



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 6, 2026 – 07:31 AM UTC

PDB ID : 6GSK / pdb_00006gsk
Title : Structure of T. thermophilus 70S ribosome complex with mRNA, tRNA^{fMet} and near-cognate tRNA^{Thr} 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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

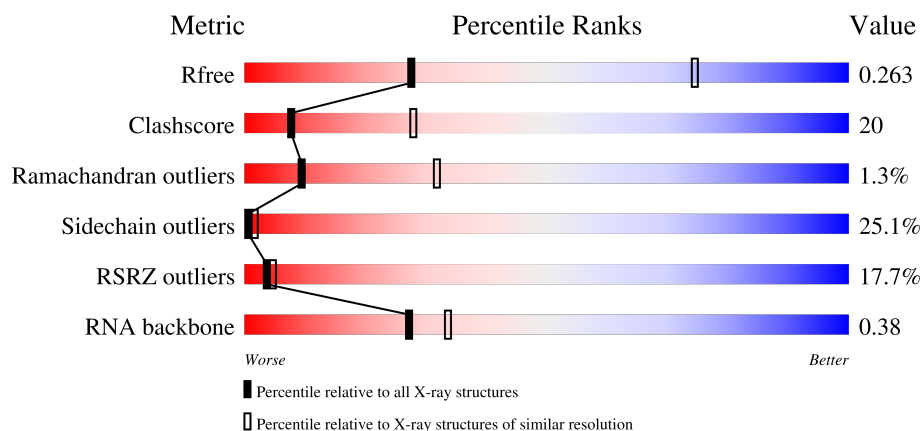
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.36 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}	180053	1099 (3.40-3.32)
Clashscore	190562	1116 (3.40-3.32)
Ramachandran outliers	187476	1101 (3.40-3.32)
Sidechain outliers	187428	1101 (3.40-3.32)
RSRZ outliers	180081	1099 (3.40-3.32)
RNA backbone	3983	1110 (3.72-3.00)

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

Mol	Chain	Length	Quality of chain
1	13	1522	24% 33% 51% 15%
1	1G	1522	15% 31% 51% 16%
2	12	256	29% 36% 31% 14% 19%
2	1E	256	15% 38% 39% 13% 10%

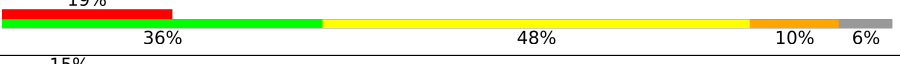
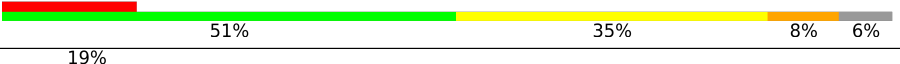
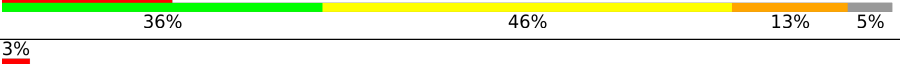
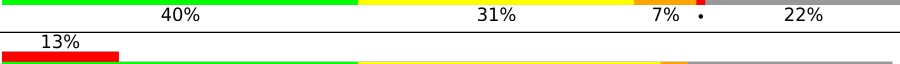
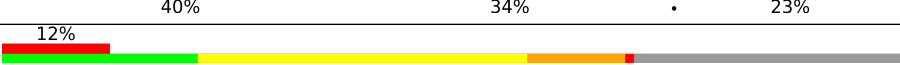
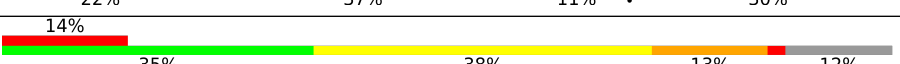
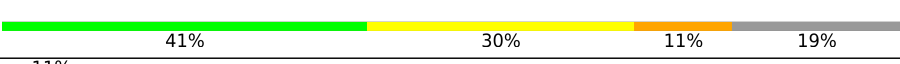
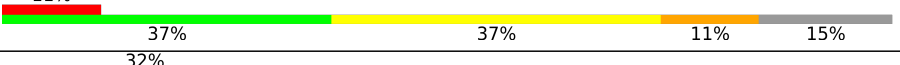
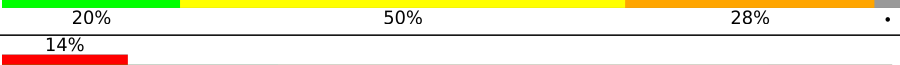
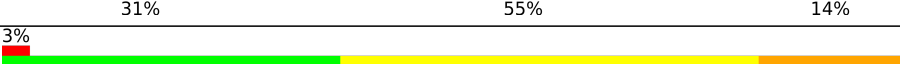
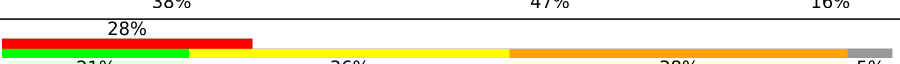
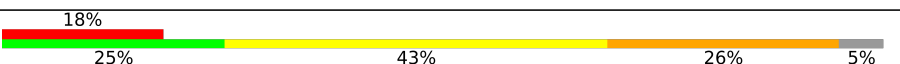
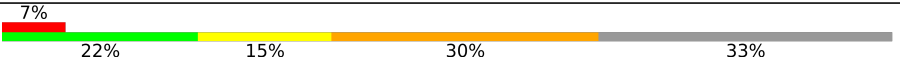
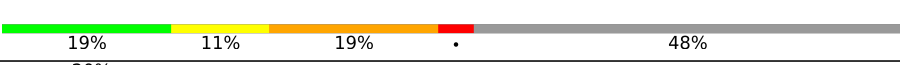
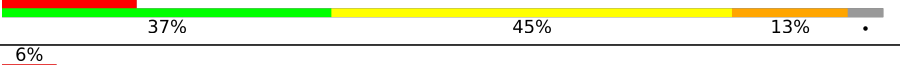
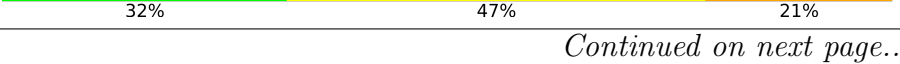
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Mol	Chain	Length	Quality of chain
3	22	239	
3	2E	239	
4	32	209	
4	3E	209	
5	42	162	
5	4E	162	
6	52	101	
6	5E	101	
7	62	156	
7	6E	156	
8	72	138	
8	7E	138	
9	82	128	
9	8E	128	
10	1A	105	
10	1I	105	
11	2A	129	
11	2I	129	
12	3A	132	
12	3I	132	
13	4A	126	
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
55	MG	13	1668	-	-	-	X
55	MG	14	3016	-	-	-	X
55	MG	14	3113	-	-	-	X
55	MG	14	3176	-	-	-	X
55	MG	14	3178	-	-	-	X
55	MG	14	3189	-	-	-	X
55	MG	1G	1618	-	-	-	X
55	MG	1G	1621	-	-	-	X
55	MG	1G	1627	-	-	-	X
55	MG	1G	1630	-	-	-	X
55	MG	1G	1640	-	-	-	X
55	MG	1G	1644	-	-	-	X
55	MG	1G	1662	-	-	-	X
55	MG	1G	1663	-	-	-	X
55	MG	1G	1667	-	-	-	X
55	MG	1G	1685	-	-	-	X
55	MG	1H	3022	-	-	-	X
55	MG	1H	3099	-	-	-	X
55	MG	1H	3102	-	-	-	X
55	MG	1H	3181	-	-	-	X
55	MG	1H	3200	-	-	-	X
55	MG	1H	3211	-	-	-	X
55	MG	1H	3245	-	-	-	X
55	MG	1H	3268	-	-	-	X
55	MG	1H	3277	-	-	-	X
56	SF4	32	302	-	-	X	-

2 Entry composition

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 (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
55	13	140	Total	Mg	0	0
			140	140		
55	5I	2	Total	Mg	0	0
			2	2		
55	8I	1	Total	Mg	0	0
			1	1		

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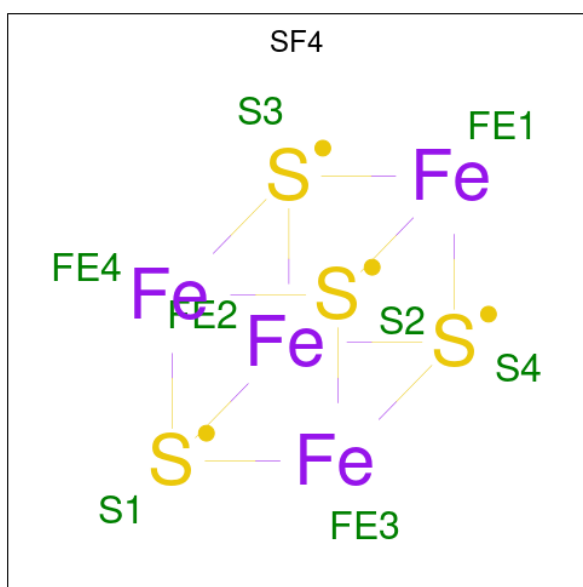
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
55	BI	1	Total 1	Mg 1	0	0
55	1F	2	Total 2	Mg 2	0	0
55	2K	1	Total 1	Mg 1	0	0
55	1H	473	Total 473	Mg 473	0	0
55	16	2	Total 2	Mg 2	0	0
55	11	1	Total 1	Mg 1	0	0
55	21	3	Total 3	Mg 3	0	0
55	41	1	Total 1	Mg 1	0	0
55	78	2	Total 2	Mg 2	0	0
55	88	3	Total 3	Mg 3	0	0
55	C8	2	Total 2	Mg 2	0	0
55	D8	1	Total 1	Mg 1	0	0
55	I8	1	Total 1	Mg 1	0	0
55	J8	1	Total 1	Mg 1	0	0
55	P8	1	Total 1	Mg 1	0	0
55	1G	126	Total 126	Mg 126	0	0
55	32	1	Total 1	Mg 1	0	0
55	42	2	Total 2	Mg 2	0	0
55	2A	1	Total 1	Mg 1	0	0
55	4A	1	Total 1	Mg 1	0	0
55	7A	1	Total 1	Mg 1	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
55	BA	1	Total 1	Mg 1	0	0
55	2L	1	Total 1	Mg 1	0	0
55	14	300	Total 300	Mg 300	0	0
55	1J	2	Total 2	Mg 2	0	0
55	29	1	Total 1	Mg 1	0	0
55	39	1	Total 1	Mg 1	0	0
55	35	1	Total 1	Mg 1	0	0
55	45	2	Total 2	Mg 2	0	0
55	85	1	Total 1	Mg 1	0	0
55	E5	1	Total 1	Mg 1	0	0
55	F5	1	Total 1	Mg 1	0	0

- Molecule 56 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe_4S_4).



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 (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
57	5I	1	Total	Zn	0	0
			1	1		
57	5A	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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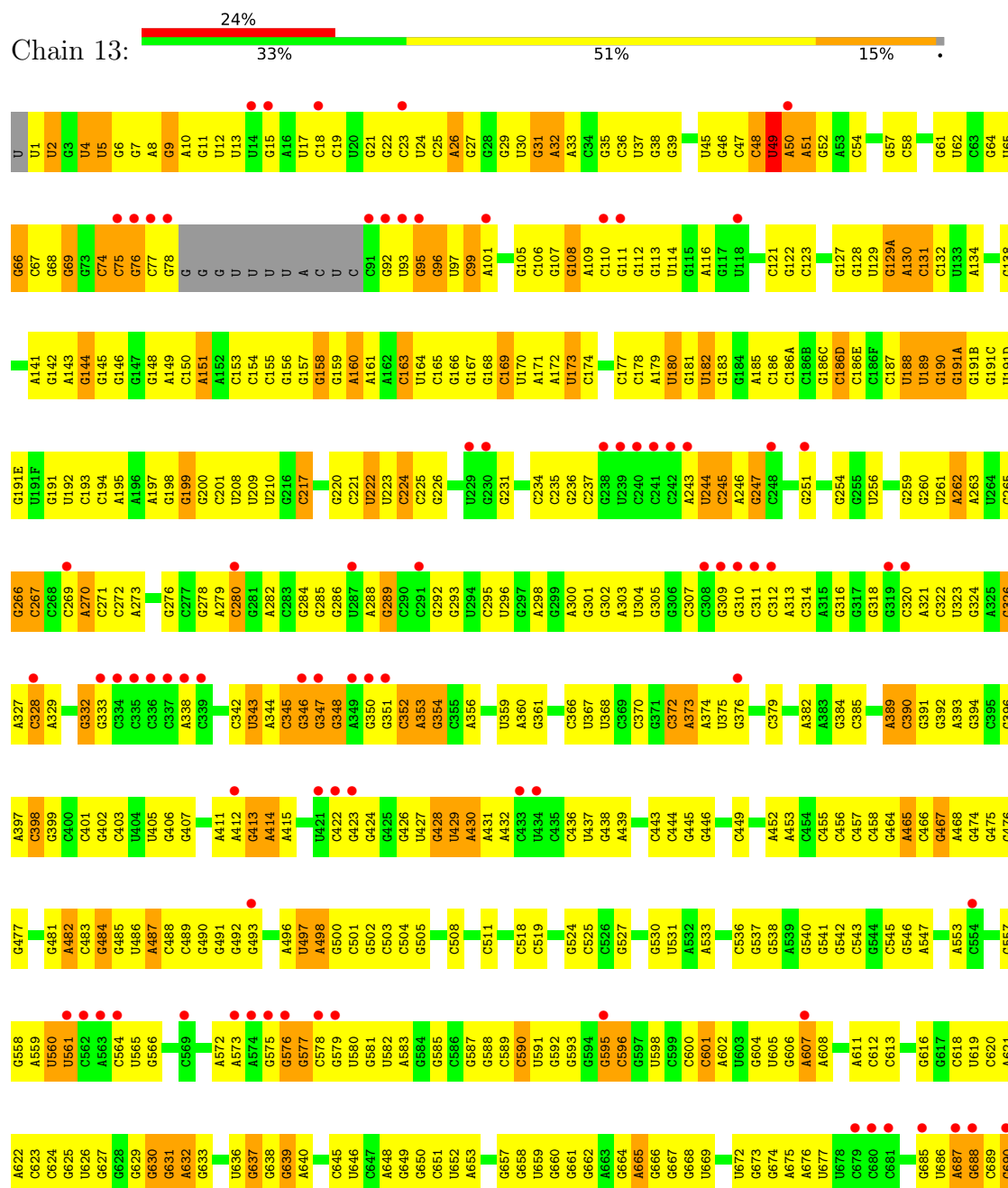
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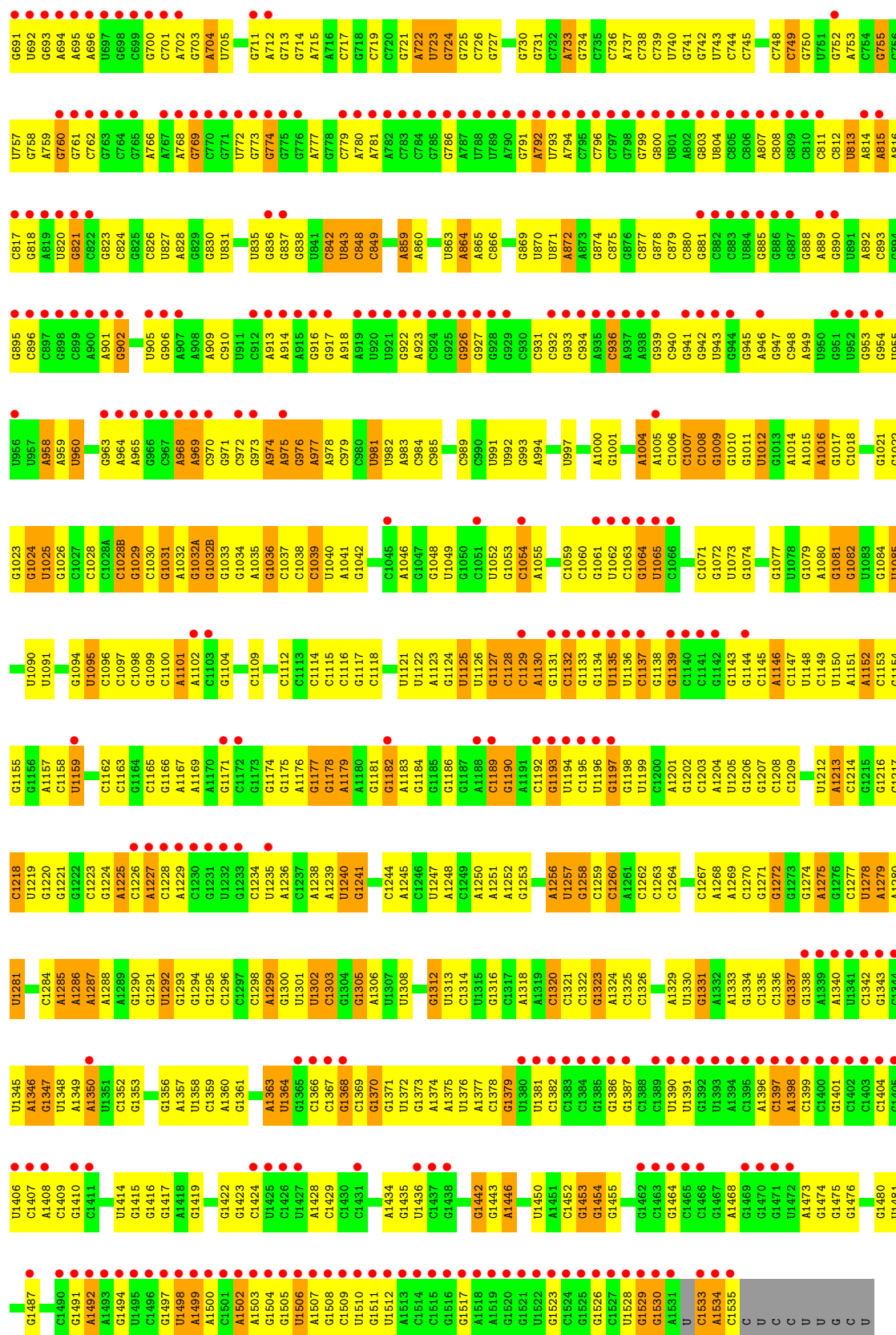
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
58	39	6	Total 6	O 6	0	0
58	35	5	Total 5	O 5	0	0
58	45	5	Total 5	O 5	0	0
58	B5	2	Total 2	O 2	0	0
58	H5	2	Total 2	O 2	0	0
58	L5	1	Total 1	O 1	0	0

3 Residue-property plots [i](#)

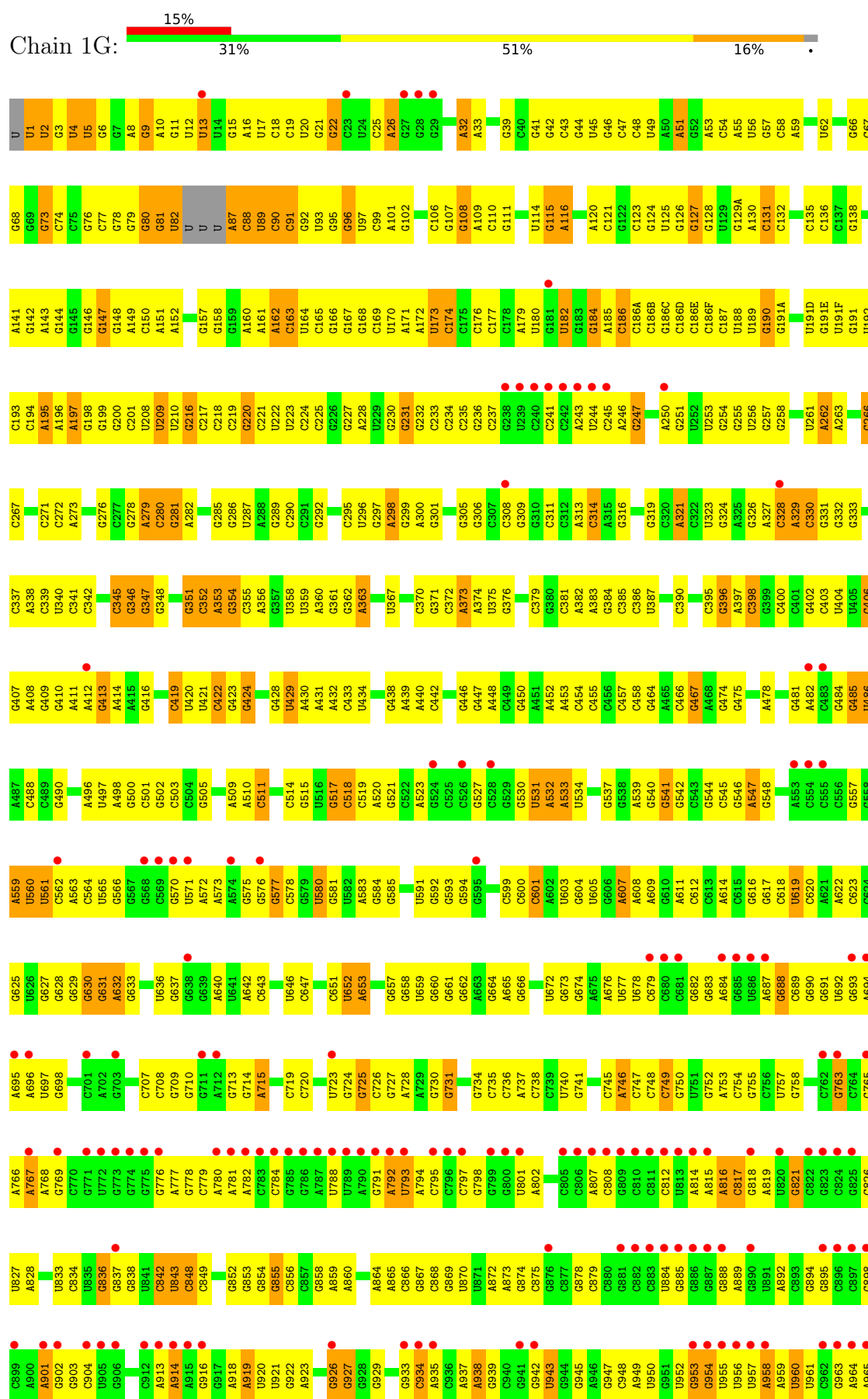
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

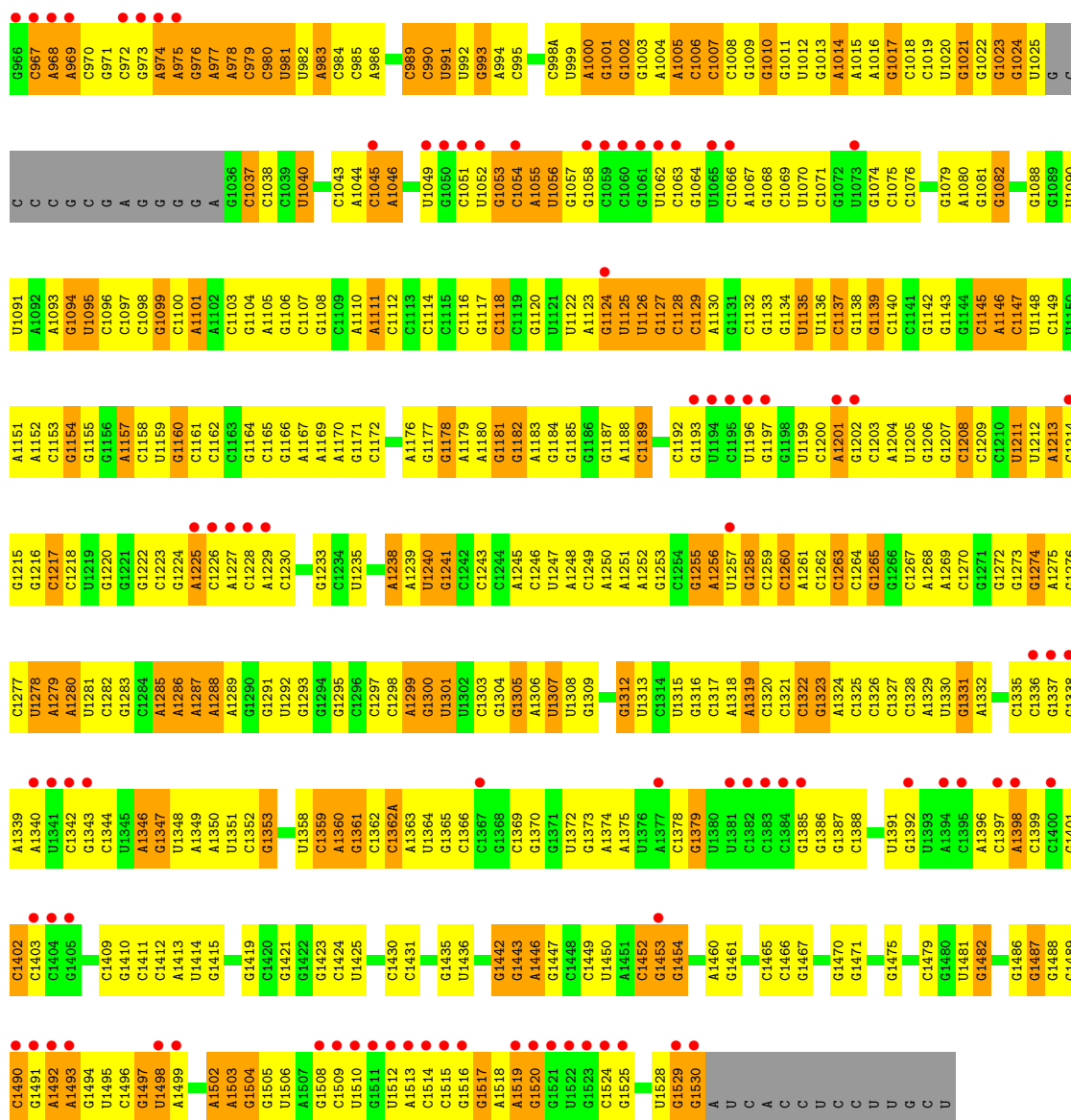
• Molecule 1: 16S ribosomal RNA



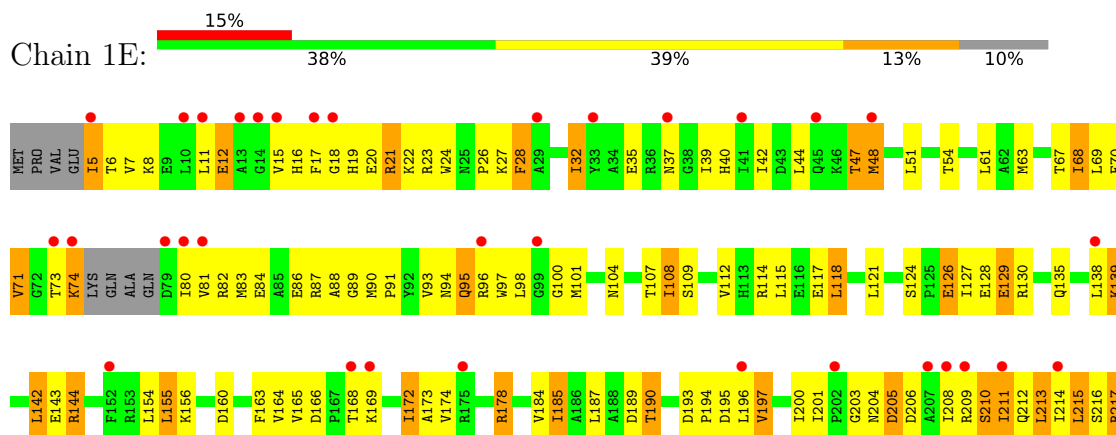


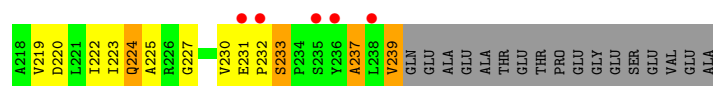
• Molecule 1: 16S ribosomal RNA



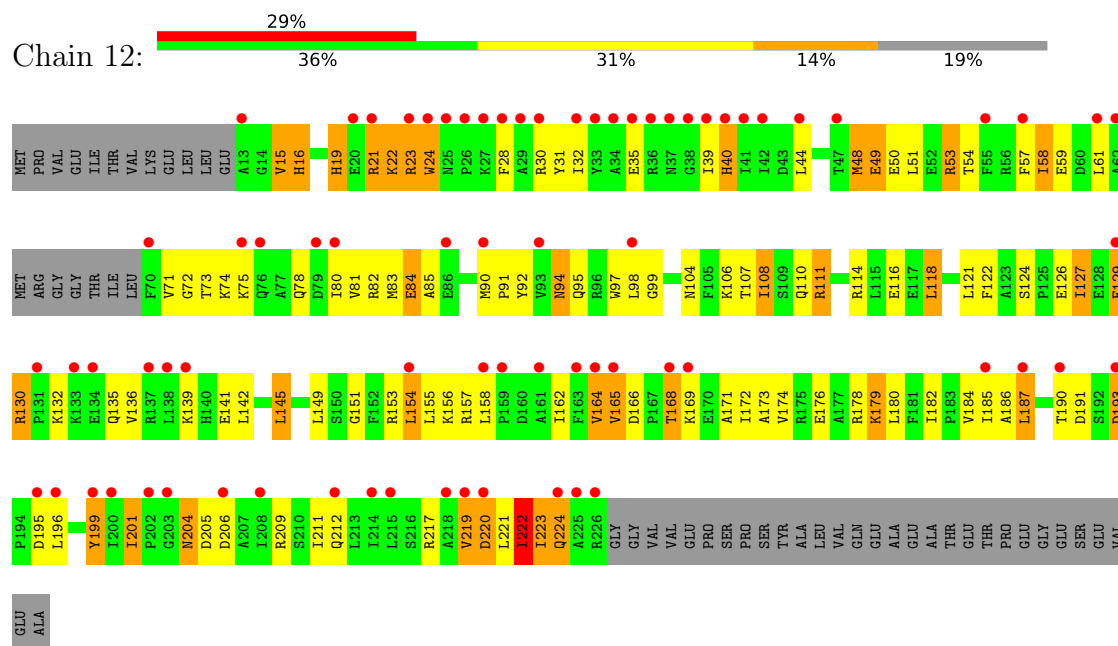


• Molecule 2: 30S ribosomal protein S2

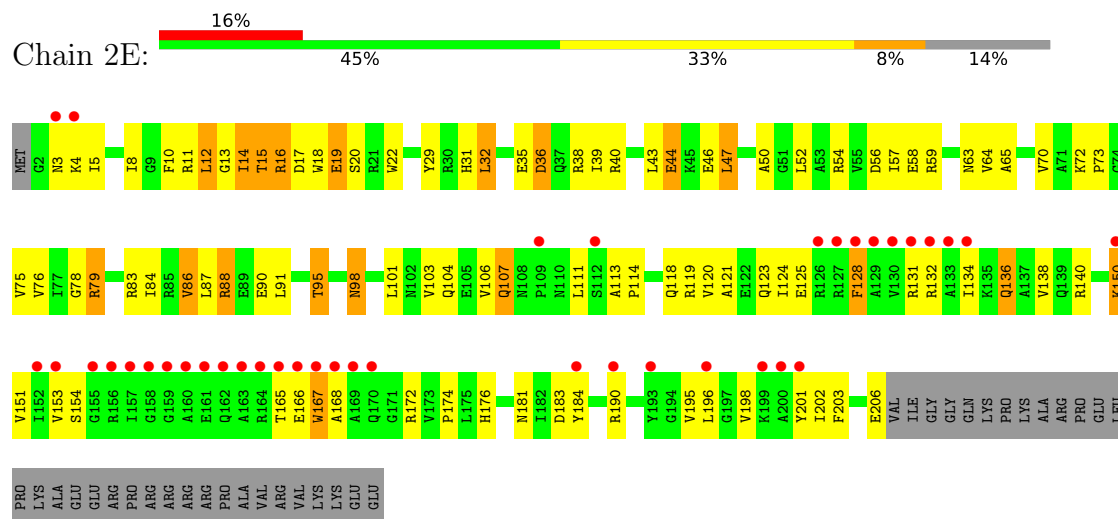




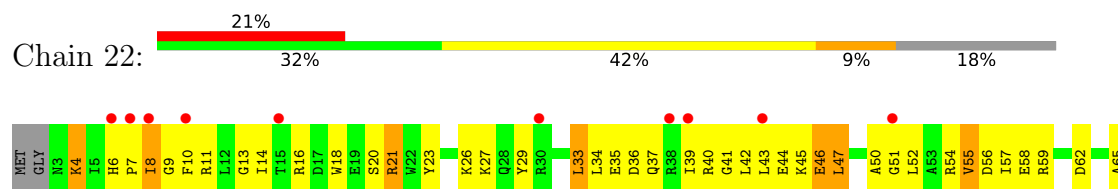
• Molecule 2: 30S ribosomal protein S2

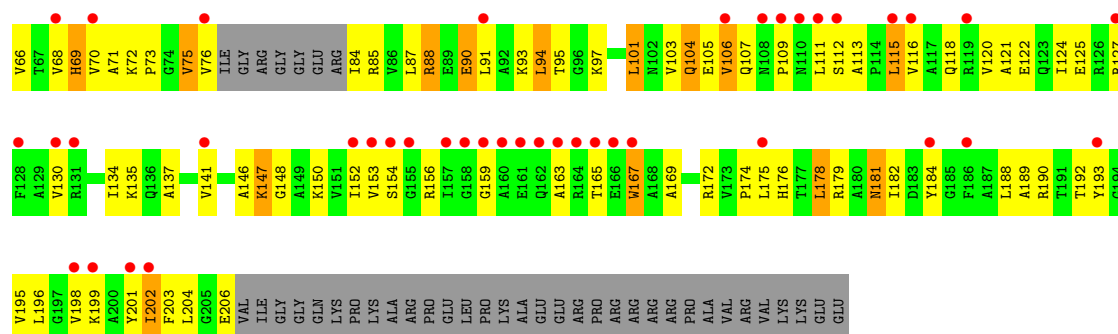


• Molecule 3: 30S ribosomal protein S3

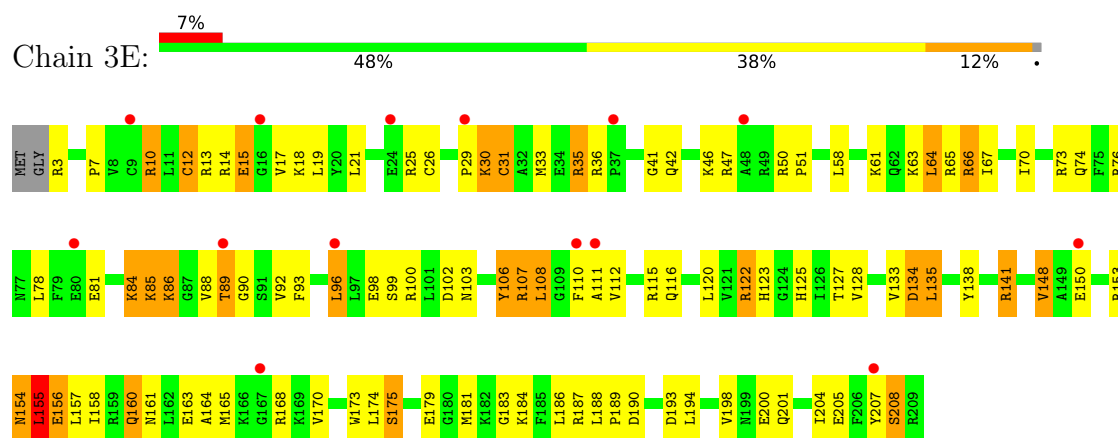


• Molecule 3: 30S ribosomal protein S3

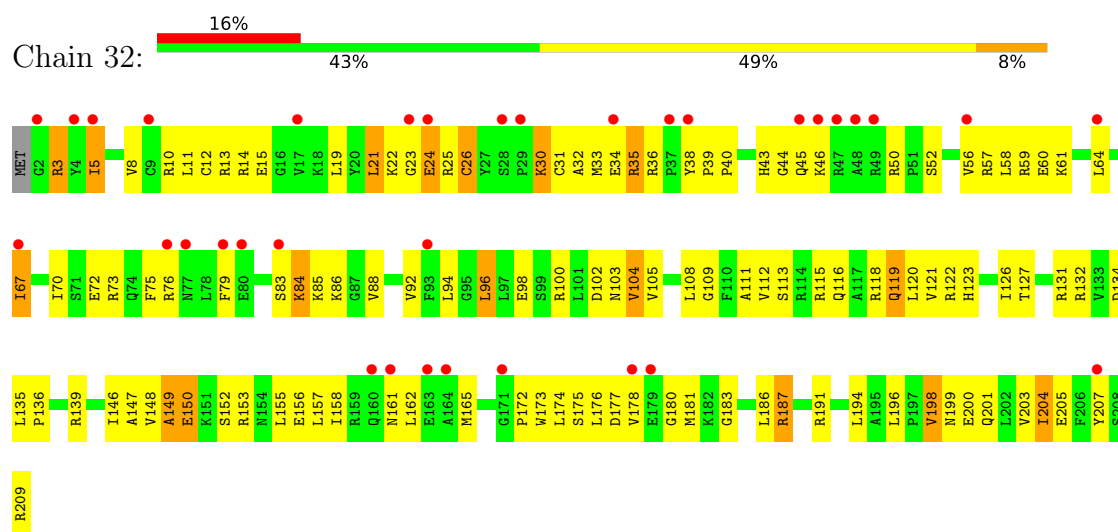




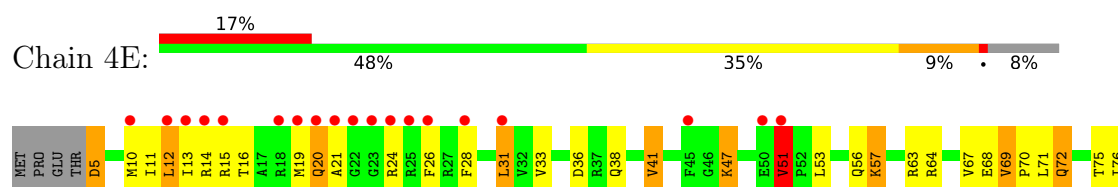
• Molecule 4: 30S ribosomal protein S4



• Molecule 4: 30S ribosomal protein S4

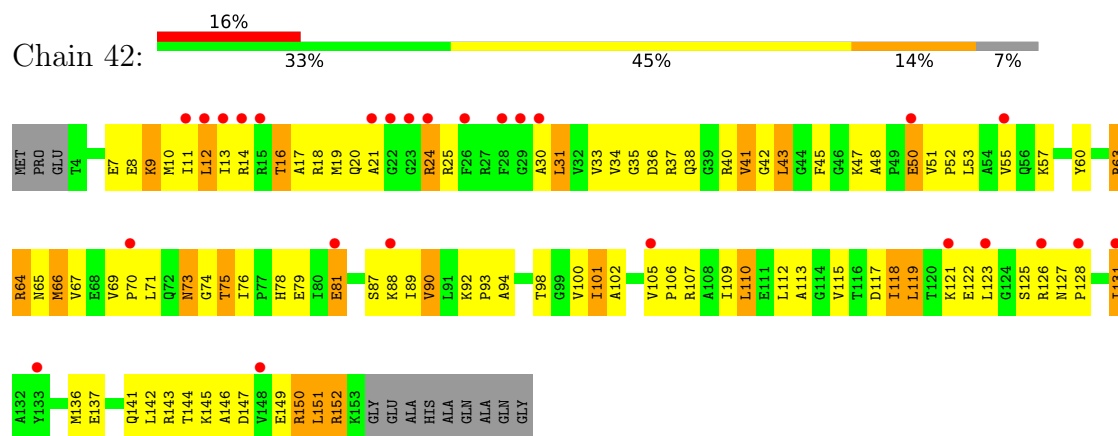


• Molecule 5: 30S ribosomal protein S5

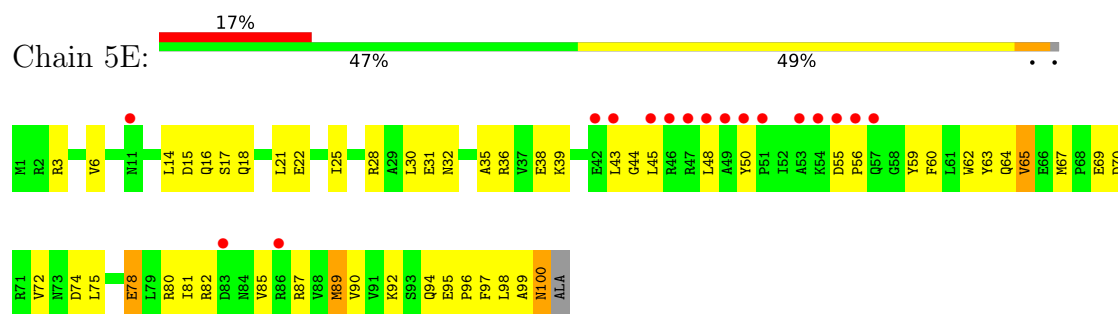




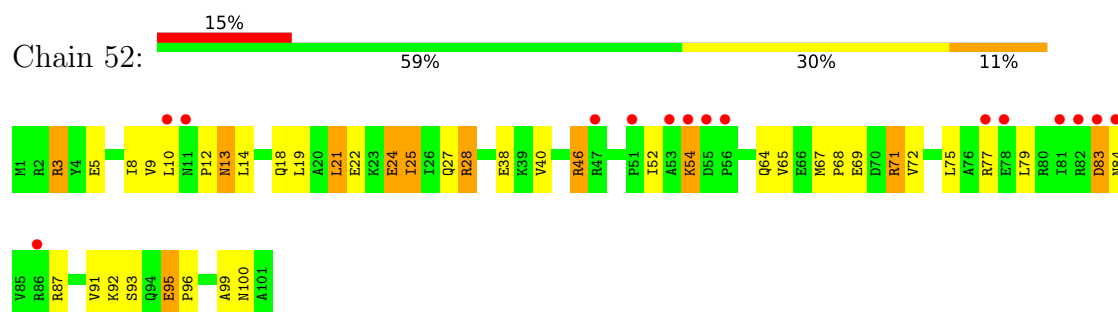
• Molecule 5: 30S ribosomal protein S5



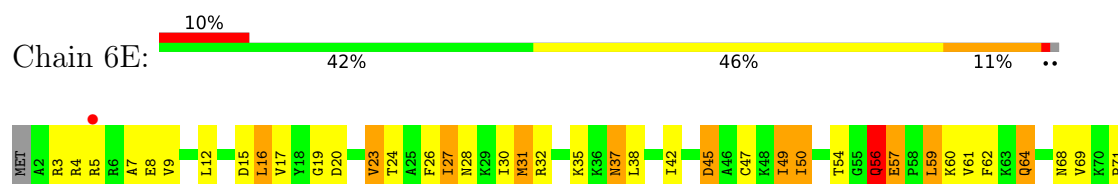
• Molecule 6: 30S ribosomal protein S6

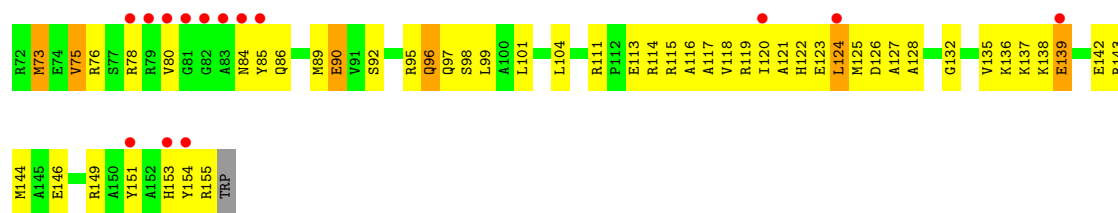


• Molecule 6: 30S ribosomal protein S6

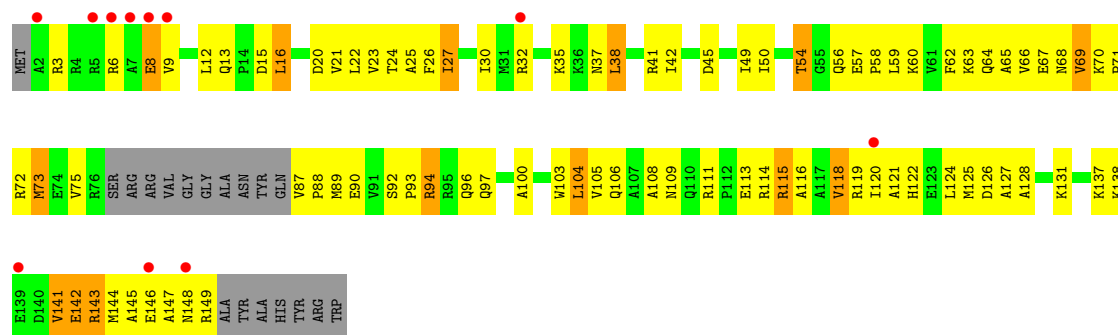


• Molecule 7: 30S ribosomal protein S7

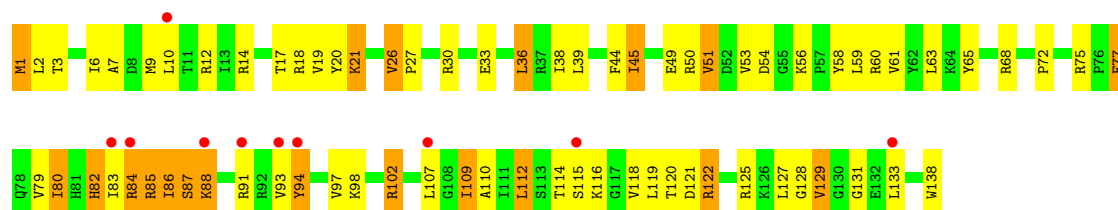




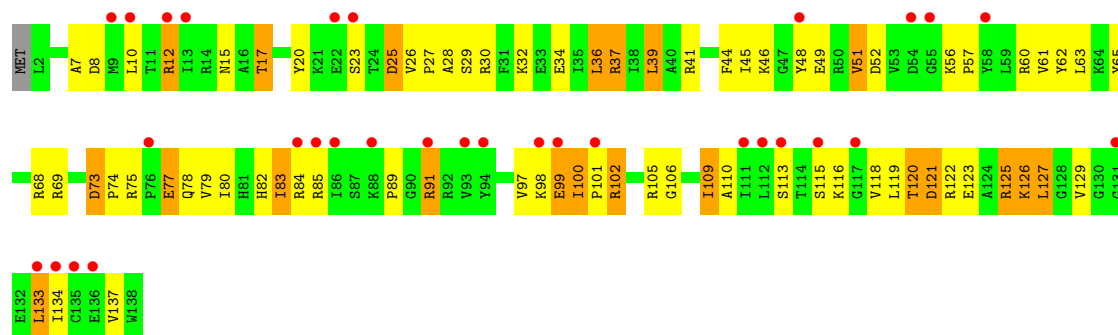
• Molecule 7: 30S ribosomal protein S7



• Molecule 8: 30S ribosomal protein S8

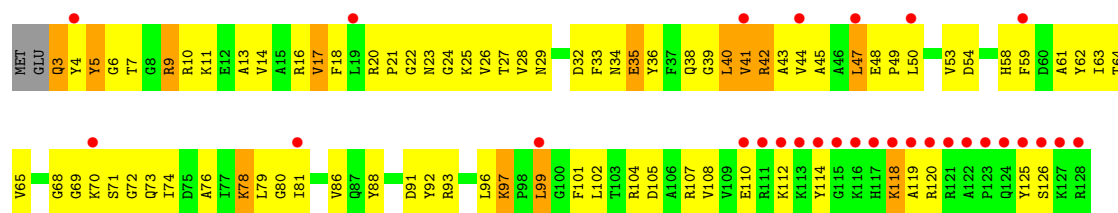


• Molecule 8: 30S ribosomal protein S8

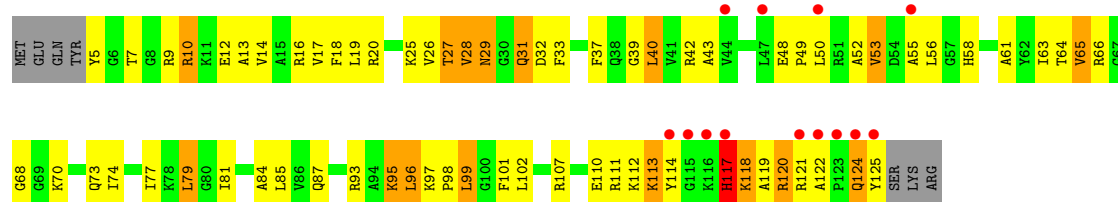


• Molecule 9: 30S ribosomal protein S9

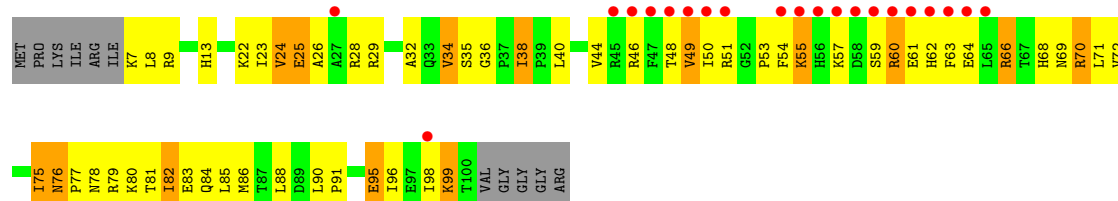




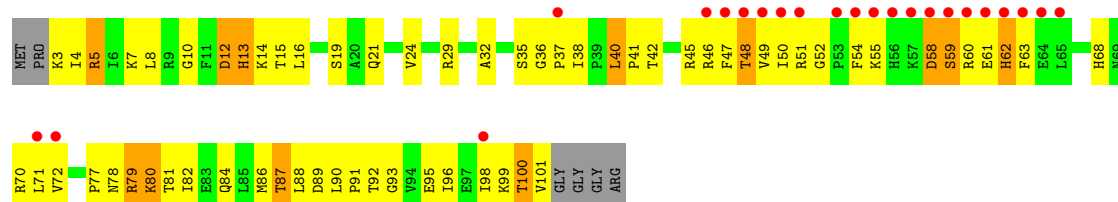
• Molecule 9: 30S ribosomal protein S9



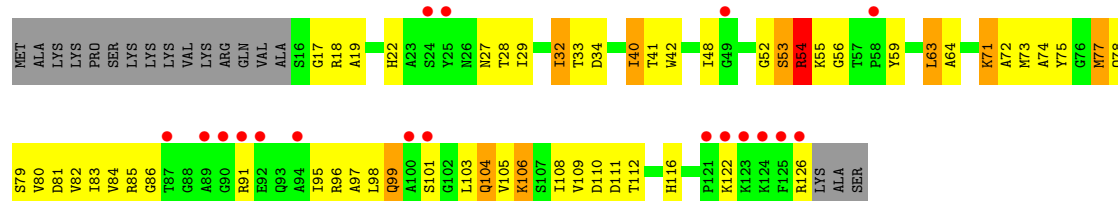
• Molecule 10: 30S ribosomal protein S10



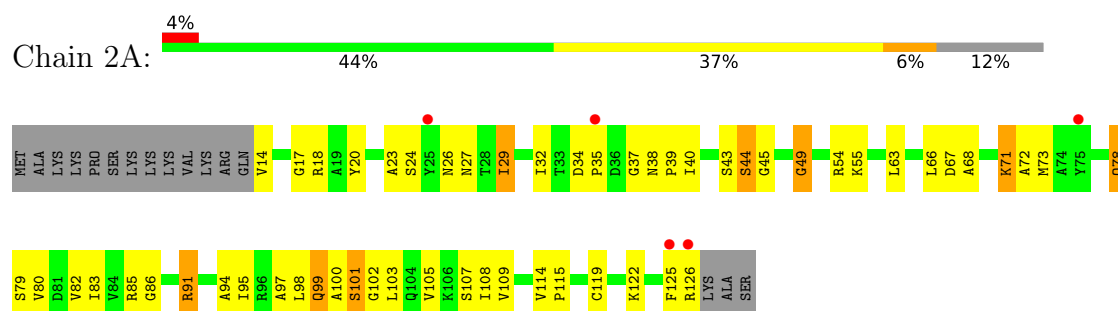
• Molecule 10: 30S ribosomal protein S10



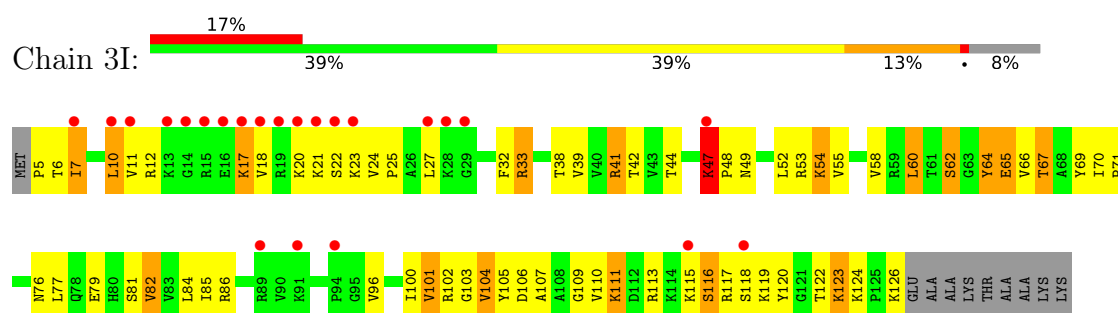
• Molecule 11: 30S ribosomal protein S11



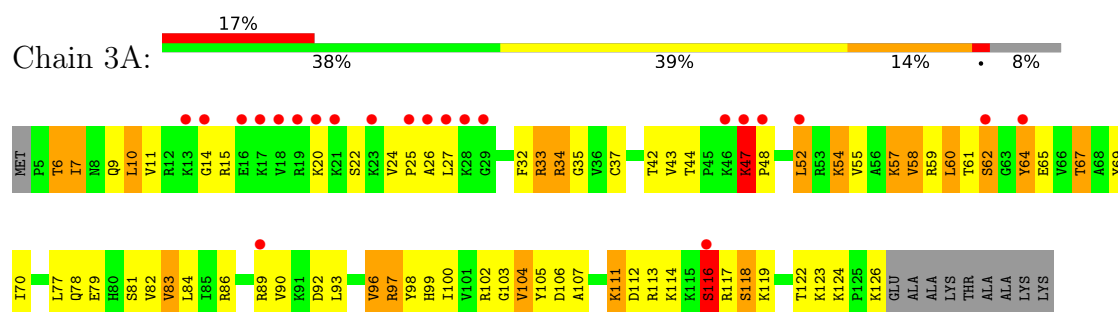
- Molecule 11: 30S ribosomal protein S11



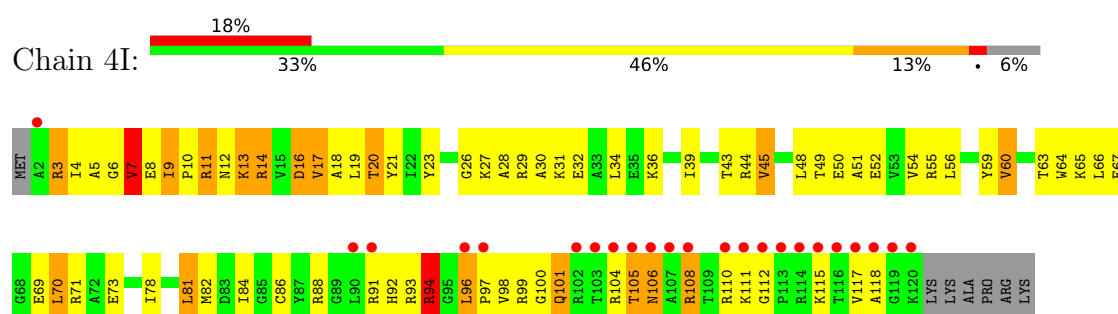
- Molecule 12: 30S ribosomal protein S12



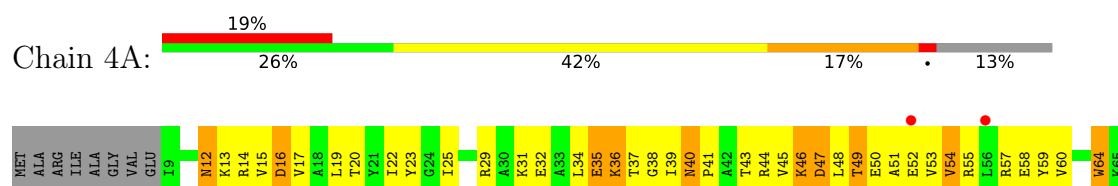
- Molecule 12: 30S ribosomal protein S12

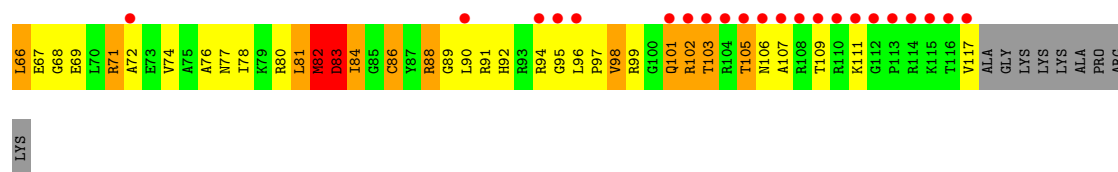


- Molecule 13: 30S ribosomal protein S13

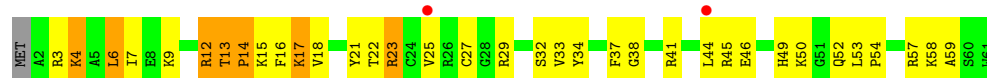


- Molecule 13: 30S ribosomal protein S13

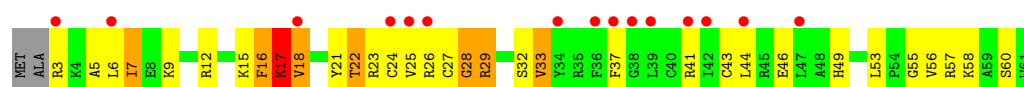
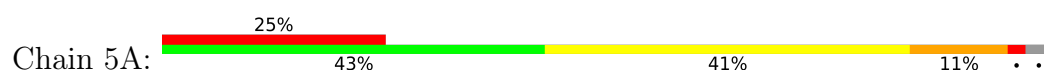




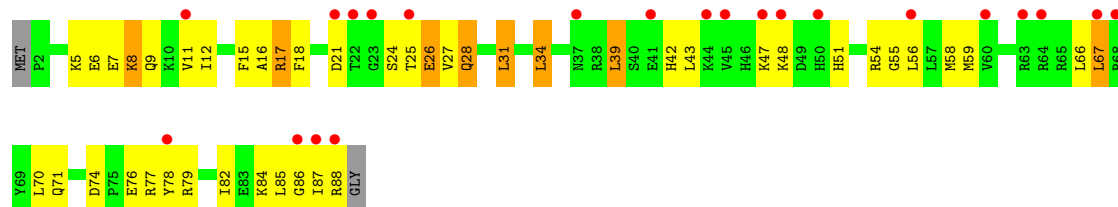
- Molecule 14: 30S ribosomal protein S14 type Z



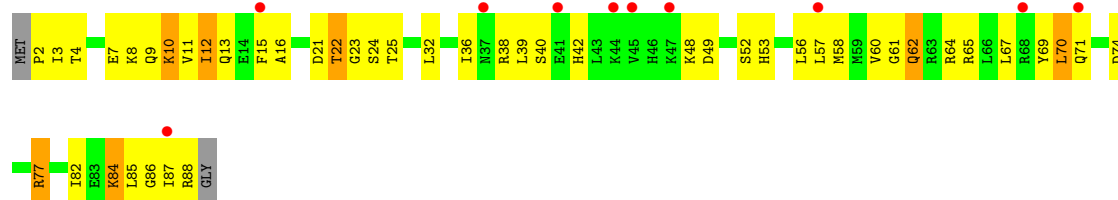
- Molecule 14: 30S ribosomal protein S14 type Z



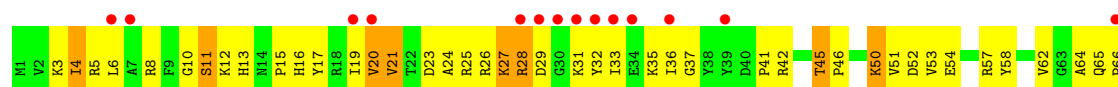
- Molecule 15: 30S ribosomal protein S15

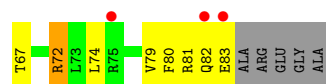


- Molecule 15: 30S ribosomal protein S15

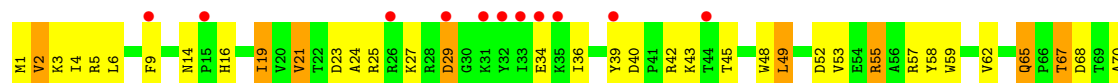


- Molecule 16: 30S ribosomal protein S16

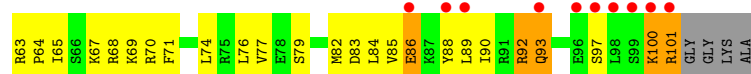
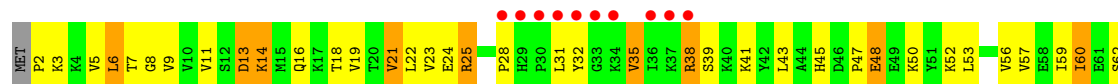




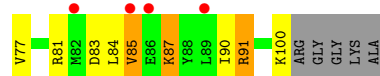
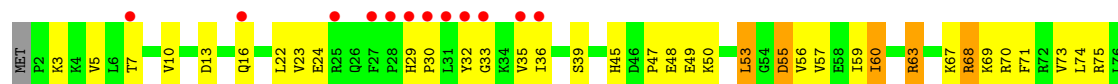
- Molecule 16: 30S ribosomal protein S16



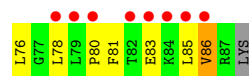
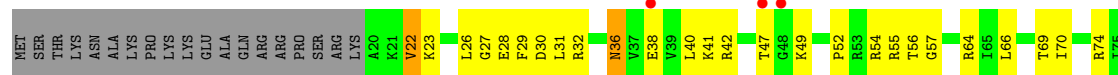
- Molecule 17: 30S ribosomal protein S17



- Molecule 17: 30S ribosomal protein S17

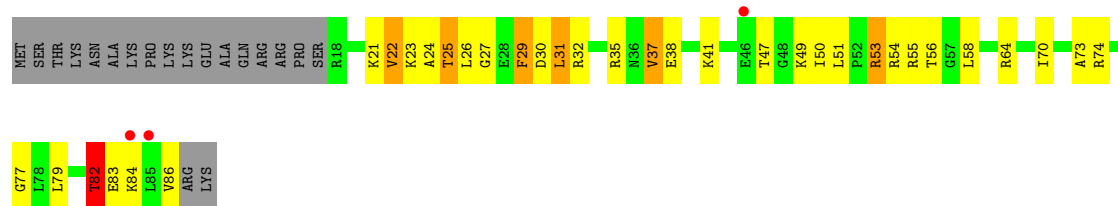


- Molecule 18: 30S ribosomal protein S18

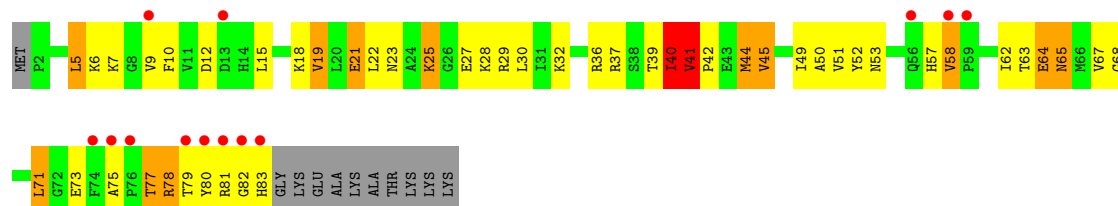


- Molecule 18: 30S ribosomal protein S18

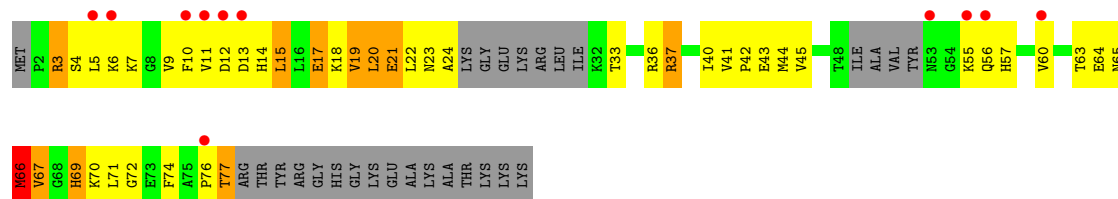
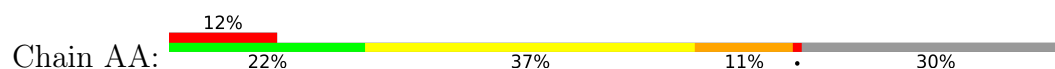




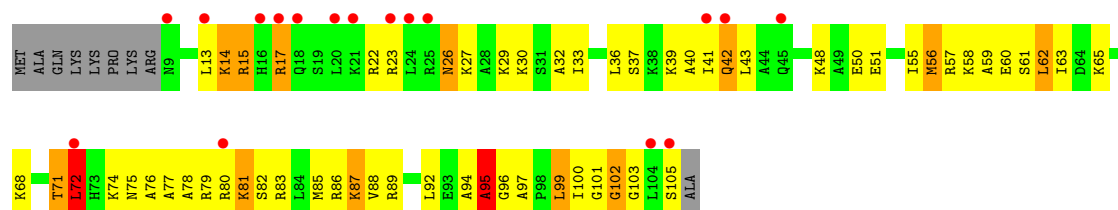
• Molecule 19: 30S ribosomal protein S19



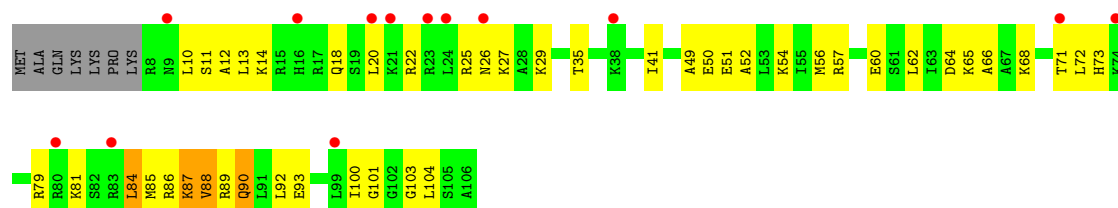
• Molecule 19: 30S ribosomal protein S19



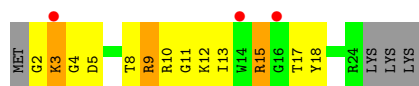
• Molecule 20: 30S ribosomal protein S20



• Molecule 20: 30S ribosomal protein S20



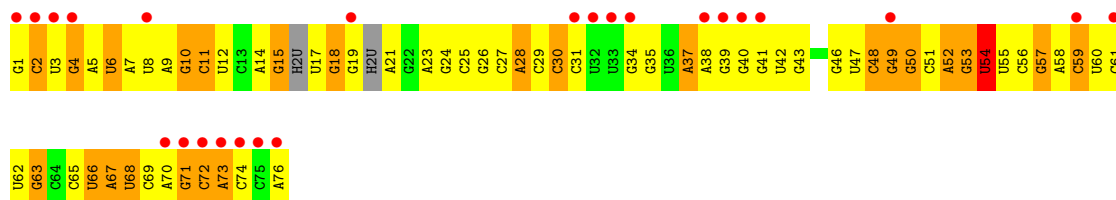
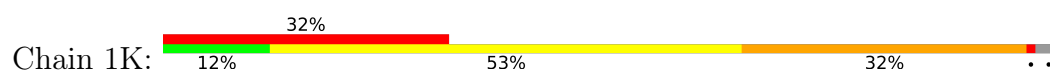
- Molecule 21: 30S ribosomal protein Thx



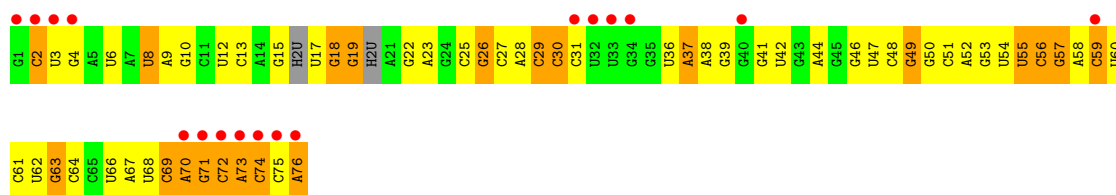
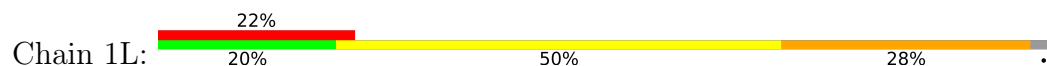
- Molecule 21: 30S ribosomal protein Thx



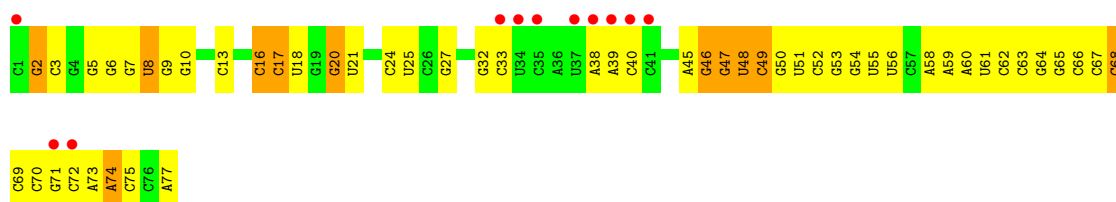
- Molecule 22: tRNA^{Thr}



- Molecule 22: tRNA^{Thr}

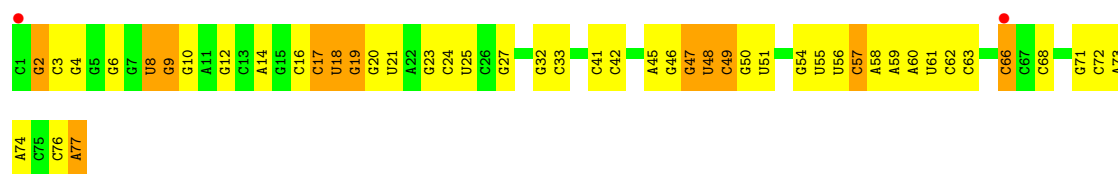


- Molecule 23: tRNA^{fMet}

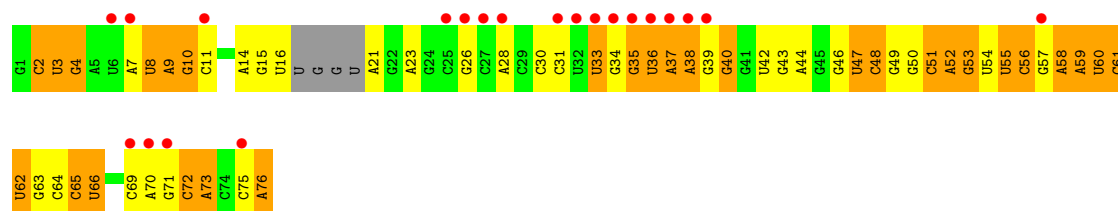
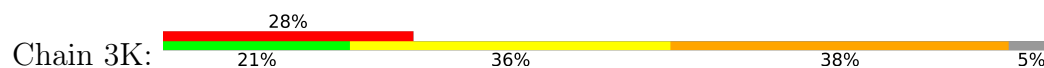


- Molecule 23: tRNA^{fMet}

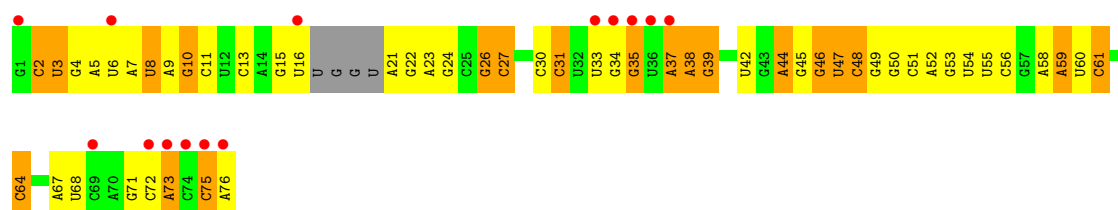




• Molecule 24: tRNAThr



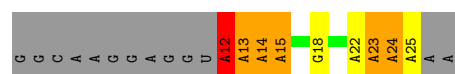
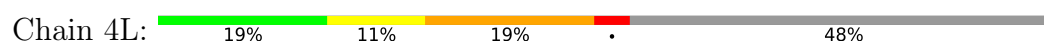
• Molecule 24: tRNAThr



• Molecule 25: mRNA

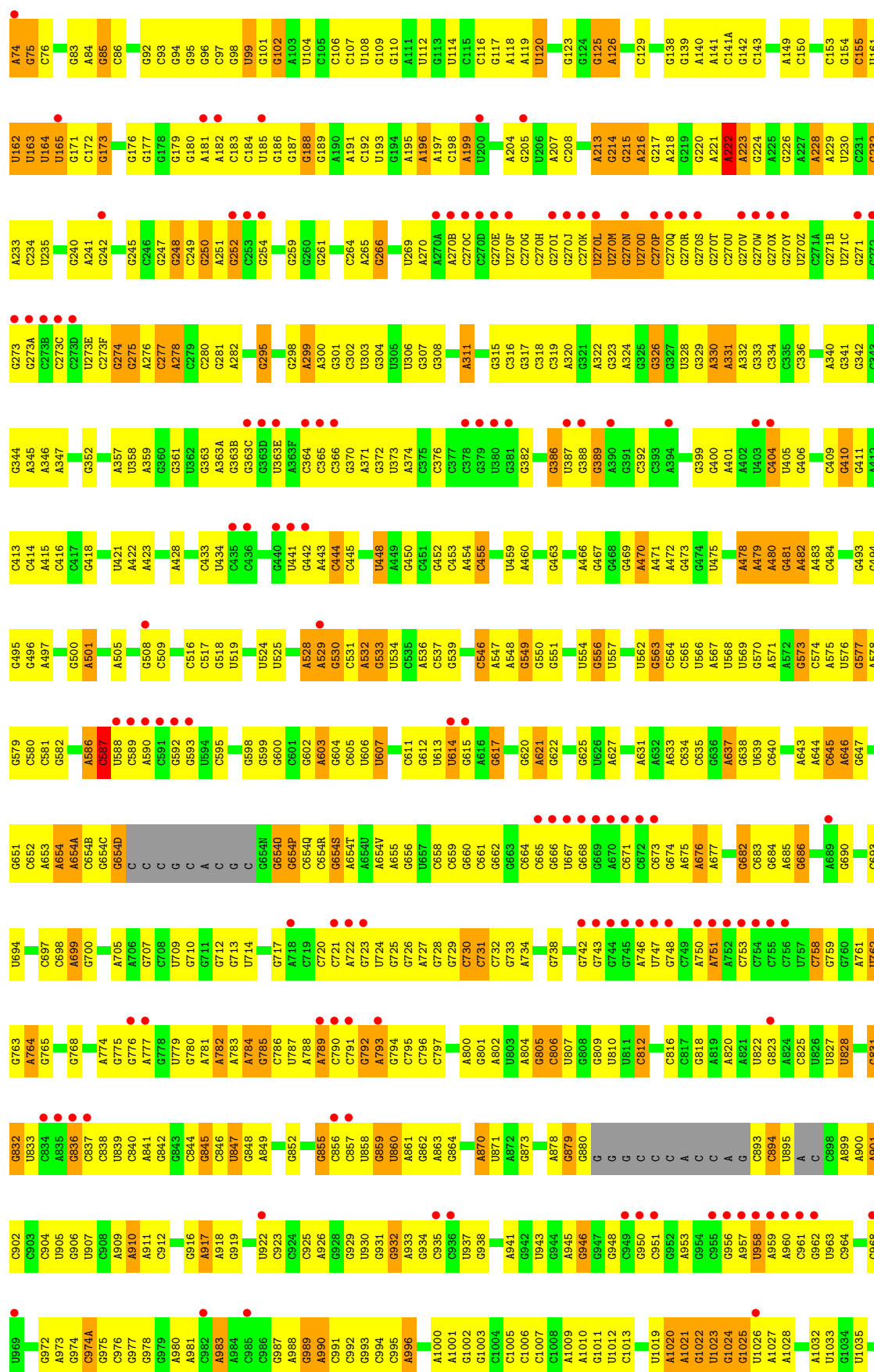


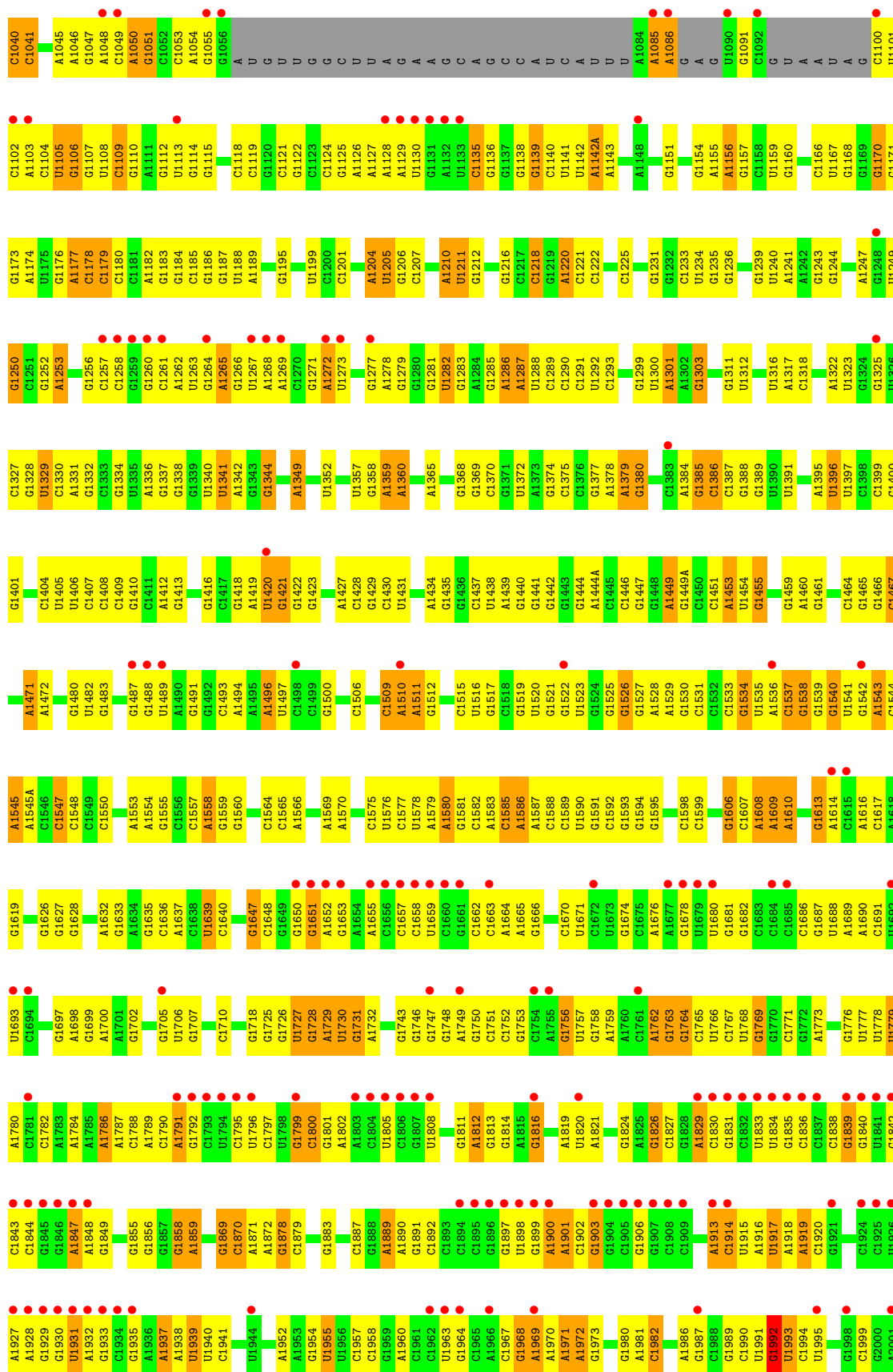
• Molecule 25: mRNA

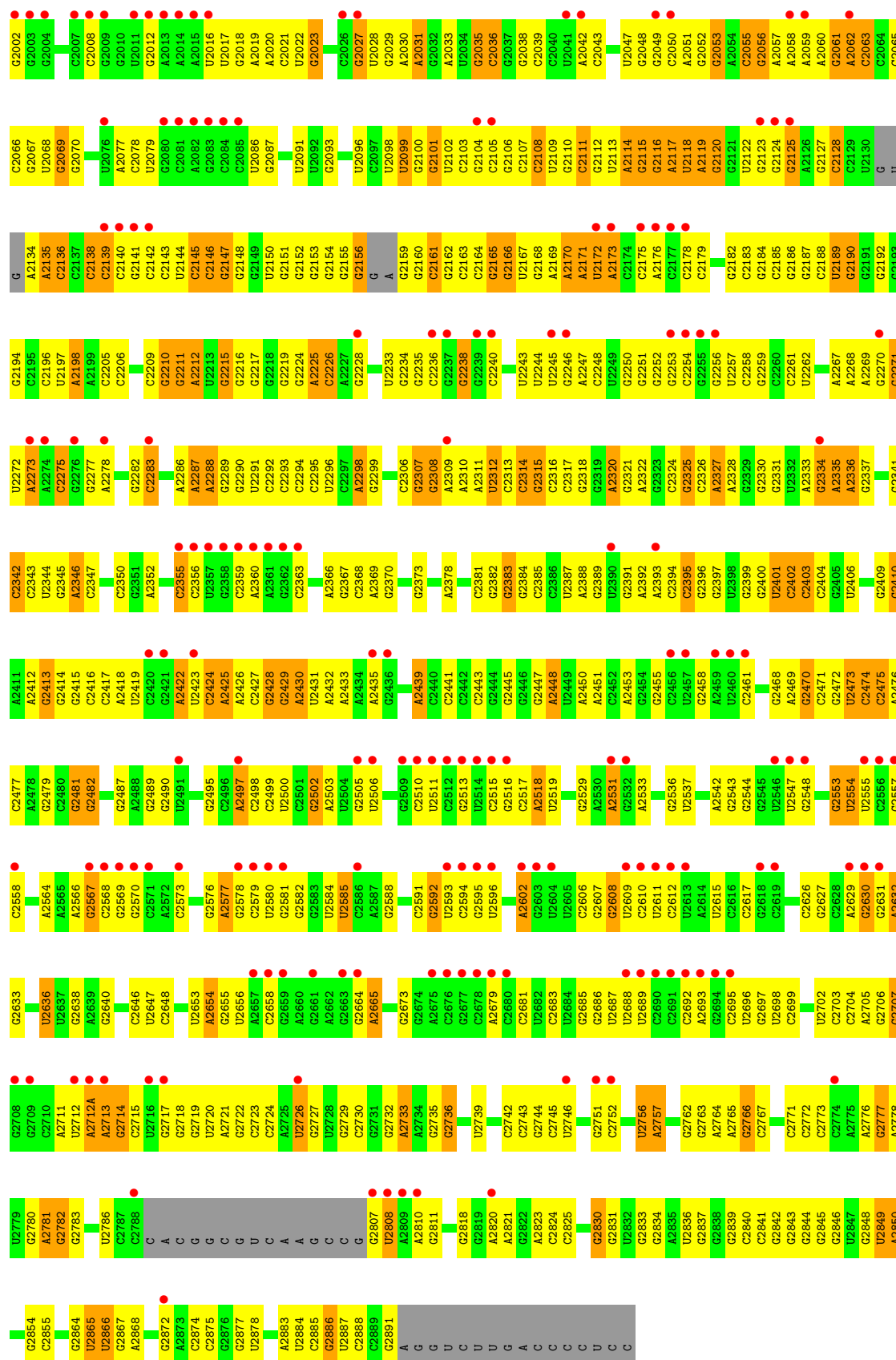


• Molecule 26: 23S ribosomal RNA

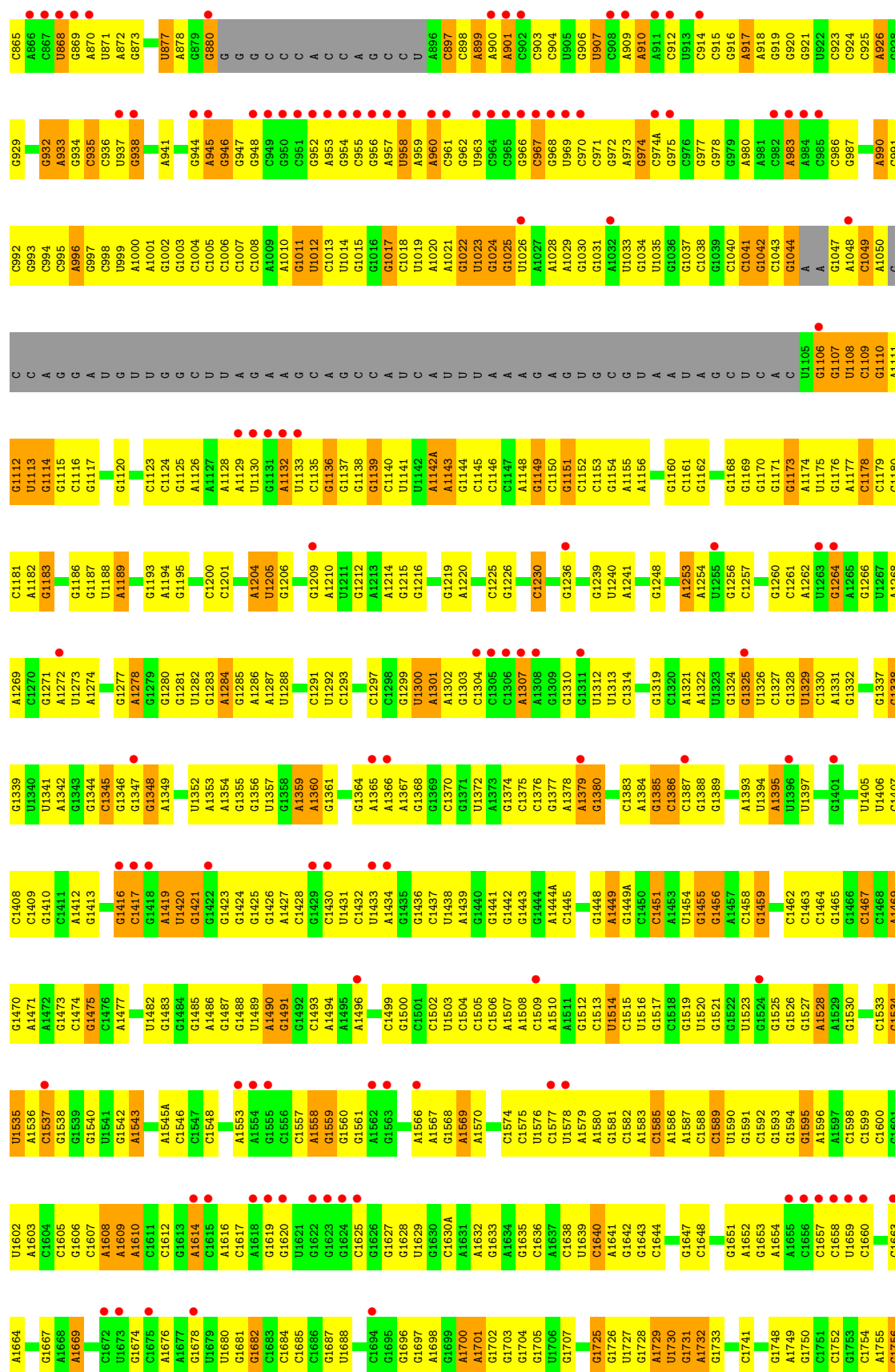


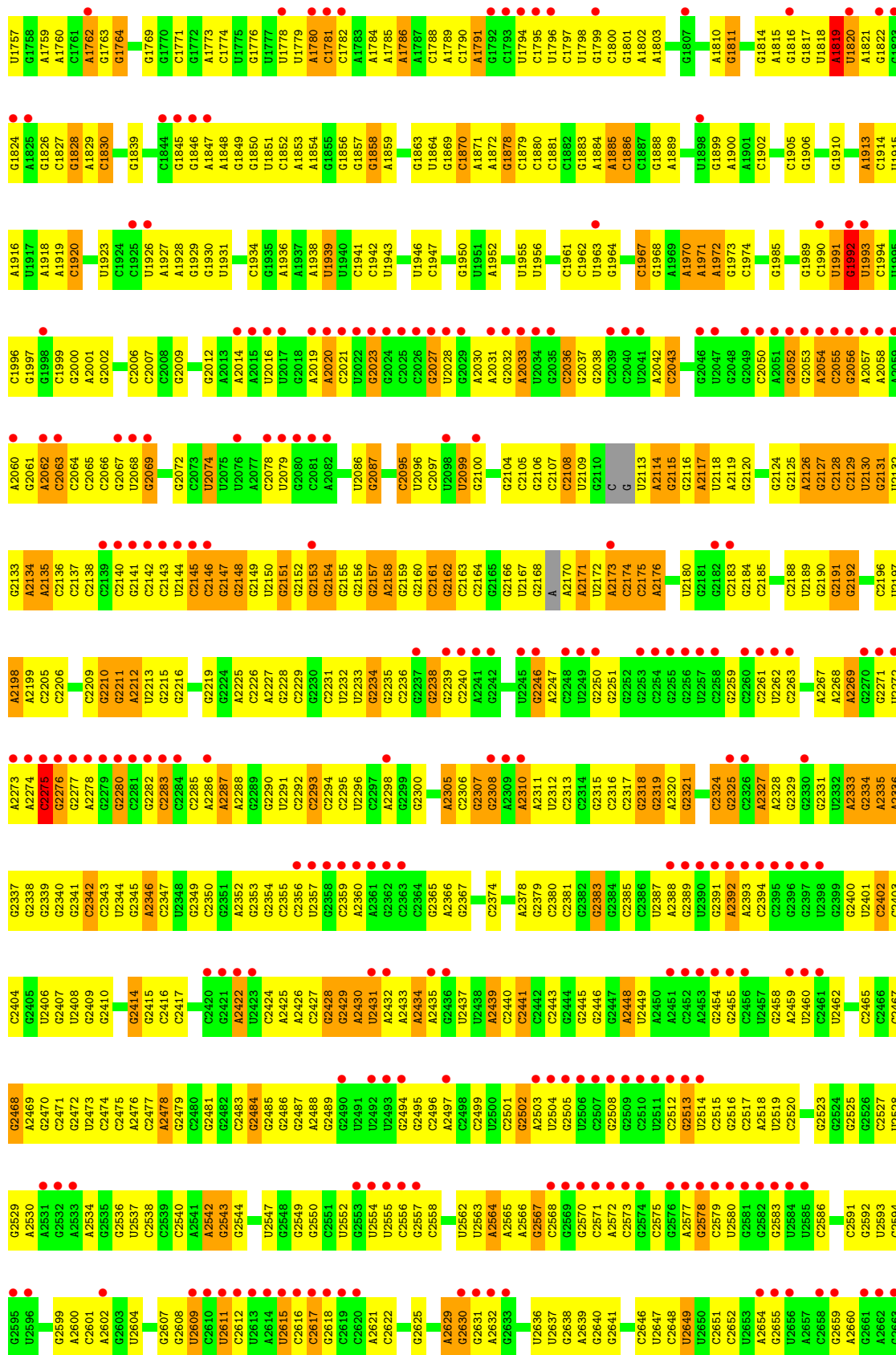


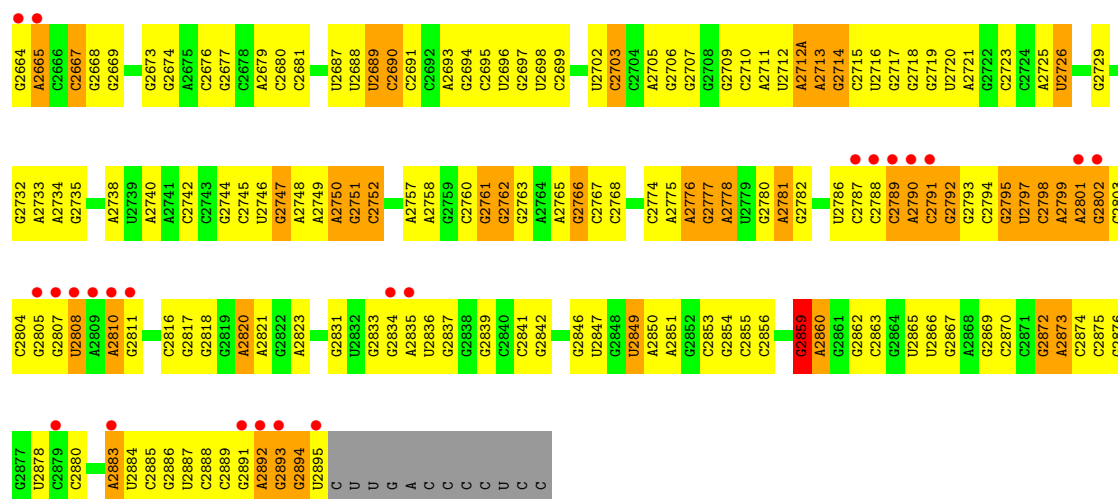




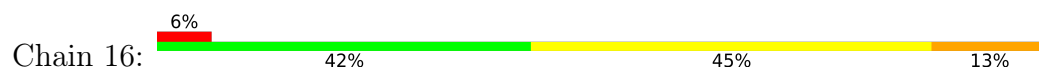








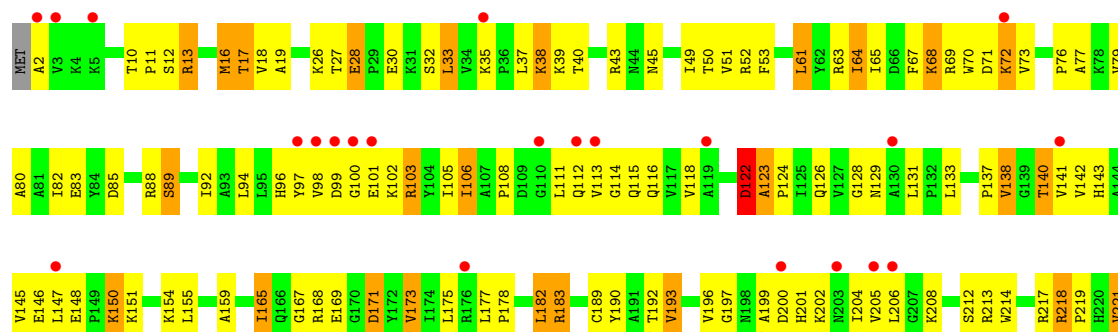
• Molecule 27: 5S ribosomal RNA

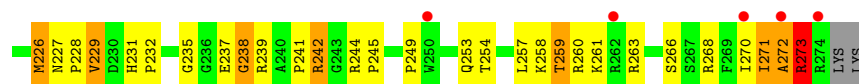


• Molecule 27: 5S ribosomal RNA

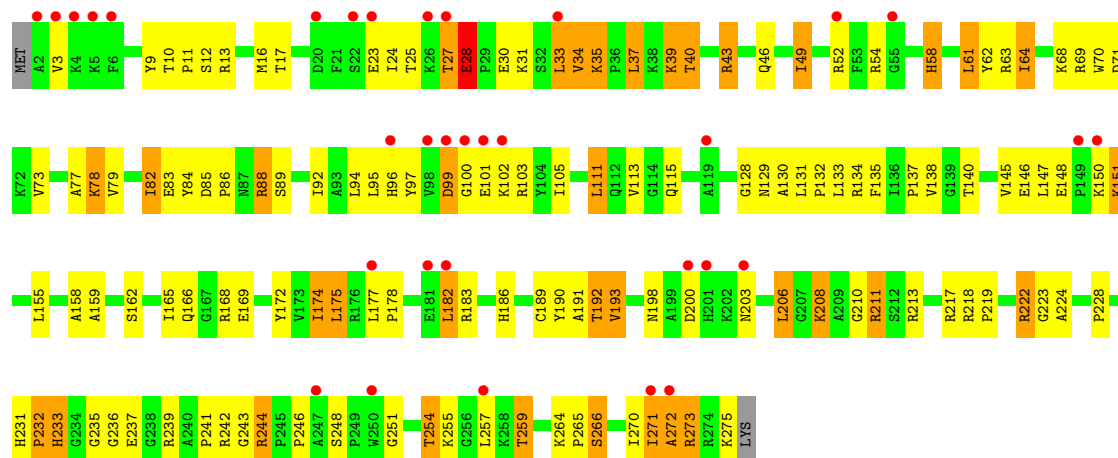


• Molecule 28: 50S ribosomal protein L2

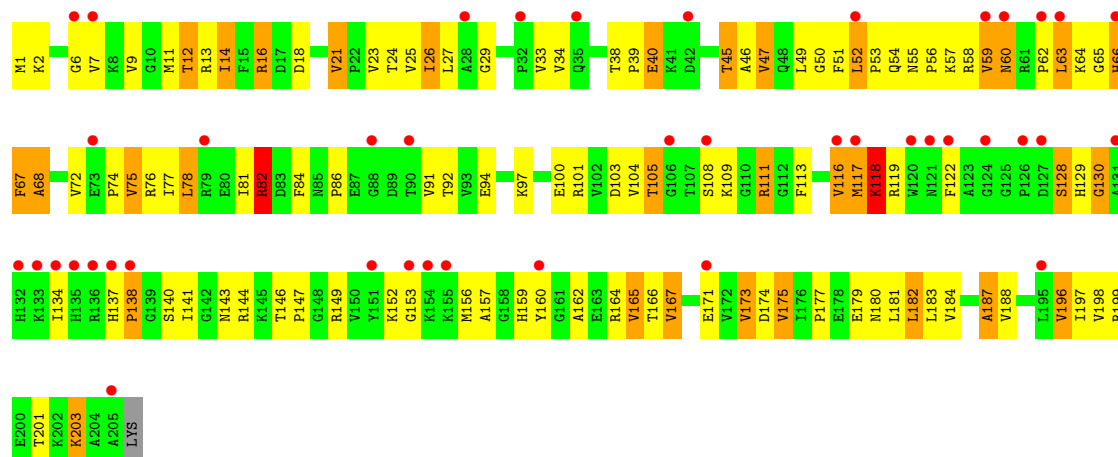
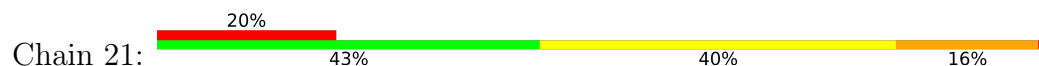




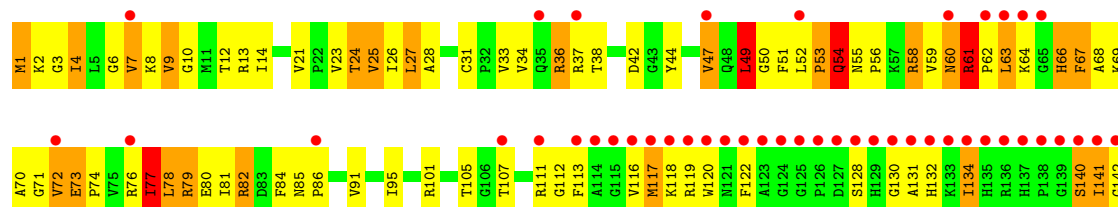
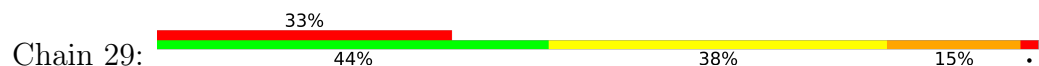
• Molecule 28: 50S ribosomal protein L2



• Molecule 29: 50S ribosomal protein L3

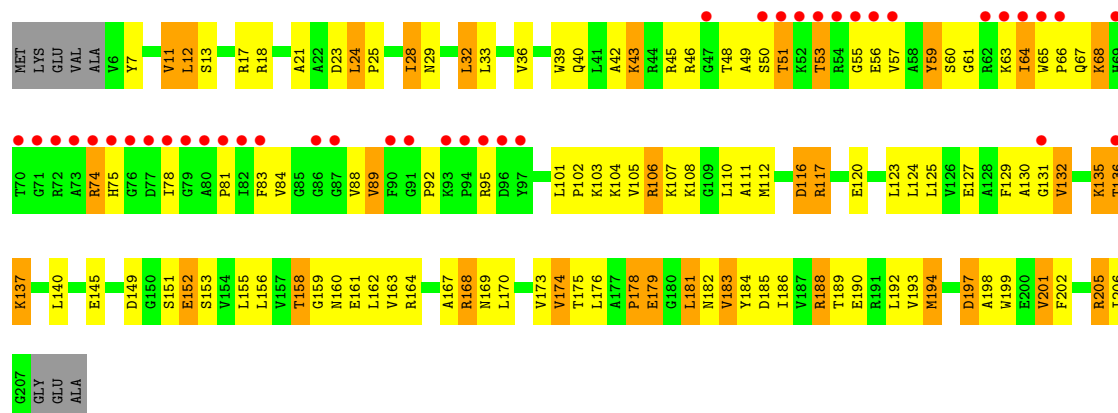


• Molecule 29: 50S ribosomal protein L3

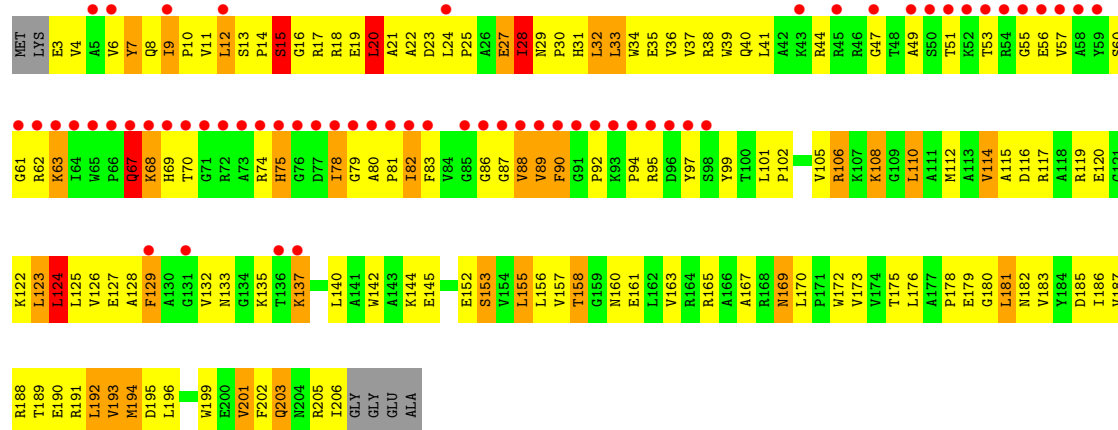




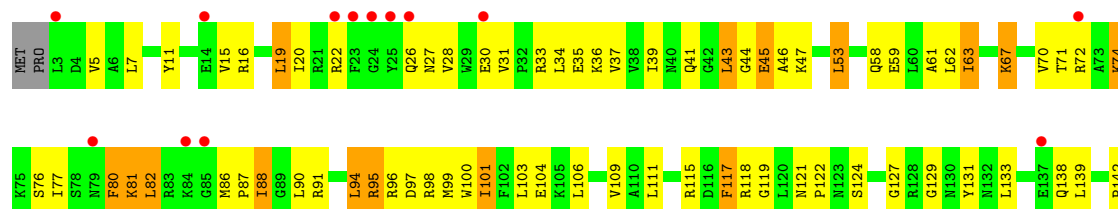
• Molecule 30: 50S ribosomal protein L4

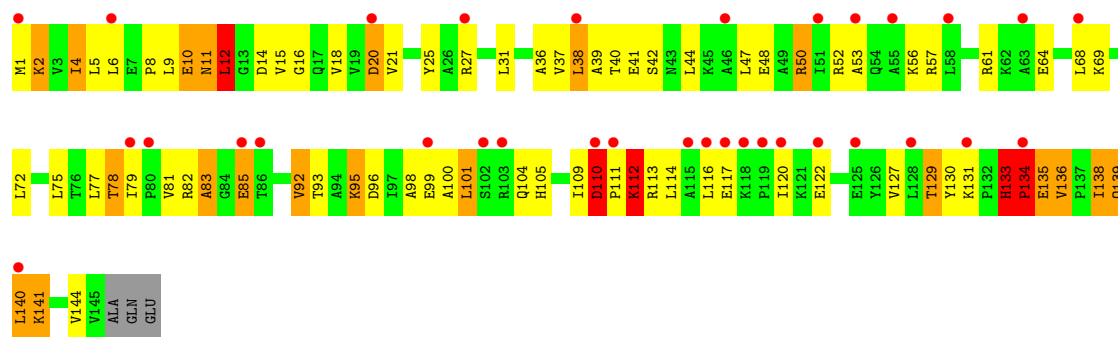


• Molecule 30: 50S ribosomal protein L4

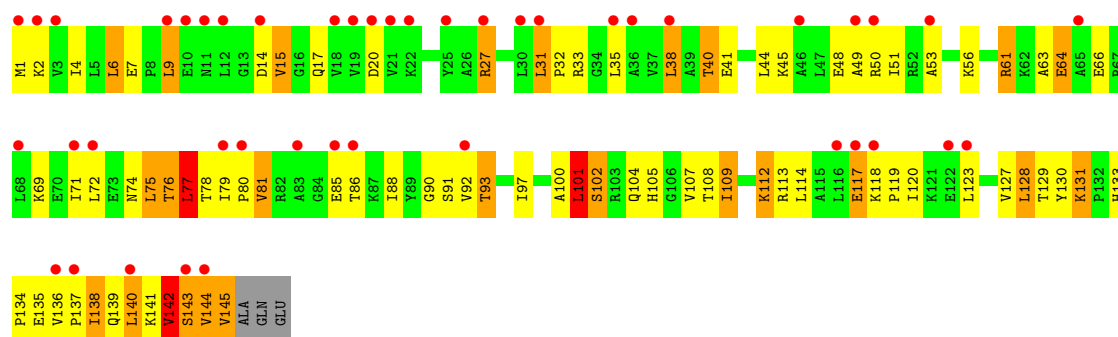
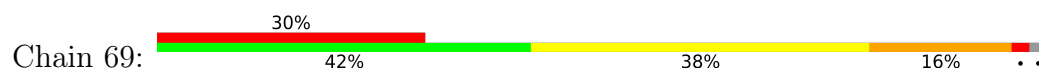


• Molecule 31: 50S ribosomal protein L5

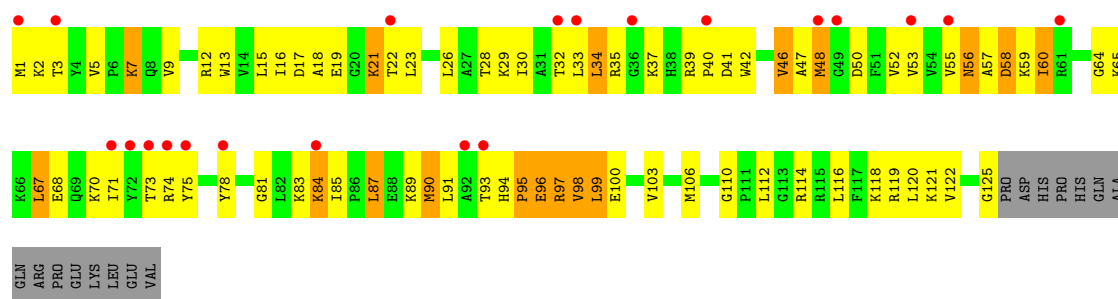




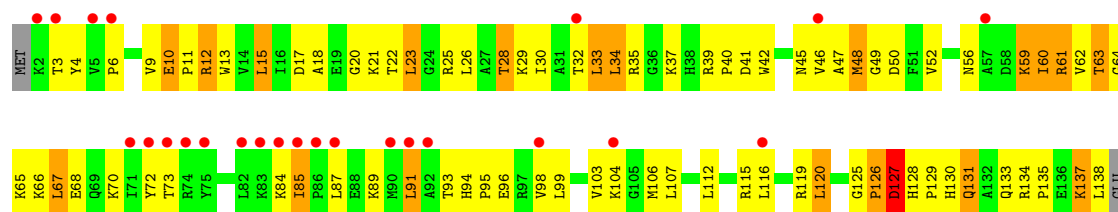
• Molecule 33: 50S ribosomal protein L9



• Molecule 34: 50S ribosomal protein L13

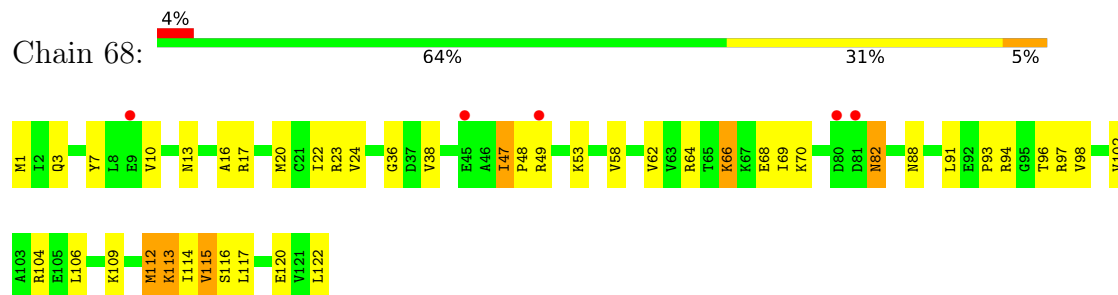


• Molecule 34: 50S ribosomal protein L13

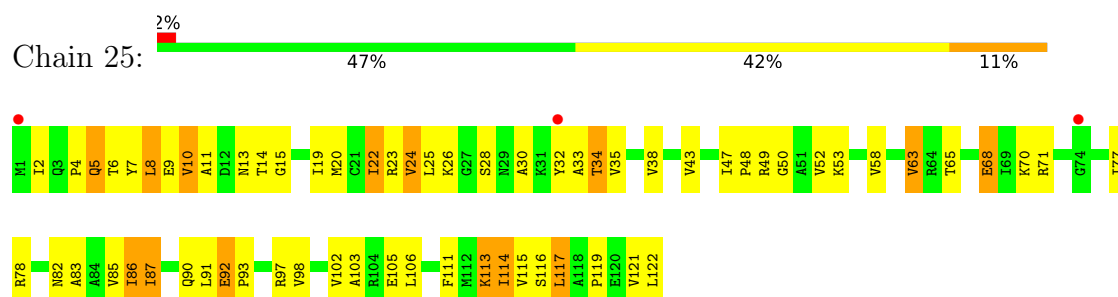


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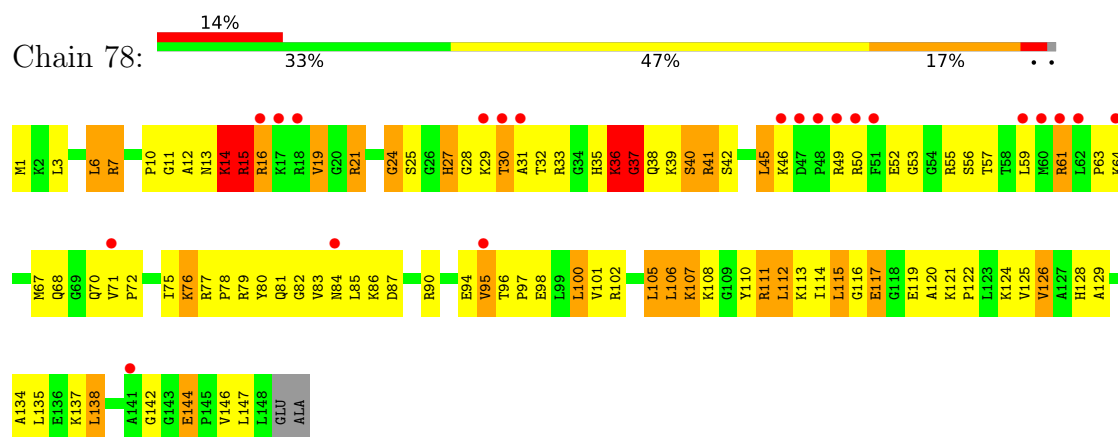
- Molecule 35: 50S ribosomal protein L14



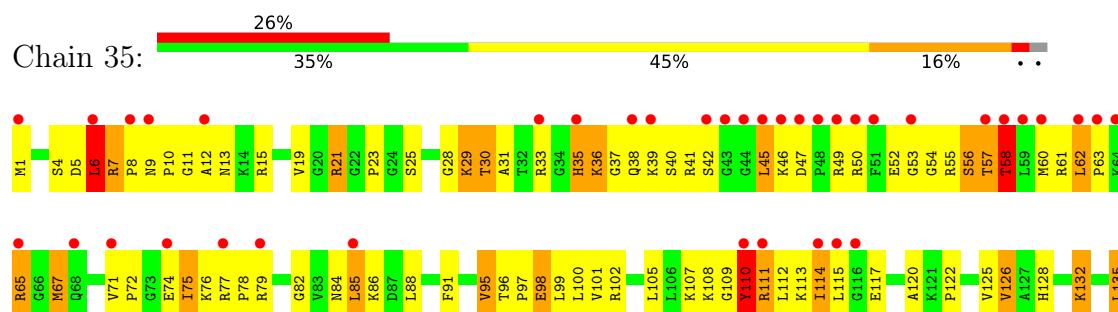
- Molecule 35: 50S ribosomal protein L14



- Molecule 36: 50S ribosomal protein L15

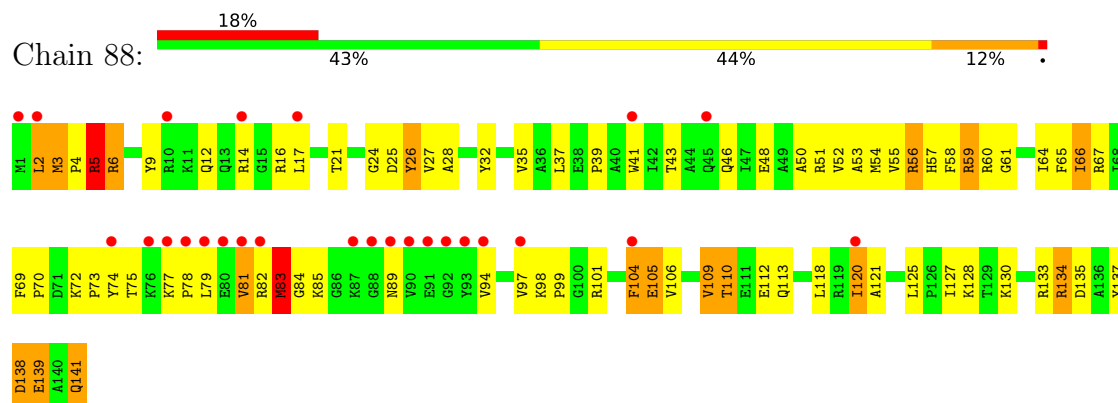


- Molecule 36: 50S ribosomal protein L15

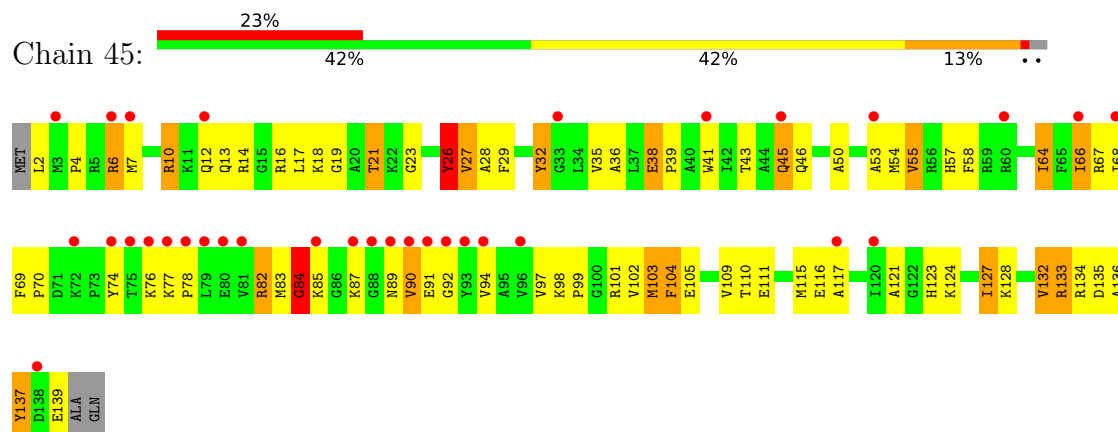




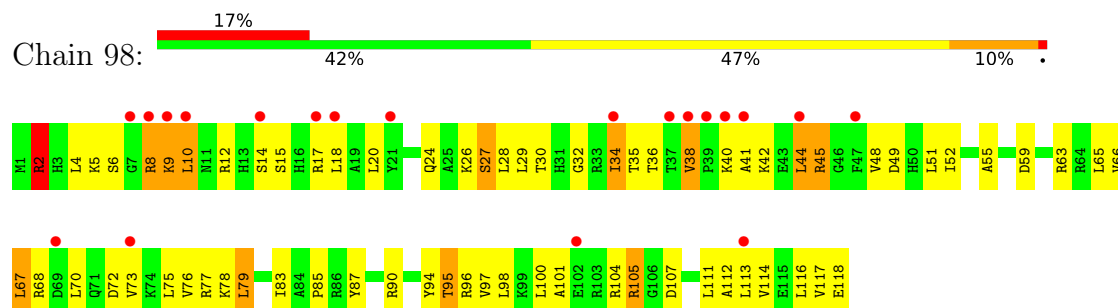
• Molecule 37: 50S ribosomal protein L16



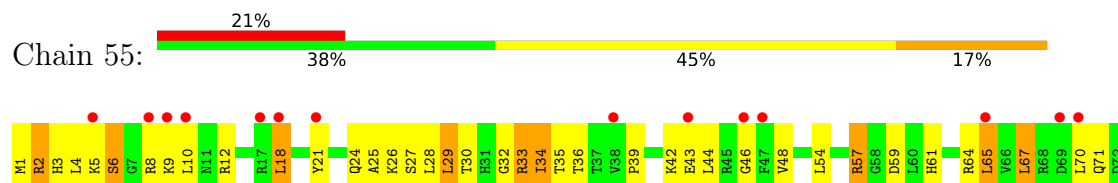
• Molecule 37: 50S ribosomal protein L16

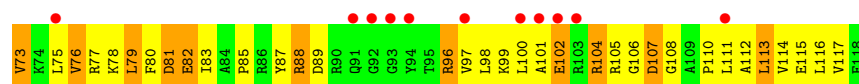


• Molecule 38: 50S ribosomal protein L17

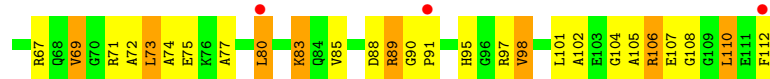
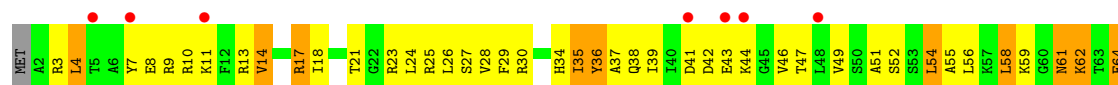


• Molecule 38: 50S ribosomal protein L17

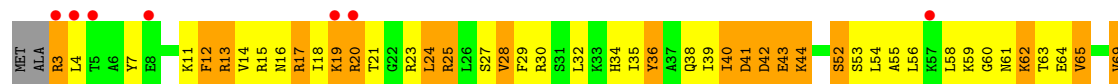




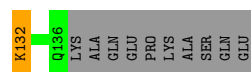
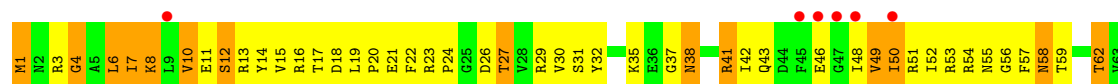
• Molecule 39: 50S ribosomal protein L18



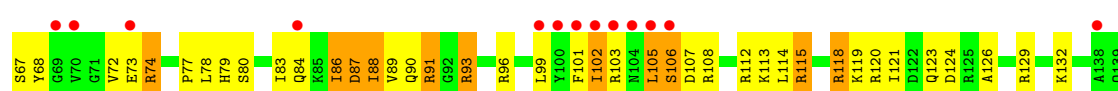
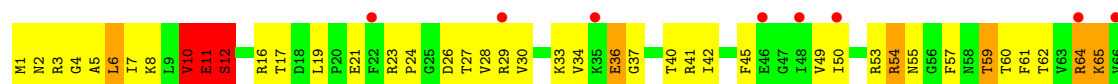
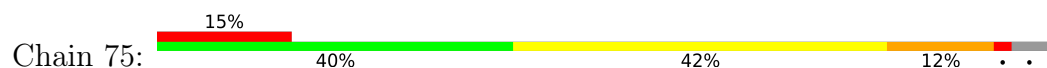
• Molecule 39: 50S ribosomal protein L18

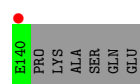


• Molecule 40: 50S ribosomal protein L19

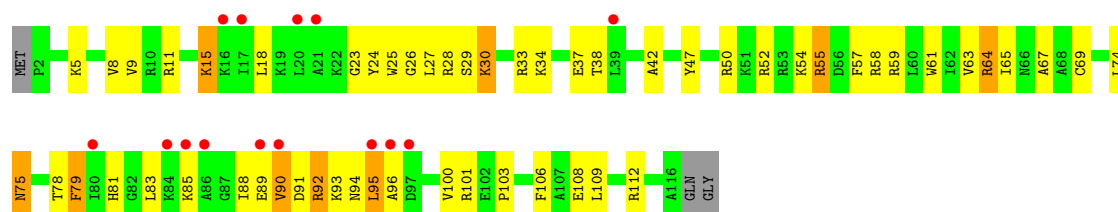


• Molecule 40: 50S ribosomal protein L19

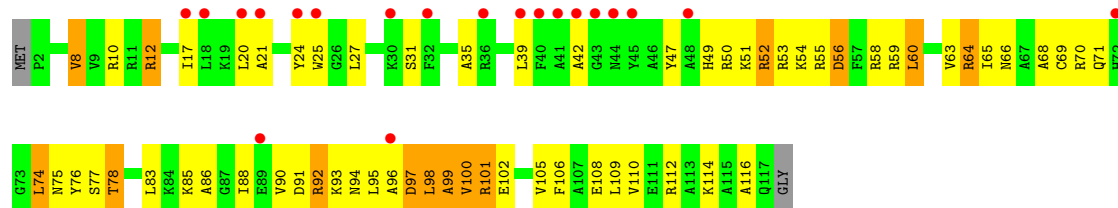




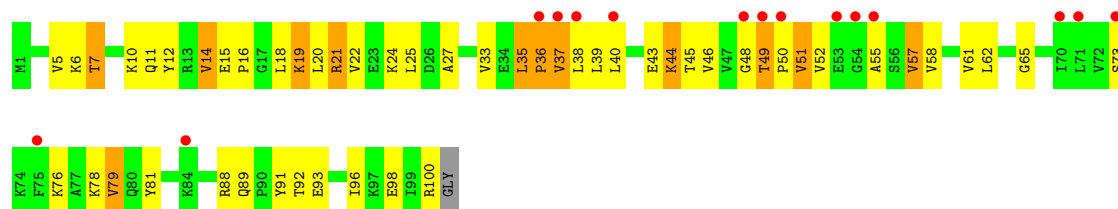
• Molecule 41: 50S ribosomal protein L20



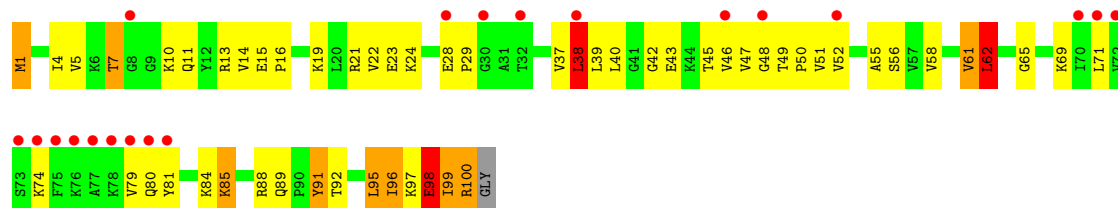
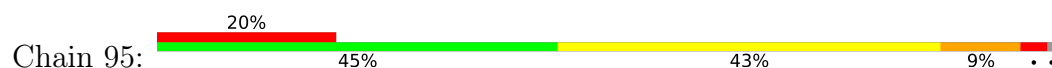
• Molecule 41: 50S ribosomal protein L20



• Molecule 42: 50S ribosomal protein L21

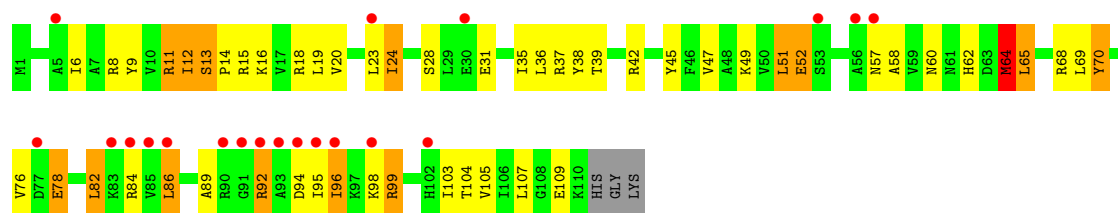


• Molecule 42: 50S ribosomal protein L21

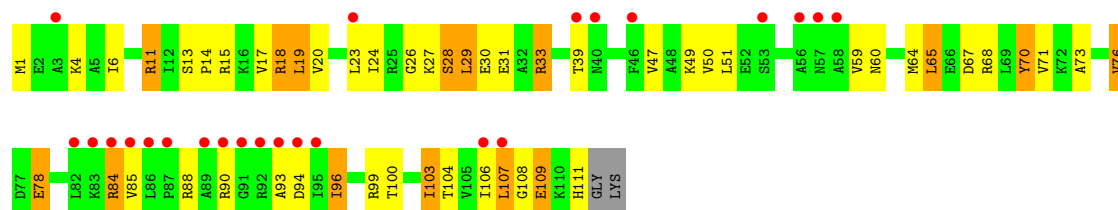


• Molecule 43: 50S ribosomal protein L22

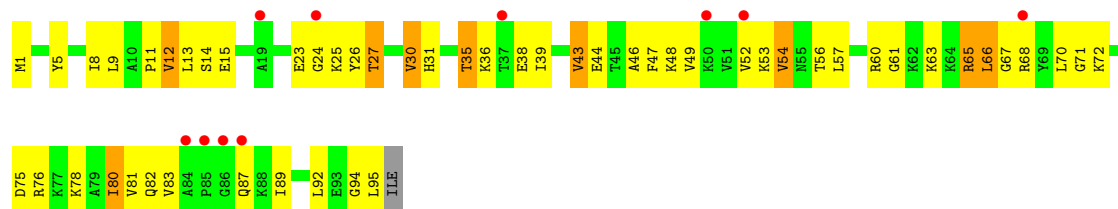
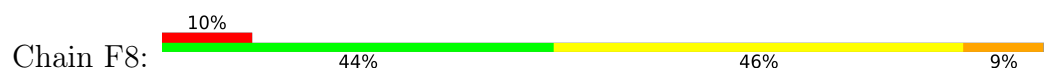




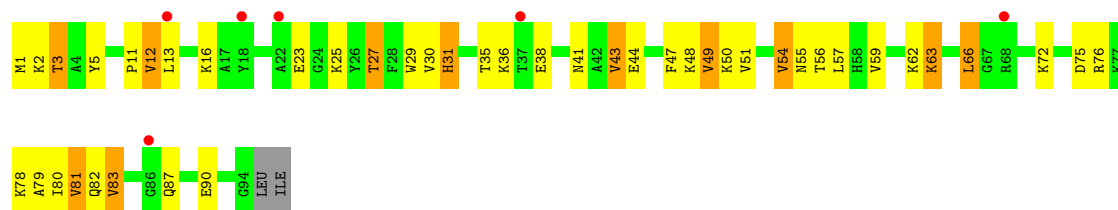
• Molecule 43: 50S ribosomal protein L22



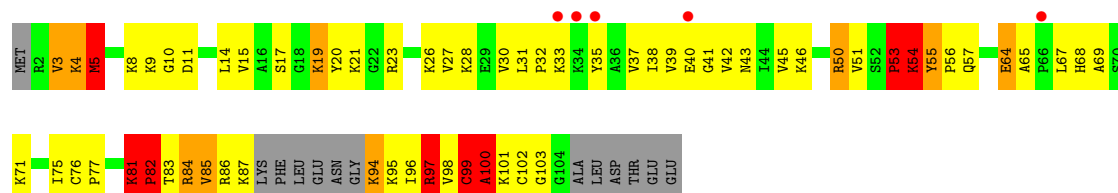
• Molecule 44: 50S ribosomal protein L23



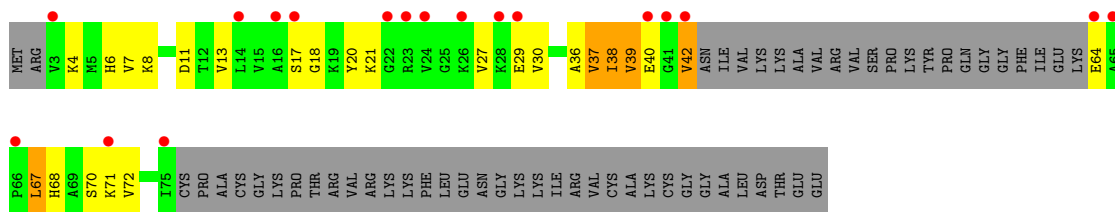
• Molecule 44: 50S ribosomal protein L23



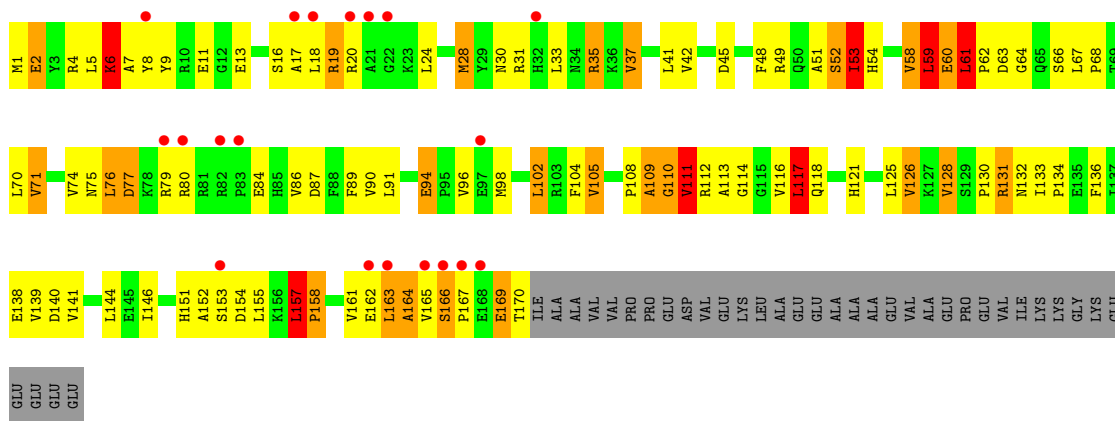
• Molecule 45: 50S ribosomal protein L24



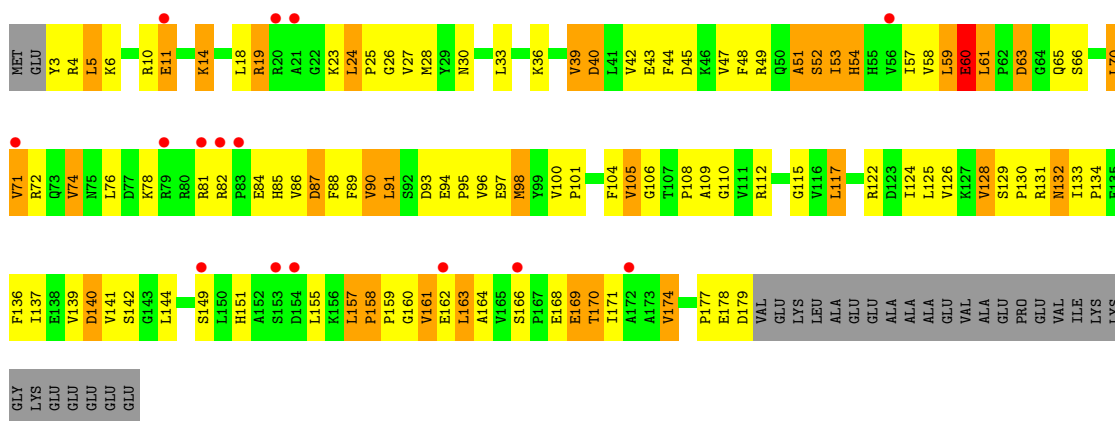
Chain C5:



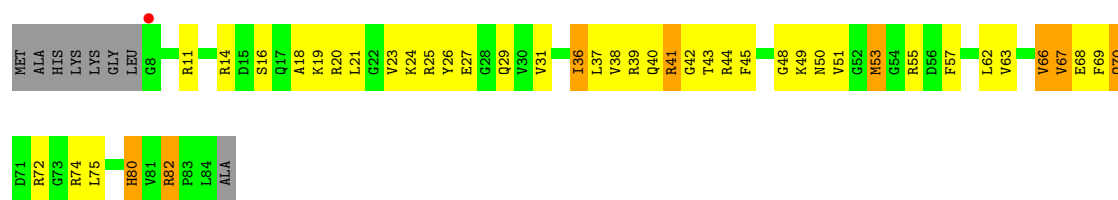
Chain H8:



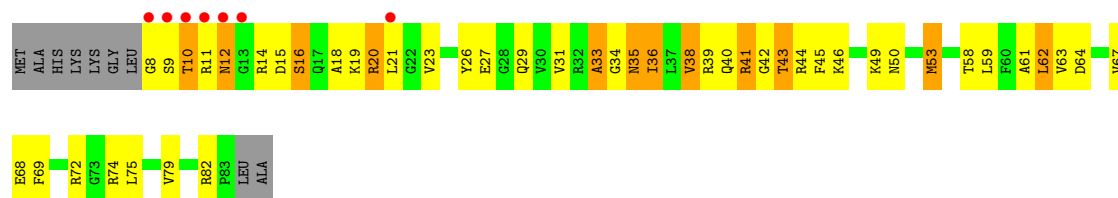
Chain D5:



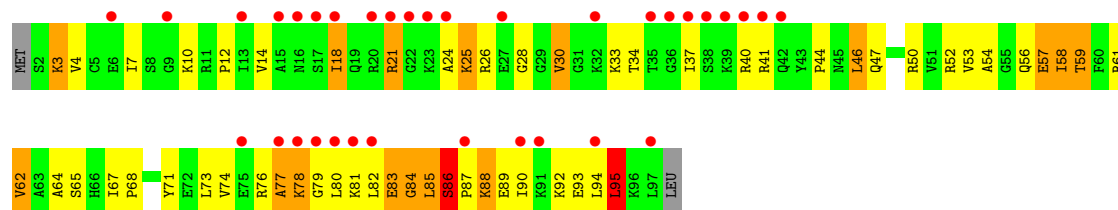
Chain I8:



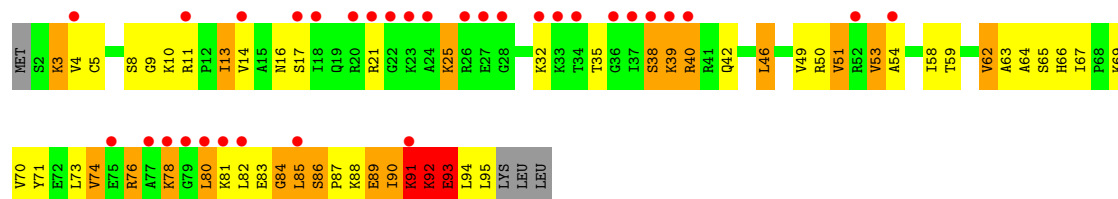
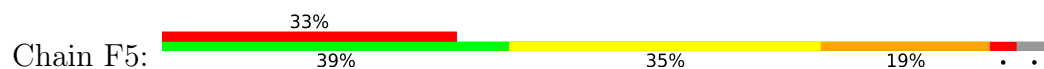
- Molecule 47: 50S ribosomal protein L27



- Molecule 48: 50S ribosomal protein L28



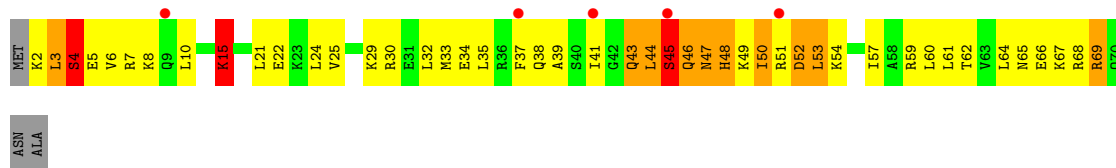
- Molecule 48: 50S ribosomal protein L28



- Molecule 49: 50S ribosomal protein L29



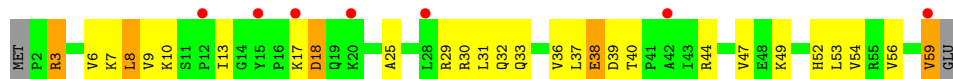
- Molecule 49: 50S ribosomal protein L29



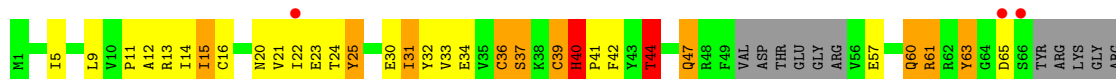
- Molecule 50: 50S ribosomal protein L30



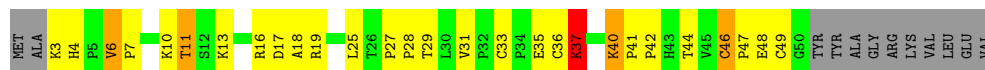
- Molecule 50: 50S ribosomal protein L30



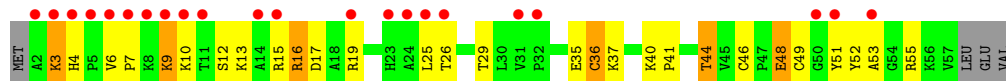
- Molecule 51: 50S ribosomal protein L31



- Molecule 52: 50S ribosomal protein L32

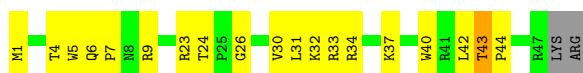


- Molecule 52: 50S ribosomal protein L32



- 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, α , β , γ	209.82Å 449.75Å 618.71Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	224.88 – 3.36 224.88 – 3.36	Depositor EDS
% Data completeness (in resolution range)	99.9 (224.88-3.36) 91.0 (224.88-3.36)	Depositor EDS
R_{merge}	0.36	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.88 (at 3.33Å)	Xtriage
Refinement program	PHENIX 1.12_2829	Depositor
R, R_{free}	0.200 , 0.264 0.202 , 0.263	Depositor DCC
R_{free} test set	2000 reflections (0.24%)	wwPDB-VP
Wilson B-factor (Å ²)	101.0	Xtriage
Anisotropy	0.195	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 181.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.89	EDS
Total number of atoms	292640	wwPDB-VP
Average B, all atoms (Å ²)	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.*

¹Intensities estimated from amplitudes.

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

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: PSU, ZN, AET, MG, 5MU, H2U, SF4

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	0.41	0/36095	0.61	5/56332 (0.0%)
1	1G	0.41	0/35850	0.62	1/55949 (0.0%)
2	12	0.34	0/1727	0.66	2/2326 (0.1%)
2	1E	0.34	0/1908	0.63	2/2573 (0.1%)
3	22	0.35	0/1569	0.68	1/2116 (0.0%)
3	2E	0.37	0/1629	0.65	1/2195 (0.0%)
4	32	0.35	0/1732	0.67	0/2318
4	3E	0.38	0/1728	0.66	0/2313
5	42	0.35	0/1156	0.58	0/1557
5	4E	0.55	1/1158 (0.1%)	0.64	0/1559
6	52	0.37	0/855	0.58	0/1154
6	5E	0.36	0/850	0.57	0/1147
7	62	0.33	0/1122	0.64	2/1500 (0.1%)
7	6E	0.37	0/1259	0.61	2/1686 (0.1%)
8	72	0.31	0/1127	0.62	0/1517
8	7E	0.34	0/1135	0.61	0/1527
9	82	0.28	0/971	0.59	0/1304
9	8E	0.34	0/1019	0.68	0/1367
10	1A	0.28	0/814	0.61	0/1095
10	1I	0.34	0/762	0.65	0/1027
11	2A	0.35	0/850	0.57	0/1150
11	2I	0.40	0/838	0.72	1/1133 (0.1%)
12	3A	0.41	0/972	0.74	0/1301
12	3I	0.50	0/972	0.76	0/1301
13	4A	0.35	0/889	0.74	1/1192 (0.1%)
13	4I	0.43	0/952	0.86	3/1277 (0.2%)
14	5A	0.36	0/495	0.77	0/657
14	5I	0.42	0/500	0.77	2/664 (0.3%)
15	6A	0.36	0/740	0.56	0/987
15	6I	0.39	0/740	0.66	0/987
16	7A	0.35	0/721	0.66	0/970
16	7I	0.39	0/716	0.63	0/963

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
17	8A	0.40	0/836	0.61	0/1117
17	8I	0.37	0/847	0.66	0/1131
18	9A	0.37	0/559	0.65	0/746
18	9I	0.37	0/554	0.57	0/739
19	AA	0.39	0/520	0.81	0/700
19	AI	0.39	0/676	0.79	2/910 (0.2%)
20	BA	0.34	0/764	0.57	0/1007
20	BI	0.38	0/748	0.63	1/986 (0.1%)
21	1B	0.28	0/192	0.58	0/252
21	1F	0.35	0/203	0.57	0/266
22	1K	0.36	0/1675	0.60	0/2608
22	1L	0.31	0/1675	0.50	0/2608
23	2K	0.42	0/1791	0.62	0/2791
23	2L	0.39	0/1791	0.62	0/2791
24	3K	0.34	0/1716	0.56	0/2668
24	3L	0.30	0/1716	0.57	0/2668
25	4K	0.51	0/440	0.79	0/684
25	4L	0.57	0/341	1.02	3/529 (0.6%)
26	14	0.50	0/67828	0.69	11/105880 (0.0%)
26	1H	0.58	0/67804	0.75	8/105829 (0.0%)
27	16	0.46	0/2928	0.72	0/4568
27	1J	0.38	0/2928	0.63	0/4568
28	11	0.58	0/2170	0.94	7/2926 (0.2%)
28	19	0.58	0/2175	0.85	3/2933 (0.1%)
29	21	0.55	1/1589 (0.1%)	0.94	4/2145 (0.2%)
29	29	0.49	0/1596	0.91	2/2153 (0.1%)
30	31	0.56	0/1620	0.81	0/2194
30	39	0.43	0/1637	0.78	4/2218 (0.2%)
31	41	0.43	0/1481	0.70	0/1994
31	49	0.36	0/1483	0.71	1/1997 (0.1%)
32	51	0.47	0/1354	0.95	8/1833 (0.4%)
32	59	0.39	0/1320	0.77	2/1787 (0.1%)
33	61	0.41	0/1146	0.85	6/1551 (0.4%)
33	69	0.37	0/1146	0.74	2/1551 (0.1%)
34	15	0.38	0/1123	0.68	0/1515
34	58	0.49	0/1017	0.83	2/1369 (0.1%)
35	25	0.46	0/942	0.72	0/1269
35	68	0.51	0/942	0.69	0/1269
36	35	0.52	0/1139	0.88	3/1514 (0.2%)
36	78	0.56	0/1144	1.01	3/1521 (0.2%)
37	45	0.50	0/1120	0.91	1/1498 (0.1%)
37	88	0.56	0/1138	0.91	5/1523 (0.3%)
38	55	0.45	0/981	0.73	0/1312

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
38	98	0.76	1/981 (0.1%)	0.76	0/1312
39	65	0.39	0/886	0.74	0/1180
39	A8	0.47	0/891	0.80	0/1187
40	75	0.46	1/1178 (0.1%)	0.77	1/1573 (0.1%)
40	B8	0.47	0/1142	0.83	1/1526 (0.1%)
41	85	0.44	0/977	0.72	0/1301
41	C8	0.53	0/968	0.77	0/1289
42	95	0.40	0/781	0.84	0/1048
42	D8	0.46	0/785	0.83	1/1052 (0.1%)
43	A5	0.46	0/897	0.70	0/1204
43	E8	0.53	0/886	0.76	0/1189
44	B5	0.48	0/749	0.73	0/1007
44	F8	0.59	0/764	0.81	0/1025
45	C5	0.51	0/401	0.93	2/535 (0.4%)
45	G8	0.62	0/745	1.12	5/993 (0.5%)
46	D5	0.36	0/1443	0.70	0/1960
46	H8	0.45	1/1395 (0.1%)	0.85	6/1890 (0.3%)
47	E5	0.47	0/611	0.83	0/814
47	I8	0.63	0/619	0.84	0/825
48	F5	0.52	0/744	0.89	2/989 (0.2%)
48	J8	0.57	0/754	0.91	3/1003 (0.3%)
49	G5	0.47	0/578	0.87	2/766 (0.3%)
49	K8	0.60	0/577	0.99	2/763 (0.3%)
50	H5	0.41	0/464	0.65	0/623
50	L8	0.48	0/464	0.81	0/623
51	M8	0.46	0/485	0.91	0/652
52	J5	0.50	0/448	0.81	0/606
52	N8	0.59	0/381	0.79	0/516
53	L5	0.55	0/414	0.88	0/547
53	P8	0.70	0/409	0.87	0/540
54	M5	0.60	0/524	0.88	2/691 (0.3%)
54	Q8	0.59	0/524	0.97	2/691 (0.3%)
All	All	0.48	5/314511 (0.0%)	0.70	130/471182 (0.0%)

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

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
38	98	38	VAL	CA-CB	18.20	1.63	1.54
5	4E	51	VAL	CA-CB	13.59	1.61	1.54
29	21	109	LYS	C-N	-7.83	1.29	1.33
46	H8	157	LEU	C-O	6.18	1.26	1.23
40	75	106	SER	CA-CB	5.52	1.70	1.53

The worst 5 of 130 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
37	45	104	PHE	N-CA-C	10.63	123.35	110.91
28	11	196	VAL	CA-C-N	-9.94	107.02	121.44
28	11	196	VAL	C-N-CA	-9.94	107.02	121.44
13	4I	7	VAL	N-CA-C	-9.23	102.80	111.48
45	G8	81	LYS	CA-C-N	8.68	147.82	127.00

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	920	0
1	1G	32028	0	16164	934	0
2	12	1696	0	1730	84	0
2	1E	1874	0	1926	95	0
3	22	1546	0	1608	106	0
3	2E	1605	0	1668	60	0
4	32	1702	0	1765	98	0
4	3E	1698	0	1761	80	0
5	42	1141	0	1198	70	0
5	4E	1142	0	1204	44	0
6	52	842	0	857	23	0
6	5E	837	0	852	34	0
7	62	1110	0	1163	71	0
7	6E	1242	0	1286	70	0
8	72	1107	0	1165	71	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	53	0
10	1I	749	0	767	55	0
11	2A	835	0	847	34	0
11	2I	823	0	833	45	0
12	3A	956	0	1046	48	0
12	3I	956	0	1046	48	0
13	4A	879	0	935	84	0
13	4I	942	0	997	64	0
14	5A	486	0	525	28	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	37	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	36	0
17	8I	834	0	904	56	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	45	0
20	BA	762	0	861	38	0
20	BI	746	0	843	58	0
21	1B	188	0	195	9	0
21	1F	199	0	208	12	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	54	0
24	3L	1537	0	779	32	0
25	4K	391	0	196	13	0
25	4L	303	0	153	10	0
26	14	60561	0	30528	1457	0
26	1H	60546	0	30528	1558	0
27	16	2617	0	1328	59	0
27	1J	2617	0	1328	89	0
28	11	2120	0	2197	117	0
28	19	2125	0	2199	119	0
29	21	1556	0	1612	96	0
29	29	1563	0	1629	99	0
30	31	1585	0	1632	95	0
30	39	1602	0	1649	124	0
31	41	1457	0	1514	80	0
31	49	1459	0	1507	95	0
32	51	1328	0	1396	71	0
32	59	1295	0	1366	86	0
33	61	1131	0	1218	49	0
33	69	1131	0	1218	58	0
34	15	1096	0	1168	72	0
34	58	995	0	1077	63	0
35	25	932	0	996	47	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
35	68	932	0	996	25	0
36	35	1122	0	1206	84	0
36	78	1127	0	1208	89	0
37	45	1099	0	1154	86	0
37	88	1117	0	1168	83	0
38	55	967	0	1033	58	0
38	98	967	0	1033	47	0
39	65	876	0	938	75	0
39	A8	881	0	943	57	0
40	75	1164	0	1221	69	0
40	B8	1128	0	1183	79	0
41	85	959	0	1019	63	0
41	C8	950	0	1011	61	0
42	95	770	0	838	44	0
42	D8	774	0	849	31	0
43	A5	886	0	948	34	0
43	E8	876	0	941	37	0
44	B5	735	0	785	33	0
44	F8	750	0	814	35	0
45	C5	396	0	444	15	0
45	G8	734	0	820	46	0
46	D5	1411	0	1436	93	0
46	H8	1365	0	1391	80	0
47	E5	603	0	620	46	0
47	I8	611	0	631	43	0
48	F5	737	0	813	56	0
48	J8	747	0	817	48	0
49	G5	576	0	625	29	0
49	K8	575	0	634	39	0
50	H5	459	0	512	15	0
50	L8	459	0	512	21	0
51	M8	475	0	465	28	0
52	J5	434	0	454	22	0
52	N8	369	0	388	36	0
53	L5	406	0	438	29	0
53	P8	401	0	436	11	0
54	M5	516	0	582	26	0
54	Q8	516	0	582	41	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	2I	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	1	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	9309	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 9309 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%)	24	52
2	1E	227/256 (89%)	184 (81%)	42 (18%)	1 (0%)	30	58
3	22	193/239 (81%)	165 (86%)	27 (14%)	1 (0%)	24	52
3	2E	203/239 (85%)	165 (81%)	36 (18%)	2 (1%)	12	38
4	32	206/209 (99%)	166 (81%)	39 (19%)	1 (0%)	24	52
4	3E	205/209 (98%)	178 (87%)	26 (13%)	1 (0%)	24	52
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%)	18	46
8	7E	136/138 (99%)	120 (88%)	14 (10%)	2 (2%)	8	29
9	82	119/128 (93%)	103 (87%)	14 (12%)	2 (2%)	7	27
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%)	5	23
11	2A	111/129 (86%)	96 (86%)	13 (12%)	2 (2%)	6	26
11	2I	109/129 (84%)	91 (84%)	17 (16%)	1 (1%)	14	41
12	3A	120/132 (91%)	94 (78%)	24 (20%)	2 (2%)	7	27
12	3I	120/132 (91%)	96 (80%)	23 (19%)	1 (1%)	16	44
13	4A	107/126 (85%)	79 (74%)	27 (25%)	1 (1%)	14	41
13	4I	117/126 (93%)	90 (77%)	25 (21%)	2 (2%)	7	27
14	5A	57/61 (93%)	44 (77%)	12 (21%)	1 (2%)	6	26
14	5I	58/61 (95%)	50 (86%)	6 (10%)	2 (3%)	3	16
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%)	9	32
20	BA	97/106 (92%)	82 (84%)	15 (16%)	0	100	100
20	BI	95/106 (90%)	72 (76%)	21 (22%)	2 (2%)	5	23
21	1B	20/27 (74%)	19 (95%)	0	1 (5%)	1	10
21	1F	21/27 (78%)	18 (86%)	2 (10%)	1 (5%)	2	11
28	11	271/276 (98%)	231 (85%)	35 (13%)	5 (2%)	6	26
28	19	272/276 (99%)	233 (86%)	39 (14%)	0	100	100
29	21	203/206 (98%)	157 (77%)	42 (21%)	4 (2%)	6	24
29	29	202/206 (98%)	145 (72%)	52 (26%)	5 (2%)	4	20
30	31	200/210 (95%)	172 (86%)	25 (12%)	3 (2%)	8	29
30	39	202/210 (96%)	155 (77%)	42 (21%)	5 (2%)	4	20
31	41	177/182 (97%)	152 (86%)	24 (14%)	1 (1%)	21	49

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
31	49	178/182 (98%)	151 (85%)	24 (14%)	3 (2%)	7	27
32	51	172/180 (96%)	132 (77%)	30 (17%)	10 (6%)	1	8
32	59	167/180 (93%)	129 (77%)	38 (23%)	0	100	100
33	61	143/148 (97%)	110 (77%)	30 (21%)	3 (2%)	5	23
33	69	143/148 (97%)	109 (76%)	30 (21%)	4 (3%)	4	19
34	15	135/140 (96%)	115 (85%)	19 (14%)	1 (1%)	18	46
34	58	123/140 (88%)	101 (82%)	20 (16%)	2 (2%)	7	28
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%)	5	23
36	78	146/150 (97%)	104 (71%)	35 (24%)	7 (5%)	2	11
37	45	136/141 (96%)	104 (76%)	29 (21%)	3 (2%)	5	23
37	88	139/141 (99%)	114 (82%)	22 (16%)	3 (2%)	5	23
38	55	116/118 (98%)	100 (86%)	15 (13%)	1 (1%)	14	41
38	98	116/118 (98%)	102 (88%)	14 (12%)	0	100	100
39	65	108/112 (96%)	83 (77%)	24 (22%)	1 (1%)	14	41
39	A8	109/112 (97%)	84 (77%)	24 (22%)	1 (1%)	14	41
40	75	138/146 (94%)	118 (86%)	18 (13%)	2 (1%)	9	30
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%)	6	26
42	95	98/101 (97%)	78 (80%)	16 (16%)	4 (4%)	2	14
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	5
46	D5	175/206 (85%)	122 (70%)	48 (27%)	5 (3%)	3	18
46	H8	168/206 (82%)	123 (73%)	38 (23%)	7 (4%)	2	13

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
47	E5	74/85 (87%)	58 (78%)	15 (20%)	1 (1%)	9	30
47	I8	75/85 (88%)	63 (84%)	12 (16%)	0	100	100
48	F5	92/98 (94%)	77 (84%)	12 (13%)	3 (3%)	3	17
48	J8	94/98 (96%)	76 (81%)	13 (14%)	5 (5%)	1	9
49	G5	67/72 (93%)	59 (88%)	7 (10%)	1 (2%)	8	29
49	K8	66/72 (92%)	56 (85%)	7 (11%)	3 (4%)	2	12
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%)	2	15
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	11
All	All	10925/11875 (92%)	9065 (83%)	1719 (16%)	141 (1%)	9	32

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%)	132 (74%)	47 (26%)	0	1

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	1E	200/220 (91%)	147 (74%)	53 (26%)	0	1
3	22	154/188 (82%)	115 (75%)	39 (25%)	0	1
3	2E	159/188 (85%)	124 (78%)	35 (22%)	1	3
4	32	180/181 (99%)	144 (80%)	36 (20%)	1	4
4	3E	180/181 (99%)	134 (74%)	46 (26%)	0	1
5	42	114/123 (93%)	82 (72%)	32 (28%)	0	1
5	4E	115/123 (94%)	84 (73%)	31 (27%)	0	1
6	52	90/90 (100%)	69 (77%)	21 (23%)	1	2
6	5E	90/90 (100%)	76 (84%)	14 (16%)	2	10
7	62	114/127 (90%)	92 (81%)	22 (19%)	1	5
7	6E	125/127 (98%)	90 (72%)	35 (28%)	0	1
8	72	118/119 (99%)	92 (78%)	26 (22%)	1	3
8	7E	119/119 (100%)	90 (76%)	29 (24%)	1	2
9	82	92/99 (93%)	68 (74%)	24 (26%)	0	1
9	8E	97/99 (98%)	75 (77%)	22 (23%)	1	3
10	1A	89/92 (97%)	67 (75%)	22 (25%)	1	2
10	1I	81/92 (88%)	63 (78%)	18 (22%)	1	3
11	2A	85/99 (86%)	70 (82%)	15 (18%)	2	8
11	2I	84/99 (85%)	67 (80%)	17 (20%)	1	4
12	3A	103/109 (94%)	69 (67%)	34 (33%)	0	0
12	3I	103/109 (94%)	71 (69%)	32 (31%)	0	1
13	4A	90/101 (89%)	61 (68%)	29 (32%)	0	0
13	4I	94/101 (93%)	68 (72%)	26 (28%)	0	1
14	5A	49/50 (98%)	35 (71%)	14 (29%)	0	1
14	5I	49/50 (98%)	39 (80%)	10 (20%)	1	4
15	6A	79/80 (99%)	69 (87%)	10 (13%)	4	17
15	6I	79/80 (99%)	61 (77%)	18 (23%)	1	3
16	7A	72/74 (97%)	59 (82%)	13 (18%)	2	7
16	7I	72/74 (97%)	54 (75%)	18 (25%)	0	2
17	8A	94/97 (97%)	79 (84%)	15 (16%)	2	10
17	8I	95/97 (98%)	72 (76%)	23 (24%)	1	2

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
18	9A	58/77 (75%)	44 (76%)	14 (24%)	1	2
18	9I	58/77 (75%)	52 (90%)	6 (10%)	7	25
19	AA	56/80 (70%)	38 (68%)	18 (32%)	0	0
19	AI	72/80 (90%)	48 (67%)	24 (33%)	0	0
20	BA	76/82 (93%)	71 (93%)	5 (7%)	15	42
20	BI	75/82 (92%)	60 (80%)	15 (20%)	1	4
21	1B	17/22 (77%)	15 (88%)	2 (12%)	5	19
21	1F	18/22 (82%)	14 (78%)	4 (22%)	1	3
28	11	214/218 (98%)	160 (75%)	54 (25%)	0	1
28	19	214/218 (98%)	159 (74%)	55 (26%)	0	1
29	21	162/166 (98%)	123 (76%)	39 (24%)	1	2
29	29	165/166 (99%)	128 (78%)	37 (22%)	1	3
30	31	161/166 (97%)	114 (71%)	47 (29%)	0	1
30	39	163/166 (98%)	116 (71%)	47 (29%)	0	1
31	41	153/156 (98%)	116 (76%)	37 (24%)	1	2
31	49	152/156 (97%)	111 (73%)	41 (27%)	0	1
32	51	143/148 (97%)	109 (76%)	34 (24%)	1	2
32	59	140/148 (95%)	88 (63%)	52 (37%)	0	0
33	61	122/124 (98%)	82 (67%)	40 (33%)	0	0
33	69	122/124 (98%)	86 (70%)	36 (30%)	0	1
34	15	116/119 (98%)	85 (73%)	31 (27%)	0	1
34	58	105/119 (88%)	76 (72%)	29 (28%)	0	1
35	25	100/100 (100%)	80 (80%)	20 (20%)	1	4
35	68	100/100 (100%)	80 (80%)	20 (20%)	1	4
36	35	114/116 (98%)	73 (64%)	41 (36%)	0	0
36	78	114/116 (98%)	78 (68%)	36 (32%)	0	1
37	45	109/111 (98%)	85 (78%)	24 (22%)	1	3
37	88	110/111 (99%)	89 (81%)	21 (19%)	1	6
38	55	101/101 (100%)	71 (70%)	30 (30%)	0	1
38	98	101/101 (100%)	78 (77%)	23 (23%)	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%)	62 (71%)	25 (29%)	0	1	
40	75	122/127 (96%)	90 (74%)	32 (26%)	0	1	
40	B8	118/127 (93%)	86 (73%)	32 (27%)	0	1	
41	85	93/94 (99%)	75 (81%)	18 (19%)	1	5	
41	C8	92/94 (98%)	80 (87%)	12 (13%)	4	16	
42	95	81/82 (99%)	63 (78%)	18 (22%)	1	3	
42	D8	82/82 (100%)	52 (63%)	30 (37%)	0	0	
43	A5	91/92 (99%)	67 (74%)	24 (26%)	0	1	
43	E8	90/92 (98%)	68 (76%)	22 (24%)	1	2	
44	B5	74/78 (95%)	58 (78%)	16 (22%)	1	3	
44	F8	77/78 (99%)	57 (74%)	20 (26%)	0	1	
45	C5	43/91 (47%)	32 (74%)	11 (26%)	0	1	
45	G8	79/91 (87%)	58 (73%)	21 (27%)	0	1	
46	D5	156/179 (87%)	114 (73%)	42 (27%)	0	1	
46	H8	151/179 (84%)	113 (75%)	38 (25%)	0	1	
47	E5	61/67 (91%)	46 (75%)	15 (25%)	1	2	
47	I8	62/67 (92%)	53 (86%)	9 (14%)	3	13	
48	F5	79/83 (95%)	53 (67%)	26 (33%)	0	0	
48	J8	79/83 (95%)	58 (73%)	21 (27%)	0	1	
49	G5	63/67 (94%)	40 (64%)	23 (36%)	0	0	
49	K8	64/67 (96%)	40 (62%)	24 (38%)	0	0	
50	H5	50/52 (96%)	35 (70%)	15 (30%)	0	1	
50	L8	50/52 (96%)	34 (68%)	16 (32%)	0	1	
51	M8	52/63 (82%)	38 (73%)	14 (27%)	0	1	
52	J5	48/52 (92%)	37 (77%)	11 (23%)	1	2	
52	N8	43/52 (83%)	36 (84%)	7 (16%)	2	10	
53	L5	38/42 (90%)	32 (84%)	6 (16%)	2	10	
53	P8	38/42 (90%)	32 (84%)	6 (16%)	2	10	
54	M5	54/55 (98%)	45 (83%)	9 (17%)	2	9	
54	Q8	54/55 (98%)	44 (82%)	10 (18%)	1	7	
All	All	9213/9831 (94%)	6905 (75%)	2308 (25%)	0	2	

5 of 2308 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
33	69	101	LEU
52	J5	55	ARG
35	25	38	VAL
33	69	86	THR
41	85	60	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 76 such sidechains are listed below:

Mol	Chain	Res	Type
31	49	26	GLN
43	A5	60	ASN
32	59	143	GLN
38	55	61	HIS
49	G5	56	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	13	1498/1522 (98%)	347 (23%)	28 (1%)
1	1G	1489/1522 (97%)	370 (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	2805/2917 (96%)	693 (24%)	36 (1%)
26	1H	2800/2917 (95%)	628 (22%)	41 (1%)
27	16	121/122 (99%)	27 (22%)	1 (0%)
27	1J	121/122 (99%)	34 (28%)	1 (0%)
All	All	9297/9634 (96%)	2306 (24%)	158 (1%)

5 of 2306 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
23	2L	48	U
26	14	1963	U
25	4L	22	A
26	14	774	A
26	14	2611	U

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	PSU	1K	55	22	18,21,22	1.30	1 (5%)	21,30,33	2.02	5 (23%)
22	H2U	1L	17	22	18,21,22	2.32	4 (22%)	19,30,33	1.64	4 (21%)
23	PSU	2K	56	23	18,21,22	1.24	2 (11%)	21,30,33	2.42	5 (23%)
23	PSU	2L	56	23	18,21,22	1.29	2 (11%)	21,30,33	1.91	3 (14%)
23	5MU	2L	55	23	19,22,23	3.89	5 (26%)	27,32,35	3.25	10 (37%)
23	5MU	2K	55	23	19,22,23	3.96	5 (26%)	27,32,35	3.25	8 (29%)
22	H2U	1K	17	22	18,21,22	2.24	4 (22%)	19,30,33	1.61	4 (21%)
22	AET	1L	37	22	32,35,36	2.70	6 (18%)	43,51,54	2.17	14 (32%)
22	PSU	1L	55	22	18,21,22	1.24	1 (5%)	21,30,33	1.81	4 (19%)
22	AET	1K	37	22	32,35,36	3.02	6 (18%)	43,51,54	2.28	14 (32%)
22	5MU	1L	54	22	19,22,23	4.09	5 (26%)	27,32,35	3.22	9 (33%)
22	5MU	1K	54	22	19,22,23	4.01	5 (26%)	27,32,35	3.36	9 (33%)

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

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	PSU	1K	55	22	-	2/7/25/26	0/2/2/2
22	H2U	1L	17	22	-	5/7/38/39	0/2/2/2
23	PSU	2K	56	23	-	0/7/25/26	0/2/2/2
23	PSU	2L	56	23	-	0/7/25/26	0/2/2/2
23	5MU	2L	55	23	-	0/7/25/26	0/2/2/2
23	5MU	2K	55	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	-	8/27/45/46	0/3/3/3
22	PSU	1L	55	22	-	3/7/25/26	0/2/2/2
22	AET	1K	37	22	-	8/27/45/46	0/3/3/3
22	5MU	1L	54	22	-	0/7/25/26	0/2/2/2
22	5MU	1K	54	22	-	4/7/25/26	0/2/2/2

The worst 5 of 46 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	1L	54	5MU	C2-N1	13.32	1.59	1.38
22	1K	54	5MU	C2-N1	13.15	1.59	1.38
22	1K	37	AET	C10-N6	12.92	1.55	1.37
23	2K	55	5MU	C2-N1	12.91	1.58	1.38
23	2L	55	5MU	C2-N1	12.22	1.57	1.38

The worst 5 of 89 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	1K	54	5MU	C5-C4-N3	10.86	124.76	115.32
23	2L	55	5MU	C5-C4-N3	10.67	124.60	115.32
22	1L	54	5MU	C5-C4-N3	9.66	123.72	115.32
23	2K	55	5MU	C5-C4-N3	9.21	123.33	115.32
23	2K	55	5MU	C6-C5-C4	7.02	123.81	118.02

There are no chirality outliers.

5 of 34 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
22	1K	17	H2U	O4'-C1'-N1-C6
22	1K	17	H2U	C2'-C1'-N1-C2

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Mol	Chain	Res	Type	Atoms
22	1K	17	H2U	C2'-C1'-N1-C6
22	1L	17	H2U	O4'-C1'-N1-C2
22	1L	17	H2U	O4'-C1'-N1-C6

There are no ring outliers.

3 monomers are involved in 7 short contacts:

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides 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	-	-	-		
56	SF4	3E	301	-	0,12,12	-	-	-		

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
24	3L	1
24	3K	1
26	1H	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, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	13	1500/1522 (98%)	1.26	371 (24%) 2 3	76, 125, 184, 245	0
1	1G	1490/1522 (97%)	0.78	227 (15%) 5 6	83, 128, 188, 248	0
2	12	207/256 (80%)	1.77	74 (35%) 1 1	161, 184, 195, 199	0
2	1E	231/256 (90%)	1.06	38 (16%) 4 5	141, 166, 184, 190	0
3	22	197/239 (82%)	1.35	51 (25%) 1 2	154, 171, 186, 191	0
3	2E	205/239 (85%)	1.12	39 (19%) 3 4	111, 131, 153, 161	0
4	32	208/209 (99%)	0.90	34 (16%) 4 5	120, 138, 152, 159	0
4	3E	207/209 (99%)	0.49	14 (6%) 23 18	110, 133, 148, 155	0
5	42	150/162 (92%)	1.15	26 (17%) 4 5	125, 140, 157, 169	0
5	4E	149/162 (91%)	1.02	28 (18%) 3 4	103, 125, 139, 144	0
6	52	101/101 (100%)	0.99	15 (14%) 5 6	115, 130, 143, 149	0
6	5E	100/101 (99%)	1.11	17 (17%) 4 5	111, 130, 143, 148	0
7	62	138/156 (88%)	0.62	11 (7%) 18 15	141, 152, 160, 165	0
7	6E	154/156 (98%)	0.94	15 (9%) 13 12	121, 144, 164, 171	0
8	72	137/138 (99%)	1.31	31 (22%) 2 3	124, 148, 161, 164	0
8	7E	138/138 (100%)	0.58	10 (7%) 21 17	114, 133, 143, 154	0
9	82	121/128 (94%)	0.81	13 (10%) 11 11	136, 172, 180, 189	0
9	8E	126/128 (98%)	1.84	29 (23%) 2 3	113, 159, 175, 182	0
10	1A	99/105 (94%)	1.79	23 (23%) 2 3	151, 177, 186, 190	0
10	1I	94/105 (89%)	1.52	21 (22%) 2 3	108, 151, 170, 173	0
11	2A	113/129 (87%)	0.60	5 (4%) 39 28	107, 132, 147, 153	0
11	2I	111/129 (86%)	1.20	18 (16%) 4 5	100, 132, 150, 165	0
12	3A	122/132 (92%)	1.16	22 (18%) 3 4	112, 126, 140, 147	0
12	3I	122/132 (92%)	0.96	23 (18%) 3 4	89, 102, 123, 138	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
13	4A	109/126 (86%)	1.65	24 (22%) 2 3	147, 174, 184, 192	0
13	4I	119/126 (94%)	1.48	23 (19%) 3 4	108, 141, 151, 161	0
14	5A	59/61 (96%)	1.63	15 (25%) 1 3	155, 172, 184, 193	0
14	5I	60/61 (98%)	0.29	2 (3%) 49 35	113, 123, 140, 142	0
15	6A	87/89 (97%)	0.74	10 (11%) 9 10	113, 133, 149, 153	0
15	6I	87/89 (97%)	1.09	22 (25%) 1 3	110, 126, 142, 148	0
16	7A	84/88 (95%)	0.91	12 (14%) 6 7	110, 128, 147, 175	0
16	7I	83/88 (94%)	1.15	17 (20%) 2 4	127, 142, 164, 175	0
17	8A	99/105 (94%)	0.88	16 (16%) 4 5	116, 127, 140, 145	0
17	8I	100/105 (95%)	1.45	20 (20%) 3 4	111, 128, 138, 139	0
18	9A	69/88 (78%)	0.25	3 (4%) 40 28	118, 135, 151, 160	0
18	9I	68/88 (77%)	0.73	11 (16%) 4 5	114, 132, 145, 153	0
19	AA	65/93 (69%)	0.92	11 (16%) 4 5	170, 188, 195, 196	0
19	AI	82/93 (88%)	0.97	13 (15%) 5 5	116, 140, 164, 171	0
20	BA	99/106 (93%)	0.85	13 (13%) 7 8	116, 133, 153, 156	0
20	BI	97/106 (91%)	1.02	17 (17%) 4 5	124, 143, 162, 165	0
21	1B	22/27 (81%)	0.22	0 100 100	138, 161, 164, 166	0
21	1F	23/27 (85%)	0.34	3 (13%) 7 8	117, 127, 134, 141	0
22	1K	70/76 (92%)	1.97	24 (34%) 1 1	118, 199, 215, 218	0
22	1L	70/76 (92%)	1.82	17 (24%) 2 3	137, 224, 235, 238	0
23	2K	75/77 (97%)	0.62	11 (14%) 6 6	84, 118, 147, 158	0
23	2L	75/77 (97%)	0.28	2 (2%) 56 41	94, 135, 158, 169	0
24	3K	72/76 (94%)	1.71	21 (29%) 1 2	88, 208, 234, 241	0
24	3L	72/76 (94%)	1.20	14 (19%) 3 4	100, 201, 226, 230	0
25	4K	18/27 (66%)	0.20	2 (11%) 10 10	96, 147, 195, 200	0
25	4L	14/27 (51%)	0.05	0 100 100	118, 164, 175, 177	0
26	14	2811/2917 (96%)	0.87	572 (20%) 3 4	64, 104, 193, 248	0
26	1H	2811/2917 (96%)	0.60	452 (16%) 4 5	56, 89, 174, 260	0
27	16	122/122 (100%)	0.35	7 (5%) 29 22	87, 112, 131, 182	0
27	1J	122/122 (100%)	0.51	13 (10%) 11 11	117, 142, 157, 190	0
28	11	273/276 (98%)	0.63	27 (9%) 13 12	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%)	0.67	33 (12%)	9	9	59, 90, 108, 119	0
29	21	205/206 (99%)	0.97	42 (20%)	2	4	66, 100, 134, 144	0
29	29	204/206 (99%)	2.24	67 (32%)	1	1	76, 114, 145, 159	0
30	31	202/210 (96%)	1.19	40 (19%)	3	4	60, 93, 126, 139	0
30	39	204/210 (97%)	2.10	60 (29%)	1	2	74, 123, 157, 170	0
31	41	179/182 (98%)	0.56	14 (7%)	19	15	105, 125, 147, 157	0
31	49	180/182 (98%)	0.72	19 (10%)	11	11	139, 158, 176, 187	0
32	51	174/180 (96%)	0.83	23 (13%)	7	8	99, 119, 132, 147	0
32	59	169/180 (93%)	2.68	83 (49%)	0	0	174, 207, 224, 229	0
33	61	145/148 (97%)	1.22	33 (22%)	2	3	97, 148, 162, 167	0
33	69	145/148 (97%)	1.73	44 (30%)	1	1	100, 142, 160, 165	0
34	15	137/140 (97%)	1.16	24 (17%)	4	5	94, 127, 154, 162	0
34	58	125/140 (89%)	0.99	21 (16%)	4	5	84, 101, 118, 135	0
35	25	122/122 (100%)	0.35	3 (2%)	58	43	82, 104, 119, 128	0
35	68	122/122 (100%)	0.35	5 (4%)	41	29	73, 94, 112, 126	0
36	35	147/150 (98%)	1.47	39 (26%)	1	2	74, 122, 150, 161	0
36	78	148/150 (98%)	0.60	21 (14%)	6	7	63, 98, 121, 128	0
37	45	138/141 (97%)	1.46	33 (23%)	2	3	91, 125, 148, 160	0
37	88	141/141 (100%)	1.31	26 (18%)	3	4	74, 98, 119, 144	0
38	55	118/118 (100%)	1.04	25 (21%)	2	4	79, 101, 115, 124	0
38	98	118/118 (100%)	0.81	20 (16%)	4	5	78, 97, 116, 131	0
39	65	110/112 (98%)	0.46	9 (8%)	17	15	116, 134, 146, 155	0
39	A8	111/112 (99%)	0.62	10 (9%)	15	13	93, 108, 124, 136	0
40	75	140/146 (95%)	1.07	22 (15%)	5	6	97, 114, 166, 177	0
40	B8	136/146 (93%)	1.18	29 (21%)	2	4	89, 108, 150, 175	0
41	85	116/118 (98%)	1.23	20 (17%)	4	5	82, 117, 146, 155	0
41	C8	115/118 (97%)	0.74	14 (12%)	8	9	68, 94, 121, 131	0
42	95	100/101 (99%)	1.16	20 (20%)	3	4	82, 141, 153, 159	0
42	D8	100/101 (99%)	0.93	15 (15%)	5	6	66, 112, 131, 136	0
43	A5	111/113 (98%)	1.32	24 (21%)	2	4	77, 95, 124, 143	0
43	E8	110/113 (97%)	1.29	20 (18%)	3	4	68, 87, 111, 124	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
44	B5	94/96 (97%)	0.44	6 (6%) 25 19	91, 104, 118, 125	0
44	F8	95/96 (98%)	0.74	10 (10%) 11 11	71, 85, 112, 122	0
45	C5	52/110 (47%)	1.78	18 (34%) 1 1	109, 122, 135, 145	0
45	G8	97/110 (88%)	0.73	5 (5%) 33 23	91, 107, 131, 142	0
46	D5	177/206 (85%)	0.68	15 (8%) 16 14	132, 166, 217, 221	0
46	H8	170/206 (82%)	0.68	19 (11%) 10 10	105, 137, 187, 195	0
47	E5	76/85 (89%)	0.57	7 (9%) 14 13	95, 109, 124, 131	0
47	I8	77/85 (90%)	0.03	1 (1%) 75 61	76, 88, 110, 120	0
48	F5	94/98 (95%)	1.84	32 (34%) 1 1	78, 104, 133, 138	0
48	J8	96/98 (97%)	1.65	34 (35%) 1 1	72, 94, 142, 152	0
49	G5	69/72 (95%)	0.58	5 (7%) 21 17	107, 128, 145, 156	0
49	K8	68/72 (94%)	1.19	16 (23%) 2 3	78, 99, 116, 136	0
50	H5	58/60 (96%)	0.78	7 (12%) 8 9	100, 121, 137, 150	0
50	L8	58/60 (96%)	0.43	4 (6%) 23 18	72, 93, 122, 124	0
51	M8	60/71 (84%)	0.50	3 (5%) 34 24	126, 154, 167, 170	0
52	J5	56/60 (93%)	1.92	22 (39%) 1 1	74, 103, 138, 151	0
52	N8	48/60 (80%)	0.49	0 100 100	64, 98, 126, 133	0
53	L5	48/49 (97%)	-0.06	3 (6%) 26 19	70, 78, 110, 114	0
53	P8	47/49 (95%)	-0.16	0 100 100	61, 68, 90, 98	0
54	M5	64/65 (98%)	0.56	4 (6%) 26 19	83, 97, 115, 126	0
54	Q8	64/65 (98%)	0.18	0 100 100	68, 83, 101, 110	0
All	All	20451/21509 (95%)	0.95	3618 (17%) 4 5	56, 119, 186, 260	0

The worst 5 of 3618 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
32	59	151	ILE	23.1
22	1L	76	A	17.9
9	8E	127	LYS	17.3
13	4I	120	LYS	16.9
9	82	115	GLY	16.7

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, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
22	PSU	1L	55	20/21	0.55	0.12	169,202,215,222	0
22	5MU	1L	54	21/22	0.56	0.14	171,182,192,193	0
22	H2U	1K	17	20/21	0.56	0.15	199,211,220,220	0
22	H2U	1L	17	20/21	0.57	0.23	213,231,237,237	0
22	5MU	1K	54	21/22	0.60	0.17	139,156,165,170	0
23	5MU	2L	55	21/22	0.68	0.11	129,139,144,146	0
22	PSU	1K	55	20/21	0.74	0.13	146,178,188,189	0
22	AET	1L	37	33/34	0.76	0.30	156,171,176,178	0
23	5MU	2K	55	21/22	0.80	0.10	118,124,135,139	0
22	AET	1K	37	33/34	0.82	0.39	112,124,147,151	0
23	PSU	2L	56	20/21	0.82	0.07	126,136,143,146	0
23	PSU	2K	56	20/21	0.84	0.09	113,119,131,132	0

6.3 Carbohydrates ⓘ

There are no oligosaccharides 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, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
55	MG	13	1663	1/1	-0.20	0.39	123,123,123,123	0
55	MG	1G	1642	1/1	-0.17	0.35	154,154,154,154	0
55	MG	1G	1630	1/1	-0.13	0.42	135,135,135,135	0
55	MG	14	3176	1/1	0.06	0.45	109,109,109,109	0
55	MG	1G	1621	1/1	0.15	0.50	115,115,115,115	0
55	MG	1H	3208	1/1	0.16	0.37	113,113,113,113	0
55	MG	14	3138	1/1	0.17	0.38	134,134,134,134	0
55	MG	14	3016	1/1	0.17	0.47	110,110,110,110	0
55	MG	1H	3277	1/1	0.25	0.43	103,103,103,103	0
55	MG	1G	1662	1/1	0.26	0.49	116,116,116,116	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
55	MG	14	3113	1/1	0.27	0.47	120,120,120,120	0
55	MG	1G	1666	1/1	0.29	0.37	136,136,136,136	0
55	MG	1H	3254	1/1	0.30	0.39	97,97,97,97	0
55	MG	13	1631	1/1	0.31	0.35	132,132,132,132	0
55	MG	13	1668	1/1	0.32	0.53	121,121,121,121	0
55	MG	14	3137	1/1	0.32	0.34	151,151,151,151	0
55	MG	1H	3246	1/1	0.35	0.39	117,117,117,117	0
55	MG	1G	1663	1/1	0.35	0.49	121,121,121,121	0
55	MG	1G	1638	1/1	0.35	0.26	151,151,151,151	0
55	MG	13	1656	1/1	0.35	0.31	124,124,124,124	0
55	MG	1G	1680	1/1	0.36	0.30	138,138,138,138	0
55	MG	13	1670	1/1	0.36	0.16	137,137,137,137	0
55	MG	13	1642	1/1	0.36	0.24	149,149,149,149	0
55	MG	14	3028	1/1	0.38	0.33	114,114,114,114	0
55	MG	1G	1669	1/1	0.40	0.23	131,131,131,131	0
55	MG	1H	3200	1/1	0.40	0.44	88,88,88,88	0
55	MG	14	3190	1/1	0.41	0.30	100,100,100,100	0
55	MG	1G	1611	1/1	0.42	0.35	112,112,112,112	0
55	MG	1H	3148	1/1	0.43	0.40	100,100,100,100	0
55	MG	14	3189	1/1	0.43	0.40	99,99,99,99	0
55	MG	14	3146	1/1	0.43	0.36	92,92,92,92	0
55	MG	13	1666	1/1	0.44	0.33	115,115,115,115	0
55	MG	13	1634	1/1	0.44	0.34	120,120,120,120	0
55	MG	1G	1639	1/1	0.45	0.38	106,106,106,106	0
55	MG	1G	1602	1/1	0.45	0.32	109,109,109,109	0
55	MG	1G	1625	1/1	0.46	0.32	118,118,118,118	0
55	MG	13	1605	1/1	0.46	0.27	122,122,122,122	0
55	MG	1G	1640	1/1	0.46	0.47	103,103,103,103	0
55	MG	13	1688	1/1	0.47	0.30	122,122,122,122	0
55	MG	13	1647	1/1	0.47	0.11	116,116,116,116	0
55	MG	1H	3034	1/1	0.48	0.35	77,77,77,77	0
55	MG	13	1628	1/1	0.48	0.32	120,120,120,120	0
55	MG	42	202	1/1	0.48	0.36	135,135,135,135	0
55	MG	1H	3221	1/1	0.48	0.32	100,100,100,100	0
55	MG	1H	3233	1/1	0.49	0.32	102,102,102,102	0
55	MG	14	3094	1/1	0.50	0.18	108,108,108,108	0
55	MG	1G	1667	1/1	0.50	0.51	101,101,101,101	0
55	MG	1G	1622	1/1	0.50	0.26	104,104,104,104	0
55	MG	1H	3213	1/1	0.50	0.38	100,100,100,100	0
55	MG	14	3069	1/1	0.51	0.25	107,107,107,107	0
55	MG	1H	3164	1/1	0.51	0.34	98,98,98,98	0
55	MG	1H	3102	1/1	0.51	0.44	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	14	3111	1/1	0.52	0.30	110,110,110,110	0
55	MG	1H	3009	1/1	0.52	0.28	95,95,95,95	0
55	MG	13	1665	1/1	0.52	0.32	115,115,115,115	0
55	MG	1H	3242	1/1	0.52	0.27	94,94,94,94	0
55	MG	1H	3015	1/1	0.53	0.35	93,93,93,93	0
55	MG	1H	3109	1/1	0.53	0.22	109,109,109,109	0
55	MG	14	3004	1/1	0.53	0.21	66,66,66,66	0
55	MG	1G	1659	1/1	0.53	0.25	99,99,99,99	0
55	MG	13	1679	1/1	0.53	0.24	111,111,111,111	0
55	MG	14	3164	1/1	0.54	0.31	95,95,95,95	0
55	MG	1H	3135	1/1	0.54	0.31	75,75,75,75	0
55	MG	1G	1636	1/1	0.54	0.29	123,123,123,123	0
55	MG	1H	3181	1/1	0.54	0.54	89,89,89,89	0
55	MG	BI	201	1/1	0.55	0.33	110,110,110,110	0
55	MG	1H	3180	1/1	0.55	0.23	112,112,112,112	0
55	MG	14	3103	1/1	0.55	0.39	113,113,113,113	0
55	MG	14	3029	1/1	0.55	0.32	99,99,99,99	0
55	MG	14	3059	1/1	0.56	0.20	105,105,105,105	0
55	MG	1H	3195	1/1	0.57	0.24	114,114,114,114	0
55	MG	1G	1645	1/1	0.57	0.29	118,118,118,118	0
55	MG	1H	3023	1/1	0.57	0.31	85,85,85,85	0
55	MG	13	1681	1/1	0.58	0.25	113,113,113,113	0
55	MG	1H	3055	1/1	0.58	0.29	91,91,91,91	0
55	MG	1H	3022	1/1	0.59	0.40	77,77,77,77	0
55	MG	1H	3144	1/1	0.59	0.27	106,106,106,106	0
55	MG	1H	3192	1/1	0.59	0.18	114,114,114,114	0
55	MG	1H	3167	1/1	0.59	0.38	93,93,93,93	0
55	MG	1H	3172	1/1	0.59	0.23	101,101,101,101	0
55	MG	13	1625	1/1	0.60	0.19	101,101,101,101	0
55	MG	13	1640	1/1	0.60	0.36	99,99,99,99	0
55	MG	1H	3110	1/1	0.61	0.22	93,93,93,93	0
55	MG	1H	3211	1/1	0.61	0.41	93,93,93,93	0
55	MG	13	1626	1/1	0.61	0.27	123,123,123,123	0
55	MG	1G	1635	1/1	0.61	0.14	139,139,139,139	0
55	MG	1H	3006	1/1	0.61	0.37	49,49,49,49	0
55	MG	1H	3037	1/1	0.62	0.24	76,76,76,76	0
55	MG	1H	3027	1/1	0.62	0.39	75,75,75,75	0
55	MG	14	3169	1/1	0.62	0.34	97,97,97,97	0
55	MG	1G	1647	1/1	0.62	0.22	120,120,120,120	0
55	MG	1G	1648	1/1	0.62	0.21	115,115,115,115	0
55	MG	14	3144	1/1	0.62	0.15	114,114,114,114	0
55	MG	1H	3223	1/1	0.63	0.17	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	13	1651	1/1	0.63	0.30	110,110,110,110	0
55	MG	1G	1665	1/1	0.63	0.33	130,130,130,130	0
55	MG	13	1660	1/1	0.64	0.29	120,120,120,120	0
55	MG	1H	3031	1/1	0.64	0.27	83,83,83,83	0
55	MG	1H	3042	1/1	0.64	0.26	96,96,96,96	0
55	MG	14	3121	1/1	0.64	0.38	94,94,94,94	0
55	MG	14	3122	1/1	0.64	0.31	103,103,103,103	0
55	MG	1G	1682	1/1	0.64	0.24	101,101,101,101	0
55	MG	14	3099	1/1	0.64	0.21	90,90,90,90	0
55	MG	13	1661	1/1	0.65	0.28	117,117,117,117	0
55	MG	1H	3196	1/1	0.65	0.15	107,107,107,107	0
55	MG	13	1613	1/1	0.65	0.35	129,129,129,129	0
55	MG	14	3007	1/1	0.65	0.28	97,97,97,97	0
55	MG	1H	3113	1/1	0.65	0.11	83,83,83,83	0
55	MG	1H	3114	1/1	0.66	0.24	92,92,92,92	0
55	MG	14	3141	1/1	0.66	0.22	104,104,104,104	0
55	MG	1H	3106	1/1	0.66	0.29	100,100,100,100	0
55	MG	1H	3174	1/1	0.66	0.14	129,129,129,129	0
55	MG	14	3151	1/1	0.66	0.28	96,96,96,96	0
55	MG	1H	3178	1/1	0.66	0.26	94,94,94,94	0
55	MG	13	1637	1/1	0.66	0.25	101,101,101,101	0
55	MG	1G	1632	1/1	0.66	0.15	127,127,127,127	0
55	MG	14	3178	1/1	0.66	0.43	98,98,98,98	0
55	MG	1H	3100	1/1	0.66	0.36	65,65,65,65	0
55	MG	1H	3049	1/1	0.66	0.22	74,74,74,74	0
55	MG	16	201	1/1	0.67	0.25	92,92,92,92	0
55	MG	13	1618	1/1	0.67	0.29	115,115,115,115	0
55	MG	1G	1685	1/1	0.67	0.40	94,94,94,94	0
55	MG	13	1632	1/1	0.68	0.36	109,109,109,109	0
55	MG	1H	3099	1/1	0.68	0.46	79,79,79,79	0
55	MG	1G	1624	1/1	0.68	0.28	94,94,94,94	0
55	MG	1G	1668	1/1	0.68	0.26	125,125,125,125	0
55	MG	1H	3206	1/1	0.68	0.37	108,108,108,108	0
55	MG	1H	3020	1/1	0.68	0.38	77,77,77,77	0
55	MG	1G	1614	1/1	0.68	0.31	123,123,123,123	0
55	MG	1G	1681	1/1	0.69	0.26	92,92,92,92	0
55	MG	13	1673	1/1	0.69	0.17	113,113,113,113	0
55	MG	14	3112	1/1	0.69	0.14	96,96,96,96	0
55	MG	1H	3168	1/1	0.69	0.35	109,109,109,109	0
55	MG	14	3048	1/1	0.69	0.23	94,94,94,94	0
55	MG	42	201	1/1	0.69	0.31	115,115,115,115	0
55	MG	1G	1644	1/1	0.69	0.44	97,97,97,97	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
55	MG	1G	1664	1/1	0.69	0.22	105,105,105,105	0
55	MG	1G	1656	1/1	0.69	0.18	115,115,115,115	0
55	MG	1H	3122	1/1	0.70	0.20	98,98,98,98	0
55	MG	13	1648	1/1	0.70	0.17	110,110,110,110	0
55	MG	1H	3268	1/1	0.70	0.45	74,74,74,74	0
55	MG	14	3010	1/1	0.70	0.39	78,78,78,78	0
55	MG	14	3183	1/1	0.70	0.25	99,99,99,99	0
55	MG	14	3184	1/1	0.70	0.38	96,96,96,96	0
55	MG	13	1639	1/1	0.70	0.24	110,110,110,110	0
55	MG	1G	1650	1/1	0.70	0.21	107,107,107,107	0
55	MG	1H	3160	1/1	0.71	0.29	81,81,81,81	0
55	MG	13	1623	1/1	0.71	0.29	112,112,112,112	0
55	MG	1H	3045	1/1	0.71	0.13	80,80,80,80	0
55	MG	1H	3071	1/1	0.72	0.14	72,72,72,72	0
55	MG	1H	3281	1/1	0.72	0.09	96,96,96,96	0
55	MG	14	3139	1/1	0.72	0.24	103,103,103,103	0
55	MG	1H	3253	1/1	0.72	0.37	98,98,98,98	0
55	MG	14	3120	1/1	0.72	0.24	106,106,106,106	0
55	MG	14	3030	1/1	0.72	0.20	110,110,110,110	0
55	MG	14	3013	1/1	0.72	0.22	96,96,96,96	0
55	MG	14	3152	1/1	0.72	0.29	90,90,90,90	0
55	MG	1H	3212	1/1	0.73	0.37	91,91,91,91	0
55	MG	1G	1649	1/1	0.73	0.16	151,151,151,151	0
55	MG	1H	3216	1/1	0.73	0.16	89,89,89,89	0
55	MG	14	3125	1/1	0.73	0.37	97,97,97,97	0
55	MG	1H	3229	1/1	0.73	0.11	70,70,70,70	0
55	MG	14	3083	1/1	0.74	0.21	105,105,105,105	0
55	MG	14	3163	1/1	0.74	0.33	102,102,102,102	0
55	MG	1H	3138	1/1	0.74	0.34	98,98,98,98	0
55	MG	1H	3265	1/1	0.74	0.25	63,63,63,63	0
55	MG	1H	3214	1/1	0.74	0.31	84,84,84,84	0
55	MG	1G	1618	1/1	0.74	0.43	98,98,98,98	0
55	MG	14	3038	1/1	0.74	0.27	91,91,91,91	0
55	MG	13	1649	1/1	0.74	0.12	127,127,127,127	0
55	MG	13	1627	1/1	0.74	0.18	94,94,94,94	0
55	MG	1H	3189	1/1	0.74	0.24	71,71,71,71	0
55	MG	1H	3187	1/1	0.75	0.25	99,99,99,99	0
55	MG	14	3003	1/1	0.75	0.30	85,85,85,85	0
55	MG	1H	3247	1/1	0.75	0.37	101,101,101,101	0
55	MG	1G	1627	1/1	0.75	0.57	122,122,122,122	0
55	MG	14	3079	1/1	0.75	0.24	100,100,100,100	0
55	MG	14	3172	1/1	0.75	0.33	100,100,100,100	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
55	MG	1H	3251	1/1	0.75	0.29	87,87,87,87	0
55	MG	1H	3238	1/1	0.75	0.16	94,94,94,94	0
55	MG	1H	3282	1/1	0.75	0.29	101,101,101,101	0
55	MG	1H	3182	1/1	0.75	0.36	114,114,114,114	0
55	MG	32	301	1/1	0.75	0.15	138,138,138,138	0
55	MG	1G	1623	1/1	0.75	0.15	161,161,161,161	0
55	MG	13	1676	1/1	0.76	0.25	104,104,104,104	0
55	MG	1G	1607	1/1	0.76	0.31	94,94,94,94	0
55	MG	1H	3199	1/1	0.76	0.32	69,69,69,69	0
55	MG	1H	3272	1/1	0.76	0.29	83,83,83,83	0
55	MG	14	3047	1/1	0.76	0.38	83,83,83,83	0
55	MG	1H	3228	1/1	0.76	0.30	86,86,86,86	0
55	MG	13	1608	1/1	0.76	0.17	131,131,131,131	0
55	MG	14	3114	1/1	0.76	0.23	101,101,101,101	0
55	MG	13	1659	1/1	0.76	0.25	105,105,105,105	0
55	MG	1H	3175	1/1	0.76	0.18	114,114,114,114	0
55	MG	1J	202	1/1	0.76	0.16	129,129,129,129	0
55	MG	1H	3065	1/1	0.77	0.31	87,87,87,87	0
55	MG	1H	3245	1/1	0.77	0.42	76,76,76,76	0
55	MG	14	3127	1/1	0.77	0.28	64,64,64,64	0
55	MG	14	3001	1/1	0.77	0.27	94,94,94,94	0
55	MG	13	1671	1/1	0.77	0.12	117,117,117,117	0
55	MG	1H	3021	1/1	0.77	0.24	78,78,78,78	0
55	MG	1H	3173	1/1	0.77	0.17	94,94,94,94	0
55	MG	13	1636	1/1	0.77	0.33	91,91,91,91	0
55	MG	14	3066	1/1	0.77	0.26	82,82,82,82	0
55	MG	1H	3137	1/1	0.77	0.22	75,75,75,75	0
55	MG	88	201	1/1	0.77	0.30	94,94,94,94	0
55	MG	45	201	1/1	0.77	0.12	121,121,121,121	0
55	MG	14	3076	1/1	0.78	0.40	90,90,90,90	0
55	MG	13	1674	1/1	0.78	0.30	109,109,109,109	0
55	MG	1G	1679	1/1	0.78	0.28	79,79,79,79	0
55	MG	14	3186	1/1	0.78	0.25	85,85,85,85	0
55	MG	14	3053	1/1	0.78	0.25	91,91,91,91	0
55	MG	1H	3218	1/1	0.78	0.22	95,95,95,95	0
55	MG	1F	102	1/1	0.78	0.10	125,125,125,125	0
55	MG	1H	3285	1/1	0.78	0.34	89,89,89,89	0
55	MG	14	3118	1/1	0.79	0.10	99,99,99,99	0
55	MG	14	3155	1/1	0.79	0.34	92,92,92,92	0
55	MG	1H	3090	1/1	0.79	0.18	88,88,88,88	0
55	MG	13	1687	1/1	0.79	0.19	88,88,88,88	0
55	MG	1H	3241	1/1	0.79	0.14	110,110,110,110	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
55	MG	14	3084	1/1	0.79	0.26	91,91,91,91	0
55	MG	1H	3064	1/1	0.79	0.23	85,85,85,85	0
55	MG	14	3136	1/1	0.79	0.14	120,120,120,120	0
55	MG	13	1675	1/1	0.79	0.10	104,104,104,104	0
55	MG	1H	3225	1/1	0.79	0.26	109,109,109,109	0
55	MG	14	3107	1/1	0.79	0.31	88,88,88,88	0
55	MG	1H	3279	1/1	0.79	0.16	81,81,81,81	0
55	MG	1H	3115	1/1	0.79	0.27	76,76,76,76	0
55	MG	14	3067	1/1	0.79	0.27	97,97,97,97	0
55	MG	13	1653	1/1	0.79	0.13	120,120,120,120	0
55	MG	13	1617	1/1	0.80	0.25	92,92,92,92	0
55	MG	1H	3127	1/1	0.80	0.25	87,87,87,87	0
55	MG	1H	3169	1/1	0.80	0.20	75,75,75,75	0
55	MG	1H	3171	1/1	0.80	0.24	91,91,91,91	0
55	MG	13	1690	1/1	0.80	0.15	123,123,123,123	0
55	MG	14	3019	1/1	0.80	0.09	85,85,85,85	0
55	MG	1H	3087	1/1	0.80	0.22	74,74,74,74	0
55	MG	14	3130	1/1	0.80	0.16	106,106,106,106	0
55	MG	14	3177	1/1	0.80	0.15	79,79,79,79	0
55	MG	14	3133	1/1	0.80	0.20	99,99,99,99	0
55	MG	1G	1658	1/1	0.80	0.23	114,114,114,114	0
55	MG	1H	3050	1/1	0.80	0.30	79,79,79,79	0
55	MG	14	3185	1/1	0.80	0.12	88,88,88,88	0
55	MG	1H	3143	1/1	0.80	0.18	89,89,89,89	0
55	MG	1H	3092	1/1	0.80	0.16	92,92,92,92	0
55	MG	13	1662	1/1	0.80	0.13	99,99,99,99	0
55	MG	13	1677	1/1	0.80	0.31	100,100,100,100	0
55	MG	39	301	1/1	0.80	0.25	109,109,109,109	0
55	MG	1H	3121	1/1	0.80	0.23	91,91,91,91	0
55	MG	1H	3057	1/1	0.81	0.17	57,57,57,57	0
55	MG	1H	3060	1/1	0.81	0.23	68,68,68,68	0
55	MG	14	3166	1/1	0.81	0.26	82,82,82,82	0
55	MG	1H	3116	1/1	0.81	0.17	91,91,91,91	0
55	MG	1H	3141	1/1	0.81	0.19	89,89,89,89	0
55	MG	1H	3191	1/1	0.81	0.30	93,93,93,93	0
55	MG	1G	1654	1/1	0.81	0.23	107,107,107,107	0
55	MG	1H	3039	1/1	0.81	0.26	73,73,73,73	0
55	MG	1G	1683	1/1	0.81	0.17	122,122,122,122	0
55	MG	1H	3219	1/1	0.81	0.26	91,91,91,91	0
55	MG	14	3110	1/1	0.81	0.30	103,103,103,103	0
55	MG	13	1630	1/1	0.81	0.15	109,109,109,109	0
55	MG	1H	3024	1/1	0.81	0.17	71,71,71,71	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
55	MG	1H	3150	1/1	0.81	0.28	79,79,79,79	0
55	MG	1H	3133	1/1	0.81	0.27	85,85,85,85	0
55	MG	1H	3161	1/1	0.81	0.18	86,86,86,86	0
55	MG	1H	3162	1/1	0.81	0.20	87,87,87,87	0
55	MG	13	1646	1/1	0.82	0.18	122,122,122,122	0
55	MG	13	1657	1/1	0.82	0.21	123,123,123,123	0
55	MG	1H	3101	1/1	0.82	0.23	89,89,89,89	0
55	MG	1H	3117	1/1	0.82	0.15	88,88,88,88	0
55	MG	14	3115	1/1	0.82	0.08	103,103,103,103	0
55	MG	78	201	1/1	0.82	0.29	90,90,90,90	0
55	MG	1H	3145	1/1	0.82	0.17	84,84,84,84	0
55	MG	1H	3085	1/1	0.82	0.21	74,74,74,74	0
55	MG	1G	1605	1/1	0.82	0.17	98,98,98,98	0
55	MG	14	3005	1/1	0.82	0.17	85,85,85,85	0
55	MG	1H	3103	1/1	0.82	0.15	77,77,77,77	0
55	MG	14	3180	1/1	0.82	0.17	81,81,81,81	0
55	MG	13	1612	1/1	0.82	0.28	85,85,85,85	0
55	MG	1H	3255	1/1	0.82	0.24	78,78,78,78	0
55	MG	14	3085	1/1	0.82	0.15	94,94,94,94	0
55	MG	14	3086	1/1	0.82	0.11	97,97,97,97	0
55	MG	1H	3048	1/1	0.82	0.23	93,93,93,93	0
55	MG	13	1645	1/1	0.82	0.15	97,97,97,97	0
55	MG	1H	3095	1/1	0.82	0.29	63,63,63,63	0
55	MG	1H	3165	1/1	0.82	0.23	90,90,90,90	0
55	MG	1H	3240	1/1	0.82	0.13	114,114,114,114	0
55	MG	13	1615	1/1	0.83	0.12	71,71,71,71	0
55	MG	1H	3086	1/1	0.83	0.12	79,79,79,79	0
55	MG	1G	1617	1/1	0.83	0.17	91,91,91,91	0
55	MG	14	3088	1/1	0.83	0.19	109,109,109,109	0
55	MG	1H	3252	1/1	0.83	0.20	69,69,69,69	0
55	MG	13	1711	1/1	0.83	0.09	154,154,154,154	0
55	MG	14	3131	1/1	0.83	0.51	88,88,88,88	0
55	MG	1H	3179	1/1	0.83	0.19	86,86,86,86	0
55	MG	14	3009	1/1	0.83	0.10	90,90,90,90	0
55	MG	1H	3017	1/1	0.83	0.27	75,75,75,75	0
55	MG	1H	3158	1/1	0.83	0.24	92,92,92,92	0
55	MG	14	3014	1/1	0.83	0.14	78,78,78,78	0
55	MG	13	1683	1/1	0.83	0.18	103,103,103,103	0
55	MG	14	3078	1/1	0.83	0.21	100,100,100,100	0
55	MG	13	1633	1/1	0.83	0.14	85,85,85,85	0
55	MG	14	3116	1/1	0.83	0.19	89,89,89,89	0
55	MG	13	1629	1/1	0.83	0.30	109,109,109,109	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
55	MG	14	3119	1/1	0.83	0.25	101,101,101,101	0
55	MG	1H	3140	1/1	0.84	0.19	80,80,80,80	0
55	MG	14	3140	1/1	0.84	0.11	86,86,86,86	0
55	MG	1G	1651	1/1	0.84	0.18	91,91,91,91	0
55	MG	1H	3205	1/1	0.84	0.35	80,80,80,80	0
55	MG	1H	3066	1/1	0.84	0.22	78,78,78,78	0
55	MG	14	3031	1/1	0.84	0.21	77,77,77,77	0
55	MG	1G	1693	1/1	0.84	0.09	148,148,148,148	0
55	MG	1G	1601	1/1	0.84	0.16	101,101,101,101	0
55	MG	14	3162	1/1	0.84	0.28	57,57,57,57	0
55	MG	1F	101	1/1	0.84	0.07	107,107,107,107	0
55	MG	1H	3081	1/1	0.84	0.20	72,72,72,72	0
55	MG	14	3057	1/1	0.84	0.15	90,90,90,90	0
55	MG	4A	201	1/1	0.84	0.15	136,136,136,136	0
55	MG	14	3117	1/1	0.84	0.14	91,91,91,91	0
55	MG	14	3062	1/1	0.84	0.23	87,87,87,87	0
55	MG	1H	3084	1/1	0.84	0.10	71,71,71,71	0
55	MG	13	1689	1/1	0.84	0.22	85,85,85,85	0
55	MG	1H	3270	1/1	0.84	0.28	62,62,62,62	0
55	MG	14	3181	1/1	0.84	0.13	71,71,71,71	0
55	MG	1H	3176	1/1	0.84	0.12	107,107,107,107	0
55	MG	1H	3194	1/1	0.84	0.18	113,113,113,113	0
55	MG	14	3008	1/1	0.84	0.13	81,81,81,81	0
55	MG	1H	3244	1/1	0.84	0.16	87,87,87,87	0
55	MG	1H	3177	1/1	0.84	0.17	82,82,82,82	0
55	MG	1G	1671	1/1	0.84	0.15	100,100,100,100	0
55	MG	1J	201	1/1	0.84	0.16	106,106,106,106	0
55	MG	1H	3002	1/1	0.84	0.21	55,55,55,55	0
55	MG	1H	3151	1/1	0.84	0.17	100,100,100,100	0
55	MG	14	3093	1/1	0.84	0.12	94,94,94,94	0
55	MG	1H	3041	1/1	0.85	0.17	65,65,65,65	0
55	MG	13	1619	1/1	0.85	0.16	86,86,86,86	0
55	MG	1G	1722	1/1	0.85	0.19	161,161,161,161	0
55	MG	1G	1629	1/1	0.85	0.16	131,131,131,131	0
55	MG	1H	3119	1/1	0.85	0.13	105,105,105,105	0
55	MG	1H	3104	1/1	0.85	0.11	74,74,74,74	0
55	MG	1H	3105	1/1	0.85	0.21	93,93,93,93	0
55	MG	14	3134	1/1	0.85	0.14	105,105,105,105	0
55	MG	13	1621	1/1	0.85	0.09	117,117,117,117	0
55	MG	1G	1606	1/1	0.85	0.11	109,109,109,109	0
55	MG	1H	3129	1/1	0.85	0.30	92,92,92,92	0
55	MG	1H	3032	1/1	0.85	0.20	66,66,66,66	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
55	MG	1H	3275	1/1	0.85	0.25	62,62,62,62	0
55	MG	1G	1616	1/1	0.85	0.22	93,93,93,93	0
55	MG	1H	3193	1/1	0.85	0.10	73,73,73,73	0
55	MG	5I	102	1/1	0.85	0.08	119,119,119,119	0
55	MG	1H	3035	1/1	0.85	0.25	71,71,71,71	0
55	MG	8I	201	1/1	0.85	0.27	107,107,107,107	0
55	MG	1H	3018	1/1	0.85	0.13	68,68,68,68	0
55	MG	1H	3436	1/1	0.85	0.17	96,96,96,96	0
55	MG	14	3036	1/1	0.86	0.24	80,80,80,80	0
55	MG	5I	101	1/1	0.86	0.09	105,105,105,105	0
55	MG	1G	1657	1/1	0.86	0.18	98,98,98,98	0
55	MG	1H	3098	1/1	0.86	0.06	54,54,54,54	0
55	MG	13	1610	1/1	0.86	0.14	130,130,130,130	0
55	MG	14	3054	1/1	0.86	0.06	113,113,113,113	0
55	MG	1H	3004	1/1	0.86	0.27	64,64,64,64	0
55	MG	2L	101	1/1	0.86	0.09	147,147,147,147	0
55	MG	1G	1634	1/1	0.86	0.17	109,109,109,109	0
55	MG	14	3167	1/1	0.86	0.18	100,100,100,100	0
55	MG	13	1635	1/1	0.86	0.24	82,82,82,82	0
55	MG	14	3171	1/1	0.86	0.24	98,98,98,98	0
55	MG	1H	3163	1/1	0.86	0.27	82,82,82,82	0
55	MG	1H	3267	1/1	0.86	0.22	67,67,67,67	0
55	MG	1H	3062	1/1	0.86	0.24	85,85,85,85	0
55	MG	1H	3207	1/1	0.86	0.20	77,77,77,77	0
55	MG	13	1694	1/1	0.86	0.26	117,117,117,117	0
55	MG	14	3128	1/1	0.86	0.15	54,54,54,54	0
55	MG	1H	3274	1/1	0.86	0.35	78,78,78,78	0
55	MG	14	3012	1/1	0.86	0.14	95,95,95,95	0
55	MG	1G	1677	1/1	0.86	0.16	110,110,110,110	0
55	MG	1H	3142	1/1	0.86	0.19	76,76,76,76	0
55	MG	1H	3088	1/1	0.86	0.32	81,81,81,81	0
55	MG	13	1602	1/1	0.86	0.09	115,115,115,115	0
55	MG	1H	3036	1/1	0.86	0.22	74,74,74,74	0
55	MG	1H	3108	1/1	0.86	0.08	58,58,58,58	0
55	MG	1H	3128	1/1	0.86	0.08	92,92,92,92	0
55	MG	1H	3249	1/1	0.86	0.10	70,70,70,70	0
55	MG	13	1686	1/1	0.87	0.10	73,73,73,73	0
55	MG	14	3090	1/1	0.87	0.10	69,69,69,69	0
55	MG	14	3015	1/1	0.87	0.22	70,70,70,70	0
55	MG	14	3142	1/1	0.87	0.14	105,105,105,105	0
55	MG	1G	1674	1/1	0.87	0.13	89,89,89,89	0
55	MG	1G	1641	1/1	0.87	0.10	107,107,107,107	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
55	MG	13	1603	1/1	0.87	0.15	85,85,85,85	0
55	MG	1H	3243	1/1	0.87	0.20	85,85,85,85	0
55	MG	1H	3126	1/1	0.87	0.16	78,78,78,78	0
55	MG	14	3161	1/1	0.87	0.10	73,73,73,73	0
55	MG	1G	1615	1/1	0.87	0.17	141,141,141,141	0
55	MG	13	1641	1/1	0.87	0.27	94,94,94,94	0
55	MG	1H	3014	1/1	0.87	0.19	64,64,64,64	0
55	MG	1H	3280	1/1	0.87	0.09	73,73,73,73	0
55	MG	13	1678	1/1	0.87	0.17	116,116,116,116	0
55	MG	1H	3222	1/1	0.87	0.21	101,101,101,101	0
55	MG	1H	3283	1/1	0.87	0.17	83,83,83,83	0
55	MG	1H	3029	1/1	0.87	0.15	68,68,68,68	0
55	MG	1H	3296	1/1	0.87	0.09	122,122,122,122	0
55	MG	14	3060	1/1	0.87	0.29	84,84,84,84	0
55	MG	1H	3405	1/1	0.87	0.12	108,108,108,108	0
55	MG	1G	1660	1/1	0.87	0.07	118,118,118,118	0
55	MG	14	3123	1/1	0.87	0.10	99,99,99,99	0
55	MG	13	1624	1/1	0.87	0.11	98,98,98,98	0
55	MG	13	1604	1/1	0.87	0.06	87,87,87,87	0
55	MG	21	301	1/1	0.87	0.08	82,82,82,82	0
55	MG	1H	3183	1/1	0.87	0.29	82,82,82,82	0
55	MG	14	3188	1/1	0.87	0.19	89,89,89,89	0
55	MG	1H	3153	1/1	0.87	0.12	91,91,91,91	0
55	MG	14	3081	1/1	0.87	0.23	88,88,88,88	0
55	MG	1H	3236	1/1	0.87	0.24	72,72,72,72	0
55	MG	1H	3155	1/1	0.87	0.11	78,78,78,78	0
55	MG	13	1622	1/1	0.87	0.20	88,88,88,88	0
55	MG	1G	1670	1/1	0.87	0.20	101,101,101,101	0
55	MG	1H	3082	1/1	0.88	0.18	77,77,77,77	0
55	MG	1H	3284	1/1	0.88	0.09	60,60,60,60	0
55	MG	13	1652	1/1	0.88	0.12	97,97,97,97	0
55	MG	1H	3294	1/1	0.88	0.23	83,83,83,83	0
55	MG	1G	1626	1/1	0.88	0.10	100,100,100,100	0
55	MG	13	1704	1/1	0.88	0.08	147,147,147,147	0
55	MG	14	3143	1/1	0.88	0.10	97,97,97,97	0
55	MG	1H	3322	1/1	0.88	0.20	124,124,124,124	0
55	MG	14	3092	1/1	0.88	0.15	81,81,81,81	0
55	MG	1H	3325	1/1	0.88	0.09	122,122,122,122	0
55	MG	1G	1631	1/1	0.88	0.17	95,95,95,95	0
55	MG	1H	3044	1/1	0.88	0.09	72,72,72,72	0
55	MG	14	3156	1/1	0.88	0.21	80,80,80,80	0
55	MG	14	3100	1/1	0.88	0.13	91,91,91,91	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
55	MG	1H	3063	1/1	0.88	0.16	63,63,63,63	0
55	MG	14	3017	1/1	0.88	0.17	83,83,83,83	0
55	MG	1H	3107	1/1	0.88	0.18	92,92,92,92	0
55	MG	13	1705	1/1	0.88	0.13	130,130,130,130	0
55	MG	1G	1672	1/1	0.88	0.19	102,102,102,102	0
55	MG	1H	3198	1/1	0.88	0.11	68,68,68,68	0
55	MG	78	202	1/1	0.88	0.09	55,55,55,55	0
55	MG	13	1643	1/1	0.88	0.08	124,124,124,124	0
55	MG	1H	3019	1/1	0.88	0.13	57,57,57,57	0
55	MG	14	3044	1/1	0.88	0.22	85,85,85,85	0
55	MG	1H	3069	1/1	0.88	0.18	77,77,77,77	0
55	MG	13	1734	1/1	0.88	0.10	133,133,133,133	0
55	MG	1H	3271	1/1	0.88	0.35	82,82,82,82	0
55	MG	1G	1646	1/1	0.88	0.18	101,101,101,101	0
55	MG	1H	3237	1/1	0.88	0.19	79,79,79,79	0
55	MG	1G	1697	1/1	0.88	0.05	172,172,172,172	0
55	MG	1H	3073	1/1	0.88	0.19	74,74,74,74	0
55	MG	1H	3079	1/1	0.88	0.23	71,71,71,71	0
55	MG	1H	3209	1/1	0.88	0.14	84,84,84,84	0
55	MG	1H	3210	1/1	0.88	0.39	90,90,90,90	0
55	MG	14	3197	1/1	0.88	0.15	114,114,114,114	0
55	MG	1H	3030	1/1	0.88	0.26	77,77,77,77	0
55	MG	1G	1655	1/1	0.88	0.26	84,84,84,84	0
55	MG	1H	3166	1/1	0.88	0.19	74,74,74,74	0
55	MG	1H	3118	1/1	0.88	0.19	89,89,89,89	0
55	MG	1H	3146	1/1	0.89	0.16	80,80,80,80	0
55	MG	14	3145	1/1	0.89	0.15	86,86,86,86	0
55	MG	1H	3008	1/1	0.89	0.31	82,82,82,82	0
55	MG	1H	3293	1/1	0.89	0.09	124,124,124,124	0
55	MG	1H	3124	1/1	0.89	0.29	69,69,69,69	0
55	MG	14	3154	1/1	0.89	0.14	65,65,65,65	0
55	MG	1H	3295	1/1	0.89	0.15	83,83,83,83	0
55	MG	1H	3139	1/1	0.89	0.24	60,60,60,60	0
55	MG	1H	3312	1/1	0.89	0.17	105,105,105,105	0
55	MG	13	1667	1/1	0.89	0.10	101,101,101,101	0
55	MG	1H	3154	1/1	0.89	0.18	61,61,61,61	0
55	MG	1H	3215	1/1	0.89	0.10	78,78,78,78	0
55	MG	14	3165	1/1	0.89	0.32	83,83,83,83	0
55	MG	1H	3269	1/1	0.89	0.25	55,55,55,55	0
55	MG	1G	1661	1/1	0.89	0.18	77,77,77,77	0
55	MG	1H	3052	1/1	0.89	0.25	64,64,64,64	0
55	MG	14	3064	1/1	0.89	0.19	80,80,80,80	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
55	MG	11	301	1/1	0.89	0.22	52,52,52,52	0
55	MG	1H	3112	1/1	0.89	0.28	68,68,68,68	0
55	MG	14	3006	1/1	0.89	0.07	91,91,91,91	0
55	MG	1H	3010	1/1	0.89	0.07	70,70,70,70	0
55	MG	14	3077	1/1	0.89	0.35	89,89,89,89	0
55	MG	1H	3184	1/1	0.89	0.19	87,87,87,87	0
55	MG	1H	3185	1/1	0.89	0.13	72,72,72,72	0
55	MG	88	203	1/1	0.89	0.42	77,77,77,77	0
55	MG	J8	101	1/1	0.89	0.25	74,74,74,74	0
55	MG	1H	3120	1/1	0.89	0.16	81,81,81,81	0
55	MG	1H	3278	1/1	0.89	0.20	75,75,75,75	0
55	MG	1H	3224	1/1	0.89	0.11	102,102,102,102	0
55	MG	1H	3248	1/1	0.89	0.22	86,86,86,86	0
55	MG	13	1672	1/1	0.89	0.12	123,123,123,123	0
55	MG	1H	3250	1/1	0.89	0.21	53,53,53,53	0
55	MG	14	3027	1/1	0.89	0.07	72,72,72,72	0
55	MG	1G	1612	1/1	0.89	0.25	85,85,85,85	0
55	MG	1H	3226	1/1	0.89	0.13	90,90,90,90	0
55	MG	85	201	1/1	0.89	0.33	72,72,72,72	0
55	MG	1H	3286	1/1	0.90	0.21	67,67,67,67	0
55	MG	1G	1604	1/1	0.90	0.14	102,102,102,102	0
55	MG	1H	3075	1/1	0.90	0.33	72,72,72,72	0
55	MG	13	1680	1/1	0.90	0.10	108,108,108,108	0
55	MG	1H	3197	1/1	0.90	0.09	77,77,77,77	0
55	MG	1G	1609	1/1	0.90	0.16	105,105,105,105	0
55	MG	1G	1678	1/1	0.90	0.24	99,99,99,99	0
55	MG	1H	3007	1/1	0.90	0.24	62,62,62,62	0
55	MG	14	3021	1/1	0.90	0.12	90,90,90,90	0
55	MG	1H	3300	1/1	0.90	0.24	104,104,104,104	0
55	MG	1H	3311	1/1	0.90	0.17	97,97,97,97	0
55	MG	1H	3097	1/1	0.90	0.15	66,66,66,66	0
55	MG	1H	3319	1/1	0.90	0.08	123,123,123,123	0
55	MG	13	1685	1/1	0.90	0.20	107,107,107,107	0
55	MG	14	3109	1/1	0.90	0.12	102,102,102,102	0
55	MG	1G	1690	1/1	0.90	0.12	144,144,144,144	0
55	MG	1H	3220	1/1	0.90	0.22	85,85,85,85	0
55	MG	14	3040	1/1	0.90	0.09	62,62,62,62	0
55	MG	14	3043	1/1	0.90	0.13	54,54,54,54	0
55	MG	1G	1620	1/1	0.90	0.09	81,81,81,81	0
55	MG	1G	1701	1/1	0.90	0.10	137,137,137,137	0
55	MG	1G	1707	1/1	0.90	0.12	122,122,122,122	0
55	MG	14	3049	1/1	0.90	0.20	80,80,80,80	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
55	MG	1H	3337	1/1	0.90	0.06	127,127,127,127	0
55	MG	1H	3397	1/1	0.90	0.08	81,81,81,81	0
55	MG	1H	3201	1/1	0.90	0.26	68,68,68,68	0
55	MG	1H	3204	1/1	0.90	0.20	80,80,80,80	0
55	MG	14	3182	1/1	0.90	0.16	88,88,88,88	0
55	MG	13	1719	1/1	0.90	0.14	107,107,107,107	0
55	MG	14	3061	1/1	0.90	0.12	92,92,92,92	0
55	MG	1H	3156	1/1	0.90	0.26	75,75,75,75	0
55	MG	14	3063	1/1	0.90	0.15	82,82,82,82	0
55	MG	1H	3067	1/1	0.90	0.19	65,65,65,65	0
55	MG	1H	3125	1/1	0.90	0.10	125,125,125,125	0
55	MG	13	1664	1/1	0.90	0.07	87,87,87,87	0
55	MG	1H	3061	1/1	0.90	0.13	66,66,66,66	0
55	MG	14	3198	1/1	0.90	0.12	109,109,109,109	0
55	MG	14	3298	1/1	0.90	0.10	103,103,103,103	0
55	MG	1H	3230	1/1	0.90	0.10	73,73,73,73	0
55	MG	1H	3040	1/1	0.90	0.18	58,58,58,58	0
55	MG	P8	101	1/1	0.90	0.12	61,61,61,61	0
55	MG	35	201	1/1	0.90	0.17	81,81,81,81	0
55	MG	1H	3089	1/1	0.90	0.23	82,82,82,82	0
55	MG	45	202	1/1	0.90	0.40	116,116,116,116	0
55	MG	14	3080	1/1	0.90	0.21	90,90,90,90	0
55	MG	F5	101	1/1	0.90	0.09	82,82,82,82	0
55	MG	BA	201	1/1	0.91	0.12	127,127,127,127	0
55	MG	13	1698	1/1	0.91	0.09	138,138,138,138	0
55	MG	14	3032	1/1	0.91	0.14	62,62,62,62	0
55	MG	14	3034	1/1	0.91	0.21	77,77,77,77	0
55	MG	1G	1633	1/1	0.91	0.28	96,96,96,96	0
55	MG	14	3082	1/1	0.91	0.12	78,78,78,78	0
55	MG	14	3124	1/1	0.91	0.07	95,95,95,95	0
55	MG	1H	3188	1/1	0.91	0.06	91,91,91,91	0
55	MG	14	3175	1/1	0.91	0.09	85,85,85,85	0
55	MG	13	1706	1/1	0.91	0.27	132,132,132,132	0
55	MG	1H	3266	1/1	0.91	0.12	64,64,64,64	0
55	MG	1G	1637	1/1	0.91	0.13	125,125,125,125	0
55	MG	14	3087	1/1	0.91	0.47	66,66,66,66	0
55	MG	1H	3190	1/1	0.91	0.09	106,106,106,106	0
55	MG	1H	3203	1/1	0.91	0.10	81,81,81,81	0
55	MG	14	3091	1/1	0.91	0.12	105,105,105,105	0
55	MG	1G	1684	1/1	0.91	0.22	89,89,89,89	0
55	MG	1H	3332	1/1	0.91	0.16	125,125,125,125	0
55	MG	1H	3170	1/1	0.91	0.13	80,80,80,80	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
55	MG	1G	1603	1/1	0.91	0.12	95,95,95,95	0
55	MG	1H	3016	1/1	0.91	0.18	62,62,62,62	0
55	MG	1H	3132	1/1	0.91	0.22	79,79,79,79	0
55	MG	1H	3077	1/1	0.91	0.22	60,60,60,60	0
55	MG	14	3108	1/1	0.91	0.26	87,87,87,87	0
55	MG	14	3202	1/1	0.91	0.14	106,106,106,106	0
55	MG	14	3214	1/1	0.91	0.10	96,96,96,96	0
55	MG	14	3285	1/1	0.91	0.15	99,99,99,99	0
55	MG	14	3296	1/1	0.91	0.07	119,119,119,119	0
55	MG	1G	1720	1/1	0.91	0.11	152,152,152,152	0
55	MG	13	1601	1/1	0.91	0.17	77,77,77,77	0
55	MG	1G	1628	1/1	0.91	0.11	118,118,118,118	0
55	MG	14	3026	1/1	0.91	0.14	76,76,76,76	0
55	MG	1H	3033	1/1	0.91	0.06	60,60,60,60	0
55	MG	1H	3111	1/1	0.91	0.18	86,86,86,86	0
55	MG	14	3072	1/1	0.91	0.20	91,91,91,91	0
55	MG	14	3075	1/1	0.91	0.09	99,99,99,99	0
55	MG	41	201	1/1	0.91	0.17	88,88,88,88	0
55	MG	1H	3096	1/1	0.92	0.14	79,79,79,79	0
55	MG	1H	3005	1/1	0.92	0.10	51,51,51,51	0
55	MG	13	1638	1/1	0.92	0.07	80,80,80,80	0
55	MG	21	302	1/1	0.92	0.11	50,50,50,50	0
55	MG	13	1710	1/1	0.92	0.20	143,143,143,143	0
55	MG	14	3071	1/1	0.92	0.16	84,84,84,84	0
55	MG	1G	1652	1/1	0.92	0.09	105,105,105,105	0
55	MG	14	3170	1/1	0.92	0.15	69,69,69,69	0
55	MG	1G	1653	1/1	0.92	0.14	103,103,103,103	0
55	MG	1H	3053	1/1	0.92	0.12	77,77,77,77	0
55	MG	13	1701	1/1	0.92	0.07	137,137,137,137	0
55	MG	1G	1691	1/1	0.92	0.12	115,115,115,115	0
55	MG	1H	3262	1/1	0.92	0.21	74,74,74,74	0
55	MG	1H	3056	1/1	0.92	0.17	46,46,46,46	0
55	MG	13	1712	1/1	0.92	0.06	96,96,96,96	0
55	MG	1G	1704	1/1	0.92	0.09	130,130,130,130	0
55	MG	1H	3083	1/1	0.92	0.32	85,85,85,85	0
55	MG	1G	1714	1/1	0.92	0.09	133,133,133,133	0
55	MG	1H	3038	1/1	0.92	0.16	83,83,83,83	0
55	MG	1H	3301	1/1	0.92	0.07	100,100,100,100	0
55	MG	13	1658	1/1	0.92	0.15	114,114,114,114	0
55	MG	1H	3025	1/1	0.92	0.25	55,55,55,55	0
55	MG	13	1724	1/1	0.92	0.06	128,128,128,128	0
55	MG	2K	101	1/1	0.92	0.22	71,71,71,71	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
55	MG	14	3191	1/1	0.92	0.12	102,102,102,102	0
55	MG	13	1695	1/1	0.92	0.06	139,139,139,139	0
55	MG	1H	3003	1/1	0.92	0.16	49,49,49,49	0
55	MG	1H	3334	1/1	0.92	0.12	94,94,94,94	0
55	MG	14	3050	1/1	0.92	0.20	54,54,54,54	0
55	MG	14	3237	1/1	0.92	0.18	96,96,96,96	0
55	MG	14	3052	1/1	0.92	0.09	64,64,64,64	0
55	MG	1H	3335	1/1	0.92	0.06	134,134,134,134	0
55	MG	14	3105	1/1	0.92	0.25	81,81,81,81	0
55	MG	14	3147	1/1	0.92	0.15	63,63,63,63	0
55	MG	14	3149	1/1	0.92	0.11	61,61,61,61	0
55	MG	1H	3046	1/1	0.92	0.14	69,69,69,69	0
55	MG	1H	3157	1/1	0.92	0.15	73,73,73,73	0
55	MG	13	1738	1/1	0.92	0.22	134,134,134,134	0
55	MG	1G	1673	1/1	0.92	0.11	93,93,93,93	0
55	MG	1H	3136	1/1	0.92	0.08	87,87,87,87	0
55	MG	1H	3450	1/1	0.92	0.07	132,132,132,132	0
55	MG	1H	3078	1/1	0.93	0.19	63,63,63,63	0
55	MG	14	3104	1/1	0.93	0.11	91,91,91,91	0
55	MG	13	1609	1/1	0.93	0.09	99,99,99,99	0
55	MG	14	3106	1/1	0.93	0.11	90,90,90,90	0
55	MG	1H	3298	1/1	0.93	0.18	89,89,89,89	0
55	MG	1H	3080	1/1	0.93	0.13	64,64,64,64	0
55	MG	1H	3011	1/1	0.93	0.11	48,48,48,48	0
55	MG	13	1620	1/1	0.93	0.06	70,70,70,70	0
55	MG	1H	3047	1/1	0.93	0.19	66,66,66,66	0
55	MG	1H	3159	1/1	0.93	0.31	79,79,79,79	0
55	MG	14	3168	1/1	0.93	0.08	72,72,72,72	0
55	MG	1H	3321	1/1	0.93	0.07	123,123,123,123	0
55	MG	13	1713	1/1	0.93	0.08	81,81,81,81	0
55	MG	13	1616	1/1	0.93	0.15	93,93,93,93	0
55	MG	1H	3276	1/1	0.93	0.11	74,74,74,74	0
55	MG	1H	3026	1/1	0.93	0.08	82,82,82,82	0
55	MG	1G	1675	1/1	0.93	0.19	77,77,77,77	0
55	MG	13	1723	1/1	0.93	0.13	103,103,103,103	0
55	MG	1H	3028	1/1	0.93	0.15	80,80,80,80	0
55	MG	14	3179	1/1	0.93	0.10	70,70,70,70	0
55	MG	1H	3378	1/1	0.93	0.09	75,75,75,75	0
55	MG	1G	1613	1/1	0.93	0.15	94,94,94,94	0
55	MG	13	1709	1/1	0.93	0.07	147,147,147,147	0
55	MG	14	3074	1/1	0.93	0.08	92,92,92,92	0
55	MG	13	1725	1/1	0.93	0.16	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	3410	1/1	0.93	0.14	95,95,95,95	0
55	MG	1H	3425	1/1	0.93	0.13	102,102,102,102	0
55	MG	13	1655	1/1	0.93	0.10	95,95,95,95	0
55	MG	14	3023	1/1	0.93	0.15	99,99,99,99	0
55	MG	14	3132	1/1	0.93	0.21	100,100,100,100	0
55	MG	14	3025	1/1	0.93	0.10	90,90,90,90	0
55	MG	1G	1619	1/1	0.93	0.08	98,98,98,98	0
55	MG	1H	3147	1/1	0.93	0.09	54,54,54,54	0
55	MG	1H	3452	1/1	0.93	0.07	108,108,108,108	0
55	MG	14	3205	1/1	0.93	0.11	118,118,118,118	0
55	MG	1H	3463	1/1	0.93	0.08	110,110,110,110	0
55	MG	1H	3468	1/1	0.93	0.23	88,88,88,88	0
55	MG	14	3269	1/1	0.93	0.13	104,104,104,104	0
55	MG	1H	3076	1/1	0.93	0.20	70,70,70,70	0
55	MG	14	3288	1/1	0.93	0.19	86,86,86,86	0
55	MG	14	3290	1/1	0.93	0.10	115,115,115,115	0
55	MG	1H	3059	1/1	0.93	0.12	78,78,78,78	0
55	MG	1G	1708	1/1	0.93	0.10	100,100,100,100	0
55	MG	14	3300	1/1	0.93	0.15	140,140,140,140	0
55	MG	1G	1712	1/1	0.93	0.06	131,131,131,131	0
55	MG	1H	3259	1/1	0.93	0.18	53,53,53,53	0
55	MG	14	3039	1/1	0.93	0.13	75,75,75,75	0
55	MG	1G	1715	1/1	0.93	0.13	126,126,126,126	0
55	MG	14	3041	1/1	0.93	0.13	61,61,61,61	0
55	MG	14	3095	1/1	0.93	0.13	88,88,88,88	0
55	MG	1H	3235	1/1	0.93	0.24	57,57,57,57	0
55	MG	E5	101	1/1	0.93	0.10	90,90,90,90	0
55	MG	1H	3131	1/1	0.93	0.22	73,73,73,73	0
55	MG	13	1692	1/1	0.94	0.08	107,107,107,107	0
55	MG	14	3018	1/1	0.94	0.21	84,84,84,84	0
55	MG	1H	3043	1/1	0.94	0.16	72,72,72,72	0
55	MG	1H	3313	1/1	0.94	0.17	112,112,112,112	0
55	MG	14	3022	1/1	0.94	0.12	91,91,91,91	0
55	MG	1G	1698	1/1	0.94	0.05	176,176,176,176	0
55	MG	1G	1699	1/1	0.94	0.08	121,121,121,121	0
55	MG	14	3173	1/1	0.94	0.07	66,66,66,66	0
55	MG	1H	3318	1/1	0.94	0.07	93,93,93,93	0
55	MG	13	1732	1/1	0.94	0.14	108,108,108,108	0
55	MG	1H	3320	1/1	0.94	0.12	127,127,127,127	0
55	MG	1H	3231	1/1	0.94	0.11	65,65,65,65	0
55	MG	1H	3232	1/1	0.94	0.10	76,76,76,76	0
55	MG	1H	3323	1/1	0.94	0.13	100,100,100,100	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
55	MG	13	1682	1/1	0.94	0.12	118,118,118,118	0
55	MG	14	3129	1/1	0.94	0.13	90,90,90,90	0
55	MG	14	3033	1/1	0.94	0.08	76,76,76,76	0
55	MG	1H	3328	1/1	0.94	0.09	114,114,114,114	0
55	MG	1H	3329	1/1	0.94	0.07	119,119,119,119	0
55	MG	1H	3130	1/1	0.94	0.08	66,66,66,66	0
55	MG	13	1606	1/1	0.94	0.09	83,83,83,83	0
55	MG	1H	3256	1/1	0.94	0.21	53,53,53,53	0
55	MG	14	3089	1/1	0.94	0.06	79,79,79,79	0
55	MG	1H	3336	1/1	0.94	0.06	127,127,127,127	0
55	MG	1H	3217	1/1	0.94	0.17	43,43,43,43	0
55	MG	1H	3340	1/1	0.94	0.06	139,139,139,139	0
55	MG	1H	3360	1/1	0.94	0.15	62,62,62,62	0
55	MG	1H	3202	1/1	0.94	0.06	87,87,87,87	0
55	MG	1H	3263	1/1	0.94	0.14	53,53,53,53	0
55	MG	14	3097	1/1	0.94	0.13	55,55,55,55	0
55	MG	14	3098	1/1	0.94	0.20	78,78,78,78	0
55	MG	1G	1676	1/1	0.94	0.16	83,83,83,83	0
55	MG	13	1708	1/1	0.94	0.07	145,145,145,145	0
55	MG	14	3148	1/1	0.94	0.13	57,57,57,57	0
55	MG	14	3291	1/1	0.94	0.15	114,114,114,114	0
55	MG	1H	3058	1/1	0.94	0.14	58,58,58,58	0
55	MG	14	3150	1/1	0.94	0.14	89,89,89,89	0
55	MG	13	1654	1/1	0.94	0.13	81,81,81,81	0
55	MG	14	3055	1/1	0.94	0.10	80,80,80,80	0
55	MG	1H	3123	1/1	0.94	0.10	79,79,79,79	0
55	MG	1H	3445	1/1	0.94	0.09	91,91,91,91	0
55	MG	1H	3149	1/1	0.94	0.10	76,76,76,76	0
55	MG	1H	3451	1/1	0.94	0.15	81,81,81,81	0
55	MG	13	1669	1/1	0.94	0.15	100,100,100,100	0
55	MG	1H	3093	1/1	0.94	0.24	70,70,70,70	0
55	MG	1H	3152	1/1	0.94	0.25	49,49,49,49	0
55	MG	14	3065	1/1	0.94	0.15	68,68,68,68	0
55	MG	1G	1689	1/1	0.95	0.06	125,125,125,125	0
55	MG	D8	201	1/1	0.95	0.11	84,84,84,84	0
55	MG	14	3153	1/1	0.95	0.12	59,59,59,59	0
55	MG	1H	3438	1/1	0.95	0.08	93,93,93,93	0
55	MG	1G	1692	1/1	0.95	0.05	118,118,118,118	0
55	MG	13	1731	1/1	0.95	0.15	79,79,79,79	0
55	MG	14	3195	1/1	0.95	0.07	67,67,67,67	0
55	MG	1G	1696	1/1	0.95	0.13	137,137,137,137	0
55	MG	1H	3264	1/1	0.95	0.08	72,72,72,72	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
55	MG	1H	3273	1/1	0.95	0.15	63,63,63,63	0
55	MG	14	3204	1/1	0.95	0.15	106,106,106,106	0
55	MG	14	3068	1/1	0.95	0.06	71,71,71,71	0
55	MG	1H	3299	1/1	0.95	0.06	84,84,84,84	0
55	MG	1G	1700	1/1	0.95	0.08	142,142,142,142	0
55	MG	14	3249	1/1	0.95	0.06	110,110,110,110	0
55	MG	1H	3341	1/1	0.95	0.05	129,129,129,129	0
55	MG	14	3272	1/1	0.95	0.06	93,93,93,93	0
55	MG	1H	3347	1/1	0.95	0.09	65,65,65,65	0
55	MG	14	3287	1/1	0.95	0.05	110,110,110,110	0
55	MG	14	3011	1/1	0.95	0.10	66,66,66,66	0
55	MG	1H	3072	1/1	0.95	0.15	53,53,53,53	0
55	MG	13	1607	1/1	0.95	0.05	110,110,110,110	0
55	MG	14	3292	1/1	0.95	0.19	103,103,103,103	0
55	MG	14	3294	1/1	0.95	0.10	117,117,117,117	0
55	MG	1H	3396	1/1	0.95	0.08	64,64,64,64	0
55	MG	1H	3091	1/1	0.95	0.16	70,70,70,70	0
55	MG	1H	3258	1/1	0.95	0.16	73,73,73,73	0
55	MG	1H	3330	1/1	0.95	0.06	78,78,78,78	0
55	MG	1H	3422	1/1	0.95	0.05	121,121,121,121	0
55	MG	14	3051	1/1	0.95	0.08	67,67,67,67	0
55	MG	1G	1725	1/1	0.95	0.12	130,130,130,130	0
55	MG	14	3020	1/1	0.95	0.06	81,81,81,81	0
55	MG	1G	1726	1/1	0.95	0.10	136,136,136,136	0
55	MG	13	1733	1/1	0.95	0.10	92,92,92,92	0
55	MG	1H	3134	1/1	0.95	0.18	61,61,61,61	0
55	MG	1G	1687	1/1	0.95	0.15	108,108,108,108	0
55	MG	13	1735	1/1	0.96	0.06	100,100,100,100	0
55	MG	13	1700	1/1	0.96	0.07	151,151,151,151	0
55	MG	1H	3094	1/1	0.96	0.09	95,95,95,95	0
55	MG	13	1740	1/1	0.96	0.07	123,123,123,123	0
55	MG	C8	202	1/1	0.96	0.21	70,70,70,70	0
55	MG	13	1693	1/1	0.96	0.10	100,100,100,100	0
55	MG	13	1702	1/1	0.96	0.08	110,110,110,110	0
55	MG	14	3174	1/1	0.96	0.08	60,60,60,60	0
55	MG	1H	3350	1/1	0.96	0.07	71,71,71,71	0
55	MG	13	1703	1/1	0.96	0.09	110,110,110,110	0
55	MG	1H	3365	1/1	0.96	0.09	82,82,82,82	0
55	MG	13	1644	1/1	0.96	0.10	109,109,109,109	0
55	MG	1H	3305	1/1	0.96	0.19	110,110,110,110	0
55	MG	1H	3308	1/1	0.96	0.05	107,107,107,107	0
55	MG	1H	3309	1/1	0.96	0.12	108,108,108,108	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
55	MG	1H	3227	1/1	0.96	0.12	61,61,61,61	0
55	MG	1G	1608	1/1	0.96	0.09	114,114,114,114	0
55	MG	14	3126	1/1	0.96	0.24	48,48,48,48	0
55	MG	1H	3419	1/1	0.96	0.09	115,115,115,115	0
55	MG	1G	1694	1/1	0.96	0.06	151,151,151,151	0
55	MG	14	3187	1/1	0.96	0.08	74,74,74,74	0
55	MG	1H	3421	1/1	0.96	0.08	113,113,113,113	0
55	MG	13	1691	1/1	0.96	0.09	113,113,113,113	0
55	MG	13	1696	1/1	0.96	0.09	117,117,117,117	0
55	MG	14	3024	1/1	0.96	0.11	51,51,51,51	0
55	MG	14	3193	1/1	0.96	0.08	87,87,87,87	0
55	MG	14	3194	1/1	0.96	0.07	132,132,132,132	0
55	MG	13	1727	1/1	0.96	0.18	100,100,100,100	0
55	MG	14	3196	1/1	0.96	0.07	85,85,85,85	0
55	MG	13	1728	1/1	0.96	0.12	114,114,114,114	0
55	MG	14	3135	1/1	0.96	0.20	91,91,91,91	0
55	MG	1H	3440	1/1	0.96	0.08	54,54,54,54	0
55	MG	1H	3442	1/1	0.96	0.05	111,111,111,111	0
55	MG	1G	1706	1/1	0.96	0.14	138,138,138,138	0
55	MG	14	3207	1/1	0.96	0.11	117,117,117,117	0
55	MG	13	1707	1/1	0.96	0.04	133,133,133,133	0
55	MG	14	3217	1/1	0.96	0.05	97,97,97,97	0
55	MG	14	3220	1/1	0.96	0.05	84,84,84,84	0
55	MG	1H	3051	1/1	0.96	0.11	95,95,95,95	0
55	MG	14	3239	1/1	0.96	0.06	106,106,106,106	0
55	MG	14	3246	1/1	0.96	0.07	105,105,105,105	0
55	MG	1H	3234	1/1	0.96	0.12	92,92,92,92	0
55	MG	14	3250	1/1	0.96	0.13	99,99,99,99	0
55	MG	14	3253	1/1	0.96	0.11	83,83,83,83	0
55	MG	14	3268	1/1	0.96	0.07	82,82,82,82	0
55	MG	13	1697	1/1	0.96	0.09	146,146,146,146	0
55	MG	1H	3453	1/1	0.96	0.11	99,99,99,99	0
55	MG	14	3276	1/1	0.96	0.06	109,109,109,109	0
55	MG	14	3281	1/1	0.96	0.10	92,92,92,92	0
55	MG	14	3284	1/1	0.96	0.07	98,98,98,98	0
55	MG	14	3035	1/1	0.96	0.11	68,68,68,68	0
55	MG	1G	1719	1/1	0.96	0.14	123,123,123,123	0
55	MG	14	3037	1/1	0.96	0.05	54,54,54,54	0
55	MG	14	3289	1/1	0.96	0.16	84,84,84,84	0
55	MG	1H	3456	1/1	0.96	0.05	111,111,111,111	0
55	MG	1G	1721	1/1	0.96	0.14	123,123,123,123	0
55	MG	13	1614	1/1	0.96	0.09	100,100,100,100	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
55	MG	14	3293	1/1	0.96	0.05	130,130,130,130	0
55	MG	14	3096	1/1	0.96	0.20	55,55,55,55	0
55	MG	14	3295	1/1	0.96	0.05	104,104,104,104	0
55	MG	1H	3465	1/1	0.96	0.07	98,98,98,98	0
55	MG	14	3042	1/1	0.96	0.12	80,80,80,80	0
55	MG	14	3299	1/1	0.96	0.09	89,89,89,89	0
55	MG	1H	3326	1/1	0.96	0.06	109,109,109,109	0
55	MG	1H	3469	1/1	0.96	0.19	110,110,110,110	0
55	MG	14	3101	1/1	0.96	0.06	88,88,88,88	0
55	MG	29	301	1/1	0.96	0.07	64,64,64,64	0
55	MG	13	1699	1/1	0.96	0.07	116,116,116,116	0
55	MG	1H	3260	1/1	0.96	0.18	53,53,53,53	0
55	MG	2A	201	1/1	0.96	0.12	101,101,101,101	0
55	MG	1H	3261	1/1	0.96	0.06	70,70,70,70	0
55	MG	1H	3074	1/1	0.96	0.15	65,65,65,65	0
55	MG	21	303	1/1	0.96	0.09	63,63,63,63	0
55	MG	1H	3239	1/1	0.96	0.07	103,103,103,103	0
55	MG	1H	3431	1/1	0.97	0.05	62,62,62,62	0
55	MG	14	3192	1/1	0.97	0.04	104,104,104,104	0
55	MG	1H	3432	1/1	0.97	0.04	71,71,71,71	0
55	MG	1H	3307	1/1	0.97	0.05	100,100,100,100	0
55	MG	14	3045	1/1	0.97	0.11	89,89,89,89	0
55	MG	14	3046	1/1	0.97	0.04	76,76,76,76	0
55	MG	1H	3346	1/1	0.97	0.06	63,63,63,63	0
55	MG	1H	3287	1/1	0.97	0.12	58,58,58,58	0
55	MG	13	1736	1/1	0.97	0.17	137,137,137,137	0
55	MG	1H	3357	1/1	0.97	0.05	89,89,89,89	0
55	MG	1H	3447	1/1	0.97	0.05	102,102,102,102	0
55	MG	14	3206	1/1	0.97	0.05	131,131,131,131	0
55	MG	1H	3449	1/1	0.97	0.19	99,99,99,99	0
55	MG	14	3102	1/1	0.97	0.07	83,83,83,83	0
55	MG	14	3215	1/1	0.97	0.11	111,111,111,111	0
55	MG	14	3216	1/1	0.97	0.06	68,68,68,68	0
55	MG	1H	3327	1/1	0.97	0.04	121,121,121,121	0
55	MG	1H	3363	1/1	0.97	0.07	61,61,61,61	0
55	MG	14	3227	1/1	0.97	0.05	79,79,79,79	0
55	MG	14	3230	1/1	0.97	0.05	76,76,76,76	0
55	MG	14	3231	1/1	0.97	0.14	65,65,65,65	0
55	MG	1H	3364	1/1	0.97	0.07	74,74,74,74	0
55	MG	14	3238	1/1	0.97	0.05	83,83,83,83	0
55	MG	14	3056	1/1	0.97	0.14	60,60,60,60	0
55	MG	14	3241	1/1	0.97	0.14	86,86,86,86	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
55	MG	14	3243	1/1	0.97	0.12	116,116,116,116	0
55	MG	14	3244	1/1	0.97	0.05	105,105,105,105	0
55	MG	1H	3070	1/1	0.97	0.13	55,55,55,55	0
55	MG	1H	3369	1/1	0.97	0.11	63,63,63,63	0
55	MG	14	3158	1/1	0.97	0.13	51,51,51,51	0
55	MG	14	3251	1/1	0.97	0.07	65,65,65,65	0
55	MG	14	3160	1/1	0.97	0.09	86,86,86,86	0
55	MG	14	3254	1/1	0.97	0.04	108,108,108,108	0
55	MG	14	3258	1/1	0.97	0.09	97,97,97,97	0
55	MG	14	3259	1/1	0.97	0.06	75,75,75,75	0
55	MG	14	3261	1/1	0.97	0.11	92,92,92,92	0
55	MG	14	3265	1/1	0.97	0.05	65,65,65,65	0
55	MG	1H	3457	1/1	0.97	0.07	133,133,133,133	0
55	MG	1H	3458	1/1	0.97	0.06	126,126,126,126	0
55	MG	14	3270	1/1	0.97	0.10	85,85,85,85	0
55	MG	1H	3461	1/1	0.97	0.04	119,119,119,119	0
55	MG	14	3274	1/1	0.97	0.04	110,110,110,110	0
55	MG	1H	3371	1/1	0.97	0.17	85,85,85,85	0
55	MG	13	1737	1/1	0.97	0.11	111,111,111,111	0
55	MG	1H	3466	1/1	0.97	0.22	111,111,111,111	0
55	MG	1H	3394	1/1	0.97	0.06	75,75,75,75	0
55	MG	14	3286	1/1	0.97	0.09	97,97,97,97	0
55	MG	1H	3013	1/1	0.97	0.08	63,63,63,63	0
55	MG	1H	3471	1/1	0.97	0.10	79,79,79,79	0
55	MG	1H	3331	1/1	0.97	0.10	109,109,109,109	0
55	MG	16	202	1/1	0.97	0.06	118,118,118,118	0
55	MG	1G	1709	1/1	0.97	0.09	127,127,127,127	0
55	MG	14	3073	1/1	0.97	0.07	69,69,69,69	0
55	MG	1G	1710	1/1	0.97	0.12	125,125,125,125	0
55	MG	1G	1711	1/1	0.97	0.18	139,139,139,139	0
55	MG	1H	3400	1/1	0.97	0.17	78,78,78,78	0
55	MG	1H	3316	1/1	0.97	0.04	115,115,115,115	0
55	MG	14	3297	1/1	0.97	0.06	115,115,115,115	0
55	MG	13	1726	1/1	0.97	0.11	103,103,103,103	0
55	MG	1G	1717	1/1	0.97	0.08	137,137,137,137	0
55	MG	1G	1718	1/1	0.97	0.12	112,112,112,112	0
55	MG	1H	3412	1/1	0.97	0.21	128,128,128,128	0
55	MG	1H	3416	1/1	0.97	0.09	119,119,119,119	0
55	MG	1H	3418	1/1	0.97	0.06	99,99,99,99	0
55	MG	13	1650	1/1	0.97	0.06	106,106,106,106	0
55	MG	13	1716	1/1	0.97	0.05	103,103,103,103	0
55	MG	1H	3001	1/1	0.97	0.07	53,53,53,53	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
55	MG	C8	201	1/1	0.97	0.09	76,76,76,76	0
55	MG	1H	3423	1/1	0.97	0.05	102,102,102,102	0
55	MG	13	1611	1/1	0.97	0.06	81,81,81,81	0
55	MG	1H	3429	1/1	0.97	0.06	92,92,92,92	0
57	ZN	5A	101	1/1	0.97	0.09	159,159,159,159	0
55	MG	1H	3370	1/1	0.98	0.06	59,59,59,59	0
55	MG	14	3203	1/1	0.98	0.07	95,95,95,95	0
55	MG	1H	3454	1/1	0.98	0.08	109,109,109,109	0
55	MG	1H	3291	1/1	0.98	0.05	98,98,98,98	0
55	MG	1H	3373	1/1	0.98	0.10	106,106,106,106	0
55	MG	1H	3310	1/1	0.98	0.08	109,109,109,109	0
55	MG	14	3212	1/1	0.98	0.09	67,67,67,67	0
55	MG	14	3213	1/1	0.98	0.04	77,77,77,77	0
55	MG	1H	3381	1/1	0.98	0.04	68,68,68,68	0
55	MG	1H	3388	1/1	0.98	0.06	56,56,56,56	0
55	MG	1H	3464	1/1	0.98	0.17	67,67,67,67	0
55	MG	1H	3393	1/1	0.98	0.07	79,79,79,79	0
55	MG	14	3218	1/1	0.98	0.09	69,69,69,69	0
55	MG	14	3219	1/1	0.98	0.06	63,63,63,63	0
55	MG	13	1729	1/1	0.98	0.06	86,86,86,86	0
55	MG	14	3223	1/1	0.98	0.05	81,81,81,81	0
55	MG	14	3224	1/1	0.98	0.04	84,84,84,84	0
55	MG	14	3226	1/1	0.98	0.03	59,59,59,59	0
55	MG	1G	1686	1/1	0.98	0.04	112,112,112,112	0
55	MG	14	3228	1/1	0.98	0.07	72,72,72,72	0
55	MG	14	3229	1/1	0.98	0.05	74,74,74,74	0
55	MG	1H	3467	1/1	0.98	0.09	106,106,106,106	0
55	MG	1G	1688	1/1	0.98	0.13	94,94,94,94	0
55	MG	14	3235	1/1	0.98	0.10	73,73,73,73	0
55	MG	1H	3186	1/1	0.98	0.05	80,80,80,80	0
55	MG	13	1714	1/1	0.98	0.10	121,121,121,121	0
55	MG	1H	3315	1/1	0.98	0.05	112,112,112,112	0
55	MG	14	3240	1/1	0.98	0.17	135,135,135,135	0
55	MG	1H	3472	1/1	0.98	0.05	64,64,64,64	0
55	MG	1H	3401	1/1	0.98	0.05	72,72,72,72	0
55	MG	1H	3403	1/1	0.98	0.11	87,87,87,87	0
55	MG	14	3245	1/1	0.98	0.03	117,117,117,117	0
55	MG	1H	3404	1/1	0.98	0.04	76,76,76,76	0
55	MG	14	3247	1/1	0.98	0.04	125,125,125,125	0
55	MG	14	3248	1/1	0.98	0.04	86,86,86,86	0
55	MG	13	1720	1/1	0.98	0.12	117,117,117,117	0
55	MG	1H	3409	1/1	0.98	0.07	63,63,63,63	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
55	MG	1H	3317	1/1	0.98	0.05	106,106,106,106	0
55	MG	14	3157	1/1	0.98	0.09	61,61,61,61	0
55	MG	1G	1643	1/1	0.98	0.13	105,105,105,105	0
55	MG	14	3257	1/1	0.98	0.13	99,99,99,99	0
55	MG	1H	3411	1/1	0.98	0.05	81,81,81,81	0
55	MG	1H	3338	1/1	0.98	0.09	105,105,105,105	0
55	MG	14	3260	1/1	0.98	0.10	110,110,110,110	0
55	MG	1H	3413	1/1	0.98	0.18	93,93,93,93	0
55	MG	1H	3297	1/1	0.98	0.07	86,86,86,86	0
55	MG	1H	3417	1/1	0.98	0.08	108,108,108,108	0
55	MG	13	1684	1/1	0.98	0.05	89,89,89,89	0
55	MG	1H	3343	1/1	0.98	0.05	56,56,56,56	0
55	MG	1H	3420	1/1	0.98	0.07	96,96,96,96	0
55	MG	14	3273	1/1	0.98	0.04	89,89,89,89	0
55	MG	I8	101	1/1	0.98	0.17	87,87,87,87	0
55	MG	14	3275	1/1	0.98	0.17	94,94,94,94	0
55	MG	1G	1713	1/1	0.98	0.15	144,144,144,144	0
55	MG	14	3278	1/1	0.98	0.04	109,109,109,109	0
55	MG	14	3279	1/1	0.98	0.05	107,107,107,107	0
55	MG	14	3280	1/1	0.98	0.06	101,101,101,101	0
55	MG	1H	3345	1/1	0.98	0.07	63,63,63,63	0
55	MG	14	3282	1/1	0.98	0.04	117,117,117,117	0
55	MG	13	1739	1/1	0.98	0.14	128,128,128,128	0
55	MG	13	1718	1/1	0.98	0.06	113,113,113,113	0
55	MG	1H	3348	1/1	0.98	0.05	54,54,54,54	0
55	MG	1H	3054	1/1	0.98	0.02	77,77,77,77	0
55	MG	1H	3430	1/1	0.98	0.05	54,54,54,54	0
55	MG	1H	3352	1/1	0.98	0.05	55,55,55,55	0
55	MG	1H	3353	1/1	0.98	0.03	59,59,59,59	0
55	MG	1G	1723	1/1	0.98	0.03	113,113,113,113	0
55	MG	1G	1724	1/1	0.98	0.05	120,120,120,120	0
55	MG	1H	3433	1/1	0.98	0.10	87,87,87,87	0
55	MG	1H	3434	1/1	0.98	0.05	59,59,59,59	0
55	MG	1H	3355	1/1	0.98	0.05	83,83,83,83	0
55	MG	1G	1610	1/1	0.98	0.07	100,100,100,100	0
55	MG	1H	3437	1/1	0.98	0.08	95,95,95,95	0
55	MG	1H	3356	1/1	0.98	0.06	59,59,59,59	0
55	MG	14	3058	1/1	0.98	0.06	95,95,95,95	0
55	MG	1H	3304	1/1	0.98	0.15	96,96,96,96	0
55	MG	7A	101	1/1	0.98	0.07	116,116,116,116	0
55	MG	1H	3324	1/1	0.98	0.06	115,115,115,115	0
55	MG	1H	3362	1/1	0.98	0.06	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	1H	3012	1/1	0.98	0.07	47,47,47,47	0
55	MG	14	3002	1/1	0.98	0.09	53,53,53,53	0
55	MG	1H	3448	1/1	0.98	0.05	72,72,72,72	0
55	MG	1H	3306	1/1	0.98	0.04	93,93,93,93	0
55	MG	1H	3257	1/1	0.98	0.14	53,53,53,53	0
55	MG	1H	3367	1/1	0.98	0.10	92,92,92,92	0
55	MG	1H	3289	1/1	0.98	0.04	102,102,102,102	0
55	MG	14	3070	1/1	0.98	0.07	72,72,72,72	0
55	MG	1H	3427	1/1	0.99	0.07	68,68,68,68	0
55	MG	1H	3428	1/1	0.99	0.07	66,66,66,66	0
55	MG	1H	3333	1/1	0.99	0.03	80,80,80,80	0
55	MG	14	3159	1/1	0.99	0.06	83,83,83,83	0
55	MG	1H	3382	1/1	0.99	0.10	93,93,93,93	0
55	MG	14	3232	1/1	0.99	0.04	59,59,59,59	0
55	MG	14	3233	1/1	0.99	0.12	89,89,89,89	0
55	MG	14	3234	1/1	0.99	0.08	82,82,82,82	0
55	MG	1H	3383	1/1	0.99	0.04	60,60,60,60	0
55	MG	14	3236	1/1	0.99	0.14	98,98,98,98	0
55	MG	1H	3384	1/1	0.99	0.04	76,76,76,76	0
55	MG	1G	1716	1/1	0.99	0.12	123,123,123,123	0
55	MG	1H	3385	1/1	0.99	0.04	63,63,63,63	0
55	MG	1H	3386	1/1	0.99	0.05	56,56,56,56	0
55	MG	1H	3435	1/1	0.99	0.02	80,80,80,80	0
55	MG	14	3242	1/1	0.99	0.03	89,89,89,89	0
55	MG	1H	3387	1/1	0.99	0.04	67,67,67,67	0
55	MG	1H	3351	1/1	0.99	0.06	70,70,70,70	0
55	MG	1H	3390	1/1	0.99	0.09	74,74,74,74	0
55	MG	1H	3439	1/1	0.99	0.04	69,69,69,69	0
55	MG	1H	3391	1/1	0.99	0.04	81,81,81,81	0
55	MG	1H	3441	1/1	0.99	0.02	64,64,64,64	0
55	MG	1H	3392	1/1	0.99	0.03	47,47,47,47	0
55	MG	1H	3443	1/1	0.99	0.03	73,73,73,73	0
55	MG	1H	3444	1/1	0.99	0.04	50,50,50,50	0
55	MG	14	3252	1/1	0.99	0.09	66,66,66,66	0
55	MG	13	1715	1/1	0.99	0.03	99,99,99,99	0
55	MG	1H	3290	1/1	0.99	0.09	79,79,79,79	0
55	MG	14	3255	1/1	0.99	0.06	80,80,80,80	0
55	MG	14	3256	1/1	0.99	0.12	87,87,87,87	0
55	MG	1H	3395	1/1	0.99	0.04	67,67,67,67	0
55	MG	1H	3354	1/1	0.99	0.03	61,61,61,61	0
55	MG	13	1721	1/1	0.99	0.05	87,87,87,87	0
55	MG	1H	3398	1/1	0.99	0.03	84,84,84,84	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
55	MG	1H	3399	1/1	0.99	0.04	86,86,86,86	0
55	MG	14	3262	1/1	0.99	0.06	60,60,60,60	0
55	MG	14	3263	1/1	0.99	0.08	76,76,76,76	0
55	MG	14	3264	1/1	0.99	0.10	88,88,88,88	0
55	MG	1H	3292	1/1	0.99	0.06	103,103,103,103	0
55	MG	14	3266	1/1	0.99	0.03	83,83,83,83	0
55	MG	14	3267	1/1	0.99	0.14	88,88,88,88	0
55	MG	1H	3302	1/1	0.99	0.04	120,120,120,120	0
55	MG	1H	3455	1/1	0.99	0.05	85,85,85,85	0
55	MG	1H	3358	1/1	0.99	0.03	60,60,60,60	0
55	MG	14	3271	1/1	0.99	0.04	56,56,56,56	0
55	MG	1H	3339	1/1	0.99	0.07	78,78,78,78	0
55	MG	1H	3314	1/1	0.99	0.02	113,113,113,113	0
55	MG	1H	3459	1/1	0.99	0.03	112,112,112,112	0
55	MG	1H	3406	1/1	0.99	0.03	70,70,70,70	0
55	MG	1H	3462	1/1	0.99	0.10	106,106,106,106	0
55	MG	14	3277	1/1	0.99	0.10	74,74,74,74	0
55	MG	1H	3407	1/1	0.99	0.04	76,76,76,76	0
55	MG	1H	3303	1/1	0.99	0.10	98,98,98,98	0
55	MG	1H	3342	1/1	0.99	0.07	60,60,60,60	0
55	MG	1H	3068	1/1	0.99	0.03	53,53,53,53	0
55	MG	1H	3366	1/1	0.99	0.15	75,75,75,75	0
55	MG	14	3283	1/1	0.99	0.06	106,106,106,106	0
55	MG	1H	3344	1/1	0.99	0.03	72,72,72,72	0
55	MG	1H	3414	1/1	0.99	0.06	82,82,82,82	0
55	MG	14	3199	1/1	0.99	0.05	97,97,97,97	0
55	MG	14	3200	1/1	0.99	0.07	70,70,70,70	0
55	MG	14	3201	1/1	0.99	0.07	101,101,101,101	0
55	MG	1H	3470	1/1	0.99	0.03	69,69,69,69	0
55	MG	1H	3415	1/1	0.99	0.05	88,88,88,88	0
55	MG	1H	3368	1/1	0.99	0.09	83,83,83,83	0
55	MG	1H	3473	1/1	0.99	0.02	74,74,74,74	0
55	MG	1G	1695	1/1	0.99	0.13	130,130,130,130	0
55	MG	13	1730	1/1	0.99	0.14	125,125,125,125	0
55	MG	14	3208	1/1	0.99	0.04	70,70,70,70	0
55	MG	14	3209	1/1	0.99	0.08	65,65,65,65	0
55	MG	14	3211	1/1	0.99	0.04	84,84,84,84	0
55	MG	13	1722	1/1	0.99	0.03	106,106,106,106	0
55	MG	13	1717	1/1	0.99	0.15	109,109,109,109	0
55	MG	1H	3372	1/1	0.99	0.17	94,94,94,94	0
55	MG	1H	3288	1/1	0.99	0.09	99,99,99,99	0
55	MG	1H	3375	1/1	0.99	0.06	65,65,65,65	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
55	MG	1G	1702	1/1	0.99	0.05	83,83,83,83	0
55	MG	1H	3349	1/1	0.99	0.05	67,67,67,67	0
55	MG	1G	1705	1/1	0.99	0.11	102,102,102,102	0
55	MG	1H	3424	1/1	0.99	0.03	68,68,68,68	0
55	MG	14	3221	1/1	0.99	0.04	67,67,67,67	0
55	MG	14	3222	1/1	0.99	0.04	67,67,67,67	0
55	MG	1H	3380	1/1	0.99	0.03	83,83,83,83	0
55	MG	1H	3426	1/1	0.99	0.13	97,97,97,97	0
56	SF4	3E	301	8/8	0.99	0.04	96,110,122,122	0
56	SF4	32	302	8/8	0.99	0.03	112,135,144,151	0
57	ZN	5I	103	1/1	0.99	0.03	109,109,109,109	0
55	MG	88	202	1/1	0.99	0.66	62,62,62,62	0
55	MG	1H	3359	1/1	1.00	0.04	51,51,51,51	0
55	MG	1H	3402	1/1	1.00	0.03	66,66,66,66	0
55	MG	1H	3376	1/1	1.00	0.02	58,58,58,58	0
55	MG	1H	3460	1/1	1.00	0.03	64,64,64,64	0
55	MG	1H	3389	1/1	1.00	0.06	68,68,68,68	0
55	MG	1G	1703	1/1	1.00	0.02	94,94,94,94	0
55	MG	14	3210	1/1	1.00	0.02	60,60,60,60	0
55	MG	1H	3377	1/1	1.00	0.03	58,58,58,58	0
55	MG	14	3225	1/1	1.00	0.05	63,63,63,63	0
55	MG	1H	3361	1/1	1.00	0.02	53,53,53,53	0
55	MG	1H	3379	1/1	1.00	0.03	76,76,76,76	0
55	MG	1H	3408	1/1	1.00	0.03	58,58,58,58	0
55	MG	1H	3374	1/1	1.00	0.03	47,47,47,47	0
55	MG	1H	3446	1/1	1.00	0.02	88,88,88,88	0

6.5 Other polymers [i](#)

There are no such residues in this entry.