



# wwPDB X-ray Structure Validation Summary Report ⓘ

May 23, 2020 – 03:18 pm BST

PDB ID : 4WR6  
Title : Complex of 70S ribosome with tRNA-Tyr and mRNA with A-A mismatch in the first position in the A-site.  
Authors : Rozov, A.; Demeshkina, N.; Yusupov, M.; Yusupova, G.  
Deposited on : 2014-10-23  
Resolution : 3.05 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	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11



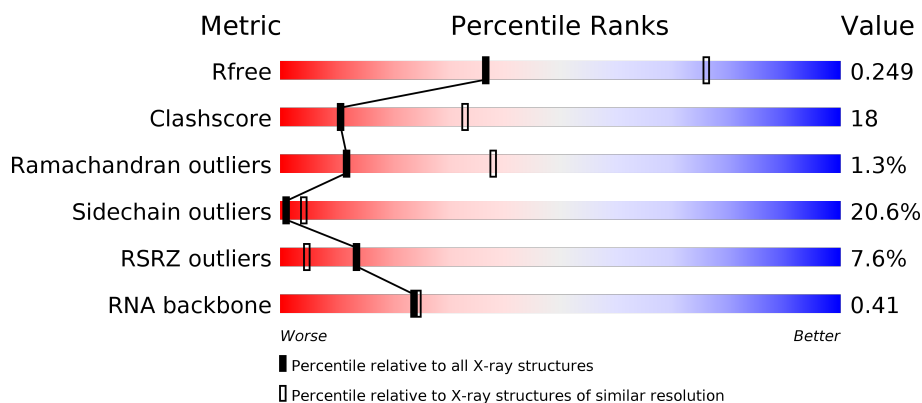
# 1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.05 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	130704	1754 (3.10-3.02)
Clashscore	141614	1864 (3.10-3.02)
Ramachandran outliers	138981	1794 (3.10-3.02)
Sidechain outliers	138945	1793 (3.10-3.02)
RSRZ outliers	127900	1713 (3.10-3.02)
RNA backbone	3102	1036 (3.32-2.80)

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 respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	13	1522	<div> <div>2%</div> <div>30% 46% 19% . .</div> </div>
2	12	256	<div> <div>3%</div> <div>37% 42% 14% 7%</div> </div>
2	1E	256	<div> <div>2%</div> <div>42% 40% 11% 7%</div> </div>
3	22	239	<div> <div>7%</div> <div>36% 41% 9% 14%</div> </div>

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Mol	Chain	Length	Quality of chain
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	
15	6I	89	

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Mol	Chain	Length	Quality of chain
16	7A	88	
16	7I	88	
17	8A	105	
17	8I	105	
18	9A	88	
18	9I	88	
19	AA	93	
19	AI	93	
20	BA	106	
20	BI	106	
21	1B	27	
21	1F	27	
22	1K	85	
22	3K	85	
23	2K	77	
24	4K	27	
25	14	2917	
25	1H	2917	
26	16	122	
26	1J	122	
27	11	276	
27	19	276	
28	21	206	
28	29	206	
29	31	210	

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Mol	Chain	Length	Quality of chain
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	
39	B8	146	
40	85	118	
40	C8	118	
41	95	101	
41	D8	101	

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Mol	Chain	Length	Quality of chain
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	
52	L5	49	
52	P8	49	
53	M5	65	
53	Q8	65	
54	1G	1522	

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Mol	Chain	Length	Quality of chain
55	1L	85	
55	3L	85	
56	2L	77	
57	4L	27	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
58	MG	14	3064	-	-	-	X
58	MG	14	3146	-	-	-	X
58	MG	14	3187	-	-	-	X
58	MG	14	3229	-	-	-	X
58	MG	14	3289	-	-	-	X
58	MG	14	3298	-	-	-	X
58	MG	14	3308	-	-	-	X
58	MG	1H	3313	-	-	-	X
58	MG	1H	3359	-	-	-	X
58	MG	1H	3365	-	-	-	X
58	MG	1H	3366	-	-	-	X
58	MG	1H	3367	-	-	-	X
58	MG	1H	3370	-	-	-	X
58	MG	1H	3373	-	-	-	X



## 2 Entry composition

There are 60 unique types of molecules in this entry. The entry contains 299318 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	1498	Total	C	N	O	P	0	0	0
			32207	14334	5973	10402	1498			

- 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			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
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			
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	119	Total	C	N	O	S	0	0	0
			884	549	168	164	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.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
14	5I	61	Total	C	N	O	S	0	0	0
			498	316	105	72	5			
14	5A	58	Total	C	N	O	S	0	0	0
			475	303	99	69	4			

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

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

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



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
16	7I	84	Total	C	N	O	S	0	0	0
			705	446	140	118	1			
16	7A	84	Total	C	N	O	S	0	0	0
			705	446	140	118	1			

- Molecule 17 is a protein called 30S ribosomal protein S17.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
17	8I	100	Total	C	N	O	S	0	0	0
			834	534	155	143	2			
17	8A	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	69	Total	C	N	O	0	0	0
			564	361	110	93			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
19	AI	83	Total	C	N	O	S	0	0	0
			665	424	124	115	2			
19	AA	82	Total	C	N	O	S	0	0	0
			640	407	118	113	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	22	Total	C	N	O	0	0	0
			188	116	44	28			

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
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	1K	85	Total	C	N	O	P	S	0	0	0
			1825	822	323	593	85	2			
22	3K	85	Total	C	N	O	P	S	0	0	0
			1825	822	323	593	85	2			

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

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
23	2K	77	Total	C	N	O	P	S	0	0	0
			1646	735	298	535	77	1			

- Molecule 24 is a RNA chain called mRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
24	4K	15	Total	C	N	O	P	0	1	0
			349	158	75	100	16			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
25	1H	2912	Total	C	N	O	P	0	0	0
			62707	27911	11722	20163	2911			
25	14	2907	Total	C	N	O	P	0	0	0
			62605	27865	11708	20126	2906			

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 26 is a RNA chain called 5S ribosomal RNA.



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
26	16	122	Total	C	N	O	P	0	0	0
			2617	1166	486	844	121			
26	1J	122	Total	C	N	O	P	0	0	0
			2617	1166	486	844	121			

- Molecule 27 is a protein called 50S ribosomal protein 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			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
31	59	171	Total	C	N	O	S	0	0	0
			1316	835	247	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			
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	138	Total	C	N	O	S	0	0	0
			1098	702	208	181	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	136	Total	C	N	O	0	0	0
			1133	705	233	195			
39	75	137	Total	C	N	O	S	0	0
			1141	710	234	196	1		

- 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	94	Total	C	N	O	S	0	0	0
			742	482	134	125	1			
43	B5	92	Total	C	N	O		0	0	0
			725	471	131	123				

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
44	G8	102	Total	C	N	O	S	0	0	0
			778	501	147	125	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	77	Total	C	N	O	S	0	0	0
			612	379	129	103	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	93	Total	C	N	O	S	0	0	0
			729	457	145	126	1			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
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	66	Total	C	N	O	S	0	0	0
			558	346	113	98	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	49	Total	C	N	O	S	0	0	0
			374	232	76	61	5			
51	J5	58	Total	C	N	O	S	0	0	0
			453	285	89	74	5			

- Molecule 52 is a protein called 50S ribosomal protein L34.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
52	P8	45	Total	C	N	O	S	0	0	0
			391	240	97	52	2			
52	L5	45	Total	C	N	O	S	0	0	0
			391	240	97	52	2			



- Molecule 53 is a protein called 50S ribosomal protein L35.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
53	Q8	62	Total	C	N	O	S	0	0	0
			448	284	86	76	2			
53	M5	60	Total	C	N	O	S	0	0	0
			480	306	98	74	2			

- Molecule 54 is a RNA chain called 16S ribosomal RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
54	1G	1498	Total	C	N	O	P	0	0	0
			32204	14334	5973	10400	1497			

- Molecule 55 is a RNA chain called tRNA-Tyr.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
55	1L	85	Total	C	N	O	P	0	0	0
			1807	807	323	592	85			
55	3L	85	Total	C	N	O	P	0	0	0
			1807	807	323	592	85			

- Molecule 56 is a RNA chain called tRNA-fMet.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
56	2L	77	Total	C	N	O	P	S	0	0
			1645	734	298	535	77	1		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
2L	18	C	U	conflict	GB 675817920

- Molecule 57 is a RNA chain called mRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
57	4L	16	Total	C	N	O	P	0	0	0
			349	158	75	100	16			

- Molecule 58 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
58	98	2	Total	Mg	0	0
			2	2		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
58	45	1	Total 1	Mg 1	0	0
58	P8	1	Total 1	Mg 1	0	0
58	85	1	Total 1	Mg 1	0	0
58	C5	1	Total 1	Mg 1	0	0
58	13	138	Total 138	Mg 138	0	0
58	1J	6	Total 6	Mg 6	0	0
58	16	13	Total 13	Mg 13	0	0
58	25	1	Total 1	Mg 1	0	0
58	21	2	Total 2	Mg 2	0	0
58	31	4	Total 4	Mg 4	0	0
58	L8	2	Total 2	Mg 2	0	0
58	I8	2	Total 2	Mg 2	0	0
58	8E	1	Total 1	Mg 1	0	0
58	L5	1	Total 1	Mg 1	0	0
58	29	3	Total 3	Mg 3	0	0
58	2K	6	Total 6	Mg 6	0	0
58	1L	1	Total 1	Mg 1	0	0
58	39	1	Total 1	Mg 1	0	0
58	1G	90	Total 90	Mg 90	0	0
58	4E	1	Total 1	Mg 1	0	0
58	11	1	Total 1	Mg 1	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
58	1H	475	Total 475	Mg 475	0	0
58	3I	1	Total 1	Mg 1	0	0
58	14	398	Total 398	Mg 398	0	0
58	78	1	Total 1	Mg 1	0	0
58	3E	1	Total 1	Mg 1	0	0
58	3L	1	Total 1	Mg 1	0	0
58	1K	1	Total 1	Mg 1	0	0
58	2L	3	Total 3	Mg 3	0	0

- Molecule 59 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
59	32	1	Total 1	Zn 1	0	0
59	3E	1	Total 1	Zn 1	0	0
59	5I	1	Total 1	Zn 1	0	0
59	5A	1	Total 1	Zn 1	0	0
59	G8	1	Total 1	Zn 1	0	0
59	C5	1	Total 1	Zn 1	0	0

- Molecule 60 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
60	13	100	Total 100	O 100	0	0
60	3E	2	Total 2	O 2	0	0
60	3I	2	Total 2	O 2	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
60	5I	1	Total O 1 1	0	0
60	7I	1	Total O 1 1	0	0
60	1K	1	Total O 1 1	0	0
60	2K	6	Total O 6 6	0	0
60	4K	2	Total O 2 2	0	0
60	1H	538	Total O 538 538	0	0
60	16	11	Total O 11 11	0	0
60	11	4	Total O 4 4	0	0
60	21	2	Total O 2 2	0	0
60	31	4	Total O 4 4	0	0
60	78	4	Total O 4 4	0	0
60	D8	1	Total O 1 1	0	0
60	F8	1	Total O 1 1	0	0
60	L8	3	Total O 3 3	0	0
60	1G	51	Total O 51 51	0	0
60	32	1	Total O 1 1	0	0
60	BA	1	Total O 1 1	0	0
60	4L	1	Total O 1 1	0	0
60	14	409	Total O 409 409	0	0
60	19	7	Total O 7 7	0	0
60	29	2	Total O 2 2	0	0

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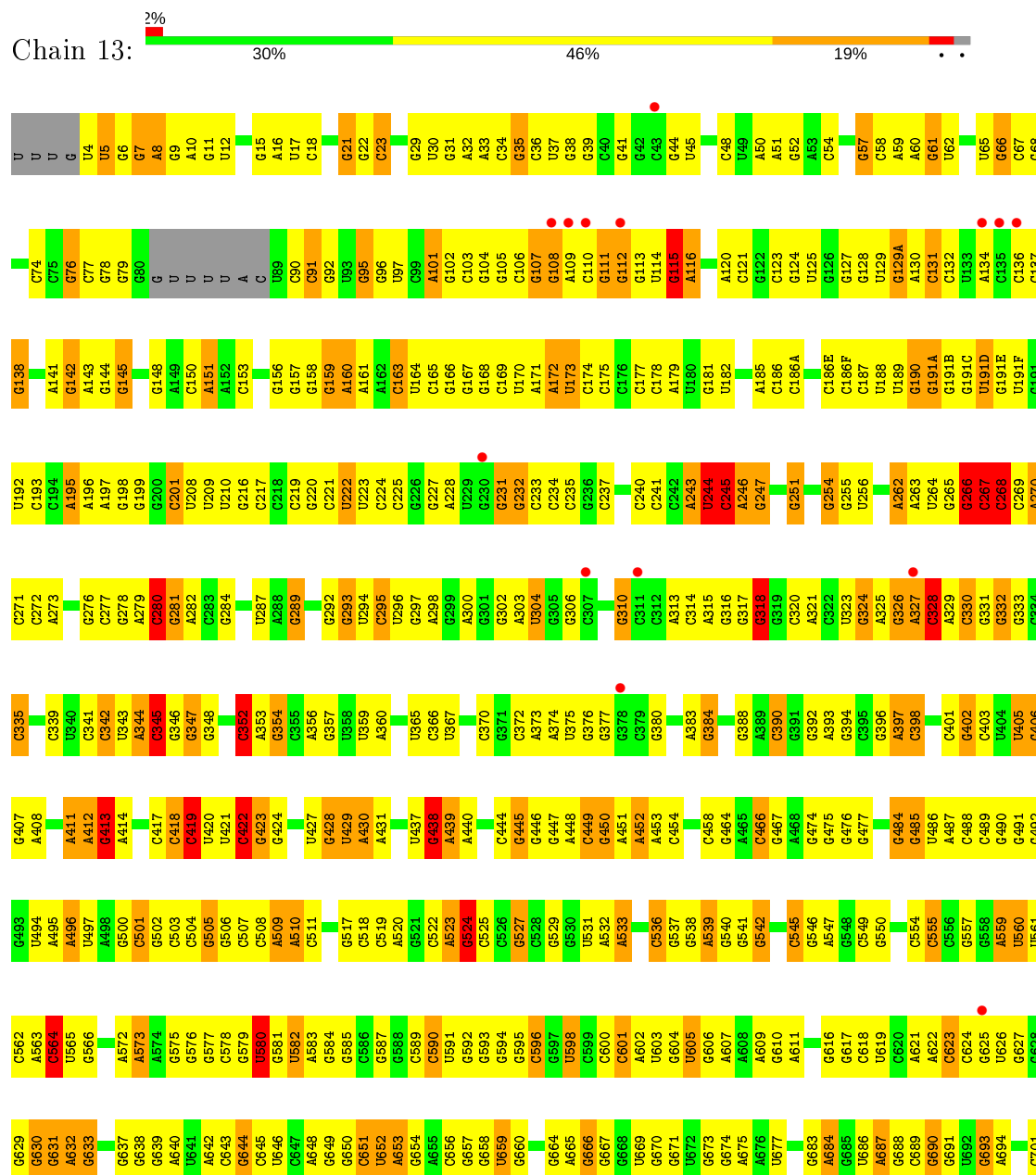
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
60	39	4	Total 4	O 4	0	0
60	35	1	Total 1	O 1	0	0
60	55	1	Total 1	O 1	0	0
60	75	1	Total 1	O 1	0	0
60	85	1	Total 1	O 1	0	0



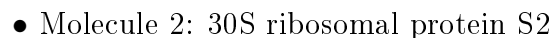
### 3 Residue-property plots

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 ( $\text{RSRZ} > 2$ ). 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

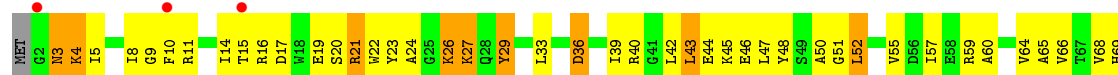




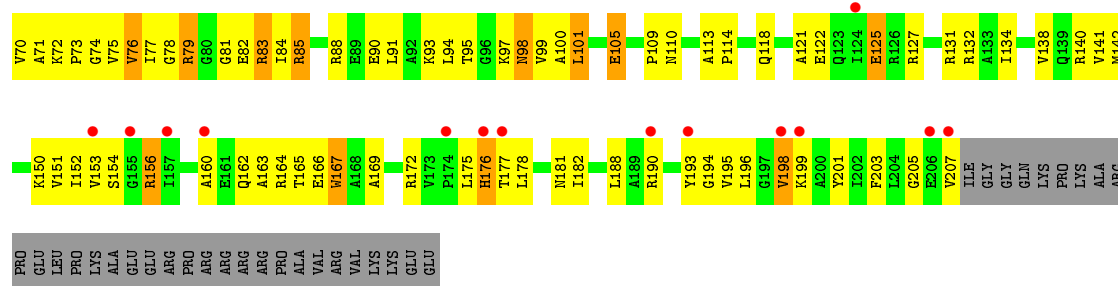


MET	PRO	VAL	E4	E5	E8	E9	L10	L11	E12	V15	H16	F17	G18	H19	E20	R21	K22	R23	W24	N25	P26	V31	I32	V33	A34	E35	I39	H40	I41	I42	D43	L44	T47	M48	L51	E52	E53	F54	F55	E59	D60	L61	A62	M63	R64	T67	L68	F69	L70	V71
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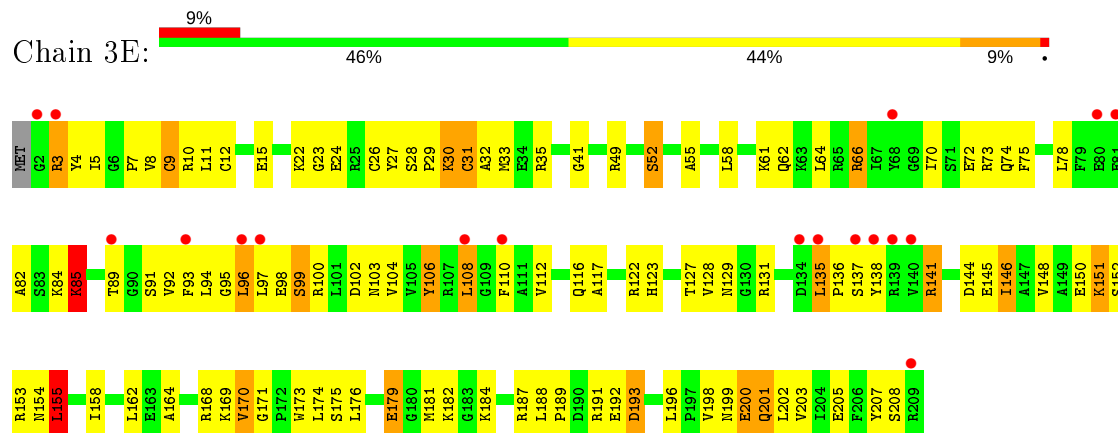




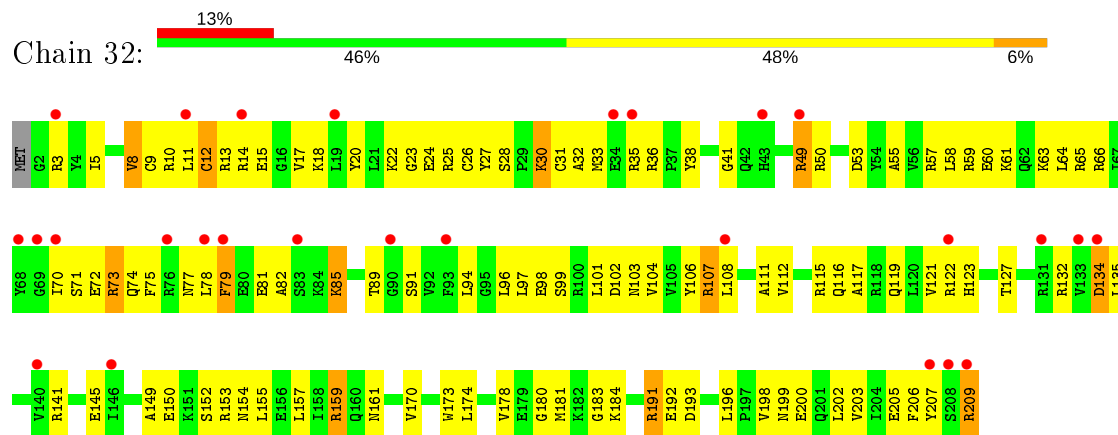




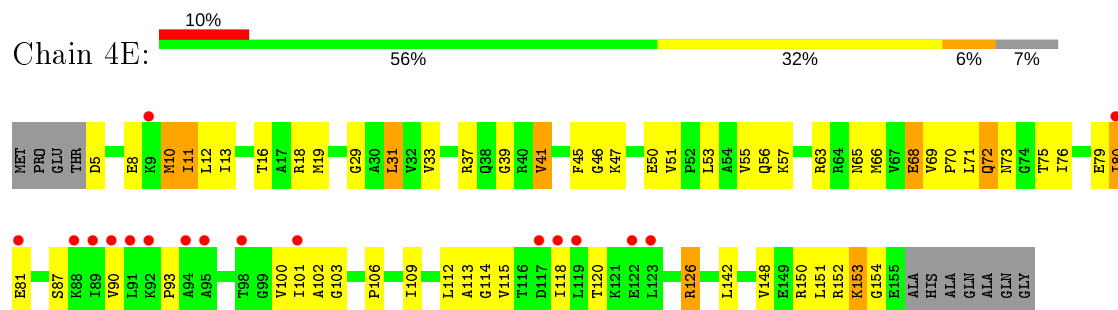
• Molecule 4: 30S ribosomal protein S4



• Molecule 4: 30S ribosomal protein S4

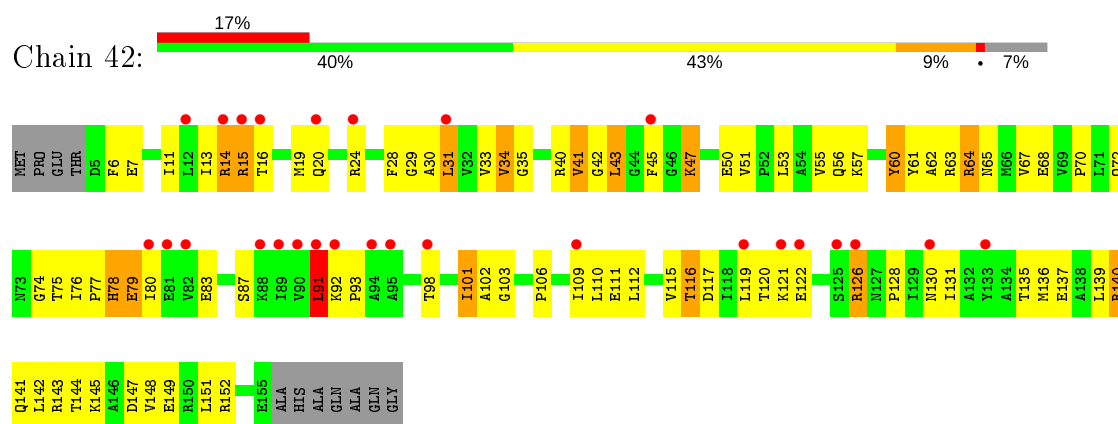


• Molecule 5: 30S ribosomal protein S5

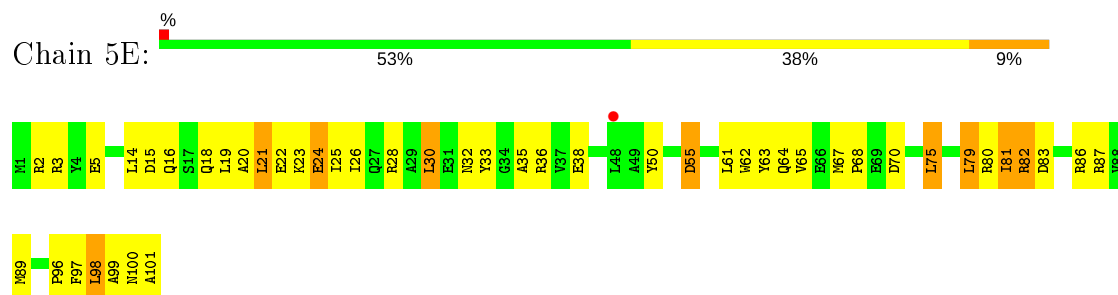


• Molecule 5: 30S ribosomal protein S5

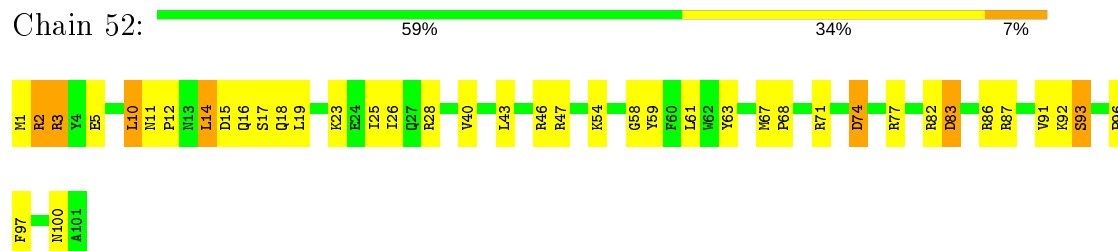




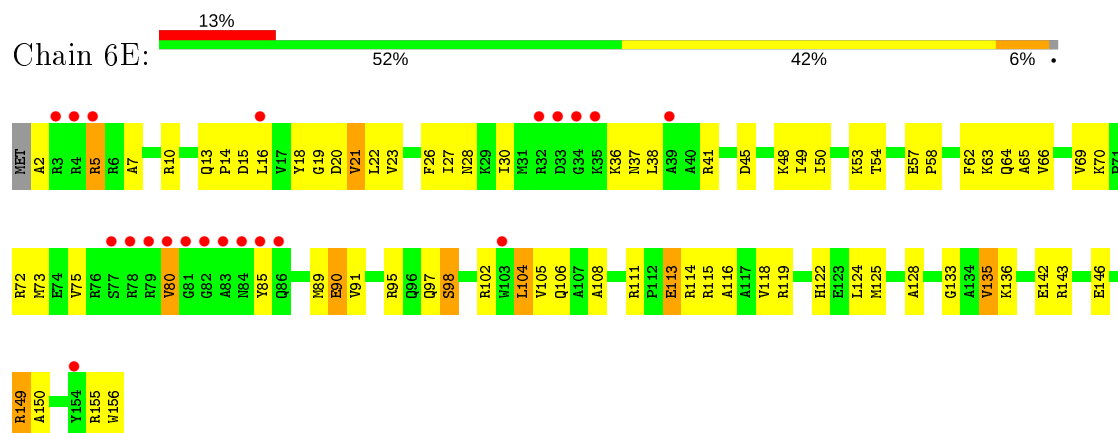
- Molecule 6: 30S ribosomal protein S6



- Molecule 6: 30S ribosomal protein S6



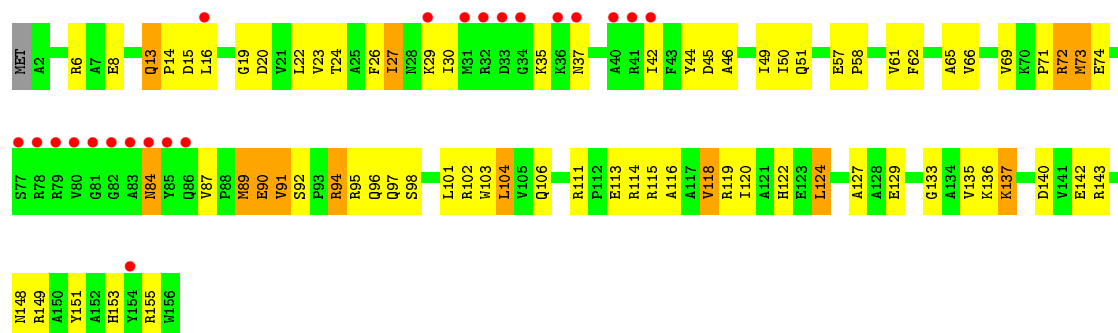
- Molecule 7: 30S ribosomal protein S7



- Molecule 7: 30S ribosomal protein S7

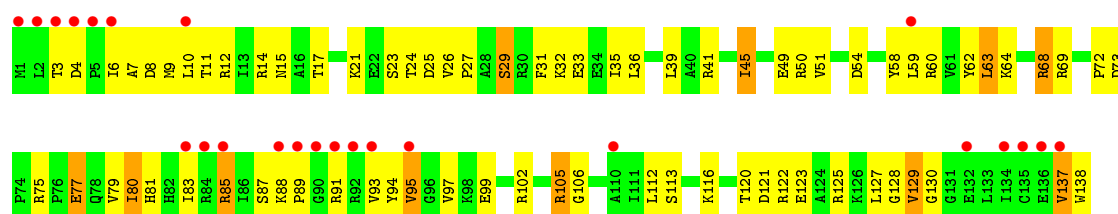


Chain 62: 



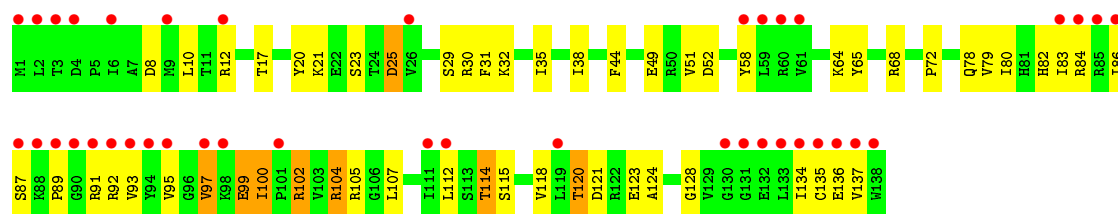
- Molecule 8: 30S ribosomal protein S8

Chain 7E: 



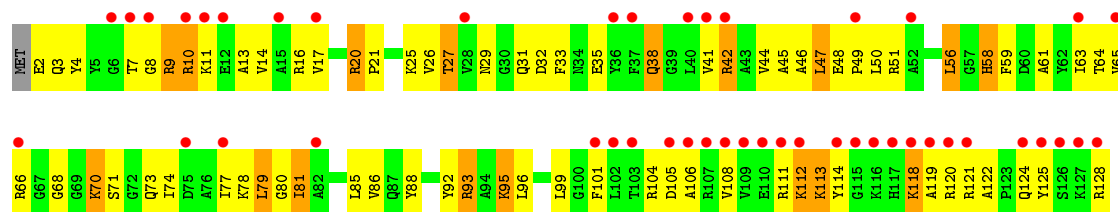
- Molecule 8: 30S ribosomal protein S8

Chain 72: 



- Molecule 9: 30S ribosomal protein S9

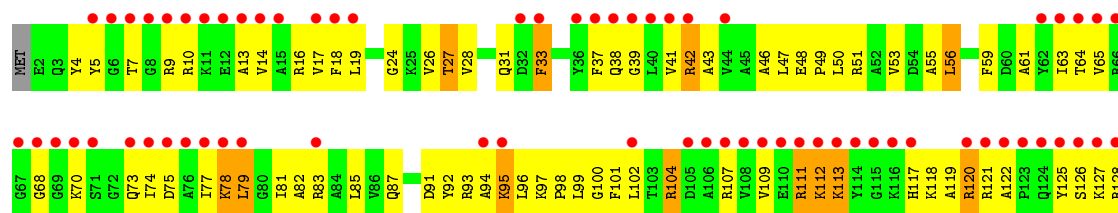
Chain 8E: 



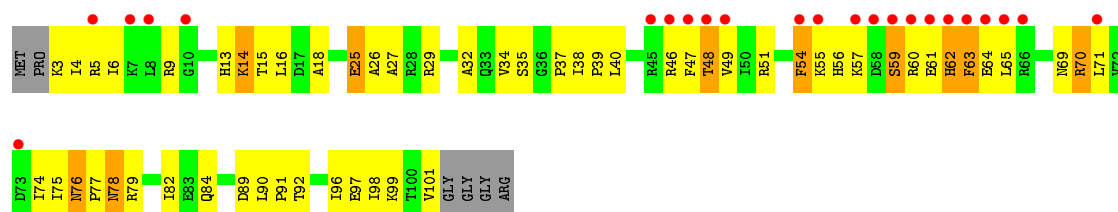
- Molecule 9: 30S ribosomal protein S9

Chain 82: 

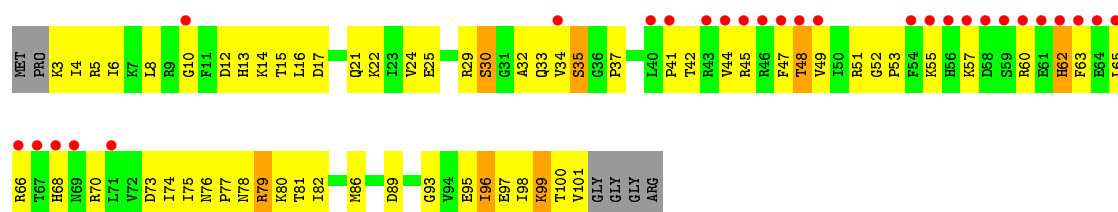




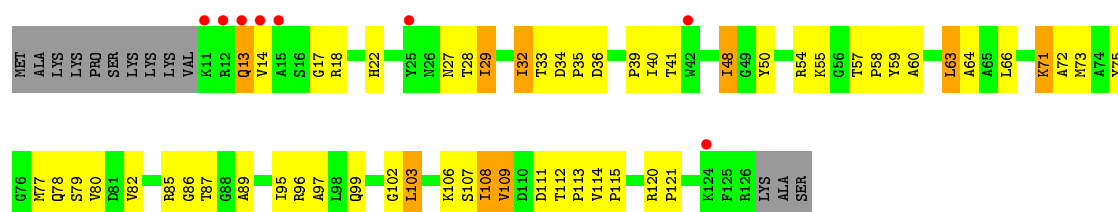
• Molecule 10: 30S ribosomal protein S10



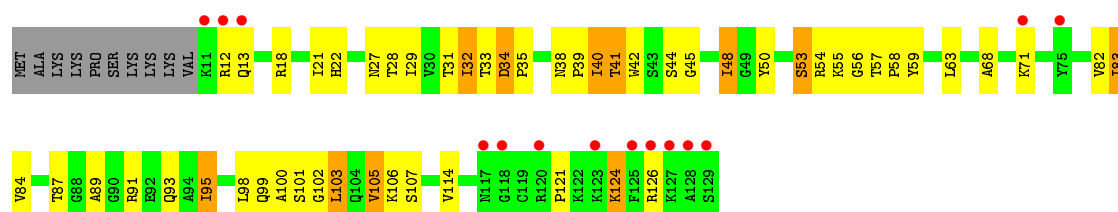
• Molecule 10: 30S ribosomal protein S10



• Molecule 11: 30S ribosomal protein S11

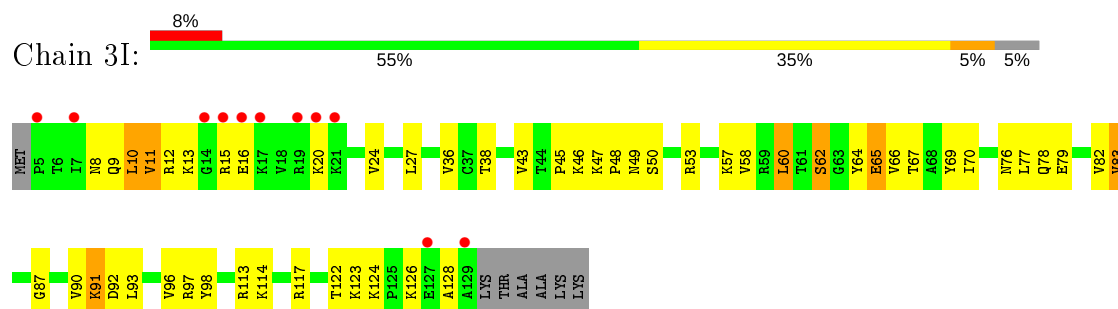


• Molecule 11: 30S ribosomal protein S11

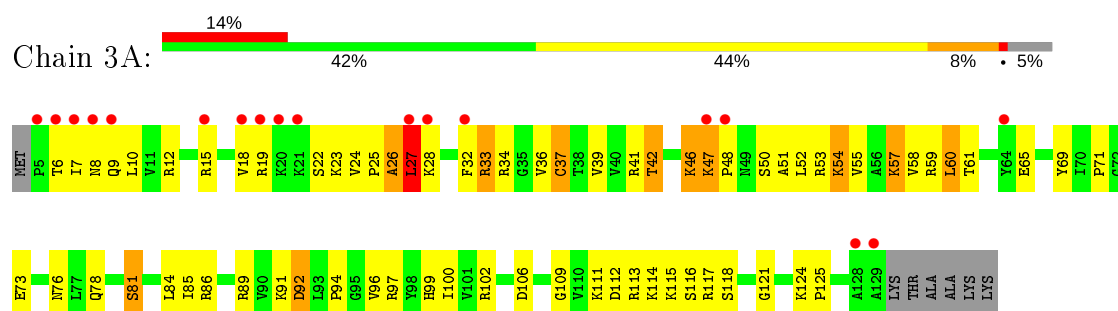




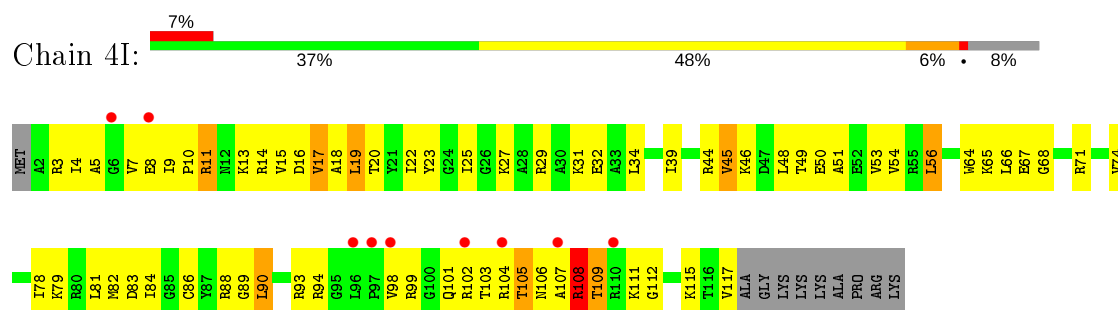
- Molecule 12: 30S ribosomal protein S12



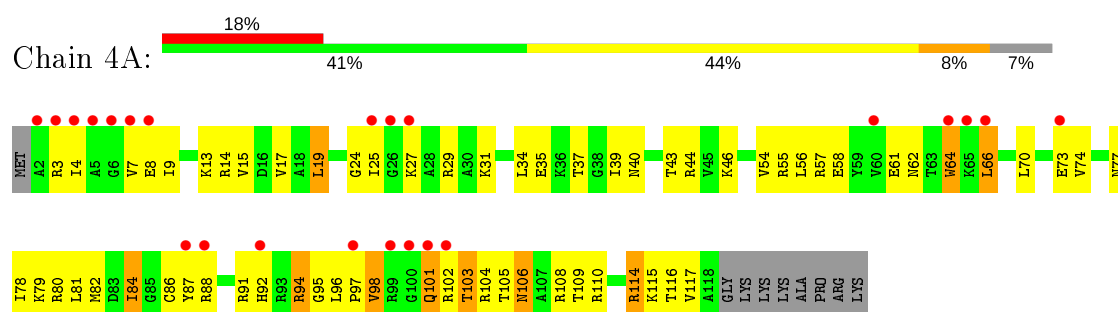
- Molecule 12: 30S ribosomal protein S12



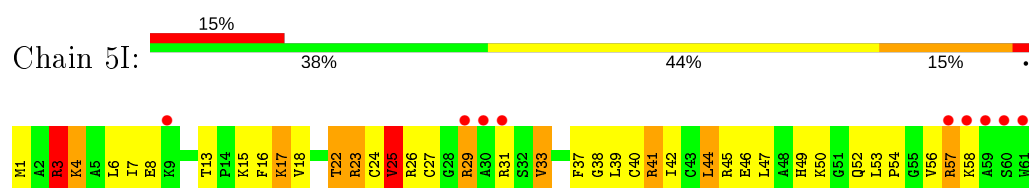
- Molecule 13: 30S ribosomal protein S13



- Molecule 13: 30S ribosomal protein S13

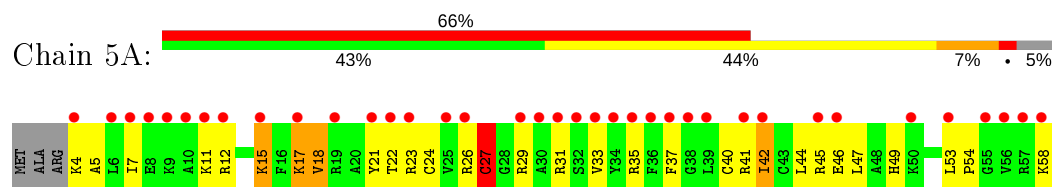


- Molecule 14: 30S ribosomal protein S14

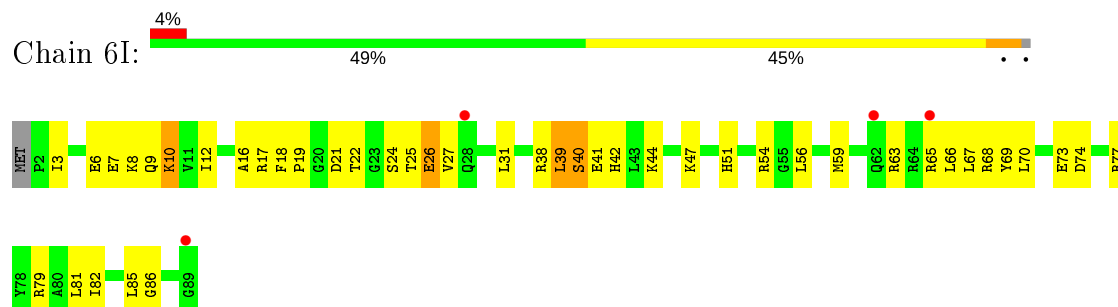




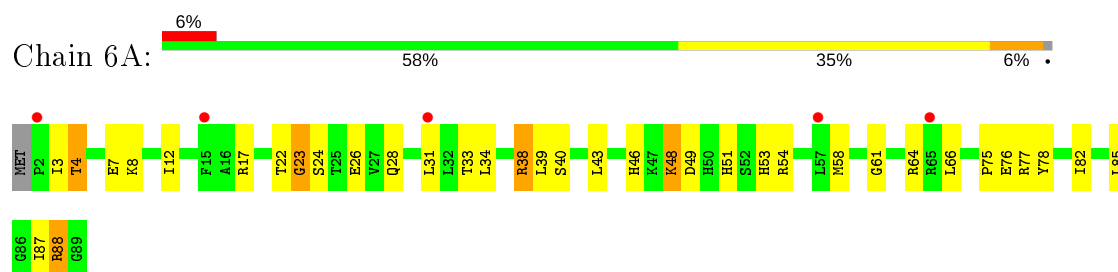
- Molecule 14: 30S ribosomal protein S14



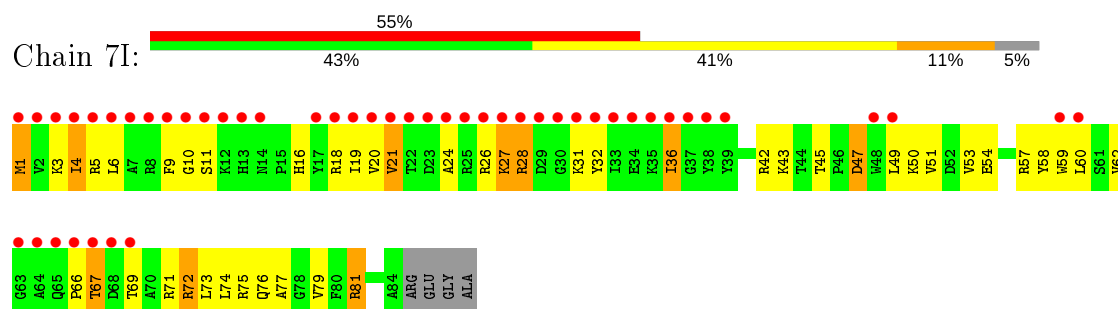
- Molecule 15: 30S ribosomal protein S15



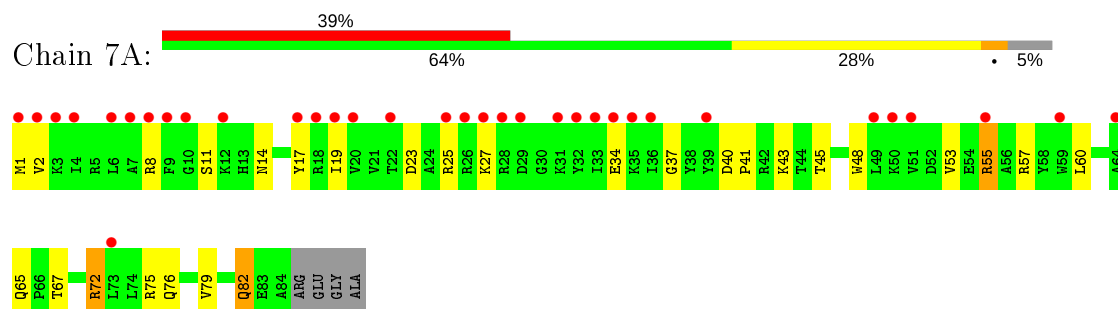
- Molecule 15: 30S ribosomal protein S15



- Molecule 16: 30S ribosomal protein S16

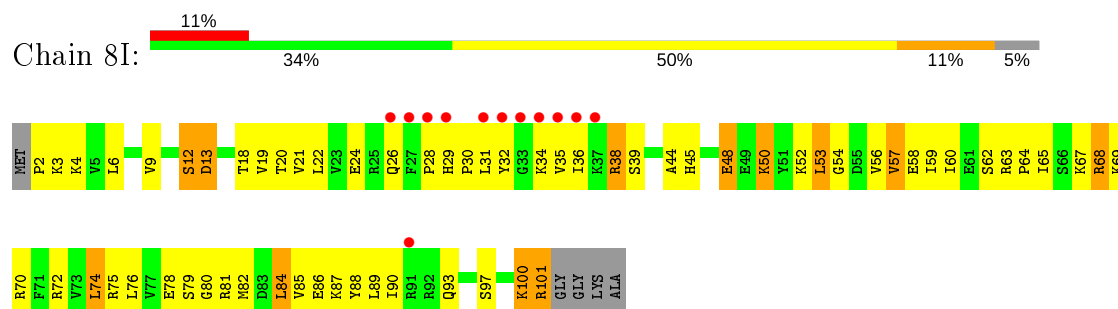


- Molecule 16: 30S ribosomal protein S16

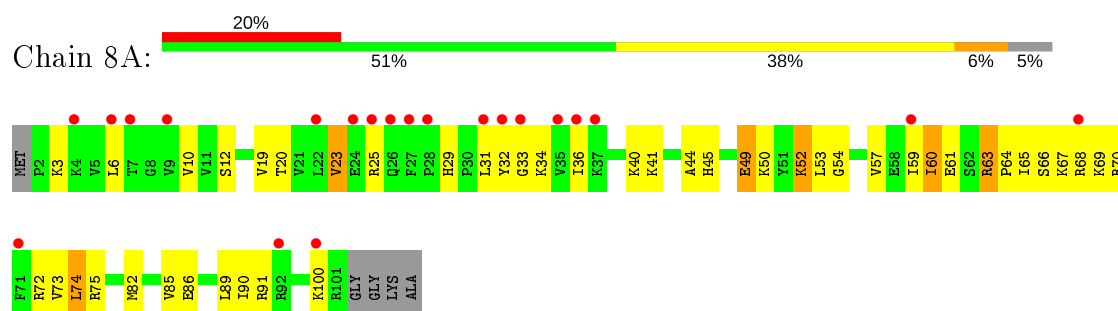




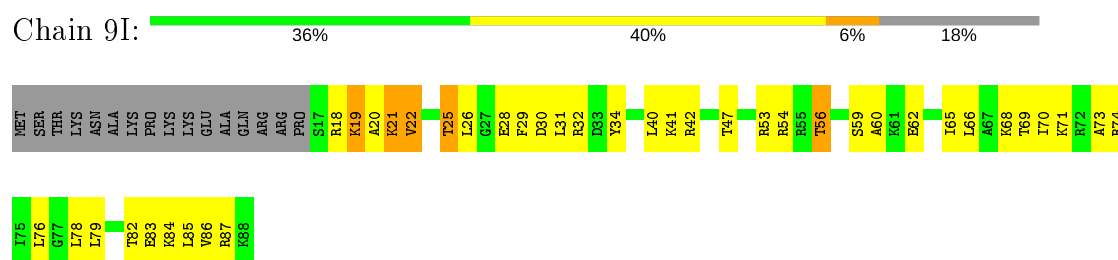
- Molecule 17: 30S ribosomal protein S17



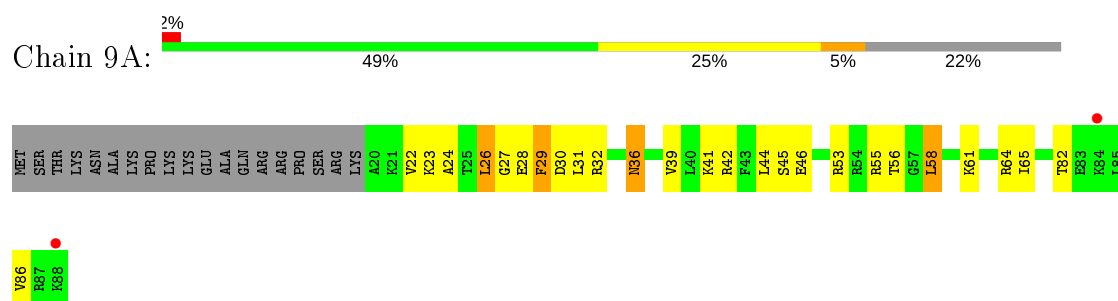
- Molecule 17: 30S ribosomal protein S17



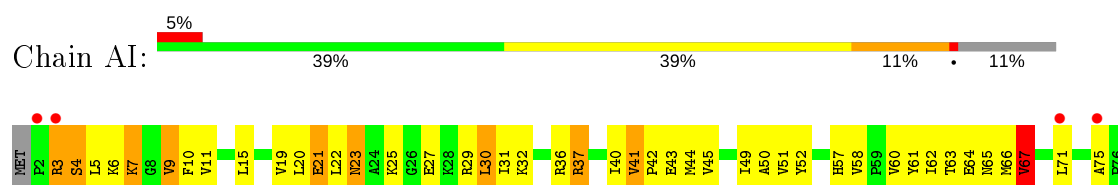
- Molecule 18: 30S ribosomal protein S18



- Molecule 18: 30S ribosomal protein S18



- Molecule 19: 30S ribosomal protein S19

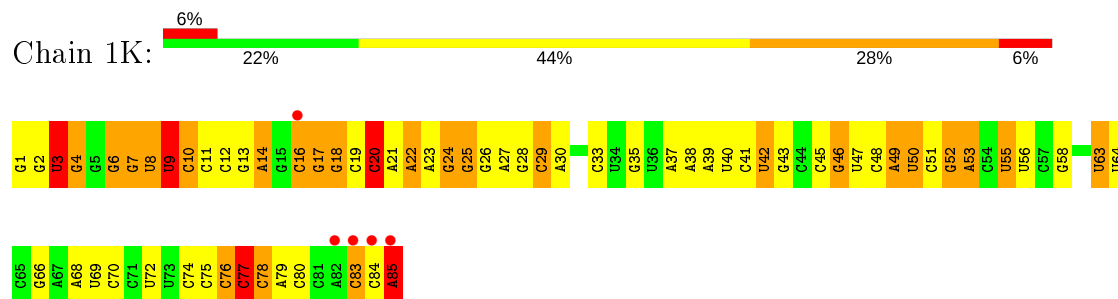




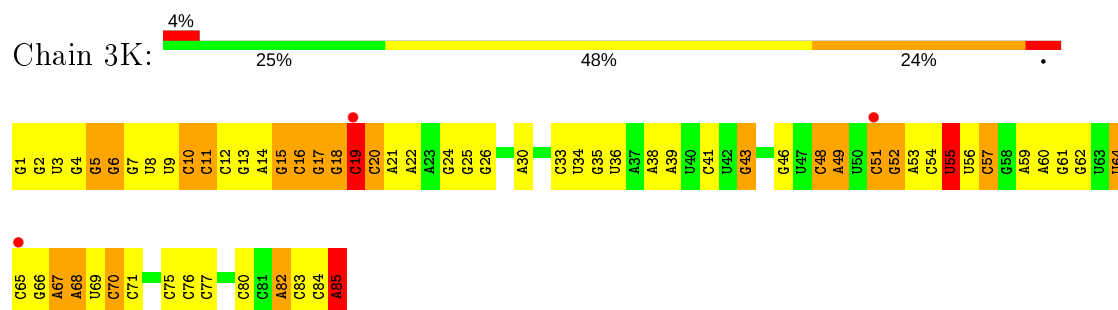




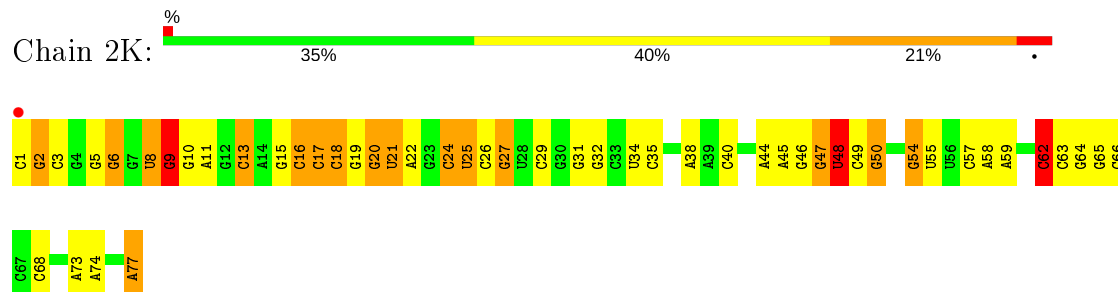
- Molecule 22: tRNA-Tyr



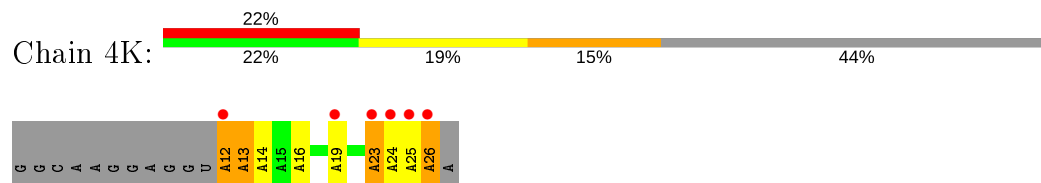
- Molecule 22: tRNA-Tyr



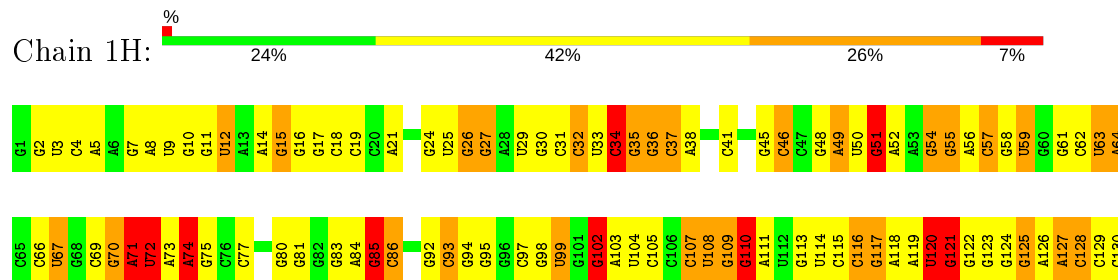
- Molecule 23: tRNA-fMet



- Molecule 24: mRNA



- Molecule 25: 23S ribosomal RNA





C1005	U943	U877	C916	C755	A689	G648	G585	C517	U448	C376	U306	U269	G131
C1006	G944	A978	C917	C756	G690	G649	A586	G518	A449	C379	G307	A270	G132
C1007	A945	G880	G918	U757	C691	G650	C587	U519	G451	U380	G308		C133
C1008	G946	G881	C692	C758	C692	G651	U588		C451	G382	G309	C270C	C134
A1009	G947	G882	A821		G693		A590	U524	G452	G381	A310	A207	G135
A1010	G948	G883	U822	A761	U694	A654	A591		C453	G382	A311	G270E	
C1011	C949	G884	G823	U762		A654A	C591	C527	A454	U383	G315	U270F	G137A
U1012	G950	C885	A824	G763	C697	G654B	G592	A528	C455	U384	G316	C270G	G138
C1013	C951	C886	C825	A764	C698	G654C	G593	A529	C456	C385	C316	C270H	G139
U1014	G952	A887	U826	G765	G700	G654D	G594	G530	A457	G386	G317	G270I	A140
A1020	G953	C888	U827	C766	G701	G654E	C531	C531	G458		C318	G270J	A141
A1021	G954	C889	U828	U767	G702	G654F	A532	A532	U459	G389	C319	G270K	A213
C1022	C955	C890	A829	G768	G703	G654G	G599	G533	A460	A390	A320	U270L	G214
U1023	A957	G892	G831	G770	A705	G654H	G600	U534	C461	C391	G321	U270M	G145
G1025	U958	C993	G832	C771		A654J	C601	C535	C462	C392	A322	G270N	C144
U1026	A959	C994	U833	C772		G654K	G602	A536	G463	C393	C323	U270O	
A1027	A960	C995	C834	C773	C708	G654L	A603	C537	U464	A394	A324	C270P	
A1028	C961	A996	A835	A774	U709	G654M	G604	G540	G465	U395	G325	C270Q	U147
A1029	G962	C997	G836	G775	G710	G654N	G605	G541	A466	G396	G326		U148
U1033	G963	C998	C837	C776		G654O	U606	C542	G467	G397	G327		A149
G1036	C964	A999	U838	A777	A716	G654P	C543	C543	A469		U328	G270T	C150
G1037	G965	U839	U839	G778	A717	G654Q	C544	C544	A470		G329	C270U	C151
U1038	G966	A901	C940	U779	G718		A608	C545	A471	C404	A331	G270V	G152
C1038	C967	C902	A841	G780	A719	G654R	A609	C546	A472	U405	A332	G270X	C153
C1040	G968	C903	G842	A781	C719	A654T		A401	G473	G406	G333	G270Y	G154
A1045	C971	C904	G843	A782		A655	C611	C547					C155
A1046	G972	U907	G944	A783	A722	G656	G612	A548	A480	G407		G271B	U163
G1047	A973	C908	C846	G784	G723	U657	U613	G549	C231	G408	A340	U271C	U164
A1048	G974	A909	U847	G785	U724	G658	G615	G550	G481	C409	G341	G271D	U165
A1049	G975	A910	U848	G786	G725	C659	A616	G551	A482	G410	G342	G272	G171
A1050	C976	A911	G949	U787	G726	G660	G617	G552	A483	G411	C343	G273	C172
A1051	G977	C912	A842	A788				U553	C484	A412	G344		C173
C1052	A980	C913	U851	A789	A727	G661	G620	U554	C485	C413	A345	U273E	G174
C1053	G978	C914	G852	C790	G728	G662	A621	G556		C414	A346	G273F	C175
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C1056	G984	A918	C856	G794	G733	U667	U626	C560	G493	A278	G352	A278	G179
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U1061	A990	A926	G862	A800	G739	C673	U568	U568	G500	A428	U358	C247	U185
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G1063	C992	G929	G864	A802	G741	A675	G570	A503	C287		G360	C249	G187
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	G939	A873	G873	U811	A751	G684	G642	U511	G442	A301	G301		A196
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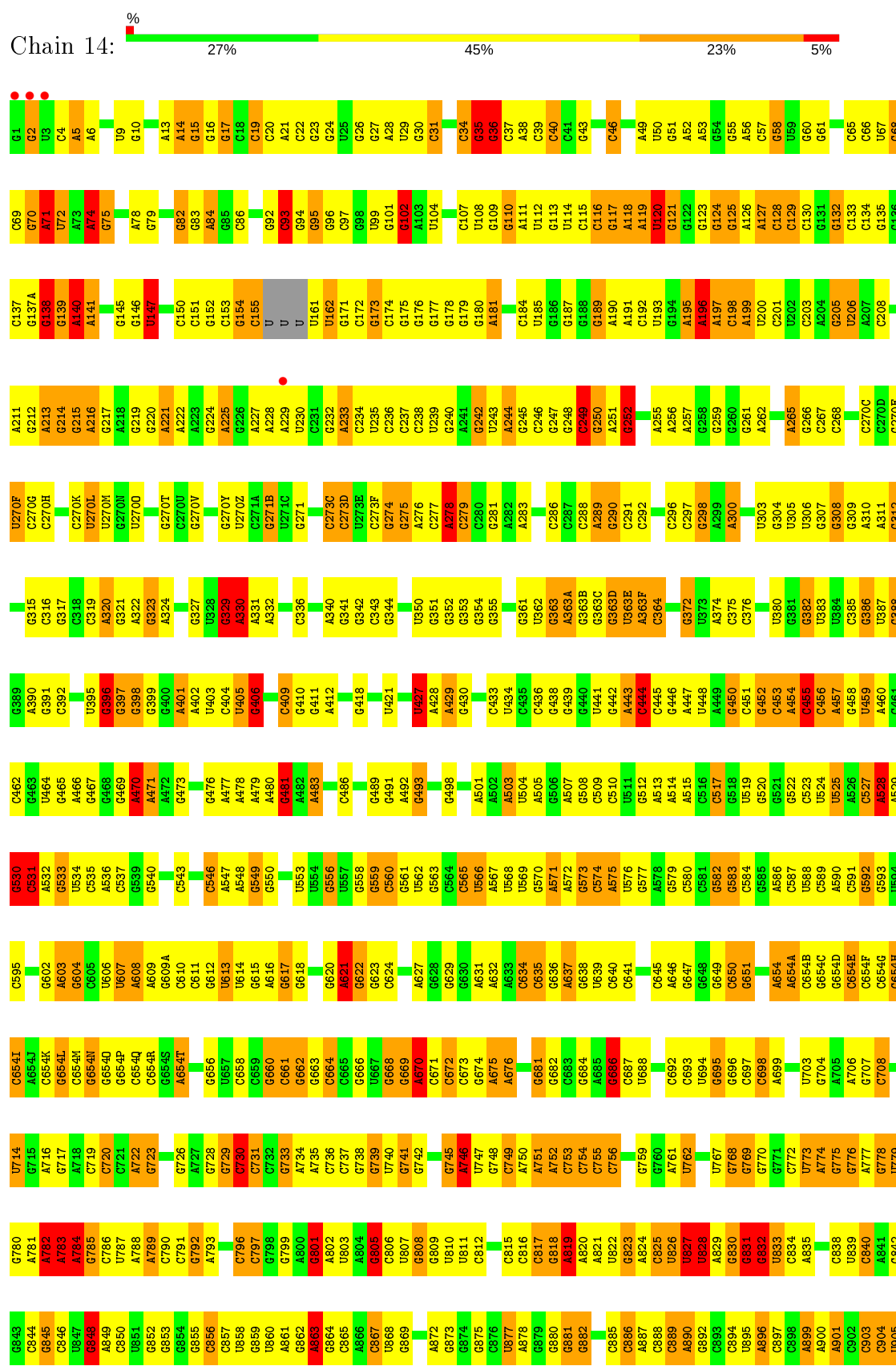
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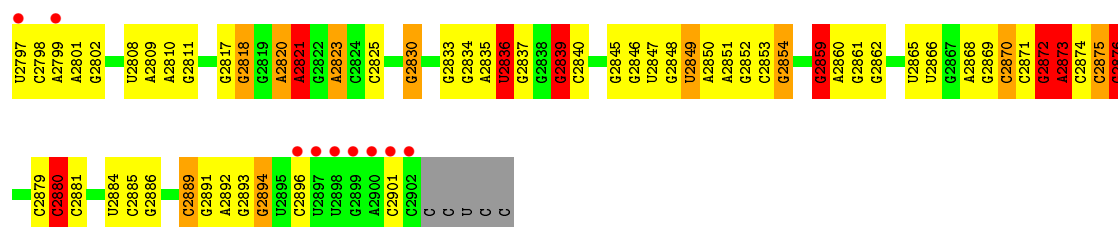


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		A1583	C1513	G1446	C1382	C1321	G1187	U1114		G987	A917
		G1585	C1515	G1447	C1383	A1322	U1188	G1115	G1051	A988	A918
		C1586	U1516	G1448	A1384	U1323	A1189	C1116	C1052	G989	G919
		A1587	G1517	G1449	G1385	G1324	G1189		C1053	A990	G920
		G1588	A1518	G1449A	C1386	G1325	G1190		C1054	C991	G921
		C1589	C1519	C1450	G1387	U1326	G1191	G1120	G1055	G992	U922
			U1520	C1451	G1388	G1327	U1263	G1121	G1056	G993	
			G1521	G1452	G1389	G1328	G1193	G1122	A1057	C994	G929
		G1593	G1522	A1453	U1390	U1329			U1058	C995	
		C1594	U1523	G1454	U1391	U1330	G1197	A1126	G1059	A996	G932
		A1596	G1524	G1455	A1392	A1331	U1198		U1060	G997	A933
		C1597	G1525	G1459	U1393	G1332	U1199	A1129	G1061	C998	G934
		G1598	G1526	A1460	U1394	G1333	C1201	U1130	G1062	U999	C935
		C1599	G1527	G1461	U1395	G1334	G1202	A1131	G1063	A1000	C936
		C1600	A1528	G1462	U1396	U1335	G1203	A1132	U1065	A1001	
		G1601	G1529	C1463		A1336	C1204	U1133	U1066	G1002	
		U1602	G1530	C1464	C1399	G1337	A1204	C1135	G1003	G940	
		A1603	C1531	G1465	G1400	G1338	U1205	G1136	A1067	C1004	A941
		C1604	G1532	G1466	G1401	G1339		G1137	G1068	G1005	G942
		G1605	G1533	C1467	C1402	U1340	U1210	G1138	A1069	C1006	U943
		C1606	G1534		C1403	U1341	U1211	G1139	U1070	C1007	G944
		G1607	U1535	G1470	C1404	A1342	U1212	C1140	G1071	C1008	A945
		U1608	A1536	A1471	U1406	G1343	A1213	U1141	A1009	G1009	G946
		A1609	G1537	G1472	C1407	C1344	G1217	U1142	C1072	G947	G948
		G1610	G1538	G1473	C1408	G1345	U1218	A1143	G1073	U1011	
		C1611	G1539	G1475	C1409	U1347	G1219	G1144	G1074	U1012	C949
		C1612			G1410	G1348	A1220			C1013	G950
		G1613	G1542	G1478	C1411	A1349	G1221	C1145	U1080	U1014	C951
		A1614	A1543	G1479	A1412	C1350		C1146	U1081	G1015	G952
		C1615	C1544	G1480	G1413	G1351	C1225	C1147	U1082	G1016	A953
		A1545	A1545A	U1482		U1352	G1226	U1148	G1017	G1017	G954
				G1483	G1416	A1353	G1269	G1149	U1083	C1018	C955
		C1617		G1484	C1417	A1354	A1227	C1150	A1084	U1019	G956
		A1618	C1548	G1485	G1418	G1355	G1228	G1151	A1086	A1020	A957
		G1619	C1549	A1486	A1419	G1356		C1152	G1087	A1021	U958
		U1621	C1549	G1487	U1420	U1357	G1231	C1153	A1088	G1022	A959
		G1622	A1554	G1488	G1421	G1358	G1232	A1155	U1089	U1023	A960
		G1623		U1489	G1422	A1359	C1233	A1156	U1090	G1024	C961
		G1624	C1557	A1490	G1423	A1360	U1234	G1157	G1091	G1025	G962
		C1625	A1558		G1424		U1235	C1158	C1092	U1026	U963
		G1626	C1559	C1493	G1425	C1363	G1236	G1159	G1093	U1027	C964
		G1627	G1560	A1494	G1426	G1364	A1237	U1159	U1094	A1028	G965
		G1628	A1495	A1496	A1427	G1365	G1238	G1160	A1095	A1029	G966
		U1629	C1564	U1497	G1428	A1366	G1239		A1096	G1030	
			C1565		G1429	A1367	U1240	G1164	U1097		C970
		A1631	A1566		C1430	G1368	U1241	U1165	A1098		C971
		G1632	G1568	G1500	U1431	G1369	A1242	C1166	G1099	G1034	G972
		G1633		C1501	C1432	C1370	G1243	G1170	C1100	A1036	G974

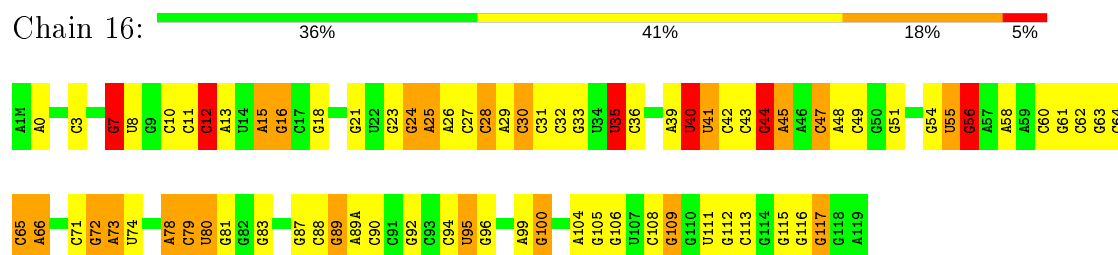




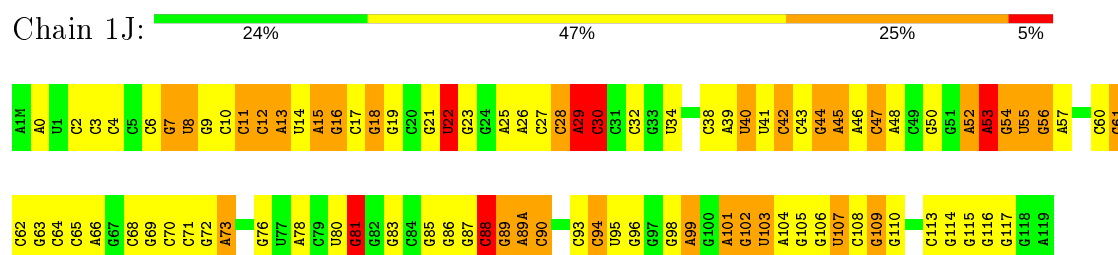




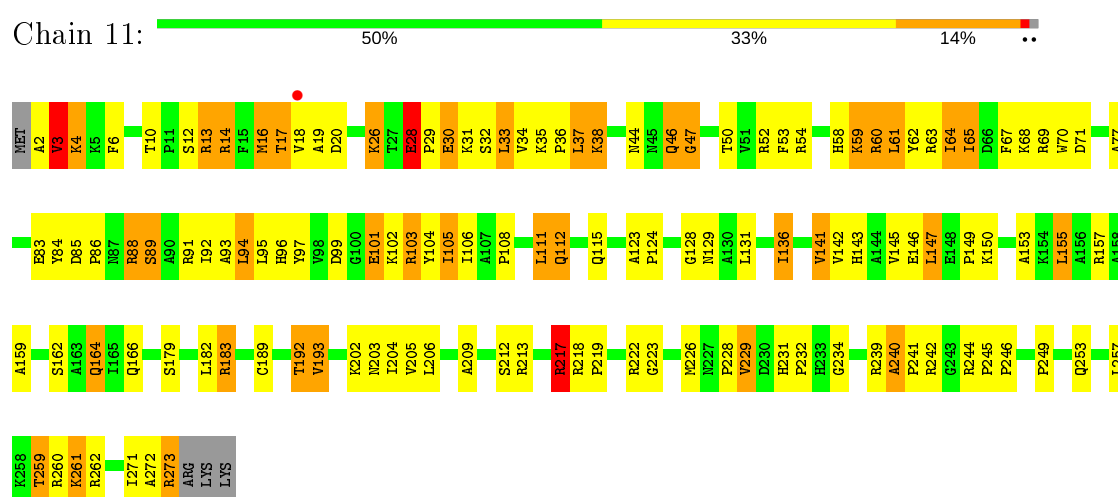
• Molecule 26: 5S ribosomal RNA



• Molecule 26: 5S ribosomal RNA



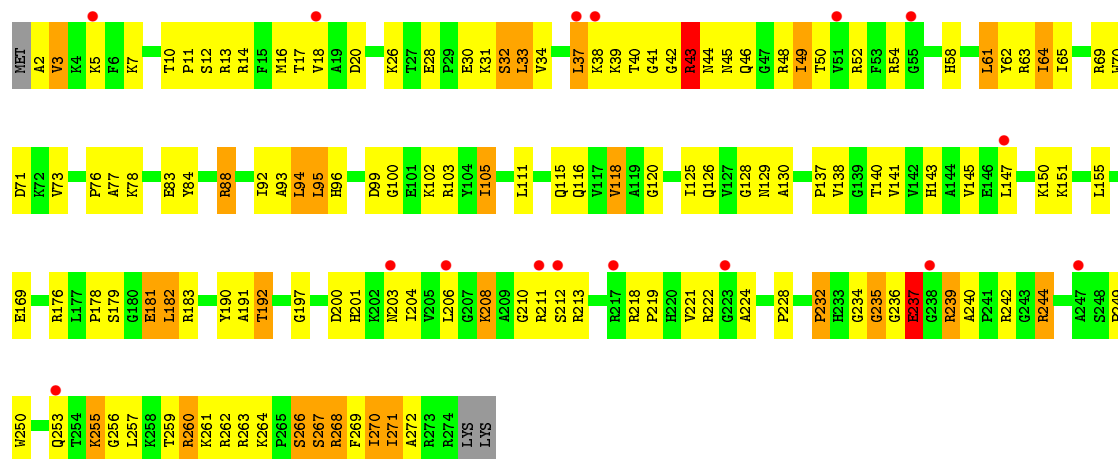
• Molecule 27: 50S ribosomal protein L2



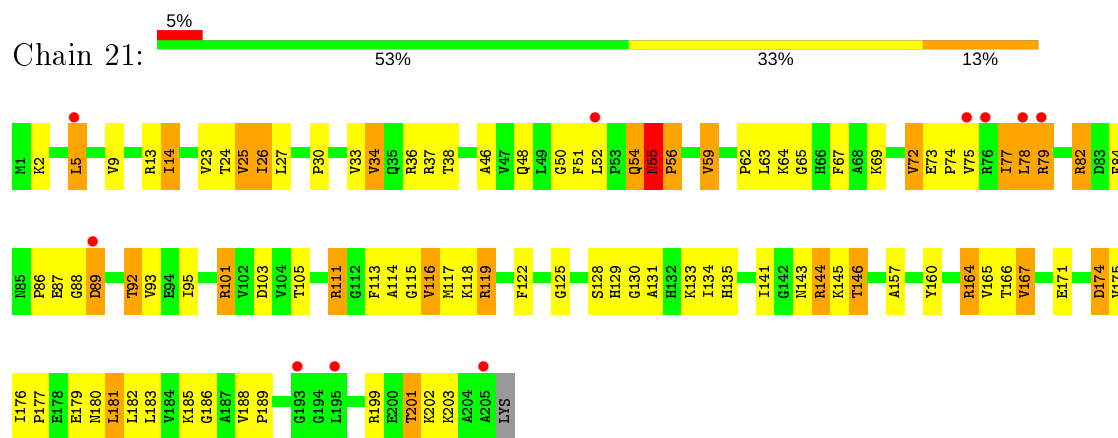
• Molecule 27: 50S ribosomal protein L2



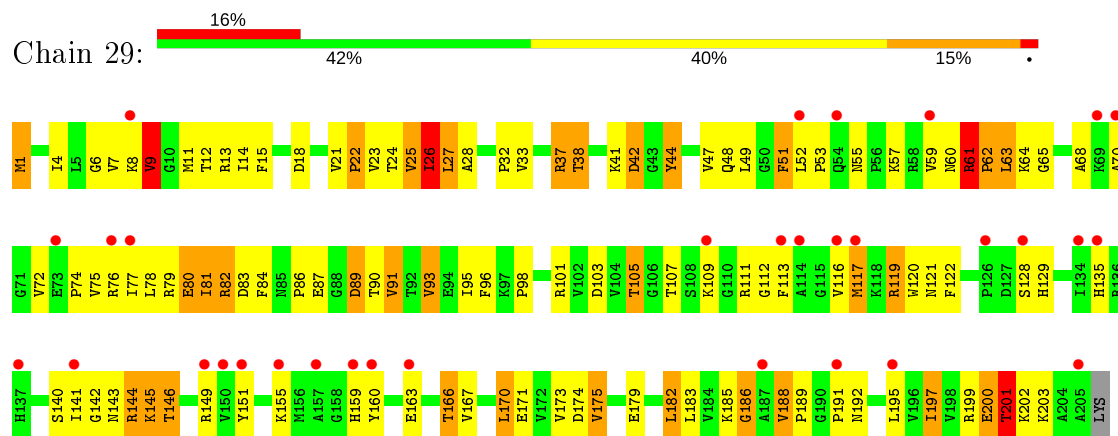




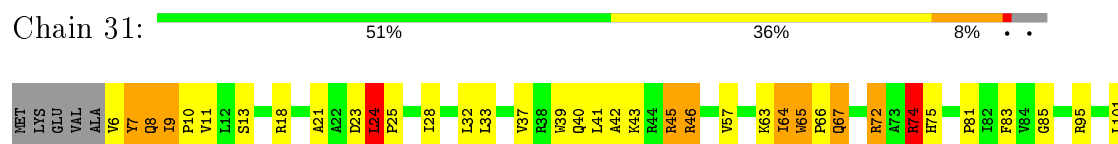
• Molecule 28: 50S ribosomal protein L3



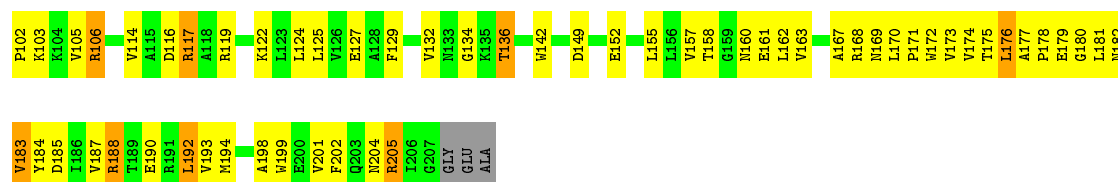
• Molecule 28: 50S ribosomal protein L3



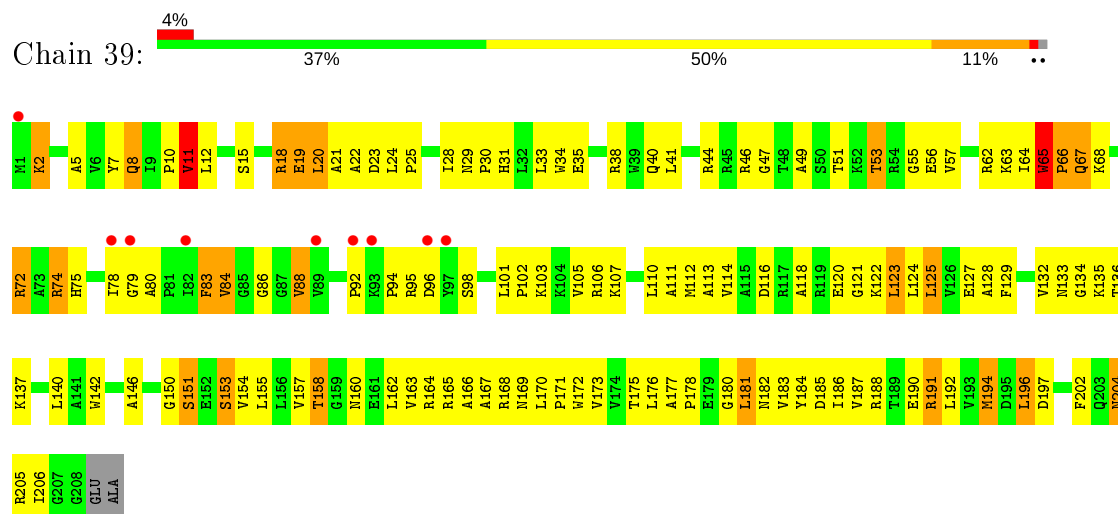
• Molecule 29: 50S ribosomal protein L4



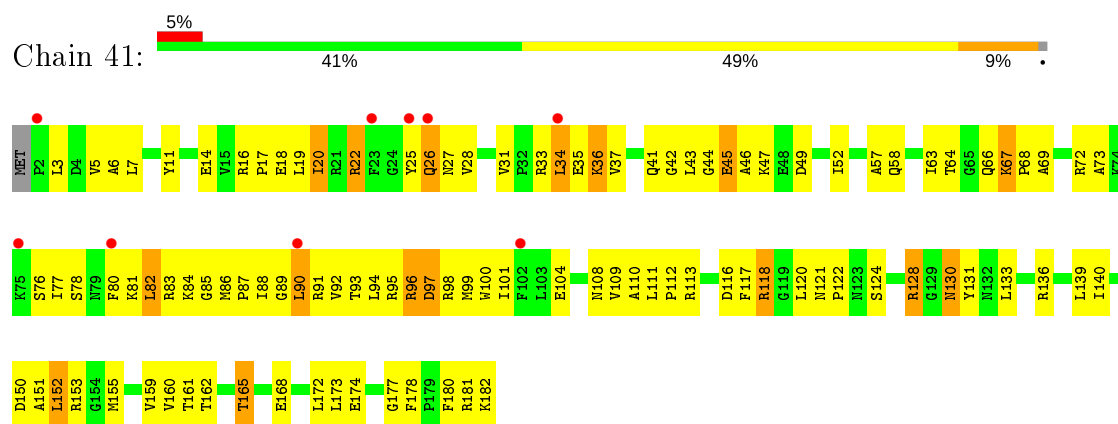




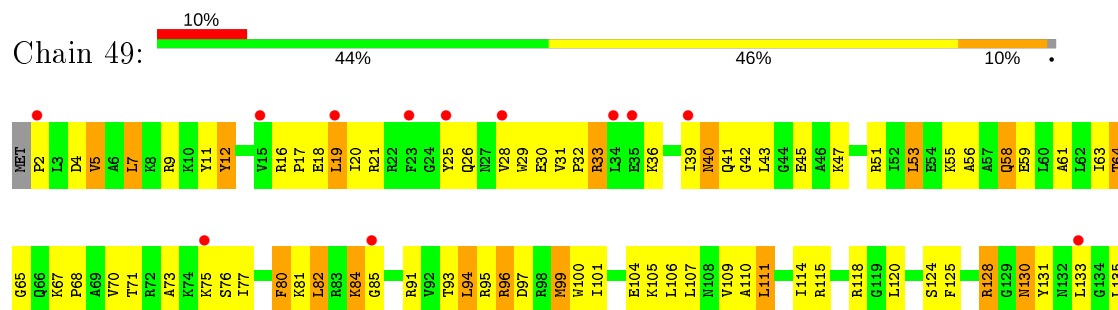
- Molecule 29: 50S ribosomal protein L4



- Molecule 30: 50S ribosomal protein L5



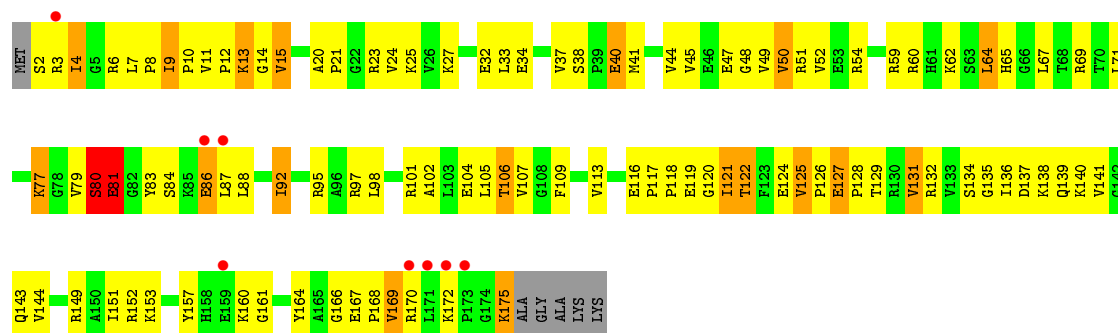
- Molecule 30: 50S ribosomal protein L5



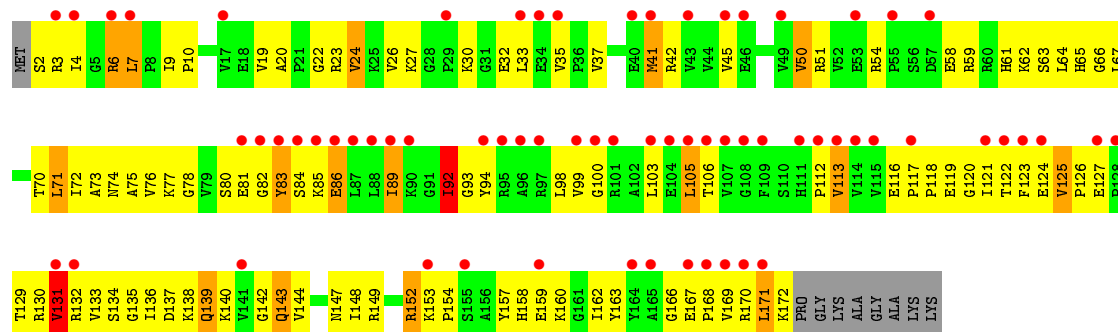




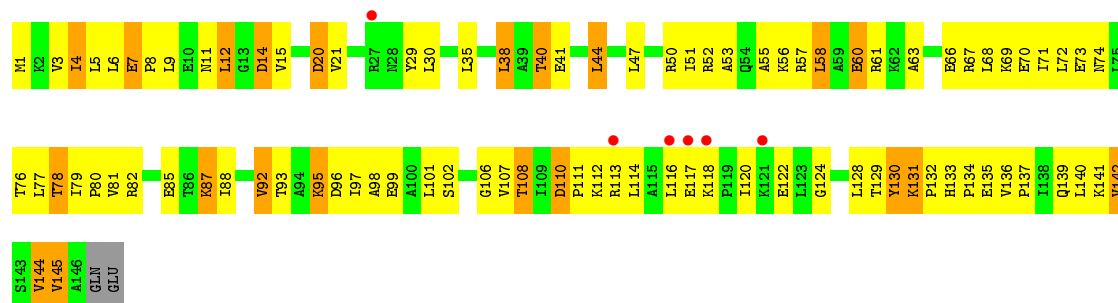
- Molecule 31: 50S ribosomal protein L6



- Molecule 31: 50S ribosomal protein L6



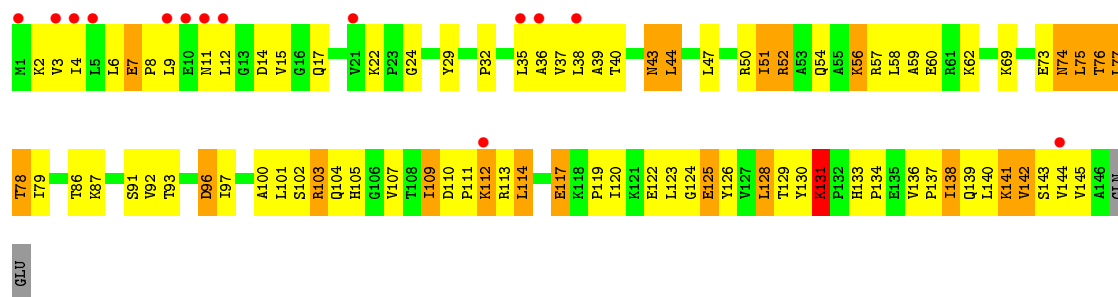
- Molecule 32: 50S ribosomal protein L9



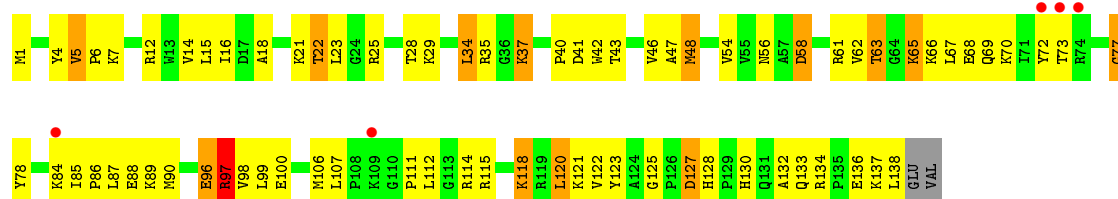
- Molecule 32: 50S ribosomal protein L9



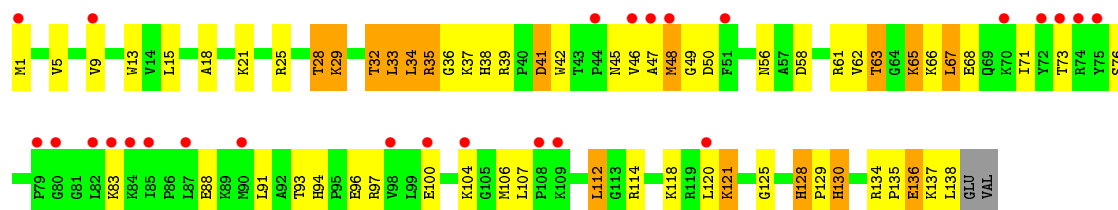




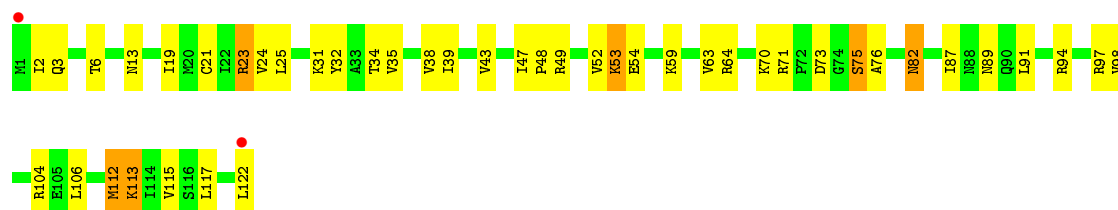
- Molecule 33: 50S ribosomal protein L13



- Molecule 33: 50S ribosomal protein L13



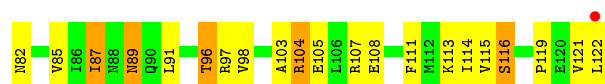
- Molecule 34: 50S ribosomal protein L14



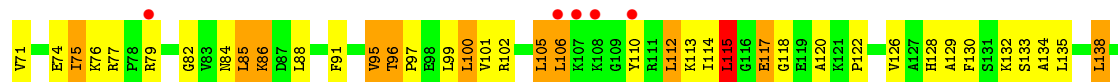
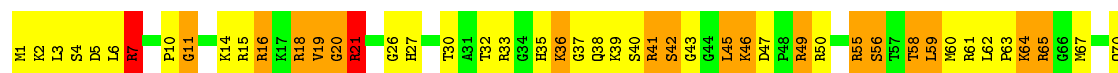
- Molecule 34: 50S ribosomal protein L14



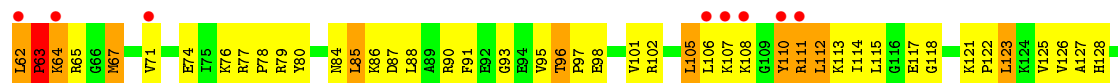
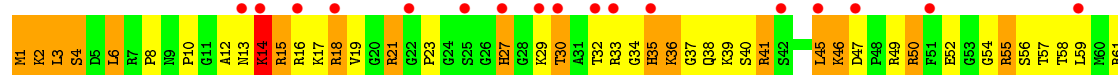




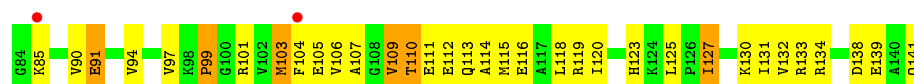
- Molecule 35: 50S ribosomal protein L15



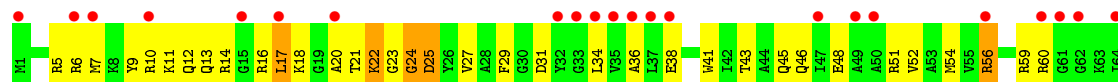
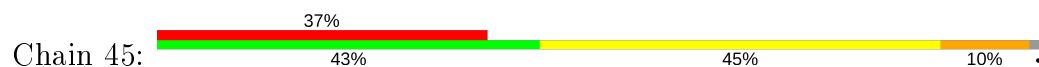
- Molecule 35: 50S ribosomal protein L15



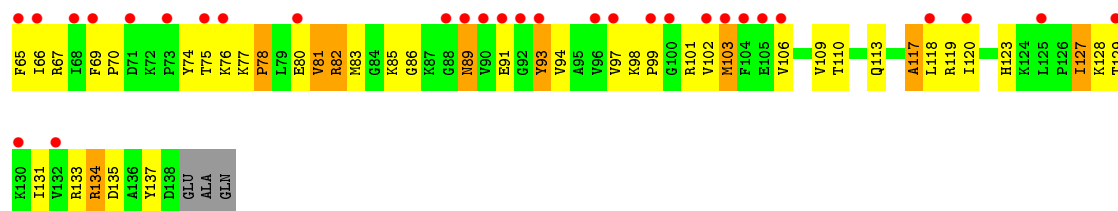
- Molecule 36: 50S ribosomal protein L16



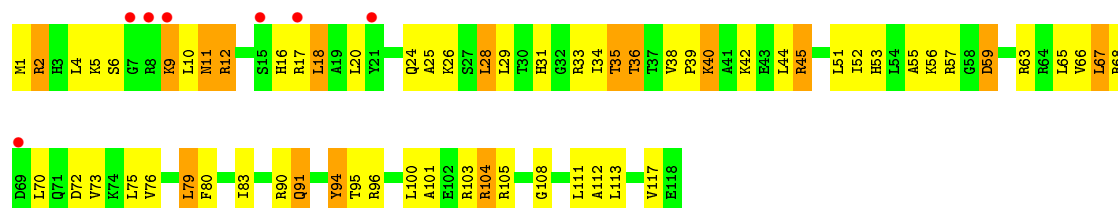
- Molecule 36: 50S ribosomal protein L16



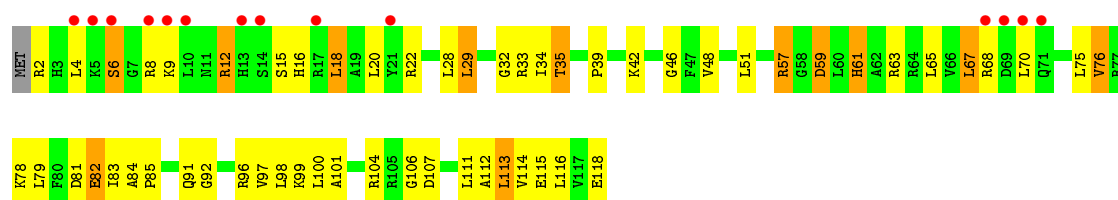




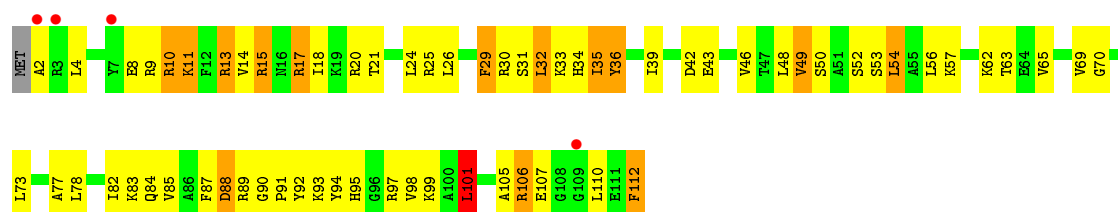
• Molecule 37: 50S ribosomal protein L17



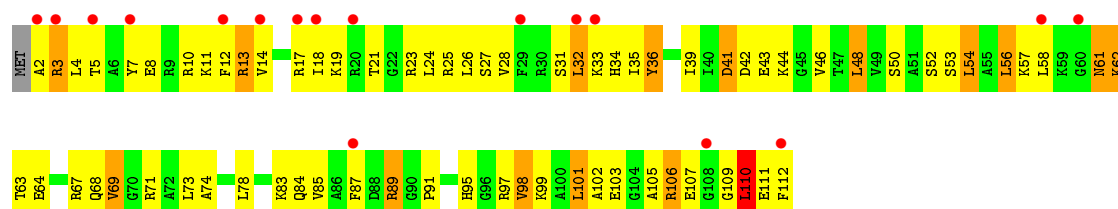
• Molecule 37: 50S ribosomal protein L17



• Molecule 38: 50S ribosomal protein L18

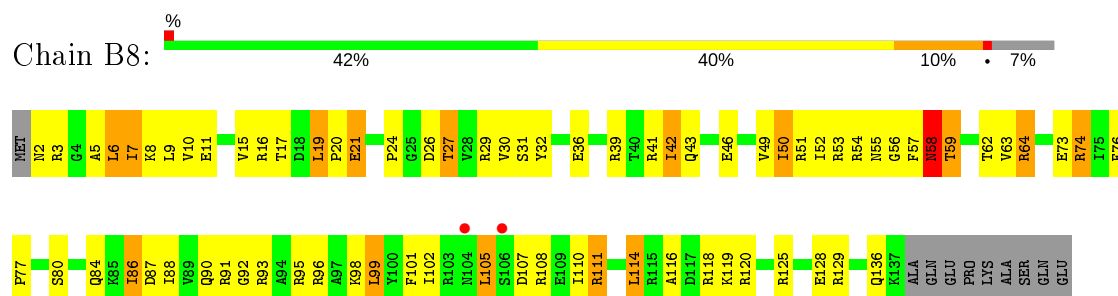


• Molecule 38: 50S ribosomal protein L18

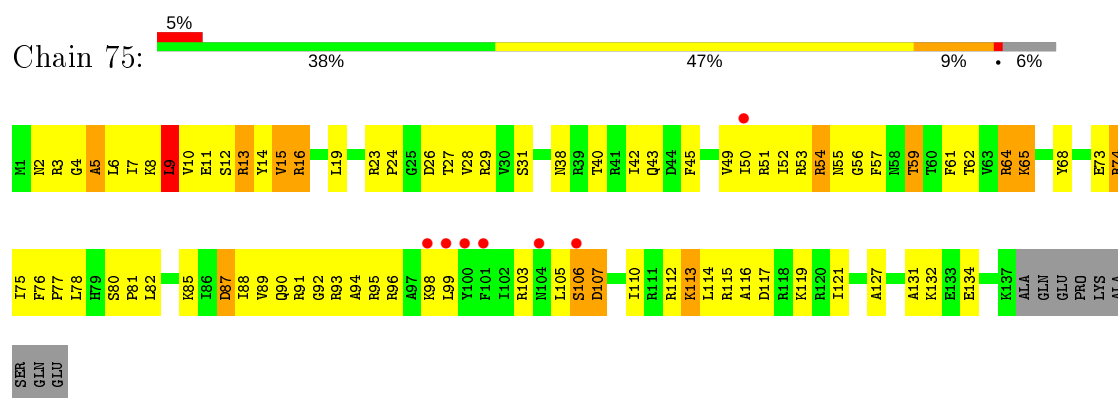




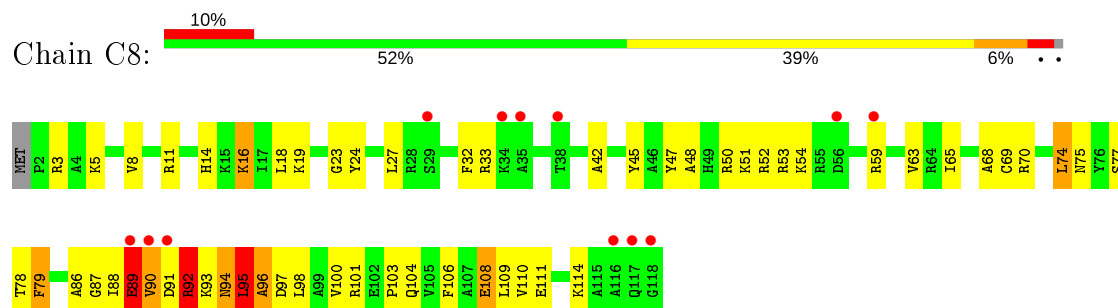
- Molecule 39: 50S ribosomal protein L19



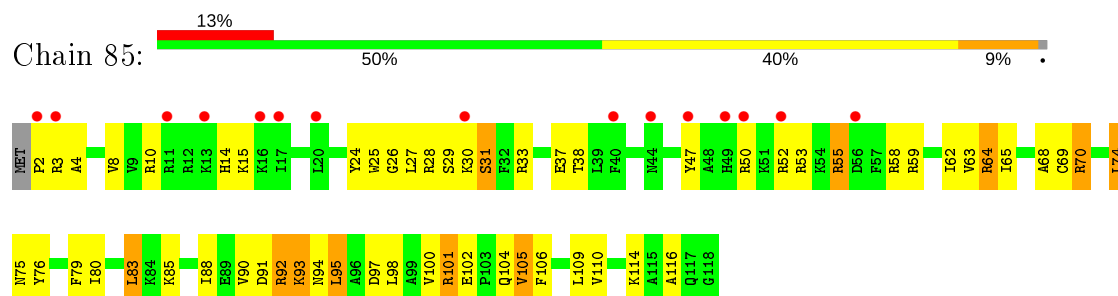
- Molecule 39: 50S ribosomal protein L19



- Molecule 40: 50S ribosomal protein L20



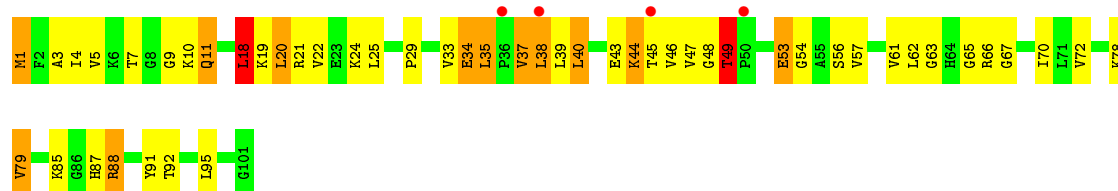
- Molecule 40: 50S ribosomal protein L20



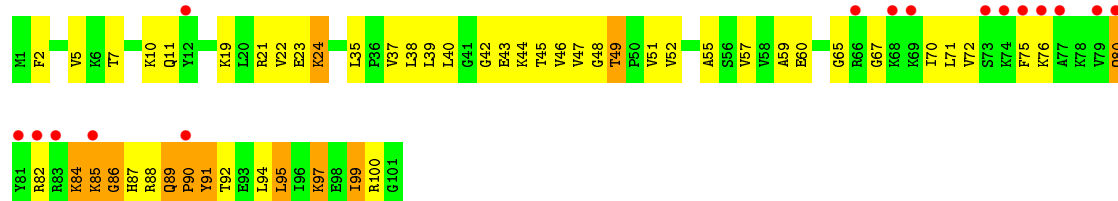
- Molecule 41: 50S ribosomal protein L21



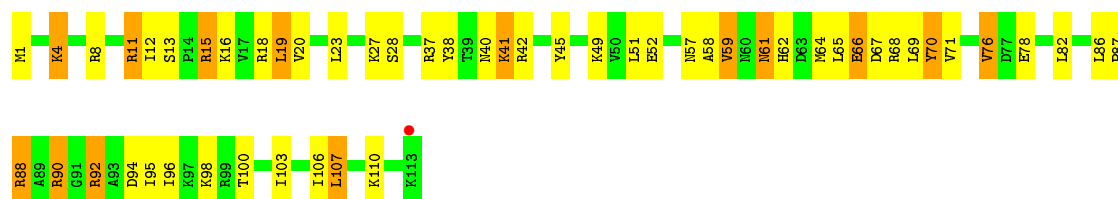




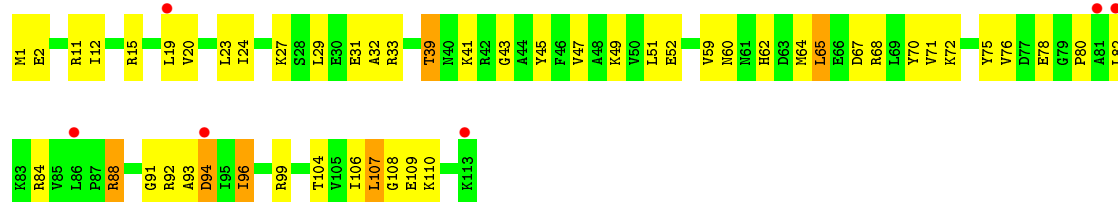
- Molecule 41: 50S ribosomal protein L21



- Molecule 42: 50S ribosomal protein L22



- Molecule 42: 50S ribosomal protein L22

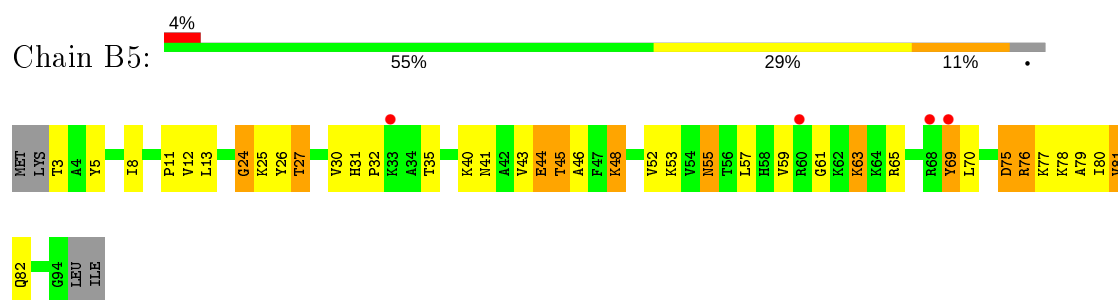


- Molecule 43: 50S ribosomal protein L23

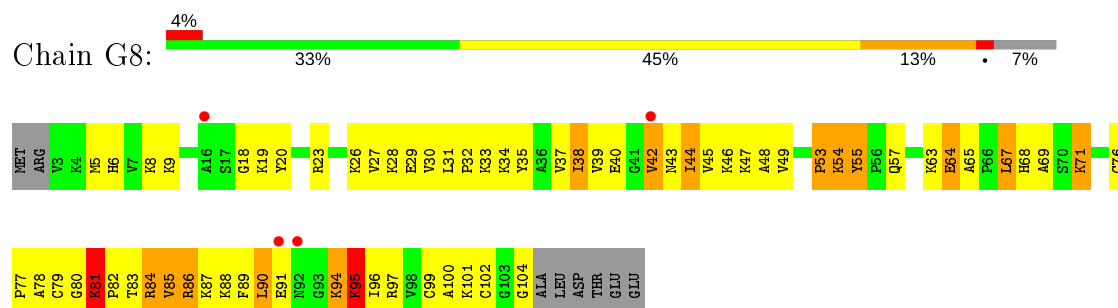


- Molecule 43: 50S ribosomal protein L23

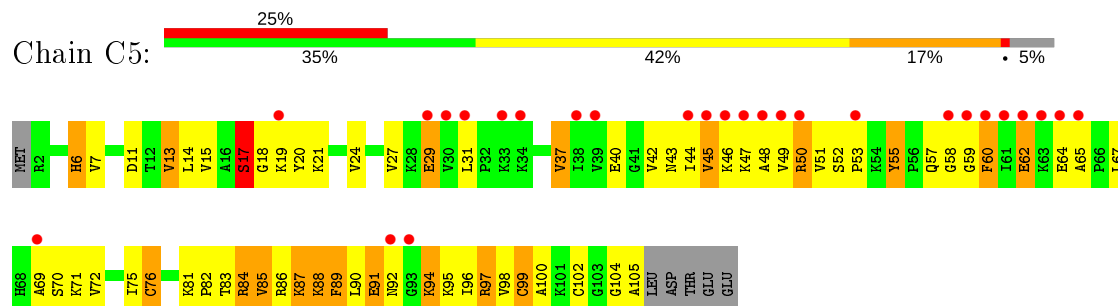




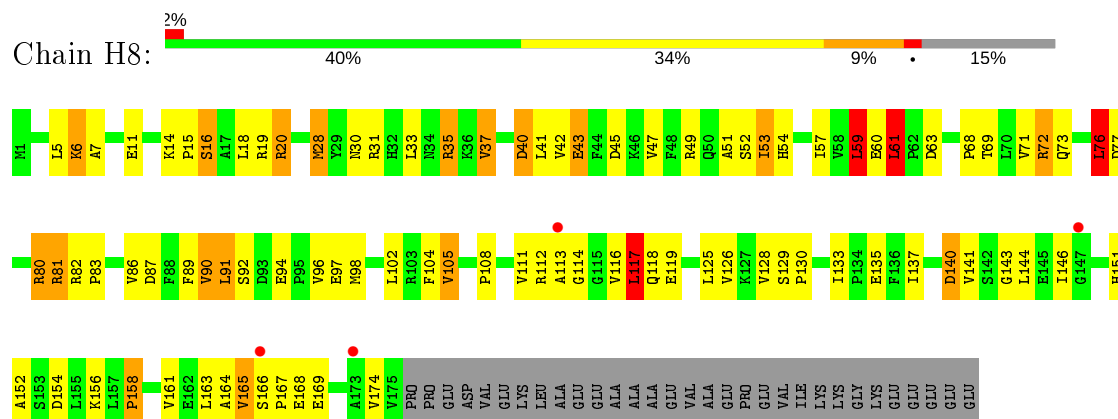
- Molecule 44: 50S ribosomal protein L24



- Molecule 44: 50S ribosomal protein L24



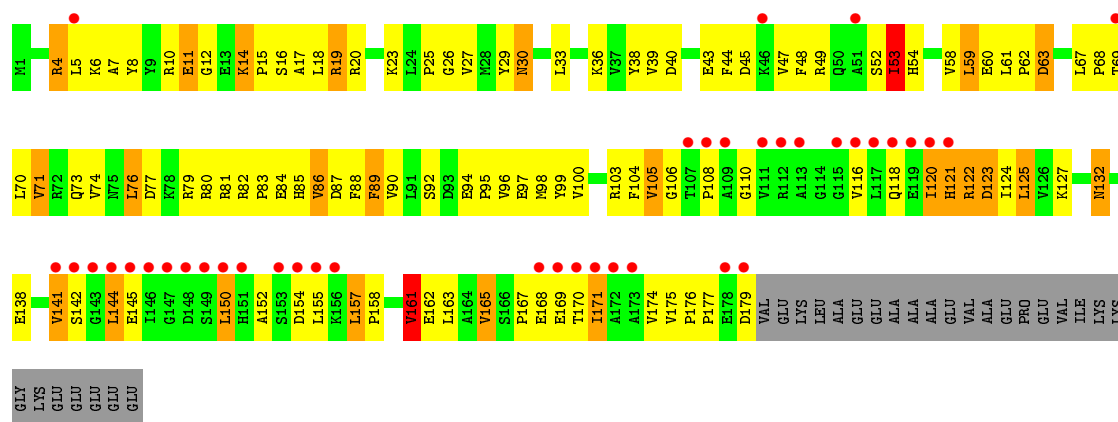
- Molecule 45: 50S ribosomal protein L25



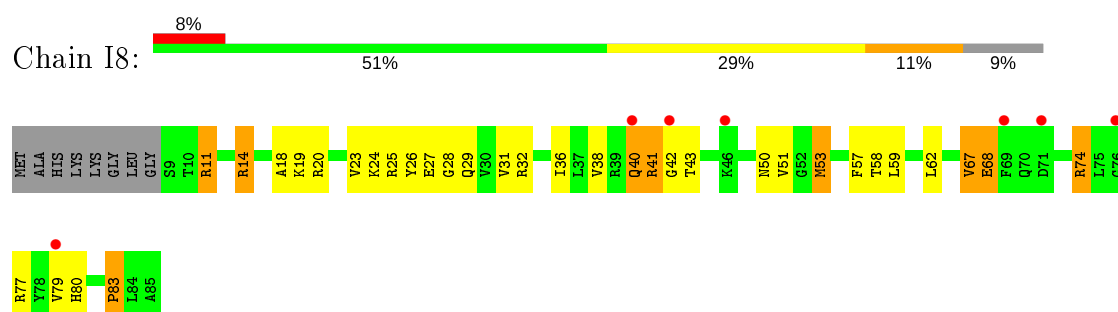
- Molecule 45: 50S ribosomal protein L25



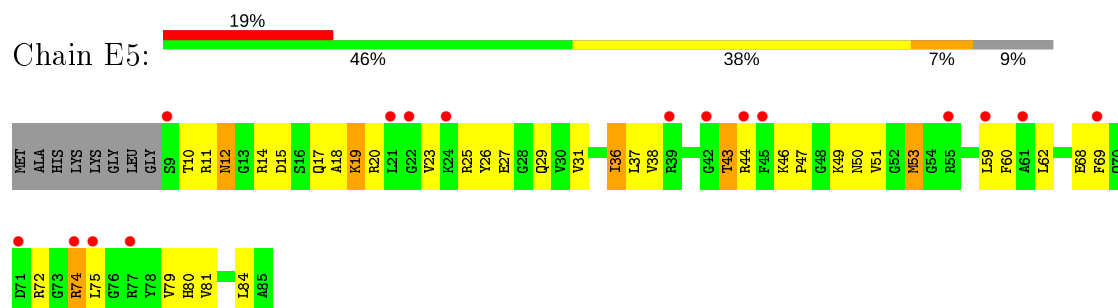




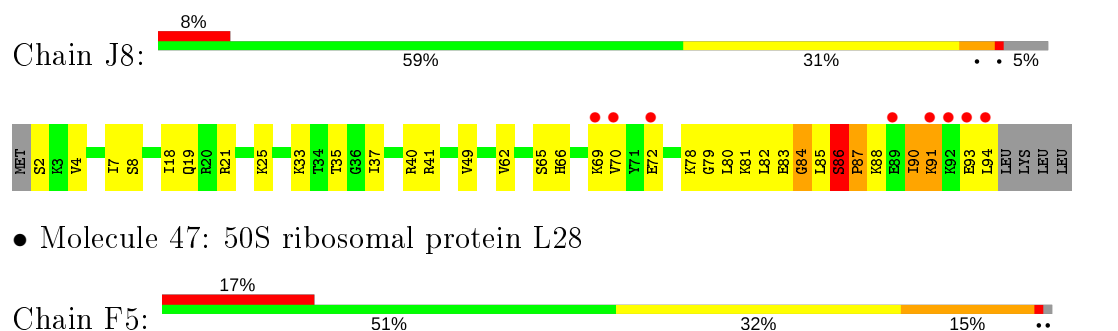
- Molecule 46: 50S ribosomal protein L27



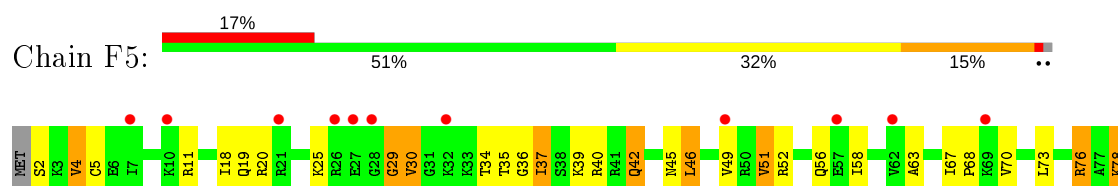
- Molecule 46: 50S ribosomal protein L27



- Molecule 47: 50S ribosomal protein L28



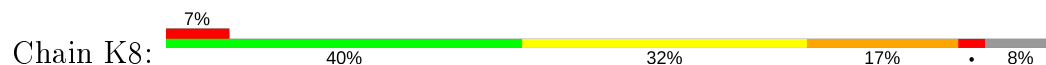
- Molecule 47: 50S ribosomal protein L28



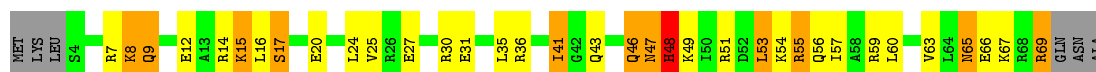




- Molecule 48: 50S ribosomal protein L29



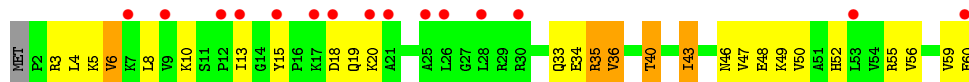
- Molecule 48: 50S ribosomal protein L29



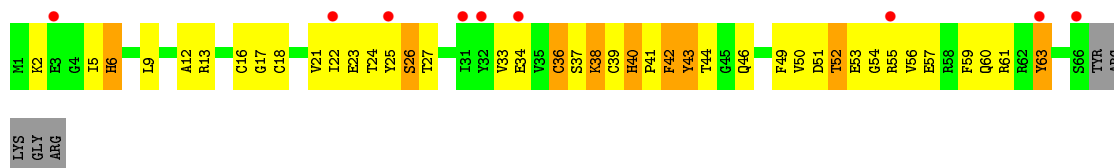
- Molecule 49: 50S ribosomal protein L30



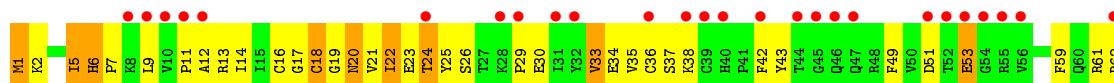
- Molecule 49: 50S ribosomal protein L30



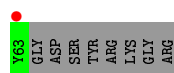
- Molecule 50: 50S ribosomal protein L31



- Molecule 50: 50S ribosomal protein L31







- Molecule 51: 50S ribosomal protein L32

Chain N8: 50% 20% 12% 18%



- Molecule 51: 50S ribosomal protein L32

Chain J5: 3% 58% 33% 5%



- Molecule 52: 50S ribosomal protein L34

Chain P8: 2% 53% 35% 8%



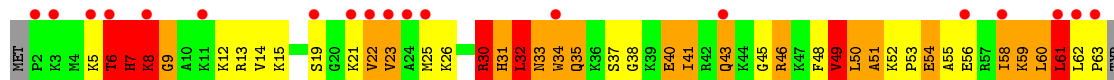
- Molecule 52: 50S ribosomal protein L34

Chain L5: 2% 51% 35% 6% 8%



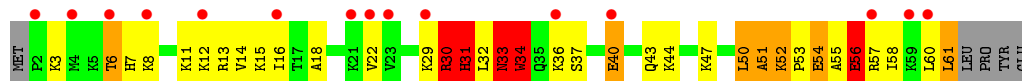
- Molecule 53: 50S ribosomal protein L35

Chain Q8: 29% 29% 29% 26% 11% 5%



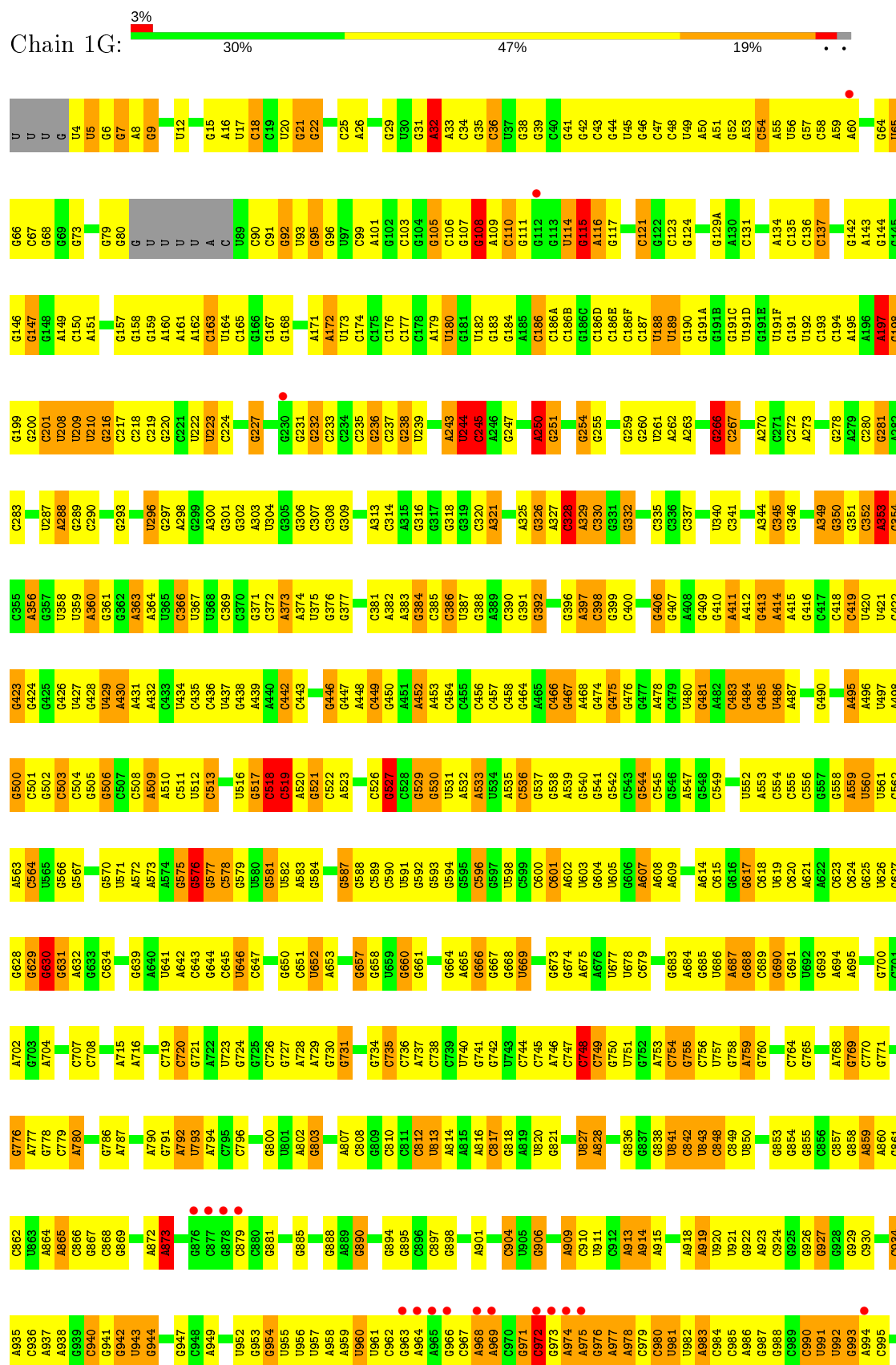
- Molecule 53: 50S ribosomal protein L35

Chain M5: 23% 38% 35% 11% 8% 8%





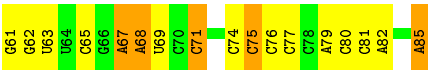
## ● Molecule 54: 16S ribosomal RNA



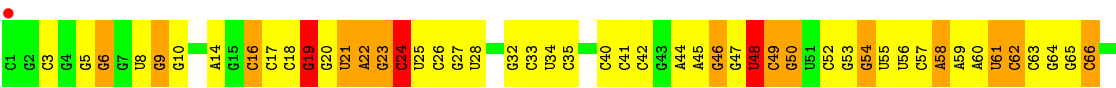








● Molecule 56: tRNA-fMet



● Molecule 57: mRNA





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	209.90Å 450.30Å 619.50Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	225.15 – 3.05 255.20 – 3.05	Depositor EDS
% Data completeness (in resolution range)	99.9 (225.15-3.05) 93.6 (255.20-3.05)	Depositor EDS
$R_{merge}$	0.42	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	0.86 (at 3.07Å)	Xtriage
Refinement program	PHENIX	Depositor
R, $R_{free}$	0.205 , 0.249 0.201 , 0.249	Depositor DCC
$R_{free}$ test set	2000 reflections (0.18%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	76.2	Xtriage
Anisotropy	0.299	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.26 , 75.4	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.42$ , $\langle L^2 \rangle = 0.25$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.89	EDS
Total number of atoms	299318	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	104.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.40% 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, OMC, ZN, OMG, MIA, MG, H2U, 4SU, 7MG, 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	0.78	10/36053 (0.0%)	1.46	488/56270 (0.9%)
2	12	0.35	0/1959	0.61	0/2642
2	1E	0.42	0/1959	0.66	1/2642 (0.0%)
3	22	0.40	0/1636	0.60	0/2205
3	2E	0.51	0/1629	0.66	0/2195
4	32	0.48	0/1732	0.71	0/2318
4	3E	0.65	3/1732 (0.2%)	0.80	2/2318 (0.1%)
5	42	0.45	0/1171	0.70	1/1576 (0.1%)
5	4E	0.55	0/1171	0.70	0/1576
6	52	0.50	0/855	0.70	0/1154
6	5E	0.56	0/855	0.74	0/1154
7	62	0.43	0/1275	0.59	0/1709
7	6E	0.46	0/1275	0.61	0/1709
8	72	0.42	0/1135	0.64	0/1527
8	7E	0.53	0/1135	0.71	0/1527
9	82	0.42	0/1028	0.63	0/1379
9	8E	0.45	0/1028	0.66	0/1379
10	1A	0.36	0/814	0.60	0/1095
10	1I	0.46	0/814	0.67	0/1095
11	2A	0.46	0/899	0.69	0/1213
11	2I	0.53	0/879	0.72	1/1187 (0.1%)
12	3A	0.52	0/991	0.81	2/1327 (0.2%)
12	3I	0.71	0/991	0.85	0/1327
13	4A	0.37	0/943	0.60	0/1265
13	4I	0.47	0/938	0.72	1/1258 (0.1%)
14	5A	0.43	0/484	0.72	0/643
14	5I	0.59	0/507	0.92	1/672 (0.1%)
15	6A	0.45	0/744	0.62	1/992 (0.1%)
15	6I	0.57	0/744	0.77	0/992
16	7A	0.51	0/721	0.71	0/970
16	7I	0.47	0/721	0.72	0/970
17	8A	0.52	1/847 (0.1%)	0.64	0/1131



Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
17	8I	0.55	0/847	0.74	0/1131
18	9A	0.50	0/569	0.69	0/757
18	9I	0.50	0/595	0.73	0/790
19	AA	0.41	0/654	0.70	0/884
19	AI	0.51	0/680	0.77	0/915
20	BA	0.48	0/764	0.76	0/1007
20	BI	0.43	0/764	0.68	0/1007
21	1B	0.48	0/221	0.65	0/288
21	1F	0.55	0/192	0.74	0/252
22	1K	0.76	0/1851	1.36	18/2877 (0.6%)
22	3K	0.64	0/1851	1.17	10/2877 (0.3%)
23	2K	0.90	1/1699 (0.1%)	1.64	40/2648 (1.5%)
24	4K	0.93	0/394	1.31	2/612 (0.3%)
25	14	0.95	72/70119 (0.1%)	1.66	1690/109464 (1.5%)
25	1H	1.12	193/70233 (0.3%)	1.89	2816/109643 (2.6%)
26	16	0.86	0/2928	1.60	51/4568 (1.1%)
26	1J	0.76	0/2928	1.48	37/4568 (0.8%)
27	11	0.83	0/2165	1.00	3/2919 (0.1%)
27	19	0.77	0/2170	0.98	6/2926 (0.2%)
28	21	0.66	0/1601	0.93	1/2160 (0.0%)
28	29	0.66	0/1601	0.89	1/2160 (0.0%)
29	31	0.79	1/1620 (0.1%)	0.90	2/2194 (0.1%)
29	39	0.62	1/1662 (0.1%)	0.84	2/2249 (0.1%)
30	41	0.55	0/1498	0.74	0/2016
30	49	0.42	0/1498	0.69	0/2016
31	51	0.60	0/1362	0.88	2/1841 (0.1%)
31	59	0.38	0/1341	0.67	1/1813 (0.1%)
32	61	0.50	0/1151	0.76	0/1558
32	69	0.47	0/1151	0.74	2/1558 (0.1%)
33	15	0.50	0/1131	0.69	0/1525
33	58	0.61	0/1131	0.84	0/1525
34	25	0.65	0/942	0.81	1/1269 (0.1%)
34	68	0.70	0/942	0.81	0/1269
35	35	0.65	0/1161	1.09	3/1544 (0.2%)
35	78	0.75	0/1161	1.06	1/1544 (0.1%)
36	45	0.68	0/1119	0.92	2/1496 (0.1%)
36	88	0.88	2/1142 (0.2%)	1.01	1/1527 (0.1%)
37	55	0.65	0/973	0.83	0/1302
37	98	0.64	0/981	0.85	0/1312
38	65	0.55	0/891	0.92	3/1187 (0.3%)
38	A8	0.65	0/891	0.89	2/1187 (0.2%)
39	75	0.60	0/1155	0.81	1/1542 (0.1%)
39	B8	0.66	0/1147	0.80	0/1532



Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
40	85	0.61	0/981	0.76	0/1306
40	C8	0.72	0/981	0.93	3/1306 (0.2%)
41	95	0.59	0/789	0.81	0/1057
41	D8	0.61	0/789	0.85	2/1057 (0.2%)
42	A5	0.74	0/910	0.82	0/1220
42	E8	0.70	0/910	0.93	3/1220 (0.2%)
43	B5	0.78	0/739	0.86	0/993
43	F8	0.82	0/756	0.95	1/1014 (0.1%)
44	C5	0.60	0/807	0.82	0/1076
44	G8	0.76	1/791 (0.1%)	0.98	3/1055 (0.3%)
45	D5	0.41	0/1460	0.67	0/1982
45	H8	0.50	0/1427	0.82	2/1935 (0.1%)
46	E5	0.64	0/620	0.85	0/827
46	I8	0.85	0/620	0.94	0/827
47	F5	0.63	0/769	0.85	0/1022
47	J8	0.77	0/736	0.93	0/978
48	G5	0.60	0/560	0.79	0/741
48	K8	0.85	1/560 (0.2%)	0.92	0/741
49	H5	0.53	0/473	0.70	0/635
49	L8	0.57	0/473	0.70	0/635
50	I5	0.43	0/527	0.73	0/709
50	M8	0.45	0/545	0.70	0/733
51	J5	0.62	0/467	0.80	0/632
51	N8	0.65	0/386	0.84	0/523
52	L5	0.82	0/399	0.94	0/526
52	P8	0.96	0/399	0.98	0/526
53	M5	0.83	1/486 (0.2%)	1.13	2/638 (0.3%)
53	Q8	1.03	0/454	1.44	4/607 (0.7%)
54	1G	0.68	1/36049 (0.0%)	1.34	271/56262 (0.5%)
55	1L	0.85	1/2018 (0.0%)	1.32	24/3142 (0.8%)
55	3L	0.67	2/2018 (0.1%)	1.25	12/3142 (0.4%)
56	2L	0.73	0/1725	1.37	12/2689 (0.4%)
57	4L	0.81	0/394	1.29	2/612 (0.3%)
All	All	0.85	291/322559 (0.1%)	1.47	5537/483244 (1.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
2	1E	0	2

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Mol	Chain	#Chirality outliers	#Planarity outliers
3	2E	0	1
4	3E	0	2
6	5E	0	1
11	2A	0	1
12	3I	0	1
13	4I	0	1
14	5A	0	1
14	5I	0	1
17	8I	0	1
19	AI	0	1
20	BA	0	1
20	BI	0	1
27	11	0	5
27	19	0	5
28	21	0	3
28	29	0	4
29	39	0	2
30	41	0	1
31	51	0	1
31	59	0	1
32	61	0	4
32	69	0	1
33	58	0	1
35	35	0	2
35	78	0	5
36	45	0	5
36	88	0	4
39	75	0	1
39	B8	0	1
40	85	0	2
40	C8	0	1
41	95	0	2
41	D8	0	1
43	B5	0	2
44	C5	0	2
44	G8	0	5
45	D5	0	1
45	H8	0	3
47	F5	0	2
47	J8	0	2
48	G5	0	3
50	M8	0	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
53	M5	0	3
53	Q8	0	4
All	All	0	95

The worst 5 of 291 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	1H	783	A	N3-C4	-12.01	1.27	1.34
25	1H	774	A	N9-C4	-10.83	1.31	1.37
25	1H	2430	A	N9-C4	-10.39	1.31	1.37
25	14	783	A	N9-C4	-9.88	1.31	1.37
25	14	774	A	N9-C4	-9.74	1.32	1.37

The worst 5 of 5537 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	1H	1899	G	N3-C4-N9	-19.08	114.55	126.00
25	1H	676	A	C2-N3-C4	-18.37	101.42	110.60
25	1H	945	A	C6-C5-N7	-18.34	119.46	132.30
25	1H	945	A	N1-C6-N6	17.84	129.30	118.60
25	1H	783	A	C2-N3-C4	-17.75	101.73	110.60

There are no chirality outliers.

5 of 95 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	1E	15	VAL	Peptide
2	1E	71	VAL	Peptide
3	2E	166	GLU	Peptide
4	3E	29	PRO	Peptide
4	3E	85	LYS	Peptide

## 5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	13	32207	0	16254	795	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	12	1924	0	1975	105	0
2	1E	1924	0	1975	91	0
3	22	1612	0	1677	104	0
3	2E	1605	0	1668	46	0
4	32	1702	0	1763	103	0
4	3E	1702	0	1763	79	0
5	42	1155	0	1213	75	0
5	4E	1155	0	1213	37	0
6	52	842	0	857	28	0
6	5E	842	0	857	44	0
7	62	1256	0	1296	57	0
7	6E	1256	0	1296	60	0
8	72	1115	0	1177	46	0
8	7E	1115	0	1177	56	0
9	82	1009	0	1037	65	0
9	8E	1009	0	1037	63	0
10	1A	801	0	849	52	0
10	1I	801	0	849	52	0
11	2A	884	0	904	39	0
11	2I	864	0	881	35	0
12	3A	975	0	1062	57	0
12	3I	975	0	1062	37	0
13	4A	933	0	992	61	0
13	4I	928	0	987	56	0
14	5A	475	0	511	31	0
14	5I	498	0	537	38	0
15	6A	733	0	771	28	0
15	6I	733	0	771	30	0
16	7A	705	0	725	15	0
16	7I	705	0	725	46	0
17	8A	834	0	904	35	0
17	8I	834	0	904	54	0
18	9A	564	0	631	21	0
18	9I	590	0	662	33	0
19	AA	640	0	633	37	0
19	AI	665	0	686	41	0
20	BA	762	0	861	36	0
20	BI	762	0	861	38	0
21	1B	217	0	234	20	0
21	1F	188	0	195	9	0
22	1K	1825	0	946	59	0
22	3K	1825	0	946	49	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
23	2K	1646	0	847	33	0
24	4K	349	0	176	13	0
25	14	62605	0	31561	1396	0
25	1H	62707	0	31610	1456	1
26	16	2617	0	1328	68	0
26	1J	2617	0	1328	93	0
27	11	2115	0	2195	124	0
27	19	2120	0	2197	103	0
28	21	1568	0	1634	94	0
28	29	1568	0	1634	108	0
29	31	1585	0	1632	81	0
29	39	1627	0	1680	101	0
30	41	1473	0	1535	86	0
30	49	1473	0	1535	74	0
31	51	1336	0	1418	82	0
31	59	1316	0	1395	79	0
32	61	1136	0	1223	61	0
32	69	1136	0	1223	62	0
33	15	1104	0	1180	50	0
33	58	1104	0	1180	66	0
34	25	932	0	996	54	0
34	68	932	0	996	26	0
35	35	1144	0	1228	108	0
35	78	1144	0	1228	99	0
36	45	1098	0	1160	66	0
36	88	1121	0	1179	56	0
37	55	959	0	1021	44	0
37	98	967	0	1033	55	0
38	65	881	0	943	67	0
38	A8	881	0	943	47	0
39	75	1141	0	1202	64	0
39	B8	1133	0	1190	64	0
40	85	963	0	1022	55	0
40	C8	963	0	1022	65	0
41	95	778	0	852	60	0
41	D8	778	0	852	34	0
42	A5	899	0	964	40	0
42	E8	899	0	964	27	0
43	B5	725	0	778	29	0
43	F8	742	0	803	44	0
44	C5	794	0	883	64	0
44	G8	778	0	863	61	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
45	D5	1428	0	1454	82	0
45	H8	1397	0	1430	57	0
46	E5	612	0	633	35	0
46	I8	612	0	633	31	0
47	F5	762	0	848	42	0
47	J8	729	0	802	23	0
48	G5	558	0	610	24	0
48	K8	558	0	610	33	0
49	H5	468	0	518	16	0
49	L8	468	0	518	20	0
50	I5	515	0	514	30	0
50	M8	533	0	526	34	0
51	J5	453	0	475	18	0
51	N8	374	0	393	22	0
52	L5	391	0	432	22	0
52	P8	391	0	432	15	0
53	M5	480	0	549	44	0
53	Q8	448	0	463	60	0
54	1G	32204	0	16256	845	1
55	1L	1807	0	920	33	0
55	3L	1807	0	920	54	0
56	2L	1645	0	843	44	0
57	4L	349	0	176	10	0
58	11	1	0	0	0	0
58	13	138	0	0	0	0
58	14	398	0	0	0	0
58	16	13	0	0	0	0
58	1G	90	0	0	0	0
58	1H	475	0	0	0	0
58	1J	6	0	0	0	0
58	1K	1	0	0	0	0
58	1L	1	0	0	0	0
58	21	2	0	0	0	0
58	25	1	0	0	0	0
58	29	3	0	0	0	0
58	2K	6	0	0	0	0
58	2L	3	0	0	0	0
58	31	4	0	0	0	0
58	39	1	0	0	0	0
58	3E	1	0	0	0	0
58	3I	1	0	0	0	0
58	3L	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
58	45	1	0	0	0	0
58	4E	1	0	0	0	0
58	78	1	0	0	0	0
58	85	1	0	0	0	0
58	8E	1	0	0	0	0
58	98	2	0	0	0	0
58	C5	1	0	0	0	0
58	I8	2	0	0	0	0
58	L5	1	0	0	0	0
58	L8	2	0	0	0	0
58	P8	1	0	0	0	0
59	32	1	0	0	0	0
59	3E	1	0	0	0	0
59	5A	1	0	0	0	0
59	5I	1	0	0	0	0
59	C5	1	0	0	0	0
59	G8	1	0	0	0	0
60	11	4	0	0	0	0
60	13	100	0	0	20	0
60	14	409	0	0	100	0
60	16	11	0	0	1	0
60	19	7	0	0	1	0
60	1G	51	0	0	14	0
60	1H	538	0	0	157	0
60	1K	1	0	0	0	0
60	21	2	0	0	0	0
60	29	2	0	0	1	0
60	2K	6	0	0	0	0
60	31	4	0	0	0	0
60	32	1	0	0	0	0
60	35	1	0	0	0	0
60	39	4	0	0	0	0
60	3E	2	0	0	0	0
60	3I	2	0	0	1	0
60	4K	2	0	0	0	0
60	4L	1	0	0	0	0
60	55	1	0	0	2	0
60	5I	1	0	0	0	0
60	75	1	0	0	0	0
60	78	4	0	0	2	0
60	7I	1	0	0	0	0
60	85	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
60	BA	1	0	0	0	0
60	D8	1	0	0	0	0
60	F8	1	0	0	0	0
60	L8	3	0	0	0	0
All	All	299318	0	199912	8796	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 18.

The worst 5 of 8796 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)
22:1K:35:QUO:N3	22:1K:35:QUO:C4	1.70	1.51
22:3K:35:QUO:C4	22:3K:35:QUO:N3	1.72	1.48
25:14:2057:A:OP2	60:14:3437:HOH:O	1.73	1.07
25:14:2032:G:N7	60:14:3594:HOH:O	1.91	1.04
25:14:2711:A:OP2	60:14:3464:HOH:O	1.72	1.04

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)
25:1H:2137:C:OP1	54:1G:999:U:O2'[4_555]	2.16	0.04

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	12	235/256 (92%)	201 (86%)	32 (14%)	2 (1%)	17	47
2	1E	235/256 (92%)	202 (86%)	31 (13%)	2 (1%)	17	47

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	22	204/239 (85%)	187 (92%)	17 (8%)	0	100	100
3	2E	203/239 (85%)	191 (94%)	12 (6%)	0	100	100
4	32	206/209 (99%)	181 (88%)	25 (12%)	0	100	100
4	3E	206/209 (99%)	191 (93%)	14 (7%)	1 (0%)	29	60
5	42	149/162 (92%)	141 (95%)	8 (5%)	0	100	100
5	4E	149/162 (92%)	145 (97%)	3 (2%)	1 (1%)	22	52
6	52	99/101 (98%)	97 (98%)	2 (2%)	0	100	100
6	5E	99/101 (98%)	94 (95%)	5 (5%)	0	100	100
7	62	153/156 (98%)	146 (95%)	7 (5%)	0	100	100
7	6E	153/156 (98%)	145 (95%)	8 (5%)	0	100	100
8	72	136/138 (99%)	127 (93%)	8 (6%)	1 (1%)	22	52
8	7E	136/138 (99%)	130 (96%)	6 (4%)	0	100	100
9	82	125/128 (98%)	116 (93%)	9 (7%)	0	100	100
9	8E	125/128 (98%)	109 (87%)	16 (13%)	0	100	100
10	1A	97/105 (92%)	90 (93%)	7 (7%)	0	100	100
10	1I	97/105 (92%)	86 (89%)	11 (11%)	0	100	100
11	2A	117/129 (91%)	106 (91%)	11 (9%)	0	100	100
11	2I	114/129 (88%)	98 (86%)	14 (12%)	2 (2%)	8	30
12	3A	123/132 (93%)	106 (86%)	14 (11%)	3 (2%)	6	23
12	3I	123/132 (93%)	106 (86%)	17 (14%)	0	100	100
13	4A	115/126 (91%)	99 (86%)	15 (13%)	1 (1%)	17	47
13	4I	114/126 (90%)	98 (86%)	16 (14%)	0	100	100
14	5A	56/61 (92%)	48 (86%)	8 (14%)	0	100	100
14	5I	59/61 (97%)	49 (83%)	9 (15%)	1 (2%)	9	32
15	6A	86/89 (97%)	78 (91%)	8 (9%)	0	100	100
15	6I	86/89 (97%)	77 (90%)	9 (10%)	0	100	100
16	7A	82/88 (93%)	73 (89%)	9 (11%)	0	100	100
16	7I	82/88 (93%)	78 (95%)	4 (5%)	0	100	100
17	8A	98/105 (93%)	91 (93%)	7 (7%)	0	100	100
17	8I	98/105 (93%)	92 (94%)	6 (6%)	0	100	100
18	9A	67/88 (76%)	61 (91%)	6 (9%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
18	9I	70/88 (80%)	63 (90%)	6 (9%)	1 (1%)	11	36
19	AA	80/93 (86%)	64 (80%)	14 (18%)	2 (2%)	5	22
19	AI	81/93 (87%)	69 (85%)	9 (11%)	3 (4%)	3	16
20	BA	97/106 (92%)	88 (91%)	9 (9%)	0	100	100
20	BI	97/106 (92%)	84 (87%)	13 (13%)	0	100	100
21	1B	23/27 (85%)	19 (83%)	4 (17%)	0	100	100
21	1F	20/27 (74%)	18 (90%)	2 (10%)	0	100	100
27	11	270/276 (98%)	249 (92%)	18 (7%)	3 (1%)	14	42
27	19	271/276 (98%)	249 (92%)	17 (6%)	5 (2%)	8	30
28	21	203/206 (98%)	175 (86%)	24 (12%)	4 (2%)	7	27
28	29	203/206 (98%)	162 (80%)	32 (16%)	9 (4%)	2	12
29	31	200/210 (95%)	178 (89%)	21 (10%)	1 (0%)	29	60
29	39	206/210 (98%)	171 (83%)	29 (14%)	6 (3%)	4	20
30	41	179/182 (98%)	158 (88%)	18 (10%)	3 (2%)	9	32
30	49	179/182 (98%)	160 (89%)	18 (10%)	1 (1%)	25	55
31	51	172/180 (96%)	139 (81%)	28 (16%)	5 (3%)	4	20
31	59	169/180 (94%)	137 (81%)	29 (17%)	3 (2%)	8	30
32	61	144/148 (97%)	117 (81%)	23 (16%)	4 (3%)	5	21
32	69	144/148 (97%)	120 (83%)	20 (14%)	4 (3%)	5	21
33	15	136/140 (97%)	122 (90%)	13 (10%)	1 (1%)	22	52
33	58	136/140 (97%)	118 (87%)	15 (11%)	3 (2%)	6	25
34	25	120/122 (98%)	113 (94%)	7 (6%)	0	100	100
34	68	120/122 (98%)	113 (94%)	7 (6%)	0	100	100
35	35	148/150 (99%)	110 (74%)	31 (21%)	7 (5%)	2	12
35	78	148/150 (99%)	119 (80%)	24 (16%)	5 (3%)	3	17
36	45	136/141 (96%)	114 (84%)	21 (15%)	1 (1%)	22	52
36	88	139/141 (99%)	113 (81%)	25 (18%)	1 (1%)	22	52
37	55	115/118 (98%)	107 (93%)	8 (7%)	0	100	100
37	98	116/118 (98%)	106 (91%)	8 (7%)	2 (2%)	9	32
38	65	109/112 (97%)	89 (82%)	19 (17%)	1 (1%)	17	47
38	A8	109/112 (97%)	89 (82%)	19 (17%)	1 (1%)	17	47

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
39	75	135/146 (92%)	116 (86%)	17 (13%)	2 (2%)	10	35
39	B8	134/146 (92%)	122 (91%)	12 (9%)	0	100	100
40	85	115/118 (98%)	106 (92%)	8 (7%)	1 (1%)	17	47
40	C8	115/118 (98%)	105 (91%)	8 (7%)	2 (2%)	9	32
41	95	99/101 (98%)	80 (81%)	17 (17%)	2 (2%)	7	27
41	D8	99/101 (98%)	95 (96%)	2 (2%)	2 (2%)	7	27
42	A5	111/113 (98%)	103 (93%)	7 (6%)	1 (1%)	17	47
42	E8	111/113 (98%)	105 (95%)	6 (5%)	0	100	100
43	B5	90/96 (94%)	87 (97%)	3 (3%)	0	100	100
43	F8	92/96 (96%)	83 (90%)	7 (8%)	2 (2%)	6	25
44	C5	102/110 (93%)	75 (74%)	24 (24%)	3 (3%)	4	20
44	G8	100/110 (91%)	81 (81%)	14 (14%)	5 (5%)	2	11
45	D5	177/206 (86%)	138 (78%)	30 (17%)	9 (5%)	2	10
45	H8	173/206 (84%)	143 (83%)	22 (13%)	8 (5%)	2	12
46	E5	75/85 (88%)	73 (97%)	1 (1%)	1 (1%)	12	38
46	I8	75/85 (88%)	63 (84%)	11 (15%)	1 (1%)	12	38
47	F5	95/98 (97%)	87 (92%)	6 (6%)	2 (2%)	7	26
47	J8	91/98 (93%)	85 (93%)	4 (4%)	2 (2%)	6	25
48	G5	64/72 (89%)	60 (94%)	2 (3%)	2 (3%)	4	19
48	K8	64/72 (89%)	59 (92%)	4 (6%)	1 (2%)	9	33
49	H5	57/60 (95%)	55 (96%)	2 (4%)	0	100	100
49	L8	57/60 (95%)	55 (96%)	2 (4%)	0	100	100
50	I5	61/71 (86%)	35 (57%)	24 (39%)	2 (3%)	4	17
50	M8	64/71 (90%)	44 (69%)	18 (28%)	2 (3%)	4	19
51	J5	56/60 (93%)	50 (89%)	5 (9%)	1 (2%)	8	30
51	N8	47/60 (78%)	43 (92%)	4 (8%)	0	100	100
52	L5	43/49 (88%)	41 (95%)	2 (5%)	0	100	100
52	P8	43/49 (88%)	41 (95%)	2 (5%)	0	100	100
53	M5	58/65 (89%)	46 (79%)	10 (17%)	2 (3%)	3	17
53	Q8	60/65 (92%)	41 (68%)	12 (20%)	7 (12%)	0	1
All	All	11230/11946 (94%)	9889 (88%)	1191 (11%)	150 (1%)	12	38



5 of 150 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
14	5I	25	VAL
18	9I	22	VAL
44	G8	81	LYS
45	H8	53	ILE
53	Q8	51	ALA

### 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%)	159 (78%)	46 (22%)	1	3
2	1E	205/220 (93%)	161 (78%)	44 (22%)	1	3
3	22	160/188 (85%)	124 (78%)	36 (22%)	1	3
3	2E	159/188 (85%)	124 (78%)	35 (22%)	1	3
4	32	180/181 (99%)	150 (83%)	30 (17%)	2	8
4	3E	180/181 (99%)	148 (82%)	32 (18%)	2	7
5	42	116/123 (94%)	93 (80%)	23 (20%)	1	5
5	4E	116/123 (94%)	97 (84%)	19 (16%)	2	9
6	52	90/90 (100%)	73 (81%)	17 (19%)	1	5
6	5E	90/90 (100%)	77 (86%)	13 (14%)	3	12
7	62	126/127 (99%)	102 (81%)	24 (19%)	1	5
7	6E	126/127 (99%)	107 (85%)	19 (15%)	3	10
8	72	119/119 (100%)	106 (89%)	13 (11%)	6	22
8	7E	119/119 (100%)	97 (82%)	22 (18%)	1	6
9	82	98/99 (99%)	78 (80%)	20 (20%)	1	4
9	8E	98/99 (99%)	76 (78%)	22 (22%)	1	3
10	1A	89/92 (97%)	70 (79%)	19 (21%)	1	4
10	1I	89/92 (97%)	73 (82%)	16 (18%)	1	6
11	2A	90/99 (91%)	74 (82%)	16 (18%)	2	7

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
11	2I	88/99 (89%)	73 (83%)	15 (17%)	2	8
12	3A	104/109 (95%)	85 (82%)	19 (18%)	1	6
12	3I	104/109 (95%)	88 (85%)	16 (15%)	2	10
13	4A	94/101 (93%)	77 (82%)	17 (18%)	1	6
13	4I	94/101 (93%)	76 (81%)	18 (19%)	1	5
14	5A	48/50 (96%)	39 (81%)	9 (19%)	1	5
14	5I	50/50 (100%)	36 (72%)	14 (28%)	0	1
15	6A	79/80 (99%)	70 (89%)	9 (11%)	5	20
15	6I	79/80 (99%)	67 (85%)	12 (15%)	3	10
16	7A	72/74 (97%)	62 (86%)	10 (14%)	3	13
16	7I	72/74 (97%)	56 (78%)	16 (22%)	1	3
17	8A	95/97 (98%)	82 (86%)	13 (14%)	3	14
17	8I	95/97 (98%)	77 (81%)	18 (19%)	1	5
18	9A	60/77 (78%)	50 (83%)	10 (17%)	2	8
18	9I	63/77 (82%)	52 (82%)	11 (18%)	2	7
19	AA	66/80 (82%)	55 (83%)	11 (17%)	2	8
19	AI	72/80 (90%)	55 (76%)	17 (24%)	1	2
20	BA	76/82 (93%)	58 (76%)	18 (24%)	1	2
20	BI	76/82 (93%)	66 (87%)	10 (13%)	4	15
21	1B	20/22 (91%)	17 (85%)	3 (15%)	3	11
21	1F	17/22 (77%)	14 (82%)	3 (18%)	2	7
27	11	214/218 (98%)	164 (77%)	50 (23%)	1	2
27	19	214/218 (98%)	170 (79%)	44 (21%)	1	4
28	21	165/166 (99%)	131 (79%)	34 (21%)	1	4
28	29	165/166 (99%)	124 (75%)	41 (25%)	0	2
29	31	161/166 (97%)	133 (83%)	28 (17%)	2	7
29	39	165/166 (99%)	129 (78%)	36 (22%)	1	3
30	41	155/156 (99%)	123 (79%)	32 (21%)	1	4
30	49	155/156 (99%)	127 (82%)	28 (18%)	1	6
31	51	145/148 (98%)	111 (77%)	34 (23%)	1	2
31	59	143/148 (97%)	114 (80%)	29 (20%)	1	4

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
32	61	122/124 (98%)	91 (75%)	31 (25%)	0	1
32	69	122/124 (98%)	89 (73%)	33 (27%)	0	1
33	15	117/119 (98%)	91 (78%)	26 (22%)	1	3
33	58	117/119 (98%)	96 (82%)	21 (18%)	2	6
34	25	100/100 (100%)	77 (77%)	23 (23%)	1	2
34	68	100/100 (100%)	84 (84%)	16 (16%)	2	9
35	35	116/116 (100%)	81 (70%)	35 (30%)	0	0
35	78	116/116 (100%)	73 (63%)	43 (37%)	0	0
36	45	109/111 (98%)	87 (80%)	22 (20%)	1	4
36	88	111/111 (100%)	89 (80%)	22 (20%)	1	5
37	55	100/101 (99%)	78 (78%)	22 (22%)	1	3
37	98	101/101 (100%)	78 (77%)	23 (23%)	1	3
38	65	87/88 (99%)	61 (70%)	26 (30%)	0	0
38	A8	87/88 (99%)	59 (68%)	28 (32%)	0	0
39	75	120/127 (94%)	94 (78%)	26 (22%)	1	3
39	B8	119/127 (94%)	89 (75%)	30 (25%)	0	1
40	85	93/94 (99%)	81 (87%)	12 (13%)	4	16
40	C8	93/94 (99%)	78 (84%)	15 (16%)	2	9
41	95	82/82 (100%)	65 (79%)	17 (21%)	1	4
41	D8	82/82 (100%)	63 (77%)	19 (23%)	1	2
42	A5	92/92 (100%)	75 (82%)	17 (18%)	1	6
42	E8	92/92 (100%)	66 (72%)	26 (28%)	0	1
43	B5	74/78 (95%)	60 (81%)	14 (19%)	1	5
43	F8	76/78 (97%)	66 (87%)	10 (13%)	4	15
44	C5	85/91 (93%)	59 (69%)	26 (31%)	0	0
44	G8	84/91 (92%)	68 (81%)	16 (19%)	1	5
45	D5	158/179 (88%)	123 (78%)	35 (22%)	1	3
45	H8	154/179 (86%)	120 (78%)	34 (22%)	1	3
46	E5	62/67 (92%)	51 (82%)	11 (18%)	2	7
46	I8	62/67 (92%)	51 (82%)	11 (18%)	2	7
47	F5	82/83 (99%)	63 (77%)	19 (23%)	1	2

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
47	J8	78/83 (94%)	66 (85%)	12 (15%)	2	10
48	G5	62/67 (92%)	49 (79%)	13 (21%)	1	4
48	K8	62/67 (92%)	42 (68%)	20 (32%)	0	0
49	H5	51/52 (98%)	40 (78%)	11 (22%)	1	3
49	L8	51/52 (98%)	42 (82%)	9 (18%)	2	7
50	I5	57/63 (90%)	43 (75%)	14 (25%)	0	2
50	M8	59/63 (94%)	47 (80%)	12 (20%)	1	4
51	J5	51/52 (98%)	45 (88%)	6 (12%)	5	18
51	N8	43/52 (83%)	34 (79%)	9 (21%)	1	4
52	L5	38/42 (90%)	33 (87%)	5 (13%)	4	15
52	P8	38/42 (90%)	30 (79%)	8 (21%)	1	4
53	M5	50/55 (91%)	37 (74%)	13 (26%)	0	1
53	Q8	42/55 (76%)	22 (52%)	20 (48%)	0	0
All	All	9458/9894 (96%)	7506 (79%)	1952 (21%)	1	4

5 of 1952 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
45	H8	168	GLU
4	32	184	LYS
44	C5	31	LEU
48	K8	14	ARG
2	12	25	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 23 such sidechains are listed below:

Mol	Chain	Res	Type
7	62	28	ASN
11	2A	26	ASN
46	E5	29	GLN
9	82	23	ASN
13	4A	77	ASN

### 5.3.3 RNA ⓘ



Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	13	1496/1522 (98%)	355 (23%)	31 (2%)
22	1K	82/85 (96%)	39 (47%)	4 (4%)
22	3K	82/85 (96%)	31 (37%)	3 (3%)
23	2K	76/77 (98%)	20 (26%)	3 (3%)
24	4K	13/27 (48%)	4 (30%)	0
25	14	2905/2917 (99%)	766 (26%)	39 (1%)
25	1H	2911/2917 (99%)	766 (26%)	56 (1%)
26	16	121/122 (99%)	26 (21%)	0
26	1J	121/122 (99%)	30 (24%)	2 (1%)
54	1G	1495/1522 (98%)	393 (26%)	37 (2%)
55	1L	84/85 (98%)	37 (44%)	4 (4%)
55	3L	84/85 (98%)	28 (33%)	3 (3%)
56	2L	76/77 (98%)	17 (22%)	2 (2%)
57	4L	15/27 (55%)	5 (33%)	1 (6%)
All	All	9561/9670 (98%)	2517 (26%)	185 (1%)

5 of 2517 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	31	G

5 of 185 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
25	1H	1992	G
54	1G	266	G
25	14	2212	A
25	1H	2171	A
25	1H	2566	A

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

25 non-standard protein/DNA/RNA residues are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the



expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z  > 2$	Counts	RMSZ	# $ Z  > 2$
23	7MG	2K	47	23	22,26,27	3.37	7 (31%)	28,39,42	2.56	11 (39%)
56	PSU	2L	56	56	17,21,22	1.10	1 (5%)	20,30,33	3.28	5 (25%)
22	OMG	1K	17	22	18,26,27	5.66	6 (33%)	20,38,41	5.42	10 (50%)
22	PSU	3K	64	22	17,21,22	1.21	2 (11%)	20,30,33	3.41	6 (30%)
22	OMG	3K	17	22	18,26,27	5.72	6 (33%)	20,38,41	5.40	7 (35%)
22	MIA	3K	38	22	24,31,32	2.72	5 (20%)	26,44,47	2.79	10 (38%)
56	5MU	2L	55	56	15,22,23	2.18	3 (20%)	16,32,35	1.87	3 (18%)
22	5MU	1K	63	22	15,22,23	2.13	3 (20%)	16,32,35	1.65	2 (12%)
56	4SU	2L	8	56	14,21,22	3.52	2 (14%)	15,30,33	1.15	2 (13%)
56	OMC	2L	33	56	15,22,23	2.31	4 (26%)	17,31,34	1.57	2 (11%)
22	PSU	1K	40	22	17,21,22	1.07	1 (5%)	20,30,33	3.34	7 (35%)
23	5MU	2K	55	23	15,22,23	2.19	3 (20%)	16,32,35	1.82	2 (12%)
22	4SU	1K	8	22	14,21,22	3.43	2 (14%)	15,30,33	1.48	2 (13%)
22	PSU	3K	40	22	17,21,22	1.13	1 (5%)	20,30,33	3.58	7 (35%)
22	MIA	1K	38	22	24,31,32	2.48	3 (12%)	26,44,47	2.83	9 (34%)
22	5MU	3K	63	22	15,22,23	2.14	3 (20%)	16,32,35	1.81	2 (12%)
23	4SU	2K	8	23	14,21,22	3.39	2 (14%)	15,30,33	0.87	0
23	PSU	2K	56	23	17,21,22	1.21	2 (11%)	20,30,33	3.14	5 (25%)
23	H2U	2K	21	23	18,21,22	2.58	4 (22%)	21,30,33	1.87	5 (23%)
22	PSU	1K	64	22	17,21,22	1.01	1 (5%)	20,30,33	3.29	5 (25%)
22	4SU	3K	8	22	14,21,22	3.21	2 (14%)	15,30,33	1.44	2 (13%)
56	H2U	2L	21	56	18,21,22	2.38	3 (16%)	21,30,33	1.69	5 (23%)
22	QUO	1K	35	24,22	28,35,36	5.53	8 (28%)	32,52,55	4.94	10 (31%)
23	OMC	2K	33	23	15,22,23	2.02	4 (26%)	17,31,34	1.82	3 (17%)
22	QUO	3K	35	22	28,35,36	5.80	9 (32%)	32,52,55	4.88	12 (37%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
23	7MG	2K	47	23	-	4/7/37/38	0/3/3/3
56	PSU	2L	56	56	-	0/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	OMG	1K	17	22	-	3/5/27/28	0/3/3/3
22	PSU	3K	64	22	-	1/7/25/26	0/2/2/2
22	OMG	3K	17	22	-	4/5/27/28	0/3/3/3
22	MIA	3K	38	22	-	6/11/33/34	0/3/3/3
56	5MU	2L	55	56	-	0/5/25/26	0/2/2/2
22	5MU	1K	63	22	-	4/5/25/26	0/2/2/2
56	4SU	2L	8	56	-	0/5/25/26	0/2/2/2
56	OMC	2L	33	56	-	0/7/27/28	0/2/2/2
22	PSU	1K	40	22	-	2/7/25/26	0/2/2/2
23	5MU	2K	55	23	-	0/5/25/26	0/2/2/2
22	4SU	1K	8	22	-	3/5/25/26	0/2/2/2
22	PSU	3K	40	22	-	1/7/25/26	0/2/2/2
22	MIA	1K	38	22	-	5/11/33/34	0/3/3/3
22	5MU	3K	63	22	-	0/5/25/26	0/2/2/2
23	4SU	2K	8	23	-	0/5/25/26	0/2/2/2
23	PSU	2K	56	23	-	0/7/25/26	0/2/2/2
23	H2U	2K	21	23	-	4/7/38/39	0/2/2/2
22	PSU	1K	64	22	-	0/7/25/26	0/2/2/2
22	4SU	3K	8	22	-	1/5/25/26	0/2/2/2
56	H2U	2L	21	56	-	3/7/38/39	0/2/2/2
22	QUO	1K	35	24,22	-	5/6/43/44	0/4/4/4
23	OMC	2K	33	23	-	0/7/27/28	0/2/2/2
22	QUO	3K	35	22	-	2/6/43/44	0/4/4/4

The worst 5 of 87 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	3K	35	QUO	C4-N3	23.67	1.72	1.35
22	1K	35	QUO	C4-N3	22.33	1.70	1.35
22	3K	17	OMG	C4-N3	16.34	1.61	1.35
22	1K	17	OMG	C4-N3	16.02	1.60	1.35
22	1K	17	OMG	C8-N7	-14.61	1.08	1.34

The worst 5 of 134 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	1K	35	QUO	C6-C5-C4	21.44	127.12	115.01
22	3K	35	QUO	C6-C5-C4	20.38	126.52	115.01
22	1K	17	OMG	C6-C5-C4	-14.63	106.83	120.80
22	3K	17	OMG	C6-C5-C4	-14.34	107.11	120.80

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Mol	Chain	Res	Type	Atoms	Z	Observed( $^{\circ}$ )	Ideal( $^{\circ}$ )
22	3K	17	OMG	C1'-N9-C4	12.69	148.94	126.64

There are no chirality outliers.

5 of 48 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
22	1K	17	OMG	O4'-C4'-C5'-O5'
22	1K	17	OMG	C1'-C2'-O2'-CM2
22	3K	17	OMG	C1'-C2'-O2'-CM2
22	3K	38	MIA	C5-C6-N6-C12
22	3K	38	MIA	N1-C6-N6-C12

There are no ring outliers.

20 monomers are involved in 43 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
23	2K	47	7MG	3	0
56	2L	56	PSU	1	0
22	1K	17	OMG	3	0
22	3K	64	PSU	1	0
22	3K	17	OMG	3	0
22	3K	38	MIA	4	0
56	2L	55	5MU	2	0
22	1K	63	5MU	2	0
56	2L	8	4SU	1	0
56	2L	33	OMC	1	0
23	2K	55	5MU	3	0
22	1K	8	4SU	1	0
22	1K	38	MIA	5	0
23	2K	8	4SU	1	0
23	2K	21	H2U	1	0
22	1K	64	PSU	2	0
22	3K	8	4SU	2	0
56	2L	21	H2U	1	0
22	1K	35	QUO	6	0
22	3K	35	QUO	2	0

## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.



## 5.6 Ligand geometry [i](#)

Of 1166 ligands modelled in this entry, 1166 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
54	1G	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	1G	1530:G	O3'	1531:A	P	3.04



## 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	1498/1522 (98%)	0.03	25 (1%) 70 46	53, 97, 184, 399	0
2	12	237/256 (92%)	-0.05	8 (3%) 45 22	130, 169, 209, 225	0
2	1E	237/256 (92%)	-0.03	5 (2%) 63 39	106, 143, 183, 208	0
3	22	206/239 (86%)	0.31	17 (8%) 11 4	131, 148, 178, 208	0
3	2E	205/239 (85%)	-0.10	2 (0%) 82 63	84, 106, 147, 160	0
4	32	208/209 (99%)	0.96	27 (12%) 3 1	94, 116, 145, 163	0
4	3E	208/209 (99%)	0.55	18 (8%) 10 3	78, 104, 133, 148	0
5	42	151/162 (93%)	0.76	27 (17%) 1 0	104, 129, 145, 174	0
5	4E	151/162 (93%)	0.59	17 (11%) 5 1	73, 99, 121, 159	0
6	52	101/101 (100%)	-0.36	0 100 100	86, 101, 124, 148	0
6	5E	101/101 (100%)	0.11	1 (0%) 82 63	82, 104, 122, 147	0
7	62	155/156 (99%)	0.61	22 (14%) 2 1	107, 125, 147, 172	0
7	6E	155/156 (99%)	0.55	21 (13%) 3 1	99, 117, 150, 172	0
8	72	138/138 (100%)	1.44	40 (28%) 0 0	103, 129, 141, 146	0
8	7E	138/138 (100%)	0.70	24 (17%) 1 0	86, 107, 122, 130	0
9	82	127/128 (99%)	2.63	67 (52%) 0 0	112, 160, 189, 195	0
9	8E	127/128 (99%)	1.72	46 (36%) 0 0	87, 138, 174, 191	0
10	1A	99/105 (94%)	1.37	28 (28%) 0 0	125, 160, 189, 204	0
10	1I	99/105 (94%)	0.87	23 (23%) 0 0	84, 135, 166, 180	0
11	2A	119/129 (92%)	1.00	14 (11%) 4 1	90, 112, 142, 222	0
11	2I	116/129 (89%)	0.53	8 (6%) 16 6	75, 106, 136, 169	0
12	3A	125/132 (94%)	0.50	18 (14%) 2 1	84, 106, 150, 179	0
12	3I	125/132 (94%)	0.35	11 (8%) 10 3	65, 74, 119, 207	0
13	4A	117/126 (92%)	0.83	23 (19%) 1 0	113, 148, 183, 198	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
13	4I	116/126 (92%)	0.29	9 (7%) 13 4	82, 125, 146, 160	0
14	5A	58/61 (95%)	3.44	40 (68%) 0 0	130, 150, 162, 165	0
14	5I	61/61 (100%)	0.87	9 (14%) 2 1	85, 96, 116, 139	0
15	6A	88/89 (98%)	0.36	5 (5%) 23 10	82, 113, 134, 140	0
15	6I	88/89 (98%)	0.46	4 (4%) 33 15	78, 99, 119, 132	0
16	7A	84/88 (95%)	1.87	34 (40%) 0 0	88, 105, 134, 165	0
16	7I	84/88 (95%)	2.62	48 (57%) 0 0	97, 113, 152, 171	0
17	8A	100/105 (95%)	0.85	21 (21%) 1 0	92, 111, 131, 172	0
17	8I	100/105 (95%)	0.60	12 (12%) 4 1	85, 103, 119, 129	0
18	9A	69/88 (78%)	0.03	2 (2%) 51 26	94, 116, 143, 162	0
18	9I	72/88 (81%)	0.13	0 100 100	87, 108, 156, 177	0
19	AA	82/93 (88%)	0.85	11 (13%) 3 1	144, 164, 200, 218	0
19	AI	83/93 (89%)	0.27	5 (6%) 21 9	93, 125, 162, 185	0
20	BA	99/106 (93%)	1.09	22 (22%) 0 0	85, 108, 139, 170	0
20	BI	99/106 (93%)	1.19	34 (34%) 0 0	107, 121, 164, 171	0
21	1B	25/27 (92%)	5.69	22 (88%) 0 0	114, 135, 154, 180	0
21	1F	22/27 (81%)	3.18	15 (68%) 0 0	96, 108, 115, 122	0
22	1K	78/85 (91%)	0.13	5 (6%) 19 7	84, 149, 162, 175	0
22	3K	78/85 (91%)	-0.27	3 (3%) 40 20	68, 166, 190, 197	0
23	2K	71/77 (92%)	-0.10	1 (1%) 75 53	65, 89, 122, 126	0
24	4K	15/27 (55%)	1.92	6 (40%) 0 0	68, 100, 173, 180	0
25	14	2907/2917 (99%)	0.05	40 (1%) 75 53	46, 81, 243, 482	0
25	1H	2912/2917 (99%)	0.08	20 (0%) 87 72	35, 69, 228, 380	0
26	16	122/122 (100%)	-0.31	0 100 100	64, 90, 115, 254	0
26	1J	122/122 (100%)	-0.43	0 100 100	79, 115, 142, 216	0
27	11	272/276 (98%)	0.19	1 (0%) 92 82	38, 61, 80, 92	0
27	19	273/276 (98%)	0.53	16 (5%) 22 9	43, 70, 87, 100	0
28	21	205/206 (99%)	0.52	10 (4%) 29 13	46, 86, 143, 168	0
28	29	205/206 (99%)	0.84	32 (15%) 2 1	56, 90, 162, 204	0
29	31	202/210 (96%)	0.08	0 100 100	41, 75, 128, 144	0
29	39	208/210 (99%)	0.20	9 (4%) 35 16	56, 99, 181, 218	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2		OWAB(Å <sup>2</sup> )	Q<0.9
30	41	181/182 (99%)	0.42	9 (4%)	28 12	81, 107, 149, 173	0
30	49	181/182 (99%)	0.47	19 (10%)	6 2	110, 135, 175, 194	0
31	51	174/180 (96%)	0.24	8 (4%)	32 15	80, 105, 120, 146	0
31	59	171/180 (95%)	1.93	67 (39%)	0 0	138, 195, 241, 262	0
32	61	146/148 (98%)	0.10	6 (4%)	37 18	72, 128, 153, 163	0
32	69	146/148 (98%)	0.36	14 (9%)	8 2	77, 127, 159, 170	0
33	15	138/140 (98%)	0.95	26 (18%)	1 0	72, 103, 140, 162	0
33	58	138/140 (98%)	0.31	5 (3%)	42 21	62, 87, 134, 151	0
34	25	122/122 (100%)	0.35	6 (4%)	29 13	62, 84, 103, 109	0
34	68	122/122 (100%)	0.11	2 (1%)	72 49	53, 73, 90, 105	0
35	35	150/150 (100%)	0.92	28 (18%)	1 0	57, 105, 148, 199	0
35	78	150/150 (100%)	0.37	6 (4%)	38 18	43, 80, 110, 179	0
36	45	138/141 (97%)	1.82	52 (37%)	0 0	72, 104, 132, 153	0
36	88	141/141 (100%)	0.58	4 (2%)	53 28	55, 77, 101, 124	0
37	55	117/118 (99%)	0.61	14 (11%)	4 1	56, 76, 93, 114	0
37	98	118/118 (100%)	0.47	7 (5%)	22 9	56, 80, 99, 114	0
38	65	111/112 (99%)	0.81	17 (15%)	2 1	88, 112, 136, 157	0
38	A8	111/112 (99%)	0.15	4 (3%)	42 21	72, 87, 122, 145	0
39	75	137/146 (93%)	0.35	7 (5%)	28 12	75, 92, 156, 208	0
39	B8	136/146 (93%)	0.15	2 (1%)	73 51	70, 91, 146, 166	0
40	85	117/118 (99%)	0.82	15 (12%)	3 1	61, 89, 141, 183	0
40	C8	117/118 (99%)	0.73	12 (10%)	6 2	49, 77, 129, 152	0
41	95	101/101 (100%)	0.66	16 (15%)	2 0	59, 129, 145, 163	0
41	D8	101/101 (100%)	0.29	4 (3%)	38 18	52, 106, 146, 167	0
42	A5	113/113 (100%)	0.56	6 (5%)	26 11	58, 71, 109, 189	0
42	E8	113/113 (100%)	0.36	1 (0%)	84 66	51, 69, 100, 167	0
43	B5	92/96 (95%)	0.18	4 (4%)	35 16	64, 79, 106, 118	0
43	F8	94/96 (97%)	-0.09	0	100 100	52, 68, 95, 109	0
44	C5	104/110 (94%)	1.28	27 (25%)	0 0	90, 118, 184, 206	0
44	G8	102/110 (92%)	0.63	4 (3%)	39 19	64, 93, 138, 169	0
45	D5	179/206 (86%)	1.12	40 (22%)	0 0	111, 159, 253, 266	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
45	H8	175/206 (84%)	-0.00	4 (2%) 60 36	83, 130, 215, 234	0
46	E5	77/85 (90%)	1.18	16 (20%) 1 0	64, 85, 108, 157	0
46	I8	77/85 (90%)	0.67	7 (9%) 9 3	53, 69, 93, 148	0
47	F5	97/98 (98%)	1.44	17 (17%) 1 0	57, 80, 139, 192	0
47	J8	93/98 (94%)	0.84	8 (8%) 10 4	48, 68, 134, 163	0
48	G5	66/72 (91%)	0.07	0 100 100	78, 100, 122, 175	0
48	K8	66/72 (91%)	0.56	5 (7%) 13 5	54, 78, 98, 148	0
49	H5	59/60 (98%)	1.41	15 (25%) 0 0	77, 97, 153, 166	0
49	L8	59/60 (98%)	0.41	1 (1%) 70 46	58, 77, 114, 136	0
50	I5	63/71 (88%)	1.98	27 (42%) 0 0	153, 212, 237, 256	0
50	M8	66/71 (92%)	0.72	9 (13%) 3 1	111, 171, 226, 241	0
51	J5	58/60 (96%)	0.31	2 (3%) 45 22	55, 84, 168, 218	0
51	N8	49/60 (81%)	0.45	0 100 100	45, 64, 135, 149	0
52	L5	45/49 (91%)	0.51	1 (2%) 62 38	47, 56, 67, 77	0
52	P8	45/49 (91%)	0.17	1 (2%) 62 38	38, 45, 58, 78	0
53	M5	60/65 (92%)	1.42	15 (25%) 0 0	66, 77, 112, 129	0
53	Q8	62/65 (95%)	1.51	19 (30%) 0 0	56, 70, 96, 108	0
54	1G	1498/1522 (98%)	0.07	40 (2%) 54 28	69, 115, 181, 370	0
55	1L	85/85 (100%)	1.93	28 (32%) 0 0	124, 157, 168, 180	0
55	3L	85/85 (100%)	0.07	2 (2%) 59 34	75, 171, 201, 208	0
56	2L	72/77 (93%)	-0.29	1 (1%) 75 53	74, 105, 136, 141	0
57	4L	16/27 (59%)	2.43	8 (50%) 0 0	93, 136, 209, 217	0
All	All	20977/21616 (97%)	0.39	1586 (7%) 13 5	35, 99, 186, 482	0

The worst 5 of 1586 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
11	2A	129	SER	23.9
47	F5	98	LEU	19.3
31	59	100	GLY	15.0
11	2A	128	ALA	14.9
47	F5	97	LEU	12.1



## 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
56	H2U	2L	21	20/21	0.72	0.21	126,132,139,144	0
22	OMG	1K	17	24/25	0.79	0.19	131,142,162,173	0
22	5MU	3K	63	21/22	0.80	0.20	141,157,163,170	0
22	PSU	3K	64	20/21	0.82	0.17	152,161,169,173	0
22	4SU	3K	8	20/21	0.83	0.11	159,163,169,172	0
22	4SU	1K	8	20/21	0.85	0.14	137,141,150,153	0
22	OMG	3K	17	24/25	0.85	0.16	155,167,174,174	0
23	H2U	2K	21	20/21	0.86	0.19	113,120,123,125	0
22	5MU	1K	63	21/22	0.89	0.18	115,124,133,139	0
56	PSU	2L	56	20/21	0.90	0.10	110,113,122,124	0
22	PSU	1K	64	20/21	0.90	0.17	116,128,135,140	0
56	4SU	2L	8	20/21	0.91	0.12	108,114,119,122	0
22	QUO	3K	35	32/33	0.91	0.25	107,114,128,136	0
22	QUO	1K	35	32/33	0.93	0.34	71,90,101,103	0
22	PSU	1K	40	20/21	0.93	0.17	75,99,107,110	0
22	MIA	1K	38	29/30	0.94	0.32	76,87,107,110	0
22	MIA	3K	38	29/30	0.94	0.18	107,114,119,123	0
23	7MG	2K	47	24/25	0.95	0.14	91,98,108,113	0
56	5MU	2L	55	21/22	0.95	0.10	109,115,121,126	0
23	PSU	2K	56	20/21	0.95	0.13	92,97,108,110	0
22	PSU	3K	40	20/21	0.96	0.11	104,112,115,117	0
23	4SU	2K	8	20/21	0.96	0.15	87,91,95,95	0
23	OMC	2K	33	21/22	0.96	0.27	70,76,81,84	0
56	OMC	2L	33	21/22	0.96	0.23	96,98,101,111	0
23	5MU	2K	55	21/22	0.97	0.15	92,101,109,115	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( $\text{\AA}^2$ )	Q<0.9
58	MG	14	3301	1/1	0.45	0.23	87,87,87,87	0
58	MG	14	3270	1/1	0.47	0.26	84,84,84,84	0
58	MG	14	3202	1/1	0.49	0.23	70,70,70,70	0
58	MG	14	3228	1/1	0.49	0.38	79,79,79,79	0
58	MG	13	1619	1/1	0.51	0.23	99,99,99,99	0
58	MG	2K	103	1/1	0.51	0.23	80,80,80,80	0
58	MG	1H	3309	1/1	0.53	0.28	83,83,83,83	0
58	MG	1G	1661	1/1	0.54	0.21	100,100,100,100	0
58	MG	14	3162	1/1	0.54	0.34	100,100,100,100	0
58	MG	14	3296	1/1	0.57	0.37	97,97,97,97	0
58	MG	14	3151	1/1	0.57	0.24	82,82,82,82	0
58	MG	1G	1633	1/1	0.58	0.20	80,80,80,80	0
58	MG	13	1707	1/1	0.58	0.27	83,83,83,83	0
58	MG	29	302	1/1	0.61	0.26	68,68,68,68	0
58	MG	1H	3359	1/1	0.62	0.56	97,97,97,97	0
58	MG	14	3316	1/1	0.62	0.28	96,96,96,96	0
58	MG	1H	3175	1/1	0.62	0.17	58,58,58,58	0
58	MG	1H	3474	1/1	0.62	0.07	84,84,84,84	0
58	MG	1H	3365	1/1	0.63	0.46	84,84,84,84	0
58	MG	13	1654	1/1	0.63	0.24	76,76,76,76	0
58	MG	1H	3106	1/1	0.63	0.25	78,78,78,78	0
58	MG	14	3398	1/1	0.65	0.21	107,107,107,107	0
58	MG	14	3085	1/1	0.67	0.32	59,59,59,59	0
58	MG	1H	3374	1/1	0.67	0.34	78,78,78,78	0
58	MG	P8	101	1/1	0.68	0.34	70,70,70,70	0
58	MG	1H	3110	1/1	0.68	0.30	58,58,58,58	0
58	MG	14	3064	1/1	0.68	0.54	63,63,63,63	0
58	MG	13	1700	1/1	0.68	0.33	96,96,96,96	0
58	MG	14	3146	1/1	0.68	0.52	88,88,88,88	0
58	MG	1H	3296	1/1	0.69	0.25	66,66,66,66	0
58	MG	1H	3313	1/1	0.69	0.40	82,82,82,82	0
58	MG	3E	301	1/1	0.70	0.24	115,115,115,115	0
58	MG	1H	3261	1/1	0.70	0.24	66,66,66,66	0
58	MG	1G	1658	1/1	0.70	0.30	104,104,104,104	0
58	MG	1H	3377	1/1	0.70	0.28	68,68,68,68	0
58	MG	1H	3210	1/1	0.70	0.27	86,86,86,86	0
58	MG	14	3212	1/1	0.70	0.28	68,68,68,68	0
58	MG	14	3185	1/1	0.70	0.15	63,63,63,63	0
58	MG	13	1717	1/1	0.70	0.31	93,93,93,93	0
58	MG	1H	3409	1/1	0.70	0.14	46,46,46,46	0
58	MG	25	201	1/1	0.71	0.26	88,88,88,88	0
58	MG	14	3164	1/1	0.71	0.12	76,76,76,76	0
58	MG	14	3306	1/1	0.71	0.23	66,66,66,66	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
58	MG	1H	3316	1/1	0.71	0.24	80,80,80,80	0
58	MG	1H	3370	1/1	0.72	0.45	83,83,83,83	0
58	MG	14	3200	1/1	0.72	0.21	85,85,85,85	0
58	MG	1G	1689	1/1	0.72	0.08	108,108,108,108	0
58	MG	13	1720	1/1	0.72	0.26	89,89,89,89	0
58	MG	1H	3291	1/1	0.73	0.25	70,70,70,70	0
58	MG	13	1677	1/1	0.73	0.11	59,59,59,59	0
58	MG	1H	3269	1/1	0.73	0.25	55,55,55,55	0
58	MG	1H	3367	1/1	0.73	0.51	88,88,88,88	0
58	MG	13	1692	1/1	0.73	0.39	80,80,80,80	0
58	MG	13	1693	1/1	0.73	0.30	87,87,87,87	0
58	MG	14	3278	1/1	0.73	0.17	67,67,67,67	0
58	MG	14	3284	1/1	0.73	0.18	70,70,70,70	0
59	ZN	G8	201	1/1	0.73	0.33	185,185,185,185	0
58	MG	14	3166	1/1	0.74	0.25	76,76,76,76	0
58	MG	1G	1612	1/1	0.74	0.24	78,78,78,78	0
58	MG	14	3387	1/1	0.74	0.09	86,86,86,86	0
58	MG	13	1680	1/1	0.74	0.25	71,71,71,71	0
58	MG	14	3302	1/1	0.74	0.25	131,131,131,131	0
58	MG	13	1713	1/1	0.74	0.24	83,83,83,83	0
58	MG	1G	1666	1/1	0.74	0.20	117,117,117,117	0
58	MG	14	3308	1/1	0.74	0.53	79,79,79,79	0
58	MG	14	3147	1/1	0.74	0.15	73,73,73,73	0
58	MG	1H	3163	1/1	0.75	0.38	78,78,78,78	0
58	MG	14	3374	1/1	0.75	0.15	87,87,87,87	0
58	MG	1H	3315	1/1	0.75	0.26	67,67,67,67	0
58	MG	1H	3263	1/1	0.76	0.20	61,61,61,61	0
58	MG	1G	1631	1/1	0.76	0.26	73,73,73,73	0
58	MG	14	3115	1/1	0.76	0.19	71,71,71,71	0
58	MG	1H	3301	1/1	0.76	0.21	75,75,75,75	0
58	MG	1H	3221	1/1	0.76	0.14	69,69,69,69	0
58	MG	1H	3303	1/1	0.76	0.26	75,75,75,75	0
58	MG	14	3254	1/1	0.76	0.21	94,94,94,94	0
58	MG	1G	1656	1/1	0.76	0.16	92,92,92,92	0
58	MG	14	3140	1/1	0.76	0.13	61,61,61,61	0
58	MG	14	3229	1/1	0.76	0.54	82,82,82,82	0
58	MG	1H	3196	1/1	0.76	0.39	71,71,71,71	0
58	MG	14	3187	1/1	0.76	0.46	88,88,88,88	0
58	MG	1H	3305	1/1	0.76	0.24	66,66,66,66	0
58	MG	13	1698	1/1	0.76	0.17	83,83,83,83	0
58	MG	1H	3373	1/1	0.76	0.48	72,72,72,72	0
58	MG	13	1716	1/1	0.77	0.16	80,80,80,80	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
58	MG	2L	102	1/1	0.77	0.19	76,76,76,76	0
58	MG	1H	3198	1/1	0.77	0.16	79,79,79,79	0
58	MG	1H	3151	1/1	0.77	0.27	56,56,56,56	0
58	MG	1G	1654	1/1	0.77	0.16	110,110,110,110	0
58	MG	1G	1685	1/1	0.77	0.07	111,111,111,111	0
58	MG	1H	3332	1/1	0.77	0.17	62,62,62,62	0
58	MG	13	1723	1/1	0.77	0.14	77,77,77,77	0
58	MG	14	3259	1/1	0.77	0.21	66,66,66,66	0
58	MG	L8	101	1/1	0.78	0.24	84,84,84,84	0
58	MG	1H	3253	1/1	0.78	0.15	47,47,47,47	0
58	MG	1H	3122	1/1	0.78	0.35	74,74,74,74	0
58	MG	1H	3357	1/1	0.78	0.38	86,86,86,86	0
58	MG	14	3107	1/1	0.78	0.24	64,64,64,64	0
58	MG	1G	1629	1/1	0.78	0.25	85,85,85,85	0
58	MG	16	208	1/1	0.78	0.31	80,80,80,80	0
58	MG	1G	1627	1/1	0.79	0.26	77,77,77,77	0
58	MG	14	3194	1/1	0.79	0.14	57,57,57,57	0
58	MG	1G	1645	1/1	0.79	0.23	78,78,78,78	0
58	MG	14	3289	1/1	0.79	0.40	75,75,75,75	0
58	MG	1H	3338	1/1	0.79	0.31	80,80,80,80	0
58	MG	1G	1679	1/1	0.79	0.22	157,157,157,157	0
58	MG	14	3141	1/1	0.79	0.17	75,75,75,75	0
58	MG	14	3397	1/1	0.79	0.10	86,86,86,86	0
58	MG	1H	3461	1/1	0.79	0.16	103,103,103,103	0
58	MG	1H	3143	1/1	0.79	0.29	66,66,66,66	0
58	MG	1H	3366	1/1	0.79	0.42	83,83,83,83	0
58	MG	14	3267	1/1	0.80	0.12	74,74,74,74	0
58	MG	14	3298	1/1	0.80	0.57	80,80,80,80	0
58	MG	1H	3469	1/1	0.80	0.10	106,106,106,106	0
58	MG	16	205	1/1	0.80	0.19	87,87,87,87	0
58	MG	14	3295	1/1	0.80	0.19	80,80,80,80	0
58	MG	39	301	1/1	0.80	0.12	60,60,60,60	0
58	MG	1H	3302	1/1	0.80	0.55	92,92,92,92	0
58	MG	13	1735	1/1	0.80	0.12	93,93,93,93	0
58	MG	13	1610	1/1	0.80	0.32	94,94,94,94	0
58	MG	13	1671	1/1	0.80	0.20	138,138,138,138	0
58	MG	1G	1657	1/1	0.80	0.39	110,110,110,110	0
58	MG	1H	3224	1/1	0.80	0.38	79,79,79,79	0
58	MG	13	1648	1/1	0.80	0.30	75,75,75,75	0
58	MG	1H	3036	1/1	0.80	0.17	67,67,67,67	0
58	MG	1H	3192	1/1	0.80	0.24	58,58,58,58	0
58	MG	1G	1677	1/1	0.80	0.18	99,99,99,99	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
58	MG	13	1737	1/1	0.80	0.15	132,132,132,132	0
58	MG	14	3325	1/1	0.80	0.30	86,86,86,86	0
59	ZN	C5	202	1/1	0.80	0.15	194,194,194,194	0
58	MG	1H	3262	1/1	0.80	0.17	56,56,56,56	0
58	MG	13	1635	1/1	0.80	0.32	77,77,77,77	0
58	MG	1H	3184	1/1	0.80	0.16	87,87,87,87	0
58	MG	1G	1620	1/1	0.80	0.14	91,91,91,91	0
58	MG	16	203	1/1	0.81	0.36	77,77,77,77	0
58	MG	13	1714	1/1	0.81	0.36	95,95,95,95	0
58	MG	13	1653	1/1	0.81	0.15	84,84,84,84	0
58	MG	14	3310	1/1	0.81	0.30	76,76,76,76	0
58	MG	16	204	1/1	0.81	0.12	75,75,75,75	0
58	MG	31	303	1/1	0.81	0.15	63,63,63,63	0
58	MG	1H	3226	1/1	0.81	0.48	66,66,66,66	0
58	MG	13	1721	1/1	0.81	0.12	59,59,59,59	0
58	MG	1G	1626	1/1	0.81	0.18	80,80,80,80	0
58	MG	14	3129	1/1	0.82	0.36	73,73,73,73	0
58	MG	1H	3437	1/1	0.82	0.13	66,66,66,66	0
58	MG	13	1622	1/1	0.82	0.17	64,64,64,64	0
58	MG	13	1612	1/1	0.82	0.15	74,74,74,74	0
58	MG	13	1708	1/1	0.82	0.24	81,81,81,81	0
58	MG	1H	3462	1/1	0.82	0.07	76,76,76,76	0
58	MG	14	3138	1/1	0.82	0.19	69,69,69,69	0
58	MG	1G	1668	1/1	0.82	0.24	76,76,76,76	0
58	MG	13	1702	1/1	0.82	0.23	77,77,77,77	0
58	MG	13	1682	1/1	0.82	0.11	78,78,78,78	0
58	MG	13	1710	1/1	0.82	0.19	77,77,77,77	0
58	MG	1H	3467	1/1	0.82	0.09	68,68,68,68	0
58	MG	1H	3297	1/1	0.82	0.22	59,59,59,59	0
58	MG	13	1660	1/1	0.82	0.20	87,87,87,87	0
58	MG	8E	201	1/1	0.82	0.21	95,95,95,95	0
58	MG	1H	3231	1/1	0.82	0.31	110,110,110,110	0
58	MG	2K	105	1/1	0.83	0.30	87,87,87,87	0
58	MG	1H	3433	1/1	0.83	0.12	53,53,53,53	0
58	MG	1H	3266	1/1	0.83	0.14	43,43,43,43	0
58	MG	1H	3217	1/1	0.83	0.34	77,77,77,77	0
58	MG	14	3132	1/1	0.83	0.08	64,64,64,64	0
58	MG	14	3262	1/1	0.83	0.21	86,86,86,86	0
58	MG	16	212	1/1	0.83	0.11	78,78,78,78	0
58	MG	1G	1640	1/1	0.83	0.27	78,78,78,78	0
58	MG	1H	3035	1/1	0.83	0.34	83,83,83,83	0
58	MG	14	3142	1/1	0.83	0.16	62,62,62,62	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
58	MG	1G	1687	1/1	0.83	0.08	106,106,106,106	0
58	MG	13	1641	1/1	0.83	0.26	68,68,68,68	0
58	MG	14	3189	1/1	0.83	0.25	71,71,71,71	0
58	MG	14	3319	1/1	0.83	0.34	96,96,96,96	0
58	MG	18	101	1/1	0.83	0.19	63,63,63,63	0
58	MG	13	1670	1/1	0.83	0.19	86,86,86,86	0
58	MG	1G	1637	1/1	0.83	0.17	75,75,75,75	0
58	MG	14	3384	1/1	0.83	0.10	71,71,71,71	0
58	MG	13	1728	1/1	0.83	0.06	101,101,101,101	0
58	MG	1H	3398	1/1	0.83	0.12	50,50,50,50	0
58	MG	14	3078	1/1	0.84	0.27	87,87,87,87	0
58	MG	1H	3304	1/1	0.84	0.39	77,77,77,77	0
58	MG	1H	3342	1/1	0.84	0.23	70,70,70,70	0
58	MG	1H	3074	1/1	0.84	0.26	58,58,58,58	0
58	MG	14	3359	1/1	0.84	0.19	73,73,73,73	0
58	MG	14	3143	1/1	0.84	0.21	64,64,64,64	0
58	MG	1H	3475	1/1	0.84	0.14	95,95,95,95	0
58	MG	14	3326	1/1	0.84	0.13	90,90,90,90	0
58	MG	14	3080	1/1	0.84	0.19	45,45,45,45	0
58	MG	1H	3195	1/1	0.84	0.28	80,80,80,80	0
58	MG	14	3156	1/1	0.84	0.33	70,70,70,70	0
58	MG	1H	3276	1/1	0.84	0.45	76,76,76,76	0
58	MG	1H	3239	1/1	0.84	0.38	76,76,76,76	0
58	MG	1H	3463	1/1	0.84	0.25	92,92,92,92	0
58	MG	1H	3465	1/1	0.84	0.09	87,87,87,87	0
58	MG	1H	3082	1/1	0.84	0.36	60,60,60,60	0
58	MG	1H	3201	1/1	0.84	0.44	87,87,87,87	0
58	MG	14	3286	1/1	0.84	0.31	84,84,84,84	0
58	MG	1G	1636	1/1	0.84	0.24	85,85,85,85	0
58	MG	14	3299	1/1	0.84	0.23	53,53,53,53	0
58	MG	1H	3238	1/1	0.84	0.31	67,67,67,67	0
58	MG	1H	3159	1/1	0.84	0.38	64,64,64,64	0
58	MG	1H	3380	1/1	0.84	0.22	69,69,69,69	0
58	MG	3I	201	1/1	0.85	0.09	59,59,59,59	0
58	MG	14	3390	1/1	0.85	0.14	70,70,70,70	0
58	MG	1J	203	1/1	0.85	0.23	75,75,75,75	0
58	MG	13	1711	1/1	0.85	0.35	89,89,89,89	0
58	MG	14	3196	1/1	0.85	0.32	82,82,82,82	0
58	MG	13	1650	1/1	0.85	0.30	76,76,76,76	0
58	MG	14	3150	1/1	0.85	0.37	70,70,70,70	0
58	MG	1H	3346	1/1	0.85	0.28	78,78,78,78	0
58	MG	1H	3285	1/1	0.85	0.26	62,62,62,62	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
58	MG	14	3170	1/1	0.85	0.12	69,69,69,69	0
58	MG	1G	1660	1/1	0.85	0.41	82,82,82,82	0
58	MG	1H	3423	1/1	0.85	0.11	71,71,71,71	0
58	MG	13	1663	1/1	0.85	0.20	68,68,68,68	0
58	MG	1H	3207	1/1	0.85	0.21	57,57,57,57	0
58	MG	14	3283	1/1	0.85	0.28	88,88,88,88	0
58	MG	14	3235	1/1	0.85	0.19	87,87,87,87	0
58	MG	13	1712	1/1	0.85	0.17	74,74,74,74	0
58	MG	13	1709	1/1	0.85	0.33	87,87,87,87	0
58	MG	1H	3225	1/1	0.85	0.34	68,68,68,68	0
58	MG	14	3034	1/1	0.85	0.30	57,57,57,57	0
58	MG	1H	3128	1/1	0.85	0.17	46,46,46,46	0
58	MG	1H	3223	1/1	0.85	0.25	63,63,63,63	0
58	MG	14	3291	1/1	0.85	0.15	77,77,77,77	0
58	MG	1G	1611	1/1	0.85	0.23	89,89,89,89	0
58	MG	13	1615	1/1	0.86	0.18	86,86,86,86	0
58	MG	1H	3300	1/1	0.86	0.30	63,63,63,63	0
58	MG	1H	3328	1/1	0.86	0.31	63,63,63,63	0
58	MG	13	1706	1/1	0.86	0.19	98,98,98,98	0
58	MG	1H	3105	1/1	0.86	0.15	59,59,59,59	0
58	MG	14	3174	1/1	0.86	0.11	78,78,78,78	0
58	MG	29	303	1/1	0.86	0.26	63,63,63,63	0
58	MG	13	1676	1/1	0.86	0.25	76,76,76,76	0
58	MG	14	3102	1/1	0.86	0.48	81,81,81,81	0
58	MG	1G	1616	1/1	0.86	0.14	56,56,56,56	0
58	MG	1H	3112	1/1	0.86	0.14	33,33,33,33	0
58	MG	1H	3288	1/1	0.86	0.28	76,76,76,76	0
58	MG	1H	3453	1/1	0.86	0.13	51,51,51,51	0
58	MG	14	3131	1/1	0.86	0.23	71,71,71,71	0
58	MG	14	3363	1/1	0.86	0.07	77,77,77,77	0
58	MG	1H	3046	1/1	0.86	0.30	82,82,82,82	0
58	MG	1H	3312	1/1	0.86	0.26	68,68,68,68	0
58	MG	1H	3137	1/1	0.86	0.21	49,49,49,49	0
58	MG	1H	3383	1/1	0.86	0.23	113,113,113,113	0
58	MG	13	1611	1/1	0.86	0.29	64,64,64,64	0
58	MG	14	3303	1/1	0.86	0.40	73,73,73,73	0
58	MG	14	3036	1/1	0.86	0.12	74,74,74,74	0
58	MG	14	3309	1/1	0.86	0.24	83,83,83,83	0
58	MG	14	3381	1/1	0.86	0.08	70,70,70,70	0
58	MG	1H	3404	1/1	0.86	0.12	56,56,56,56	0
58	MG	14	3086	1/1	0.86	0.19	69,69,69,69	0
58	MG	13	1694	1/1	0.86	0.15	82,82,82,82	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
58	MG	14	3168	1/1	0.86	0.27	79,79,79,79	0
58	MG	14	3245	1/1	0.86	0.14	69,69,69,69	0
58	MG	14	3030	1/1	0.86	0.17	91,91,91,91	0
58	MG	14	3197	1/1	0.86	0.18	85,85,85,85	0
58	MG	13	1642	1/1	0.86	0.17	59,59,59,59	0
58	MG	1G	1624	1/1	0.86	0.31	89,89,89,89	0
58	MG	1H	3244	1/1	0.87	0.42	75,75,75,75	0
58	MG	1G	1625	1/1	0.87	0.20	90,90,90,90	0
58	MG	14	3188	1/1	0.87	0.25	79,79,79,79	0
58	MG	14	3389	1/1	0.87	0.09	73,73,73,73	0
58	MG	13	1684	1/1	0.87	0.27	96,96,96,96	0
58	MG	1G	1664	1/1	0.87	0.34	88,88,88,88	0
58	MG	1H	3324	1/1	0.87	0.42	86,86,86,86	0
58	MG	14	3275	1/1	0.87	0.15	70,70,70,70	0
58	MG	1H	3320	1/1	0.87	0.24	59,59,59,59	0
58	MG	1H	3040	1/1	0.87	0.16	62,62,62,62	0
58	MG	14	3238	1/1	0.87	0.14	83,83,83,83	0
58	MG	14	3268	1/1	0.87	0.25	88,88,88,88	0
58	MG	1H	3197	1/1	0.87	0.23	61,61,61,61	0
58	MG	16	209	1/1	0.87	0.27	59,59,59,59	0
58	MG	1H	3064	1/1	0.87	0.18	55,55,55,55	0
58	MG	13	1699	1/1	0.87	0.45	71,71,71,71	0
58	MG	14	3161	1/1	0.87	0.27	88,88,88,88	0
58	MG	1G	1647	1/1	0.87	0.27	83,83,83,83	0
58	MG	1H	3363	1/1	0.87	0.46	98,98,98,98	0
58	MG	1H	3222	1/1	0.87	0.36	82,82,82,82	0
58	MG	14	3261	1/1	0.87	0.39	68,68,68,68	0
58	MG	14	3327	1/1	0.87	0.29	86,86,86,86	0
58	MG	14	3089	1/1	0.87	0.08	72,72,72,72	0
58	MG	31	301	1/1	0.87	0.23	56,56,56,56	0
58	MG	1H	3382	1/1	0.87	0.21	80,80,80,80	0
58	MG	14	3195	1/1	0.87	0.33	81,81,81,81	0
58	MG	1G	1621	1/1	0.87	0.15	81,81,81,81	0
58	MG	14	3365	1/1	0.87	0.12	67,67,67,67	0
58	MG	14	3130	1/1	0.87	0.28	68,68,68,68	0
58	MG	78	201	1/1	0.88	0.21	53,53,53,53	0
58	MG	1H	3178	1/1	0.88	0.49	69,69,69,69	0
58	MG	1H	3158	1/1	0.88	0.26	69,69,69,69	0
58	MG	1H	3254	1/1	0.88	0.22	73,73,73,73	0
58	MG	1G	1635	1/1	0.88	0.21	86,86,86,86	0
58	MG	14	3288	1/1	0.88	0.15	66,66,66,66	0
58	MG	1H	3341	1/1	0.88	0.51	86,86,86,86	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
58	MG	1H	3115	1/1	0.88	0.20	48,48,48,48	0
58	MG	1H	3323	1/1	0.88	0.16	61,61,61,61	0
58	MG	13	1722	1/1	0.88	0.11	101,101,101,101	0
58	MG	13	1662	1/1	0.88	0.09	81,81,81,81	0
58	MG	1H	3072	1/1	0.88	0.20	62,62,62,62	0
58	MG	14	3249	1/1	0.88	0.61	49,49,49,49	0
58	MG	14	3204	1/1	0.88	0.14	48,48,48,48	0
58	MG	1H	3164	1/1	0.88	0.23	78,78,78,78	0
58	MG	1H	3429	1/1	0.88	0.13	49,49,49,49	0
58	MG	1H	3347	1/1	0.88	0.31	64,64,64,64	0
58	MG	13	1637	1/1	0.88	0.40	73,73,73,73	0
58	MG	1H	3339	1/1	0.88	0.42	78,78,78,78	0
58	MG	1H	3378	1/1	0.88	0.21	68,68,68,68	0
58	MG	14	3277	1/1	0.88	0.18	73,73,73,73	0
58	MG	1H	3408	1/1	0.88	0.11	47,47,47,47	0
58	MG	21	302	1/1	0.88	0.18	69,69,69,69	0
58	MG	1K	101	1/1	0.88	0.21	84,84,84,84	0
58	MG	13	1719	1/1	0.88	0.11	89,89,89,89	0
58	MG	2L	103	1/1	0.88	0.12	102,102,102,102	0
58	MG	16	213	1/1	0.88	0.13	82,82,82,82	0
58	MG	1H	3290	1/1	0.88	0.18	66,66,66,66	0
58	MG	14	3210	1/1	0.88	0.32	79,79,79,79	0
58	MG	1H	3336	1/1	0.88	0.34	66,66,66,66	0
58	MG	1H	3168	1/1	0.88	0.17	64,64,64,64	0
58	MG	1H	3161	1/1	0.88	0.28	68,68,68,68	0
58	MG	13	1703	1/1	0.88	0.27	71,71,71,71	0
58	MG	14	3216	1/1	0.88	0.20	83,83,83,83	0
58	MG	14	3176	1/1	0.88	0.19	71,71,71,71	0
58	MG	14	3163	1/1	0.88	0.43	71,71,71,71	0
58	MG	1H	3228	1/1	0.89	0.33	83,83,83,83	0
58	MG	L8	102	1/1	0.89	0.23	67,67,67,67	0
58	MG	1G	1630	1/1	0.89	0.19	71,71,71,71	0
58	MG	13	1687	1/1	0.89	0.20	82,82,82,82	0
58	MG	1H	3452	1/1	0.89	0.07	71,71,71,71	0
58	MG	1H	3171	1/1	0.89	0.43	89,89,89,89	0
58	MG	1H	3140	1/1	0.89	0.25	59,59,59,59	0
58	MG	1G	1628	1/1	0.89	0.21	64,64,64,64	0
58	MG	14	3250	1/1	0.89	0.15	70,70,70,70	0
58	MG	1H	3432	1/1	0.89	0.12	77,77,77,77	0
58	MG	14	3305	1/1	0.89	0.19	59,59,59,59	0
58	MG	1H	3447	1/1	0.89	0.14	47,47,47,47	0
58	MG	14	3020	1/1	0.89	0.17	63,63,63,63	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
58	MG	14	3287	1/1	0.89	0.43	112,112,112,112	0
58	MG	1H	3084	1/1	0.89	0.14	59,59,59,59	0
58	MG	13	1649	1/1	0.89	0.45	83,83,83,83	0
58	MG	C5	201	1/1	0.89	0.29	105,105,105,105	0
58	MG	1H	3358	1/1	0.89	0.44	92,92,92,92	0
58	MG	13	1614	1/1	0.89	0.22	65,65,65,65	0
58	MG	13	1667	1/1	0.89	0.33	59,59,59,59	0
58	MG	1H	3317	1/1	0.89	0.27	73,73,73,73	0
58	MG	13	1651	1/1	0.89	0.11	63,63,63,63	0
58	MG	13	1639	1/1	0.89	0.17	69,69,69,69	0
58	MG	1H	3185	1/1	0.89	0.45	77,77,77,77	0
58	MG	13	1674	1/1	0.89	0.09	81,81,81,81	0
58	MG	14	3255	1/1	0.89	0.35	69,69,69,69	0
58	MG	1H	3049	1/1	0.89	0.24	56,56,56,56	0
58	MG	13	1688	1/1	0.89	0.19	101,101,101,101	0
58	MG	13	1655	1/1	0.89	0.28	78,78,78,78	0
58	MG	1H	3287	1/1	0.89	0.37	62,62,62,62	0
58	MG	1H	3426	1/1	0.89	0.09	39,39,39,39	0
58	MG	1H	3375	1/1	0.89	0.54	94,94,94,94	0
58	MG	1H	3454	1/1	0.89	0.08	65,65,65,65	0
58	MG	1H	3071	1/1	0.89	0.27	52,52,52,52	0
58	MG	14	3386	1/1	0.89	0.09	83,83,83,83	0
58	MG	1G	1675	1/1	0.89	0.24	83,83,83,83	0
58	MG	14	3239	1/1	0.89	0.15	64,64,64,64	0
58	MG	1H	3033	1/1	0.89	0.41	82,82,82,82	0
58	MG	1H	3229	1/1	0.89	0.21	61,61,61,61	0
58	MG	11	301	1/1	0.89	0.22	39,39,39,39	0
58	MG	1H	3066	1/1	0.89	0.23	71,71,71,71	0
58	MG	13	1718	1/1	0.89	0.29	113,113,113,113	0
58	MG	1H	3245	1/1	0.89	0.26	69,69,69,69	0
58	MG	4E	201	1/1	0.89	0.29	76,76,76,76	0
58	MG	1H	3271	1/1	0.89	0.35	77,77,77,77	0
58	MG	13	1673	1/1	0.90	0.26	70,70,70,70	0
58	MG	1H	3169	1/1	0.90	0.17	58,58,58,58	0
58	MG	14	3290	1/1	0.90	0.18	74,74,74,74	0
58	MG	1G	1634	1/1	0.90	0.24	87,87,87,87	0
58	MG	13	1738	1/1	0.90	0.08	112,112,112,112	0
58	MG	1H	3088	1/1	0.90	0.30	56,56,56,56	0
58	MG	1H	3132	1/1	0.90	0.21	63,63,63,63	0
58	MG	1H	3258	1/1	0.90	0.25	55,55,55,55	0
58	MG	14	3370	1/1	0.90	0.06	75,75,75,75	0
58	MG	1G	1665	1/1	0.90	0.27	77,77,77,77	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
58	MG	1H	3100	1/1	0.90	0.38	46,46,46,46	0
58	MG	1H	3205	1/1	0.90	0.33	71,71,71,71	0
58	MG	14	3234	1/1	0.90	0.08	56,56,56,56	0
58	MG	14	3133	1/1	0.90	0.13	58,58,58,58	0
58	MG	14	3322	1/1	0.90	0.18	73,73,73,73	0
58	MG	1H	3308	1/1	0.90	0.35	82,82,82,82	0
58	MG	1H	3032	1/1	0.90	0.25	71,71,71,71	0
58	MG	1G	1655	1/1	0.90	0.18	112,112,112,112	0
58	MG	1H	3170	1/1	0.90	0.28	65,65,65,65	0
58	MG	14	3293	1/1	0.90	0.13	71,71,71,71	0
58	MG	1H	3141	1/1	0.90	0.10	70,70,70,70	0
58	MG	1H	3349	1/1	0.90	0.20	62,62,62,62	0
58	MG	1H	3364	1/1	0.90	0.56	90,90,90,90	0
58	MG	14	3059	1/1	0.90	0.40	65,65,65,65	0
58	MG	1H	3232	1/1	0.90	0.26	70,70,70,70	0
58	MG	1H	3314	1/1	0.90	0.36	86,86,86,86	0
58	MG	14	3148	1/1	0.90	0.20	79,79,79,79	0
58	MG	1H	3456	1/1	0.90	0.09	87,87,87,87	0
58	MG	1G	1667	1/1	0.90	0.14	84,84,84,84	0
58	MG	1H	3142	1/1	0.90	0.23	59,59,59,59	0
58	MG	1H	3267	1/1	0.90	0.14	57,57,57,57	0
58	MG	1H	3299	1/1	0.90	0.34	60,60,60,60	0
58	MG	1G	1610	1/1	0.90	0.17	95,95,95,95	0
58	MG	1H	3348	1/1	0.90	0.15	64,64,64,64	0
58	MG	13	1685	1/1	0.90	0.26	65,65,65,65	0
58	MG	14	3380	1/1	0.90	0.09	90,90,90,90	0
58	MG	13	1725	1/1	0.90	0.07	85,85,85,85	0
58	MG	16	207	1/1	0.90	0.40	76,76,76,76	0
58	MG	14	3182	1/1	0.90	0.23	61,61,61,61	0
58	MG	14	3335	1/1	0.90	0.11	71,71,71,71	0
58	MG	1H	3464	1/1	0.90	0.08	88,88,88,88	0
58	MG	1H	3282	1/1	0.90	0.51	85,85,85,85	0
58	MG	1H	3233	1/1	0.90	0.27	65,65,65,65	0
58	MG	14	3198	1/1	0.90	0.31	84,84,84,84	0
58	MG	1G	1676	1/1	0.90	0.31	105,105,105,105	0
58	MG	1H	3189	1/1	0.90	0.36	73,73,73,73	0
58	MG	1H	3325	1/1	0.91	0.22	67,67,67,67	0
58	MG	1G	1613	1/1	0.91	0.33	81,81,81,81	0
58	MG	1H	3451	1/1	0.91	0.11	84,84,84,84	0
58	MG	13	1690	1/1	0.91	0.18	66,66,66,66	0
58	MG	1H	3458	1/1	0.91	0.15	68,68,68,68	0
58	MG	14	3388	1/1	0.91	0.12	88,88,88,88	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
58	MG	16	211	1/1	0.91	0.26	80,80,80,80	0
58	MG	14	3346	1/1	0.91	0.07	63,63,63,63	0
58	MG	14	3276	1/1	0.91	0.25	75,75,75,75	0
58	MG	1H	3176	1/1	0.91	0.28	70,70,70,70	0
58	MG	1G	1690	1/1	0.91	0.30	98,98,98,98	0
58	MG	1H	3275	1/1	0.91	0.14	53,53,53,53	0
58	MG	1G	1673	1/1	0.91	0.36	94,94,94,94	0
58	MG	1H	3279	1/1	0.91	0.21	77,77,77,77	0
58	MG	14	3222	1/1	0.91	0.26	58,58,58,58	0
58	MG	31	304	1/1	0.91	0.11	48,48,48,48	0
58	MG	1H	3418	1/1	0.91	0.19	52,52,52,52	0
58	MG	1H	3191	1/1	0.91	0.14	68,68,68,68	0
58	MG	1H	3098	1/1	0.91	0.17	44,44,44,44	0
58	MG	1G	1641	1/1	0.91	0.09	94,94,94,94	0
58	MG	13	1652	1/1	0.91	0.21	60,60,60,60	0
58	MG	14	3098	1/1	0.91	0.39	67,67,67,67	0
58	MG	45	201	1/1	0.91	0.16	59,59,59,59	0
58	MG	1G	1603	1/1	0.91	0.12	71,71,71,71	0
58	MG	1H	3376	1/1	0.91	0.28	78,78,78,78	0
58	MG	1H	3436	1/1	0.91	0.11	87,87,87,87	0
58	MG	14	3266	1/1	0.91	0.22	72,72,72,72	0
58	MG	L5	400	1/1	0.91	0.15	70,70,70,70	0
58	MG	1G	1678	1/1	0.91	0.32	92,92,92,92	0
58	MG	13	1659	1/1	0.91	0.27	85,85,85,85	0
58	MG	14	3345	1/1	0.91	0.13	63,63,63,63	0
58	MG	14	3323	1/1	0.91	0.21	85,85,85,85	0
58	MG	1H	3129	1/1	0.91	0.32	58,58,58,58	0
58	MG	13	1656	1/1	0.91	0.13	72,72,72,72	0
58	MG	14	3248	1/1	0.91	0.10	65,65,65,65	0
58	MG	1H	3248	1/1	0.91	0.20	88,88,88,88	0
58	MG	1H	3215	1/1	0.91	0.20	52,52,52,52	0
58	MG	14	3251	1/1	0.91	0.19	80,80,80,80	0
58	MG	1H	3444	1/1	0.91	0.08	90,90,90,90	0
58	MG	13	1679	1/1	0.91	0.34	96,96,96,96	0
58	MG	14	3046	1/1	0.91	0.24	73,73,73,73	0
58	MG	1H	3188	1/1	0.91	0.29	60,60,60,60	0
58	MG	14	3145	1/1	0.91	0.17	65,65,65,65	0
58	MG	13	1630	1/1	0.91	0.30	70,70,70,70	0
58	MG	14	3029	1/1	0.92	0.11	77,77,77,77	0
58	MG	1H	3180	1/1	0.92	0.14	63,63,63,63	0
58	MG	14	3233	1/1	0.92	0.19	66,66,66,66	0
58	MG	14	3315	1/1	0.92	0.16	67,67,67,67	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
58	MG	14	3314	1/1	0.92	0.27	59,59,59,59	0
58	MG	1H	3330	1/1	0.92	0.16	74,74,74,74	0
58	MG	1J	204	1/1	0.92	0.28	88,88,88,88	0
58	MG	16	202	1/1	0.92	0.30	63,63,63,63	0
58	MG	1H	3052	1/1	0.92	0.23	63,63,63,63	0
58	MG	1H	3087	1/1	0.92	0.16	61,61,61,61	0
58	MG	14	3304	1/1	0.92	0.34	63,63,63,63	0
58	MG	1H	3186	1/1	0.92	0.33	52,52,52,52	0
58	MG	1H	3427	1/1	0.92	0.10	55,55,55,55	0
58	MG	98	202	1/1	0.92	0.20	90,90,90,90	0
58	MG	14	3208	1/1	0.92	0.16	58,58,58,58	0
58	MG	14	3108	1/1	0.92	0.20	55,55,55,55	0
58	MG	1H	3218	1/1	0.92	0.28	57,57,57,57	0
58	MG	14	3087	1/1	0.92	0.23	41,41,41,41	0
58	MG	1H	3213	1/1	0.92	0.18	63,63,63,63	0
58	MG	14	3263	1/1	0.92	0.12	84,84,84,84	0
58	MG	14	3368	1/1	0.92	0.10	64,64,64,64	0
58	MG	14	3015	1/1	0.92	0.14	76,76,76,76	0
58	MG	1H	3089	1/1	0.92	0.14	68,68,68,68	0
58	MG	14	3336	1/1	0.92	0.11	48,48,48,48	0
58	MG	1H	3199	1/1	0.92	0.26	63,63,63,63	0
58	MG	1H	3327	1/1	0.92	0.34	80,80,80,80	0
58	MG	13	1633	1/1	0.92	0.16	54,54,54,54	0
58	MG	1G	1638	1/1	0.92	0.31	80,80,80,80	0
58	MG	14	3329	1/1	0.92	0.10	56,56,56,56	0
58	MG	1G	1648	1/1	0.92	0.30	95,95,95,95	0
58	MG	1G	1653	1/1	0.92	0.13	77,77,77,77	0
58	MG	14	3178	1/1	0.92	0.10	85,85,85,85	0
58	MG	1H	3242	1/1	0.92	0.34	66,66,66,66	0
58	MG	1H	3091	1/1	0.92	0.21	62,62,62,62	0
58	MG	1H	3352	1/1	0.92	0.36	81,81,81,81	0
58	MG	1H	3234	1/1	0.92	0.45	85,85,85,85	0
58	MG	14	3224	1/1	0.92	0.28	59,59,59,59	0
58	MG	1H	3381	1/1	0.92	0.26	90,90,90,90	0
58	MG	1H	3194	1/1	0.92	0.20	55,55,55,55	0
58	MG	1H	3068	1/1	0.92	0.31	63,63,63,63	0
58	MG	13	1705	1/1	0.92	0.32	127,127,127,127	0
58	MG	14	3274	1/1	0.92	0.47	77,77,77,77	0
58	MG	13	1730	1/1	0.92	0.09	88,88,88,88	0
58	MG	1H	3083	1/1	0.92	0.26	71,71,71,71	0
58	MG	14	3321	1/1	0.92	0.38	86,86,86,86	0
58	MG	1G	1670	1/1	0.92	0.18	86,86,86,86	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
58	MG	1G	1686	1/1	0.92	0.09	83,83,83,83	0
58	MG	1H	3177	1/1	0.92	0.20	47,47,47,47	0
58	MG	14	3392	1/1	0.92	0.11	61,61,61,61	0
58	MG	1H	3150	1/1	0.92	0.17	48,48,48,48	0
58	MG	1H	3211	1/1	0.92	0.36	59,59,59,59	0
58	MG	1H	3095	1/1	0.92	0.15	47,47,47,47	0
58	MG	1H	3094	1/1	0.92	0.24	53,53,53,53	0
58	MG	1H	3240	1/1	0.92	0.62	86,86,86,86	0
58	MG	1H	3070	1/1	0.92	0.26	55,55,55,55	0
58	MG	1H	3157	1/1	0.92	0.20	48,48,48,48	0
58	MG	1H	3410	1/1	0.92	0.08	59,59,59,59	0
58	MG	13	1638	1/1	0.92	0.22	78,78,78,78	0
58	MG	14	3352	1/1	0.92	0.11	73,73,73,73	0
58	MG	1G	1650	1/1	0.92	0.27	68,68,68,68	0
58	MG	14	3307	1/1	0.92	0.08	62,62,62,62	0
58	MG	1H	3319	1/1	0.92	0.18	50,50,50,50	0
58	MG	1H	3256	1/1	0.93	0.17	57,57,57,57	0
58	MG	13	1657	1/1	0.93	0.23	74,74,74,74	0
58	MG	1H	3179	1/1	0.93	0.31	71,71,71,71	0
58	MG	1H	3200	1/1	0.93	0.25	73,73,73,73	0
58	MG	1H	3385	1/1	0.93	0.14	49,49,49,49	0
58	MG	1H	3414	1/1	0.93	0.10	50,50,50,50	0
58	MG	14	3231	1/1	0.93	0.27	75,75,75,75	0
58	MG	1H	3044	1/1	0.93	0.15	50,50,50,50	0
58	MG	1H	3041	1/1	0.93	0.14	51,51,51,51	0
58	MG	14	3240	1/1	0.93	0.17	71,71,71,71	0
58	MG	1H	3435	1/1	0.93	0.08	70,70,70,70	0
58	MG	1H	3108	1/1	0.93	0.49	56,56,56,56	0
58	MG	1H	3125	1/1	0.93	0.24	46,46,46,46	0
58	MG	1J	205	1/1	0.93	0.27	75,75,75,75	0
58	MG	1H	3173	1/1	0.93	0.24	68,68,68,68	0
58	MG	14	3177	1/1	0.93	0.13	70,70,70,70	0
58	MG	1H	3246	1/1	0.93	0.46	79,79,79,79	0
58	MG	13	1640	1/1	0.93	0.19	65,65,65,65	0
58	MG	1H	3360	1/1	0.93	0.34	73,73,73,73	0
58	MG	1H	3333	1/1	0.93	0.20	63,63,63,63	0
58	MG	14	3257	1/1	0.93	0.18	63,63,63,63	0
58	MG	1H	3247	1/1	0.93	0.48	73,73,73,73	0
58	MG	1G	1623	1/1	0.93	0.16	96,96,96,96	0
58	MG	1H	3172	1/1	0.93	0.37	56,56,56,56	0
59	ZN	5A	101	1/1	0.93	0.13	132,132,132,132	0
58	MG	1H	3152	1/1	0.93	0.19	62,62,62,62	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
58	MG	14	3124	1/1	0.93	0.15	43,43,43,43	0
58	MG	14	3095	1/1	0.93	0.11	52,52,52,52	0
58	MG	1H	3407	1/1	0.93	0.12	60,60,60,60	0
58	MG	14	3128	1/1	0.93	0.41	79,79,79,79	0
58	MG	13	1631	1/1	0.93	0.21	64,64,64,64	0
58	MG	1H	3270	1/1	0.93	0.34	76,76,76,76	0
58	MG	1G	1674	1/1	0.93	0.21	136,136,136,136	0
58	MG	13	1704	1/1	0.93	0.21	130,130,130,130	0
58	MG	13	1658	1/1	0.93	0.29	73,73,73,73	0
58	MG	1G	1606	1/1	0.93	0.07	92,92,92,92	0
58	MG	13	1697	1/1	0.93	0.13	90,90,90,90	0
58	MG	1H	3165	1/1	0.93	0.20	68,68,68,68	0
58	MG	1H	3241	1/1	0.93	0.18	65,65,65,65	0
58	MG	14	3317	1/1	0.93	0.30	65,65,65,65	0
58	MG	1H	3037	1/1	0.93	0.20	47,47,47,47	0
58	MG	1J	206	1/1	0.93	0.14	109,109,109,109	0
58	MG	1H	3073	1/1	0.93	0.26	52,52,52,52	0
58	MG	14	3171	1/1	0.93	0.17	65,65,65,65	0
58	MG	13	1695	1/1	0.93	0.30	75,75,75,75	0
58	MG	14	3155	1/1	0.93	0.17	57,57,57,57	0
58	MG	14	3165	1/1	0.93	0.19	65,65,65,65	0
58	MG	1H	3204	1/1	0.93	0.24	72,72,72,72	0
58	MG	85	201	1/1	0.93	0.29	64,64,64,64	0
58	MG	14	3320	1/1	0.93	0.14	61,61,61,61	0
58	MG	1H	3331	1/1	0.93	0.28	72,72,72,72	0
58	MG	1H	3292	1/1	0.93	0.90	50,50,50,50	0
58	MG	14	3247	1/1	0.93	0.48	64,64,64,64	0
58	MG	1H	3362	1/1	0.93	0.20	105,105,105,105	0
58	MG	1G	1608	1/1	0.93	0.25	81,81,81,81	0
58	MG	13	1729	1/1	0.93	0.08	85,85,85,85	0
58	MG	1H	3182	1/1	0.93	0.49	73,73,73,73	0
58	MG	14	3226	1/1	0.93	0.18	74,74,74,74	0
58	MG	14	3206	1/1	0.93	0.18	56,56,56,56	0
58	MG	1H	3344	1/1	0.93	0.35	71,71,71,71	0
58	MG	1H	3340	1/1	0.93	0.23	51,51,51,51	0
58	MG	2K	106	1/1	0.93	0.07	87,87,87,87	0
58	MG	14	3232	1/1	0.93	0.13	73,73,73,73	0
58	MG	14	3366	1/1	0.93	0.13	76,76,76,76	0
58	MG	1H	3351	1/1	0.93	0.19	62,62,62,62	0
58	MG	13	1669	1/1	0.93	0.21	70,70,70,70	0
58	MG	1G	1632	1/1	0.93	0.28	64,64,64,64	0
58	MG	1H	3202	1/1	0.93	0.33	60,60,60,60	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
58	MG	16	206	1/1	0.93	0.18	78,78,78,78	0
58	MG	1H	3075	1/1	0.93	0.13	41,41,41,41	0
58	MG	1H	3406	1/1	0.93	0.16	53,53,53,53	0
58	MG	1H	3294	1/1	0.93	0.22	70,70,70,70	0
58	MG	14	3153	1/1	0.93	0.30	104,104,104,104	0
58	MG	14	3324	1/1	0.93	0.17	83,83,83,83	0
58	MG	14	3181	1/1	0.93	0.23	81,81,81,81	0
58	MG	1H	3400	1/1	0.93	0.14	58,58,58,58	0
58	MG	1H	3146	1/1	0.93	0.17	62,62,62,62	0
58	MG	14	3062	1/1	0.93	0.17	51,51,51,51	0
58	MG	14	3175	1/1	0.94	0.32	64,64,64,64	0
58	MG	14	3344	1/1	0.94	0.09	60,60,60,60	0
58	MG	1H	3119	1/1	0.94	0.20	55,55,55,55	0
58	MG	1H	3394	1/1	0.94	0.15	47,47,47,47	0
58	MG	14	3213	1/1	0.94	0.13	55,55,55,55	0
58	MG	1H	3446	1/1	0.94	0.07	60,60,60,60	0
58	MG	1G	1652	1/1	0.94	0.20	91,91,91,91	0
58	MG	1H	3289	1/1	0.94	0.18	63,63,63,63	0
58	MG	14	3118	1/1	0.94	0.19	40,40,40,40	0
58	MG	14	3253	1/1	0.94	0.14	83,83,83,83	0
58	MG	14	3011	1/1	0.94	0.17	48,48,48,48	0
58	MG	14	3134	1/1	0.94	0.14	54,54,54,54	0
58	MG	14	3211	1/1	0.94	0.16	60,60,60,60	0
58	MG	1H	3216	1/1	0.94	0.22	68,68,68,68	0
58	MG	1H	3193	1/1	0.94	0.18	52,52,52,52	0
58	MG	1H	3417	1/1	0.94	0.12	51,51,51,51	0
58	MG	1H	3113	1/1	0.94	0.31	37,37,37,37	0
58	MG	1H	3167	1/1	0.94	0.26	65,65,65,65	0
58	MG	14	3063	1/1	0.94	0.20	51,51,51,51	0
58	MG	14	3027	1/1	0.94	0.23	76,76,76,76	0
58	MG	1H	3131	1/1	0.94	0.21	60,60,60,60	0
58	MG	14	3159	1/1	0.94	0.21	63,63,63,63	0
58	MG	13	1681	1/1	0.94	0.06	71,71,71,71	0
58	MG	21	301	1/1	0.94	0.14	46,46,46,46	0
58	MG	1H	3354	1/1	0.94	0.29	80,80,80,80	0
58	MG	14	3367	1/1	0.94	0.08	49,49,49,49	0
58	MG	1H	3457	1/1	0.94	0.09	81,81,81,81	0
58	MG	14	3125	1/1	0.94	0.14	42,42,42,42	0
58	MG	1H	3104	1/1	0.94	0.16	47,47,47,47	0
58	MG	14	3048	1/1	0.94	0.22	66,66,66,66	0
58	MG	14	3158	1/1	0.94	0.14	72,72,72,72	0
58	MG	14	3144	1/1	0.94	0.27	75,75,75,75	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
58	MG	1H	3286	1/1	0.94	0.25	67,67,67,67	0
58	MG	1H	3153	1/1	0.94	0.29	58,58,58,58	0
58	MG	1H	3372	1/1	0.94	0.21	78,78,78,78	0
58	MG	14	3184	1/1	0.94	0.26	60,60,60,60	0
58	MG	1H	3103	1/1	0.94	0.29	47,47,47,47	0
58	MG	1H	3174	1/1	0.94	0.14	51,51,51,51	0
58	MG	2K	102	1/1	0.94	0.20	78,78,78,78	0
58	MG	14	3077	1/1	0.94	0.21	68,68,68,68	0
58	MG	1H	3209	1/1	0.94	0.18	57,57,57,57	0
58	MG	14	3117	1/1	0.94	0.11	52,52,52,52	0
58	MG	1H	3206	1/1	0.94	0.23	65,65,65,65	0
58	MG	14	3292	1/1	0.94	0.17	109,109,109,109	0
58	MG	14	3167	1/1	0.94	0.17	61,61,61,61	0
58	MG	14	3300	1/1	0.94	0.09	81,81,81,81	0
58	MG	14	3026	1/1	0.94	0.09	76,76,76,76	0
58	MG	1H	3099	1/1	0.94	0.15	37,37,37,37	0
58	MG	1H	3139	1/1	0.94	0.19	48,48,48,48	0
58	MG	1H	3166	1/1	0.94	0.25	58,58,58,58	0
58	MG	13	1645	1/1	0.94	0.14	65,65,65,65	0
58	MG	14	3105	1/1	0.94	0.12	65,65,65,65	0
58	MG	14	3356	1/1	0.94	0.17	78,78,78,78	0
58	MG	1H	3455	1/1	0.94	0.13	58,58,58,58	0
58	MG	14	3281	1/1	0.94	0.62	67,67,67,67	0
58	MG	1H	3190	1/1	0.94	0.16	50,50,50,50	0
58	MG	14	3127	1/1	0.94	0.17	55,55,55,55	0
58	MG	1H	3337	1/1	0.94	0.40	67,67,67,67	0
58	MG	1H	3379	1/1	0.94	0.21	85,85,85,85	0
58	MG	1H	3353	1/1	0.94	0.20	93,93,93,93	0
58	MG	1H	3329	1/1	0.94	0.38	74,74,74,74	0
58	MG	14	3375	1/1	0.94	0.07	65,65,65,65	0
58	MG	3L	101	1/1	0.94	0.30	81,81,81,81	0
58	MG	14	3347	1/1	0.94	0.09	49,49,49,49	0
58	MG	14	3076	1/1	0.94	0.13	59,59,59,59	0
58	MG	13	1668	1/1	0.94	0.29	69,69,69,69	0
58	MG	1H	3280	1/1	0.94	0.14	44,44,44,44	0
58	MG	1H	3136	1/1	0.94	0.24	53,53,53,53	0
58	MG	14	3362	1/1	0.94	0.17	70,70,70,70	0
58	MG	14	3280	1/1	0.94	0.12	51,51,51,51	0
58	MG	13	1683	1/1	0.94	0.10	94,94,94,94	0
58	MG	14	3025	1/1	0.94	0.20	79,79,79,79	0
58	MG	1H	3081	1/1	0.94	0.37	67,67,67,67	0
58	MG	14	3230	1/1	0.94	0.12	63,63,63,63	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
58	MG	1G	1669	1/1	0.94	0.29	131,131,131,131	0
58	MG	14	3053	1/1	0.94	0.12	57,57,57,57	0
58	MG	14	3050	1/1	0.94	0.17	55,55,55,55	0
58	MG	14	3120	1/1	0.94	0.10	84,84,84,84	0
58	MG	14	3183	1/1	0.94	0.13	60,60,60,60	0
58	MG	1H	3183	1/1	0.94	0.23	56,56,56,56	0
58	MG	1H	3284	1/1	0.94	0.10	72,72,72,72	0
58	MG	14	3264	1/1	0.94	0.24	69,69,69,69	0
58	MG	1H	3272	1/1	0.94	0.46	88,88,88,88	0
58	MG	14	3209	1/1	0.94	0.12	63,63,63,63	0
58	MG	1G	1662	1/1	0.94	0.18	78,78,78,78	0
58	MG	14	3382	1/1	0.94	0.14	60,60,60,60	0
58	MG	14	3214	1/1	0.94	0.22	54,54,54,54	0
58	MG	1G	1672	1/1	0.94	0.10	91,91,91,91	0
58	MG	14	3241	1/1	0.94	0.10	72,72,72,72	0
58	MG	14	3112	1/1	0.94	0.26	86,86,86,86	0
58	MG	1H	3109	1/1	0.94	0.15	37,37,37,37	0
58	MG	1H	3473	1/1	0.94	0.07	99,99,99,99	0
58	MG	1H	3441	1/1	0.94	0.12	40,40,40,40	0
58	MG	1H	3402	1/1	0.94	0.07	58,58,58,58	0
58	MG	13	1632	1/1	0.94	0.10	45,45,45,45	0
58	MG	1G	1688	1/1	0.94	0.17	105,105,105,105	0
58	MG	14	3056	1/1	0.94	0.12	73,73,73,73	0
58	MG	13	1625	1/1	0.94	0.25	58,58,58,58	0
58	MG	14	3252	1/1	0.94	0.11	71,71,71,71	0
58	MG	1H	3061	1/1	0.94	0.20	51,51,51,51	0
58	MG	13	1626	1/1	0.94	0.24	80,80,80,80	0
58	MG	1H	3273	1/1	0.94	0.12	66,66,66,66	0
58	MG	1G	1642	1/1	0.94	0.12	80,80,80,80	0
58	MG	13	1627	1/1	0.94	0.44	72,72,72,72	0
58	MG	1H	3133	1/1	0.94	0.21	43,43,43,43	0
58	MG	1H	3220	1/1	0.94	0.22	64,64,64,64	0
58	MG	1H	3311	1/1	0.95	0.18	58,58,58,58	0
58	MG	14	3100	1/1	0.95	0.47	62,62,62,62	0
58	MG	1H	3393	1/1	0.95	0.11	47,47,47,47	0
58	MG	98	201	1/1	0.95	0.28	64,64,64,64	0
58	MG	14	3342	1/1	0.95	0.10	51,51,51,51	0
58	MG	14	3285	1/1	0.95	0.18	74,74,74,74	0
58	MG	14	3201	1/1	0.95	0.42	49,49,49,49	0
58	MG	14	3060	1/1	0.95	0.17	67,67,67,67	0
58	MG	1H	3155	1/1	0.95	0.14	41,41,41,41	0
58	MG	14	3172	1/1	0.95	0.21	64,64,64,64	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
58	MG	1H	3384	1/1	0.95	0.13	38,38,38,38	0
58	MG	1H	3405	1/1	0.95	0.10	41,41,41,41	0
58	MG	1H	3343	1/1	0.95	0.28	62,62,62,62	0
58	MG	1G	1684	1/1	0.95	0.08	81,81,81,81	0
58	MG	14	3334	1/1	0.95	0.18	48,48,48,48	0
58	MG	14	3179	1/1	0.95	0.45	63,63,63,63	0
58	MG	1H	3208	1/1	0.95	0.43	70,70,70,70	0
58	MG	1H	3077	1/1	0.95	0.22	47,47,47,47	0
58	MG	14	3126	1/1	0.95	0.29	78,78,78,78	0
58	MG	14	3136	1/1	0.95	0.11	50,50,50,50	0
58	MG	14	3186	1/1	0.95	0.27	65,65,65,65	0
58	MG	1G	1646	1/1	0.95	0.20	117,117,117,117	0
58	MG	14	3099	1/1	0.95	0.41	75,75,75,75	0
58	MG	1H	3187	1/1	0.95	0.24	64,64,64,64	0
58	MG	14	3338	1/1	0.95	0.06	61,61,61,61	0
58	MG	14	3340	1/1	0.95	0.15	60,60,60,60	0
58	MG	1H	3057	1/1	0.95	0.23	60,60,60,60	0
58	MG	1H	3415	1/1	0.95	0.12	48,48,48,48	0
58	MG	1H	3085	1/1	0.95	0.33	48,48,48,48	0
58	MG	14	3028	1/1	0.95	0.16	76,76,76,76	0
58	MG	14	3082	1/1	0.95	0.18	54,54,54,54	0
58	MG	1H	3422	1/1	0.95	0.13	63,63,63,63	0
58	MG	14	3258	1/1	0.95	0.41	68,68,68,68	0
58	MG	14	3332	1/1	0.95	0.14	62,62,62,62	0
58	MG	1H	3014	1/1	0.95	0.18	33,33,33,33	0
58	MG	14	3383	1/1	0.95	0.12	70,70,70,70	0
58	MG	1H	3227	1/1	0.95	0.15	63,63,63,63	0
58	MG	1H	3047	1/1	0.95	0.43	84,84,84,84	0
58	MG	1H	3281	1/1	0.95	0.21	65,65,65,65	0
58	MG	1J	202	1/1	0.95	0.43	84,84,84,84	0
58	MG	1H	3390	1/1	0.95	0.09	41,41,41,41	0
58	MG	14	3358	1/1	0.95	0.12	51,51,51,51	0
58	MG	1H	3123	1/1	0.95	0.10	32,32,32,32	0
58	MG	13	1724	1/1	0.95	0.07	87,87,87,87	0
58	MG	1G	1607	1/1	0.95	0.08	92,92,92,92	0
58	MG	1H	3391	1/1	0.95	0.08	47,47,47,47	0
58	MG	1G	1663	1/1	0.95	0.20	105,105,105,105	0
58	MG	13	1727	1/1	0.95	0.14	69,69,69,69	0
58	MG	2K	104	1/1	0.95	0.21	72,72,72,72	0
58	MG	13	1678	1/1	0.95	0.28	92,92,92,92	0
58	MG	1H	3045	1/1	0.95	0.19	90,90,90,90	0
58	MG	14	3097	1/1	0.95	0.22	51,51,51,51	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
58	MG	1H	3274	1/1	0.95	0.14	59,59,59,59	0
58	MG	1H	3006	1/1	0.95	0.14	42,42,42,42	0
58	MG	1H	3117	1/1	0.95	0.30	54,54,54,54	0
58	MG	14	3106	1/1	0.95	0.13	57,57,57,57	0
58	MG	14	3313	1/1	0.95	0.17	81,81,81,81	0
58	MG	13	1646	1/1	0.95	0.12	63,63,63,63	0
58	MG	1H	3361	1/1	0.95	0.33	112,112,112,112	0
58	MG	1H	3369	1/1	0.95	0.33	54,54,54,54	0
58	MG	1H	3438	1/1	0.95	0.06	71,71,71,71	0
58	MG	1H	3268	1/1	0.95	0.25	65,65,65,65	0
58	MG	1H	3116	1/1	0.95	0.21	52,52,52,52	0
58	MG	1H	3060	1/1	0.95	0.39	59,59,59,59	0
58	MG	14	3396	1/1	0.95	0.28	75,75,75,75	0
58	MG	1H	3053	1/1	0.95	0.28	33,33,33,33	0
58	MG	2L	101	1/1	0.95	0.19	69,69,69,69	0
58	MG	14	3341	1/1	0.95	0.04	71,71,71,71	0
58	MG	14	3068	1/1	0.95	0.20	54,54,54,54	0
58	MG	14	3236	1/1	0.95	0.11	71,71,71,71	0
58	MG	1H	3063	1/1	0.95	0.25	45,45,45,45	0
58	MG	1H	3460	1/1	0.95	0.12	53,53,53,53	0
58	MG	1G	1649	1/1	0.95	0.19	78,78,78,78	0
58	MG	1H	3148	1/1	0.95	0.28	57,57,57,57	0
58	MG	13	1608	1/1	0.95	0.20	77,77,77,77	0
58	MG	18	102	1/1	0.95	0.24	49,49,49,49	0
58	MG	14	3055	1/1	0.95	0.18	55,55,55,55	0
58	MG	14	3157	1/1	0.95	0.35	63,63,63,63	0
58	MG	13	1736	1/1	0.95	0.14	97,97,97,97	0
58	MG	1H	3431	1/1	0.95	0.08	57,57,57,57	0
58	MG	1H	3102	1/1	0.95	0.18	44,44,44,44	0
58	MG	13	1664	1/1	0.95	0.26	71,71,71,71	0
58	MG	14	3311	1/1	0.95	0.13	66,66,66,66	0
58	MG	1G	1609	1/1	0.95	0.15	81,81,81,81	0
58	MG	1H	3430	1/1	0.95	0.06	69,69,69,69	0
58	MG	14	3010	1/1	0.95	0.18	48,48,48,48	0
58	MG	14	3022	1/1	0.95	0.28	80,80,80,80	0
58	MG	16	201	1/1	0.95	0.23	75,75,75,75	0
58	MG	13	1686	1/1	0.95	0.17	89,89,89,89	0
58	MG	1H	3277	1/1	0.95	0.18	70,70,70,70	0
58	MG	1G	1605	1/1	0.95	0.12	78,78,78,78	0
58	MG	14	3220	1/1	0.95	0.16	66,66,66,66	0
58	MG	14	3219	1/1	0.95	0.13	68,68,68,68	0
58	MG	1G	1671	1/1	0.95	0.13	85,85,85,85	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
58	MG	14	3038	1/1	0.95	0.29	71,71,71,71	0
58	MG	14	3169	1/1	0.95	0.29	91,91,91,91	0
58	MG	14	3294	1/1	0.96	0.31	90,90,90,90	0
58	MG	1H	3413	1/1	0.96	0.07	40,40,40,40	0
58	MG	1G	1682	1/1	0.96	0.10	75,75,75,75	0
58	MG	1H	3154	1/1	0.96	0.32	52,52,52,52	0
58	MG	13	1665	1/1	0.96	0.20	82,82,82,82	0
58	MG	1H	3219	1/1	0.96	0.27	61,61,61,61	0
58	MG	14	3070	1/1	0.96	0.19	62,62,62,62	0
58	MG	1H	3255	1/1	0.96	0.12	40,40,40,40	0
58	MG	14	3225	1/1	0.96	0.15	68,68,68,68	0
58	MG	1G	1615	1/1	0.96	0.19	82,82,82,82	0
58	MG	1G	1659	1/1	0.96	0.10	76,76,76,76	0
58	MG	1H	3080	1/1	0.96	0.25	67,67,67,67	0
58	MG	1H	3012	1/1	0.96	0.22	58,58,58,58	0
58	MG	13	1618	1/1	0.96	0.31	92,92,92,92	0
58	MG	14	3357	1/1	0.96	0.16	48,48,48,48	0
58	MG	1H	3130	1/1	0.96	0.31	67,67,67,67	0
58	MG	1H	3018	1/1	0.96	0.29	48,48,48,48	0
58	MG	14	3369	1/1	0.96	0.13	69,69,69,69	0
58	MG	14	3350	1/1	0.96	0.13	61,61,61,61	0
58	MG	14	3007	1/1	0.96	0.13	42,42,42,42	0
58	MG	1H	3038	1/1	0.96	0.16	46,46,46,46	0
58	MG	1H	3101	1/1	0.96	0.25	30,30,30,30	0
58	MG	14	3215	1/1	0.96	0.27	60,60,60,60	0
58	MG	13	1647	1/1	0.96	0.30	47,47,47,47	0
58	MG	1H	3321	1/1	0.96	0.27	80,80,80,80	0
58	MG	14	3207	1/1	0.96	0.17	53,53,53,53	0
58	MG	14	3040	1/1	0.96	0.17	61,61,61,61	0
58	MG	14	3376	1/1	0.96	0.11	87,87,87,87	0
58	MG	1H	3386	1/1	0.96	0.16	39,39,39,39	0
58	MG	14	3379	1/1	0.96	0.10	51,51,51,51	0
58	MG	14	3092	1/1	0.96	0.16	59,59,59,59	0
58	MG	1G	1644	1/1	0.96	0.20	83,83,83,83	0
58	MG	13	1613	1/1	0.96	0.14	66,66,66,66	0
58	MG	14	3282	1/1	0.96	0.25	62,62,62,62	0
58	MG	1H	3306	1/1	0.96	0.23	54,54,54,54	0
58	MG	1H	3260	1/1	0.96	0.32	48,48,48,48	0
58	MG	1G	1622	1/1	0.96	0.12	113,113,113,113	0
58	MG	14	3279	1/1	0.96	0.09	67,67,67,67	0
58	MG	14	3244	1/1	0.96	0.42	61,61,61,61	0
58	MG	1H	3043	1/1	0.96	0.26	62,62,62,62	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
58	MG	13	1732	1/1	0.96	0.08	79,79,79,79	0
58	MG	1H	3127	1/1	0.96	0.30	75,75,75,75	0
58	MG	14	3193	1/1	0.96	0.23	60,60,60,60	0
58	MG	14	3243	1/1	0.96	0.15	68,68,68,68	0
58	MG	1H	3388	1/1	0.96	0.14	39,39,39,39	0
58	MG	13	1606	1/1	0.96	0.17	70,70,70,70	0
58	MG	1H	3345	1/1	0.96	0.19	75,75,75,75	0
58	MG	1H	3214	1/1	0.96	0.27	53,53,53,53	0
58	MG	14	3057	1/1	0.96	0.23	62,62,62,62	0
58	MG	1G	1639	1/1	0.96	0.24	110,110,110,110	0
58	MG	1H	3243	1/1	0.96	0.28	50,50,50,50	0
58	MG	13	1696	1/1	0.96	0.35	81,81,81,81	0
58	MG	1H	3419	1/1	0.96	0.11	37,37,37,37	0
58	MG	14	3371	1/1	0.96	0.08	59,59,59,59	0
58	MG	14	3203	1/1	0.96	0.23	47,47,47,47	0
58	MG	1H	3259	1/1	0.96	0.19	46,46,46,46	0
58	MG	14	3373	1/1	0.96	0.06	65,65,65,65	0
58	MG	1H	3005	1/1	0.96	0.23	53,53,53,53	0
58	MG	14	3139	1/1	0.96	0.35	68,68,68,68	0
58	MG	1H	3392	1/1	0.96	0.10	60,60,60,60	0
58	MG	1H	3257	1/1	0.96	0.17	55,55,55,55	0
58	MG	1H	3326	1/1	0.96	0.15	92,92,92,92	0
58	MG	1H	3368	1/1	0.96	0.15	72,72,72,72	0
58	MG	14	3096	1/1	0.96	0.11	61,61,61,61	0
58	MG	14	3052	1/1	0.96	0.15	52,52,52,52	0
58	MG	1H	3334	1/1	0.96	0.14	55,55,55,55	0
58	MG	14	3395	1/1	0.96	0.08	64,64,64,64	0
58	MG	14	3024	1/1	0.96	0.14	70,70,70,70	0
58	MG	1H	3265	1/1	0.96	0.15	66,66,66,66	0
58	MG	14	3180	1/1	0.96	0.26	75,75,75,75	0
58	MG	14	3330	1/1	0.96	0.14	58,58,58,58	0
58	MG	1H	3156	1/1	0.96	0.16	44,44,44,44	0
58	MG	14	3205	1/1	0.96	0.14	44,44,44,44	0
58	MG	14	3385	1/1	0.96	0.15	71,71,71,71	0
58	MG	1H	3396	1/1	0.96	0.13	55,55,55,55	0
58	MG	1G	1602	1/1	0.96	0.21	64,64,64,64	0
58	MG	1G	1683	1/1	0.96	0.11	81,81,81,81	0
58	MG	1H	3278	1/1	0.96	0.14	75,75,75,75	0
58	MG	14	3037	1/1	0.96	0.08	72,72,72,72	0
58	MG	1H	3097	1/1	0.96	0.22	47,47,47,47	0
58	MG	14	3256	1/1	0.96	0.27	80,80,80,80	0
58	MG	13	1602	1/1	0.96	0.22	71,71,71,71	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
58	MG	14	3237	1/1	0.96	0.11	48,48,48,48	0
58	MG	14	3273	1/1	0.96	0.11	64,64,64,64	0
58	MG	13	1726	1/1	0.96	0.10	75,75,75,75	0
58	MG	1H	3065	1/1	0.96	0.19	72,72,72,72	0
58	MG	1H	3050	1/1	0.96	0.29	59,59,59,59	0
58	MG	1H	3120	1/1	0.96	0.18	63,63,63,63	0
58	MG	14	3312	1/1	0.97	0.09	89,89,89,89	0
58	MG	1H	3059	1/1	0.97	0.35	55,55,55,55	0
58	MG	14	3328	1/1	0.97	0.16	55,55,55,55	0
58	MG	14	3149	1/1	0.97	0.23	69,69,69,69	0
58	MG	1H	3371	1/1	0.97	0.16	59,59,59,59	0
58	MG	13	1675	1/1	0.97	0.22	63,63,63,63	0
58	MG	1H	3162	1/1	0.97	0.39	57,57,57,57	0
58	MG	14	3160	1/1	0.97	0.19	80,80,80,80	0
58	MG	14	3217	1/1	0.97	0.39	79,79,79,79	0
58	MG	1G	1617	1/1	0.97	0.16	96,96,96,96	0
58	MG	14	3035	1/1	0.97	0.20	76,76,76,76	0
58	MG	1H	3449	1/1	0.97	0.08	74,74,74,74	0
58	MG	14	3072	1/1	0.97	0.30	56,56,56,56	0
58	MG	14	3269	1/1	0.97	0.17	78,78,78,78	0
58	MG	1H	3401	1/1	0.97	0.10	71,71,71,71	0
58	MG	1H	3003	1/1	0.97	0.35	30,30,30,30	0
58	MG	14	3012	1/1	0.97	0.27	66,66,66,66	0
58	MG	14	3227	1/1	0.97	0.29	51,51,51,51	0
58	MG	13	1607	1/1	0.97	0.23	69,69,69,69	0
58	MG	14	3394	1/1	0.97	0.07	94,94,94,94	0
58	MG	14	3218	1/1	0.97	0.16	89,89,89,89	0
58	MG	1H	3355	1/1	0.97	0.21	73,73,73,73	0
58	MG	1H	3249	1/1	0.97	0.18	53,53,53,53	0
58	MG	1H	3235	1/1	0.97	0.12	53,53,53,53	0
58	MG	1H	3468	1/1	0.97	0.07	59,59,59,59	0
58	MG	1H	3145	1/1	0.97	0.33	53,53,53,53	0
58	MG	14	3393	1/1	0.97	0.07	71,71,71,71	0
58	MG	14	3083	1/1	0.97	0.22	58,58,58,58	0
58	MG	14	3391	1/1	0.97	0.11	93,93,93,93	0
58	MG	14	3039	1/1	0.97	0.14	45,45,45,45	0
58	MG	1H	3293	1/1	0.97	0.12	56,56,56,56	0
58	MG	1G	1681	1/1	0.97	0.40	85,85,85,85	0
58	MG	1H	3030	1/1	0.97	0.19	40,40,40,40	0
58	MG	14	3101	1/1	0.97	0.18	60,60,60,60	0
58	MG	14	3353	1/1	0.97	0.06	57,57,57,57	0
58	MG	13	1628	1/1	0.97	0.25	43,43,43,43	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
58	MG	1G	1618	1/1	0.97	0.20	86,86,86,86	0
58	MG	14	3104	1/1	0.97	0.26	42,42,42,42	0
58	MG	14	3348	1/1	0.97	0.07	42,42,42,42	0
58	MG	1H	3031	1/1	0.97	0.22	60,60,60,60	0
58	MG	1H	3283	1/1	0.97	0.20	59,59,59,59	0
58	MG	14	3192	1/1	0.97	0.18	74,74,74,74	0
58	MG	14	3361	1/1	0.97	0.08	52,52,52,52	0
58	MG	14	3318	1/1	0.97	0.06	81,81,81,81	0
58	MG	1H	3470	1/1	0.97	0.10	64,64,64,64	0
58	MG	1H	3001	1/1	0.97	0.15	44,44,44,44	0
58	MG	1H	3019	1/1	0.97	0.28	38,38,38,38	0
58	MG	14	3081	1/1	0.97	0.18	52,52,52,52	0
58	MG	1H	3004	1/1	0.97	0.35	33,33,33,33	0
58	MG	14	3019	1/1	0.97	0.13	69,69,69,69	0
58	MG	1H	3144	1/1	0.97	0.26	47,47,47,47	0
58	MG	1H	3252	1/1	0.97	0.11	36,36,36,36	0
58	MG	14	3221	1/1	0.97	0.17	66,66,66,66	0
58	MG	14	3045	1/1	0.97	0.16	44,44,44,44	0
58	MG	1H	3026	1/1	0.97	0.19	45,45,45,45	0
58	MG	14	3343	1/1	0.97	0.09	49,49,49,49	0
58	MG	1H	3011	1/1	0.97	0.19	50,50,50,50	0
58	MG	1H	3212	1/1	0.97	0.32	80,80,80,80	0
58	MG	1H	3025	1/1	0.97	0.28	47,47,47,47	0
58	MG	1H	3295	1/1	0.97	0.27	51,51,51,51	0
58	MG	1H	3251	1/1	0.97	0.18	33,33,33,33	0
58	MG	1H	3237	1/1	0.97	0.12	44,44,44,44	0
58	MG	1G	1651	1/1	0.97	0.26	71,71,71,71	0
58	MG	1H	3086	1/1	0.97	0.40	52,52,52,52	0
58	MG	1H	3397	1/1	0.97	0.10	51,51,51,51	0
58	MG	14	3004	1/1	0.97	0.15	50,50,50,50	0
58	MG	1J	201	1/1	0.97	0.16	100,100,100,100	0
58	MG	14	3246	1/1	0.97	0.21	76,76,76,76	0
58	MG	14	3377	1/1	0.97	0.15	66,66,66,66	0
58	MG	14	3084	1/1	0.97	0.21	54,54,54,54	0
58	MG	14	3119	1/1	0.97	0.32	75,75,75,75	0
58	MG	1H	3009	1/1	0.97	0.23	42,42,42,42	0
58	MG	1H	3264	1/1	0.97	0.19	47,47,47,47	0
58	MG	14	3023	1/1	0.97	0.12	46,46,46,46	0
58	MG	1H	3389	1/1	0.97	0.10	49,49,49,49	0
58	MG	14	3116	1/1	0.97	0.12	57,57,57,57	0
58	MG	14	3114	1/1	0.97	0.20	65,65,65,65	0
58	MG	1H	3149	1/1	0.97	0.21	42,42,42,42	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
58	MG	14	3006	1/1	0.97	0.13	46,46,46,46	0
58	MG	14	3355	1/1	0.97	0.12	43,43,43,43	0
58	MG	1H	3021	1/1	0.97	0.20	43,43,43,43	0
58	MG	1H	3027	1/1	0.97	0.28	36,36,36,36	0
58	MG	14	3173	1/1	0.97	0.12	78,78,78,78	0
58	MG	14	3122	1/1	0.97	0.24	54,54,54,54	0
58	MG	13	1634	1/1	0.97	0.20	52,52,52,52	0
58	MG	14	3090	1/1	0.97	0.23	65,65,65,65	0
58	MG	14	3372	1/1	0.97	0.08	59,59,59,59	0
58	MG	14	3113	1/1	0.97	0.10	46,46,46,46	0
58	MG	14	3047	1/1	0.97	0.17	71,71,71,71	0
58	MG	14	3061	1/1	0.97	0.23	43,43,43,43	0
58	MG	14	3079	1/1	0.97	0.20	55,55,55,55	0
58	MG	14	3135	1/1	0.97	0.14	67,67,67,67	0
58	MG	1H	3138	1/1	0.97	0.44	62,62,62,62	0
58	MG	1H	3020	1/1	0.97	0.22	38,38,38,38	0
58	MG	14	3223	1/1	0.97	0.18	44,44,44,44	0
58	MG	14	3109	1/1	0.97	0.21	60,60,60,60	0
58	MG	13	1616	1/1	0.97	0.18	59,59,59,59	0
58	MG	14	3265	1/1	0.97	0.19	55,55,55,55	0
58	MG	14	3031	1/1	0.97	0.25	56,56,56,56	0
58	MG	14	3044	1/1	0.97	0.14	40,40,40,40	0
58	MG	14	3016	1/1	0.97	0.15	53,53,53,53	0
58	MG	14	3021	1/1	0.97	0.16	51,51,51,51	0
58	MG	14	3339	1/1	0.97	0.09	60,60,60,60	0
58	MG	14	3002	1/1	0.97	0.21	43,43,43,43	0
58	MG	1H	3203	1/1	0.97	0.14	68,68,68,68	0
58	MG	1H	3350	1/1	0.97	0.34	62,62,62,62	0
58	MG	14	3199	1/1	0.97	0.22	66,66,66,66	0
58	MG	1G	1614	1/1	0.97	0.17	73,73,73,73	0
58	MG	13	1661	1/1	0.97	0.29	82,82,82,82	0
58	MG	16	210	1/1	0.97	0.14	63,63,63,63	0
58	MG	13	1666	1/1	0.97	0.34	81,81,81,81	0
58	MG	14	3088	1/1	0.97	0.20	47,47,47,47	0
58	MG	1H	3121	1/1	0.97	0.26	41,41,41,41	0
58	MG	1G	1619	1/1	0.97	0.18	88,88,88,88	0
58	MG	1G	1680	1/1	0.97	0.12	83,83,83,83	0
58	MG	1H	3412	1/1	0.97	0.10	48,48,48,48	0
58	MG	1H	3307	1/1	0.97	0.12	64,64,64,64	0
58	MG	14	3190	1/1	0.97	0.21	65,65,65,65	0
58	MG	14	3271	1/1	0.97	0.11	58,58,58,58	0
58	MG	1H	3048	1/1	0.98	0.18	52,52,52,52	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
58	MG	13	1604	1/1	0.98	0.14	65,65,65,65	0
58	MG	1H	3092	1/1	0.98	0.26	65,65,65,65	0
58	MG	1H	3118	1/1	0.98	0.17	36,36,36,36	0
58	MG	14	3017	1/1	0.98	0.22	49,49,49,49	0
58	MG	13	1623	1/1	0.98	0.27	56,56,56,56	0
58	MG	1H	3069	1/1	0.98	0.43	69,69,69,69	0
58	MG	1H	3472	1/1	0.98	0.07	75,75,75,75	0
58	MG	1H	3434	1/1	0.98	0.12	42,42,42,42	0
58	MG	1H	3078	1/1	0.98	0.22	41,41,41,41	0
58	MG	13	1629	1/1	0.98	0.32	45,45,45,45	0
58	MG	14	3049	1/1	0.98	0.13	47,47,47,47	0
58	MG	1G	1601	1/1	0.98	0.22	77,77,77,77	0
58	MG	31	302	1/1	0.98	0.08	57,57,57,57	0
58	MG	1H	3090	1/1	0.98	0.27	45,45,45,45	0
58	MG	1H	3411	1/1	0.98	0.11	43,43,43,43	0
58	MG	1H	3395	1/1	0.98	0.17	40,40,40,40	0
58	MG	1H	3250	1/1	0.98	0.20	41,41,41,41	0
58	MG	1H	3024	1/1	0.98	0.21	40,40,40,40	0
58	MG	13	1689	1/1	0.98	0.10	70,70,70,70	0
58	MG	14	3121	1/1	0.98	0.15	64,64,64,64	0
58	MG	13	1601	1/1	0.98	0.21	59,59,59,59	0
58	MG	13	1605	1/1	0.98	0.11	77,77,77,77	0
58	MG	14	3297	1/1	0.98	0.11	60,60,60,60	0
58	MG	14	3354	1/1	0.98	0.11	57,57,57,57	0
58	MG	14	3094	1/1	0.98	0.21	40,40,40,40	0
58	MG	14	3067	1/1	0.98	0.20	54,54,54,54	0
58	MG	14	3378	1/1	0.98	0.08	73,73,73,73	0
58	MG	1H	3007	1/1	0.98	0.34	45,45,45,45	0
58	MG	14	3001	1/1	0.98	0.27	50,50,50,50	0
58	MG	14	3033	1/1	0.98	0.15	56,56,56,56	0
58	MG	14	3137	1/1	0.98	0.19	65,65,65,65	0
58	MG	1G	1643	1/1	0.98	0.09	83,83,83,83	0
58	MG	14	3351	1/1	0.98	0.17	60,60,60,60	0
58	MG	14	3003	1/1	0.98	0.19	49,49,49,49	0
58	MG	1H	3471	1/1	0.98	0.11	54,54,54,54	0
58	MG	13	1644	1/1	0.98	0.14	56,56,56,56	0
58	MG	1H	3440	1/1	0.98	0.07	59,59,59,59	0
58	MG	13	1733	1/1	0.98	0.10	61,61,61,61	0
58	MG	13	1603	1/1	0.98	0.12	61,61,61,61	0
58	MG	1H	3134	1/1	0.98	0.21	45,45,45,45	0
58	MG	14	3154	1/1	0.98	0.17	80,80,80,80	0
58	MG	14	3066	1/1	0.98	0.18	54,54,54,54	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
58	MG	13	1621	1/1	0.98	0.23	59,59,59,59	0
58	MG	14	3123	1/1	0.98	0.15	59,59,59,59	0
58	MG	1H	3310	1/1	0.98	0.16	79,79,79,79	0
58	MG	1H	3062	1/1	0.98	0.21	66,66,66,66	0
58	MG	1H	3298	1/1	0.98	0.36	94,94,94,94	0
58	MG	13	1617	1/1	0.98	0.27	87,87,87,87	0
58	MG	14	3242	1/1	0.98	0.12	55,55,55,55	0
58	MG	1H	3424	1/1	0.98	0.08	48,48,48,48	0
58	MG	29	301	1/1	0.98	0.19	46,46,46,46	0
58	MG	1H	3076	1/1	0.98	0.15	53,53,53,53	0
58	MG	14	3071	1/1	0.98	0.27	38,38,38,38	0
58	MG	1H	3135	1/1	0.98	0.28	52,52,52,52	0
58	MG	13	1715	1/1	0.98	0.08	78,78,78,78	0
58	MG	1H	3421	1/1	0.98	0.10	43,43,43,43	0
58	MG	1H	3126	1/1	0.98	0.24	46,46,46,46	0
58	MG	1H	3056	1/1	0.98	0.19	59,59,59,59	0
58	MG	13	1731	1/1	0.98	0.11	85,85,85,85	0
58	MG	14	3042	1/1	0.98	0.18	46,46,46,46	0
58	MG	1G	1604	1/1	0.98	0.12	84,84,84,84	0
58	MG	1H	3079	1/1	0.98	0.32	55,55,55,55	0
58	MG	1H	3096	1/1	0.98	0.21	40,40,40,40	0
58	MG	1H	3008	1/1	0.98	0.30	37,37,37,37	0
58	MG	1H	3058	1/1	0.98	0.23	50,50,50,50	0
58	MG	1H	3399	1/1	0.98	0.08	58,58,58,58	0
58	MG	14	3073	1/1	0.98	0.30	37,37,37,37	0
58	MG	13	1701	1/1	0.98	0.21	74,74,74,74	0
58	MG	13	1620	1/1	0.98	0.11	64,64,64,64	0
58	MG	1H	3107	1/1	0.98	0.32	54,54,54,54	0
58	MG	1H	3403	1/1	0.98	0.11	69,69,69,69	0
58	MG	13	1691	1/1	0.98	0.14	71,71,71,71	0
59	ZN	3E	302	1/1	0.98	0.37	89,89,89,89	0
58	MG	1H	3111	1/1	0.98	0.11	53,53,53,53	0
58	MG	13	1672	1/1	0.98	0.29	56,56,56,56	0
58	MG	1H	3034	1/1	0.98	0.22	71,71,71,71	0
58	MG	14	3191	1/1	0.98	0.22	66,66,66,66	0
58	MG	14	3111	1/1	0.98	0.19	63,63,63,63	0
58	MG	1H	3181	1/1	0.98	0.30	71,71,71,71	0
58	MG	14	3333	1/1	0.98	0.21	54,54,54,54	0
58	MG	14	3152	1/1	0.98	0.18	72,72,72,72	0
58	MG	13	1609	1/1	0.98	0.19	72,72,72,72	0
58	MG	14	3337	1/1	0.98	0.10	49,49,49,49	0
58	MG	1H	3387	1/1	0.98	0.12	38,38,38,38	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
58	MG	1H	3230	1/1	0.98	0.23	47,47,47,47	0
58	MG	1H	3013	1/1	0.98	0.28	46,46,46,46	0
58	MG	14	3008	1/1	0.98	0.21	55,55,55,55	0
58	MG	14	3331	1/1	0.98	0.09	53,53,53,53	0
58	MG	1H	3428	1/1	0.98	0.10	38,38,38,38	0
58	MG	1L	101	1/1	0.98	0.17	71,71,71,71	0
58	MG	1H	3028	1/1	0.98	0.18	51,51,51,51	0
58	MG	1H	3039	1/1	0.98	0.31	76,76,76,76	0
58	MG	14	3364	1/1	0.98	0.11	45,45,45,45	0
58	MG	14	3032	1/1	0.98	0.22	54,54,54,54	0
58	MG	14	3018	1/1	0.98	0.16	79,79,79,79	0
58	MG	1H	3160	1/1	0.98	0.17	64,64,64,64	0
58	MG	14	3360	1/1	0.98	0.07	55,55,55,55	0
58	MG	1H	3042	1/1	0.98	0.17	48,48,48,48	0
58	MG	1H	3466	1/1	0.98	0.12	51,51,51,51	0
58	MG	1H	3356	1/1	0.98	0.34	55,55,55,55	0
58	MG	14	3041	1/1	0.98	0.12	35,35,35,35	0
58	MG	13	1636	1/1	0.98	0.22	65,65,65,65	0
59	ZN	5I	101	1/1	0.99	0.19	88,88,88,88	0
58	MG	14	3110	1/1	0.99	0.17	44,44,44,44	0
58	MG	1H	3054	1/1	0.99	0.27	57,57,57,57	0
58	MG	14	3014	1/1	0.99	0.19	61,61,61,61	0
58	MG	2K	101	1/1	0.99	0.21	55,55,55,55	0
58	MG	14	3005	1/1	0.99	0.24	49,49,49,49	0
58	MG	1H	3459	1/1	0.99	0.07	65,65,65,65	0
58	MG	1H	3322	1/1	0.99	0.23	39,39,39,39	0
58	MG	14	3058	1/1	0.99	0.20	61,61,61,61	0
58	MG	1H	3335	1/1	0.99	0.17	47,47,47,47	0
59	ZN	32	301	1/1	0.99	0.34	103,103,103,103	0
58	MG	13	1734	1/1	0.99	0.09	76,76,76,76	0
58	MG	1H	3236	1/1	0.99	0.12	52,52,52,52	0
58	MG	1H	3016	1/1	0.99	0.30	45,45,45,45	0
58	MG	14	3043	1/1	0.99	0.21	47,47,47,47	0
58	MG	1H	3318	1/1	0.99	0.10	50,50,50,50	0
58	MG	1H	3147	1/1	0.99	0.20	57,57,57,57	0
58	MG	14	3093	1/1	0.99	0.11	63,63,63,63	0
58	MG	1H	3448	1/1	0.99	0.12	50,50,50,50	0
58	MG	1H	3010	1/1	0.99	0.33	33,33,33,33	0
58	MG	14	3260	1/1	0.99	0.12	57,57,57,57	0
58	MG	1H	3450	1/1	0.99	0.05	79,79,79,79	0
58	MG	1H	3439	1/1	0.99	0.06	70,70,70,70	0
58	MG	1H	3114	1/1	0.99	0.16	40,40,40,40	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
58	MG	14	3272	1/1	0.99	0.14	72,72,72,72	0
58	MG	1H	3023	1/1	0.99	0.25	40,40,40,40	0
58	MG	1H	3445	1/1	0.99	0.11	40,40,40,40	0
58	MG	1H	3029	1/1	0.99	0.21	50,50,50,50	0
58	MG	1H	3017	1/1	0.99	0.17	52,52,52,52	0
58	MG	1H	3093	1/1	0.99	0.39	38,38,38,38	0
58	MG	14	3074	1/1	0.99	0.28	41,41,41,41	0
58	MG	1H	3067	1/1	0.99	0.15	53,53,53,53	0
58	MG	14	3349	1/1	0.99	0.12	57,57,57,57	0
58	MG	14	3103	1/1	0.99	0.22	36,36,36,36	0
58	MG	1H	3002	1/1	0.99	0.19	38,38,38,38	0
58	MG	1H	3443	1/1	0.99	0.12	55,55,55,55	0
58	MG	13	1643	1/1	0.99	0.22	50,50,50,50	0
58	MG	1H	3425	1/1	0.99	0.10	43,43,43,43	0
58	MG	1H	3051	1/1	0.99	0.38	57,57,57,57	0
58	MG	14	3091	1/1	0.99	0.26	50,50,50,50	0
58	MG	1H	3055	1/1	0.99	0.36	41,41,41,41	0
58	MG	14	3009	1/1	0.99	0.16	49,49,49,49	0
58	MG	1H	3420	1/1	0.99	0.14	37,37,37,37	0
58	MG	13	1624	1/1	0.99	0.26	85,85,85,85	0
58	MG	1H	3124	1/1	0.99	0.20	43,43,43,43	0
58	MG	1H	3442	1/1	0.99	0.06	60,60,60,60	0
58	MG	14	3075	1/1	0.99	0.19	53,53,53,53	0
58	MG	1H	3015	1/1	0.99	0.27	46,46,46,46	0
58	MG	1H	3416	1/1	0.99	0.12	51,51,51,51	0
58	MG	14	3065	1/1	0.99	0.29	39,39,39,39	0
58	MG	14	3069	1/1	0.99	0.26	75,75,75,75	0
58	MG	1H	3022	1/1	0.99	0.17	39,39,39,39	0
58	MG	14	3051	1/1	0.99	0.09	52,52,52,52	0
58	MG	14	3013	1/1	0.99	0.18	56,56,56,56	0
58	MG	14	3054	1/1	0.99	0.15	48,48,48,48	0

## 6.5 Other polymers

There are no such residues in this entry.