



# wwPDB X-ray Structure Validation Summary Report ⓘ

May 21, 2020 – 05:29 am BST

PDB ID : 6GSK  
Title : Structure of T. thermophilus 70S ribosome complex with mRNA, tRNA<sup>fMet</sup> and near-cognate tRNA<sup>Thr</sup> in the A-site  
Authors : Rozov, A.; Yusupov, M.; Yusupova, G.  
Deposited on : 2018-06-14  
Resolution : 3.36 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

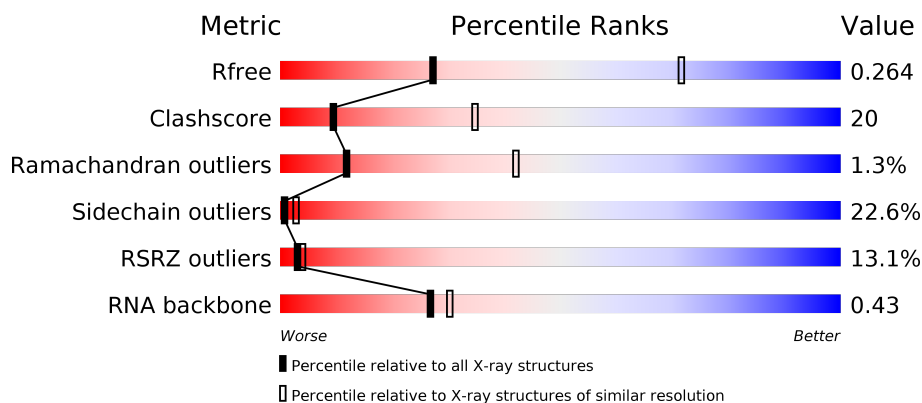
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.36 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	1558 (3.42-3.30)
Clashscore	141614	1627 (3.42-3.30)
Ramachandran outliers	138981	1599 (3.42-3.30)
Sidechain outliers	138945	1598 (3.42-3.30)
RSRZ outliers	127900	1507 (3.42-3.30)
RNA backbone	3102	1023 (3.80-2.92)

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% 49% 17%</div> </div>
1	1G	1522	<div> <div>%</div> <div>28% 48% 20%</div> </div>
2	12	256	<div> <div>4%</div> <div>38% 32% 11% 19%</div> </div>
2	1E	256	<div> <div>%</div> <div>39% 39% 12% 10%</div> </div>

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

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Mol	Chain	Length	Quality of chain
15	6I	89	
16	7A	88	
16	7I	88	
17	8A	105	
17	8I	105	
18	9A	88	
18	9I	88	
19	AA	93	
19	AI	93	
20	BA	106	
20	BI	106	
21	1B	27	
21	1F	27	
22	1K	76	
22	1L	76	
23	2K	77	
23	2L	77	
24	3K	76	
24	3L	76	
25	4K	27	
25	4L	27	
26	14	2917	
26	1H	2917	
27	16	122	
27	1J	122	

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Mol	Chain	Length	Quality of chain
28	11	276	
28	19	276	
29	21	206	
29	29	206	
30	31	210	
30	39	210	
31	41	182	
31	49	182	
32	51	180	
32	59	180	
33	61	148	
33	69	148	
34	15	140	
34	58	140	
35	25	122	
35	68	122	
36	35	150	
36	78	150	
37	45	141	
37	88	141	
38	55	118	
38	98	118	
39	65	112	
39	A8	112	
40	75	146	

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Mol	Chain	Length	Quality of chain
40	B8	146	
41	85	118	
41	C8	118	
42	95	101	
42	D8	101	
43	A5	113	
43	E8	113	
44	B5	96	
44	F8	96	
45	C5	110	
45	G8	110	
46	D5	206	
46	H8	206	
47	E5	85	
47	I8	85	
48	F5	98	
48	J8	98	
49	G5	72	
49	K8	72	
50	H5	60	
50	L8	60	
51	M8	71	
52	J5	60	
52	N8	60	
53	L5	49	

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

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
22	H2U	1L	17	-	-	-	X
55	MG	13	1638	-	-	-	X
55	MG	13	1674	-	-	-	X
55	MG	13	1686	-	-	-	X
55	MG	13	1705	-	-	-	X
55	MG	14	3009	-	-	-	X
55	MG	14	3041	-	-	-	X
55	MG	14	3092	-	-	-	X
55	MG	14	3094	-	-	-	X
55	MG	14	3112	-	-	-	X
55	MG	14	3133	-	-	-	X
55	MG	14	3135	-	-	-	X
55	MG	14	3177	-	-	-	X
55	MG	14	3185	-	-	-	X
55	MG	1G	1618	-	-	-	X
55	MG	1G	1621	-	-	-	X
55	MG	1G	1650	-	-	-	X
55	MG	1G	1662	-	-	-	X
55	MG	1G	1663	-	-	-	X
55	MG	1G	1670	-	-	-	X
55	MG	1H	3045	-	-	-	X
55	MG	1H	3107	-	-	-	X
55	MG	1H	3142	-	-	-	X
55	MG	1H	3149	-	-	-	X
55	MG	1H	3181	-	-	-	X
55	MG	1H	3185	-	-	-	X
55	MG	1H	3212	-	-	-	X
55	MG	1H	3223	-	-	-	X
55	MG	1H	3226	-	-	-	X
55	MG	1H	3229	-	-	-	X
55	MG	1H	3241	-	-	-	X
55	MG	1H	3274	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
55	MG	1H	3275	-	-	-	X
55	MG	35	201	-	-	-	X
55	MG	5I	101	-	-	-	X
55	MG	8I	201	-	-	-	X
56	SF4	32	302	-	-	X	-



## 2 Entry composition [i](#)

There are 58 unique types of molecules in this entry. The entry contains 292640 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	1500	Total	C	N	O	P	0	0	0
			32246	14352	5978	10416	1500			
1	1G	1490	Total	C	N	O	P	0	0	0
			32028	14255	5932	10351	1490			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
13	1542	G	U	conflict	GB 55771382
1G	1542	G	U	conflict	GB 55771382

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	1E	231	Total	C	N	O	S	0	0	0
			1874	1199	334	336	5			
2	12	207	Total	C	N	O	S	0	0	0
			1696	1083	306	303	4			

- 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	197	Total	C	N	O	S	0	0	0
			1546	978	299	268	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	3E	207	Total	C	N	O	S	0	0	0
			1698	1064	338	289	7			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
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	149	Total	C	N	O	S	0	0	0
			1142	722	216	200	4			
5	42	150	Total	C	N	O	S	0	0	0
			1141	719	217	201	4			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	5E	100	Total	C	N	O	S	0	0	0
			837	528	154	152	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	154	Total	C	N	O	S	0	0	0
			1242	770	250	216	6			
7	62	138	Total	C	N	O	S	0	0	0
			1110	689	221	194	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	137	Total	C	N	O	S	0	0	0
			1107	700	214	191	2			

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
9	8E	126	Total	C	N	O	0	0	0
			1000	634	196	170			
9	82	121	Total	C	N	O	0	0	0
			953	605	186	162			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	1I	94	Total	C	N	O	S	0	0	0
			749	468	147	133	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	111	Total	C	N	O	S	0	0	0
			823	512	154	154	3			
11	2A	113	Total	C	N	O	S	0	0	0
			835	520	156	156	3			

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	4I	119	Total	C	N	O	S	0	0	0
			942	582	194	164	2			
13	4A	109	Total	C	N	O	S	0	0	0
			879	544	181	152	2			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
14	5I	60	Total	C	N	O	S	0	0	0
			491	312	104	71	4			
14	5A	59	Total	C	N	O	S	0	0	0
			486	309	103	70	4			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
15	6I	87	Total	C	N	O	S	0	0	0
			729	457	146	124	2			
15	6A	87	Total	C	N	O	S	0	0	0
			729	457	146	124	2			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
16	7I	83	Total	C	N	O	S	0	0	0
			700	443	139	117	1			
16	7A	84	Total	C	N	O	S	0	0	0
			705	446	140	118	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
17	8I	100	Total	C	N	O	S	0	0	0
			834	534	155	143	2			
17	8A	99	Total	C	N	O	S	0	0	0
			823	528	151	142	2			

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
18	9I	68	Total	C	N	O	0	0	0
			549	352	105	92			
18	9A	69	Total	C	N	O	0	0	0
			554	355	106	93			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
19	AI	82	Total	C	N	O	S	0	0	0
			661	422	123	114	2			
19	AA	65	Total	C	N	O	S	0	0	0
			510	324	92	92	2			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
20	BI	97	Total	C	N	O	S	0	0	0
			746	461	157	126	2			

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

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
21	1F	23	Total	C	N	O	0	0	0
			199	122	48	29			
21	1B	22	Total	C	N	O	0	0	0
			188	116	44	28			

- Molecule 22 is a RNA chain called tRNAThr.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
22	1K	74	Total	C	N	O	P	0	0	0
			1593	712	285	522	74			
22	1L	74	Total	C	N	O	P	0	0	0
			1593	712	285	522	74			

- Molecule 23 is a RNA chain called tRNAfMet.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
23	2K	77	Total	C	N	O	P	0	0	0
			1644	733	297	537	77			
23	2L	77	Total	C	N	O	P	0	0	0
			1644	733	297	537	77			

- Molecule 24 is a RNA chain called tRNAThr.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
24	3K	72	Total	C	N	O	P	0	0	0
			1537	686	276	503	72			
24	3L	72	Total	C	N	O	P	0	0	0
			1537	686	276	503	72			

- Molecule 25 is a RNA chain called mRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
25	4K	18	Total	C	N	O	P	0	0	0
			391	176	79	118	18			
25	4L	14	Total	C	N	O	P	0	0	0
			303	137	62	90	14			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
26	1H	2811	Total	C	N	O	P	0	0	0
			60546	26946	11325	19464	2811			
26	14	2811	Total	C	N	O	P	0	0	0
			60561	26951	11337	19462	2811			

There are 14 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
1H	161	U	UNK	conflict	GB 55771382
1H	654A	A	G	conflict	GB 55771382
1H	654E	C	G	conflict	GB 55771382
1H	654P	G	C	conflict	GB 55771382
1H	654T	A	C	conflict	GB 55771382
1H	1058	U	G	conflict	GB 55771382
1H	1080	A	C	conflict	GB 55771382
14	158	U	UNK	conflict	GB 55771382
14	654A	A	G	conflict	GB 55771382
14	654E	C	G	conflict	GB 55771382
14	654P	G	C	conflict	GB 55771382
14	654T	A	C	conflict	GB 55771382
14	1058	U	G	conflict	GB 55771382
14	1080	A	C	conflict	GB 55771382

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
28	11	273	Total	C	N	O	S	0	0	0
			2120	1338	421	358	3			
28	19	274	Total	C	N	O	S	0	0	0
			2125	1341	422	359	3			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
29	21	205	Total	C	N	O	S	0	0	0
			1556	984	297	269	6			
29	29	204	Total	C	N	O	S	0	0	0
			1563	988	299	270	6			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
30	31	202	Total	C	N	O	S	0	0	0
			1585	1011	297	275	2			
30	39	204	Total	C	N	O	S	0	0	0
			1602	1022	299	279	2			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
31	41	179	Total	C	N	O	S	0	0	0
			1457	931	265	257	4			
31	49	180	Total	C	N	O	S	0	0	0
			1459	931	266	258	4			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
32	51	174	Total	C	N	O	S	0	0	0
			1328	842	249	236	1			
32	59	169	Total	C	N	O	S	0	0	0
			1295	823	241	230	1			

- Molecule 33 is a protein called 50S ribosomal protein L9.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
33	61	145	Total	C	N	O	S	0	0	0
			1131	723	200	207	1			
33	69	145	Total	C	N	O	S	0	0	0
			1131	723	200	207	1			

- Molecule 34 is a protein called 50S ribosomal protein L13.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
34	58	125	Total	C	N	O	S	0	0	0
			995	645	183	163	4			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
34	15	137	Total	C	N	O	S	0	0	0
			1096	707	205	181	3			

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
36	78	148	Total	C	N	O	S	0	0	0
			1127	701	230	193	3			
36	35	147	Total	C	N	O	S	0	0	0
			1122	698	229	192	3			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
37	88	141	Total	C	N	O	S	0	0	0
			1117	712	211	187	7			
37	45	138	Total	C	N	O	S	0	0	0
			1099	702	208	183	6			

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

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

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
39	A8	111	Total	C	N	O	0	0	0
			881	556	176	149			
39	65	110	Total	C	N	O	0	0	0
			876	553	175	148			



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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
40	B8	136	Total	C	N	O	S	0	0	0
			1128	702	231	194	1			
40	75	140	Total	C	N	O	S	0	0	0
			1164	723	238	202	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
41	C8	115	Total	C	N	O	S	0	0	0
			950	603	199	147	1			
41	85	116	Total	C	N	O	S	0	0	0
			959	608	201	149	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
42	D8	100	Total	C	N	O	S	0	0	0
			774	499	141	133	1			
42	95	100	Total	C	N	O	S	0	0	0
			770	496	140	133	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
43	E8	110	Total	C	N	O	S	0	0	0
			876	552	171	151	2			
43	A5	111	Total	C	N	O	S	0	0	0
			886	558	174	152	2			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
44	F8	95	Total	C	N	O	S	0	0	0
			750	488	135	126	1			
44	B5	94	Total	C	N	O		0	0	0
			735	477	133	125				

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
45	G8	97	Total	C	N	O	S	0	0	0
			734	472	140	117	5			
45	C5	52	Total	C	N	O	S	0	0	0
			396	258	72	65	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
46	H8	170	Total	C	N	O	S	0	0	0
			1365	870	246	246	3			
46	D5	177	Total	C	N	O	S	0	0	0
			1411	901	253	255	2			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
47	I8	77	Total	C	N	O	S	0	0	0
			611	378	129	103	1			
47	E5	76	Total	C	N	O	S	0	0	0
			603	372	128	102	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
48	J8	96	Total	C	N	O	S	0	0	0
			747	469	148	129	1			
48	F5	94	Total	C	N	O	S	0	0	0
			737	463	146	127	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
49	K8	68	Total	C	N	O	S	0	0	0
			575	358	116	100	1			
49	G5	69	Total	C	N	O	S	0	0	0
			576	358	116	101	1			

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
50	L8	58	Total	C	N	O	0	0	0
			459	293	89	77			

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
50	H5	58	Total	C	N	O	0	0	0
			459	293	89	77			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
51	M8	60	Total	C	N	O	S	0	0	0
			475	300	84	86	5			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
52	N8	48	Total	C	N	O	S	0	0	0
			369	229	75	60	5			
52	J5	56	Total	C	N	O	S	0	0	0
			434	272	87	70	5			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
53	P8	47	Total	C	N	O	S	0	0	0
			401	246	99	54	2			
53	L5	48	Total	C	N	O	S	0	0	0
			406	249	100	55	2			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
54	Q8	64	Total	C	N	O	S	0	0	0
			516	331	102	81	2			
54	M5	64	Total	C	N	O	S	0	0	0
			516	331	102	81	2			

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
55	45	2	Total	Mg	0	0
			2	2		
55	BA	1	Total	Mg	0	0
			1	1		
55	P8	1	Total	Mg	0	0
			1	1		

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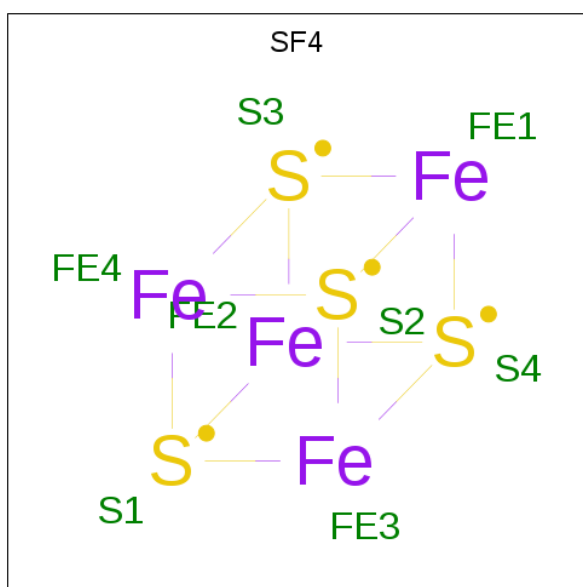
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
55	85	1	Total 1	Mg 1	0	0
55	32	1	Total 1	Mg 1	0	0
55	13	140	Total 140	Mg 140	0	0
55	1J	2	Total 2	Mg 2	0	0
55	5I	2	Total 2	Mg 2	0	0
55	35	1	Total 1	Mg 1	0	0
55	C8	2	Total 2	Mg 2	0	0
55	BI	1	Total 1	Mg 1	0	0
55	16	2	Total 2	Mg 2	0	0
55	42	2	Total 2	Mg 2	0	0
55	21	3	Total 3	Mg 3	0	0
55	2K	1	Total 1	Mg 1	0	0
55	8I	1	Total 1	Mg 1	0	0
55	I8	1	Total 1	Mg 1	0	0
55	D8	1	Total 1	Mg 1	0	0
55	29	1	Total 1	Mg 1	0	0
55	7A	1	Total 1	Mg 1	0	0
55	78	2	Total 2	Mg 2	0	0
55	J8	1	Total 1	Mg 1	0	0
55	4A	1	Total 1	Mg 1	0	0
55	39	1	Total 1	Mg 1	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
55	1G	126	Total 126	Mg 126	0	0
55	11	1	Total 1	Mg 1	0	0
55	1H	473	Total 473	Mg 473	0	0
55	F5	1	Total 1	Mg 1	0	0
55	E5	1	Total 1	Mg 1	0	0
55	88	3	Total 3	Mg 3	0	0
55	14	300	Total 300	Mg 300	0	0
55	1F	2	Total 2	Mg 2	0	0
55	2A	1	Total 1	Mg 1	0	0
55	41	1	Total 1	Mg 1	0	0
55	2L	1	Total 1	Mg 1	0	0

- Molecule 56 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe<sub>4</sub>S<sub>4</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
56	3E	1	Total	Fe	S	0	0
			8	4	4		
56	32	1	Total	Fe	S	0	0
			8	4	4		

- Molecule 57 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
57	5A	1	Total	Zn	0	0
			1	1		
57	5I	1	Total	Zn	0	0
			1	1		

- Molecule 58 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
58	13	274	Total	O	0	0
			274	274		
58	4E	6	Total	O	0	0
			6	6		
58	8E	1	Total	O	0	0
			1	1		
58	1I	2	Total	O	0	0
			2	2		
58	3I	1	Total	O	0	0
			1	1		
58	4I	2	Total	O	0	0
			2	2		
58	5I	1	Total	O	0	0
			1	1		
58	7I	3	Total	O	0	0
			3	3		
58	1F	1	Total	O	0	0
			1	1		
58	1K	1	Total	O	0	0
			1	1		
58	1H	1010	Total	O	0	0
			1010	1010		
58	16	8	Total	O	0	0
			8	8		
58	11	8	Total	O	0	0
			8	8		
58	21	4	Total	O	0	0
			4	4		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
58	31	5	Total 5	O 5	0	0
58	58	1	Total 1	O 1	0	0
58	78	8	Total 8	O 8	0	0
58	98	1	Total 1	O 1	0	0
58	D8	1	Total 1	O 1	0	0
58	E8	1	Total 1	O 1	0	0
58	G8	1	Total 1	O 1	0	0
58	I8	3	Total 3	O 3	0	0
58	J8	2	Total 2	O 2	0	0
58	L8	3	Total 3	O 3	0	0
58	Q8	2	Total 2	O 2	0	0
58	1G	240	Total 240	O 240	0	0
58	32	1	Total 1	O 1	0	0
58	42	1	Total 1	O 1	0	0
58	7A	4	Total 4	O 4	0	0
58	BA	2	Total 2	O 2	0	0
58	2L	6	Total 6	O 6	0	0
58	4L	1	Total 1	O 1	0	0
58	14	586	Total 586	O 586	0	0
58	19	7	Total 7	O 7	0	0
58	29	2	Total 2	O 2	0	0

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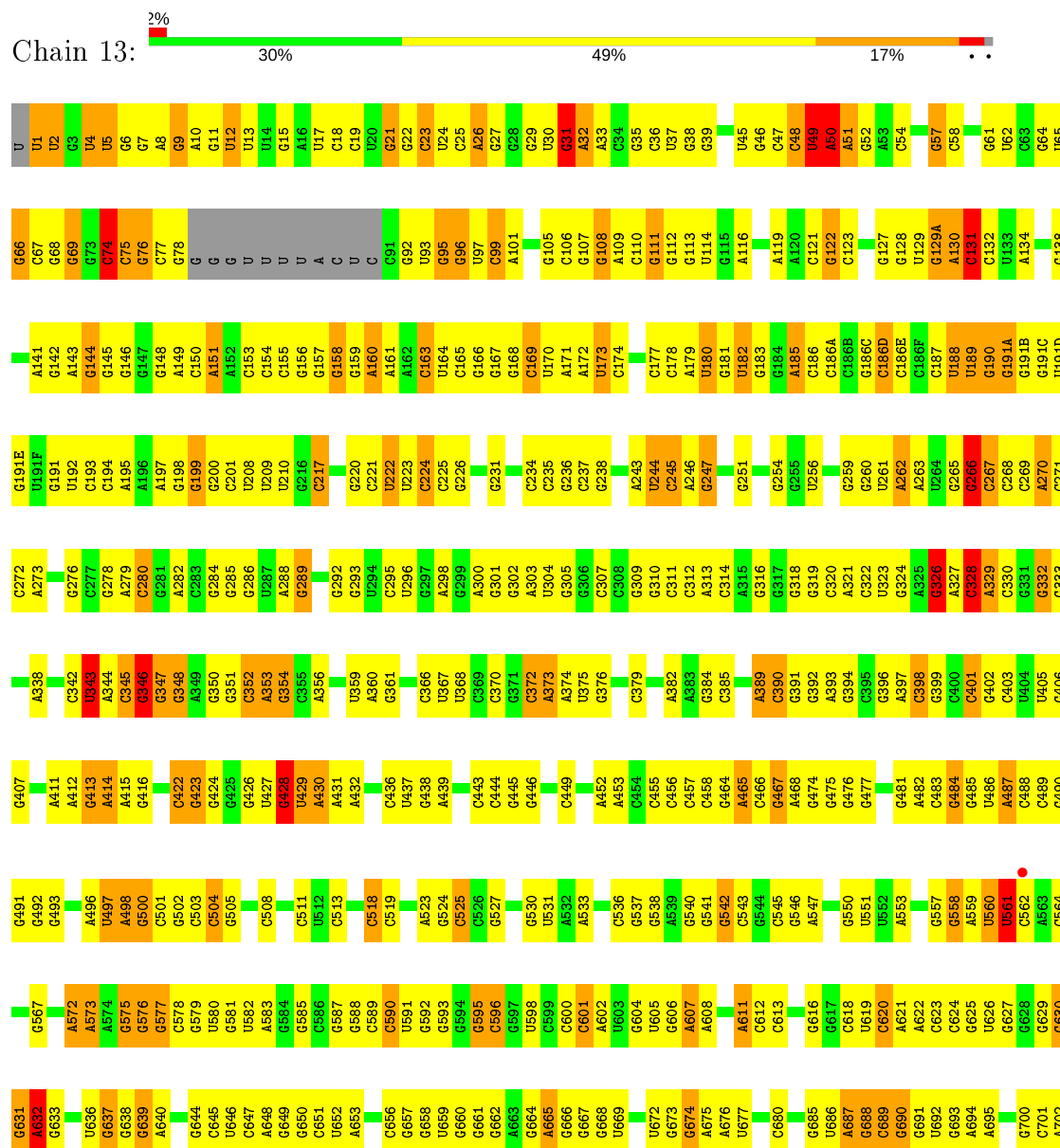
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
58	39	6	Total 6	O 6	0	0
58	35	5	Total 5	O 5	0	0
58	45	5	Total 5	O 5	0	0
58	B5	2	Total 2	O 2	0	0
58	H5	2	Total 2	O 2	0	0
58	L5	1	Total 1	O 1	0	0

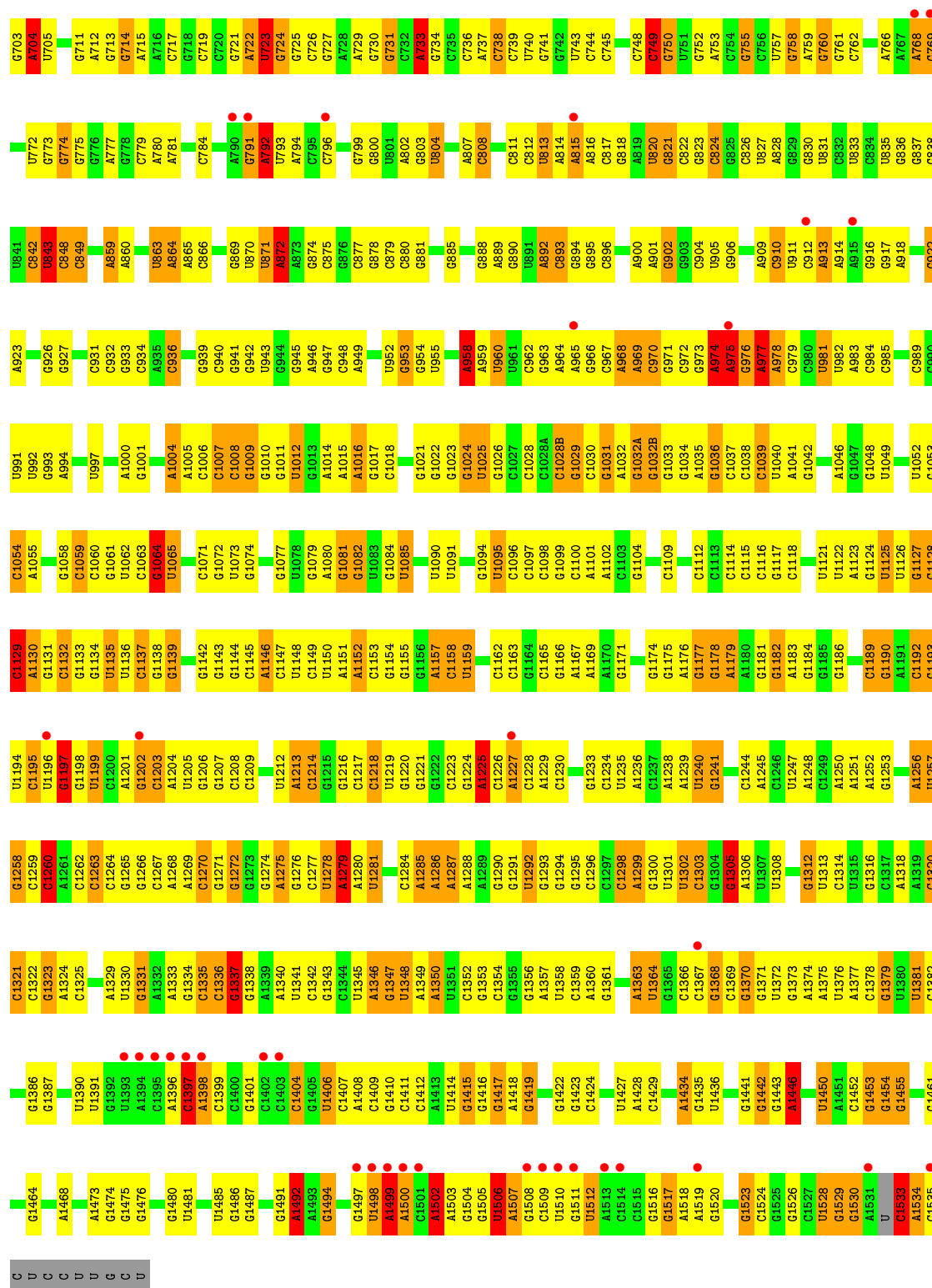


### 3 Residue-property plots

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.

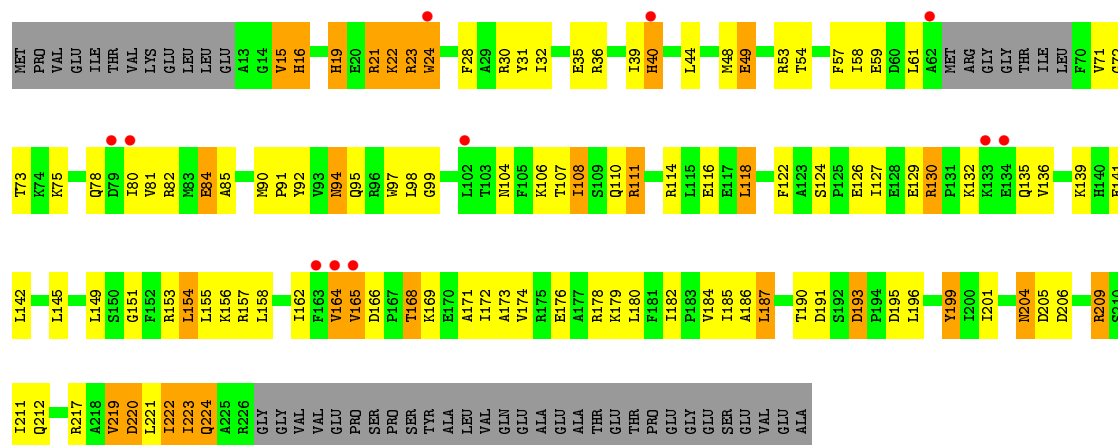
#### • Molecule 1: 16S ribosomal RNA



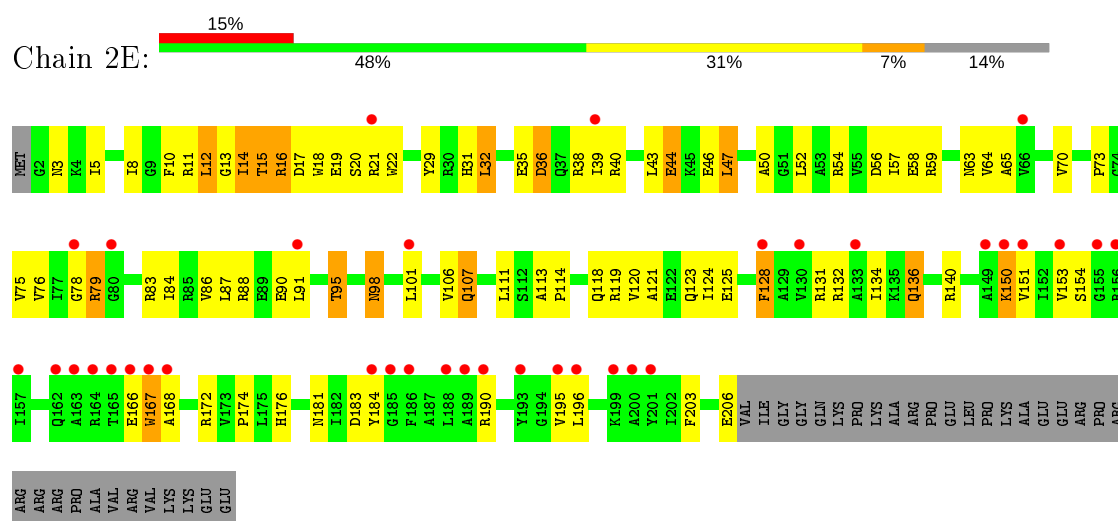




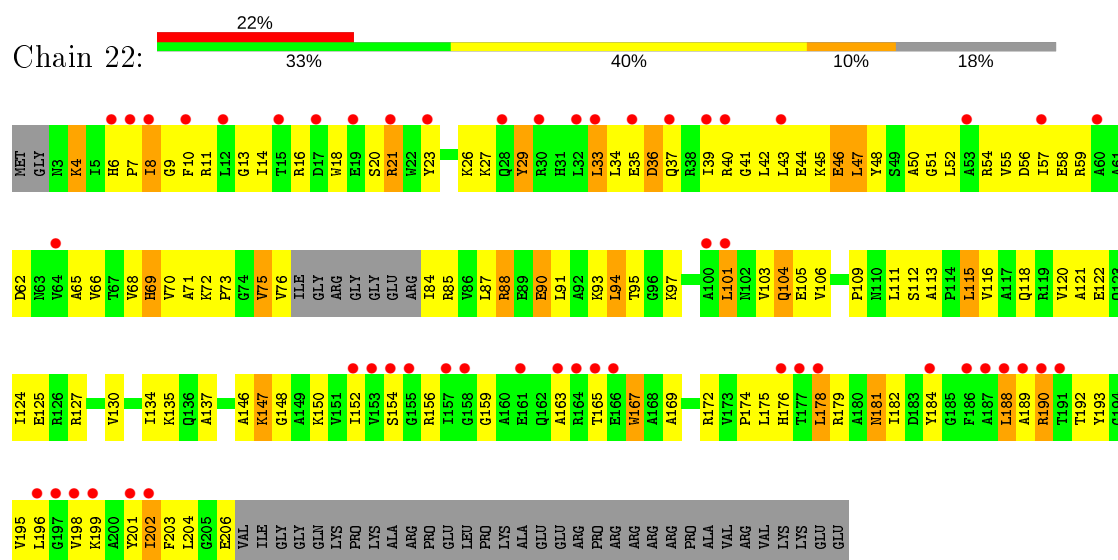




• Molecule 3: 30S ribosomal protein S3

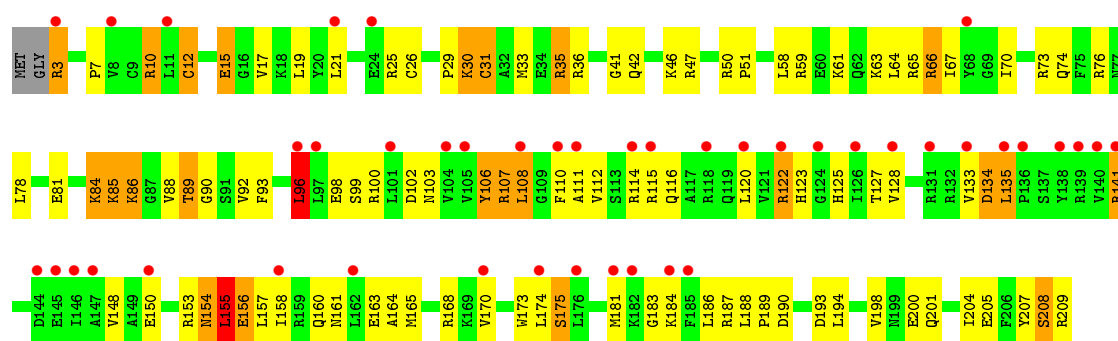


• Molecule 3: 30S ribosomal protein S3




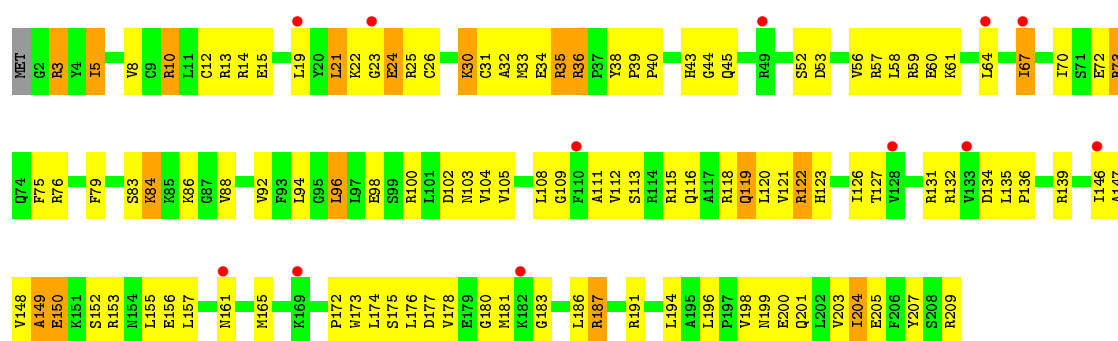
• Molecule 4: 30S ribosomal protein S4

Chain 3E: 



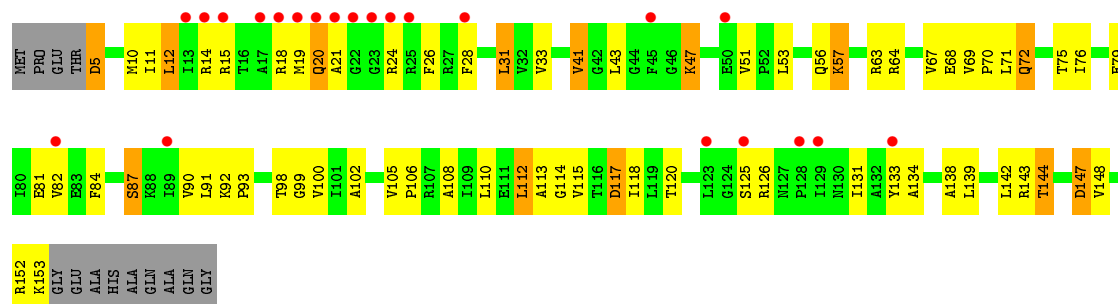
• Molecule 4: 30S ribosomal protein S4

Chain 32: 



• Molecule 5: 30S ribosomal protein S5

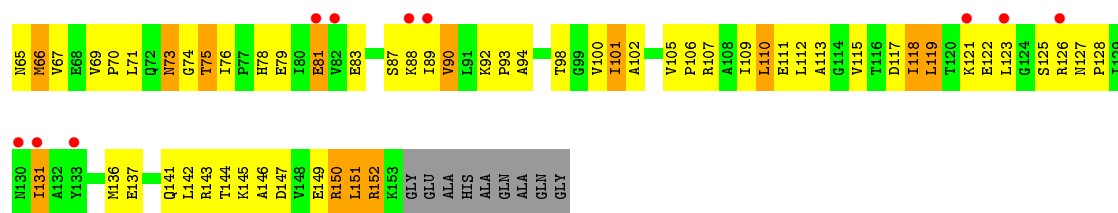
Chain 4E: 



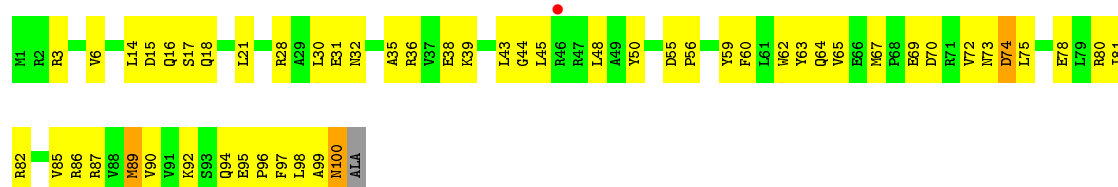
• Molecule 5: 30S ribosomal protein S5

Chain 42: 

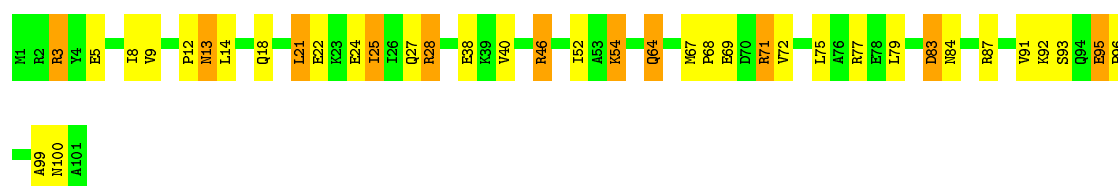




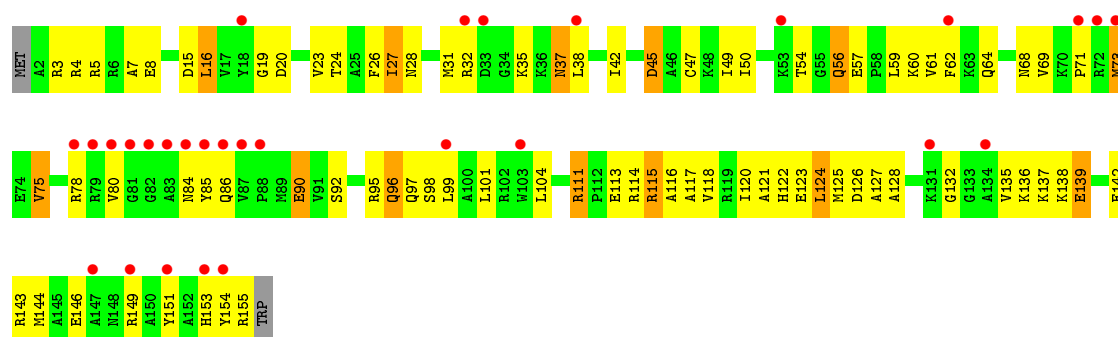
• Molecule 6: 30S ribosomal protein S6



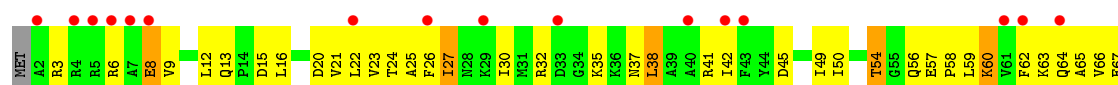
• Molecule 6: 30S ribosomal protein S6

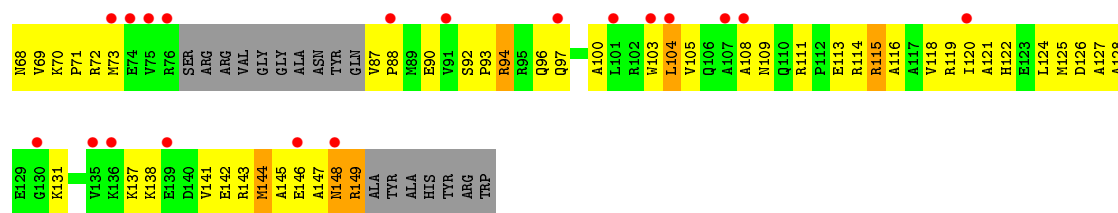


• Molecule 7: 30S ribosomal protein S7

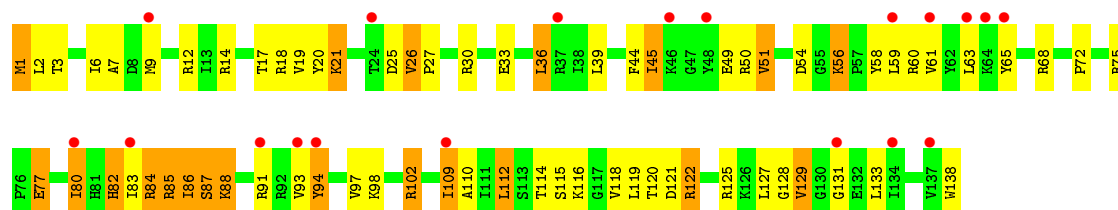


• Molecule 7: 30S ribosomal protein S7

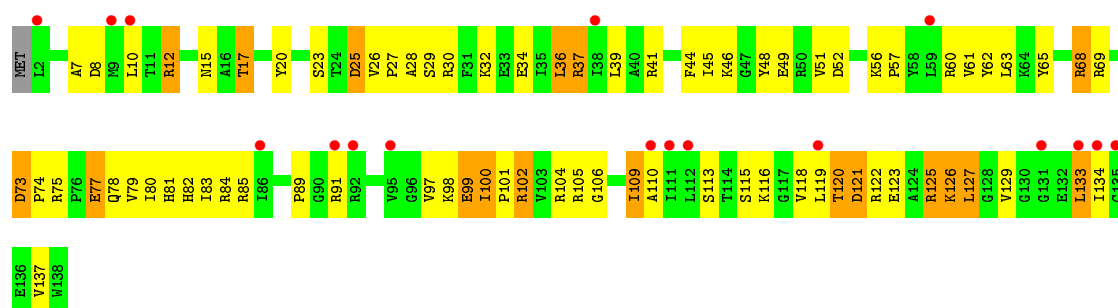
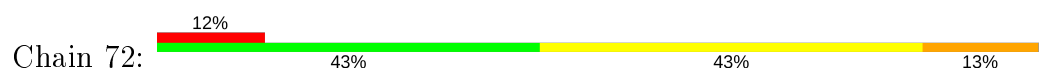




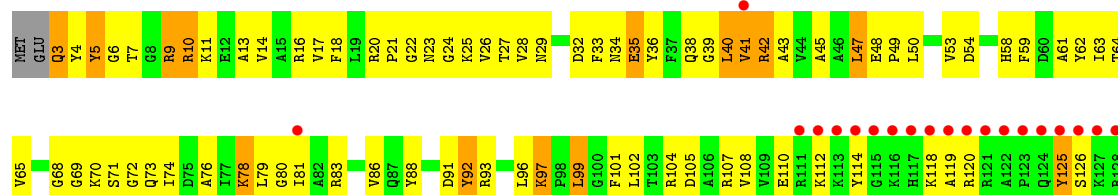
• Molecule 8: 30S ribosomal protein S8



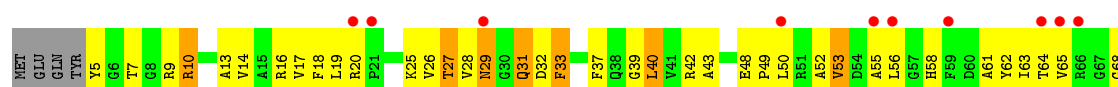
• Molecule 8: 30S ribosomal protein S8



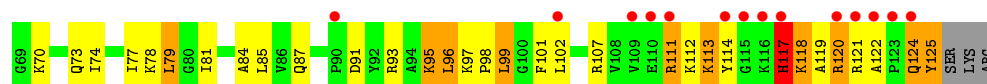
• Molecule 9: 30S ribosomal protein S9



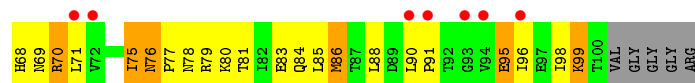
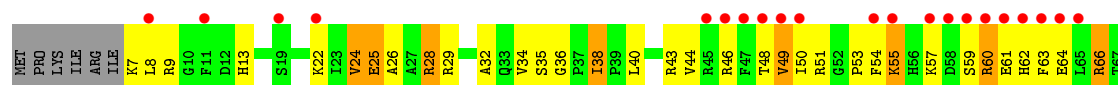
• Molecule 9: 30S ribosomal protein S9



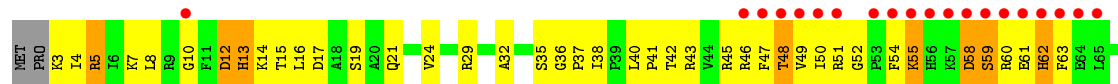




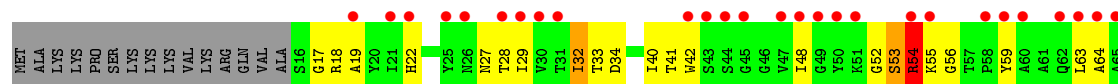
- Molecule 10: 30S ribosomal protein S10



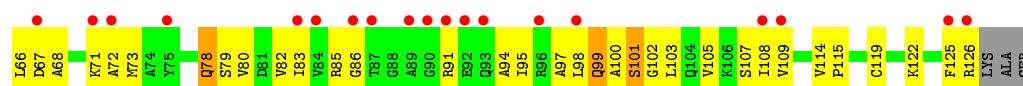
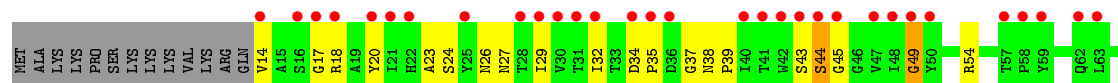
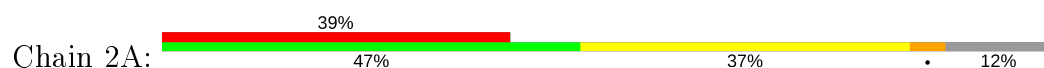
- Molecule 10: 30S ribosomal protein S10



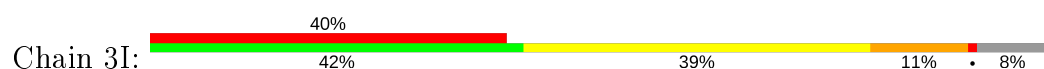
- Molecule 11: 30S ribosomal protein S11

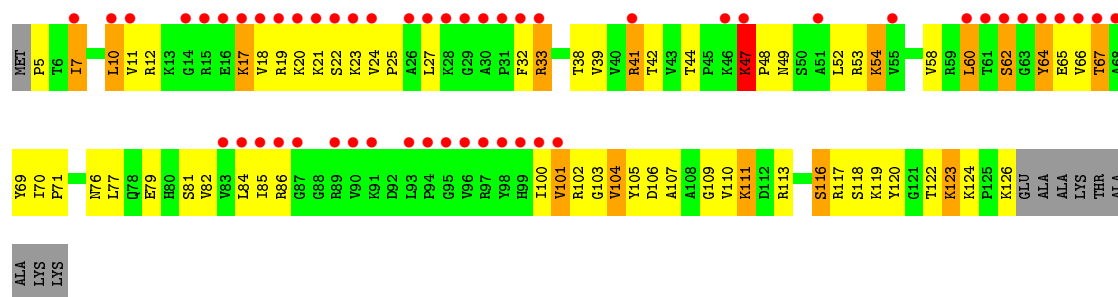


- Molecule 11: 30S ribosomal protein S11



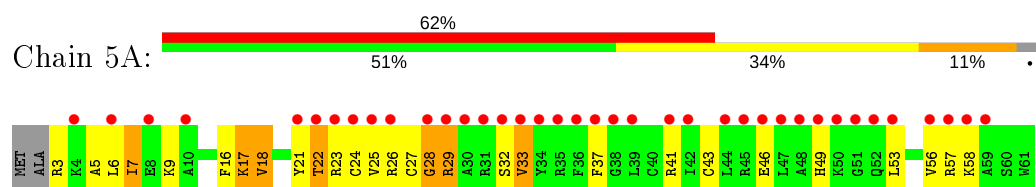
- Molecule 12: 30S ribosomal protein S12



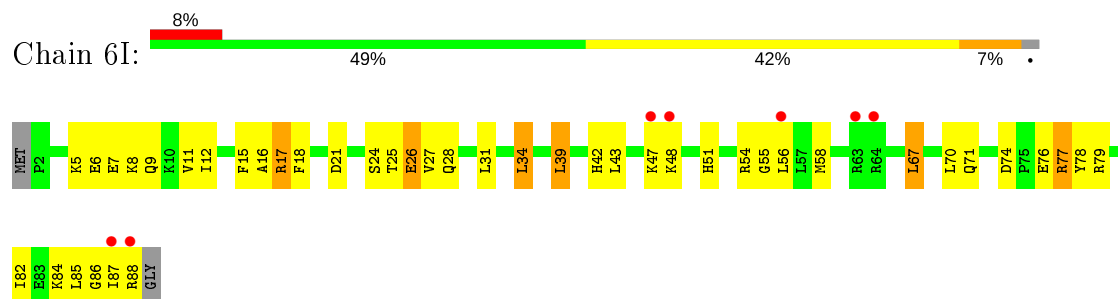


- Molecule 12: 30S ribosomal protein S12

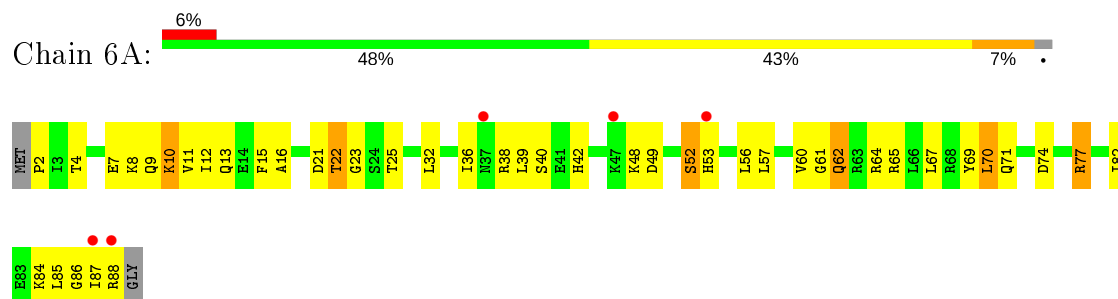




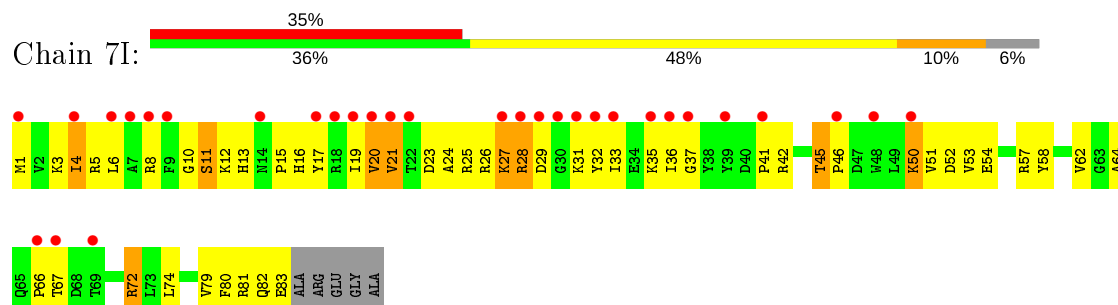
- Molecule 15: 30S ribosomal protein S15



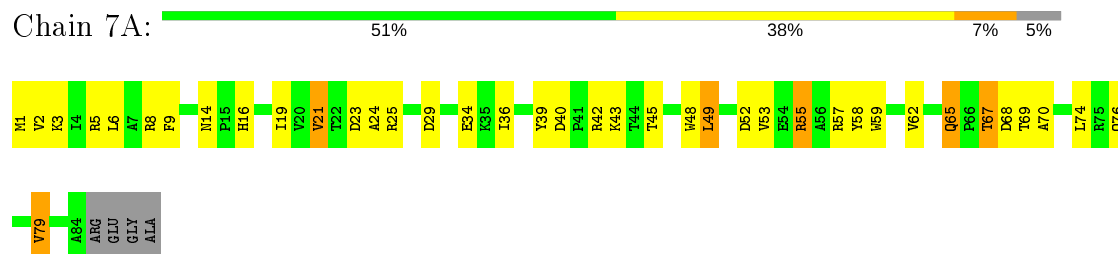
- Molecule 15: 30S ribosomal protein S15



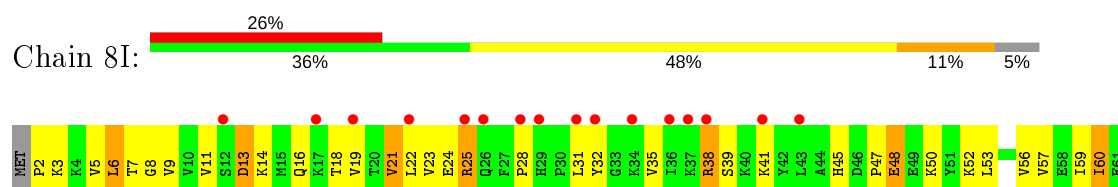
- Molecule 16: 30S ribosomal protein S16



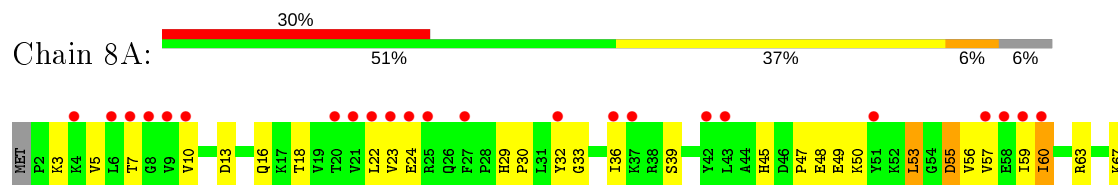
- Molecule 16: 30S ribosomal protein S16



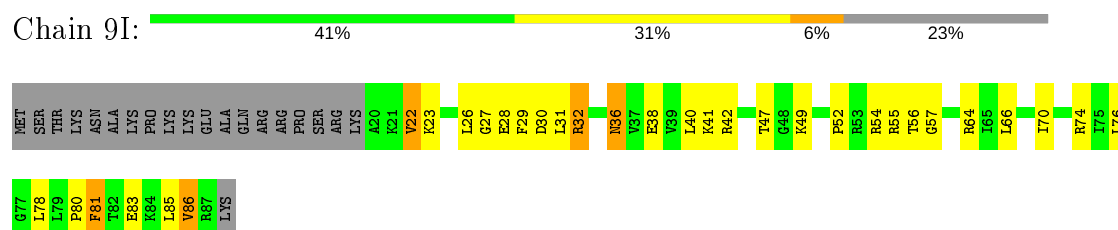
- Molecule 17: 30S ribosomal protein S17



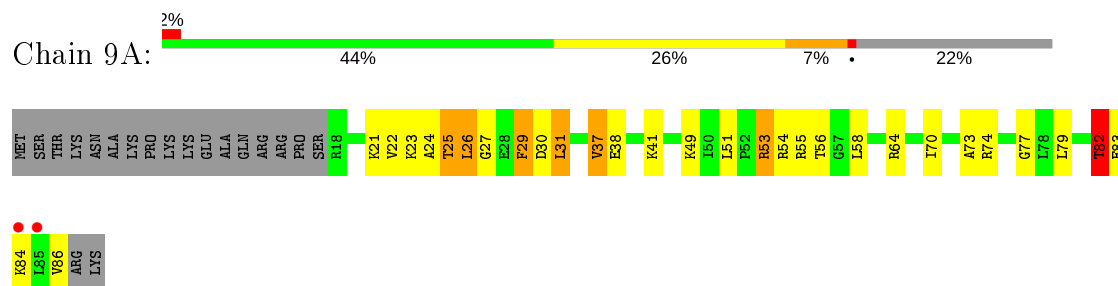
- Molecule 17: 30S ribosomal protein S17



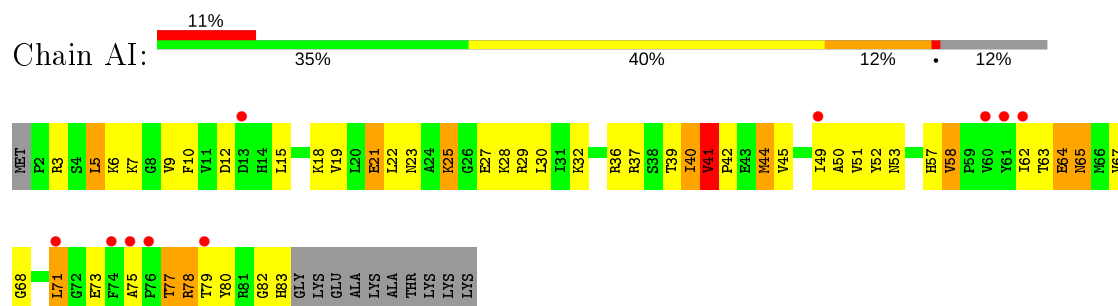
- Molecule 18: 30S ribosomal protein S18



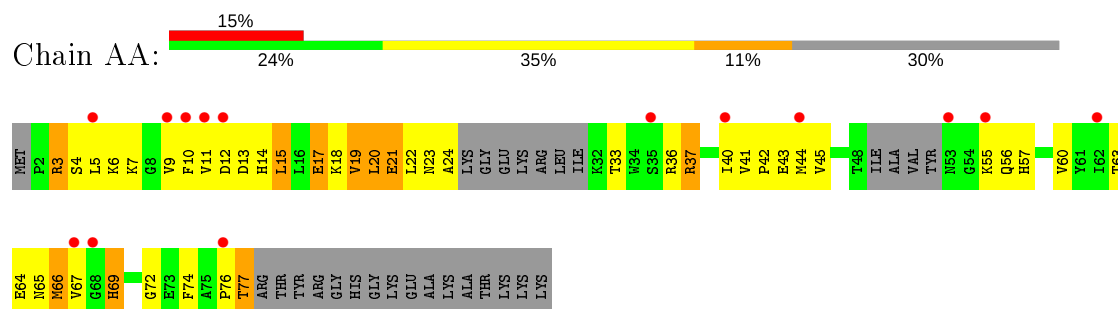
- Molecule 18: 30S ribosomal protein S18



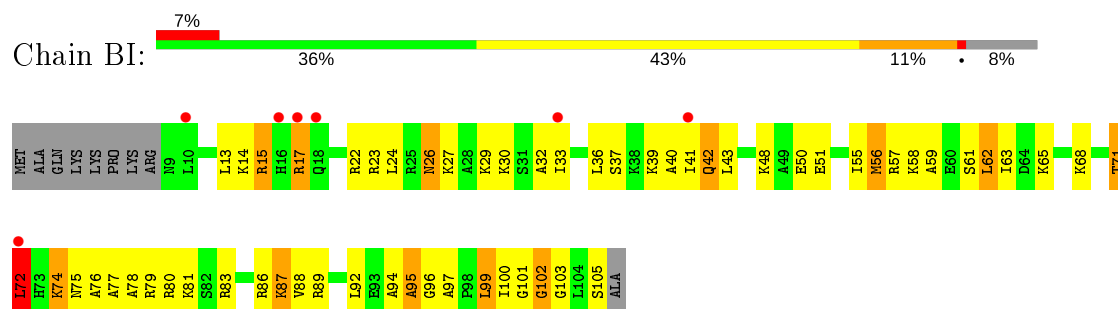
- Molecule 19: 30S ribosomal protein S19



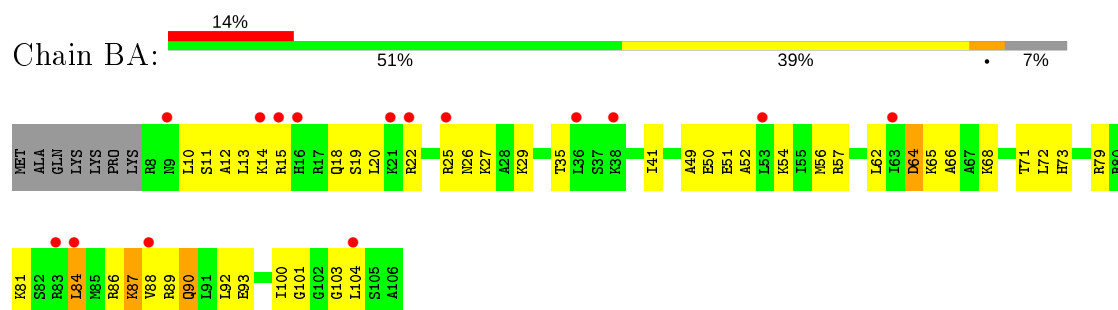
- Molecule 19: 30S ribosomal protein S19



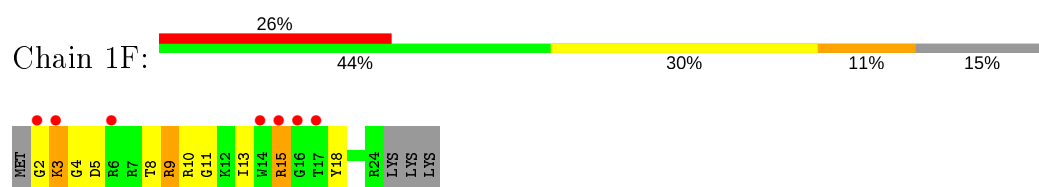
- Molecule 20: 30S ribosomal protein S20



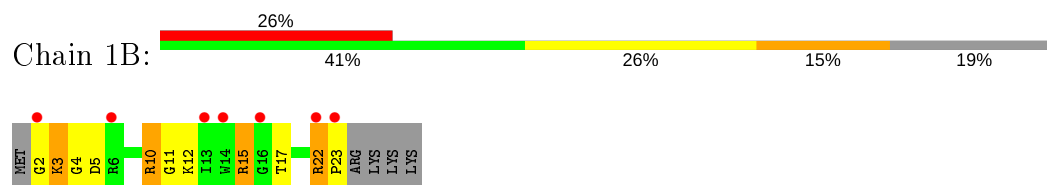
- Molecule 20: 30S ribosomal protein S20



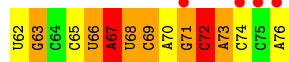
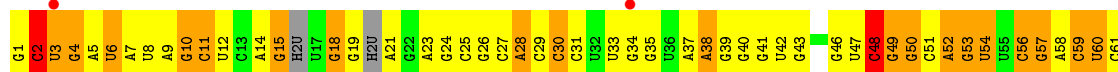
- Molecule 21: 30S ribosomal protein Thx



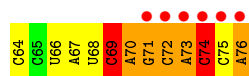
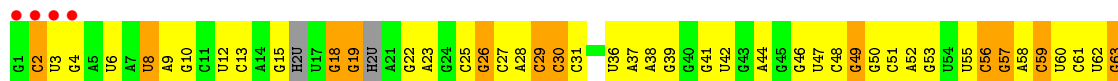
- Molecule 21: 30S ribosomal protein Thx



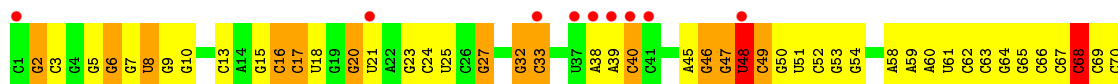
- Molecule 22: tRNAThr



• Molecule 22: tRNAThr



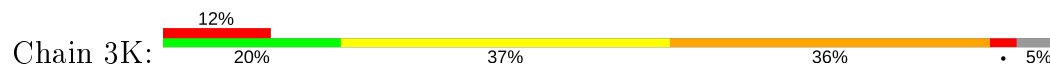
• Molecule 23: tRNAfMet



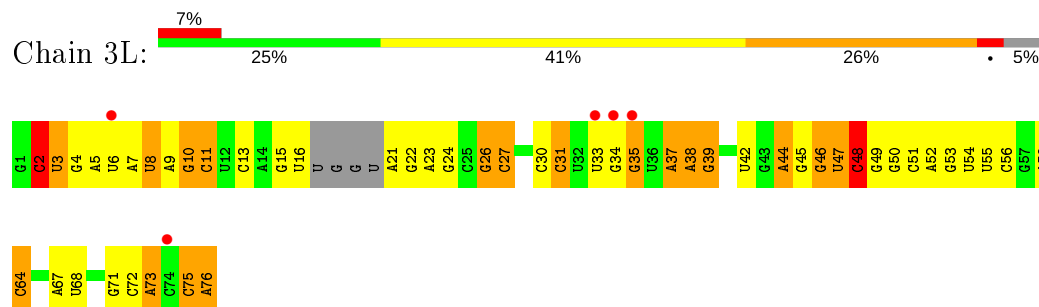
• Molecule 23: tRNAfMet



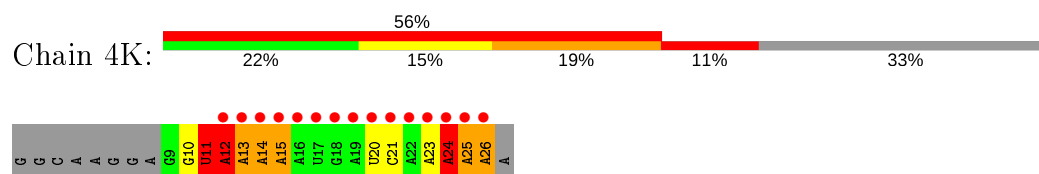
• Molecule 24: tRNAThr



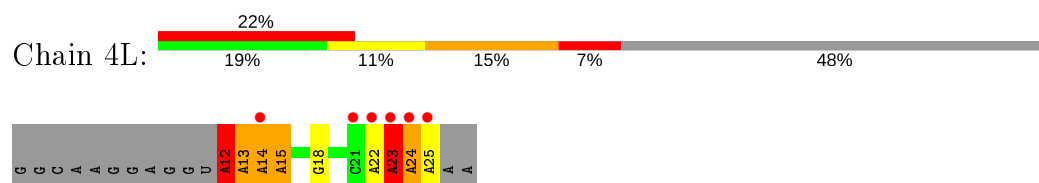
- Molecule 24: tRNA<sup>Thr</sup>



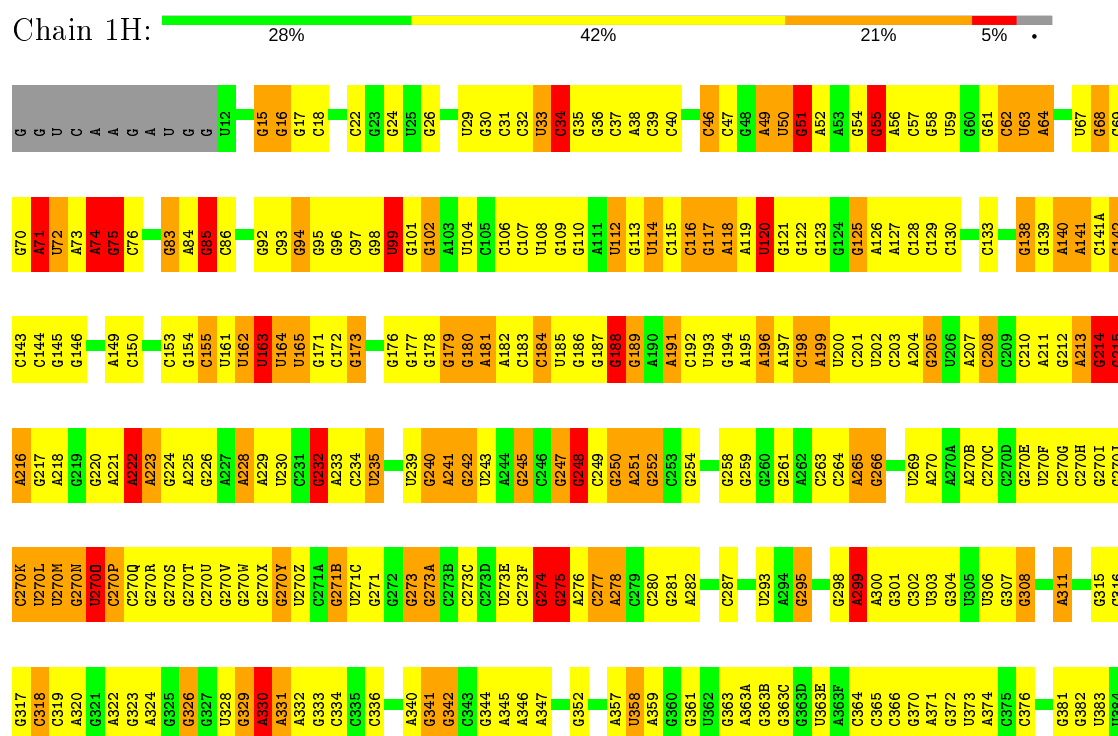
- Molecule 25: mRNA



- Molecule 25: mRNA



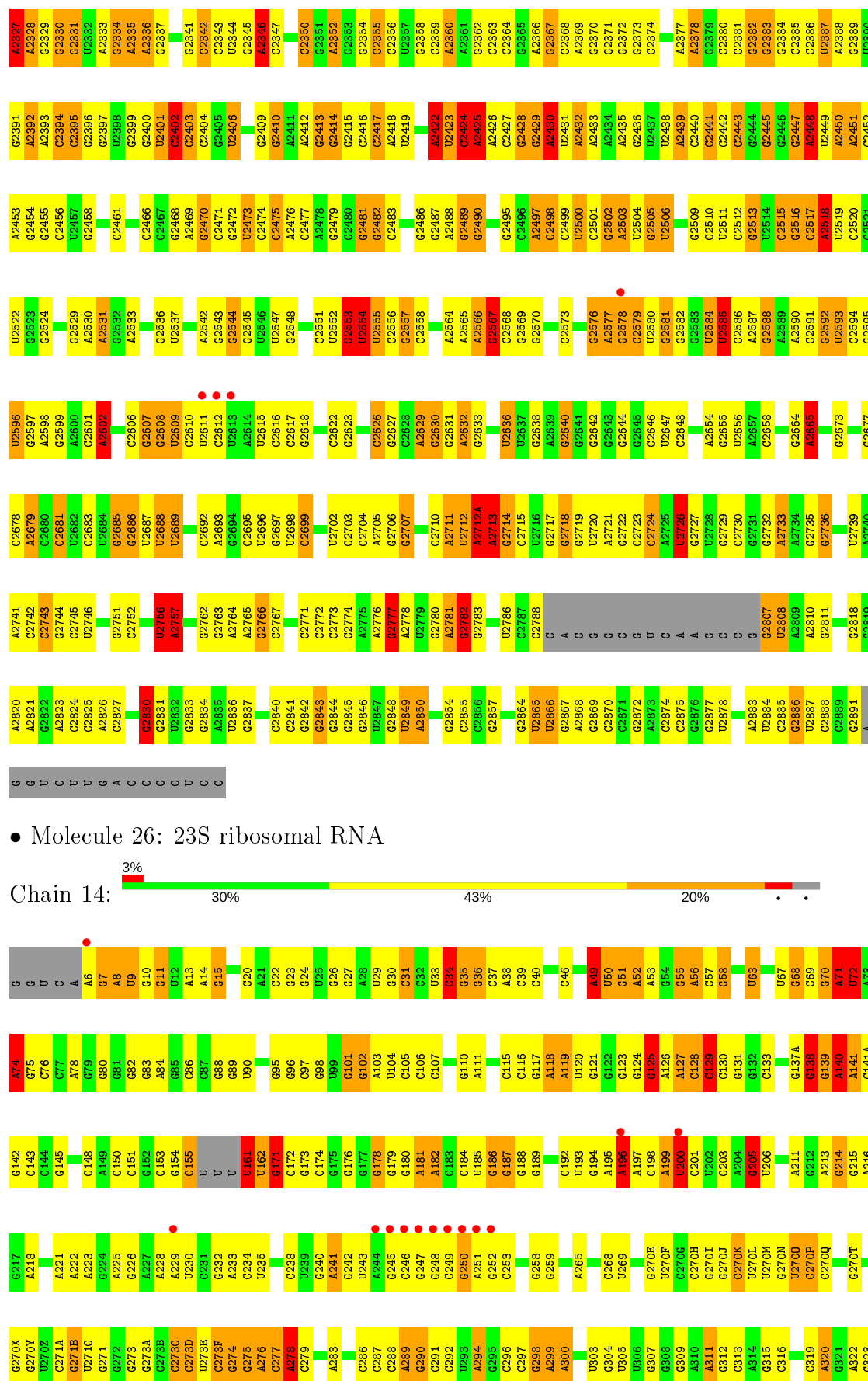
- Molecule 26: 23S ribosomal RNA









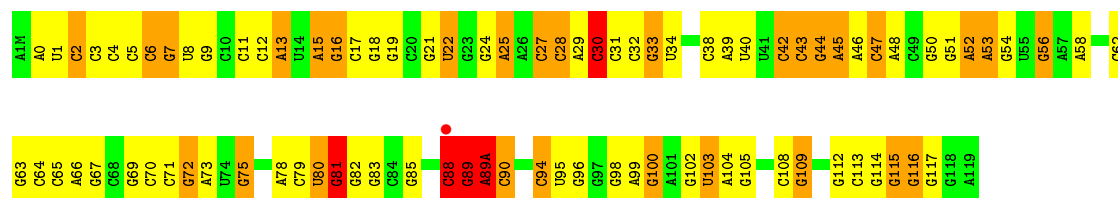


• Molecule 26: 23S ribosomal RNA

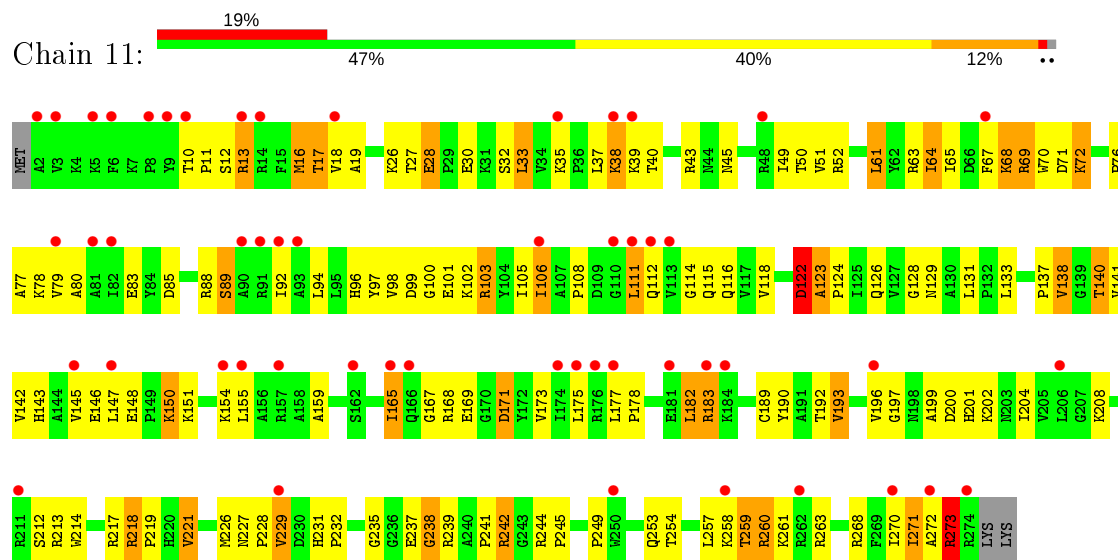


G2115	G2116	A2042	A1970	C1902	A1819	C1754	G1667	A1603	G1538	G1473	G1441	G1344	U1273
G2116	G2117	C2043	A1971	C1905	U1820	A1755	A1683	C1604	G1539	C1474	A1412	C1345	A1274
A2118	A1972	G1906	G1973	G1906	A1821	G1756	A1669	C1605	G1540	G1476	G1413	G1346	G1277
A2119	C1974	G1975	C1974	C1909	A1825	A1759	C1670	C1606	G1542	A1477	G1416	G1348	A1278
C2120	U1976	G2082	U1976	G1910	G1826	A1760	G1672	A1609	C1544	U1482	G1418	C1349	G1279
G2124	G2053	G2053	A1981	A1913	G1828	A1762	U1673	C1611	A1545	G1483	A1419	C1350	G1280
G2125	A2054	C2055	A1982	C1914	A1829	G1763	A1674	C1612	A1546	G1484	G1422	U1282	U1281
A2126	C2056	G2056	A1983	U1915	G1830	A1676	A1675	G1613	C1547	A1486	G1421	A1283	A1284
G2127	A2057	A2057	G1831	G1916	G1832	A1677	A1678	G1614	C1548	G1487	G1423	G1285	G1286
C2128	A2058	G2058	U1917	U1917	U1833	A1678	A1679	C1615	U1549	G1488	G1424	G1356	A1287
C2129	A2059	A2059	A1918	A1918	U1833	G1769	U1679	A1616	A1553	U1489	G1425	U1357	U1288
U2130	A2060	G2060	A1919	A1919	U1833	G1770	U1680	C1617	A1554	A1490	G1426	G1358	G1291
G2131	G2061	C2061	C1920	C1920	C1836	G1771	G1681	A1618	G1555	A1491	A1427	A1359	A1360
U2132	C2062	A2062	A1990	U1923	G1839	A1773	C1683	G1619	A1558	G1492	G1428	G1361	G1292
A2133	C2063	G2063	U1991	G1924	G1840	C1774	C1684	U1621	G1559	A1494	U1430	C1293	C1293
A2134	C2064	C2064	G1982	G1925	U1841	U1775	C1685	G1622	G1560	A1495	U1431	G1364	G1297
A2135	G1983	G1983	U1993	C1926	U1842	U1776	C1686	G1623	G1561	A1496	U1432	A1367	G1298
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C2147	A2077	A2077	C2008	A1937	A1854	A1788	G1703	G1635	A1575	A1510	G1445	G1380	U1313
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G2152	C2081	C2081	G2011	C1941	G1858	A1791	G1707	U1638	A1579	U1516	G1491	A1384	A1321
G2153	A2012	A2012	G2012	C1942	A1859	U1794	C1712	U1639	A1580	G1517	G1492	G1385	A1322
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G2155	C2085	U2086	U2016	U1946	U1864	U1796	G1726	G1642	A1582	G1519	U1455	G1388	G1325
G2156	G2087	G2087	G2016	C1947	G1869	C1797	U1727	G1643	A1583	U1520	G1456	G1389	U1326
G2157	G2087	G2087	U2016	G1948	C1870	U1798	G1728	C1644	G1585	G1521	A1457	U1327	C1327
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G2159	G2087	G2087	A2019	G1949	A1872	G1800	A1730	C1648	A1587	G1523	G1459	U1394	U1329
C2160	U2096	C2097	A2020	G1950	G1878	G1801	U1731	G1651	A1588	G1524	G1460	A1395	U1330
C2161	C2097	U2098	C2021	U1951	G1879	A1802	G1732	A1652	A1589	G1525	C1462	U1396	A1331
G2162	U2098	U2098	G2022	A1952	G1880	C1879	A1733	G1653	G1590	G1526	G1463	U1397	G1332
C2164	G2100	G2100	G2023	U1955	C1881	U1905	A1734	A1654	A1591	G1527	C1464	C1403	G1337
G2165	G2104	G2104	G2027	U1956	G1882	G1806	C1735	C1657	A1592	G1528	G1465	C1404	G1338
U2166	C2105	C2105	U2028	G1957	G1883	G1807	C1736	G1658	A1593	G1529	G1466	A1405	G1339
U2167	G2106	G2106	G2029	C1958	A1884	U1908	C1737	A1661	G1594	A1530	G1467	U1406	U1340
A	C2107	C2107	A2031	C1961	C1885	A1809	C1738	G1662	A1595	G1531	C1468	U1407	U1341
G2170	G2107	G2107	G2032	C1962	C1886	A1810	C1742	C1663	A1596	G1532	G1469	C1408	G1342
U2171	C2108	C2108	A2033	U1963	C1887	G1811	C1743	A1664	A1597	G1533	G1470	U1336	G1343
U2172	G2109	G2109	G2034	U1964	A1889	G1814	C1744	C1665	A1598	G1534	A1471	C1409	
A2173	G2110	G2110	G2035	G1964	A1899	A1815	U1748	G1661	C1599	G1535	A1472	G1410	
C2174	G2111	G2111	G2036	C1967	G1899	A1816	A1749	C1662	A1599	G1536			
G2175	U2113	U2113	G2037	G1967	A1900	G1817	C1751	C1663	C1600	U1537			
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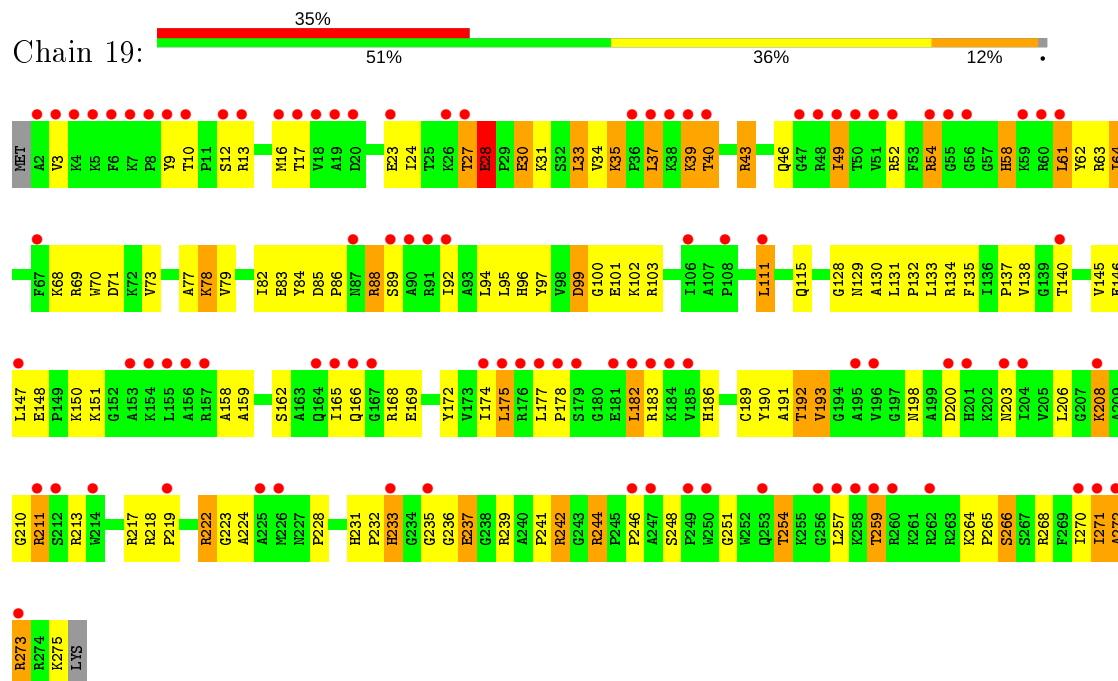




• Molecule 28: 50S ribosomal protein L2

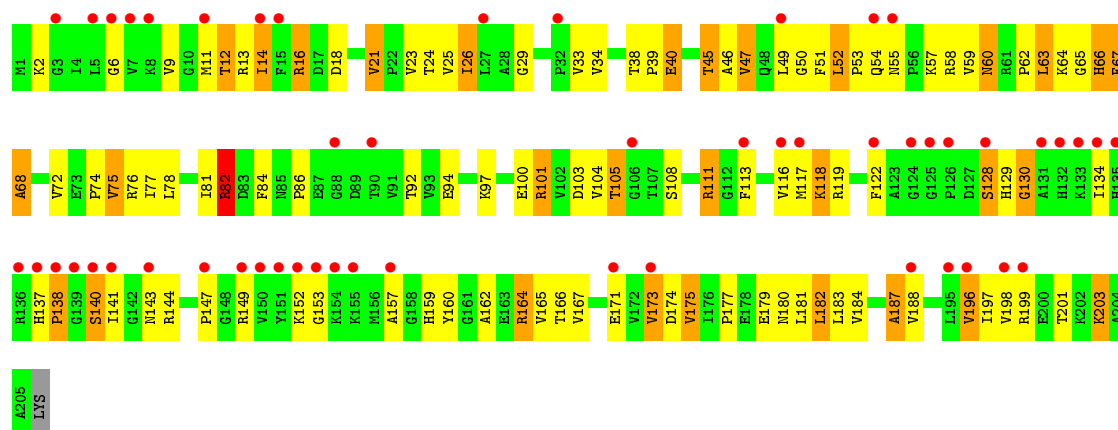


• Molecule 28: 50S ribosomal protein L2

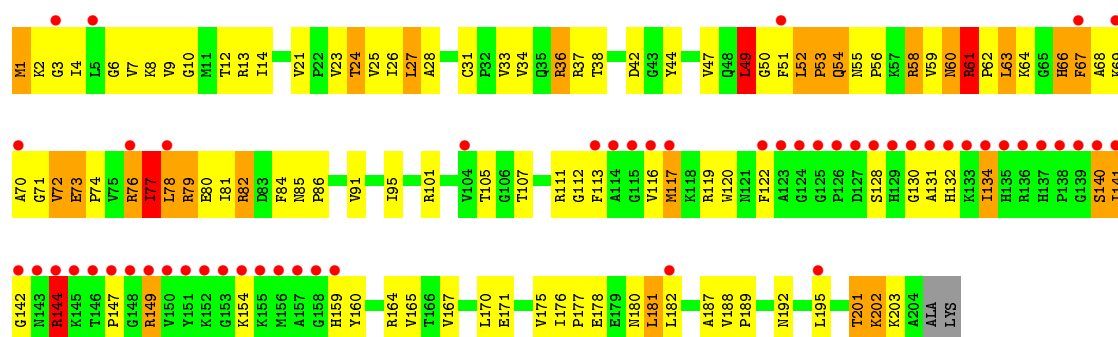


• Molecule 29: 50S ribosomal protein L3

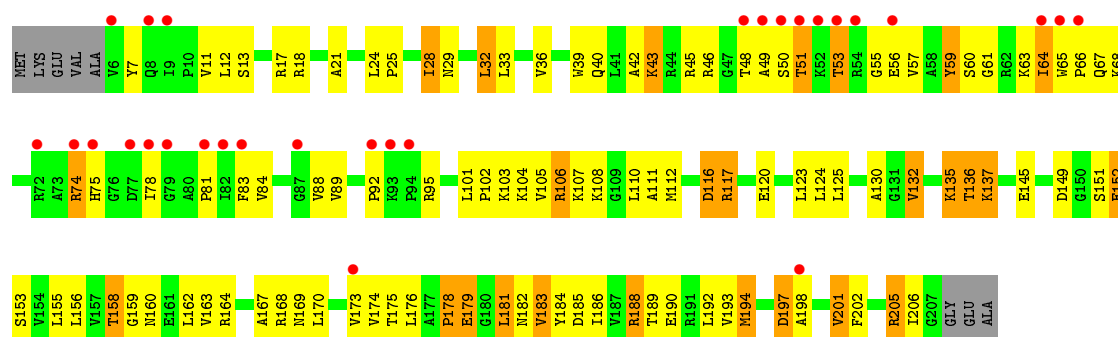
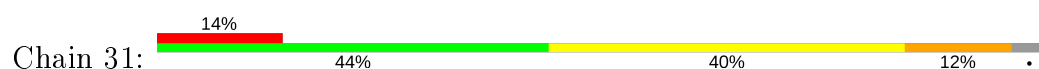




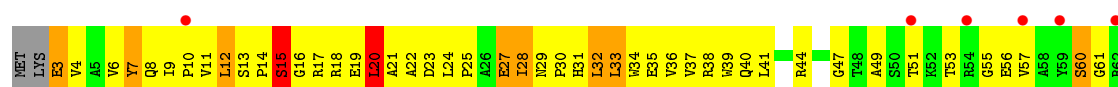
• Molecule 29: 50S ribosomal protein L3

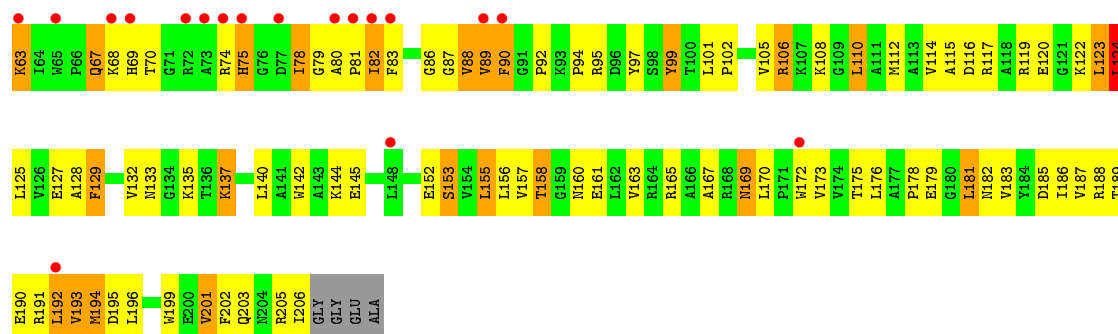


• Molecule 30: 50S ribosomal protein L4

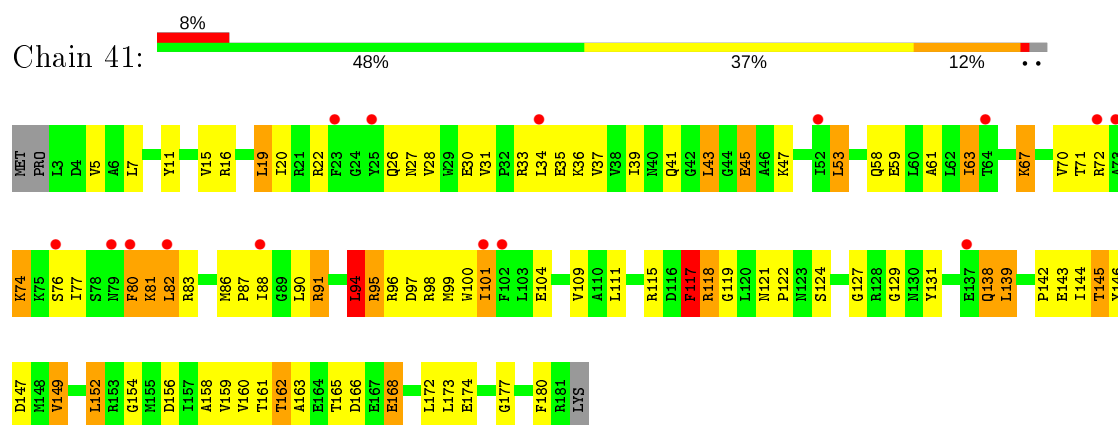


• Molecule 30: 50S ribosomal protein L4

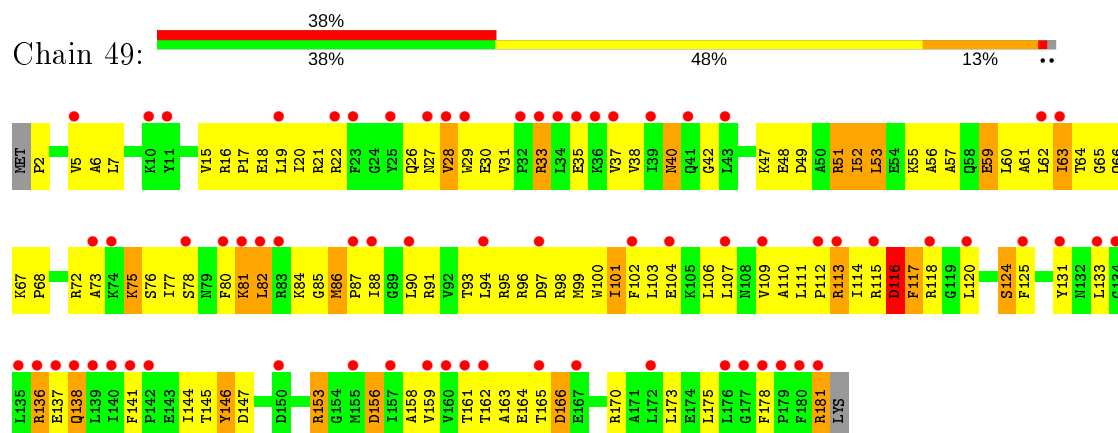




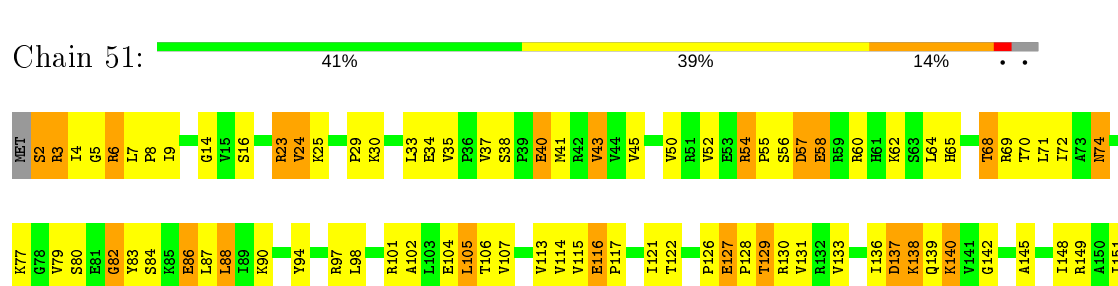
• Molecule 31: 50S ribosomal protein L5



• Molecule 31: 50S ribosomal protein L5



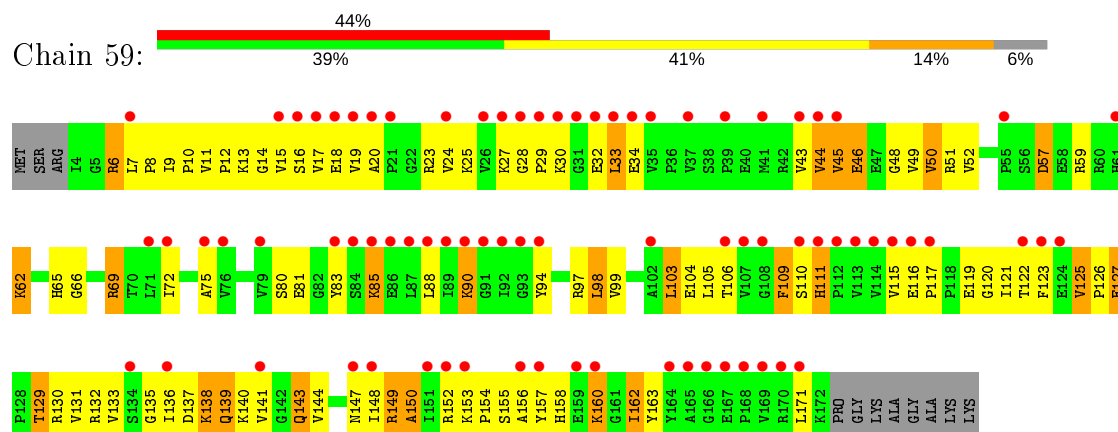
• Molecule 32: 50S ribosomal protein L6



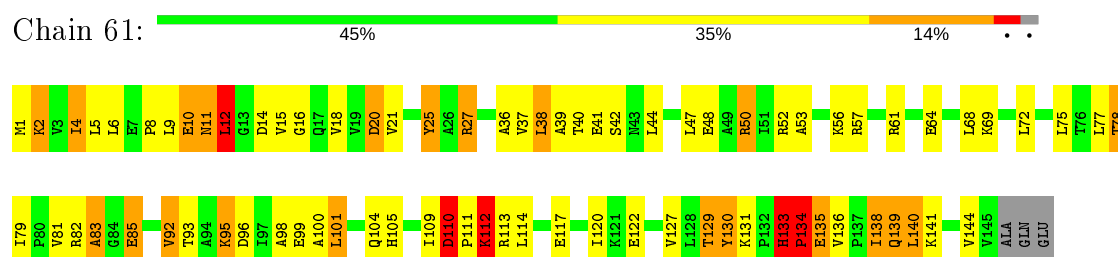




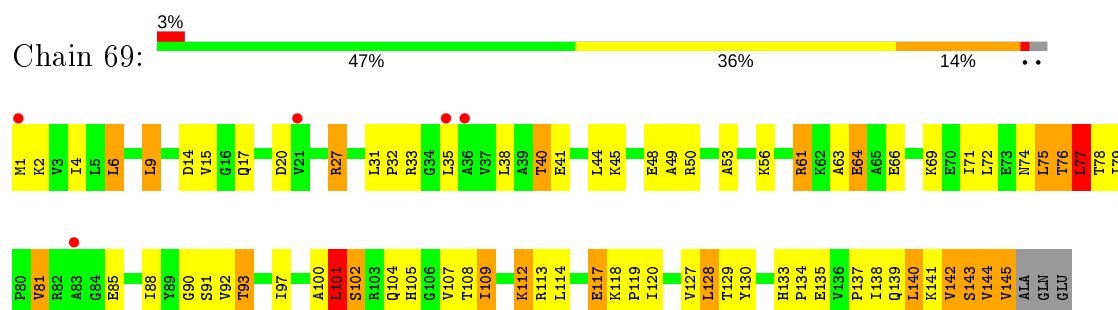
- Molecule 32: 50S ribosomal protein L6



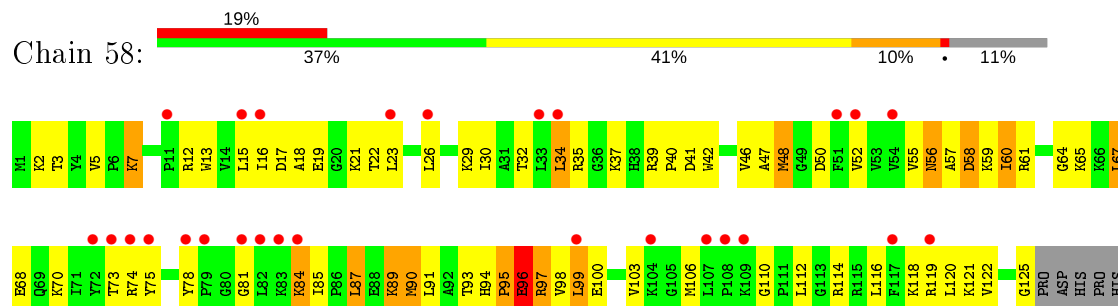
- Molecule 33: 50S ribosomal protein L9



- Molecule 33: 50S ribosomal protein L9

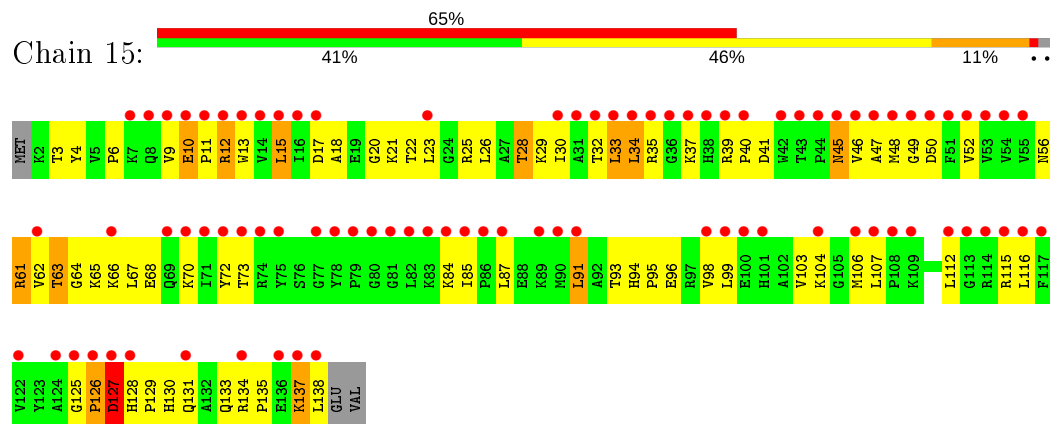


- Molecule 34: 50S ribosomal protein L13

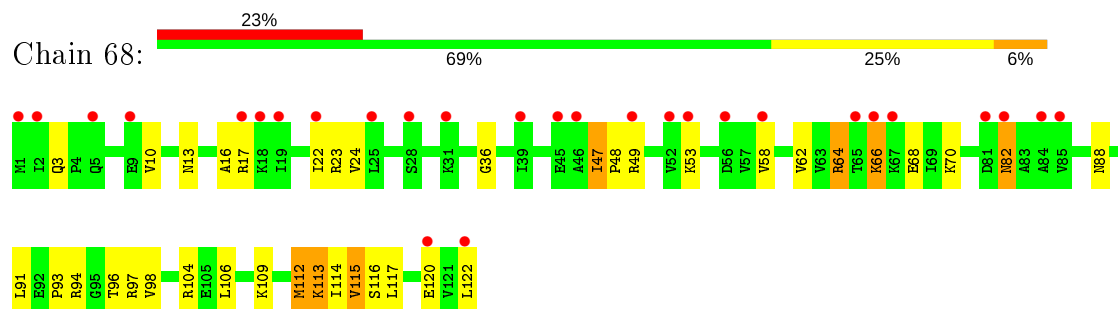


GLN  
ALA  
GLN  
ARG  
PRO  
GLU  
LYS  
LEU  
VAL

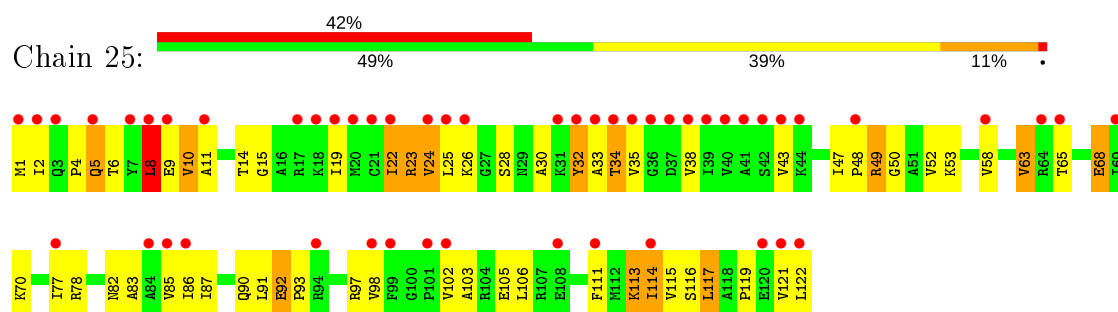
• Molecule 34: 50S ribosomal protein L13



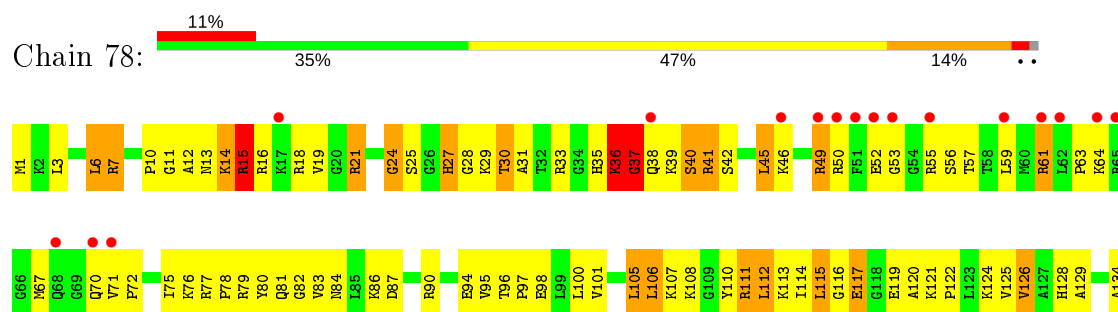
• Molecule 35: 50S ribosomal protein L14



• Molecule 35: 50S ribosomal protein L14

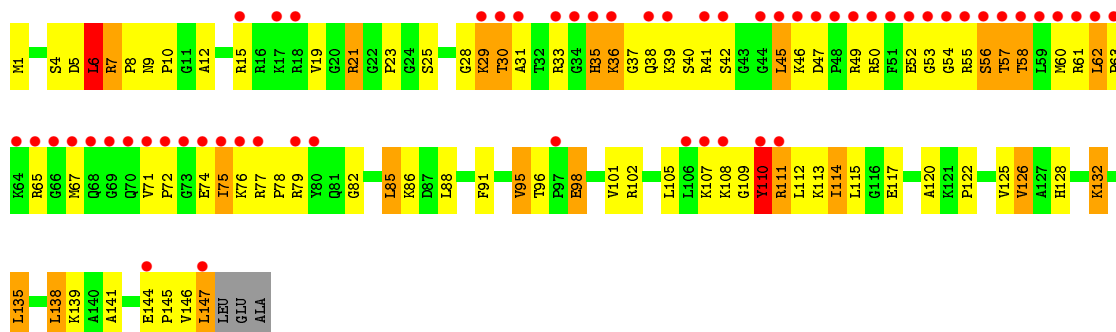


• Molecule 36: 50S ribosomal protein L15

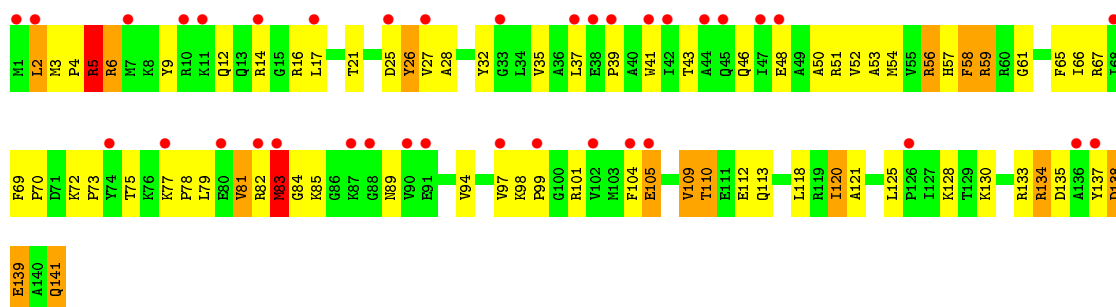




• Molecule 36: 50S ribosomal protein L15



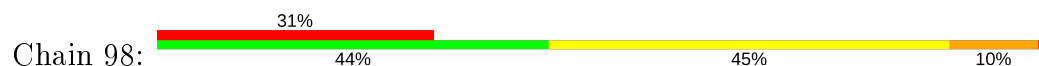
• Molecule 37: 50S ribosomal protein L16

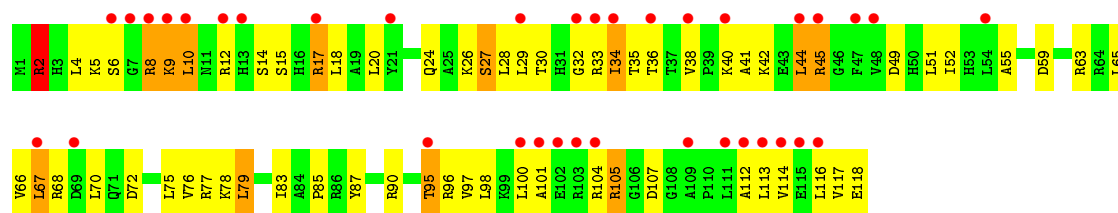


• Molecule 37: 50S ribosomal protein L16

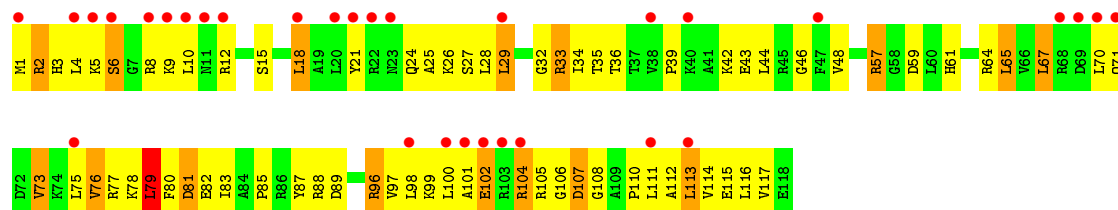


• Molecule 38: 50S ribosomal protein L17

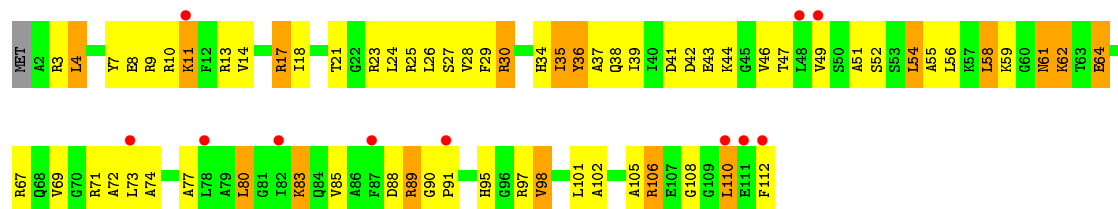
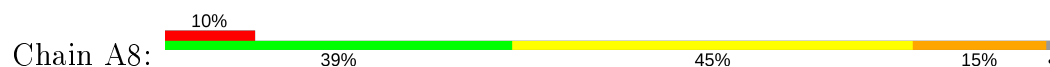




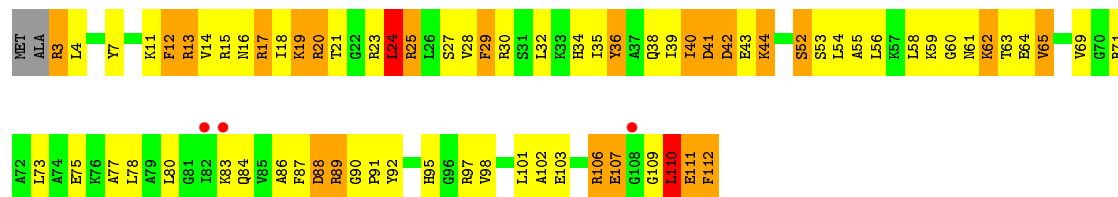
• Molecule 38: 50S ribosomal protein L17



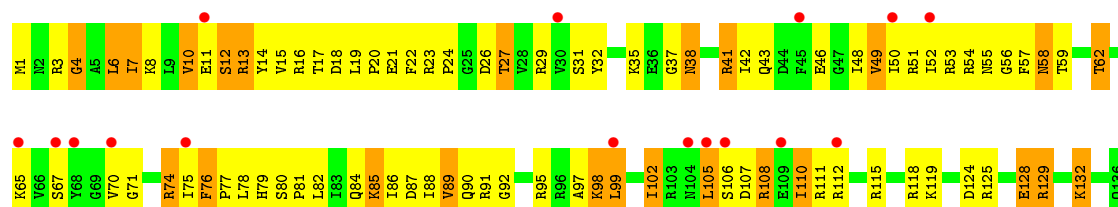
• Molecule 39: 50S ribosomal protein L18



• Molecule 39: 50S ribosomal protein L18

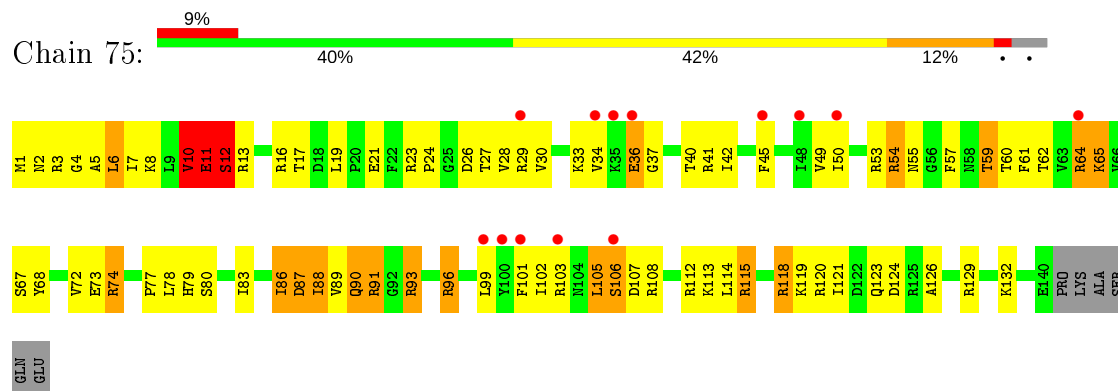


• Molecule 40: 50S ribosomal protein L19

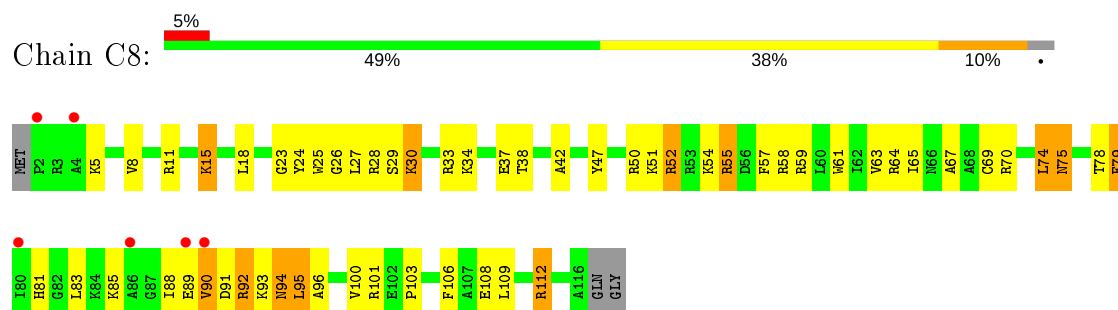


LYS  
ALA  
GLN  
GLU  
PRO  
LYS  
ALA  
SER  
GLN  
GLU

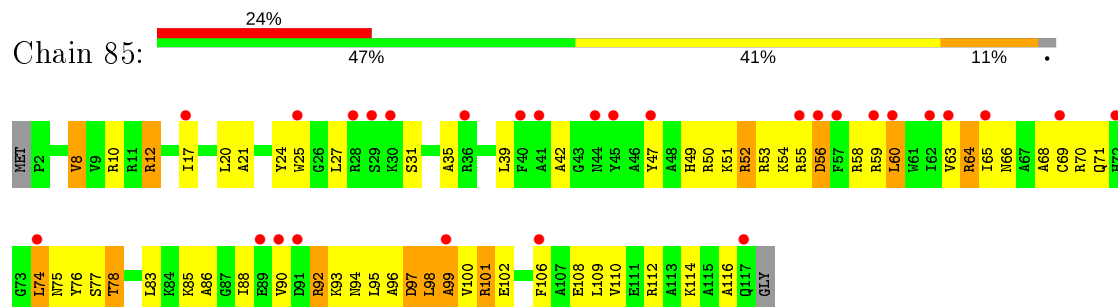
- Molecule 40: 50S ribosomal protein L19



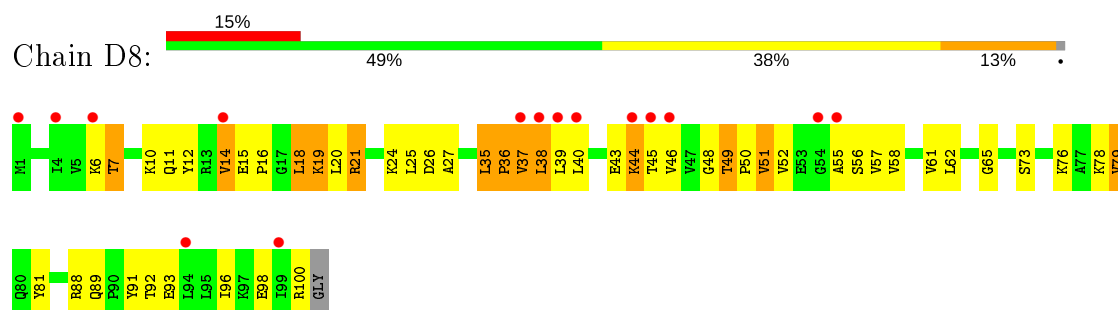
- Molecule 41: 50S ribosomal protein L20



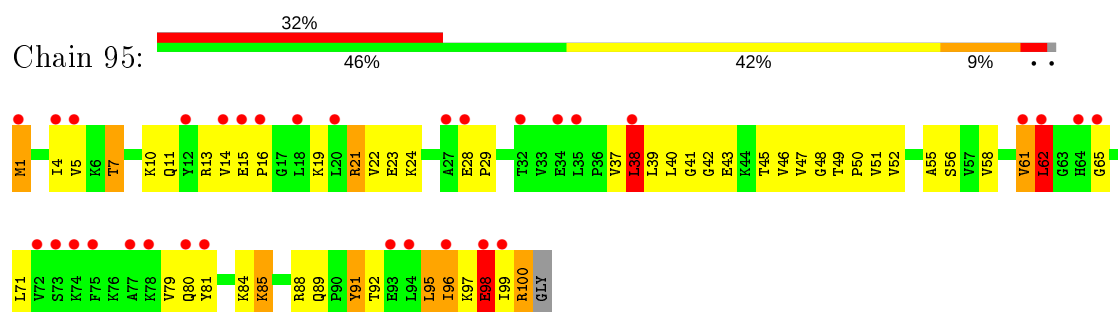
- Molecule 41: 50S ribosomal protein L20



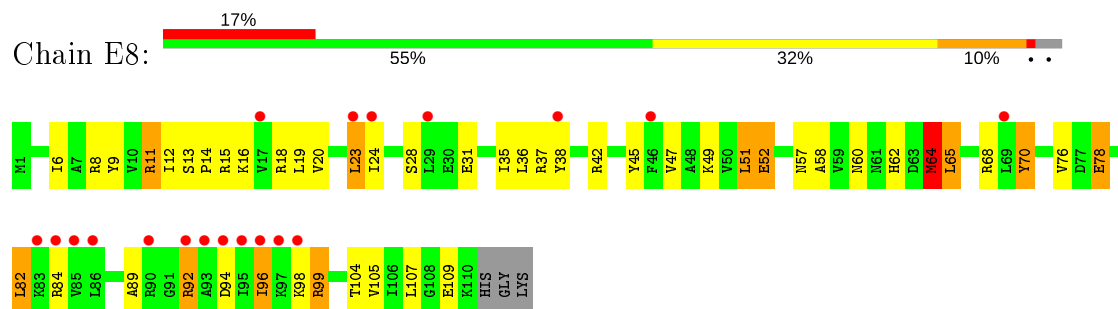
- Molecule 42: 50S ribosomal protein L21



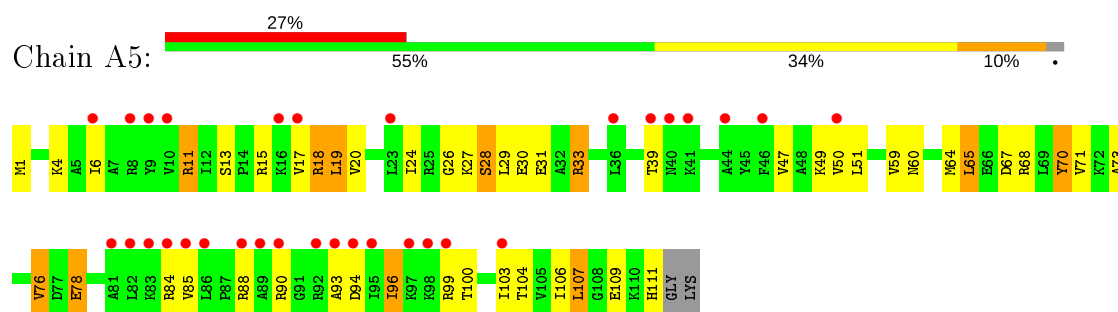
- Molecule 42: 50S ribosomal protein L21



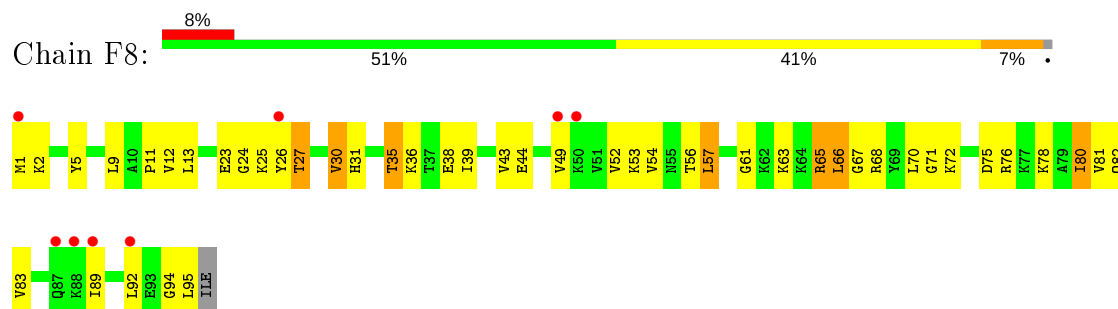
- Molecule 43: 50S ribosomal protein L22



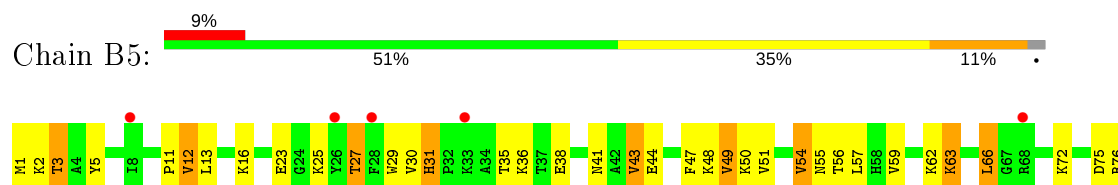
- Molecule 43: 50S ribosomal protein L22

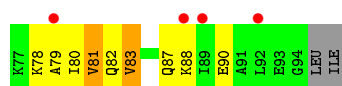


- Molecule 44: 50S ribosomal protein L23



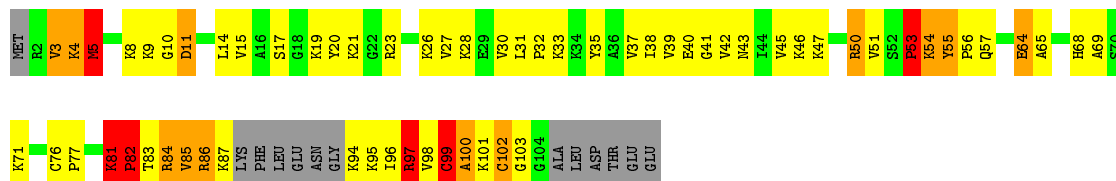
- Molecule 44: 50S ribosomal protein L23





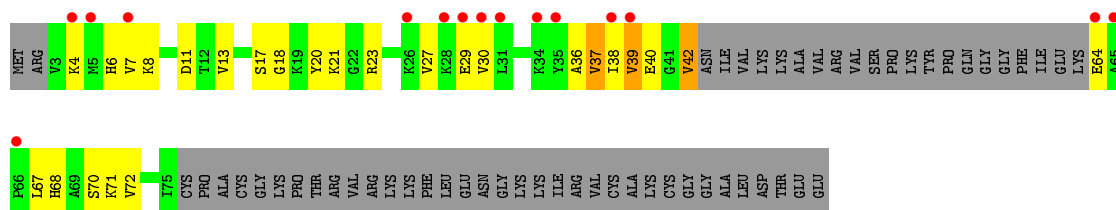
- Molecule 45: 50S ribosomal protein L24

Chain G8: 31% 41% 11% 5% 12%



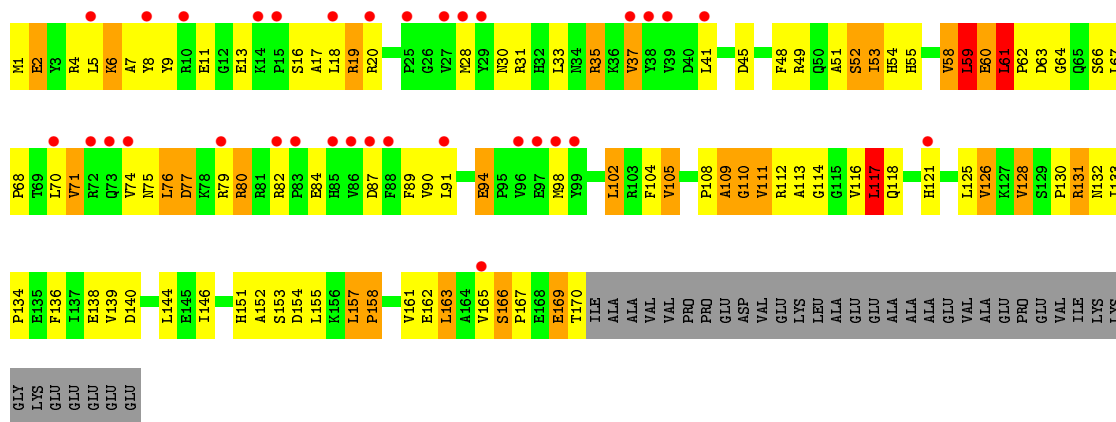
- Molecule 45: 50S ribosomal protein L24

Chain C5: 14% 24% 21% 53%



- Molecule 46: 50S ribosomal protein L25

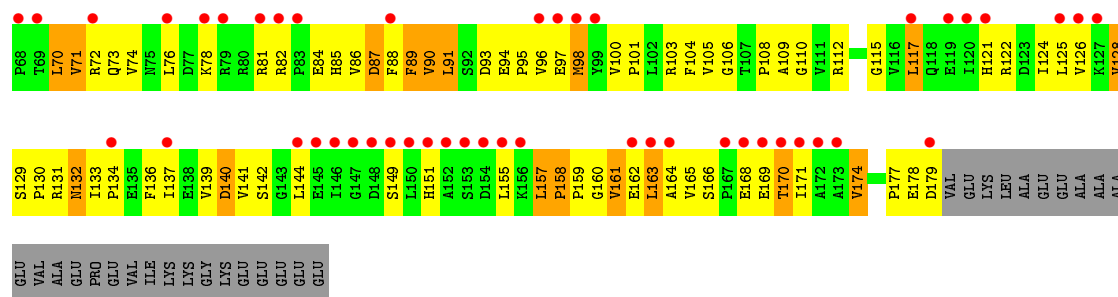
Chain H8: 16% 34% 33% 13% 17%



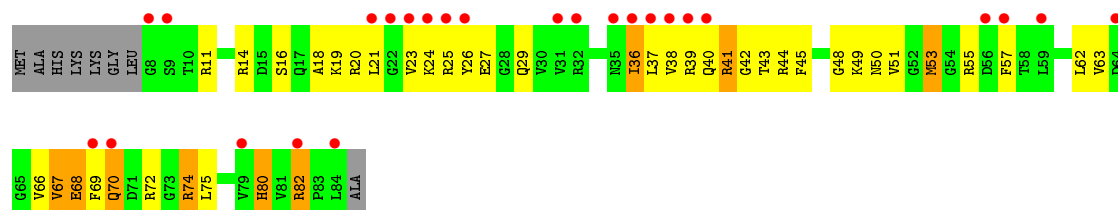
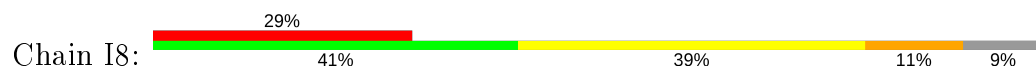
- Molecule 46: 50S ribosomal protein L25

Chain D5: 34% 31% 40% 14% 14%

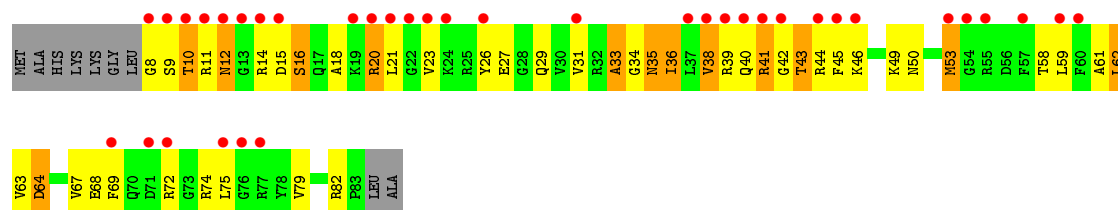




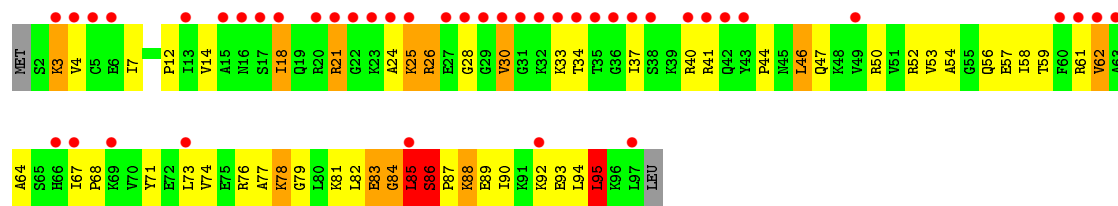
• Molecule 47: 50S ribosomal protein L27



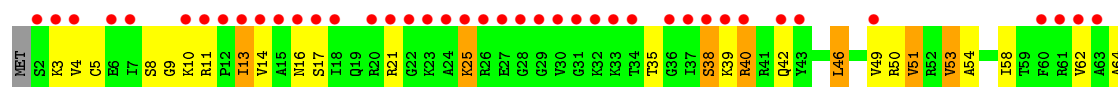
• Molecule 47: 50S ribosomal protein L27



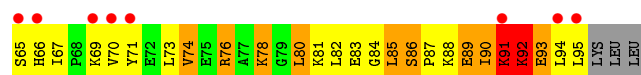
• Molecule 48: 50S ribosomal protein L28



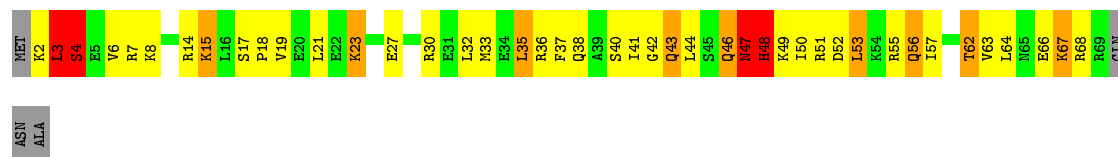
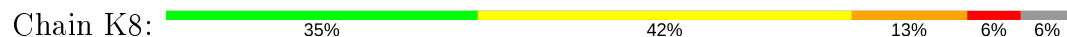
• Molecule 48: 50S ribosomal protein L28







- Molecule 49: 50S ribosomal protein L29



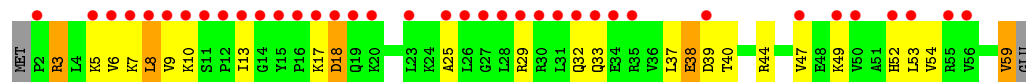
- Molecule 49: 50S ribosomal protein L29



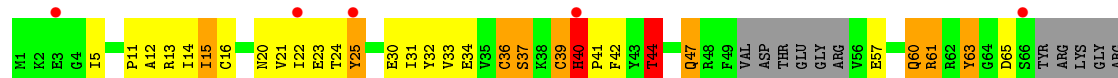
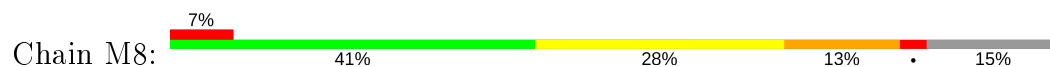
- Molecule 50: 50S ribosomal protein L30



- Molecule 50: 50S ribosomal protein L30



- Molecule 51: 50S ribosomal protein L31



- Molecule 52: 50S ribosomal protein L32





- Molecule 52: 50S ribosomal protein L32



- Molecule 53: 50S ribosomal protein L34



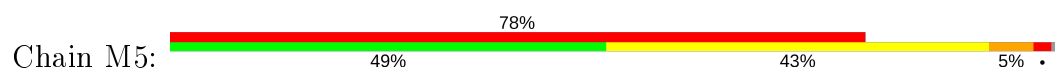
- Molecule 53: 50S ribosomal protein L34



- Molecule 54: 50S ribosomal protein L35



- Molecule 54: 50S ribosomal protein L35



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	209.82Å 449.75Å 618.71Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	224.88 – 3.36 309.36 – 3.36	Depositor EDS
% Data completeness (in resolution range)	99.9 (224.88-3.36) 91.0 (309.36-3.36)	Depositor EDS
$R_{merge}$	0.36	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	0.88 (at 3.33Å)	Xtriage
Refinement program	PHENIX 1.12 _2829	Depositor
R, $R_{free}$	0.200 , 0.264 0.200 , 0.264	Depositor DCC
$R_{free}$ test set	1998 reflections (0.24%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	101.0	Xtriage
Anisotropy	0.195	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.25 , 75.7	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.46$ , $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.88	EDS
Total number of atoms	292640	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	120.0	wwPDB-VP

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

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

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

## 5 Model quality ⓘ

### 5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: 5MU, ZN, AET, H2U, SF4, MG, 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	0.73	4/36095 (0.0%)	1.32	286/56332 (0.5%)
1	1G	0.74	5/35850 (0.0%)	1.34	316/55949 (0.6%)
2	12	0.37	0/1727	0.60	1/2326 (0.0%)
2	1E	0.38	0/1908	0.58	1/2573 (0.0%)
3	22	0.38	0/1569	0.63	1/2116 (0.0%)
3	2E	0.42	0/1629	0.62	0/2195
4	32	0.41	0/1732	0.64	0/2318
4	3E	0.44	0/1728	0.61	1/2313 (0.0%)
5	42	0.42	0/1156	0.58	0/1557
5	4E	0.43	0/1158	0.64	0/1559
6	52	0.47	0/855	0.60	0/1154
6	5E	0.42	0/850	0.59	0/1147
7	62	0.40	0/1122	0.58	0/1500
7	6E	0.42	0/1259	0.55	0/1686
8	72	0.36	0/1127	0.58	0/1517
8	7E	0.40	0/1135	0.62	0/1527
9	82	0.35	0/971	0.59	0/1304
9	8E	0.41	0/1019	0.63	0/1367
10	1A	0.32	0/814	0.57	0/1095
10	1I	0.38	0/762	0.60	0/1027
11	2A	0.43	0/850	0.58	0/1150
11	2I	0.45	0/838	0.68	0/1133
12	3A	0.46	0/972	0.68	0/1301
12	3I	0.52	0/972	0.73	0/1301
13	4A	0.37	0/889	0.71	1/1192 (0.1%)
13	4I	0.47	0/952	0.70	0/1277
14	5A	0.42	0/495	0.64	0/657
14	5I	0.53	0/500	0.70	1/664 (0.2%)
15	6A	0.41	0/740	0.57	0/987
15	6I	0.41	0/740	0.58	0/987
16	7A	0.41	0/721	0.68	0/970
16	7I	0.43	0/716	0.60	0/963

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
17	8A	0.49	0/836	0.62	0/1117
17	8I	0.46	0/847	0.63	0/1131
18	9A	0.44	0/559	0.67	1/746 (0.1%)
18	9I	0.43	0/554	0.60	0/739
19	AA	0.41	0/520	0.74	0/700
19	AI	0.44	0/676	0.70	0/910
20	BA	0.37	0/764	0.57	0/1007
20	BI	0.38	0/748	0.62	1/986 (0.1%)
21	1B	0.32	0/192	0.57	0/252
21	1F	0.40	0/203	0.57	0/266
22	1K	0.59	0/1675	1.31	16/2608 (0.6%)
22	1L	0.50	0/1675	1.10	5/2608 (0.2%)
23	2K	0.77	0/1791	1.35	13/2791 (0.5%)
23	2L	0.68	0/1791	1.30	12/2791 (0.4%)
24	3K	0.59	0/1716	1.22	7/2668 (0.3%)
24	3L	0.53	0/1716	1.20	9/2668 (0.3%)
25	4K	0.96	1/440 (0.2%)	1.40	5/684 (0.7%)
25	4L	0.90	0/341	1.59	4/529 (0.8%)
26	14	0.91	46/67828 (0.1%)	1.54	1168/105880 (1.1%)
26	1H	1.07	92/67804 (0.1%)	1.69	1740/105829 (1.6%)
27	16	0.82	1/2928 (0.0%)	1.57	51/4568 (1.1%)
27	1J	0.67	1/2928 (0.0%)	1.34	26/4568 (0.6%)
28	11	0.60	0/2170	0.81	3/2926 (0.1%)
28	19	0.66	3/2175 (0.1%)	0.77	1/2933 (0.0%)
29	21	0.56	0/1589	0.82	0/2145
29	29	0.51	0/1596	0.78	2/2153 (0.1%)
30	31	0.62	0/1620	0.76	1/2194 (0.0%)
30	39	0.50	0/1637	0.71	1/2218 (0.0%)
31	41	0.46	0/1481	0.70	2/1994 (0.1%)
31	49	0.41	0/1483	0.63	1/1997 (0.1%)
32	51	0.48	0/1354	0.84	2/1833 (0.1%)
32	59	0.38	0/1320	0.67	0/1787
33	61	0.43	0/1146	0.77	4/1551 (0.3%)
33	69	0.41	0/1146	0.69	0/1551
34	15	0.43	0/1123	0.64	0/1515
34	58	0.55	0/1017	0.74	0/1369
35	25	0.53	0/942	0.72	1/1269 (0.1%)
35	68	0.56	0/942	0.69	0/1269
36	35	0.54	0/1139	0.81	1/1514 (0.1%)
36	78	0.60	0/1144	0.93	2/1521 (0.1%)
37	45	0.52	0/1120	0.78	0/1498
37	88	0.60	0/1138	0.83	0/1523
38	55	0.45	0/981	0.74	1/1312 (0.1%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
38	98	0.51	0/981	0.74	1/1312 (0.1%)
39	65	0.43	0/886	0.71	2/1180 (0.2%)
39	A8	0.51	0/891	0.73	0/1187
40	75	0.60	1/1178 (0.1%)	0.71	1/1573 (0.1%)
40	B8	0.51	0/1142	0.74	1/1526 (0.1%)
41	85	0.50	0/977	0.69	0/1301
41	C8	0.59	0/968	0.74	1/1289 (0.1%)
42	95	0.46	0/781	0.80	2/1048 (0.2%)
42	D8	0.56	0/785	0.81	2/1052 (0.2%)
43	A5	0.51	0/897	0.69	0/1204
43	E8	0.61	0/886	0.75	1/1189 (0.1%)
44	B5	0.54	0/749	0.70	0/1007
44	F8	0.64	0/764	0.76	0/1025
45	C5	0.60	0/401	0.74	0/535
45	G8	0.65	0/745	0.89	2/993 (0.2%)
46	D5	0.40	0/1443	0.69	2/1960 (0.1%)
46	H8	0.44	0/1395	0.76	1/1890 (0.1%)
47	E5	0.50	0/611	0.77	0/814
47	I8	0.70	1/619 (0.2%)	0.81	0/825
48	F5	0.56	0/744	0.81	0/989
48	J8	0.62	0/754	0.91	2/1003 (0.2%)
49	G5	0.52	0/578	0.73	1/766 (0.1%)
49	K8	0.64	0/577	0.89	2/763 (0.3%)
50	H5	0.45	0/464	0.62	0/623
50	L8	0.51	0/464	0.77	0/623
51	M8	0.53	0/485	0.78	0/652
52	J5	0.52	0/448	0.71	0/606
52	N8	0.59	0/381	0.71	0/516
53	L5	0.56	0/414	0.75	0/547
53	P8	0.70	0/409	0.84	1/540 (0.2%)
54	M5	0.64	1/524 (0.2%)	0.83	0/691
54	Q8	0.61	0/524	0.84	1/691 (0.1%)
All	All	0.80	156/314511 (0.0%)	1.35	3711/471182 (0.8%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
2	12	0	5
2	1E	0	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
3	2E	0	1
4	32	0	1
4	3E	0	2
5	4E	0	1
9	82	0	1
9	8E	0	3
10	1A	0	1
10	1I	0	1
11	2A	0	1
11	2I	0	2
12	3A	0	4
12	3I	0	2
13	4A	0	6
13	4I	0	3
14	5A	0	1
18	9A	0	1
19	AA	0	4
19	AI	0	1
20	BA	0	1
20	BI	0	1
28	11	0	4
28	19	0	2
29	21	0	7
29	29	0	10
30	31	0	1
30	39	0	4
31	41	0	1
31	49	0	1
32	51	0	5
32	59	0	1
33	61	0	5
33	69	0	5
34	15	0	1
34	58	0	2
35	68	0	1
36	35	0	3
36	78	0	9
37	45	0	5
37	88	0	3
38	98	0	2
39	65	0	1
39	A8	0	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
40	75	0	2
40	B8	0	2
41	85	0	2
41	C8	0	4
42	95	0	4
42	D8	0	2
43	E8	0	1
44	B5	0	1
45	C5	0	2
45	G8	0	7
46	D5	0	5
46	H8	0	7
47	I8	0	1
48	F5	0	3
48	J8	0	2
49	G5	0	4
49	K8	0	4
51	M8	0	4
52	N8	0	1
54	M5	0	2
54	Q8	0	2
All	All	0	180

The worst 5 of 156 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
40	75	106	SER	CA-CB	11.86	1.70	1.52
26	14	2593	U	C4-O4	11.75	1.33	1.23
26	1H	676	A	N9-C4	-10.05	1.31	1.37
26	1H	774	A	N9-C4	-10.02	1.31	1.37
26	1H	783	A	N7-C5	-8.90	1.33	1.39

The worst 5 of 3711 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	1H	1899	G	N3-C4-N9	-20.44	113.73	126.00
26	1H	1962	C	N1-C2-O2	17.31	129.29	118.90
26	1H	774	A	C2-N3-C4	-16.57	102.32	110.60
26	1H	34	C	O5'-P-OP1	-15.77	91.51	105.70
26	1H	1899	G	N9-C4-C5	15.75	111.70	105.40

There are no chirality outliers.



5 of 180 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	1E	210	SER	Peptide
3	2E	14	ILE	Peptide
4	3E	155	LEU	Peptide
4	3E	29	PRO	Peptide
5	4E	114	GLY	Peptide

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

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	13	32246	0	16277	909	0
1	1G	32028	0	16164	936	0
2	12	1696	0	1730	80	0
2	1E	1874	0	1926	92	0
3	22	1546	0	1608	104	0
3	2E	1605	0	1668	59	0
4	32	1702	0	1765	95	0
4	3E	1698	0	1761	78	0
5	42	1141	0	1198	66	0
5	4E	1142	0	1204	43	0
6	52	842	0	857	23	0
6	5E	837	0	852	33	0
7	62	1110	0	1163	67	0
7	6E	1242	0	1286	65	0
8	72	1107	0	1165	69	0
8	7E	1115	0	1177	53	0
9	82	953	0	983	59	0
9	8E	1000	0	1031	73	0
10	1A	801	0	849	52	0
10	1I	749	0	767	54	0
11	2A	835	0	847	33	0
11	2I	823	0	833	42	0
12	3A	956	0	1046	48	0
12	3I	956	0	1046	47	0
13	4A	879	0	935	81	0
13	4I	942	0	997	60	0
14	5A	486	0	525	25	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
14	5I	491	0	530	28	0
15	6A	729	0	768	35	0
15	6I	729	0	768	41	0
16	7A	705	0	725	34	0
16	7I	700	0	720	43	0
17	8A	823	0	891	37	0
17	8I	834	0	904	53	0
18	9A	554	0	609	22	0
18	9I	549	0	607	28	0
19	AA	510	0	507	36	0
19	AI	661	0	683	42	0
20	BA	762	0	861	34	0
20	BI	746	0	843	56	0
21	1B	188	0	195	9	0
21	1F	199	0	208	10	0
22	1K	1593	0	813	52	0
22	1L	1593	0	813	28	0
23	2K	1644	0	838	34	0
23	2L	1644	0	838	32	0
24	3K	1537	0	779	55	0
24	3L	1537	0	779	32	0
25	4K	391	0	196	12	0
25	4L	303	0	153	10	0
26	14	60561	0	30528	1446	0
26	1H	60546	0	30528	1548	0
27	16	2617	0	1328	57	0
27	1J	2617	0	1328	89	0
28	11	2120	0	2197	108	0
28	19	2125	0	2199	115	0
29	21	1556	0	1612	90	0
29	29	1563	0	1629	94	0
30	31	1585	0	1632	88	0
30	39	1602	0	1649	119	0
31	41	1457	0	1514	76	0
31	49	1459	0	1507	91	0
32	51	1328	0	1396	69	0
32	59	1295	0	1366	85	0
33	61	1131	0	1218	49	0
33	69	1131	0	1218	56	0
34	15	1096	0	1168	69	0
34	58	995	0	1077	61	0
35	25	932	0	996	45	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
35	68	932	0	996	21	0
36	35	1122	0	1206	84	0
36	78	1127	0	1208	87	0
37	45	1099	0	1154	77	0
37	88	1117	0	1168	79	0
38	55	967	0	1033	56	0
38	98	967	0	1033	42	0
39	65	876	0	938	74	0
39	A8	881	0	943	53	0
40	75	1164	0	1221	69	0
40	B8	1128	0	1183	78	0
41	85	959	0	1019	61	0
41	C8	950	0	1011	58	0
42	95	770	0	838	43	0
42	D8	774	0	849	32	0
43	A5	886	0	948	33	0
43	E8	876	0	941	35	0
44	B5	735	0	785	33	0
44	F8	750	0	814	30	0
45	C5	396	0	444	15	0
45	G8	734	0	820	48	0
46	D5	1411	0	1436	92	0
46	H8	1365	0	1391	77	0
47	E5	603	0	620	45	0
47	I8	611	0	631	43	0
48	F5	737	0	813	53	0
48	J8	747	0	817	45	0
49	G5	576	0	625	28	0
49	K8	575	0	634	37	0
50	H5	459	0	512	15	0
50	L8	459	0	512	21	0
51	M8	475	0	465	27	0
52	J5	434	0	454	22	0
52	N8	369	0	388	36	0
53	L5	406	0	438	28	0
53	P8	401	0	436	10	0
54	M5	516	0	582	26	0
54	Q8	516	0	582	38	0
55	11	1	0	0	0	0
55	13	140	0	0	0	0
55	14	300	0	0	0	0
55	16	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
55	1F	2	0	0	0	0
55	1G	126	0	0	0	0
55	1H	473	0	0	0	0
55	1J	2	0	0	0	0
55	21	3	0	0	0	0
55	29	1	0	0	0	0
55	2A	1	0	0	0	0
55	2K	1	0	0	0	0
55	2L	1	0	0	0	0
55	32	1	0	0	0	0
55	35	1	0	0	0	0
55	39	1	0	0	0	0
55	41	1	0	0	0	0
55	42	2	0	0	0	0
55	45	2	0	0	0	0
55	4A	1	0	0	0	0
55	5I	2	0	0	0	0
55	78	2	0	0	0	0
55	7A	1	0	0	0	0
55	85	1	0	0	0	0
55	88	3	0	0	0	0
55	8I	1	0	0	0	0
55	BA	1	0	0	0	0
55	BI	1	0	0	0	0
55	C8	2	0	0	0	0
55	D8	1	0	0	0	0
55	E5	1	0	0	0	0
55	F5	1	0	0	0	0
55	I8	1	0	0	0	0
55	J8	1	0	0	0	0
55	P8	1	0	0	0	0
56	32	8	0	0	2	0
56	3E	8	0	0	1	0
57	5A	1	0	0	0	0
57	5I	1	0	0	0	0
58	11	8	0	0	1	0
58	13	274	0	0	53	0
58	14	586	0	0	117	0
58	16	8	0	0	0	0
58	19	7	0	0	2	0
58	1F	1	0	0	0	0
58	1G	240	0	0	24	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
58	1H	1010	0	0	224	0
58	1I	2	0	0	0	0
58	1K	1	0	0	0	0
58	2I	4	0	0	0	0
58	29	2	0	0	0	0
58	2L	6	0	0	0	0
58	3I	5	0	0	0	0
58	32	1	0	0	0	0
58	35	5	0	0	0	0
58	39	6	0	0	0	0
58	3I	1	0	0	0	0
58	42	1	0	0	0	0
58	45	5	0	0	0	0
58	4E	6	0	0	0	0
58	4I	2	0	0	0	0
58	4L	1	0	0	0	0
58	58	1	0	0	0	0
58	5I	1	0	0	0	0
58	78	8	0	0	0	0
58	7A	4	0	0	0	0
58	7I	3	0	0	0	0
58	8E	1	0	0	0	0
58	98	1	0	0	0	0
58	B5	2	0	0	0	0
58	BA	2	0	0	0	0
58	D8	1	0	0	0	0
58	E8	1	0	0	0	0
58	G8	1	0	0	0	0
58	H5	2	0	0	1	0
58	I8	3	0	0	1	0
58	J8	2	0	0	0	0
58	L5	1	0	0	0	0
58	L8	3	0	0	1	0
58	Q8	2	0	0	1	0
All	All	292640	0	194666	9118	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 20.

The worst 5 of 9118 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:1H:2714:G:OP2	58:1H:3519:HOH:O	1.69	1.07
26:1H:452:G:OP2	58:1H:3521:HOH:O	1.74	1.05
26:1H:1665:A:OP2	58:1H:3520:HOH:O	1.72	1.05
26:14:2499:C:OP2	58:14:3407:HOH:O	1.75	1.04
26:1H:990:A:OP2	58:1H:3522:HOH:O	1.76	1.04

There are no symmetry-related clashes.

## 5.3 Torsion angles ⓘ

### 5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	12	203/256 (79%)	156 (77%)	46 (23%)	1 (0%)	29	63
2	1E	227/256 (89%)	184 (81%)	42 (18%)	1 (0%)	34	68
3	22	193/239 (81%)	165 (86%)	27 (14%)	1 (0%)	29	63
3	2E	203/239 (85%)	165 (81%)	36 (18%)	2 (1%)	15	49
4	32	206/209 (99%)	166 (81%)	39 (19%)	1 (0%)	29	63
4	3E	205/209 (98%)	178 (87%)	26 (13%)	1 (0%)	29	63
5	42	148/162 (91%)	137 (93%)	11 (7%)	0	100	100
5	4E	147/162 (91%)	137 (93%)	10 (7%)	0	100	100
6	52	99/101 (98%)	90 (91%)	9 (9%)	0	100	100
6	5E	98/101 (97%)	90 (92%)	8 (8%)	0	100	100
7	62	134/156 (86%)	123 (92%)	11 (8%)	0	100	100
7	6E	152/156 (97%)	135 (89%)	17 (11%)	0	100	100
8	72	135/138 (98%)	122 (90%)	12 (9%)	1 (1%)	22	56
8	7E	136/138 (99%)	120 (88%)	14 (10%)	2 (2%)	10	39
9	82	119/128 (93%)	103 (87%)	14 (12%)	2 (2%)	9	36
9	8E	124/128 (97%)	103 (83%)	21 (17%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
10	1A	97/105 (92%)	81 (84%)	16 (16%)	0	100	100
10	1I	92/105 (88%)	80 (87%)	10 (11%)	2 (2%)	6	32
11	2A	111/129 (86%)	96 (86%)	13 (12%)	2 (2%)	8	35
11	2I	109/129 (84%)	91 (84%)	17 (16%)	1 (1%)	17	51
12	3A	120/132 (91%)	94 (78%)	24 (20%)	2 (2%)	9	36
12	3I	120/132 (91%)	96 (80%)	23 (19%)	1 (1%)	19	53
13	4A	107/126 (85%)	79 (74%)	27 (25%)	1 (1%)	17	51
13	4I	117/126 (93%)	90 (77%)	25 (21%)	2 (2%)	9	36
14	5A	57/61 (93%)	44 (77%)	12 (21%)	1 (2%)	8	35
14	5I	58/61 (95%)	50 (86%)	6 (10%)	2 (3%)	3	23
15	6A	85/89 (96%)	79 (93%)	6 (7%)	0	100	100
15	6I	85/89 (96%)	74 (87%)	11 (13%)	0	100	100
16	7A	82/88 (93%)	73 (89%)	9 (11%)	0	100	100
16	7I	81/88 (92%)	72 (89%)	9 (11%)	0	100	100
17	8A	97/105 (92%)	88 (91%)	9 (9%)	0	100	100
17	8I	98/105 (93%)	81 (83%)	17 (17%)	0	100	100
18	9A	67/88 (76%)	60 (90%)	7 (10%)	0	100	100
18	9I	66/88 (75%)	59 (89%)	7 (11%)	0	100	100
19	AA	59/93 (63%)	46 (78%)	13 (22%)	0	100	100
19	AI	80/93 (86%)	67 (84%)	12 (15%)	1 (1%)	12	42
20	BA	97/106 (92%)	82 (84%)	15 (16%)	0	100	100
20	BI	95/106 (90%)	72 (76%)	21 (22%)	2 (2%)	7	32
21	1B	20/27 (74%)	19 (95%)	0	1 (5%)	2	15
21	1F	21/27 (78%)	18 (86%)	2 (10%)	1 (5%)	2	16
28	11	271/276 (98%)	231 (85%)	35 (13%)	5 (2%)	8	35
28	19	272/276 (99%)	233 (86%)	39 (14%)	0	100	100
29	21	203/206 (98%)	157 (77%)	42 (21%)	4 (2%)	7	33
29	29	202/206 (98%)	145 (72%)	52 (26%)	5 (2%)	5	29
30	31	200/210 (95%)	172 (86%)	25 (12%)	3 (2%)	10	39
30	39	202/210 (96%)	155 (77%)	42 (21%)	5 (2%)	5	29
31	41	177/182 (97%)	152 (86%)	24 (14%)	1 (1%)	25	59

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
31	49	178/182 (98%)	151 (85%)	24 (14%)	3 (2%)	9	36
32	51	172/180 (96%)	132 (77%)	30 (17%)	10 (6%)	1	12
32	59	167/180 (93%)	129 (77%)	38 (23%)	0	100	100
33	61	143/148 (97%)	110 (77%)	30 (21%)	3 (2%)	7	32
33	69	143/148 (97%)	109 (76%)	30 (21%)	4 (3%)	5	26
34	15	135/140 (96%)	115 (85%)	19 (14%)	1 (1%)	22	56
34	58	123/140 (88%)	101 (82%)	20 (16%)	2 (2%)	9	38
35	25	120/122 (98%)	110 (92%)	10 (8%)	0	100	100
35	68	120/122 (98%)	114 (95%)	6 (5%)	0	100	100
36	35	145/150 (97%)	117 (81%)	25 (17%)	3 (2%)	7	32
36	78	146/150 (97%)	104 (71%)	35 (24%)	7 (5%)	2	16
37	45	136/141 (96%)	104 (76%)	29 (21%)	3 (2%)	6	32
37	88	139/141 (99%)	114 (82%)	22 (16%)	3 (2%)	6	32
38	55	116/118 (98%)	100 (86%)	15 (13%)	1 (1%)	17	51
38	98	116/118 (98%)	102 (88%)	14 (12%)	0	100	100
39	65	108/112 (96%)	83 (77%)	24 (22%)	1 (1%)	17	51
39	A8	109/112 (97%)	84 (77%)	24 (22%)	1 (1%)	17	51
40	75	138/146 (94%)	118 (86%)	18 (13%)	2 (1%)	11	40
40	B8	134/146 (92%)	104 (78%)	30 (22%)	0	100	100
41	85	114/118 (97%)	92 (81%)	22 (19%)	0	100	100
41	C8	113/118 (96%)	100 (88%)	11 (10%)	2 (2%)	8	35
42	95	98/101 (97%)	78 (80%)	16 (16%)	4 (4%)	3	19
42	D8	98/101 (97%)	83 (85%)	15 (15%)	0	100	100
43	A5	109/113 (96%)	96 (88%)	13 (12%)	0	100	100
43	E8	108/113 (96%)	97 (90%)	11 (10%)	0	100	100
44	B5	92/96 (96%)	79 (86%)	13 (14%)	0	100	100
44	F8	93/96 (97%)	83 (89%)	10 (11%)	0	100	100
45	C5	48/110 (44%)	36 (75%)	12 (25%)	0	100	100
45	G8	93/110 (84%)	67 (72%)	19 (20%)	7 (8%)	1	7
46	D5	175/206 (85%)	122 (70%)	48 (27%)	5 (3%)	4	26
46	H8	168/206 (82%)	123 (73%)	38 (23%)	7 (4%)	3	19

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
47	E5	74/85 (87%)	58 (78%)	15 (20%)	1 (1%)	11	40
47	I8	75/85 (88%)	63 (84%)	12 (16%)	0	100	100
48	F5	92/98 (94%)	77 (84%)	12 (13%)	3 (3%)	4	24
48	J8	94/98 (96%)	76 (81%)	13 (14%)	5 (5%)	2	14
49	G5	67/72 (93%)	59 (88%)	7 (10%)	1 (2%)	10	39
49	K8	66/72 (92%)	56 (85%)	7 (11%)	3 (4%)	2	17
50	H5	56/60 (93%)	51 (91%)	5 (9%)	0	100	100
50	L8	56/60 (93%)	51 (91%)	5 (9%)	0	100	100
51	M8	56/71 (79%)	36 (64%)	18 (32%)	2 (4%)	3	22
52	J5	54/60 (90%)	46 (85%)	8 (15%)	0	100	100
52	N8	46/60 (77%)	41 (89%)	5 (11%)	0	100	100
53	L5	46/49 (94%)	45 (98%)	1 (2%)	0	100	100
53	P8	45/49 (92%)	39 (87%)	6 (13%)	0	100	100
54	M5	62/65 (95%)	55 (89%)	7 (11%)	0	100	100
54	Q8	62/65 (95%)	45 (73%)	14 (23%)	3 (5%)	2	16
All	All	10925/11875 (92%)	9065 (83%)	1719 (16%)	141 (1%)	12	42

5 of 141 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
32	51	157	TYR
33	61	134	PRO
34	58	96	GLU
36	78	36	LYS
36	78	37	GLY

### 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	179/220 (81%)	139 (78%)	40 (22%)	1	3

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	1E	200/220 (91%)	151 (76%)	49 (24%)	0	2
3	22	154/188 (82%)	115 (75%)	39 (25%)	0	2
3	2E	159/188 (85%)	132 (83%)	27 (17%)	2	9
4	32	180/181 (99%)	147 (82%)	33 (18%)	1	6
4	3E	180/181 (99%)	135 (75%)	45 (25%)	0	2
5	42	114/123 (93%)	78 (68%)	36 (32%)	0	1
5	4E	115/123 (94%)	87 (76%)	28 (24%)	0	2
6	52	90/90 (100%)	72 (80%)	18 (20%)	1	4
6	5E	90/90 (100%)	76 (84%)	14 (16%)	2	11
7	62	114/127 (90%)	95 (83%)	19 (17%)	2	9
7	6E	125/127 (98%)	100 (80%)	25 (20%)	1	4
8	72	118/119 (99%)	93 (79%)	25 (21%)	1	3
8	7E	119/119 (100%)	93 (78%)	26 (22%)	1	3
9	82	92/99 (93%)	67 (73%)	25 (27%)	0	1
9	8E	97/99 (98%)	74 (76%)	23 (24%)	1	2
10	1A	89/92 (97%)	66 (74%)	23 (26%)	0	2
10	1I	81/92 (88%)	64 (79%)	17 (21%)	1	4
11	2A	85/99 (86%)	76 (89%)	9 (11%)	6	26
11	2I	84/99 (85%)	71 (84%)	13 (16%)	2	12
12	3A	103/109 (94%)	72 (70%)	31 (30%)	0	1
12	3I	103/109 (94%)	76 (74%)	27 (26%)	0	2
13	4A	90/101 (89%)	64 (71%)	26 (29%)	0	1
13	4I	94/101 (93%)	70 (74%)	24 (26%)	0	2
14	5A	49/50 (98%)	38 (78%)	11 (22%)	1	3
14	5I	49/50 (98%)	41 (84%)	8 (16%)	2	10
15	6A	79/80 (99%)	72 (91%)	7 (9%)	9	34
15	6I	79/80 (99%)	65 (82%)	14 (18%)	2	7
16	7A	72/74 (97%)	61 (85%)	11 (15%)	2	12
16	7I	72/74 (97%)	54 (75%)	18 (25%)	0	2
17	8A	94/97 (97%)	82 (87%)	12 (13%)	4	18
17	8I	95/97 (98%)	73 (77%)	22 (23%)	1	2

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
18	9A	58/77 (75%)	49 (84%)	9 (16%)	2	12
18	9I	58/77 (75%)	51 (88%)	7 (12%)	5	20
19	AA	56/80 (70%)	42 (75%)	14 (25%)	0	2
19	AI	72/80 (90%)	51 (71%)	21 (29%)	0	1
20	BA	76/82 (93%)	69 (91%)	7 (9%)	9	32
20	BI	75/82 (92%)	60 (80%)	15 (20%)	1	4
21	1B	17/22 (77%)	14 (82%)	3 (18%)	2	7
21	1F	18/22 (82%)	15 (83%)	3 (17%)	2	9
28	11	214/218 (98%)	161 (75%)	53 (25%)	0	2
28	19	214/218 (98%)	164 (77%)	50 (23%)	1	2
29	21	162/166 (98%)	127 (78%)	35 (22%)	1	3
29	29	165/166 (99%)	134 (81%)	31 (19%)	1	6
30	31	161/166 (97%)	125 (78%)	36 (22%)	1	3
30	39	163/166 (98%)	120 (74%)	43 (26%)	0	1
31	41	153/156 (98%)	117 (76%)	36 (24%)	1	2
31	49	152/156 (97%)	114 (75%)	38 (25%)	0	2
32	51	143/148 (97%)	108 (76%)	35 (24%)	0	2
32	59	140/148 (95%)	98 (70%)	42 (30%)	0	1
33	61	122/124 (98%)	84 (69%)	38 (31%)	0	1
33	69	122/124 (98%)	96 (79%)	26 (21%)	1	3
34	15	116/119 (98%)	89 (77%)	27 (23%)	1	2
34	58	105/119 (88%)	80 (76%)	25 (24%)	0	2
35	25	100/100 (100%)	80 (80%)	20 (20%)	1	4
35	68	100/100 (100%)	82 (82%)	18 (18%)	1	7
36	35	114/116 (98%)	80 (70%)	34 (30%)	0	1
36	78	114/116 (98%)	85 (75%)	29 (25%)	0	2
37	45	109/111 (98%)	85 (78%)	24 (22%)	1	3
37	88	110/111 (99%)	91 (83%)	19 (17%)	2	8
38	55	101/101 (100%)	74 (73%)	27 (27%)	0	1
38	98	101/101 (100%)	79 (78%)	22 (22%)	1	3
39	65	87/88 (99%)	60 (69%)	27 (31%)	0	1

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
39	A8	87/88 (99%)	64 (74%)	23 (26%)	0	1
40	75	122/127 (96%)	89 (73%)	33 (27%)	0	1
40	B8	118/127 (93%)	88 (75%)	30 (25%)	0	2
41	85	93/94 (99%)	77 (83%)	16 (17%)	2	8
41	C8	92/94 (98%)	77 (84%)	15 (16%)	2	10
42	95	81/82 (99%)	64 (79%)	17 (21%)	1	4
42	D8	82/82 (100%)	54 (66%)	28 (34%)	0	1
43	A5	91/92 (99%)	72 (79%)	19 (21%)	1	4
43	E8	90/92 (98%)	74 (82%)	16 (18%)	2	7
44	B5	74/78 (95%)	57 (77%)	17 (23%)	1	2
44	F8	77/78 (99%)	61 (79%)	16 (21%)	1	4
45	C5	43/91 (47%)	32 (74%)	11 (26%)	0	2
45	G8	79/91 (87%)	60 (76%)	19 (24%)	0	2
46	D5	156/179 (87%)	115 (74%)	41 (26%)	0	2
46	H8	151/179 (84%)	117 (78%)	34 (22%)	1	3
47	E5	61/67 (91%)	45 (74%)	16 (26%)	0	2
47	I8	62/67 (92%)	54 (87%)	8 (13%)	4	17
48	F5	79/83 (95%)	59 (75%)	20 (25%)	0	2
48	J8	79/83 (95%)	60 (76%)	19 (24%)	0	2
49	G5	63/67 (94%)	44 (70%)	19 (30%)	0	1
49	K8	64/67 (96%)	44 (69%)	20 (31%)	0	1
50	H5	50/52 (96%)	38 (76%)	12 (24%)	0	2
50	L8	50/52 (96%)	35 (70%)	15 (30%)	0	1
51	M8	52/63 (82%)	40 (77%)	12 (23%)	1	2
52	J5	48/52 (92%)	37 (77%)	11 (23%)	1	2
52	N8	43/52 (83%)	37 (86%)	6 (14%)	3	15
53	L5	38/42 (90%)	34 (90%)	4 (10%)	7	26
53	P8	38/42 (90%)	33 (87%)	5 (13%)	4	17
54	M5	54/55 (98%)	45 (83%)	9 (17%)	2	9
54	Q8	54/55 (98%)	45 (83%)	9 (17%)	2	9
All	All	9213/9831 (94%)	7134 (77%)	2079 (23%)	1	3

5 of 2079 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
46	H8	105	VAL
5	42	13	ILE
44	B5	23	GLU
48	J8	30	VAL
2	12	39	ILE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 30 such sidechains are listed below:

Mol	Chain	Res	Type
4	32	119	GLN
13	4A	40	ASN
40	75	79	HIS
10	1A	84	GLN
13	4A	101	GLN

### 5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	13	1498/1522 (98%)	346 (23%)	28 (1%)
1	1G	1489/1522 (97%)	369 (24%)	32 (2%)
22	1K	71/76 (93%)	37 (52%)	2 (2%)
22	1L	71/76 (93%)	41 (57%)	3 (4%)
23	2K	76/77 (98%)	20 (26%)	1 (1%)
23	2L	76/77 (98%)	19 (25%)	3 (3%)
24	3K	69/76 (90%)	38 (55%)	2 (2%)
24	3L	69/76 (90%)	36 (52%)	2 (2%)
25	4K	17/27 (62%)	10 (58%)	3 (17%)
25	4L	14/27 (51%)	6 (42%)	3 (21%)
26	14	2804/2917 (96%)	688 (24%)	36 (1%)
26	1H	2800/2917 (95%)	623 (22%)	41 (1%)
27	16	121/122 (99%)	27 (22%)	1 (0%)
27	1J	121/122 (99%)	34 (28%)	1 (0%)
All	All	9296/9634 (96%)	2294 (24%)	158 (1%)

5 of 2294 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	13	2	U
1	13	4	U
1	13	5	U

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Mol	Chain	Res	Type
1	13	6	G
1	13	9	G

5 of 158 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
26	1H	2062	A
1	1G	367	U
26	14	2211	G
26	1H	2225	A
1	1G	80	G

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

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

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
22	AET	1K	37	22	25,35,36	3.23	4 (16%)	26,51,54	2.21	5 (19%)
22	5MU	1K	54	22	15,22,23	2.18	3 (20%)	16,32,35	1.64	2 (12%)
22	5MU	1L	54	22	15,22,23	2.19	3 (20%)	16,32,35	1.81	2 (12%)
23	5MU	2K	55	23	15,22,23	2.19	3 (20%)	16,32,35	1.94	2 (12%)
22	PSU	1L	55	22	17,21,22	1.05	2 (11%)	20,30,33	3.22	6 (30%)
23	5MU	2L	55	23	15,22,23	2.18	3 (20%)	16,32,35	1.78	2 (12%)
22	PSU	1K	55	22	17,21,22	1.08	1 (5%)	20,30,33	3.09	6 (30%)
23	PSU	2K	56	23	17,21,22	1.24	2 (11%)	20,30,33	2.94	6 (30%)
22	H2U	1K	17	22	18,21,22	2.18	4 (22%)	21,30,33	2.01	4 (19%)
22	AET	1L	37	22	25,35,36	2.90	5 (20%)	26,51,54	1.99	6 (23%)
22	H2U	1L	17	22	18,21,22	2.26	4 (22%)	21,30,33	1.88	4 (19%)
23	PSU	2L	56	23	17,21,22	1.32	2 (11%)	20,30,33	3.32	5 (25%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	AET	1K	37	22	-	7/19/45/46	0/3/3/3
22	5MU	1K	54	22	-	3/5/25/26	0/2/2/2
22	5MU	1L	54	22	-	0/5/25/26	0/2/2/2
23	5MU	2K	55	23	-	0/5/25/26	0/2/2/2
22	PSU	1L	55	22	-	2/7/25/26	0/2/2/2
23	5MU	2L	55	23	-	0/5/25/26	0/2/2/2
22	PSU	1K	55	22	-	2/7/25/26	0/2/2/2
23	PSU	2K	56	23	-	0/7/25/26	0/2/2/2
22	H2U	1K	17	22	-	4/7/38/39	0/2/2/2
22	AET	1L	37	22	-	7/19/45/46	0/3/3/3
22	H2U	1L	17	22	-	5/7/38/39	0/2/2/2
23	PSU	2L	56	23	-	0/7/25/26	0/2/2/2

The worst 5 of 36 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	1K	37	AET	C10-N6	12.68	1.55	1.37
22	1L	37	AET	C10-N6	11.01	1.52	1.37
22	1K	37	AET	C10-N11	7.64	1.52	1.35
22	1L	37	AET	C10-N11	7.04	1.51	1.35
22	1L	17	H2U	C2-N1	6.95	1.45	1.35

The worst 5 of 50 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	2L	56	PSU	N1-C2-N3	-11.32	119.43	128.43
22	1L	55	PSU	N1-C2-N3	-10.83	119.82	128.43
22	1K	55	PSU	N1-C2-N3	-9.77	120.66	128.43
23	2K	56	PSU	N1-C2-N3	-8.90	121.36	128.43
22	1K	37	AET	N3-C2-N1	-6.85	117.98	128.68

There are no chirality outliers.

5 of 30 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
22	1K	37	AET	C5-C6-N6-C10
22	1K	37	AET	N1-C6-N6-C10

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Mol	Chain	Res	Type	Atoms
22	1K	37	AET	C13-C12-C14-O14
22	1K	54	5MU	C2'-C1'-N1-C6
22	1K	54	5MU	C3'-C4'-C5'-O5'

There are no ring outliers.

3 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
22	1K	37	AET	4	0
22	1K	54	5MU	1	0
22	1L	37	AET	2	0

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 1086 ligands modelled in this entry, 1084 are monoatomic - leaving 2 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
56	SF4	32	302	4	0,12,12	0.00	-	-		
56	SF4	3E	301	-	0,12,12	0.00	-	-		

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
56	SF4	32	302	4	-	-	0/6/5/5
56	SF4	3E	301	-	-	-	0/6/5/5



There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
56	32	302	SF4	2	0
56	3E	301	SF4	1	0

## 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
26	1H	1
24	3K	1
24	3L	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	3L	48:C	O3'	49:G	P	5.47
1	3K	48:C	O3'	49:G	P	4.84
1	1H	1053:C	O3'	1054:A	P	3.77

## 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	1500/1522 (98%)	0.00	37 (2%) 57 59	76, 125, 184, 245	0
1	1G	1490/1522 (97%)	-0.24	16 (1%) 80 84	83, 128, 188, 248	0
2	12	207/256 (80%)	0.14	11 (5%) 26 28	161, 184, 195, 199	0
2	1E	231/256 (90%)	-0.18	2 (0%) 84 87	141, 166, 184, 190	0
3	22	197/239 (82%)	1.16	52 (26%) 0 0	154, 171, 186, 191	0
3	2E	205/239 (85%)	0.79	36 (17%) 1 1	111, 131, 153, 161	0
4	32	208/209 (99%)	0.40	12 (5%) 23 25	120, 138, 152, 159	0
4	3E	207/209 (99%)	1.13	44 (21%) 0 1	110, 133, 148, 155	0
5	42	150/162 (92%)	0.42	19 (12%) 3 4	125, 140, 157, 169	0
5	4E	149/162 (91%)	0.78	22 (14%) 2 2	103, 125, 139, 144	0
6	52	101/101 (100%)	-0.06	0 100 100	115, 130, 143, 149	0
6	5E	100/101 (99%)	0.05	1 (1%) 82 86	111, 130, 143, 148	0
7	62	138/156 (88%)	1.35	35 (25%) 0 0	141, 152, 160, 165	0
7	6E	154/156 (98%)	1.13	29 (18%) 1 1	121, 144, 164, 171	0
8	72	137/138 (99%)	0.59	17 (12%) 4 4	124, 148, 161, 165	0
8	7E	138/138 (100%)	0.77	19 (13%) 2 3	114, 133, 143, 154	0
9	82	121/128 (94%)	1.01	24 (19%) 1 1	136, 172, 181, 189	0
9	8E	126/128 (98%)	0.59	20 (15%) 1 2	113, 159, 175, 182	0
10	1A	99/105 (94%)	0.88	21 (21%) 0 1	151, 177, 186, 190	0
10	1I	94/105 (89%)	0.97	28 (29%) 0 0	108, 151, 170, 173	0
11	2A	113/129 (87%)	2.03	50 (44%) 0 0	107, 132, 147, 153	0
11	2I	111/129 (86%)	2.17	55 (49%) 0 0	100, 132, 150, 165	0
12	3A	122/132 (92%)	1.70	50 (40%) 0 0	112, 126, 140, 147	0
12	3I	122/132 (92%)	1.86	53 (43%) 0 0	89, 102, 123, 138	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
13	4A	109/126 (86%)	1.07	33 (30%) 0 0	147, 174, 184, 192	0
13	4I	119/126 (94%)	0.56	21 (17%) 1 1	108, 141, 151, 161	0
14	5A	59/61 (96%)	4.09	38 (64%) 0 0	155, 172, 184, 193	0
14	5I	60/61 (98%)	1.83	27 (45%) 0 0	113, 123, 140, 142	0
15	6A	87/89 (97%)	0.23	5 (5%) 23 26	113, 133, 149, 153	0
15	6I	87/89 (97%)	0.43	7 (8%) 12 14	110, 126, 142, 148	0
16	7A	84/88 (95%)	-0.12	0 100 100	110, 128, 147, 175	0
16	7I	83/88 (94%)	1.60	31 (37%) 0 0	127, 142, 164, 175	0
17	8A	99/105 (94%)	1.47	32 (32%) 0 0	116, 127, 141, 145	0
17	8I	100/105 (95%)	1.19	27 (27%) 0 0	111, 128, 138, 139	0
18	9A	69/88 (78%)	0.03	2 (2%) 51 54	118, 135, 151, 160	0
18	9I	68/88 (77%)	0.16	0 100 100	114, 132, 145, 153	0
19	AA	65/93 (69%)	1.08	14 (21%) 0 1	170, 188, 195, 196	0
19	AI	82/93 (88%)	0.53	10 (12%) 4 4	116, 140, 164, 171	0
20	BA	99/106 (93%)	0.87	15 (15%) 2 2	116, 133, 153, 156	0
20	BI	97/106 (91%)	0.59	7 (7%) 15 18	124, 143, 162, 165	0
21	1B	22/27 (81%)	1.34	7 (31%) 0 0	138, 161, 164, 166	0
21	1F	23/27 (85%)	0.93	7 (30%) 0 0	117, 127, 134, 141	0
22	1K	70/76 (92%)	0.28	6 (8%) 10 12	118, 199, 215, 218	0
22	1L	70/76 (92%)	0.65	10 (14%) 2 3	137, 224, 235, 238	0
23	2K	75/77 (97%)	0.79	9 (12%) 4 5	84, 118, 147, 158	0
23	2L	75/77 (97%)	0.38	4 (5%) 26 28	94, 135, 158, 169	0
24	3K	72/76 (94%)	0.65	9 (12%) 3 4	88, 208, 234, 241	0
24	3L	72/76 (94%)	-0.01	5 (6%) 16 19	100, 201, 226, 230	0
25	4K	18/27 (66%)	3.49	15 (83%) 0 0	96, 147, 195, 200	0
25	4L	14/27 (51%)	2.16	6 (42%) 0 0	118, 164, 175, 177	0
26	14	2811/2917 (96%)	0.11	85 (3%) 50 53	64, 105, 193, 248	0
26	1H	2811/2917 (96%)	-0.00	12 (0%) 92 94	56, 89, 174, 260	0
27	16	122/122 (100%)	-0.36	0 100 100	87, 112, 131, 182	0
27	1J	122/122 (100%)	-0.43	1 (0%) 86 89	117, 142, 157, 190	0
28	11	273/276 (98%)	1.06	52 (19%) 1 1	57, 82, 102, 113	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å²)		Q<0.9	
28	19	274/276 (99%)	1.58	97 (35%)	0	0	59, 90, 108, 119	0
29	21	205/206 (99%)	1.23	52 (25%)	0	0	66, 100, 134, 144	0
29	29	204/206 (99%)	1.23	54 (26%)	0	0	76, 114, 145, 159	0
30	31	202/210 (96%)	0.84	29 (14%)	2	3	60, 93, 126, 139	0
30	39	204/210 (97%)	0.46	24 (11%)	4	5	74, 123, 157, 170	0
31	41	179/182 (98%)	0.52	15 (8%)	11	13	105, 125, 147, 157	0
31	49	180/182 (98%)	1.87	70 (38%)	0	0	139, 158, 176, 187	0
32	51	174/180 (96%)	0.02	0	100	100	99, 119, 132, 147	0
32	59	169/180 (93%)	2.42	79 (46%)	0	0	174, 207, 224, 229	0
33	61	145/148 (97%)	-0.27	0	100	100	97, 148, 162, 167	0
33	69	145/148 (97%)	0.01	5 (3%)	45	47	100, 142, 160, 165	0
34	15	137/140 (97%)	2.89	91 (66%)	0	0	94, 127, 154, 162	0
34	58	125/140 (89%)	1.12	27 (21%)	0	1	84, 101, 118, 135	0
35	25	122/122 (100%)	1.71	51 (41%)	0	0	82, 104, 119, 128	0
35	68	122/122 (100%)	1.19	28 (22%)	0	0	73, 94, 112, 126	0
36	35	147/150 (98%)	1.68	58 (39%)	0	0	74, 122, 150, 161	0
36	78	148/150 (98%)	0.54	17 (11%)	4	5	63, 98, 121, 128	0
37	45	138/141 (97%)	3.03	84 (60%)	0	0	91, 125, 148, 160	0
37	88	141/141 (100%)	1.28	37 (26%)	0	0	74, 98, 119, 144	0
38	55	118/118 (100%)	1.15	31 (26%)	0	0	79, 101, 115, 124	0
38	98	118/118 (100%)	1.50	36 (30%)	0	0	78, 97, 116, 131	0
39	65	110/112 (98%)	0.14	3 (2%)	54	57	116, 134, 146, 155	0
39	A8	111/112 (99%)	0.78	11 (9%)	7	8	93, 108, 124, 136	0
40	75	140/146 (95%)	0.67	13 (9%)	8	10	97, 114, 166, 177	0
40	B8	136/146 (93%)	0.70	16 (11%)	4	5	89, 108, 150, 175	0
41	85	116/118 (98%)	1.27	28 (24%)	0	0	82, 117, 146, 155	0
41	C8	115/118 (97%)	0.53	6 (5%)	27	29	68, 94, 121, 131	0
42	95	100/101 (99%)	1.53	32 (32%)	0	0	82, 141, 153, 159	0
42	D8	100/101 (99%)	0.92	15 (15%)	2	2	66, 112, 131, 136	0
43	A5	111/113 (98%)	1.38	31 (27%)	0	0	77, 95, 124, 143	0
43	E8	110/113 (97%)	1.04	19 (17%)	1	1	68, 87, 111, 124	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
44	B5	94/96 (97%)	0.76	9 (9%) 8 10	91, 104, 118, 125	0
44	F8	95/96 (98%)	0.63	8 (8%) 11 13	71, 85, 112, 122	0
45	C5	52/110 (47%)	1.51	15 (28%) 0 0	109, 122, 135, 145	0
45	G8	97/110 (88%)	-0.02	0 100 100	91, 107, 131, 142	0
46	D5	177/206 (85%)	1.82	70 (39%) 0 0	132, 166, 217, 221	0
46	H8	170/206 (82%)	0.99	33 (19%) 1 1	105, 137, 187, 195	0
47	E5	76/85 (89%)	2.58	37 (48%) 0 0	95, 109, 124, 131	0
47	I8	77/85 (90%)	1.67	25 (32%) 0 0	76, 88, 110, 120	0
48	F5	94/98 (95%)	2.16	49 (52%) 0 0	78, 104, 133, 138	0
48	J8	96/98 (97%)	1.86	43 (44%) 0 0	72, 94, 142, 152	0
49	G5	69/72 (95%)	0.22	3 (4%) 35 38	107, 128, 145, 156	0
49	K8	68/72 (94%)	0.39	0 100 100	78, 99, 116, 136	0
50	H5	58/60 (96%)	2.74	37 (63%) 0 0	100, 121, 137, 150	0
50	L8	58/60 (96%)	0.67	6 (10%) 6 7	72, 93, 122, 124	0
51	M8	60/71 (84%)	0.19	5 (8%) 11 13	126, 154, 167, 170	0
52	J5	56/60 (93%)	1.52	20 (35%) 0 0	74, 103, 138, 151	0
52	N8	48/60 (80%)	0.91	7 (14%) 2 2	64, 98, 126, 133	0
53	L5	48/49 (97%)	1.70	14 (29%) 0 0	70, 78, 110, 114	0
53	P8	47/49 (95%)	0.69	5 (10%) 6 7	61, 68, 90, 98	0
54	M5	64/65 (98%)	3.63	51 (79%) 0 0	83, 97, 115, 126	0
54	Q8	64/65 (98%)	2.00	35 (54%) 0 0	68, 83, 101, 110	0
All	All	20451/21509 (95%)	0.58	2681 (13%) 3 4	56, 119, 186, 260	0

The worst 5 of 2681 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
14	5A	38	GLY	16.2
32	59	93	GLY	14.9
22	1L	76	A	14.8
47	E5	9	SER	13.8
14	5A	39	LEU	13.7

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

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
22	H2U	1L	17	20/21	0.26	0.77	213,231,237,237	0
22	H2U	1K	17	20/21	0.45	0.40	199,211,220,220	0
22	PSU	1L	55	20/21	0.79	0.11	169,202,215,222	0
22	5MU	1L	54	21/22	0.85	0.11	171,182,192,193	0
22	AET	1L	37	33/34	0.88	0.42	156,171,176,178	0
22	PSU	1K	55	20/21	0.89	0.12	146,178,188,189	0
22	AET	1K	37	33/34	0.90	0.45	112,124,147,151	0
22	5MU	1K	54	21/22	0.90	0.15	139,156,165,170	0
23	PSU	2L	56	20/21	0.90	0.19	126,136,143,146	0
23	PSU	2K	56	20/21	0.91	0.11	113,119,131,132	0
23	5MU	2L	55	21/22	0.94	0.24	129,139,144,146	0
23	5MU	2K	55	21/22	0.95	0.12	118,124,135,139	0

## 6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 6.4 Ligands ⓘ

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
55	MG	1H	3180	1/1	0.04	0.26	112,112,112,112	0
55	MG	14	3139	1/1	0.24	0.32	103,103,103,103	0
55	MG	1H	3049	1/1	0.26	0.36	74,74,74,74	0
55	MG	14	3094	1/1	0.27	0.43	108,108,108,108	0
55	MG	1G	1650	1/1	0.37	0.83	107,107,107,107	0
55	MG	1H	3241	1/1	0.39	0.58	110,110,110,110	0
55	MG	13	1675	1/1	0.40	0.33	104,104,104,104	0
55	MG	1H	3223	1/1	0.41	0.70	99,99,99,99	0
55	MG	1H	3045	1/1	0.41	0.42	80,80,80,80	0
55	MG	1G	1656	1/1	0.45	0.36	115,115,115,115	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
55	MG	1H	3212	1/1	0.48	0.50	91,91,91,91	0
55	MG	14	3177	1/1	0.49	0.57	79,79,79,79	0
55	MG	E5	101	1/1	0.49	0.32	90,90,90,90	0
55	MG	1H	3009	1/1	0.50	0.14	95,95,95,95	0
55	MG	1H	3178	1/1	0.50	0.27	94,94,94,94	0
55	MG	13	1603	1/1	0.50	0.12	85,85,85,85	0
55	MG	1G	1701	1/1	0.51	0.24	137,137,137,137	0
55	MG	13	1711	1/1	0.52	0.22	154,154,154,154	0
55	MG	13	1647	1/1	0.52	0.21	116,116,116,116	0
55	MG	14	3116	1/1	0.52	0.17	89,89,89,89	0
55	MG	1G	1663	1/1	0.52	0.47	121,121,121,121	0
55	MG	14	3144	1/1	0.53	0.38	114,114,114,114	0
55	MG	1G	1668	1/1	0.54	0.38	125,125,125,125	0
55	MG	14	3176	1/1	0.54	0.27	109,109,109,109	0
55	MG	14	3004	1/1	0.54	0.22	66,66,66,66	0
55	MG	1H	3107	1/1	0.54	0.41	92,92,92,92	0
55	MG	1H	3229	1/1	0.55	0.70	70,70,70,70	0
55	MG	14	3184	1/1	0.55	0.30	96,96,96,96	0
55	MG	13	1670	1/1	0.56	0.20	137,137,137,137	0
55	MG	1H	3017	1/1	0.56	0.33	75,75,75,75	0
55	MG	13	1668	1/1	0.56	0.15	121,121,121,121	0
55	MG	1H	3165	1/1	0.56	0.38	90,90,90,90	0
55	MG	14	3069	1/1	0.57	0.35	107,107,107,107	0
55	MG	1H	3137	1/1	0.57	0.32	75,75,75,75	0
55	MG	42	202	1/1	0.58	0.23	135,135,135,135	0
55	MG	1G	1693	1/1	0.58	0.09	148,148,148,148	0
55	MG	14	3186	1/1	0.59	0.37	85,85,85,85	0
55	MG	1G	1651	1/1	0.59	0.24	91,91,91,91	0
55	MG	1G	1714	1/1	0.59	0.20	133,133,133,133	0
55	MG	14	3185	1/1	0.59	1.15	88,88,88,88	0
55	MG	1H	3114	1/1	0.60	0.29	92,92,92,92	0
55	MG	1H	3166	1/1	0.60	0.28	74,74,74,74	0
55	MG	1G	1722	1/1	0.60	0.12	161,161,161,161	0
55	MG	1G	1671	1/1	0.62	0.24	100,100,100,100	0
55	MG	13	1638	1/1	0.62	0.58	80,80,80,80	0
55	MG	1H	3111	1/1	0.62	0.29	86,86,86,86	0
55	MG	1H	3175	1/1	0.63	0.37	114,114,114,114	0
55	MG	14	3190	1/1	0.63	0.30	100,100,100,100	0
55	MG	1H	3113	1/1	0.63	0.39	83,83,83,83	0
55	MG	14	3122	1/1	0.63	0.40	103,103,103,103	0
55	MG	1H	3185	1/1	0.63	0.64	72,72,72,72	0
55	MG	14	3112	1/1	0.64	1.17	96,96,96,96	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
55	MG	14	3164	1/1	0.64	0.39	95,95,95,95	0
55	MG	1H	3034	1/1	0.64	0.27	77,77,77,77	0
55	MG	35	201	1/1	0.64	0.95	81,81,81,81	0
55	MG	1G	1618	1/1	0.64	0.45	98,98,98,98	0
55	MG	13	1641	1/1	0.64	0.21	94,94,94,94	0
55	MG	1H	3133	1/1	0.65	0.27	85,85,85,85	0
55	MG	13	1671	1/1	0.65	0.22	117,117,117,117	0
55	MG	13	1629	1/1	0.65	0.24	109,109,109,109	0
55	MG	1H	3181	1/1	0.65	0.52	89,89,89,89	0
55	MG	1H	3096	1/1	0.65	0.19	79,79,79,79	0
55	MG	1G	1662	1/1	0.65	0.49	116,116,116,116	0
55	MG	1H	3121	1/1	0.66	0.23	91,91,91,91	0
55	MG	14	3296	1/1	0.66	0.10	119,119,119,119	0
55	MG	14	3125	1/1	0.66	0.24	97,97,97,97	0
55	MG	1G	1667	1/1	0.66	0.23	101,101,101,101	0
55	MG	1G	1683	1/1	0.66	0.26	122,122,122,122	0
55	MG	14	3099	1/1	0.66	0.30	90,90,90,90	0
55	MG	1H	3085	1/1	0.67	0.27	74,74,74,74	0
55	MG	14	3012	1/1	0.67	0.28	95,95,95,95	0
55	MG	1H	3179	1/1	0.67	0.32	86,86,86,86	0
55	MG	14	3141	1/1	0.67	0.21	104,104,104,104	0
55	MG	14	3170	1/1	0.67	0.26	69,69,69,69	0
55	MG	1H	3214	1/1	0.67	0.17	84,84,84,84	0
55	MG	1H	3127	1/1	0.67	0.25	87,87,87,87	0
55	MG	45	201	1/1	0.67	0.16	121,121,121,121	0
55	MG	1H	3315	1/1	0.68	0.08	112,112,112,112	0
55	MG	1H	3226	1/1	0.68	1.28	90,90,90,90	0
55	MG	1G	1657	1/1	0.68	0.23	98,98,98,98	0
55	MG	13	1663	1/1	0.68	0.21	123,123,123,123	0
55	MG	1G	1640	1/1	0.68	0.20	103,103,103,103	0
55	MG	1H	3452	1/1	0.68	0.12	108,108,108,108	0
55	MG	14	3194	1/1	0.68	0.17	132,132,132,132	0
55	MG	13	1679	1/1	0.69	0.36	111,111,111,111	0
55	MG	14	3016	1/1	0.69	0.27	110,110,110,110	0
55	MG	1G	1646	1/1	0.69	0.31	101,101,101,101	0
55	MG	14	3082	1/1	0.69	0.34	78,78,78,78	0
55	MG	14	3027	1/1	0.69	0.28	72,72,72,72	0
55	MG	1H	3119	1/1	0.69	0.36	105,105,105,105	0
55	MG	1G	1620	1/1	0.69	0.17	81,81,81,81	0
55	MG	13	1705	1/1	0.70	0.53	130,130,130,130	0
55	MG	14	3009	1/1	0.70	0.66	90,90,90,90	0
55	MG	1H	3149	1/1	0.70	0.44	76,76,76,76	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
55	MG	14	3169	1/1	0.71	0.21	97,97,97,97	0
55	MG	13	1681	1/1	0.71	0.27	113,113,113,113	0
55	MG	1H	3244	1/1	0.71	0.31	87,87,87,87	0
55	MG	1H	3088	1/1	0.71	0.34	81,81,81,81	0
55	MG	1H	3457	1/1	0.72	0.17	133,133,133,133	0
55	MG	1H	3252	1/1	0.72	0.24	69,69,69,69	0
55	MG	1H	3024	1/1	0.72	0.20	71,71,71,71	0
55	MG	14	3107	1/1	0.72	0.23	88,88,88,88	0
55	MG	1G	1659	1/1	0.72	0.14	99,99,99,99	0
55	MG	14	3182	1/1	0.72	0.36	88,88,88,88	0
55	MG	14	3110	1/1	0.72	0.37	103,103,103,103	0
55	MG	14	3029	1/1	0.72	0.13	99,99,99,99	0
55	MG	1G	1682	1/1	0.72	0.16	101,101,101,101	0
55	MG	14	3001	1/1	0.72	0.17	94,94,94,94	0
55	MG	1G	1647	1/1	0.72	0.21	120,120,120,120	0
55	MG	1H	3254	1/1	0.72	0.35	97,97,97,97	0
55	MG	14	3121	1/1	0.72	0.38	94,94,94,94	0
55	MG	1H	3148	1/1	0.72	0.31	100,100,100,100	0
55	MG	1H	3340	1/1	0.72	0.18	139,139,139,139	0
55	MG	1H	3164	1/1	0.72	0.24	98,98,98,98	0
55	MG	1H	3274	1/1	0.72	0.51	78,78,78,78	0
55	MG	1H	3145	1/1	0.73	0.34	84,84,84,84	0
55	MG	13	1636	1/1	0.73	0.17	91,91,91,91	0
55	MG	1H	3312	1/1	0.73	0.23	105,105,105,105	0
55	MG	13	1708	1/1	0.73	0.32	145,145,145,145	0
55	MG	13	1627	1/1	0.73	0.19	94,94,94,94	0
55	MG	14	3188	1/1	0.73	0.32	89,89,89,89	0
55	MG	1G	1644	1/1	0.73	0.27	97,97,97,97	0
55	MG	1G	1660	1/1	0.73	0.17	118,118,118,118	0
55	MG	5I	101	1/1	0.73	0.75	105,105,105,105	0
55	MG	14	3060	1/1	0.73	0.33	84,84,84,84	0
55	MG	13	1639	1/1	0.74	0.18	110,110,110,110	0
55	MG	1G	1621	1/1	0.74	0.50	115,115,115,115	0
55	MG	8I	201	1/1	0.74	1.37	107,107,107,107	0
55	MG	1H	3310	1/1	0.74	0.10	109,109,109,109	0
55	MG	1G	1706	1/1	0.74	0.11	138,138,138,138	0
55	MG	1G	1661	1/1	0.74	0.23	77,77,77,77	0
55	MG	13	1686	1/1	0.75	0.59	73,73,73,73	0
55	MG	14	3041	1/1	0.75	0.56	61,61,61,61	0
55	MG	1G	1629	1/1	0.75	0.11	131,131,131,131	0
55	MG	14	3083	1/1	0.75	0.27	105,105,105,105	0
55	MG	1H	3337	1/1	0.75	0.08	127,127,127,127	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
55	MG	1H	3138	1/1	0.75	0.35	98,98,98,98	0
55	MG	1H	3269	1/1	0.75	0.34	55,55,55,55	0
55	MG	1H	3253	1/1	0.75	0.33	98,98,98,98	0
55	MG	1G	1627	1/1	0.75	0.27	122,122,122,122	0
55	MG	1G	1669	1/1	0.76	0.33	131,131,131,131	0
55	MG	13	1724	1/1	0.76	0.09	128,128,128,128	0
55	MG	14	3062	1/1	0.76	0.26	87,87,87,87	0
55	MG	14	3113	1/1	0.76	0.21	120,120,120,120	0
55	MG	1H	3141	1/1	0.76	0.34	89,89,89,89	0
55	MG	1G	1670	1/1	0.76	0.59	101,101,101,101	0
55	MG	1H	3142	1/1	0.76	0.43	76,76,76,76	0
55	MG	1G	1604	1/1	0.76	0.12	102,102,102,102	0
55	MG	13	1630	1/1	0.76	0.23	109,109,109,109	0
55	MG	1H	3465	1/1	0.76	0.07	98,98,98,98	0
55	MG	13	1673	1/1	0.76	0.25	113,113,113,113	0
55	MG	1H	3091	1/1	0.76	0.24	70,70,70,70	0
55	MG	1H	3301	1/1	0.76	0.11	100,100,100,100	0
55	MG	1H	3205	1/1	0.77	0.33	80,80,80,80	0
55	MG	45	202	1/1	0.77	0.33	116,116,116,116	0
55	MG	1H	3163	1/1	0.77	0.22	82,82,82,82	0
55	MG	1H	3279	1/1	0.77	0.31	81,81,81,81	0
55	MG	14	3178	1/1	0.77	0.30	98,98,98,98	0
55	MG	14	3298	1/1	0.77	0.12	103,103,103,103	0
55	MG	21	301	1/1	0.77	0.14	82,82,82,82	0
55	MG	1H	3300	1/1	0.77	0.32	104,104,104,104	0
55	MG	14	3079	1/1	0.77	0.22	100,100,100,100	0
55	MG	14	3108	1/1	0.78	0.20	87,87,87,87	0
55	MG	14	3010	1/1	0.78	0.22	78,78,78,78	0
55	MG	1G	1630	1/1	0.78	0.21	135,135,135,135	0
55	MG	1G	1623	1/1	0.78	0.07	161,161,161,161	0
55	MG	1H	3033	1/1	0.78	0.28	60,60,60,60	0
55	MG	1H	3419	1/1	0.78	0.09	115,115,115,115	0
55	MG	13	1674	1/1	0.78	0.49	109,109,109,109	0
55	MG	13	1648	1/1	0.78	0.19	110,110,110,110	0
55	MG	14	3026	1/1	0.78	0.15	76,76,76,76	0
55	MG	1H	3278	1/1	0.78	0.24	75,75,75,75	0
55	MG	1H	3050	1/1	0.78	0.36	79,79,79,79	0
55	MG	1G	1685	1/1	0.79	0.33	94,94,94,94	0
55	MG	1H	3275	1/1	0.79	0.47	62,62,62,62	0
55	MG	1H	3246	1/1	0.79	0.37	117,117,117,117	0
55	MG	13	1701	1/1	0.79	0.26	137,137,137,137	0
55	MG	14	3133	1/1	0.79	0.43	99,99,99,99	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
55	MG	14	3092	1/1	0.79	0.69	81,81,81,81	0
55	MG	14	3135	1/1	0.79	1.38	91,91,91,91	0
55	MG	1G	1715	1/1	0.79	0.25	126,126,126,126	0
55	MG	1H	3199	1/1	0.79	0.35	69,69,69,69	0
55	MG	14	3098	1/1	0.79	0.35	78,78,78,78	0
55	MG	14	3290	1/1	0.79	0.12	115,115,115,115	0
55	MG	1G	1606	1/1	0.79	0.18	109,109,109,109	0
55	MG	13	1664	1/1	0.79	0.37	87,87,87,87	0
55	MG	1H	3143	1/1	0.80	0.25	89,89,89,89	0
55	MG	13	1738	1/1	0.80	0.25	134,134,134,134	0
55	MG	1G	1645	1/1	0.80	0.27	118,118,118,118	0
55	MG	1H	3208	1/1	0.80	0.22	113,113,113,113	0
55	MG	1G	1697	1/1	0.80	0.10	172,172,172,172	0
55	MG	13	1733	1/1	0.80	0.14	92,92,92,92	0
55	MG	1G	1637	1/1	0.80	0.09	125,125,125,125	0
55	MG	1G	1649	1/1	0.80	0.21	151,151,151,151	0
55	MG	1H	3273	1/1	0.80	0.27	63,63,63,63	0
55	MG	14	3081	1/1	0.80	0.40	88,88,88,88	0
55	MG	1H	3176	1/1	0.80	0.18	107,107,107,107	0
55	MG	13	1652	1/1	0.80	0.27	97,97,97,97	0
55	MG	13	1631	1/1	0.81	0.36	132,132,132,132	0
55	MG	1H	3067	1/1	0.81	0.34	65,65,65,65	0
55	MG	14	3163	1/1	0.81	0.32	102,102,102,102	0
55	MG	1H	3174	1/1	0.81	0.64	129,129,129,129	0
55	MG	88	203	1/1	0.81	0.93	77,77,77,77	0
55	MG	13	1624	1/1	0.81	0.17	98,98,98,98	0
55	MG	1H	3281	1/1	0.81	0.36	96,96,96,96	0
55	MG	1G	1652	1/1	0.81	0.14	105,105,105,105	0
55	MG	13	1676	1/1	0.82	0.20	104,104,104,104	0
55	MG	13	1706	1/1	0.82	0.30	132,132,132,132	0
55	MG	1G	1632	1/1	0.82	0.20	127,127,127,127	0
55	MG	13	1606	1/1	0.82	0.31	83,83,83,83	0
55	MG	14	3078	1/1	0.82	0.11	100,100,100,100	0
55	MG	1G	1641	1/1	0.82	0.13	107,107,107,107	0
55	MG	1H	3331	1/1	0.82	0.18	109,109,109,109	0
55	MG	14	3137	1/1	0.82	0.34	151,151,151,151	0
55	MG	1H	3183	1/1	0.82	0.55	82,82,82,82	0
55	MG	1H	3139	1/1	0.82	0.26	60,60,60,60	0
55	MG	1G	1603	1/1	0.82	0.16	95,95,95,95	0
55	MG	1G	1614	1/1	0.82	0.27	123,123,123,123	0
55	MG	1H	3202	1/1	0.82	0.50	87,87,87,87	0
55	MG	13	1602	1/1	0.82	0.18	115,115,115,115	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
55	MG	14	3138	1/1	0.82	0.39	134,134,134,134	0
55	MG	14	3109	1/1	0.82	0.28	102,102,102,102	0
55	MG	1G	1692	1/1	0.83	0.09	118,118,118,118	0
55	MG	13	1739	1/1	0.83	0.12	128,128,128,128	0
55	MG	14	3076	1/1	0.83	0.44	90,90,90,90	0
55	MG	1H	3325	1/1	0.83	0.18	122,122,122,122	0
55	MG	1H	3255	1/1	0.83	0.30	78,78,78,78	0
55	MG	1H	3423	1/1	0.83	0.09	102,102,102,102	0
55	MG	14	3019	1/1	0.83	0.11	85,85,85,85	0
55	MG	1H	3154	1/1	0.83	0.20	61,61,61,61	0
55	MG	1G	1723	1/1	0.83	0.08	113,113,113,113	0
55	MG	1H	3249	1/1	0.83	0.23	70,70,70,70	0
55	MG	1H	3037	1/1	0.83	0.11	76,76,76,76	0
55	MG	14	3189	1/1	0.83	0.27	99,99,99,99	0
55	MG	1H	3126	1/1	0.83	0.36	78,78,78,78	0
55	MG	1H	3090	1/1	0.83	0.21	88,88,88,88	0
55	MG	1H	3216	1/1	0.83	0.36	89,89,89,89	0
55	MG	1G	1681	1/1	0.83	0.26	92,92,92,92	0
55	MG	1H	3128	1/1	0.83	0.26	92,92,92,92	0
55	MG	1H	3144	1/1	0.83	0.21	106,106,106,106	0
55	MG	1H	3207	1/1	0.83	0.30	77,77,77,77	0
55	MG	1H	3021	1/1	0.83	0.11	78,78,78,78	0
55	MG	13	1637	1/1	0.83	0.18	101,101,101,101	0
55	MG	1H	3029	1/1	0.83	0.21	68,68,68,68	0
55	MG	1H	3221	1/1	0.83	0.20	100,100,100,100	0
55	MG	1H	3237	1/1	0.83	0.19	79,79,79,79	0
55	MG	1H	3104	1/1	0.84	0.51	74,74,74,74	0
55	MG	1H	3238	1/1	0.84	0.15	94,94,94,94	0
55	MG	1H	3093	1/1	0.84	0.37	70,70,70,70	0
55	MG	1H	3184	1/1	0.84	0.17	87,87,87,87	0
55	MG	1G	1648	1/1	0.84	0.24	115,115,115,115	0
55	MG	1G	1611	1/1	0.84	0.38	112,112,112,112	0
55	MG	1H	3200	1/1	0.84	0.38	88,88,88,88	0
55	MG	13	1640	1/1	0.84	0.22	99,99,99,99	0
55	MG	14	3063	1/1	0.84	0.29	82,82,82,82	0
55	MG	1H	3320	1/1	0.84	0.25	127,127,127,127	0
55	MG	13	1695	1/1	0.84	0.14	139,139,139,139	0
55	MG	1H	3335	1/1	0.84	0.28	134,134,134,134	0
55	MG	1G	1725	1/1	0.84	0.09	130,130,130,130	0
55	MG	13	1736	1/1	0.84	0.15	137,137,137,137	0
55	MG	1H	3182	1/1	0.84	0.53	114,114,114,114	0
55	MG	1H	3313	1/1	0.84	0.26	112,112,112,112	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
55	MG	1H	3001	1/1	0.84	0.21	53,53,53,53	0
55	MG	1H	3421	1/1	0.84	0.14	113,113,113,113	0
55	MG	14	3291	1/1	0.84	0.24	114,114,114,114	0
55	MG	1H	3422	1/1	0.84	0.06	121,121,121,121	0
55	MG	1H	3196	1/1	0.84	0.56	107,107,107,107	0
55	MG	14	3111	1/1	0.84	0.46	110,110,110,110	0
55	MG	14	3088	1/1	0.84	0.17	109,109,109,109	0
55	MG	14	3191	1/1	0.85	0.19	102,102,102,102	0
55	MG	1H	3445	1/1	0.85	0.19	91,91,91,91	0
55	MG	1G	1622	1/1	0.85	0.18	104,104,104,104	0
55	MG	1H	3463	1/1	0.85	0.06	110,110,110,110	0
55	MG	13	1702	1/1	0.85	0.17	110,110,110,110	0
55	MG	1G	1684	1/1	0.85	0.37	89,89,89,89	0
55	MG	14	3013	1/1	0.85	0.18	96,96,96,96	0
55	MG	1H	3330	1/1	0.85	0.11	78,78,78,78	0
55	MG	1H	3071	1/1	0.85	0.55	72,72,72,72	0
55	MG	14	3011	1/1	0.85	0.29	66,66,66,66	0
55	MG	1H	3449	1/1	0.85	0.17	99,99,99,99	0
55	MG	1G	1699	1/1	0.85	0.31	121,121,121,121	0
55	MG	1H	3040	1/1	0.85	0.23	58,58,58,58	0
55	MG	1H	3027	1/1	0.85	0.12	75,75,75,75	0
55	MG	14	3114	1/1	0.85	0.24	101,101,101,101	0
55	MG	1G	1713	1/1	0.85	0.10	144,144,144,144	0
55	MG	14	3143	1/1	0.85	0.19	97,97,97,97	0
55	MG	13	1656	1/1	0.85	0.13	124,124,124,124	0
55	MG	14	3284	1/1	0.85	0.10	98,98,98,98	0
55	MG	14	3106	1/1	0.85	1.18	90,90,90,90	0
55	MG	1H	3256	1/1	0.85	0.26	53,53,53,53	0
55	MG	1H	3394	1/1	0.86	0.15	75,75,75,75	0
55	MG	1H	3302	1/1	0.86	0.11	120,120,120,120	0
55	MG	13	1607	1/1	0.86	0.22	110,110,110,110	0
55	MG	13	1723	1/1	0.86	0.13	103,103,103,103	0
55	MG	13	1688	1/1	0.86	0.16	122,122,122,122	0
55	MG	1H	3418	1/1	0.86	0.09	99,99,99,99	0
55	MG	1G	1708	1/1	0.86	0.21	100,100,100,100	0
55	MG	1H	3055	1/1	0.86	0.39	91,91,91,91	0
55	MG	14	3165	1/1	0.86	0.55	83,83,83,83	0
55	MG	14	3145	1/1	0.86	0.19	86,86,86,86	0
55	MG	1H	3161	1/1	0.86	0.33	86,86,86,86	0
55	MG	1H	3328	1/1	0.86	0.21	114,114,114,114	0
55	MG	1H	3405	1/1	0.86	0.12	108,108,108,108	0
55	MG	1H	3456	1/1	0.86	0.10	111,111,111,111	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
55	MG	1H	3264	1/1	0.86	0.19	72,72,72,72	0
55	MG	14	3105	1/1	0.86	0.25	81,81,81,81	0
55	MG	1H	3153	1/1	0.86	0.44	91,91,91,91	0
55	MG	13	1634	1/1	0.86	0.26	120,120,120,120	0
55	MG	1H	3451	1/1	0.86	0.23	81,81,81,81	0
55	MG	14	3136	1/1	0.86	0.40	120,120,120,120	0
55	MG	13	1653	1/1	0.86	0.46	120,120,120,120	0
55	MG	1H	3311	1/1	0.86	0.32	97,97,97,97	0
55	MG	14	3257	1/1	0.86	0.14	99,99,99,99	0
55	MG	1H	3022	1/1	0.86	0.29	77,77,77,77	0
55	MG	1G	1690	1/1	0.86	0.05	144,144,144,144	0
55	MG	1H	3018	1/1	0.86	0.20	68,68,68,68	0
55	MG	4A	201	1/1	0.86	0.15	136,136,136,136	0
55	MG	1H	3168	1/1	0.86	0.23	109,109,109,109	0
55	MG	1G	1642	1/1	0.86	0.43	154,154,154,154	0
55	MG	1H	3268	1/1	0.86	0.43	74,74,74,74	0
55	MG	1H	3284	1/1	0.87	0.19	60,60,60,60	0
55	MG	1H	3065	1/1	0.87	0.38	87,87,87,87	0
55	MG	1H	3019	1/1	0.87	0.31	57,57,57,57	0
55	MG	1H	3106	1/1	0.87	0.15	100,100,100,100	0
55	MG	1H	3134	1/1	0.87	0.38	61,61,61,61	0
55	MG	13	1617	1/1	0.87	0.22	92,92,92,92	0
55	MG	13	1704	1/1	0.87	0.26	147,147,147,147	0
55	MG	F5	101	1/1	0.87	0.27	82,82,82,82	0
55	MG	1G	1674	1/1	0.87	0.11	89,89,89,89	0
55	MG	14	3292	1/1	0.87	0.27	103,103,103,103	0
55	MG	13	1722	1/1	0.87	0.13	106,106,106,106	0
55	MG	1G	1711	1/1	0.87	0.07	139,139,139,139	0
55	MG	1H	3322	1/1	0.87	0.53	124,124,124,124	0
55	MG	1J	201	1/1	0.87	0.16	106,106,106,106	0
55	MG	1G	1601	1/1	0.87	0.12	101,101,101,101	0
55	MG	1H	3123	1/1	0.87	0.22	79,79,79,79	0
55	MG	14	3254	1/1	0.87	0.10	108,108,108,108	0
55	MG	1H	3462	1/1	0.87	0.08	106,106,106,106	0
55	MG	1H	3373	1/1	0.87	0.12	106,106,106,106	0
55	MG	1H	3416	1/1	0.87	0.07	119,119,119,119	0
55	MG	14	3119	1/1	0.87	0.23	101,101,101,101	0
55	MG	BI	201	1/1	0.87	0.24	110,110,110,110	0
55	MG	1H	3191	1/1	0.87	0.12	93,93,93,93	0
55	MG	14	3214	1/1	0.87	0.27	96,96,96,96	0
55	MG	1H	3172	1/1	0.87	0.12	101,101,101,101	0
55	MG	14	3146	1/1	0.87	0.25	92,92,92,92	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
55	MG	13	1690	1/1	0.87	0.32	123,123,123,123	0
55	MG	13	1651	1/1	0.87	0.30	110,110,110,110	0
55	MG	14	3142	1/1	0.87	0.38	105,105,105,105	0
55	MG	1H	3074	1/1	0.87	0.27	65,65,65,65	0
55	MG	1H	3346	1/1	0.87	0.12	63,63,63,63	0
55	MG	1H	3293	1/1	0.87	0.10	124,124,124,124	0
55	MG	1H	3210	1/1	0.87	0.61	90,90,90,90	0
55	MG	13	1709	1/1	0.87	0.35	147,147,147,147	0
55	MG	14	3085	1/1	0.87	1.14	94,94,94,94	0
55	MG	13	1740	1/1	0.87	0.21	123,123,123,123	0
55	MG	1H	3195	1/1	0.87	0.13	114,114,114,114	0
55	MG	14	3021	1/1	0.88	0.49	90,90,90,90	0
55	MG	14	3207	1/1	0.88	0.26	117,117,117,117	0
55	MG	14	3286	1/1	0.88	0.08	97,97,97,97	0
55	MG	1G	1724	1/1	0.88	0.13	120,120,120,120	0
55	MG	1H	3122	1/1	0.88	0.24	98,98,98,98	0
55	MG	13	1616	1/1	0.88	0.21	93,93,93,93	0
55	MG	14	3018	1/1	0.88	0.72	84,84,84,84	0
55	MG	13	1678	1/1	0.88	0.74	116,116,116,116	0
55	MG	13	1735	1/1	0.88	0.10	100,100,100,100	0
55	MG	14	3090	1/1	0.88	0.31	69,69,69,69	0
55	MG	14	3080	1/1	0.88	0.23	90,90,90,90	0
55	MG	1H	3115	1/1	0.88	0.32	76,76,76,76	0
55	MG	14	3028	1/1	0.88	0.27	114,114,114,114	0
55	MG	1H	3231	1/1	0.88	0.18	65,65,65,65	0
55	MG	1G	1666	1/1	0.88	0.48	136,136,136,136	0
55	MG	1H	3129	1/1	0.88	0.34	92,92,92,92	0
55	MG	1H	3189	1/1	0.88	0.26	71,71,71,71	0
55	MG	1H	3198	1/1	0.88	0.25	68,68,68,68	0
55	MG	14	3250	1/1	0.88	0.22	99,99,99,99	0
55	MG	1H	3204	1/1	0.88	0.28	80,80,80,80	0
55	MG	1H	3332	1/1	0.88	0.25	125,125,125,125	0
55	MG	1H	3193	1/1	0.88	0.27	73,73,73,73	0
55	MG	14	3006	1/1	0.88	0.16	91,91,91,91	0
55	MG	1H	3118	1/1	0.88	0.15	89,89,89,89	0
55	MG	13	1685	1/1	0.88	0.22	107,107,107,107	0
55	MG	1H	3192	1/1	0.88	0.15	114,114,114,114	0
55	MG	1H	3240	1/1	0.88	0.54	114,114,114,114	0
55	MG	1G	1720	1/1	0.88	0.09	152,152,152,152	0
55	MG	14	3289	1/1	0.88	0.13	84,84,84,84	0
55	MG	1H	3324	1/1	0.89	0.39	115,115,115,115	0
55	MG	1H	3353	1/1	0.89	0.09	59,59,59,59	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
55	MG	1H	3044	1/1	0.89	0.60	72,72,72,72	0
55	MG	14	3162	1/1	0.89	0.30	57,57,57,57	0
55	MG	14	3285	1/1	0.89	0.16	99,99,99,99	0
55	MG	13	1666	1/1	0.89	0.10	115,115,115,115	0
55	MG	14	3217	1/1	0.89	0.09	97,97,97,97	0
55	MG	13	1628	1/1	0.89	0.35	120,120,120,120	0
55	MG	78	202	1/1	0.89	0.35	55,55,55,55	0
55	MG	1G	1612	1/1	0.89	0.24	85,85,85,85	0
55	MG	1H	3285	1/1	0.89	0.26	89,89,89,89	0
55	MG	13	1619	1/1	0.89	0.19	86,86,86,86	0
55	MG	1H	3006	1/1	0.89	0.36	49,49,49,49	0
55	MG	13	1614	1/1	0.89	0.13	100,100,100,100	0
55	MG	1H	3155	1/1	0.89	0.32	78,78,78,78	0
55	MG	1G	1665	1/1	0.89	0.28	130,130,130,130	0
55	MG	1G	1635	1/1	0.89	0.14	139,139,139,139	0
55	MG	1H	3110	1/1	0.89	0.28	93,93,93,93	0
55	MG	13	1661	1/1	0.89	0.39	117,117,117,117	0
55	MG	1H	3436	1/1	0.89	0.31	96,96,96,96	0
55	MG	1H	3397	1/1	0.89	0.07	81,81,81,81	0
55	MG	1G	1607	1/1	0.89	0.30	94,94,94,94	0
55	MG	13	1633	1/1	0.89	0.24	85,85,85,85	0
55	MG	1G	1639	1/1	0.89	0.12	106,106,106,106	0
55	MG	14	3204	1/1	0.89	0.13	106,106,106,106	0
55	MG	1H	3197	1/1	0.89	0.27	77,77,77,77	0
55	MG	1H	3461	1/1	0.89	0.17	119,119,119,119	0
55	MG	1H	3081	1/1	0.89	0.27	72,72,72,72	0
55	MG	13	1698	1/1	0.89	0.27	138,138,138,138	0
55	MG	1H	3041	1/1	0.89	0.14	65,65,65,65	0
55	MG	1H	3280	1/1	0.89	0.28	73,73,73,73	0
55	MG	1H	3447	1/1	0.89	0.08	102,102,102,102	0
55	MG	1H	3224	1/1	0.89	0.13	102,102,102,102	0
55	MG	1H	3383	1/1	0.89	0.11	60,60,60,60	0
55	MG	14	3140	1/1	0.89	0.17	86,86,86,86	0
55	MG	14	3172	1/1	0.89	0.29	100,100,100,100	0
55	MG	1H	3117	1/1	0.89	0.15	88,88,88,88	0
55	MG	16	202	1/1	0.89	0.14	118,118,118,118	0
55	MG	1H	3083	1/1	0.89	0.40	85,85,85,85	0
55	MG	14	3003	1/1	0.89	0.11	85,85,85,85	0
55	MG	1H	3334	1/1	0.89	0.17	94,94,94,94	0
55	MG	1H	3211	1/1	0.89	0.34	93,93,93,93	0
55	MG	1H	3147	1/1	0.89	0.30	54,54,54,54	0
55	MG	13	1622	1/1	0.90	0.17	88,88,88,88	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
55	MG	14	3132	1/1	0.90	0.96	100,100,100,100	0
55	MG	1H	3151	1/1	0.90	0.28	100,100,100,100	0
55	MG	14	3243	1/1	0.90	0.11	116,116,116,116	0
55	MG	13	1608	1/1	0.90	0.12	131,131,131,131	0
55	MG	1H	3283	1/1	0.90	0.41	83,83,83,83	0
55	MG	1H	3243	1/1	0.90	0.20	85,85,85,85	0
55	MG	14	3202	1/1	0.90	0.22	106,106,106,106	0
55	MG	1H	3156	1/1	0.90	0.31	75,75,75,75	0
55	MG	14	3246	1/1	0.90	0.12	105,105,105,105	0
55	MG	1H	3336	1/1	0.90	0.08	127,127,127,127	0
55	MG	1H	3260	1/1	0.90	0.23	53,53,53,53	0
55	MG	13	1696	1/1	0.90	0.14	117,117,117,117	0
55	MG	42	201	1/1	0.90	0.28	115,115,115,115	0
55	MG	1H	3160	1/1	0.90	0.21	81,81,81,81	0
55	MG	13	1655	1/1	0.90	0.15	95,95,95,95	0
55	MG	14	3020	1/1	0.90	0.39	81,81,81,81	0
55	MG	1H	3038	1/1	0.90	0.18	83,83,83,83	0
55	MG	13	1713	1/1	0.90	0.12	81,81,81,81	0
55	MG	1H	3396	1/1	0.90	0.14	64,64,64,64	0
55	MG	13	1621	1/1	0.90	0.14	117,117,117,117	0
55	MG	1G	1679	1/1	0.90	0.23	79,79,79,79	0
55	MG	13	1697	1/1	0.90	0.06	146,146,146,146	0
55	MG	13	1605	1/1	0.90	0.26	122,122,122,122	0
55	MG	13	1707	1/1	0.90	0.18	133,133,133,133	0
55	MG	1H	3384	1/1	0.90	0.10	76,76,76,76	0
55	MG	14	3059	1/1	0.90	0.25	105,105,105,105	0
55	MG	1H	3031	1/1	0.90	0.25	83,83,83,83	0
55	MG	1H	3455	1/1	0.90	0.13	85,85,85,85	0
55	MG	1H	3131	1/1	0.90	0.24	73,73,73,73	0
55	MG	14	3084	1/1	0.90	0.26	91,91,91,91	0
55	MG	13	1680	1/1	0.90	0.21	108,108,108,108	0
55	MG	1H	3412	1/1	0.90	0.19	128,128,128,128	0
55	MG	1F	101	1/1	0.90	0.12	107,107,107,107	0
55	MG	1H	3410	1/1	0.90	0.13	95,95,95,95	0
55	MG	14	3220	1/1	0.90	0.09	84,84,84,84	0
55	MG	1H	3003	1/1	0.90	0.14	49,49,49,49	0
55	MG	1H	3136	1/1	0.90	0.43	87,87,87,87	0
55	MG	13	1604	1/1	0.91	0.26	87,87,87,87	0
55	MG	88	202	1/1	0.91	0.98	62,62,62,62	0
55	MG	1G	1655	1/1	0.91	0.13	84,84,84,84	0
55	MG	1H	3420	1/1	0.91	0.10	96,96,96,96	0
55	MG	1H	3348	1/1	0.91	0.12	54,54,54,54	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
55	MG	1H	3030	1/1	0.91	0.47	77,77,77,77	0
55	MG	13	1718	1/1	0.91	0.07	113,113,113,113	0
55	MG	1G	1609	1/1	0.91	0.49	105,105,105,105	0
55	MG	1G	1675	1/1	0.91	0.20	77,77,77,77	0
55	MG	13	1643	1/1	0.91	0.23	124,124,124,124	0
55	MG	1G	1712	1/1	0.91	0.14	131,131,131,131	0
55	MG	1H	3140	1/1	0.91	0.25	80,80,80,80	0
55	MG	1H	3169	1/1	0.91	0.47	75,75,75,75	0
55	MG	1H	3473	1/1	0.91	0.09	74,74,74,74	0
55	MG	1H	3454	1/1	0.91	0.21	109,109,109,109	0
55	MG	1H	3162	1/1	0.91	0.18	87,87,87,87	0
55	MG	14	3279	1/1	0.91	0.07	107,107,107,107	0
55	MG	2A	201	1/1	0.91	0.09	101,101,101,101	0
55	MG	14	3061	1/1	0.91	0.30	92,92,92,92	0
55	MG	14	3007	1/1	0.91	0.15	97,97,97,97	0
55	MG	1H	3203	1/1	0.91	0.27	81,81,81,81	0
55	MG	1H	3187	1/1	0.91	0.26	99,99,99,99	0
55	MG	14	3077	1/1	0.91	0.25	89,89,89,89	0
55	MG	41	201	1/1	0.91	0.17	88,88,88,88	0
55	MG	1H	3130	1/1	0.91	0.36	66,66,66,66	0
55	MG	1H	3309	1/1	0.91	0.10	108,108,108,108	0
55	MG	1H	3417	1/1	0.91	0.13	108,108,108,108	0
55	MG	14	3152	1/1	0.91	0.24	90,90,90,90	0
55	MG	1H	3291	1/1	0.91	0.09	98,98,98,98	0
55	MG	13	1712	1/1	0.91	0.11	96,96,96,96	0
55	MG	1H	3190	1/1	0.91	0.11	106,106,106,106	0
55	MG	1G	1638	1/1	0.91	0.11	151,151,151,151	0
55	MG	1H	3329	1/1	0.91	0.09	119,119,119,119	0
55	MG	1H	3466	1/1	0.91	0.19	111,111,111,111	0
55	MG	1G	1626	1/1	0.91	0.13	100,100,100,100	0
55	MG	1H	3437	1/1	0.91	0.21	95,95,95,95	0
55	MG	14	3161	1/1	0.91	0.18	73,73,73,73	0
55	MG	14	3248	1/1	0.91	0.09	86,86,86,86	0
55	MG	1H	3317	1/1	0.91	0.05	106,106,106,106	0
55	MG	1G	1686	1/1	0.91	0.31	112,112,112,112	0
55	MG	1H	3308	1/1	0.91	0.22	107,107,107,107	0
55	MG	13	1642	1/1	0.91	0.06	149,149,149,149	0
55	MG	13	1714	1/1	0.91	0.07	121,121,121,121	0
55	MG	13	1677	1/1	0.91	0.23	100,100,100,100	0
55	MG	1G	1696	1/1	0.91	0.08	137,137,137,137	0
55	MG	1H	3064	1/1	0.92	0.30	85,85,85,85	0
55	MG	1H	3272	1/1	0.92	0.37	83,83,83,83	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
55	MG	14	3151	1/1	0.92	0.22	96,96,96,96	0
55	MG	14	3195	1/1	0.92	0.14	67,67,67,67	0
55	MG	14	3265	1/1	0.92	0.09	65,65,65,65	0
55	MG	1H	3007	1/1	0.92	0.23	62,62,62,62	0
55	MG	14	3244	1/1	0.92	0.08	105,105,105,105	0
55	MG	13	1726	1/1	0.92	0.21	103,103,103,103	0
55	MG	1H	3305	1/1	0.92	0.21	110,110,110,110	0
55	MG	14	3044	1/1	0.92	0.17	85,85,85,85	0
55	MG	13	1601	1/1	0.92	0.15	77,77,77,77	0
55	MG	1H	3296	1/1	0.92	0.17	122,122,122,122	0
55	MG	1J	202	1/1	0.92	0.13	129,129,129,129	0
55	MG	14	3272	1/1	0.92	0.08	93,93,93,93	0
55	MG	13	1644	1/1	0.92	0.14	109,109,109,109	0
55	MG	14	3193	1/1	0.92	0.08	87,87,87,87	0
55	MG	13	1657	1/1	0.92	0.14	123,123,123,123	0
55	MG	14	3237	1/1	0.92	0.22	96,96,96,96	0
55	MG	13	1618	1/1	0.92	0.17	115,115,115,115	0
55	MG	1H	3271	1/1	0.92	0.23	82,82,82,82	0
55	MG	13	1687	1/1	0.92	0.27	88,88,88,88	0
55	MG	1G	1694	1/1	0.92	0.08	151,151,151,151	0
55	MG	13	1720	1/1	0.92	0.13	117,117,117,117	0
55	MG	1H	3158	1/1	0.92	0.18	92,92,92,92	0
55	MG	1H	3167	1/1	0.92	0.40	93,93,93,93	0
55	MG	14	3104	1/1	0.92	0.12	91,91,91,91	0
55	MG	1H	3105	1/1	0.92	0.16	93,93,93,93	0
55	MG	14	3117	1/1	0.92	0.17	91,91,91,91	0
55	MG	1H	3341	1/1	0.92	0.09	129,129,129,129	0
55	MG	14	3253	1/1	0.92	0.16	83,83,83,83	0
55	MG	1H	3292	1/1	0.92	0.07	103,103,103,103	0
55	MG	14	3183	1/1	0.92	0.31	99,99,99,99	0
55	MG	1H	3344	1/1	0.92	0.07	72,72,72,72	0
55	MG	1H	3103	1/1	0.92	0.18	77,77,77,77	0
55	MG	13	1710	1/1	0.92	0.34	143,143,143,143	0
55	MG	1H	3319	1/1	0.92	0.07	123,123,123,123	0
55	MG	14	3120	1/1	0.92	0.22	106,106,106,106	0
55	MG	1H	3448	1/1	0.92	0.10	72,72,72,72	0
55	MG	14	3241	1/1	0.92	0.08	86,86,86,86	0
55	MG	14	3206	1/1	0.92	0.32	131,131,131,131	0
55	MG	1G	1716	1/1	0.92	0.08	123,123,123,123	0
55	MG	13	1610	1/1	0.92	0.08	130,130,130,130	0
55	MG	1H	3431	1/1	0.92	0.10	62,62,62,62	0
55	MG	14	3216	1/1	0.92	0.10	68,68,68,68	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
55	MG	14	3072	1/1	0.92	0.18	91,91,91,91	0
55	MG	1H	3404	1/1	0.92	0.11	76,76,76,76	0
55	MG	14	3270	1/1	0.92	0.17	85,85,85,85	0
55	MG	14	3036	1/1	0.92	0.18	80,80,80,80	0
55	MG	14	3115	1/1	0.92	0.23	103,103,103,103	0
55	MG	1G	1634	1/1	0.92	0.06	109,109,109,109	0
55	MG	1H	3403	1/1	0.92	0.10	87,87,87,87	0
55	MG	14	3300	1/1	0.92	0.14	140,140,140,140	0
55	MG	1H	3028	1/1	0.92	0.15	80,80,80,80	0
55	MG	1H	3248	1/1	0.92	0.33	86,86,86,86	0
55	MG	1G	1615	1/1	0.92	0.21	141,141,141,141	0
55	MG	13	1620	1/1	0.92	0.14	70,70,70,70	0
55	MG	1G	1687	1/1	0.92	0.12	108,108,108,108	0
55	MG	1H	3135	1/1	0.92	0.26	75,75,75,75	0
55	MG	14	3198	1/1	0.92	0.34	109,109,109,109	0
55	MG	1G	1700	1/1	0.93	0.20	142,142,142,142	0
55	MG	14	3181	1/1	0.93	0.65	71,71,71,71	0
55	MG	1F	102	1/1	0.93	0.92	125,125,125,125	0
55	MG	14	3293	1/1	0.93	0.11	130,130,130,130	0
55	MG	14	3123	1/1	0.93	0.23	99,99,99,99	0
55	MG	1H	3258	1/1	0.93	0.22	73,73,73,73	0
55	MG	14	3245	1/1	0.93	0.07	117,117,117,117	0
55	MG	1H	3051	1/1	0.93	0.19	95,95,95,95	0
55	MG	1H	3014	1/1	0.93	0.25	64,64,64,64	0
55	MG	1H	3426	1/1	0.93	0.27	97,97,97,97	0
55	MG	1H	3206	1/1	0.93	0.23	108,108,108,108	0
55	MG	1H	3188	1/1	0.93	0.17	91,91,91,91	0
55	MG	2L	101	1/1	0.93	0.15	147,147,147,147	0
55	MG	14	3030	1/1	0.93	0.25	110,110,110,110	0
55	MG	14	3071	1/1	0.93	0.13	84,84,84,84	0
55	MG	1G	1718	1/1	0.93	0.14	112,112,112,112	0
55	MG	14	3014	1/1	0.93	0.18	78,78,78,78	0
55	MG	14	3149	1/1	0.93	0.12	61,61,61,61	0
55	MG	13	1737	1/1	0.93	0.20	111,111,111,111	0
55	MG	14	3168	1/1	0.93	0.22	72,72,72,72	0
55	MG	1H	3267	1/1	0.93	0.31	67,67,67,67	0
55	MG	1H	3170	1/1	0.93	0.51	80,80,80,80	0
55	MG	14	3294	1/1	0.93	0.09	117,117,117,117	0
55	MG	1H	3004	1/1	0.93	0.21	64,64,64,64	0
55	MG	14	3236	1/1	0.93	0.11	98,98,98,98	0
55	MG	1H	3438	1/1	0.93	0.13	93,93,93,93	0
55	MG	13	1654	1/1	0.93	0.26	81,81,81,81	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
55	MG	1H	3458	1/1	0.93	0.06	126,126,126,126	0
55	MG	13	1700	1/1	0.93	0.07	151,151,151,151	0
55	MG	1H	3427	1/1	0.93	0.15	68,68,68,68	0
55	MG	14	3048	1/1	0.93	0.26	94,94,94,94	0
55	MG	14	3287	1/1	0.93	0.10	110,110,110,110	0
55	MG	1H	3401	1/1	0.93	0.15	72,72,72,72	0
55	MG	1H	3087	1/1	0.93	0.30	74,74,74,74	0
55	MG	14	3268	1/1	0.93	0.06	82,82,82,82	0
55	MG	32	301	1/1	0.93	0.12	138,138,138,138	0
55	MG	1H	3099	1/1	0.93	0.34	79,79,79,79	0
55	MG	1H	3052	1/1	0.93	0.16	64,64,64,64	0
55	MG	1G	1717	1/1	0.93	0.07	137,137,137,137	0
55	MG	1H	3069	1/1	0.93	0.23	77,77,77,77	0
55	MG	13	1719	1/1	0.93	0.08	107,107,107,107	0
55	MG	13	1635	1/1	0.93	0.40	82,82,82,82	0
55	MG	1H	3173	1/1	0.93	0.14	94,94,94,94	0
55	MG	1H	3450	1/1	0.93	0.10	132,132,132,132	0
55	MG	1H	3321	1/1	0.93	0.24	123,123,123,123	0
55	MG	14	3258	1/1	0.93	0.06	97,97,97,97	0
55	MG	14	3047	1/1	0.93	0.37	83,83,83,83	0
55	MG	1G	1698	1/1	0.93	0.23	176,176,176,176	0
55	MG	14	3118	1/1	0.93	0.15	99,99,99,99	0
55	MG	14	3179	1/1	0.93	0.21	70,70,70,70	0
55	MG	1G	1676	1/1	0.93	0.10	83,83,83,83	0
55	MG	13	1669	1/1	0.93	0.09	100,100,100,100	0
55	MG	88	201	1/1	0.93	0.10	94,94,94,94	0
55	MG	14	3130	1/1	0.93	0.08	106,106,106,106	0
55	MG	1G	1673	1/1	0.93	0.42	93,93,93,93	0
55	MG	13	1734	1/1	0.93	0.33	133,133,133,133	0
55	MG	1H	3440	1/1	0.93	0.14	54,54,54,54	0
55	MG	14	3064	1/1	0.93	0.32	80,80,80,80	0
55	MG	14	3171	1/1	0.94	0.20	98,98,98,98	0
55	MG	14	3205	1/1	0.94	0.22	118,118,118,118	0
55	MG	1H	3385	1/1	0.94	0.09	63,63,63,63	0
55	MG	13	1692	1/1	0.94	0.17	107,107,107,107	0
55	MG	14	3233	1/1	0.94	0.10	89,89,89,89	0
55	MG	13	1691	1/1	0.94	0.16	113,113,113,113	0
55	MG	1H	3286	1/1	0.94	0.26	67,67,67,67	0
55	MG	1H	3095	1/1	0.94	0.35	63,63,63,63	0
55	MG	39	301	1/1	0.94	0.18	109,109,109,109	0
55	MG	14	3224	1/1	0.94	0.09	84,84,84,84	0
55	MG	14	3134	1/1	0.94	0.59	105,105,105,105	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
55	MG	1H	3102	1/1	0.94	0.30	105,105,105,105	0
55	MG	13	1665	1/1	0.94	0.20	115,115,115,115	0
55	MG	1H	3303	1/1	0.94	0.11	98,98,98,98	0
55	MG	1G	1707	1/1	0.94	0.20	122,122,122,122	0
55	MG	1H	3345	1/1	0.94	0.10	63,63,63,63	0
55	MG	14	3103	1/1	0.94	0.26	113,113,113,113	0
55	MG	1H	3132	1/1	0.94	0.25	79,79,79,79	0
55	MG	1H	3053	1/1	0.94	0.17	77,77,77,77	0
55	MG	14	3173	1/1	0.94	0.34	66,66,66,66	0
55	MG	14	3288	1/1	0.94	0.40	86,86,86,86	0
55	MG	1G	1636	1/1	0.94	0.17	123,123,123,123	0
55	MG	1H	3247	1/1	0.94	0.17	101,101,101,101	0
55	MG	14	3175	1/1	0.94	0.14	85,85,85,85	0
55	MG	1H	3057	1/1	0.94	0.25	57,57,57,57	0
55	MG	14	3197	1/1	0.94	0.29	114,114,114,114	0
55	MG	1H	3282	1/1	0.94	0.41	101,101,101,101	0
55	MG	14	3022	1/1	0.94	0.47	91,91,91,91	0
55	MG	1H	3043	1/1	0.94	0.14	72,72,72,72	0
55	MG	1H	3277	1/1	0.94	0.38	103,103,103,103	0
55	MG	1H	3020	1/1	0.94	0.12	77,77,77,77	0
55	MG	1H	3100	1/1	0.94	0.28	65,65,65,65	0
55	MG	1G	1633	1/1	0.94	0.41	96,96,96,96	0
55	MG	13	1662	1/1	0.94	0.08	99,99,99,99	0
55	MG	1H	3467	1/1	0.94	0.05	106,106,106,106	0
55	MG	1H	3347	1/1	0.94	0.18	65,65,65,65	0
55	MG	1H	3295	1/1	0.94	0.29	83,83,83,83	0
55	MG	1H	3360	1/1	0.94	0.20	62,62,62,62	0
55	MG	1H	3005	1/1	0.94	0.18	51,51,51,51	0
55	MG	14	3160	1/1	0.94	0.40	86,86,86,86	0
55	MG	14	3091	1/1	0.94	0.19	105,105,105,105	0
55	MG	14	3087	1/1	0.94	0.79	66,66,66,66	0
55	MG	D8	201	1/1	0.94	0.40	84,84,84,84	0
55	MG	16	201	1/1	0.94	0.22	92,92,92,92	0
55	MG	1H	3042	1/1	0.94	0.25	96,96,96,96	0
55	MG	1H	3350	1/1	0.94	0.14	71,71,71,71	0
55	MG	13	1725	1/1	0.94	0.15	119,119,119,119	0
55	MG	1H	3382	1/1	0.94	0.12	93,93,93,93	0
55	MG	14	3227	1/1	0.94	0.11	79,79,79,79	0
55	MG	1H	3375	1/1	0.94	0.09	65,65,65,65	0
55	MG	14	3024	1/1	0.94	0.12	51,51,51,51	0
55	MG	14	3129	1/1	0.94	0.16	90,90,90,90	0
55	MG	1H	3304	1/1	0.94	0.16	96,96,96,96	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
55	MG	1H	3066	1/1	0.94	0.33	78,78,78,78	0
55	MG	13	1609	1/1	0.94	0.12	99,99,99,99	0
55	MG	14	3215	1/1	0.94	0.10	111,111,111,111	0
55	MG	1H	3400	1/1	0.94	0.30	78,78,78,78	0
55	MG	1H	3297	1/1	0.94	0.19	86,86,86,86	0
55	MG	14	3093	1/1	0.94	0.12	94,94,94,94	0
55	MG	1H	3094	1/1	0.94	0.15	95,95,95,95	0
55	MG	1H	3318	1/1	0.94	0.12	93,93,93,93	0
55	MG	14	3032	1/1	0.94	0.16	62,62,62,62	0
55	MG	1G	1689	1/1	0.94	0.19	125,125,125,125	0
55	MG	13	1672	1/1	0.94	0.15	123,123,123,123	0
55	MG	1H	3352	1/1	0.94	0.09	55,55,55,55	0
55	MG	14	3247	1/1	0.94	0.15	125,125,125,125	0
55	MG	14	3278	1/1	0.94	0.11	109,109,109,109	0
55	MG	14	3251	1/1	0.94	0.11	65,65,65,65	0
55	MG	1H	3242	1/1	0.94	0.27	94,94,94,94	0
55	MG	1G	1719	1/1	0.94	0.10	123,123,123,123	0
55	MG	1H	3201	1/1	0.94	0.16	68,68,68,68	0
55	MG	1H	3232	1/1	0.94	0.28	76,76,76,76	0
55	MG	13	1649	1/1	0.94	0.54	127,127,127,127	0
55	MG	14	3192	1/1	0.94	0.06	104,104,104,104	0
55	MG	1H	3026	1/1	0.94	0.72	82,82,82,82	0
55	MG	1H	3409	1/1	0.95	0.13	63,63,63,63	0
55	MG	13	1659	1/1	0.95	0.18	105,105,105,105	0
55	MG	1H	3011	1/1	0.95	0.17	48,48,48,48	0
55	MG	1H	3120	1/1	0.95	0.27	81,81,81,81	0
55	MG	14	3034	1/1	0.95	0.19	77,77,77,77	0
55	MG	1G	1710	1/1	0.95	0.07	125,125,125,125	0
55	MG	1H	3054	1/1	0.95	0.08	77,77,77,77	0
55	MG	14	3231	1/1	0.95	0.31	65,65,65,65	0
55	MG	P8	101	1/1	0.95	0.27	61,61,61,61	0
55	MG	1H	3469	1/1	0.95	0.20	110,110,110,110	0
55	MG	13	1684	1/1	0.95	0.12	89,89,89,89	0
55	MG	1H	3002	1/1	0.95	0.20	55,55,55,55	0
55	MG	14	3180	1/1	0.95	0.25	81,81,81,81	0
55	MG	1H	3245	1/1	0.95	0.51	76,76,76,76	0
55	MG	1H	3086	1/1	0.95	0.26	79,79,79,79	0
55	MG	13	1732	1/1	0.95	0.22	108,108,108,108	0
55	MG	14	3017	1/1	0.95	0.15	83,83,83,83	0
55	MG	13	1615	1/1	0.95	0.13	71,71,71,71	0
55	MG	14	3196	1/1	0.95	0.10	85,85,85,85	0
55	MG	14	3240	1/1	0.95	0.09	135,135,135,135	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
55	MG	13	1717	1/1	0.95	0.13	109,109,109,109	0
55	MG	1H	3228	1/1	0.95	0.43	86,86,86,86	0
55	MG	7A	101	1/1	0.95	0.12	116,116,116,116	0
55	MG	1G	1726	1/1	0.95	0.09	136,136,136,136	0
55	MG	1G	1658	1/1	0.95	0.19	114,114,114,114	0
55	MG	1H	3236	1/1	0.95	0.15	72,72,72,72	0
55	MG	14	3261	1/1	0.95	0.20	92,92,92,92	0
55	MG	13	1683	1/1	0.95	0.21	103,103,103,103	0
55	MG	1H	3355	1/1	0.95	0.09	83,83,83,83	0
55	MG	1H	3063	1/1	0.95	0.24	63,63,63,63	0
55	MG	1H	3012	1/1	0.95	0.13	47,47,47,47	0
55	MG	1H	3276	1/1	0.95	0.21	74,74,74,74	0
55	MG	1H	3217	1/1	0.95	0.24	43,43,43,43	0
55	MG	1G	1695	1/1	0.95	0.07	130,130,130,130	0
55	MG	1G	1625	1/1	0.95	0.30	118,118,118,118	0
55	MG	14	3127	1/1	0.95	0.27	64,64,64,64	0
55	MG	1H	3010	1/1	0.95	0.39	70,70,70,70	0
55	MG	1H	3159	1/1	0.95	0.27	79,79,79,79	0
55	MG	1H	3008	1/1	0.95	0.21	82,82,82,82	0
55	MG	14	3056	1/1	0.95	0.22	60,60,60,60	0
55	MG	13	1699	1/1	0.95	0.12	116,116,116,116	0
55	MG	1H	3316	1/1	0.95	0.05	115,115,115,115	0
55	MG	1H	3213	1/1	0.95	0.17	100,100,100,100	0
55	MG	1H	3046	1/1	0.95	0.19	69,69,69,69	0
55	MG	13	1613	1/1	0.95	0.22	129,129,129,129	0
55	MG	13	1645	1/1	0.95	0.13	97,97,97,97	0
55	MG	1H	3288	1/1	0.95	0.04	99,99,99,99	0
55	MG	14	3038	1/1	0.95	0.18	91,91,91,91	0
55	MG	14	3153	1/1	0.95	0.20	59,59,59,59	0
55	MG	1H	3225	1/1	0.95	0.21	109,109,109,109	0
55	MG	14	3274	1/1	0.95	0.09	110,110,110,110	0
55	MG	14	3280	1/1	0.95	0.12	101,101,101,101	0
55	MG	1H	3381	1/1	0.95	0.18	68,68,68,68	0
55	MG	1G	1678	1/1	0.95	0.34	99,99,99,99	0
55	MG	14	3053	1/1	0.95	0.22	91,91,91,91	0
55	MG	1H	3411	1/1	0.95	0.12	81,81,81,81	0
55	MG	14	3259	1/1	0.95	0.10	75,75,75,75	0
55	MG	1H	3393	1/1	0.95	0.09	79,79,79,79	0
55	MG	1H	3078	1/1	0.95	0.24	63,63,63,63	0
55	MG	1H	3251	1/1	0.95	0.38	87,87,87,87	0
55	MG	1H	3298	1/1	0.95	0.30	89,89,89,89	0
55	MG	14	3230	1/1	0.95	0.09	76,76,76,76	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
55	MG	14	3226	1/1	0.95	0.12	59,59,59,59	0
55	MG	1H	3371	1/1	0.95	0.18	85,85,85,85	0
55	MG	1H	3442	1/1	0.95	0.14	111,111,111,111	0
55	MG	14	3262	1/1	0.95	0.07	60,60,60,60	0
55	MG	1H	3058	1/1	0.95	0.23	58,58,58,58	0
55	MG	1G	1677	1/1	0.95	0.23	110,110,110,110	0
55	MG	14	3033	1/1	0.95	0.11	76,76,76,76	0
55	MG	14	3015	1/1	0.95	0.15	70,70,70,70	0
55	MG	1H	3047	1/1	0.95	0.22	66,66,66,66	0
55	MG	1H	3235	1/1	0.95	0.25	57,57,57,57	0
55	MG	14	3263	1/1	0.95	0.17	76,76,76,76	0
55	MG	13	1667	1/1	0.95	0.13	101,101,101,101	0
55	MG	14	3281	1/1	0.95	0.16	92,92,92,92	0
55	MG	14	3238	1/1	0.95	0.07	83,83,83,83	0
55	MG	14	3050	1/1	0.95	0.23	54,54,54,54	0
55	MG	14	3008	1/1	0.95	0.11	81,81,81,81	0
55	MG	1H	3299	1/1	0.95	0.10	84,84,84,84	0
55	MG	13	1728	1/1	0.95	0.09	114,114,114,114	0
55	MG	1H	3351	1/1	0.96	0.14	70,70,70,70	0
55	MG	1H	3432	1/1	0.96	0.07	71,71,71,71	0
55	MG	1H	3270	1/1	0.96	0.35	62,62,62,62	0
55	MG	14	3199	1/1	0.96	0.09	97,97,97,97	0
55	MG	13	1730	1/1	0.96	0.18	125,125,125,125	0
55	MG	1H	3433	1/1	0.96	0.09	87,87,87,87	0
55	MG	1H	3089	1/1	0.96	0.28	82,82,82,82	0
55	MG	1G	1709	1/1	0.96	0.06	127,127,127,127	0
55	MG	1H	3413	1/1	0.96	0.17	93,93,93,93	0
55	MG	1H	3365	1/1	0.96	0.11	82,82,82,82	0
55	MG	1H	3434	1/1	0.96	0.09	59,59,59,59	0
55	MG	1H	3349	1/1	0.96	0.10	67,67,67,67	0
55	MG	14	3025	1/1	0.96	0.13	90,90,90,90	0
55	MG	1H	3061	1/1	0.96	0.18	66,66,66,66	0
55	MG	14	3276	1/1	0.96	0.10	109,109,109,109	0
55	MG	1H	3101	1/1	0.96	0.20	89,89,89,89	0
55	MG	14	3212	1/1	0.96	0.09	67,67,67,67	0
55	MG	1H	3326	1/1	0.96	0.09	109,109,109,109	0
55	MG	14	3297	1/1	0.96	0.11	115,115,115,115	0
55	MG	1H	3364	1/1	0.96	0.10	74,74,74,74	0
55	MG	14	3208	1/1	0.96	0.15	70,70,70,70	0
55	MG	14	3156	1/1	0.96	0.28	80,80,80,80	0
55	MG	2K	101	1/1	0.96	0.31	71,71,71,71	0
55	MG	5I	102	1/1	0.96	0.43	119,119,119,119	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
55	MG	1H	3323	1/1	0.96	0.20	100,100,100,100	0
55	MG	13	1646	1/1	0.96	0.17	122,122,122,122	0
55	MG	1G	1721	1/1	0.96	0.09	123,123,123,123	0
55	MG	1H	3333	1/1	0.96	0.08	80,80,80,80	0
55	MG	14	3222	1/1	0.96	0.09	67,67,67,67	0
55	MG	14	3209	1/1	0.96	0.13	65,65,65,65	0
55	MG	BA	201	1/1	0.96	0.11	127,127,127,127	0
55	MG	14	3167	1/1	0.96	0.17	100,100,100,100	0
55	MG	14	3147	1/1	0.96	0.17	63,63,63,63	0
55	MG	1G	1628	1/1	0.96	0.21	118,118,118,118	0
55	MG	14	3239	1/1	0.96	0.13	106,106,106,106	0
55	MG	14	3100	1/1	0.96	0.10	91,91,91,91	0
55	MG	1H	3357	1/1	0.96	0.08	89,89,89,89	0
55	MG	1G	1688	1/1	0.96	0.11	94,94,94,94	0
55	MG	1G	1619	1/1	0.96	0.17	98,98,98,98	0
55	MG	14	3073	1/1	0.96	0.18	69,69,69,69	0
55	MG	1H	3016	1/1	0.96	0.09	62,62,62,62	0
55	MG	1H	3116	1/1	0.96	0.12	91,91,91,91	0
55	MG	1H	3377	1/1	0.96	0.11	58,58,58,58	0
55	MG	14	3101	1/1	0.96	0.17	88,88,88,88	0
55	MG	1H	3443	1/1	0.96	0.09	73,73,73,73	0
55	MG	1H	3079	1/1	0.96	0.34	71,71,71,71	0
55	MG	1H	3062	1/1	0.96	0.21	85,85,85,85	0
55	MG	13	1626	1/1	0.96	0.16	123,123,123,123	0
55	MG	1G	1617	1/1	0.96	0.18	91,91,91,91	0
55	MG	1H	3386	1/1	0.96	0.10	56,56,56,56	0
55	MG	14	3203	1/1	0.96	0.08	95,95,95,95	0
55	MG	1H	3290	1/1	0.96	0.17	79,79,79,79	0
55	MG	1H	3425	1/1	0.96	0.16	102,102,102,102	0
55	MG	13	1660	1/1	0.96	0.12	120,120,120,120	0
55	MG	14	3040	1/1	0.96	0.23	62,62,62,62	0
55	MG	1H	3073	1/1	0.96	0.22	74,74,74,74	0
55	MG	1H	3060	1/1	0.96	0.32	68,68,68,68	0
55	MG	14	3043	1/1	0.96	0.28	54,54,54,54	0
55	MG	14	3067	1/1	0.96	0.17	97,97,97,97	0
55	MG	1G	1602	1/1	0.96	0.09	109,109,109,109	0
55	MG	14	3283	1/1	0.96	0.05	106,106,106,106	0
55	MG	29	301	1/1	0.96	0.14	64,64,64,64	0
55	MG	14	3095	1/1	0.96	0.31	88,88,88,88	0
55	MG	14	3086	1/1	0.96	0.51	97,97,97,97	0
55	MG	1G	1704	1/1	0.96	0.16	130,130,130,130	0
55	MG	1H	3327	1/1	0.96	0.08	121,121,121,121	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
55	MG	1H	3092	1/1	0.96	0.18	92,92,92,92	0
55	MG	14	3158	1/1	0.96	0.22	51,51,51,51	0
55	MG	14	3005	1/1	0.96	0.28	85,85,85,85	0
55	MG	1H	3056	1/1	0.96	0.22	46,46,46,46	0
55	MG	1H	3262	1/1	0.96	0.27	74,74,74,74	0
55	MG	14	3211	1/1	0.96	0.08	84,84,84,84	0
55	MG	14	3065	1/1	0.96	0.19	68,68,68,68	0
55	MG	13	1716	1/1	0.96	0.05	103,103,103,103	0
55	MG	14	3299	1/1	0.96	0.21	89,89,89,89	0
55	MG	1H	3390	1/1	0.96	0.09	74,74,74,74	0
55	MG	1H	3259	1/1	0.96	0.30	53,53,53,53	0
55	MG	1H	3070	1/1	0.96	0.20	55,55,55,55	0
55	MG	13	1693	1/1	0.96	0.28	100,100,100,100	0
55	MG	1H	3109	1/1	0.96	0.11	109,109,109,109	0
55	MG	21	303	1/1	0.96	0.13	63,63,63,63	0
55	MG	13	1703	1/1	0.96	0.17	110,110,110,110	0
55	MG	85	201	1/1	0.96	0.40	72,72,72,72	0
55	MG	1H	3398	1/1	0.96	0.07	84,84,84,84	0
55	MG	14	3174	1/1	0.96	0.39	60,60,60,60	0
55	MG	1H	3374	1/1	0.96	0.11	47,47,47,47	0
55	MG	1H	3380	1/1	0.96	0.07	83,83,83,83	0
55	MG	1H	3157	1/1	0.96	0.38	73,73,73,73	0
55	MG	14	3260	1/1	0.96	0.20	110,110,110,110	0
55	MG	1G	1705	1/1	0.96	0.10	102,102,102,102	0
55	MG	1H	3468	1/1	0.96	0.51	88,88,88,88	0
55	MG	1G	1613	1/1	0.96	0.19	94,94,94,94	0
55	MG	13	1632	1/1	0.96	0.47	109,109,109,109	0
55	MG	14	3229	1/1	0.96	0.12	74,74,74,74	0
55	MG	14	3218	1/1	0.97	0.12	69,69,69,69	0
55	MG	1H	3370	1/1	0.97	0.13	59,59,59,59	0
55	MG	1H	3430	1/1	0.97	0.12	54,54,54,54	0
55	MG	14	3037	1/1	0.97	0.10	54,54,54,54	0
55	MG	1H	3453	1/1	0.97	0.13	99,99,99,99	0
55	MG	1H	3048	1/1	0.97	0.34	93,93,93,93	0
55	MG	1G	1631	1/1	0.97	0.09	95,95,95,95	0
55	MG	1H	3362	1/1	0.97	0.11	69,69,69,69	0
55	MG	1H	3356	1/1	0.97	0.11	59,59,59,59	0
55	MG	1H	3035	1/1	0.97	0.17	71,71,71,71	0
55	MG	1H	3367	1/1	0.97	0.11	92,92,92,92	0
55	MG	1H	3441	1/1	0.97	0.09	64,64,64,64	0
55	MG	1H	3108	1/1	0.97	0.42	58,58,58,58	0
55	MG	1H	3439	1/1	0.97	0.09	69,69,69,69	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
55	MG	14	3273	1/1	0.97	0.09	89,89,89,89	0
55	MG	13	1623	1/1	0.97	0.35	112,112,112,112	0
55	MG	14	3267	1/1	0.97	0.11	88,88,88,88	0
55	MG	1H	3444	1/1	0.97	0.10	50,50,50,50	0
55	MG	14	3155	1/1	0.97	0.38	92,92,92,92	0
55	MG	1H	3013	1/1	0.97	0.22	63,63,63,63	0
55	MG	1H	3338	1/1	0.97	0.30	105,105,105,105	0
55	MG	14	3249	1/1	0.97	0.07	110,110,110,110	0
55	MG	1H	3435	1/1	0.97	0.06	80,80,80,80	0
55	MG	1H	3230	1/1	0.97	0.24	73,73,73,73	0
55	MG	1H	3389	1/1	0.97	0.09	68,68,68,68	0
55	MG	1H	3414	1/1	0.97	0.08	82,82,82,82	0
55	MG	1G	1672	1/1	0.97	0.18	102,102,102,102	0
55	MG	14	3131	1/1	0.97	0.59	88,88,88,88	0
55	MG	14	3269	1/1	0.97	0.18	104,104,104,104	0
55	MG	1H	3152	1/1	0.97	0.29	49,49,49,49	0
55	MG	1H	3363	1/1	0.97	0.11	61,61,61,61	0
55	MG	14	3275	1/1	0.97	0.16	94,94,94,94	0
55	MG	1H	3294	1/1	0.97	0.59	83,83,83,83	0
55	MG	14	3054	1/1	0.97	0.07	113,113,113,113	0
55	MG	1H	3471	1/1	0.97	0.11	79,79,79,79	0
55	MG	1G	1702	1/1	0.97	0.13	83,83,83,83	0
55	MG	1H	3395	1/1	0.97	0.07	67,67,67,67	0
55	MG	14	3051	1/1	0.97	0.21	67,67,67,67	0
55	MG	1H	3314	1/1	0.97	0.07	113,113,113,113	0
55	MG	14	3089	1/1	0.97	0.16	79,79,79,79	0
55	MG	1H	3209	1/1	0.97	0.37	84,84,84,84	0
57	ZN	5A	101	1/1	0.97	0.07	159,159,159,159	0
55	MG	1H	3424	1/1	0.97	0.07	68,68,68,68	0
55	MG	1H	3266	1/1	0.97	0.19	64,64,64,64	0
55	MG	1H	3032	1/1	0.97	0.24	66,66,66,66	0
55	MG	1G	1653	1/1	0.97	0.17	103,103,103,103	0
55	MG	1H	3361	1/1	0.97	0.07	53,53,53,53	0
55	MG	1H	3289	1/1	0.97	0.20	102,102,102,102	0
55	MG	14	3223	1/1	0.97	0.09	81,81,81,81	0
55	MG	1H	3080	1/1	0.97	0.24	64,64,64,64	0
55	MG	14	3213	1/1	0.97	0.12	77,77,77,77	0
55	MG	1H	3097	1/1	0.97	0.29	66,66,66,66	0
55	MG	1H	3306	1/1	0.97	0.06	93,93,93,93	0
55	MG	14	3068	1/1	0.97	0.10	71,71,71,71	0
55	MG	1H	3366	1/1	0.97	0.14	75,75,75,75	0
55	MG	1H	3459	1/1	0.97	0.21	112,112,112,112	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
55	MG	14	3221	1/1	0.97	0.11	67,67,67,67	0
55	MG	14	3166	1/1	0.97	0.24	82,82,82,82	0
55	MG	13	1611	1/1	0.97	0.14	81,81,81,81	0
55	MG	1H	3146	1/1	0.97	0.10	80,80,80,80	0
55	MG	1H	3307	1/1	0.97	0.07	100,100,100,100	0
55	MG	1H	3075	1/1	0.97	0.23	72,72,72,72	0
55	MG	1H	3039	1/1	0.97	0.20	73,73,73,73	0
55	MG	1G	1664	1/1	0.97	0.10	105,105,105,105	0
55	MG	13	1689	1/1	0.97	0.43	85,85,85,85	0
55	MG	14	3023	1/1	0.97	0.05	99,99,99,99	0
55	MG	1H	3388	1/1	0.97	0.15	56,56,56,56	0
55	MG	1H	3415	1/1	0.97	0.06	88,88,88,88	0
55	MG	14	3235	1/1	0.97	0.21	73,73,73,73	0
55	MG	11	301	1/1	0.97	0.23	52,52,52,52	0
55	MG	1H	3023	1/1	0.97	0.21	85,85,85,85	0
55	MG	1H	3359	1/1	0.97	0.12	51,51,51,51	0
55	MG	1H	3227	1/1	0.97	0.14	61,61,61,61	0
55	MG	J8	101	1/1	0.97	0.43	74,74,74,74	0
55	MG	1H	3369	1/1	0.97	0.15	63,63,63,63	0
55	MG	13	1612	1/1	0.97	0.24	85,85,85,85	0
55	MG	1G	1605	1/1	0.97	0.17	98,98,98,98	0
55	MG	1H	3464	1/1	0.97	0.12	67,67,67,67	0
55	MG	1H	3077	1/1	0.97	0.18	60,60,60,60	0
55	MG	1G	1691	1/1	0.97	0.19	115,115,115,115	0
55	MG	14	3255	1/1	0.97	0.15	80,80,80,80	0
55	MG	14	3187	1/1	0.97	0.14	74,74,74,74	0
55	MG	14	3282	1/1	0.97	0.09	117,117,117,117	0
55	MG	1H	3407	1/1	0.98	0.06	76,76,76,76	0
55	MG	1H	3215	1/1	0.98	0.25	78,78,78,78	0
55	MG	1H	3379	1/1	0.98	0.10	76,76,76,76	0
55	MG	I8	101	1/1	0.98	0.19	87,87,87,87	0
55	MG	1H	3076	1/1	0.98	0.23	70,70,70,70	0
55	MG	1H	3218	1/1	0.98	0.16	95,95,95,95	0
55	MG	14	3052	1/1	0.98	0.15	64,64,64,64	0
55	MG	1H	3186	1/1	0.98	0.30	80,80,80,80	0
55	MG	1H	3059	1/1	0.98	0.15	78,78,78,78	0
55	MG	14	3055	1/1	0.98	0.12	80,80,80,80	0
55	MG	13	1731	1/1	0.98	0.25	79,79,79,79	0
55	MG	14	3157	1/1	0.98	0.19	61,61,61,61	0
55	MG	1H	3171	1/1	0.98	0.14	91,91,91,91	0
55	MG	1H	3150	1/1	0.98	0.24	79,79,79,79	0
55	MG	1G	1608	1/1	0.98	0.07	114,114,114,114	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
55	MG	1H	3222	1/1	0.98	0.11	101,101,101,101	0
55	MG	1H	3339	1/1	0.98	0.11	78,78,78,78	0
55	MG	78	201	1/1	0.98	0.37	90,90,90,90	0
55	MG	14	3225	1/1	0.98	0.09	63,63,63,63	0
55	MG	14	3264	1/1	0.98	0.17	88,88,88,88	0
55	MG	13	1727	1/1	0.98	0.26	100,100,100,100	0
55	MG	14	3126	1/1	0.98	0.24	48,48,48,48	0
55	MG	1H	3084	1/1	0.98	0.19	71,71,71,71	0
55	MG	1H	3406	1/1	0.98	0.08	70,70,70,70	0
55	MG	14	3201	1/1	0.98	0.08	101,101,101,101	0
55	MG	1H	3124	1/1	0.98	0.39	69,69,69,69	0
55	MG	1H	3378	1/1	0.98	0.12	75,75,75,75	0
55	MG	1G	1703	1/1	0.98	0.10	94,94,94,94	0
55	MG	1H	3025	1/1	0.98	0.16	55,55,55,55	0
55	MG	1G	1654	1/1	0.98	0.12	107,107,107,107	0
55	MG	14	3219	1/1	0.98	0.10	63,63,63,63	0
55	MG	14	3159	1/1	0.98	0.13	83,83,83,83	0
55	MG	1H	3343	1/1	0.98	0.14	56,56,56,56	0
55	MG	13	1694	1/1	0.98	0.43	117,117,117,117	0
55	MG	1H	3399	1/1	0.98	0.13	86,86,86,86	0
55	MG	14	3252	1/1	0.98	0.16	66,66,66,66	0
55	MG	1H	3219	1/1	0.98	0.15	91,91,91,91	0
55	MG	13	1682	1/1	0.98	0.18	118,118,118,118	0
55	MG	1H	3387	1/1	0.98	0.11	67,67,67,67	0
55	MG	1H	3402	1/1	0.98	0.13	66,66,66,66	0
55	MG	14	3046	1/1	0.98	0.12	76,76,76,76	0
55	MG	1G	1680	1/1	0.98	0.26	138,138,138,138	0
55	MG	14	3271	1/1	0.98	0.07	56,56,56,56	0
55	MG	1H	3263	1/1	0.98	0.23	53,53,53,53	0
55	MG	1H	3408	1/1	0.98	0.13	58,58,58,58	0
55	MG	14	3295	1/1	0.98	0.11	104,104,104,104	0
55	MG	14	3277	1/1	0.98	0.09	74,74,74,74	0
55	MG	1G	1616	1/1	0.98	0.16	93,93,93,93	0
55	MG	14	3154	1/1	0.98	0.35	65,65,65,65	0
55	MG	14	3124	1/1	0.98	0.13	95,95,95,95	0
55	MG	14	3228	1/1	0.98	0.14	72,72,72,72	0
55	MG	14	3070	1/1	0.98	0.21	72,72,72,72	0
55	MG	1H	3460	1/1	0.98	0.07	64,64,64,64	0
55	MG	1H	3036	1/1	0.98	0.13	74,74,74,74	0
55	MG	14	3234	1/1	0.98	0.21	82,82,82,82	0
55	MG	1H	3342	1/1	0.98	0.12	60,60,60,60	0
55	MG	1H	3358	1/1	0.98	0.10	60,60,60,60	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
55	MG	1H	3125	1/1	0.98	0.09	125,125,125,125	0
55	MG	14	3096	1/1	0.98	0.29	55,55,55,55	0
55	MG	1H	3472	1/1	0.98	0.19	64,64,64,64	0
55	MG	1H	3177	1/1	0.98	0.13	82,82,82,82	0
55	MG	1H	3446	1/1	0.98	0.10	88,88,88,88	0
55	MG	1H	3391	1/1	0.98	0.08	81,81,81,81	0
55	MG	1H	3234	1/1	0.98	0.29	92,92,92,92	0
55	MG	14	3128	1/1	0.98	0.19	54,54,54,54	0
55	MG	14	3039	1/1	0.98	0.18	75,75,75,75	0
55	MG	13	1729	1/1	0.98	0.09	86,86,86,86	0
55	MG	1H	3250	1/1	0.98	0.32	53,53,53,53	0
55	MG	13	1715	1/1	0.98	0.10	99,99,99,99	0
55	MG	14	3242	1/1	0.98	0.05	89,89,89,89	0
55	MG	1H	3470	1/1	0.98	0.13	69,69,69,69	0
55	MG	1H	3368	1/1	0.98	0.10	83,83,83,83	0
55	MG	1H	3233	1/1	0.98	0.29	102,102,102,102	0
55	MG	14	3042	1/1	0.98	0.17	80,80,80,80	0
55	MG	14	3266	1/1	0.98	0.07	83,83,83,83	0
55	MG	1H	3112	1/1	0.98	0.21	68,68,68,68	0
55	MG	1H	3220	1/1	0.98	0.18	85,85,85,85	0
55	MG	14	3075	1/1	0.98	0.17	99,99,99,99	0
55	MG	1H	3265	1/1	0.98	0.36	63,63,63,63	0
55	MG	14	3031	1/1	0.98	0.31	77,77,77,77	0
55	MG	1H	3261	1/1	0.98	0.17	70,70,70,70	0
55	MG	14	3066	1/1	0.98	0.31	82,82,82,82	0
55	MG	1H	3098	1/1	0.98	0.17	54,54,54,54	0
55	MG	14	3002	1/1	0.98	0.15	53,53,53,53	0
55	MG	14	3058	1/1	0.98	0.15	95,95,95,95	0
55	MG	13	1625	1/1	0.98	0.26	101,101,101,101	0
55	MG	1H	3429	1/1	0.98	0.07	92,92,92,92	0
55	MG	1G	1610	1/1	0.98	0.13	100,100,100,100	0
55	MG	14	3049	1/1	0.98	0.20	80,80,80,80	0
55	MG	1G	1643	1/1	0.98	0.31	105,105,105,105	0
55	MG	C8	201	1/1	0.98	0.37	76,76,76,76	0
55	MG	14	3256	1/1	0.99	0.13	87,87,87,87	0
55	MG	1H	3392	1/1	0.99	0.10	47,47,47,47	0
55	MG	21	302	1/1	0.99	0.17	50,50,50,50	0
55	MG	1H	3068	1/1	0.99	0.14	53,53,53,53	0
55	MG	1H	3082	1/1	0.99	0.22	77,77,77,77	0
55	MG	14	3150	1/1	0.99	0.15	89,89,89,89	0
55	MG	13	1721	1/1	0.99	0.08	87,87,87,87	0
55	MG	1H	3287	1/1	0.99	0.18	58,58,58,58	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
55	MG	C8	202	1/1	0.99	0.39	70,70,70,70	0
55	MG	14	3200	1/1	0.99	0.07	70,70,70,70	0
55	MG	1H	3072	1/1	0.99	0.26	53,53,53,53	0
55	MG	14	3148	1/1	0.99	0.22	57,57,57,57	0
55	MG	14	3035	1/1	0.99	0.17	68,68,68,68	0
56	SF4	3E	301	8/8	0.99	0.20	96,110,122,122	0
55	MG	1H	3428	1/1	0.99	0.14	66,66,66,66	0
55	MG	14	3074	1/1	0.99	0.16	92,92,92,92	0
55	MG	14	3097	1/1	0.99	0.25	55,55,55,55	0
55	MG	14	3045	1/1	0.99	0.14	89,89,89,89	0
55	MG	14	3232	1/1	0.99	0.11	59,59,59,59	0
55	MG	1H	3372	1/1	0.99	0.19	94,94,94,94	0
55	MG	14	3057	1/1	0.99	0.24	90,90,90,90	0
57	ZN	5I	103	1/1	0.99	0.12	109,109,109,109	0
55	MG	13	1650	1/1	0.99	0.19	106,106,106,106	0
56	SF4	32	302	8/8	0.99	0.20	112,135,144,151	0
55	MG	1H	3354	1/1	0.99	0.08	61,61,61,61	0
55	MG	1G	1624	1/1	0.99	0.14	94,94,94,94	0
55	MG	14	3210	1/1	0.99	0.14	60,60,60,60	0
55	MG	1H	3015	1/1	0.99	0.16	93,93,93,93	0
55	MG	13	1658	1/1	0.99	0.11	114,114,114,114	0
55	MG	1H	3376	1/1	0.99	0.09	58,58,58,58	0
55	MG	14	3102	1/1	0.99	0.14	83,83,83,83	0
55	MG	1H	3239	1/1	0.99	0.24	103,103,103,103	0
55	MG	1H	3194	1/1	0.99	0.20	113,113,113,113	0
55	MG	1H	3257	1/1	1.00	0.22	53,53,53,53	0

## 6.5 Other polymers ⓘ

There are no such residues in this entry.