84	0
55	MG	1G	1660	1/1	0.83	0.10	87,87,87,87	0
55	MG	1H	3493	1/1	0.83	0.08	103,103,103,103	0
55	MG	1H	3260	1/1	0.83	0.22	70,70,70,70	0
55	MG	1H	3075	1/1	0.83	0.53	87,87,87,87	0
55	MG	1H	3103	1/1	0.83	0.41	71,71,71,71	0
55	MG	1G	1664	1/1	0.83	0.28	104,104,104,104	0
55	MG	1H	3118	1/1	0.83	0.37	83,83,83,83	0
55	MG	14	3323	1/1	0.83	0.25	87,87,87,87	0
55	MG	C5	201	1/1	0.83	0.26	86,86,86,86	0
55	MG	1H	3284	1/1	0.83	0.42	73,73,73,73	0
55	MG	1G	1727	1/1	0.83	0.24	104,104,104,104	0
55	MG	14	3317	1/1	0.83	0.36	83,83,83,83	0
55	MG	13	1646	1/1	0.83	0.39	90,90,90,90	0
55	MG	13	1702	1/1	0.83	0.24	147,147,147,147	0
55	MG	14	3295	1/1	0.83	0.18	72,72,72,72	0
55	MG	13	1655	1/1	0.83	0.31	92,92,92,92	0
55	MG	1G	1624	1/1	0.83	0.33	78,78,78,78	0
55	MG	14	3302	1/1	0.83	0.26	91,91,91,91	0
55	MG	1H	3175	1/1	0.84	0.54	74,74,74,74	0
55	MG	1H	3182	1/1	0.84	0.12	70,70,70,70	0
55	MG	1H	3032	1/1	0.84	0.35	95,95,95,95	0
55	MG	1J	203	1/1	0.84	0.10	92,92,92,92	0
55	MG	1H	3520	1/1	0.84	0.06	103,103,103,103	0
55	MG	14	3338	1/1	0.84	0.17	78,78,78,78	0
55	MG	14	3088	1/1	0.84	0.35	70,70,70,70	0
55	MG	1H	3200	1/1	0.84	0.29	99,99,99,99	0
55	MG	1G	1627	1/1	0.84	0.46	93,93,93,93	0
55	MG	1G	1674	1/1	0.84	0.34	111,111,111,111	0
55	MG	1H	3517	1/1	0.84	0.06	113,113,113,113	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
55	MG	1G	1671	1/1	0.84	0.15	92,92,92,92	0
55	MG	1G	1689	1/1	0.84	0.26	90,90,90,90	0
55	MG	14	3298	1/1	0.84	0.32	69,69,69,69	0
55	MG	14	3103	1/1	0.84	0.25	58,58,58,58	0
55	MG	1G	1642	1/1	0.84	0.26	87,87,87,87	0
55	MG	14	3210	1/1	0.84	0.15	68,68,68,68	0
55	MG	1H	3510	1/1	0.84	0.05	111,111,111,111	0
55	MG	1G	1667	1/1	0.84	0.31	103,103,103,103	0
55	MG	1H	3344	1/1	0.84	0.32	84,84,84,84	0
55	MG	1H	3157	1/1	0.84	0.28	79,79,79,79	0
55	MG	1H	3376	1/1	0.84	0.46	94,94,94,94	0
55	MG	1H	3482	1/1	0.84	0.10	70,70,70,70	0
55	MG	1H	3391	1/1	0.84	0.37	92,92,92,92	0
55	MG	1H	3508	1/1	0.84	0.06	119,119,119,119	0
55	MG	14	3324	1/1	0.84	0.36	101,101,101,101	0
55	MG	14	3105	1/1	0.84	0.38	72,72,72,72	0
55	MG	1H	3281	1/1	0.84	0.52	80,80,80,80	0
55	MG	1H	3268	1/1	0.84	0.39	100,100,100,100	0
55	MG	13	1613	1/1	0.84	0.29	99,99,99,99	0
55	MG	14	3188	1/1	0.84	0.37	76,76,76,76	0
55	MG	13	1618	1/1	0.84	0.29	96,96,96,96	0
55	MG	14	3181	1/1	0.85	0.29	70,70,70,70	0
55	MG	1H	3124	1/1	0.85	0.33	59,59,59,59	0
55	MG	1H	3359	1/1	0.85	0.14	77,77,77,77	0
55	MG	7E	201	1/1	0.85	0.33	83,83,83,83	0
55	MG	14	3285	1/1	0.85	0.31	93,93,93,93	0
55	MG	1H	3269	1/1	0.85	0.33	82,82,82,82	0
55	MG	1G	1684	1/1	0.85	0.41	99,99,99,99	0
55	MG	14	3326	1/1	0.85	0.16	90,90,90,90	0
55	MG	14	3461	1/1	0.85	0.09	82,82,82,82	0
55	MG	14	3279	1/1	0.85	0.44	84,84,84,84	0
55	MG	13	1692	1/1	0.85	0.44	132,132,132,132	0
55	MG	14	3221	1/1	0.85	0.12	76,76,76,76	0
55	MG	1H	3477	1/1	0.85	0.12	74,74,74,74	0
55	MG	14	3288	1/1	0.85	0.07	171,171,171,171	0
55	MG	14	3360	1/1	0.85	0.19	74,74,74,74	0
55	MG	14	3121	1/1	0.85	0.20	54,54,54,54	0
55	MG	1G	1650	1/1	0.85	0.26	90,90,90,90	0
55	MG	1H	3499	1/1	0.85	0.09	111,111,111,111	0
55	MG	1H	3318	1/1	0.85	0.16	75,75,75,75	0
55	MG	13	1667	1/1	0.85	0.43	94,94,94,94	0
55	MG	1H	3266	1/1	0.85	0.33	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	1G	1632	1/1	0.85	0.30	79,79,79,79	0
55	MG	1H	3199	1/1	0.85	0.19	72,72,72,72	0
55	MG	1H	3291	1/1	0.85	0.19	68,68,68,68	0
55	MG	13	1658	1/1	0.85	0.37	108,108,108,108	0
55	MG	1H	3164	1/1	0.85	0.46	90,90,90,90	0
55	MG	13	1637	1/1	0.85	0.50	90,90,90,90	0
55	MG	1H	3066	1/1	0.85	0.41	70,70,70,70	0
55	MG	14	3274	1/1	0.85	0.11	69,69,69,69	0
55	MG	14	3376	1/1	0.85	0.10	66,66,66,66	0
55	MG	1H	3256	1/1	0.85	0.19	78,78,78,78	0
55	MG	1H	3213	1/1	0.85	0.24	84,84,84,84	0
55	MG	1H	3065	1/1	0.85	0.34	64,64,64,64	0
55	MG	14	3356	1/1	0.85	0.23	195,195,195,195	0
55	MG	14	3093	1/1	0.85	0.24	84,84,84,84	0
55	MG	1G	1672	1/1	0.85	0.28	79,79,79,79	0
55	MG	14	3185	1/1	0.85	0.34	90,90,90,90	0
55	MG	14	3163	1/1	0.85	0.23	80,80,80,80	0
55	MG	14	3036	1/1	0.85	0.29	91,91,91,91	0
55	MG	1H	3399	1/1	0.85	0.22	77,77,77,77	0
55	MG	14	3304	1/1	0.85	0.45	99,99,99,99	0
55	MG	14	3106	1/1	0.85	0.44	75,75,75,75	0
55	MG	14	3420	1/1	0.85	0.07	89,89,89,89	0
55	MG	14	3343	1/1	0.86	0.30	86,86,86,86	0
55	MG	14	3265	1/1	0.86	0.38	76,76,76,76	0
55	MG	1G	1640	1/1	0.86	0.45	107,107,107,107	0
55	MG	13	1714	1/1	0.86	0.57	117,117,117,117	0
55	MG	14	3267	1/1	0.86	0.12	90,90,90,90	0
55	MG	14	3313	1/1	0.86	0.14	86,86,86,86	0
55	MG	13	1682	1/1	0.86	0.43	85,85,85,85	0
55	MG	1G	1707	1/1	0.86	0.42	90,90,90,90	0
55	MG	1H	3509	1/1	0.86	0.07	85,85,85,85	0
55	MG	14	3293	1/1	0.86	0.15	75,75,75,75	0
55	MG	16	210	1/1	0.86	0.15	96,96,96,96	0
55	MG	1H	3300	1/1	0.86	0.30	77,77,77,77	0
55	MG	13	1605	1/1	0.86	0.17	84,84,84,84	0
55	MG	13	1686	1/1	0.86	0.39	85,85,85,85	0
55	MG	1G	1658	1/1	0.86	0.14	99,99,99,99	0
55	MG	1H	3064	1/1	0.86	0.35	70,70,70,70	0
55	MG	1H	3069	1/1	0.86	0.28	51,51,51,51	0
55	MG	1G	1635	1/1	0.86	0.48	70,70,70,70	0
55	MG	13	1707	1/1	0.86	0.26	100,100,100,100	0
55	MG	14	3464	1/1	0.86	0.06	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	3239	1/1	0.86	0.32	74,74,74,74	0
55	MG	1H	3181	1/1	0.86	0.33	62,62,62,62	0
55	MG	14	3140	1/1	0.86	0.38	77,77,77,77	0
55	MG	1H	3369	1/1	0.86	0.14	94,94,94,94	0
55	MG	1H	3314	1/1	0.86	0.38	97,97,97,97	0
55	MG	14	3054	1/1	0.86	0.35	81,81,81,81	0
55	MG	11	301	1/1	0.86	0.21	54,54,54,54	0
55	MG	1J	209	1/1	0.86	0.09	128,128,128,128	0
55	MG	1H	3235	1/1	0.86	0.52	88,88,88,88	0
55	MG	14	3442	1/1	0.86	0.04	107,107,107,107	0
55	MG	13	1705	1/1	0.86	0.30	76,76,76,76	0
55	MG	14	3037	1/1	0.86	0.34	71,71,71,71	0
55	MG	19	301	1/1	0.86	0.21	67,67,67,67	0
55	MG	13	1661	1/1	0.86	0.42	95,95,95,95	0
55	MG	1H	3148	1/1	0.86	0.18	86,86,86,86	0
55	MG	1G	1704	1/1	0.86	0.23	117,117,117,117	0
55	MG	14	3310	1/1	0.86	0.49	75,75,75,75	0
55	MG	1G	1678	1/1	0.86	0.35	102,102,102,102	0
55	MG	14	3280	1/1	0.86	0.24	75,75,75,75	0
55	MG	14	3378	1/1	0.86	0.14	78,78,78,78	0
55	MG	1G	1700	1/1	0.87	0.35	94,94,94,94	0
55	MG	1H	3204	1/1	0.87	0.44	83,83,83,83	0
55	MG	1H	3038	1/1	0.87	0.20	59,59,59,59	0
55	MG	2L	104	1/1	0.87	0.07	93,93,93,93	0
55	MG	1G	1720	1/1	0.87	0.31	95,95,95,95	0
55	MG	1H	3227	1/1	0.87	0.28	76,76,76,76	0
55	MG	14	3179	1/1	0.87	0.33	88,88,88,88	0
55	MG	1H	3410	1/1	0.87	0.10	52,52,52,52	0
55	MG	13	1678	1/1	0.87	0.35	104,104,104,104	0
55	MG	14	3462	1/1	0.87	0.04	130,130,130,130	0
55	MG	1H	3329	1/1	0.87	0.40	85,85,85,85	0
55	MG	14	3199	1/1	0.87	0.23	60,60,60,60	0
55	MG	14	3085	1/1	0.87	0.31	72,72,72,72	0
55	MG	1H	3041	1/1	0.87	0.22	63,63,63,63	0
55	MG	1G	1710	1/1	0.87	0.23	101,101,101,101	0
55	MG	1H	3211	1/1	0.87	0.37	79,79,79,79	0
55	MG	14	3184	1/1	0.87	0.23	71,71,71,71	0
55	MG	14	3117	1/1	0.87	0.33	93,93,93,93	0
55	MG	1H	3068	1/1	0.87	0.25	61,61,61,61	0
55	MG	1G	1652	1/1	0.87	0.33	82,82,82,82	0
55	MG	14	3271	1/1	0.87	0.20	82,82,82,82	0
55	MG	13	1607	1/1	0.87	0.34	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	I8	103	1/1	0.87	0.39	92,92,92,92	0
55	MG	14	3208	1/1	0.87	0.23	88,88,88,88	0
55	MG	1G	1609	1/1	0.87	0.37	99,99,99,99	0
55	MG	1H	3238	1/1	0.87	0.56	82,82,82,82	0
55	MG	2K	105	1/1	0.87	0.21	76,76,76,76	0
55	MG	1H	3309	1/1	0.87	0.24	85,85,85,85	0
55	MG	1H	3194	1/1	0.87	0.32	68,68,68,68	0
55	MG	1H	3374	1/1	0.87	0.31	67,67,67,67	0
55	MG	14	3268	1/1	0.87	0.38	85,85,85,85	0
55	MG	13	1614	1/1	0.87	0.24	95,95,95,95	0
55	MG	14	3438	1/1	0.87	0.08	83,83,83,83	0
55	MG	14	3126	1/1	0.87	0.32	83,83,83,83	0
55	MG	13	1710	1/1	0.88	0.13	103,103,103,103	0
55	MG	14	3234	1/1	0.88	0.16	51,51,51,51	0
55	MG	14	3284	1/1	0.88	0.23	95,95,95,95	0
55	MG	1H	3277	1/1	0.88	0.33	74,74,74,74	0
55	MG	1G	1673	1/1	0.88	0.22	88,88,88,88	0
55	MG	14	3342	1/1	0.88	0.45	94,94,94,94	0
55	MG	1H	3176	1/1	0.88	0.38	73,73,73,73	0
55	MG	1H	3078	1/1	0.88	0.30	71,71,71,71	0
55	MG	1H	3177	1/1	0.88	0.21	69,69,69,69	0
55	MG	1H	3092	1/1	0.88	0.43	62,62,62,62	0
55	MG	13	1685	1/1	0.88	0.12	89,89,89,89	0
55	MG	14	3205	1/1	0.88	0.40	70,70,70,70	0
55	MG	1H	3305	1/1	0.88	0.17	104,104,104,104	0
55	MG	1G	1614	1/1	0.88	0.28	92,92,92,92	0
55	MG	1H	3504	1/1	0.88	0.07	80,80,80,80	0
55	MG	14	3457	1/1	0.88	0.06	125,125,125,125	0
55	MG	14	3100	1/1	0.88	0.21	79,79,79,79	0
55	MG	14	3362	1/1	0.88	0.29	111,111,111,111	0
55	MG	1H	3502	1/1	0.88	0.06	148,148,148,148	0
55	MG	25	201	1/1	0.88	0.08	111,111,111,111	0
55	MG	14	3099	1/1	0.88	0.22	67,67,67,67	0
55	MG	14	3433	1/1	0.88	0.07	87,87,87,87	0
55	MG	14	3197	1/1	0.88	0.26	81,81,81,81	0
55	MG	14	3196	1/1	0.88	0.10	60,60,60,60	0
55	MG	14	3358	1/1	0.88	0.17	85,85,85,85	0
55	MG	1H	3491	1/1	0.88	0.14	52,52,52,52	0
55	MG	1G	1655	1/1	0.88	0.33	74,74,74,74	0
55	MG	1G	1607	1/1	0.88	0.28	95,95,95,95	0
55	MG	1H	3104	1/1	0.88	0.18	85,85,85,85	0
55	MG	15	201	1/1	0.88	0.16	99,99,99,99	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
55	MG	16	207	1/1	0.88	0.46	85,85,85,85	0
55	MG	13	1632	1/1	0.88	0.49	74,74,74,74	0
55	MG	1H	3170	1/1	0.88	0.42	89,89,89,89	0
55	MG	13	1615	1/1	0.88	0.37	98,98,98,98	0
55	MG	1G	1687	1/1	0.88	0.25	79,79,79,79	0
55	MG	13	1625	1/1	0.88	0.46	95,95,95,95	0
55	MG	14	3149	1/1	0.88	0.18	66,66,66,66	0
55	MG	1H	3401	1/1	0.88	0.26	67,67,67,67	0
55	MG	1H	3258	1/1	0.88	0.50	91,91,91,91	0
55	MG	1G	1615	1/1	0.88	0.19	78,78,78,78	0
55	MG	1H	3262	1/1	0.88	0.09	71,71,71,71	0
55	MG	14	3224	1/1	0.88	0.16	112,112,112,112	0
55	MG	13	1652	1/1	0.88	0.30	88,88,88,88	0
55	MG	14	3260	1/1	0.88	0.31	99,99,99,99	0
55	MG	1H	3029	1/1	0.89	0.24	71,71,71,71	0
55	MG	1G	1626	1/1	0.89	0.26	107,107,107,107	0
55	MG	16	212	1/1	0.89	0.13	85,85,85,85	0
55	MG	1H	3037	1/1	0.89	0.33	60,60,60,60	0
55	MG	16	213	1/1	0.89	0.15	113,113,113,113	0
55	MG	1H	3372	1/1	0.89	0.38	94,94,94,94	0
55	MG	1G	1662	1/1	0.89	0.41	84,84,84,84	0
55	MG	1H	3390	1/1	0.89	0.36	88,88,88,88	0
55	MG	1H	3316	1/1	0.89	0.23	61,61,61,61	0
55	MG	13	1674	1/1	0.89	0.36	106,106,106,106	0
55	MG	1H	3154	1/1	0.89	0.45	79,79,79,79	0
55	MG	1H	3332	1/1	0.89	0.47	87,87,87,87	0
55	MG	1H	3513	1/1	0.89	0.08	116,116,116,116	0
55	MG	13	1722	1/1	0.89	0.18	101,101,101,101	0
55	MG	14	3370	1/1	0.89	0.27	75,75,75,75	0
55	MG	1H	3008	1/1	0.89	0.30	44,44,44,44	0
55	MG	14	3152	1/1	0.89	0.31	72,72,72,72	0
55	MG	14	3020	1/1	0.89	0.33	72,72,72,72	0
55	MG	1H	3184	1/1	0.89	0.47	85,85,85,85	0
55	MG	1J	202	1/1	0.89	0.45	90,90,90,90	0
55	MG	1G	1668	1/1	0.89	0.27	82,82,82,82	0
55	MG	14	3081	1/1	0.89	0.32	70,70,70,70	0
55	MG	1H	3512	1/1	0.89	0.08	115,115,115,115	0
55	MG	14	3455	1/1	0.89	0.11	108,108,108,108	0
55	MG	13	1653	1/1	0.89	0.35	104,104,104,104	0
55	MG	13	1701	1/1	0.89	0.33	100,100,100,100	0
55	MG	14	3425	1/1	0.89	0.08	96,96,96,96	0
55	MG	14	3080	1/1	0.89	0.52	81,81,81,81	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
55	MG	14	3136	1/1	0.89	0.39	75,75,75,75	0
55	MG	1G	1724	1/1	0.89	0.21	99,99,99,99	0
55	MG	1H	3310	1/1	0.89	0.41	72,72,72,72	0
55	MG	1H	3381	1/1	0.89	0.61	62,62,62,62	0
55	MG	14	3187	1/1	0.89	0.41	94,94,94,94	0
55	MG	14	3350	1/1	0.89	0.29	77,77,77,77	0
55	MG	1G	1651	1/1	0.89	0.39	96,96,96,96	0
55	MG	14	3144	1/1	0.89	0.47	98,98,98,98	0
55	MG	1H	3273	1/1	0.89	0.39	103,103,103,103	0
55	MG	14	3167	1/1	0.89	0.20	83,83,83,83	0
55	MG	14	3463	1/1	0.89	0.11	130,130,130,130	0
55	MG	1H	3093	1/1	0.89	0.48	82,82,82,82	0
55	MG	1H	3201	1/1	0.89	0.41	66,66,66,66	0
55	MG	1H	3131	1/1	0.89	0.33	75,75,75,75	0
55	MG	1H	3280	1/1	0.89	0.18	70,70,70,70	0
55	MG	Q8	102	1/1	0.89	0.31	81,81,81,81	0
55	MG	1H	3393	1/1	0.89	0.14	62,62,62,62	0
55	MG	1H	3179	1/1	0.89	0.17	60,60,60,60	0
55	MG	13	1676	1/1	0.89	0.37	84,84,84,84	0
55	MG	13	1736	1/1	0.89	0.08	132,132,132,132	0
55	MG	14	3074	1/1	0.89	0.16	47,47,47,47	0
55	MG	13	1650	1/1	0.89	0.40	88,88,88,88	0
55	MG	1H	3443	1/1	0.89	0.09	75,75,75,75	0
55	MG	1H	3212	1/1	0.89	0.22	78,78,78,78	0
55	MG	14	3241	1/1	0.89	0.30	89,89,89,89	0
55	MG	13	1662	1/1	0.89	0.26	86,86,86,86	0
55	MG	13	1651	1/1	0.89	0.31	73,73,73,73	0
55	MG	1H	3500	1/1	0.89	0.06	65,65,65,65	0
55	MG	1H	3278	1/1	0.89	0.45	76,76,76,76	0
55	MG	14	3369	1/1	0.89	0.21	78,78,78,78	0
55	MG	14	3001	1/1	0.89	0.24	70,70,70,70	0
55	MG	14	3019	1/1	0.89	0.34	68,68,68,68	0
55	MG	I8	102	1/1	0.89	0.38	65,65,65,65	0
55	MG	1G	1723	1/1	0.89	0.24	98,98,98,98	0
55	MG	1H	3486	1/1	0.89	0.07	79,79,79,79	0
55	MG	14	3414	1/1	0.89	0.10	56,56,56,56	0
55	MG	1G	1733	1/1	0.90	0.09	93,93,93,93	0
55	MG	14	3315	1/1	0.90	0.38	85,85,85,85	0
55	MG	1H	3034	1/1	0.90	0.14	54,54,54,54	0
55	MG	1H	3165	1/1	0.90	0.40	74,74,74,74	0
55	MG	1H	3522	1/1	0.90	0.15	68,68,68,68	0
55	MG	14	3424	1/1	0.90	0.08	81,81,81,81	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
55	MG	14	3333	1/1	0.90	0.15	89,89,89,89	0
55	MG	1H	3163	1/1	0.90	0.29	82,82,82,82	0
55	MG	1H	3362	1/1	0.90	0.41	103,103,103,103	0
55	MG	1G	1675	1/1	0.90	0.26	99,99,99,99	0
55	MG	1G	1643	1/1	0.90	0.31	106,106,106,106	0
55	MG	14	3439	1/1	0.90	0.07	101,101,101,101	0
55	MG	1G	1744	1/1	0.90	0.08	128,128,128,128	0
55	MG	14	3246	1/1	0.90	0.21	83,83,83,83	0
55	MG	14	3138	1/1	0.90	0.29	58,58,58,58	0
55	MG	13	1696	1/1	0.90	0.19	86,86,86,86	0
55	MG	1H	3084	1/1	0.90	0.32	62,62,62,62	0
55	MG	1H	3063	1/1	0.90	0.32	63,63,63,63	0
55	MG	98	201	1/1	0.90	0.34	89,89,89,89	0
55	MG	14	3364	1/1	0.90	0.09	68,68,68,68	0
55	MG	1G	1696	1/1	0.90	0.11	92,92,92,92	0
55	MG	14	3217	1/1	0.90	0.26	55,55,55,55	0
55	MG	1H	3272	1/1	0.90	0.31	76,76,76,76	0
55	MG	16	205	1/1	0.90	0.09	109,109,109,109	0
55	MG	14	3056	1/1	0.90	0.29	75,75,75,75	0
55	MG	14	3341	1/1	0.90	0.18	95,95,95,95	0
55	MG	1H	3334	1/1	0.90	0.23	108,108,108,108	0
55	MG	1G	1630	1/1	0.90	0.42	81,81,81,81	0
55	MG	14	3328	1/1	0.90	0.42	115,115,115,115	0
55	MG	14	3227	1/1	0.90	0.23	80,80,80,80	0
55	MG	13	1665	1/1	0.90	0.10	90,90,90,90	0
55	MG	14	3290	1/1	0.90	0.33	77,77,77,77	0
55	MG	14	3017	1/1	0.90	0.25	83,83,83,83	0
55	MG	1H	3304	1/1	0.90	0.36	82,82,82,82	0
55	MG	88	201	1/1	0.90	0.25	98,98,98,98	0
55	MG	1G	1633	1/1	0.90	0.48	80,80,80,80	0
55	MG	1H	3254	1/1	0.90	0.20	69,69,69,69	0
55	MG	14	3242	1/1	0.90	0.33	86,86,86,86	0
55	MG	14	3172	1/1	0.90	0.19	85,85,85,85	0
55	MG	1H	3324	1/1	0.90	0.26	66,66,66,66	0
55	MG	14	3299	1/1	0.90	0.42	100,100,100,100	0
55	MG	14	3385	1/1	0.90	0.13	73,73,73,73	0
55	MG	1G	1734	1/1	0.90	0.07	81,81,81,81	0
55	MG	1H	3108	1/1	0.90	0.38	77,77,77,77	0
55	MG	14	3270	1/1	0.90	0.39	76,76,76,76	0
55	MG	1H	3335	1/1	0.90	0.41	70,70,70,70	0
55	MG	1H	3226	1/1	0.90	0.30	114,114,114,114	0
55	MG	14	3294	1/1	0.90	0.11	81,81,81,81	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
55	MG	13	1681	1/1	0.90	0.39	104,104,104,104	0
55	MG	1G	1706	1/1	0.90	0.35	86,86,86,86	0
55	MG	14	3319	1/1	0.90	0.09	89,89,89,89	0
55	MG	1H	3245	1/1	0.90	0.34	86,86,86,86	0
55	MG	1H	3368	1/1	0.91	0.45	72,72,72,72	0
55	MG	1G	1670	1/1	0.91	0.32	92,92,92,92	0
55	MG	14	3327	1/1	0.91	0.43	110,110,110,110	0
55	MG	14	3115	1/1	0.91	0.16	58,58,58,58	0
55	MG	14	3278	1/1	0.91	0.27	84,84,84,84	0
55	MG	1H	3296	1/1	0.91	0.33	84,84,84,84	0
55	MG	14	3363	1/1	0.91	0.14	61,61,61,61	0
55	MG	1H	3285	1/1	0.91	0.09	89,89,89,89	0
55	MG	1H	3247	1/1	0.91	0.28	51,51,51,51	0
55	MG	14	3372	1/1	0.91	0.37	96,96,96,96	0
55	MG	13	1616	1/1	0.91	0.22	141,141,141,141	0
55	MG	13	1727	1/1	0.91	0.12	108,108,108,108	0
55	MG	14	3125	1/1	0.91	0.42	88,88,88,88	0
55	MG	13	1628	1/1	0.91	0.35	71,71,71,71	0
55	MG	14	3023	1/1	0.91	0.13	72,72,72,72	0
55	MG	1H	3389	1/1	0.91	0.40	101,101,101,101	0
55	MG	1H	3169	1/1	0.91	0.46	83,83,83,83	0
55	MG	14	3355	1/1	0.91	0.24	73,73,73,73	0
55	MG	14	3253	1/1	0.91	0.24	105,105,105,105	0
55	MG	14	3402	1/1	0.91	0.07	82,82,82,82	0
55	MG	14	3131	1/1	0.91	0.18	66,66,66,66	0
55	MG	1H	3384	1/1	0.91	0.60	108,108,108,108	0
55	MG	14	3078	1/1	0.91	0.26	60,60,60,60	0
55	MG	1H	3255	1/1	0.91	0.21	92,92,92,92	0
55	MG	1G	1622	1/1	0.91	0.29	86,86,86,86	0
55	MG	1H	3109	1/1	0.91	0.29	76,76,76,76	0
55	MG	1H	3408	1/1	0.91	0.12	54,54,54,54	0
55	MG	13	1704	1/1	0.91	0.20	87,87,87,87	0
55	MG	1H	3400	1/1	0.91	0.34	84,84,84,84	0
55	MG	1H	3345	1/1	0.91	0.29	67,67,67,67	0
55	MG	14	3413	1/1	0.91	0.12	70,70,70,70	0
55	MG	14	3450	1/1	0.91	0.14	105,105,105,105	0
55	MG	1H	3252	1/1	0.91	0.34	98,98,98,98	0
55	MG	1H	3073	1/1	0.91	0.26	77,77,77,77	0
55	MG	1H	3022	1/1	0.91	0.14	60,60,60,60	0
55	MG	14	3109	1/1	0.91	0.36	85,85,85,85	0
55	MG	14	3177	1/1	0.91	0.38	76,76,76,76	0
55	MG	1H	3361	1/1	0.91	0.22	155,155,155,155	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
55	MG	1J	201	1/1	0.91	0.24	100,100,100,100	0
55	MG	1H	3141	1/1	0.91	0.24	65,65,65,65	0
55	MG	1H	3056	1/1	0.91	0.47	68,68,68,68	0
55	MG	14	3094	1/1	0.91	0.34	81,81,81,81	0
55	MG	14	3257	1/1	0.91	0.22	75,75,75,75	0
55	MG	14	3428	1/1	0.91	0.09	69,69,69,69	0
55	MG	1H	3094	1/1	0.91	0.32	60,60,60,60	0
55	MG	1H	3049	1/1	0.91	0.33	71,71,71,71	0
55	MG	14	3212	1/1	0.91	0.14	66,66,66,66	0
55	MG	14	3320	1/1	0.91	0.40	88,88,88,88	0
55	MG	14	3409	1/1	0.91	0.07	64,64,64,64	0
55	MG	1H	3290	1/1	0.91	0.41	80,80,80,80	0
55	MG	1H	3337	1/1	0.91	0.28	94,94,94,94	0
55	MG	14	3026	1/1	0.91	0.19	78,78,78,78	0
55	MG	1G	1665	1/1	0.91	0.15	69,69,69,69	0
55	MG	14	3366	1/1	0.91	0.43	99,99,99,99	0
55	MG	1G	1659	1/1	0.91	0.20	107,107,107,107	0
55	MG	14	3374	1/1	0.91	0.17	52,52,52,52	0
55	MG	14	3334	1/1	0.91	0.24	84,84,84,84	0
55	MG	14	3124	1/1	0.91	0.19	56,56,56,56	0
55	MG	13	1664	1/1	0.91	0.59	93,93,93,93	0
55	MG	14	3446	1/1	0.91	0.07	87,87,87,87	0
55	MG	1H	3160	1/1	0.92	0.43	68,68,68,68	0
55	MG	1H	3236	1/1	0.92	0.47	89,89,89,89	0
55	MG	13	1603	1/1	0.92	0.20	96,96,96,96	0
55	MG	14	3275	1/1	0.92	0.38	90,90,90,90	0
55	MG	1H	3343	1/1	0.92	0.16	90,90,90,90	0
55	MG	14	3434	1/1	0.92	0.11	98,98,98,98	0
55	MG	2L	103	1/1	0.92	0.09	130,130,130,130	0
55	MG	1G	1731	1/1	0.92	0.13	110,110,110,110	0
55	MG	1G	1745	1/1	0.92	0.15	93,93,93,93	0
55	MG	14	3176	1/1	0.92	0.26	63,63,63,63	0
55	MG	Q8	101	1/1	0.92	0.30	99,99,99,99	0
55	MG	1H	3246	1/1	0.92	0.13	48,48,48,48	0
55	MG	1H	3005	1/1	0.92	0.26	44,44,44,44	0
55	MG	1H	3122	1/1	0.92	0.12	82,82,82,82	0
55	MG	14	3276	1/1	0.92	0.18	73,73,73,73	0
55	MG	14	3248	1/1	0.92	0.34	78,78,78,78	0
55	MG	14	3014	1/1	0.92	0.29	84,84,84,84	0
55	MG	1H	3348	1/1	0.92	0.24	88,88,88,88	0
55	MG	13	1642	1/1	0.92	0.46	66,66,66,66	0
55	MG	1G	1698	1/1	0.92	0.26	96,96,96,96	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
55	MG	1H	3288	1/1	0.92	0.25	72,72,72,72	0
55	MG	1H	3138	1/1	0.92	0.50	87,87,87,87	0
55	MG	1H	3448	1/1	0.92	0.11	63,63,63,63	0
55	MG	14	3092	1/1	0.92	0.48	70,70,70,70	0
55	MG	1G	1641	1/1	0.92	0.41	83,83,83,83	0
55	MG	1G	1714	1/1	0.92	0.24	98,98,98,98	0
55	MG	1H	3219	1/1	0.92	0.32	72,72,72,72	0
55	MG	14	3233	1/1	0.92	0.26	67,67,67,67	0
55	MG	14	3432	1/1	0.92	0.12	100,100,100,100	0
55	MG	14	3225	1/1	0.92	0.21	75,75,75,75	0
55	MG	1H	3130	1/1	0.92	0.28	69,69,69,69	0
55	MG	1H	3210	1/1	0.92	0.41	79,79,79,79	0
55	MG	1G	1742	1/1	0.92	0.05	112,112,112,112	0
55	MG	14	3375	1/1	0.92	0.17	51,51,51,51	0
55	MG	1H	3048	1/1	0.92	0.23	58,58,58,58	0
55	MG	14	3120	1/1	0.92	0.43	54,54,54,54	0
55	MG	14	3139	1/1	0.92	0.39	69,69,69,69	0
55	MG	14	3021	1/1	0.92	0.12	63,63,63,63	0
55	MG	1H	3257	1/1	0.92	0.43	83,83,83,83	0
55	MG	1H	3143	1/1	0.92	0.28	73,73,73,73	0
55	MG	13	1620	1/1	0.92	0.36	66,66,66,66	0
55	MG	1J	205	1/1	0.92	0.36	122,122,122,122	0
55	MG	1G	1712	1/1	0.92	0.17	109,109,109,109	0
55	MG	14	3071	1/1	0.92	0.21	62,62,62,62	0
55	MG	16	206	1/1	0.92	0.09	101,101,101,101	0
55	MG	1H	3365	1/1	0.92	0.28	86,86,86,86	0
55	MG	1G	1644	1/1	0.92	0.25	115,115,115,115	0
55	MG	13	1721	1/1	0.92	0.11	88,88,88,88	0
55	MG	1H	3189	1/1	0.92	0.12	83,83,83,83	0
55	MG	13	1726	1/1	0.92	0.13	89,89,89,89	0
55	MG	1H	3373	1/1	0.92	0.47	79,79,79,79	0
55	MG	14	3160	1/1	0.92	0.21	74,74,74,74	0
55	MG	1H	3156	1/1	0.92	0.31	72,72,72,72	0
55	MG	1G	1608	1/1	0.92	0.23	85,85,85,85	0
55	MG	1H	3515	1/1	0.92	0.07	106,106,106,106	0
55	MG	1G	1746	1/1	0.92	0.13	134,134,134,134	0
55	MG	14	3352	1/1	0.92	0.45	93,93,93,93	0
55	MG	1H	3476	1/1	0.92	0.15	59,59,59,59	0
55	MG	14	3226	1/1	0.92	0.12	55,55,55,55	0
55	MG	1H	3224	1/1	0.92	0.50	83,83,83,83	0
55	MG	14	3437	1/1	0.92	0.06	85,85,85,85	0
55	MG	1H	3046	1/1	0.92	0.34	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	3453	1/1	0.92	0.07	76,76,76,76	0
55	MG	14	3254	1/1	0.92	0.37	85,85,85,85	0
55	MG	1H	3117	1/1	0.92	0.35	75,75,75,75	0
55	MG	14	3346	1/1	0.92	0.29	84,84,84,84	0
55	MG	14	3401	1/1	0.92	0.06	82,82,82,82	0
55	MG	1H	3183	1/1	0.92	0.31	63,63,63,63	0
55	MG	14	3178	1/1	0.92	0.27	81,81,81,81	0
55	MG	14	3337	1/1	0.92	0.25	105,105,105,105	0
55	MG	14	3222	1/1	0.92	0.28	79,79,79,79	0
55	MG	13	1663	1/1	0.92	0.29	105,105,105,105	0
55	MG	21	301	1/1	0.92	0.31	58,58,58,58	0
55	MG	14	3322	1/1	0.92	0.09	70,70,70,70	0
55	MG	1H	3338	1/1	0.92	0.10	78,78,78,78	0
55	MG	1H	3434	1/1	0.92	0.11	60,60,60,60	0
55	MG	13	1633	1/1	0.92	0.31	79,79,79,79	0
55	MG	1H	3208	1/1	0.92	0.45	69,69,69,69	0
55	MG	1H	3358	1/1	0.92	0.12	98,98,98,98	0
55	MG	13	1673	1/1	0.92	0.26	109,109,109,109	0
55	MG	1H	3449	1/1	0.92	0.22	94,94,94,94	0
55	MG	1H	3347	1/1	0.93	0.32	72,72,72,72	0
55	MG	14	3213	1/1	0.93	0.32	68,68,68,68	0
55	MG	1H	3230	1/1	0.93	0.40	71,71,71,71	0
55	MG	13	1687	1/1	0.93	0.25	77,77,77,77	0
55	MG	13	1690	1/1	0.93	0.13	118,118,118,118	0
55	MG	14	3443	1/1	0.93	0.05	103,103,103,103	0
55	MG	55	201	1/1	0.93	0.26	68,68,68,68	0
55	MG	14	3042	1/1	0.93	0.29	67,67,67,67	0
55	MG	14	3214	1/1	0.93	0.24	66,66,66,66	0
55	MG	1H	3153	1/1	0.93	0.38	86,86,86,86	0
55	MG	14	3441	1/1	0.93	0.09	86,86,86,86	0
55	MG	1H	3326	1/1	0.93	0.11	78,78,78,78	0
55	MG	14	3421	1/1	0.93	0.05	82,82,82,82	0
55	MG	1H	3506	1/1	0.93	0.09	110,110,110,110	0
55	MG	1H	3414	1/1	0.93	0.15	59,59,59,59	0
55	MG	14	3351	1/1	0.93	0.24	87,87,87,87	0
55	MG	14	3089	1/1	0.93	0.39	71,71,71,71	0
55	MG	14	3430	1/1	0.93	0.10	67,67,67,67	0
55	MG	1H	3431	1/1	0.93	0.14	70,70,70,70	0
55	MG	1G	1737	1/1	0.93	0.07	114,114,114,114	0
55	MG	14	3051	1/1	0.93	0.27	62,62,62,62	0
55	MG	1H	3302	1/1	0.93	0.66	74,74,74,74	0
55	MG	14	3173	1/1	0.93	0.30	70,70,70,70	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
55	MG	1G	1648	1/1	0.93	0.25	89,89,89,89	0
55	MG	1H	3438	1/1	0.93	0.09	60,60,60,60	0
55	MG	13	1604	1/1	0.93	0.10	86,86,86,86	0
55	MG	1H	3271	1/1	0.93	0.09	90,90,90,90	0
55	MG	14	3195	1/1	0.93	0.25	65,65,65,65	0
55	MG	14	3365	1/1	0.93	0.19	78,78,78,78	0
55	MG	21	302	1/1	0.93	0.22	68,68,68,68	0
55	MG	1H	3320	1/1	0.93	0.61	109,109,109,109	0
55	MG	14	3256	1/1	0.93	0.35	67,67,67,67	0
55	MG	14	3129	1/1	0.93	0.39	70,70,70,70	0
55	MG	13	1634	1/1	0.93	0.35	73,73,73,73	0
55	MG	14	3130	1/1	0.93	0.20	72,72,72,72	0
55	MG	14	3162	1/1	0.93	0.42	71,71,71,71	0
55	MG	1H	3233	1/1	0.93	0.16	72,72,72,72	0
55	MG	1H	3250	1/1	0.93	0.09	73,73,73,73	0
55	MG	1H	3243	1/1	0.93	0.17	52,52,52,52	0
55	MG	1G	1645	1/1	0.93	0.12	79,79,79,79	0
55	MG	14	3394	1/1	0.93	0.06	89,89,89,89	0
55	MG	14	3059	1/1	0.93	0.30	60,60,60,60	0
55	MG	13	1672	1/1	0.93	0.23	119,119,119,119	0
55	MG	1H	3114	1/1	0.93	0.08	56,56,56,56	0
55	MG	13	1703	1/1	0.93	0.62	147,147,147,147	0
55	MG	1H	3110	1/1	0.93	0.24	47,47,47,47	0
55	MG	14	3456	1/1	0.93	0.06	102,102,102,102	0
55	MG	1H	3306	1/1	0.93	0.15	83,83,83,83	0
55	MG	14	3211	1/1	0.93	0.30	77,77,77,77	0
55	MG	14	3151	1/1	0.93	0.48	78,78,78,78	0
55	MG	14	3359	1/1	0.93	0.10	89,89,89,89	0
55	MG	1G	1604	1/1	0.93	0.15	78,78,78,78	0
55	MG	13	1623	1/1	0.93	0.21	107,107,107,107	0
55	MG	1H	3229	1/1	0.93	0.12	54,54,54,54	0
55	MG	1H	3042	1/1	0.93	0.12	95,95,95,95	0
55	MG	1H	3195	1/1	0.93	0.19	79,79,79,79	0
55	MG	1G	1680	1/1	0.93	0.39	88,88,88,88	0
55	MG	13	1622	1/1	0.93	0.42	74,74,74,74	0
55	MG	1H	3442	1/1	0.93	0.16	43,43,43,43	0
55	MG	1G	1605	1/1	0.93	0.21	92,92,92,92	0
55	MG	1H	3144	1/1	0.93	0.40	69,69,69,69	0
55	MG	14	3069	1/1	0.93	0.43	96,96,96,96	0
55	MG	1G	1617	1/1	0.93	0.38	71,71,71,71	0
55	MG	14	3435	1/1	0.93	0.07	95,95,95,95	0
55	MG	14	3198	1/1	0.93	0.23	70,70,70,70	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
55	MG	3I	201	1/1	0.93	0.20	80,80,80,80	0
55	MG	14	3416	1/1	0.93	0.12	52,52,52,52	0
55	MG	13	1691	1/1	0.93	0.49	83,83,83,83	0
55	MG	13	1732	1/1	0.93	0.13	128,128,128,128	0
55	MG	1G	1690	1/1	0.93	0.32	98,98,98,98	0
55	MG	1H	3060	1/1	0.94	0.26	80,80,80,80	0
55	MG	1H	3087	1/1	0.94	0.22	49,49,49,49	0
55	MG	1H	3127	1/1	0.94	0.41	60,60,60,60	0
55	MG	1H	3416	1/1	0.94	0.17	71,71,71,71	0
55	MG	14	3238	1/1	0.94	0.41	81,81,81,81	0
55	MG	1G	1637	1/1	0.94	0.35	71,71,71,71	0
55	MG	1H	3059	1/1	0.94	0.26	83,83,83,83	0
55	MG	1H	3380	1/1	0.94	0.45	88,88,88,88	0
55	MG	14	3266	1/1	0.94	0.43	88,88,88,88	0
55	MG	1H	3371	1/1	0.94	0.16	62,62,62,62	0
55	MG	14	3170	1/1	0.94	0.19	79,79,79,79	0
55	MG	1G	1695	1/1	0.94	0.10	86,86,86,86	0
55	MG	14	3018	1/1	0.94	0.08	64,64,64,64	0
55	MG	1H	3427	1/1	0.94	0.08	107,107,107,107	0
55	MG	14	3083	1/1	0.94	0.41	68,68,68,68	0
55	MG	14	3426	1/1	0.94	0.07	91,91,91,91	0
55	MG	1H	3016	1/1	0.94	0.29	56,56,56,56	0
55	MG	1H	3102	1/1	0.94	0.33	49,49,49,49	0
55	MG	14	3045	1/1	0.94	0.22	41,41,41,41	0
55	MG	1H	3331	1/1	0.94	0.23	84,84,84,84	0
55	MG	14	3145	1/1	0.94	0.28	78,78,78,78	0
55	MG	1G	1717	1/1	0.94	0.16	107,107,107,107	0
55	MG	1H	3490	1/1	0.94	0.06	89,89,89,89	0
55	MG	1H	3067	1/1	0.94	0.18	47,47,47,47	0
55	MG	1H	3248	1/1	0.94	0.33	61,61,61,61	0
55	MG	1H	3402	1/1	0.94	0.17	77,77,77,77	0
55	MG	14	3029	1/1	0.94	0.33	51,51,51,51	0
55	MG	1H	3079	1/1	0.94	0.38	66,66,66,66	0
55	MG	1H	3100	1/1	0.94	0.43	61,61,61,61	0
55	MG	14	3066	1/1	0.94	0.17	63,63,63,63	0
55	MG	14	3075	1/1	0.94	0.27	52,52,52,52	0
55	MG	14	3231	1/1	0.94	0.28	76,76,76,76	0
55	MG	13	1639	1/1	0.94	0.29	66,66,66,66	0
55	MG	13	1629	1/1	0.94	0.35	60,60,60,60	0
55	MG	14	3396	1/1	0.94	0.11	67,67,67,67	0
55	MG	1H	3378	1/1	0.94	0.09	91,91,91,91	0
55	MG	13	1717	1/1	0.94	0.12	66,66,66,66	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
55	MG	14	3400	1/1	0.94	0.13	65,65,65,65	0
55	MG	1H	3080	1/1	0.94	0.26	62,62,62,62	0
55	MG	1H	3126	1/1	0.94	0.42	61,61,61,61	0
55	MG	14	3451	1/1	0.94	0.13	74,74,74,74	0
55	MG	16	215	1/1	0.94	0.09	93,93,93,93	0
55	MG	1G	1729	1/1	0.94	0.05	93,93,93,93	0
55	MG	14	3458	1/1	0.94	0.10	108,108,108,108	0
55	MG	13	1679	1/1	0.94	0.34	80,80,80,80	0
55	MG	1H	3478	1/1	0.94	0.08	82,82,82,82	0
55	MG	14	3249	1/1	0.94	0.24	87,87,87,87	0
55	MG	1H	3429	1/1	0.94	0.11	71,71,71,71	0
55	MG	1G	1611	1/1	0.94	0.15	132,132,132,132	0
55	MG	14	3332	1/1	0.94	0.27	83,83,83,83	0
55	MG	14	3030	1/1	0.94	0.32	60,60,60,60	0
55	MG	1H	3484	1/1	0.94	0.06	118,118,118,118	0
55	MG	1H	3223	1/1	0.94	0.34	97,97,97,97	0
55	MG	F5	101	1/1	0.94	0.33	77,77,77,77	0
55	MG	1H	3145	1/1	0.94	0.26	46,46,46,46	0
55	MG	14	3090	1/1	0.94	0.37	70,70,70,70	0
55	MG	13	1735	1/1	0.94	0.04	106,106,106,106	0
55	MG	14	3460	1/1	0.94	0.06	112,112,112,112	0
55	MG	1G	1697	1/1	0.94	0.41	85,85,85,85	0
55	MG	1H	3437	1/1	0.94	0.12	66,66,66,66	0
55	MG	14	3153	1/1	0.94	0.44	82,82,82,82	0
55	MG	14	3052	1/1	0.94	0.37	65,65,65,65	0
55	MG	13	1720	1/1	0.94	0.09	129,129,129,129	0
55	MG	1H	3461	1/1	0.94	0.12	54,54,54,54	0
55	MG	1H	3392	1/1	0.94	0.29	73,73,73,73	0
55	MG	1H	3090	1/1	0.94	0.26	47,47,47,47	0
55	MG	1H	3107	1/1	0.94	0.46	81,81,81,81	0
55	MG	1H	3035	1/1	0.94	0.26	75,75,75,75	0
55	MG	1H	3001	1/1	0.94	0.40	50,50,50,50	0
55	MG	1H	3496	1/1	0.94	0.11	78,78,78,78	0
55	MG	1H	3136	1/1	0.94	0.56	85,85,85,85	0
55	MG	1H	3354	1/1	0.94	0.43	88,88,88,88	0
55	MG	1H	3483	1/1	0.94	0.05	84,84,84,84	0
55	MG	13	1641	1/1	0.94	0.29	67,67,67,67	0
55	MG	1H	3115	1/1	0.94	0.27	51,51,51,51	0
55	MG	1G	1735	1/1	0.94	0.08	96,96,96,96	0
55	MG	1G	1649	1/1	0.94	0.37	93,93,93,93	0
55	MG	13	1669	1/1	0.94	0.46	77,77,77,77	0
55	MG	14	3039	1/1	0.94	0.15	67,67,67,67	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
55	MG	14	3180	1/1	0.95	0.41	82,82,82,82	0
55	MG	13	1612	1/1	0.95	0.32	102,102,102,102	0
55	MG	1H	3466	1/1	0.95	0.15	59,59,59,59	0
55	MG	14	3348	1/1	0.95	0.18	65,65,65,65	0
55	MG	1G	1661	1/1	0.95	0.38	76,76,76,76	0
55	MG	1H	3472	1/1	0.95	0.07	82,82,82,82	0
55	MG	1G	1711	1/1	0.95	0.30	73,73,73,73	0
55	MG	1H	3007	1/1	0.95	0.33	62,62,62,62	0
55	MG	16	202	1/1	0.95	0.26	84,84,84,84	0
55	MG	14	3033	1/1	0.95	0.30	71,71,71,71	0
55	MG	1H	3460	1/1	0.95	0.06	87,87,87,87	0
55	MG	1H	3409	1/1	0.95	0.12	62,62,62,62	0
55	MG	1H	3054	1/1	0.95	0.39	51,51,51,51	0
55	MG	1H	3428	1/1	0.95	0.10	74,74,74,74	0
55	MG	1G	1657	1/1	0.95	0.29	87,87,87,87	0
55	MG	13	1718	1/1	0.95	0.12	85,85,85,85	0
55	MG	14	3247	1/1	0.95	0.07	79,79,79,79	0
55	MG	14	3204	1/1	0.95	0.36	70,70,70,70	0
55	MG	1H	3155	1/1	0.95	0.28	38,38,38,38	0
55	MG	1H	3321	1/1	0.95	0.48	79,79,79,79	0
55	MG	14	3041	1/1	0.95	0.32	58,58,58,58	0
55	MG	1H	3471	1/1	0.95	0.08	71,71,71,71	0
55	MG	1H	3055	1/1	0.95	0.47	77,77,77,77	0
55	MG	14	3118	1/1	0.95	0.22	84,84,84,84	0
55	MG	1H	3057	1/1	0.95	0.26	84,84,84,84	0
55	MG	1G	1612	1/1	0.95	0.06	84,84,84,84	0
55	MG	13	1659	1/1	0.95	0.33	102,102,102,102	0
55	MG	14	3229	1/1	0.95	0.21	64,64,64,64	0
55	MG	1H	3459	1/1	0.95	0.08	75,75,75,75	0
55	MG	1H	3287	1/1	0.95	0.38	78,78,78,78	0
55	MG	1H	3267	1/1	0.95	0.27	57,57,57,57	0
55	MG	14	3371	1/1	0.95	0.24	84,84,84,84	0
55	MG	1H	3028	1/1	0.95	0.17	53,53,53,53	0
55	MG	14	3245	1/1	0.95	0.40	64,64,64,64	0
55	MG	14	3070	1/1	0.95	0.34	66,66,66,66	0
55	MG	1G	1681	1/1	0.95	0.36	88,88,88,88	0
55	MG	14	3146	1/1	0.95	0.39	64,64,64,64	0
55	MG	14	3044	1/1	0.95	0.16	43,43,43,43	0
55	MG	14	3061	1/1	0.95	0.32	70,70,70,70	0
55	MG	1H	3439	1/1	0.95	0.09	92,92,92,92	0
55	MG	1G	1747	1/1	0.95	0.26	86,86,86,86	0
55	MG	1H	3251	1/1	0.95	0.32	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	2K	101	1/1	0.95	0.25	118,118,118,118	0
55	MG	1H	3098	1/1	0.95	0.21	42,42,42,42	0
55	MG	13	1654	1/1	0.95	0.39	72,72,72,72	0
55	MG	14	3380	1/1	0.95	0.12	79,79,79,79	0
55	MG	1G	1621	1/1	0.95	0.20	91,91,91,91	0
55	MG	1H	3112	1/1	0.95	0.47	73,73,73,73	0
55	MG	1G	1603	1/1	0.95	0.35	76,76,76,76	0
55	MG	1G	1619	1/1	0.95	0.34	73,73,73,73	0
55	MG	14	3454	1/1	0.95	0.14	106,106,106,106	0
55	MG	1H	3077	1/1	0.95	0.28	59,59,59,59	0
55	MG	14	3046	1/1	0.95	0.27	75,75,75,75	0
55	MG	1H	3125	1/1	0.95	0.36	73,73,73,73	0
56	ZN	5A	101	1/1	0.95	0.11	133,133,133,133	0
55	MG	14	3028	1/1	0.95	0.25	77,77,77,77	0
55	MG	16	201	1/1	0.95	0.15	110,110,110,110	0
55	MG	13	1724	1/1	0.95	0.14	107,107,107,107	0
55	MG	14	3133	1/1	0.95	0.35	71,71,71,71	0
55	MG	1H	3289	1/1	0.95	0.16	78,78,78,78	0
55	MG	14	3137	1/1	0.95	0.30	69,69,69,69	0
55	MG	1H	3475	1/1	0.95	0.09	70,70,70,70	0
55	MG	13	1670	1/1	0.95	0.11	106,106,106,106	0
55	MG	14	3110	1/1	0.95	0.34	63,63,63,63	0
55	MG	14	3192	1/1	0.95	0.09	56,56,56,56	0
55	MG	14	3091	1/1	0.95	0.35	81,81,81,81	0
55	MG	14	3395	1/1	0.95	0.11	65,65,65,65	0
55	MG	14	3165	1/1	0.95	0.18	74,74,74,74	0
55	MG	1H	3425	1/1	0.95	0.13	61,61,61,61	0
55	MG	13	1601	1/1	0.95	0.21	103,103,103,103	0
55	MG	1H	3383	1/1	0.95	0.12	60,60,60,60	0
55	MG	14	3068	1/1	0.95	0.33	66,66,66,66	0
55	MG	14	3429	1/1	0.95	0.10	77,77,77,77	0
55	MG	14	3108	1/1	0.95	0.36	85,85,85,85	0
55	MG	1H	3404	1/1	0.95	0.30	80,80,80,80	0
55	MG	14	3025	1/1	0.95	0.35	86,86,86,86	0
55	MG	1H	3274	1/1	0.95	0.44	71,71,71,71	0
55	MG	1H	3129	1/1	0.95	0.14	63,63,63,63	0
55	MG	14	3264	1/1	0.95	0.28	84,84,84,84	0
55	MG	1H	3395	1/1	0.95	0.41	76,76,76,76	0
55	MG	2L	101	1/1	0.95	0.21	77,77,77,77	0
55	MG	1H	3006	1/1	0.95	0.27	67,67,67,67	0
55	MG	14	3101	1/1	0.95	0.24	65,65,65,65	0
55	MG	14	3379	1/1	0.95	0.11	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	14	3098	1/1	0.95	0.33	46,46,46,46	0
56	ZN	32	302	1/1	0.95	0.33	111,111,111,111	0
55	MG	14	3215	1/1	0.95	0.28	76,76,76,76	0
55	MG	13	1627	1/1	0.95	0.48	65,65,65,65	0
55	MG	1H	3202	1/1	0.95	0.13	94,94,94,94	0
55	MG	1H	3433	1/1	0.96	0.12	54,54,54,54	0
55	MG	14	3383	1/1	0.96	0.08	81,81,81,81	0
55	MG	13	1675	1/1	0.96	0.42	85,85,85,85	0
55	MG	1H	3494	1/1	0.96	0.10	81,81,81,81	0
55	MG	1H	3435	1/1	0.96	0.12	76,76,76,76	0
55	MG	1H	3161	1/1	0.96	0.28	69,69,69,69	0
55	MG	14	3427	1/1	0.96	0.07	75,75,75,75	0
55	MG	1H	3214	1/1	0.96	0.31	64,64,64,64	0
55	MG	14	3194	1/1	0.96	0.13	46,46,46,46	0
55	MG	14	3251	1/1	0.96	0.26	67,67,67,67	0
55	MG	1H	3191	1/1	0.96	0.51	64,64,64,64	0
55	MG	1H	3074	1/1	0.96	0.34	82,82,82,82	0
55	MG	1H	3403	1/1	0.96	0.07	111,111,111,111	0
55	MG	14	3407	1/1	0.96	0.09	83,83,83,83	0
55	MG	14	3340	1/1	0.96	0.22	79,79,79,79	0
55	MG	14	3027	1/1	0.96	0.17	71,71,71,71	0
55	MG	1H	3097	1/1	0.96	0.39	70,70,70,70	0
55	MG	14	3408	1/1	0.96	0.11	56,56,56,56	0
55	MG	14	3024	1/1	0.96	0.23	49,49,49,49	0
55	MG	1G	1713	1/1	0.96	0.23	107,107,107,107	0
55	MG	14	3344	1/1	0.96	0.14	95,95,95,95	0
55	MG	1H	3299	1/1	0.96	0.22	57,57,57,57	0
55	MG	14	3022	1/1	0.96	0.26	60,60,60,60	0
55	MG	1H	3020	1/1	0.96	0.30	52,52,52,52	0
55	MG	3A	201	1/1	0.96	0.17	81,81,81,81	0
55	MG	1H	3308	1/1	0.96	0.23	106,106,106,106	0
55	MG	14	3202	1/1	0.96	0.48	74,74,74,74	0
55	MG	14	3111	1/1	0.96	0.10	54,54,54,54	0
55	MG	14	3040	1/1	0.96	0.34	69,69,69,69	0
55	MG	1H	3052	1/1	0.96	0.33	73,73,73,73	0
55	MG	14	3209	1/1	0.96	0.29	88,88,88,88	0
55	MG	1H	3317	1/1	0.96	0.33	63,63,63,63	0
55	MG	1H	3166	1/1	0.96	0.24	67,67,67,67	0
55	MG	14	3047	1/1	0.96	0.27	57,57,57,57	0
55	MG	1H	3275	1/1	0.96	0.26	69,69,69,69	0
55	MG	14	3393	1/1	0.96	0.12	53,53,53,53	0
55	MG	1H	3171	1/1	0.96	0.46	82,82,82,82	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
55	MG	1H	3328	1/1	0.96	0.45	85,85,85,85	0
55	MG	16	214	1/1	0.96	0.07	86,86,86,86	0
55	MG	1G	1616	1/1	0.96	0.12	62,62,62,62	0
55	MG	13	1729	1/1	0.96	0.07	112,112,112,112	0
55	MG	14	3250	1/1	0.96	0.26	70,70,70,70	0
55	MG	1H	3455	1/1	0.96	0.13	47,47,47,47	0
55	MG	1H	3444	1/1	0.96	0.14	59,59,59,59	0
55	MG	14	3447	1/1	0.96	0.04	102,102,102,102	0
55	MG	1H	3187	1/1	0.96	0.36	83,83,83,83	0
55	MG	1H	3489	1/1	0.96	0.13	67,67,67,67	0
55	MG	1H	3242	1/1	0.96	0.20	45,45,45,45	0
55	MG	14	3031	1/1	0.96	0.30	73,73,73,73	0
55	MG	1H	3498	1/1	0.96	0.07	77,77,77,77	0
55	MG	13	1730	1/1	0.96	0.10	115,115,115,115	0
55	MG	1G	1606	1/1	0.96	0.20	80,80,80,80	0
55	MG	1G	1625	1/1	0.96	0.30	85,85,85,85	0
55	MG	1H	3261	1/1	0.96	0.41	72,72,72,72	0
55	MG	13	1606	1/1	0.96	0.27	92,92,92,92	0
55	MG	1H	3507	1/1	0.96	0.19	62,62,62,62	0
55	MG	14	3193	1/1	0.96	0.21	56,56,56,56	0
55	MG	1H	3516	1/1	0.96	0.07	88,88,88,88	0
55	MG	14	3316	1/1	0.96	0.14	70,70,70,70	0
55	MG	14	3189	1/1	0.96	0.32	63,63,63,63	0
55	MG	1H	3432	1/1	0.96	0.14	68,68,68,68	0
55	MG	1H	3045	1/1	0.96	0.34	88,88,88,88	0
55	MG	13	1683	1/1	0.96	0.12	122,122,122,122	0
55	MG	14	3055	1/1	0.96	0.32	61,61,61,61	0
55	MG	1H	3128	1/1	0.96	0.42	63,63,63,63	0
55	MG	1H	3436	1/1	0.96	0.09	94,94,94,94	0
55	MG	1H	3021	1/1	0.96	0.29	51,51,51,51	0
55	MG	14	3201	1/1	0.96	0.21	61,61,61,61	0
55	MG	1H	3382	1/1	0.96	0.20	79,79,79,79	0
55	MG	1H	3441	1/1	0.96	0.08	63,63,63,63	0
55	MG	13	1648	1/1	0.96	0.37	105,105,105,105	0
55	MG	14	3399	1/1	0.96	0.07	82,82,82,82	0
55	MG	14	3440	1/1	0.96	0.05	101,101,101,101	0
55	MG	1G	1634	1/1	0.96	0.37	80,80,80,80	0
55	MG	1H	3222	1/1	0.96	0.37	65,65,65,65	0
55	MG	1H	3420	1/1	0.96	0.12	52,52,52,52	0
55	MG	1H	3225	1/1	0.96	0.46	77,77,77,77	0
55	MG	29	301	1/1	0.96	0.25	72,72,72,72	0
55	MG	1H	3479	1/1	0.96	0.17	58,58,58,58	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
55	MG	1H	3279	1/1	0.96	0.37	96,96,96,96	0
55	MG	1H	3147	1/1	0.96	0.45	60,60,60,60	0
55	MG	13	1719	1/1	0.96	0.07	94,94,94,94	0
55	MG	1H	3270	1/1	0.97	0.15	84,84,84,84	0
55	MG	14	3339	1/1	0.97	0.28	74,74,74,74	0
55	MG	1H	3295	1/1	0.97	0.31	87,87,87,87	0
55	MG	14	3084	1/1	0.97	0.10	73,73,73,73	0
55	MG	1H	3367	1/1	0.97	0.10	67,67,67,67	0
55	MG	14	3097	1/1	0.97	0.32	54,54,54,54	0
55	MG	1H	3047	1/1	0.97	0.27	76,76,76,76	0
55	MG	14	3067	1/1	0.97	0.29	71,71,71,71	0
55	MG	14	3387	1/1	0.97	0.12	58,58,58,58	0
55	MG	1H	3424	1/1	0.97	0.11	58,58,58,58	0
55	MG	1G	1666	1/1	0.97	0.38	72,72,72,72	0
55	MG	14	3397	1/1	0.97	0.15	70,70,70,70	0
55	MG	1H	3031	1/1	0.97	0.31	82,82,82,82	0
55	MG	14	3243	1/1	0.97	0.22	78,78,78,78	0
55	MG	14	3391	1/1	0.97	0.12	62,62,62,62	0
55	MG	1H	3454	1/1	0.97	0.09	49,49,49,49	0
55	MG	1J	207	1/1	0.97	0.07	88,88,88,88	0
55	MG	1G	1743	1/1	0.97	0.18	105,105,105,105	0
55	MG	1H	3198	1/1	0.97	0.42	77,77,77,77	0
55	MG	14	3444	1/1	0.97	0.04	90,90,90,90	0
55	MG	14	3448	1/1	0.97	0.06	87,87,87,87	0
55	MG	13	1626	1/1	0.97	0.39	65,65,65,65	0
55	MG	14	3004	1/1	0.97	0.25	57,57,57,57	0
55	MG	1H	3430	1/1	0.97	0.10	76,76,76,76	0
55	MG	14	3062	1/1	0.97	0.32	72,72,72,72	0
55	MG	14	3183	1/1	0.97	0.40	56,56,56,56	0
55	MG	1H	3217	1/1	0.97	0.65	92,92,92,92	0
55	MG	1H	3487	1/1	0.97	0.04	81,81,81,81	0
55	MG	14	3114	1/1	0.97	0.23	56,56,56,56	0
55	MG	14	3418	1/1	0.97	0.13	72,72,72,72	0
55	MG	1H	3015	1/1	0.97	0.38	46,46,46,46	0
55	MG	14	3382	1/1	0.97	0.12	55,55,55,55	0
55	MG	14	3452	1/1	0.97	0.07	100,100,100,100	0
55	MG	1H	3012	1/1	0.97	0.37	57,57,57,57	0
55	MG	14	3010	1/1	0.97	0.21	47,47,47,47	0
55	MG	1H	3036	1/1	0.97	0.27	70,70,70,70	0
55	MG	1H	3026	1/1	0.97	0.31	66,66,66,66	0
55	MG	1H	3023	1/1	0.97	0.35	55,55,55,55	0
55	MG	1H	3453	1/1	0.97	0.12	42,42,42,42	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
55	MG	14	3122	1/1	0.97	0.25	61,61,61,61	0
55	MG	14	3232	1/1	0.97	0.28	98,98,98,98	0
55	MG	14	3207	1/1	0.97	0.30	77,77,77,77	0
55	MG	13	1636	1/1	0.97	0.31	88,88,88,88	0
55	MG	1H	3237	1/1	0.97	0.38	67,67,67,67	0
55	MG	14	3060	1/1	0.97	0.35	64,64,64,64	0
55	MG	14	3116	1/1	0.97	0.36	49,49,49,49	0
55	MG	14	3104	1/1	0.97	0.31	59,59,59,59	0
55	MG	1H	3241	1/1	0.97	0.23	69,69,69,69	0
55	MG	1H	3445	1/1	0.97	0.13	59,59,59,59	0
55	MG	1H	3249	1/1	0.97	0.53	66,66,66,66	0
55	MG	14	3203	1/1	0.97	0.27	55,55,55,55	0
55	MG	1H	3470	1/1	0.97	0.08	74,74,74,74	0
55	MG	14	3240	1/1	0.97	0.16	95,95,95,95	0
55	MG	1G	1730	1/1	0.97	0.14	82,82,82,82	0
55	MG	1H	3081	1/1	0.97	0.37	73,73,73,73	0
55	MG	1G	1628	1/1	0.97	0.20	90,90,90,90	0
55	MG	14	3007	1/1	0.97	0.29	58,58,58,58	0
55	MG	14	3005	1/1	0.97	0.29	52,52,52,52	0
55	MG	1H	3192	1/1	0.97	0.29	87,87,87,87	0
55	MG	1H	3011	1/1	0.97	0.35	54,54,54,54	0
55	MG	29	302	1/1	0.97	0.26	51,51,51,51	0
55	MG	1G	1716	1/1	0.97	0.08	110,110,110,110	0
55	MG	14	3403	1/1	0.97	0.11	69,69,69,69	0
55	MG	1G	1682	1/1	0.97	0.15	87,87,87,87	0
55	MG	14	3237	1/1	0.97	0.34	74,74,74,74	0
55	MG	14	3415	1/1	0.97	0.06	62,62,62,62	0
55	MG	1H	3123	1/1	0.97	0.14	78,78,78,78	0
55	MG	1H	3264	1/1	0.97	0.40	100,100,100,100	0
55	MG	14	3043	1/1	0.97	0.36	62,62,62,62	0
55	MG	1H	3423	1/1	0.97	0.11	61,61,61,61	0
55	MG	14	3419	1/1	0.97	0.06	94,94,94,94	0
55	MG	1H	3413	1/1	0.97	0.10	44,44,44,44	0
55	MG	1H	3467	1/1	0.97	0.18	72,72,72,72	0
55	MG	1H	3040	1/1	0.97	0.34	71,71,71,71	0
55	MG	1H	3463	1/1	0.97	0.15	52,52,52,52	0
55	MG	1H	3082	1/1	0.97	0.38	72,72,72,72	0
56	ZN	5I	101	1/1	0.97	0.14	116,116,116,116	0
55	MG	1H	3418	1/1	0.97	0.10	63,63,63,63	0
55	MG	1G	1601	1/1	0.97	0.25	76,76,76,76	0
55	MG	1H	3142	1/1	0.97	0.25	74,74,74,74	0
55	MG	1H	3412	1/1	0.97	0.14	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	3107	1/1	0.97	0.43	80,80,80,80	0
55	MG	1H	3456	1/1	0.97	0.15	51,51,51,51	0
55	MG	13	1619	1/1	0.97	0.40	74,74,74,74	0
55	MG	1H	3111	1/1	0.97	0.34	71,71,71,71	0
55	MG	1G	1715	1/1	0.97	0.21	106,106,106,106	0
55	MG	1G	1631	1/1	0.97	0.27	90,90,90,90	0
55	MG	14	3405	1/1	0.97	0.08	64,64,64,64	0
55	MG	14	3003	1/1	0.97	0.26	47,47,47,47	0
55	MG	14	3086	1/1	0.97	0.28	51,51,51,51	0
55	MG	1H	3083	1/1	0.97	0.33	58,58,58,58	0
55	MG	1H	3061	1/1	0.97	0.43	71,71,71,71	0
55	MG	1G	1732	1/1	0.97	0.05	113,113,113,113	0
55	MG	14	3008	1/1	0.97	0.31	53,53,53,53	0
55	MG	14	3388	1/1	0.97	0.13	61,61,61,61	0
55	MG	1H	3053	1/1	0.97	0.20	61,61,61,61	0
55	MG	13	1631	1/1	0.97	0.16	60,60,60,60	0
55	MG	1G	1736	1/1	0.97	0.11	94,94,94,94	0
55	MG	1H	3151	1/1	0.97	0.44	76,76,76,76	0
55	MG	13	1723	1/1	0.97	0.08	86,86,86,86	0
55	MG	1H	3451	1/1	0.98	0.09	54,54,54,54	0
55	MG	1H	3158	1/1	0.98	0.21	71,71,71,71	0
55	MG	1G	1602	1/1	0.98	0.41	75,75,75,75	0
55	MG	1H	3018	1/1	0.98	0.21	50,50,50,50	0
55	MG	1H	3419	1/1	0.98	0.14	48,48,48,48	0
55	MG	1H	3421	1/1	0.98	0.14	52,52,52,52	0
55	MG	14	3417	1/1	0.98	0.12	51,51,51,51	0
55	MG	14	3016	1/1	0.98	0.17	63,63,63,63	0
55	MG	13	1602	1/1	0.98	0.21	78,78,78,78	0
55	MG	1H	3101	1/1	0.98	0.14	50,50,50,50	0
55	MG	1H	3089	1/1	0.98	0.34	38,38,38,38	0
55	MG	14	3347	1/1	0.98	0.17	83,83,83,83	0
55	MG	14	3009	1/1	0.98	0.28	58,58,58,58	0
55	MG	14	3095	1/1	0.98	0.20	65,65,65,65	0
55	MG	14	3057	1/1	0.98	0.42	54,54,54,54	0
55	MG	14	3404	1/1	0.98	0.05	79,79,79,79	0
55	MG	13	1609	1/1	0.98	0.23	83,83,83,83	0
55	MG	1H	3492	1/1	0.98	0.11	83,83,83,83	0
55	MG	13	1716	1/1	0.98	0.17	74,74,74,74	0
55	MG	14	3006	1/1	0.98	0.33	56,56,56,56	0
55	MG	1H	3481	1/1	0.98	0.12	64,64,64,64	0
55	MG	1H	3002	1/1	0.98	0.33	53,53,53,53	0
55	MG	14	3058	1/1	0.98	0.20	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	13	1728	1/1	0.98	0.07	76,76,76,76	0
55	MG	14	3423	1/1	0.98	0.09	84,84,84,84	0
55	MG	1H	3072	1/1	0.98	0.33	75,75,75,75	0
55	MG	1H	3206	1/1	0.98	0.44	72,72,72,72	0
55	MG	1H	3133	1/1	0.98	0.15	49,49,49,49	0
55	MG	1H	3010	1/1	0.98	0.40	66,66,66,66	0
55	MG	14	3072	1/1	0.98	0.35	54,54,54,54	0
55	MG	1H	3095	1/1	0.98	0.38	46,46,46,46	0
55	MG	14	3164	1/1	0.98	0.26	60,60,60,60	0
55	MG	13	1630	1/1	0.98	0.18	61,61,61,61	0
55	MG	1H	3440	1/1	0.98	0.07	91,91,91,91	0
56	ZN	3E	302	1/1	0.98	0.35	102,102,102,102	0
55	MG	14	3422	1/1	0.98	0.10	53,53,53,53	0
55	MG	2K	102	1/1	0.98	0.44	93,93,93,93	0
55	MG	1H	3062	1/1	0.98	0.18	48,48,48,48	0
55	MG	14	3012	1/1	0.98	0.30	53,53,53,53	0
55	MG	1H	3019	1/1	0.98	0.34	61,61,61,61	0
55	MG	14	3398	1/1	0.98	0.13	83,83,83,83	0
55	MG	14	3390	1/1	0.98	0.10	52,52,52,52	0
55	MG	1H	3017	1/1	0.98	0.33	47,47,47,47	0
55	MG	14	3216	1/1	0.98	0.29	72,72,72,72	0
55	MG	14	3381	1/1	0.98	0.13	52,52,52,52	0
55	MG	14	3050	1/1	0.98	0.15	65,65,65,65	0
55	MG	1H	3505	1/1	0.98	0.07	69,69,69,69	0
55	MG	1H	3411	1/1	0.98	0.14	67,67,67,67	0
55	MG	1H	3521	1/1	0.98	0.09	47,47,47,47	0
55	MG	1H	3099	1/1	0.98	0.47	52,52,52,52	0
55	MG	1H	3113	1/1	0.98	0.27	40,40,40,40	0
55	MG	1H	3464	1/1	0.98	0.14	52,52,52,52	0
55	MG	1H	3091	1/1	0.98	0.41	59,59,59,59	0
55	MG	14	3035	1/1	0.98	0.37	57,57,57,57	0
55	MG	14	3386	1/1	0.98	0.12	56,56,56,56	0
55	MG	14	3465	1/1	0.98	0.32	64,64,64,64	0
55	MG	1H	3485	1/1	0.98	0.15	75,75,75,75	0
55	MG	14	3112	1/1	0.98	0.33	68,68,68,68	0
55	MG	14	3063	1/1	0.98	0.35	51,51,51,51	0
55	MG	14	3011	1/1	0.98	0.33	47,47,47,47	0
55	MG	1H	3050	1/1	0.98	0.40	47,47,47,47	0
55	MG	1G	1623	1/1	0.98	0.28	87,87,87,87	0
55	MG	14	3015	1/1	0.98	0.17	64,64,64,64	0
55	MG	1H	3474	1/1	0.98	0.10	79,79,79,79	0
55	MG	14	3065	1/1	0.98	0.32	50,50,50,50	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
55	MG	1H	3473	1/1	0.98	0.06	64,64,64,64	0
55	MG	1H	3319	1/1	0.98	0.21	60,60,60,60	0
55	MG	14	3049	1/1	0.98	0.12	55,55,55,55	0
55	MG	1H	3447	1/1	0.98	0.09	62,62,62,62	0
55	MG	1H	3014	1/1	0.98	0.31	51,51,51,51	0
55	MG	1H	3228	1/1	0.98	0.32	63,63,63,63	0
55	MG	14	3392	1/1	0.98	0.10	54,54,54,54	0
55	MG	1H	3468	1/1	0.98	0.12	59,59,59,59	0
55	MG	14	3410	1/1	0.98	0.16	58,58,58,58	0
55	MG	1H	3446	1/1	0.98	0.10	52,52,52,52	0
55	MG	1H	3025	1/1	0.98	0.40	80,80,80,80	0
55	MG	14	3412	1/1	0.98	0.16	49,49,49,49	0
55	MG	14	3048	1/1	0.98	0.20	55,55,55,55	0
55	MG	14	3406	1/1	0.98	0.11	61,61,61,61	0
55	MG	14	3032	1/1	0.98	0.24	64,64,64,64	0
55	MG	1H	3009	1/1	0.98	0.38	44,44,44,44	0
55	MG	14	3411	1/1	0.98	0.10	63,63,63,63	0
55	MG	13	1725	1/1	0.98	0.11	99,99,99,99	0
55	MG	1H	3415	1/1	0.99	0.13	50,50,50,50	0
55	MG	1H	3462	1/1	0.99	0.14	49,49,49,49	0
55	MG	14	3013	1/1	0.99	0.23	56,56,56,56	0
55	MG	14	3102	1/1	0.99	0.21	61,61,61,61	0
55	MG	1H	3417	1/1	0.99	0.11	40,40,40,40	0
55	MG	1H	3137	1/1	0.99	0.26	60,60,60,60	0
55	MG	14	3002	1/1	0.99	0.23	67,67,67,67	0
55	MG	1H	3003	1/1	0.99	0.34	54,54,54,54	0
55	MG	1H	3480	1/1	0.99	0.12	47,47,47,47	0
55	MG	14	3389	1/1	0.99	0.17	53,53,53,53	0
55	MG	14	3259	1/1	0.99	0.29	82,82,82,82	0
55	MG	1G	1728	1/1	0.99	0.13	73,73,73,73	0
55	MG	14	3053	1/1	0.99	0.33	59,59,59,59	0
55	MG	1H	3071	1/1	0.99	0.36	51,51,51,51	0
55	MG	1H	3085	1/1	0.99	0.20	63,63,63,63	0
55	MG	1H	3070	1/1	0.99	0.27	60,60,60,60	0
55	MG	1H	3004	1/1	0.99	0.39	49,49,49,49	0
55	MG	14	3073	1/1	0.99	0.26	58,58,58,58	0
55	MG	1H	3458	1/1	0.99	0.15	70,70,70,70	0
55	MG	1H	3024	1/1	0.99	0.15	61,61,61,61	0
55	MG	14	3445	1/1	0.99	0.10	58,58,58,58	0
55	MG	1G	1647	1/1	0.99	0.25	80,80,80,80	0
55	MG	13	1739	1/1	0.99	0.22	90,90,90,90	0
55	MG	1H	3450	1/1	0.99	0.22	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	14	3377	1/1	0.99	0.10	57,57,57,57	0
55	MG	14	3384	1/1	0.99	0.09	54,54,54,54	0
55	MG	14	3077	1/1	0.99	0.30	61,61,61,61	0
55	MG	1H	3013	1/1	0.99	0.30	47,47,47,47	0
55	MG	1H	3426	1/1	0.99	0.10	67,67,67,67	0
55	MG	14	3223	1/1	0.99	0.20	64,64,64,64	0
55	MG	G8	201	1/1	0.99	0.14	77,77,77,77	0
55	MG	14	3076	1/1	0.99	0.32	47,47,47,47	0
55	MG	1H	3422	1/1	0.99	0.07	56,56,56,56	0
55	MG	1H	3051	1/1	0.99	0.24	47,47,47,47	0
55	MG	14	3064	1/1	0.99	0.34	52,52,52,52	0
55	MG	1H	3503	1/1	1.00	0.10	57,57,57,57	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.