wwPDB X-ray Structure Validation Summary Report (i)

Mar 24, 2026 – 12:31 PM UTC

PDB ID	:	6GSJ / pdb_00006gsj
Title	:	Structure of T. thermophilus 70S ribosome complex with mRNA, tRNAfMet and cognate tRNAThr in the A-site
Authors	:	Rozov, A.; Yusupov, M.; Yusupova, G.
Deposited on	:	2018-06-14
Resolution	:	2.96 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 (i) 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 (1)) were used in the production of this report:

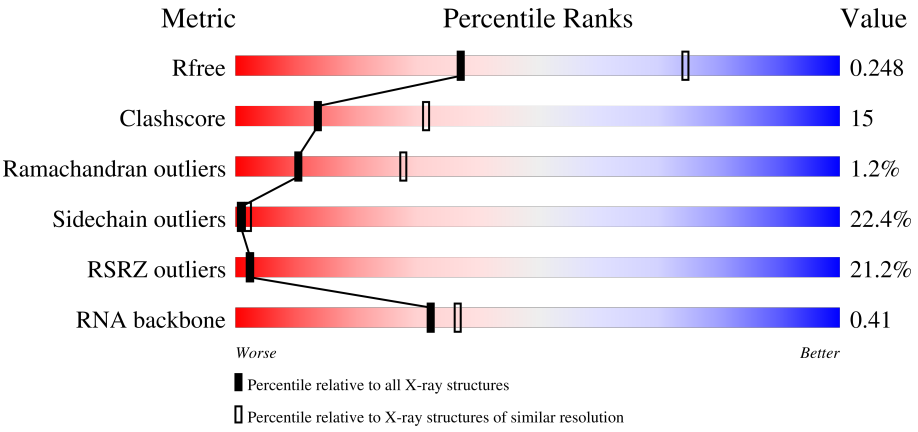
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry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

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.96 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	1130 (2.98-2.94)
Clashscore	190562	1157 (2.98-2.94)
Ramachandran outliers	187476	1101 (2.98-2.94)
Sidechain outliers	187428	1101 (2.98-2.94)
RSRZ outliers	180081	1130 (2.98-2.94)
RNA backbone	3983	1046 (3.16-2.76)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments 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 <=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	20% 45% 40% 13% •
1	1G	1522	17% 48% 38% 12% •
2	12	256	34% 30% 38% 11% • 19%
2	1E	256	20% 38% 38% 13% • 10%

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Mol	Chain	Length	Quality of chain
3	22	239	33% 37% 36% 10% 18%
3	2E	239	24% 54% 28% 5% 14%
4	32	209	22% 54% 35% 9%
4	3E	209	16% 52% 39% 8%
5	42	162	28% 42% 38% 13% 7%
5	4E	162	18% 56% 28% 8% 8%
6	52	101	24% 65% 26% 9%
6	5E	101	20% 66% 28% 5%
7	62	156	29% 45% 38% 6% 12%
7	6E	156	15% 57% 33% 8%
8	72	138	27% 54% 34% 11%
8	7E	138	9% 55% 30% 14%
9	82	128	25% 43% 41% 9% 5%
9	8E	128	24% 43% 45% 11%
10	1A	105	42% 35% 47% 12% 6%
10	1I	105	32% 51% 28% 10% 10%
11	2A	129	12% 51% 29% 7% 12%
11	2I	129	12% 47% 30% 8% 14%
12	3A	132	26% 51% 32% 10% 8%
12	3I	132	21% 47% 38% 8% 8%
13	4A	126	26% 35% 37% 13% 13%
13	4I	126	17% 40% 40% 13% 6%
14	5A	61	36% 39% 41% 16%
14	5I	61	11% 46% 39% 13%
15	6A	89	9% 75% 22%

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Mol	Chain	Length	Quality of chain
15	6I	89	20% 54% 35% 9%
16	7A	88	5% 63% 30% 5%
16	7I	88	16% 50% 39% 6% 6%
17	8A	105	13% 61% 28% 6% 6%
17	8I	105	20% 55% 30% 9% 5%
18	9A	88	3% 48% 22% 9% 22%
18	9I	88	14% 39% 33% 6% 23%
19	AA	93	29% 22% 31% 14% 30%
19	AI	93	11% 43% 33% 11% 11%
20	BA	106	21% 62% 28% 7%
20	BI	106	26% 38% 46% 8% 8%
21	1B	27	4% 37% 41% 19%
21	1F	27	7% 44% 37% 15%
22	1K	76	34% 20% 46% 30%
22	1L	76	34% 22% 37% 38%
23	2K	77	23% 56% 34% 9%
23	2L	77	16% 42% 42% 13%
24	3K	76	34% 24% 42% 29% 5%
25	4K	27	11% 26% 11% 30% 33%
25	4L	27	19% 7% 22% 48%
26	14	2917	17% 48% 38% 10%
26	1H	2917	15% 51% 37% 10%
27	16	122	6% 50% 42% 7%
27	1J	122	7% 39% 43% 18%
28	11	276	9% 63% 27% 7%

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Mol	Chain	Length	Quality of chain
28	19	276	11% 60% 30% 9%
29	21	206	27% 50% 34% 14%
29	29	206	38% 49% 35% 14%
30	31	210	16% 55% 35% 6%
30	39	210	35% 40% 40% 15%
31	41	182	25% 46% 42% 11%
31	49	182	20% 47% 41% 10%
32	51	180	23% 54% 29% 11%
32	59	180	63% 35% 44% 14% 6%
33	61	148	21% 46% 36% 13%
33	69	148	36% 49% 39% 10%
34	15	140	27% 52% 32% 14%
34	58	140	19% 48% 36% 11%
35	25	122	11% 60% 33% 7%
35	68	122	6% 66% 28% 6%
36	35	150	41% 44% 34% 20%
36	78	150	33% 42% 45% 9%
37	45	141	36% 48% 35% 14%
37	88	141	32% 52% 37% 11%
38	55	118	19% 49% 36% 14%
38	98	118	33% 44% 47% 9%
39	65	112	16% 32% 52% 14%
39	A8	112	11% 40% 45% 14%
40	75	146	21% 45% 40% 10%
40	B8	146	34% 41% 38% 13% 7%

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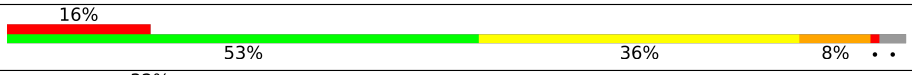
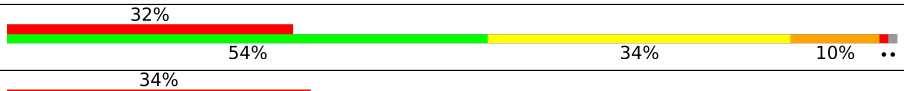
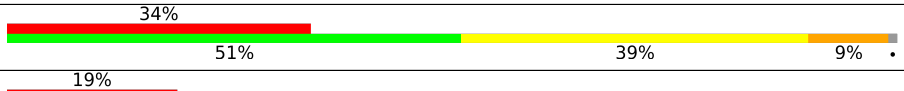
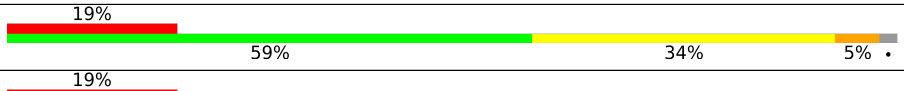
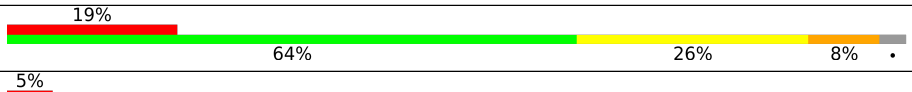
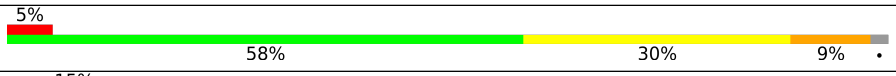
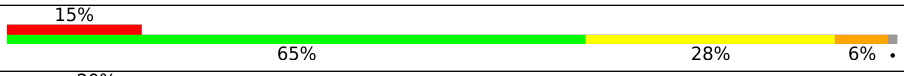
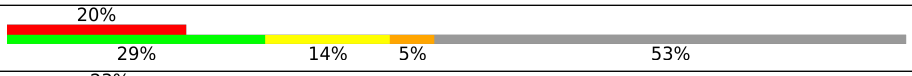
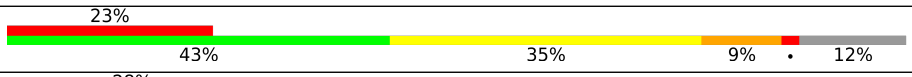
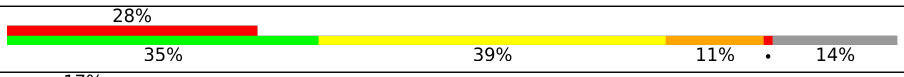
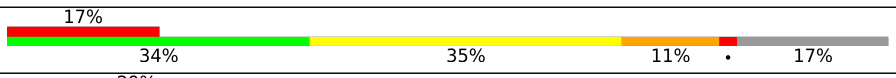
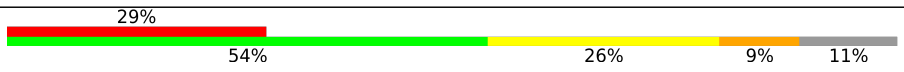
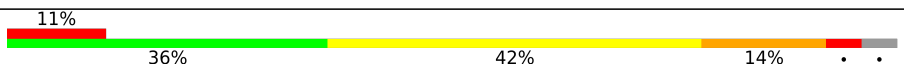
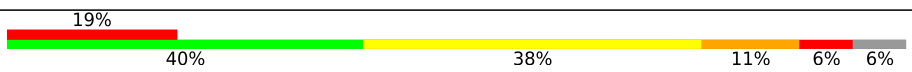
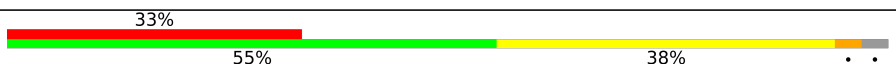
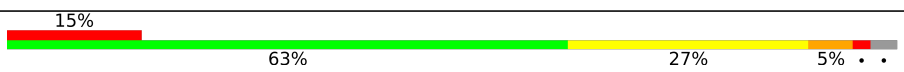
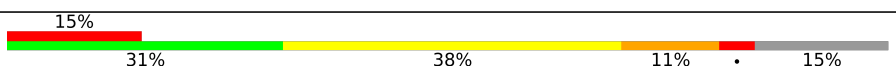
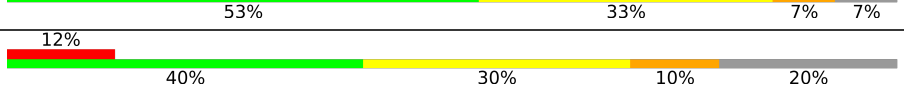
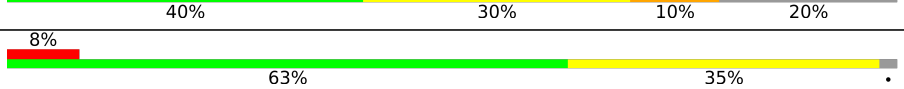
Mol	Chain	Length	Quality of chain
41	85	118	
41	C8	118	
42	95	101	
42	D8	101	
43	A5	113	
43	E8	113	
44	B5	96	
44	F8	96	
45	C5	110	
45	G8	110	
46	D5	206	
46	H8	206	
47	E5	85	
47	I8	85	
48	F5	98	
48	J8	98	
49	G5	72	
49	K8	72	
50	H5	60	
50	L8	60	
51	M8	71	
52	J5	60	
52	N8	60	
53	L5	49	
53	P8	49	

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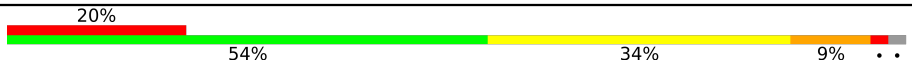
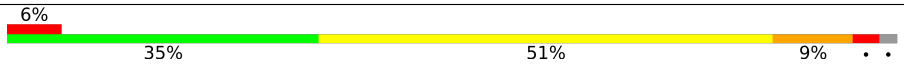
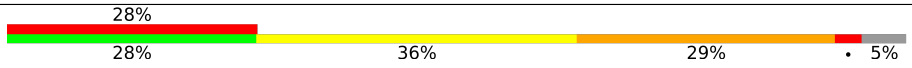
Mol	Chain	Length	Quality of chain
54	M5	65	
54	Q8	65	
55	3L	76	

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
56	MG	13	1632	-	-	-	X
56	MG	13	1665	-	-	-	X
56	MG	13	1666	-	-	-	X
56	MG	13	1668	-	-	-	X
56	MG	13	1684	-	-	-	X
56	MG	13	1686	-	-	-	X
56	MG	13	1741	-	-	-	X
56	MG	14	3029	-	-	-	X
56	MG	14	3041	-	-	-	X
56	MG	14	3042	-	-	-	X
56	MG	14	3077	-	-	-	X
56	MG	14	3096	-	-	-	X
56	MG	14	3210	-	-	-	X
56	MG	14	3245	-	-	-	X
56	MG	14	3248	-	-	-	X
56	MG	14	3268	-	-	-	X
56	MG	14	3272	-	-	-	X
56	MG	14	3280	-	-	-	X
56	MG	14	3285	-	-	-	X
56	MG	14	3298	-	-	-	X
56	MG	16	206	-	-	-	X
56	MG	16	209	-	-	-	X
56	MG	16	210	-	-	-	X
56	MG	1G	1626	-	-	-	X
56	MG	1G	1646	-	-	-	X
56	MG	1G	1690	-	-	-	X
56	MG	1G	1701	-	-	-	X
56	MG	1H	3026	-	-	-	X
56	MG	1H	3041	-	-	-	X
56	MG	1H	3054	-	-	-	X
56	MG	1H	3101	-	-	-	X
56	MG	1H	3129	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
56	MG	1H	3153	-	-	-	X
56	MG	1H	3165	-	-	-	X
56	MG	1H	3198	-	-	-	X
56	MG	1H	3205	-	-	-	X
56	MG	1H	3227	-	-	-	X
56	MG	1H	3238	-	-	-	X
56	MG	1H	3269	-	-	-	X
56	MG	1H	3276	-	-	-	X
56	MG	1H	3303	-	-	-	X
56	MG	1H	3328	-	-	-	X
56	MG	1H	3334	-	-	-	X
56	MG	1H	3356	-	-	-	X
56	MG	1H	3386	-	-	-	X
56	MG	1H	3401	-	-	-	X
56	MG	1H	3405	-	-	-	X
56	MG	1H	3421	-	-	-	X
56	MG	1J	201	-	-	-	X
56	MG	35	203	-	-	-	X
56	MG	88	201	-	-	-	X

2 Entry composition (i)

There are 59 unique types of molecules in this entry. The entry contains 294252 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			

- 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			
4	32	207	Total	C	N	O	S	0	0	0
			1698	1064	338	289	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			

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	2I	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	83	Total	C	N	O	S	0	0	0
			665	424	124	115	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			
20	BA	103	Total	C	N	O	S	0	0	0
			778	481	163	132	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	S	0	0	0
			1646	735	297	536	77	1			
23	2L	77	Total	C	N	O	P	S	0	0	0
			1646	735	297	536	77	1			

- 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			

- Molecule 25 is a RNA chain called RNA (27-MER).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
25	4K	18	Total	C	N	O	P	0	0	0
			391	176	80	117	18			
25	4L	14	Total	C	N	O	P	0	0	0
			303	137	63	89	14			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
26	1H	2850	Total	C	N	O	P	0	0	0
			61381	27319	11475	19737	2850			
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			
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			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
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			
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 a RNA chain called tRNAThr.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
55	3L	72	Total	C	N	O	P	0	0	0
			1538	687	276	503	72			

- Molecule 56 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
56	13	205	Total	Mg	0	0
			205	205		
56	3E	1	Total	Mg	0	0
			1	1		
56	5E	1	Total	Mg	0	0
			1	1		
56	2I	1	Total	Mg	0	0
			1	1		
56	5I	2	Total	Mg	0	0
			2	2		

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
56	8I	1	Total Mg 1 1	0	0
56	BI	2	Total Mg 2 2	0	0
56	1K	1	Total Mg 1 1	0	0
56	2K	2	Total Mg 2 2	0	0
56	1H	622	Total Mg 622 622	0	0
56	16	15	Total Mg 15 15	0	0
56	11	1	Total Mg 1 1	0	0
56	21	4	Total Mg 4 4	0	0
56	31	2	Total Mg 2 2	0	0
56	41	1	Total Mg 1 1	0	0
56	68	2	Total Mg 2 2	0	0
56	78	2	Total Mg 2 2	0	0
56	88	3	Total Mg 3 3	0	0
56	98	1	Total Mg 1 1	0	0
56	D8	1	Total Mg 1 1	0	0
56	I8	2	Total Mg 2 2	0	0
56	P8	1	Total Mg 1 1	0	0
56	Q8	1	Total Mg 1 1	0	0
56	1G	155	Total Mg 155 155	0	0
56	42	1	Total Mg 1 1	0	0
56	2A	1	Total Mg 1 1	0	0

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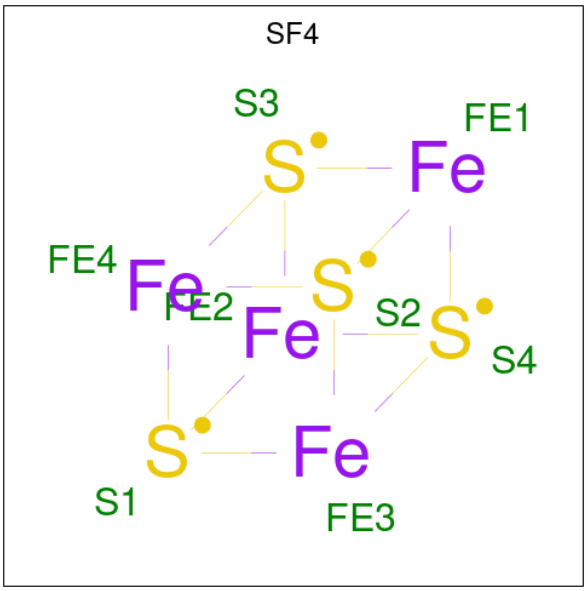
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
56	4A	1	Total Mg 1 1	0	0
56	9A	1	Total Mg 1 1	0	0
56	BA	2	Total Mg 2 2	0	0
56	1B	1	Total Mg 1 1	0	0
56	2L	2	Total Mg 2 2	0	0
56	4L	1	Total Mg 1 1	0	0
56	14	435	Total Mg 435 435	0	0
56	1J	6	Total Mg 6 6	0	0
56	19	1	Total Mg 1 1	0	0
56	29	3	Total Mg 3 3	0	0
56	39	1	Total Mg 1 1	0	0
56	25	1	Total Mg 1 1	0	0
56	35	3	Total Mg 3 3	0	0
56	45	2	Total Mg 2 2	0	0
56	55	1	Total Mg 1 1	0	0
56	85	1	Total Mg 1 1	0	0
56	E5	1	Total Mg 1 1	0	0

- Molecule 57 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe_4S_4).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
57	3E	1	Total Fe S 8 4 4	0	0
57	32	1	Total Fe S 8 4 4	0	0

- Molecule 58 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
58	5I	1	Total Zn 1 1	0	0
58	5A	1	Total Zn 1 1	0	0

- Molecule 59 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
59	13	339	Total O 339 339	0	0
59	1E	1	Total O 1 1	0	0
59	3E	2	Total O 2 2	0	0
59	4E	2	Total O 2 2	0	0
59	6E	1	Total O 1 1	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
59	8E	2	Total O 2 2	0	0
59	1I	3	Total O 3 3	0	0
59	3I	1	Total O 1 1	0	0
59	4I	2	Total O 2 2	0	0
59	5I	1	Total O 1 1	0	0
59	6I	1	Total O 1 1	0	0
59	7I	3	Total O 3 3	0	0
59	1F	2	Total O 2 2	0	0
59	1K	1	Total O 1 1	0	0
59	4K	2	Total O 2 2	0	0
59	1H	1047	Total O 1047 1047	0	0
59	16	19	Total O 19 19	0	0
59	11	11	Total O 11 11	0	0
59	21	8	Total O 8 8	0	0
59	31	7	Total O 7 7	0	0
59	58	3	Total O 3 3	0	0
59	78	6	Total O 6 6	0	0
59	D8	1	Total O 1 1	0	0
59	E8	1	Total O 1 1	0	0
59	G8	1	Total O 1 1	0	0
59	I8	2	Total O 2 2	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
59	J8	1	Total O 1 1	0	0
59	L8	4	Total O 4 4	0	0
59	P8	1	Total O 1 1	0	0
59	Q8	2	Total O 2 2	0	0
59	1G	289	Total O 289 289	0	0
59	32	2	Total O 2 2	0	0
59	42	1	Total O 1 1	0	0
59	52	4	Total O 4 4	0	0
59	1A	1	Total O 1 1	0	0
59	7A	4	Total O 4 4	0	0
59	9A	2	Total O 2 2	0	0
59	BA	2	Total O 2 2	0	0
59	2L	6	Total O 6 6	0	0
59	4L	3	Total O 3 3	0	0
59	14	730	Total O 730 730	0	0
59	19	10	Total O 10 10	0	0
59	29	2	Total O 2 2	0	0
59	39	5	Total O 5 5	0	0
59	15	1	Total O 1 1	0	0
59	25	6	Total O 6 6	0	0
59	35	6	Total O 6 6	0	0

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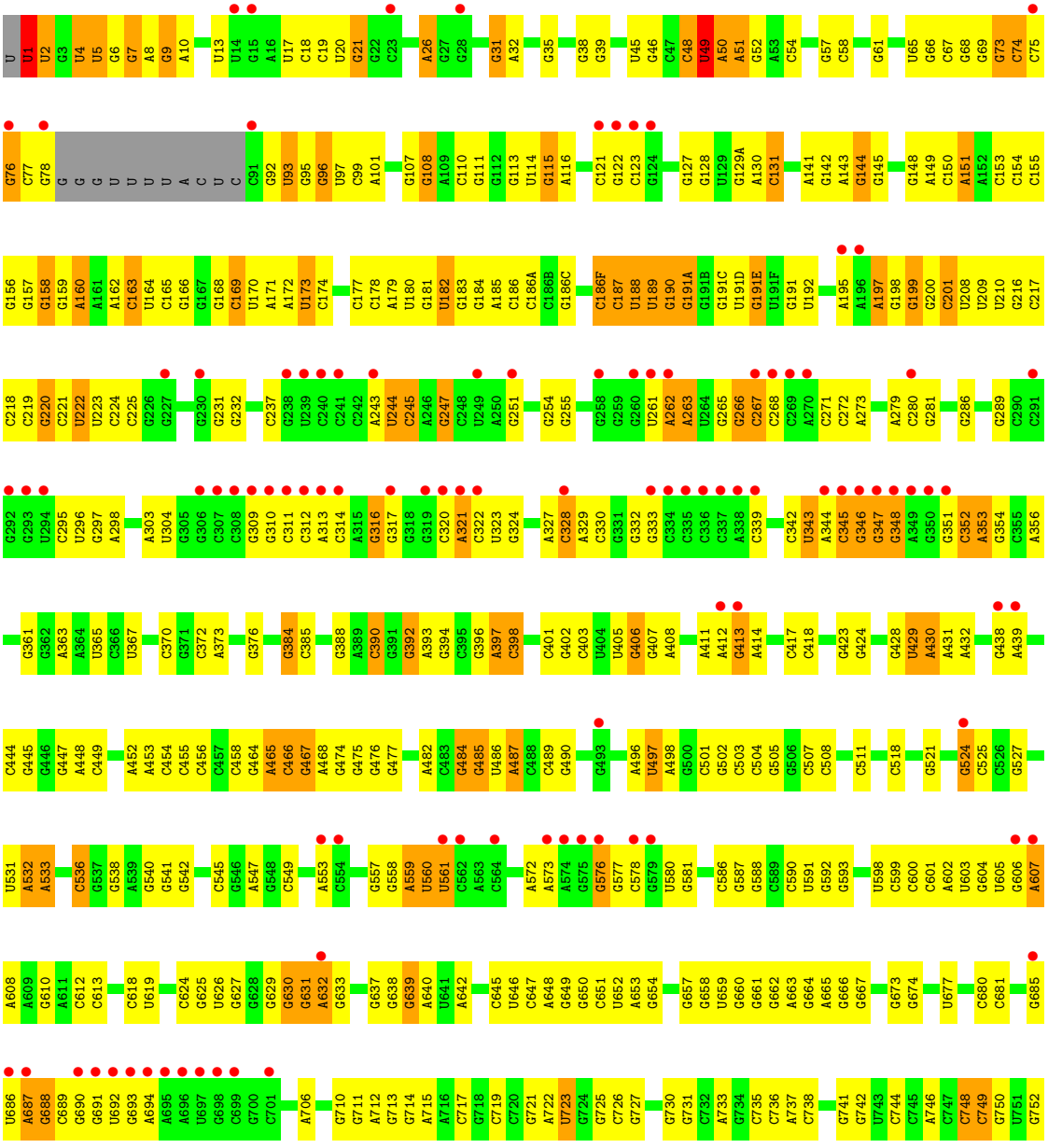
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
59	45	4	Total O 4 4	0	0
59	75	1	Total O 1 1	0	0
59	95	1	Total O 1 1	0	0
59	B5	3	Total O 3 3	0	0
59	H5	3	Total O 3 3	0	0
59	M5	2	Total O 2 2	0	0

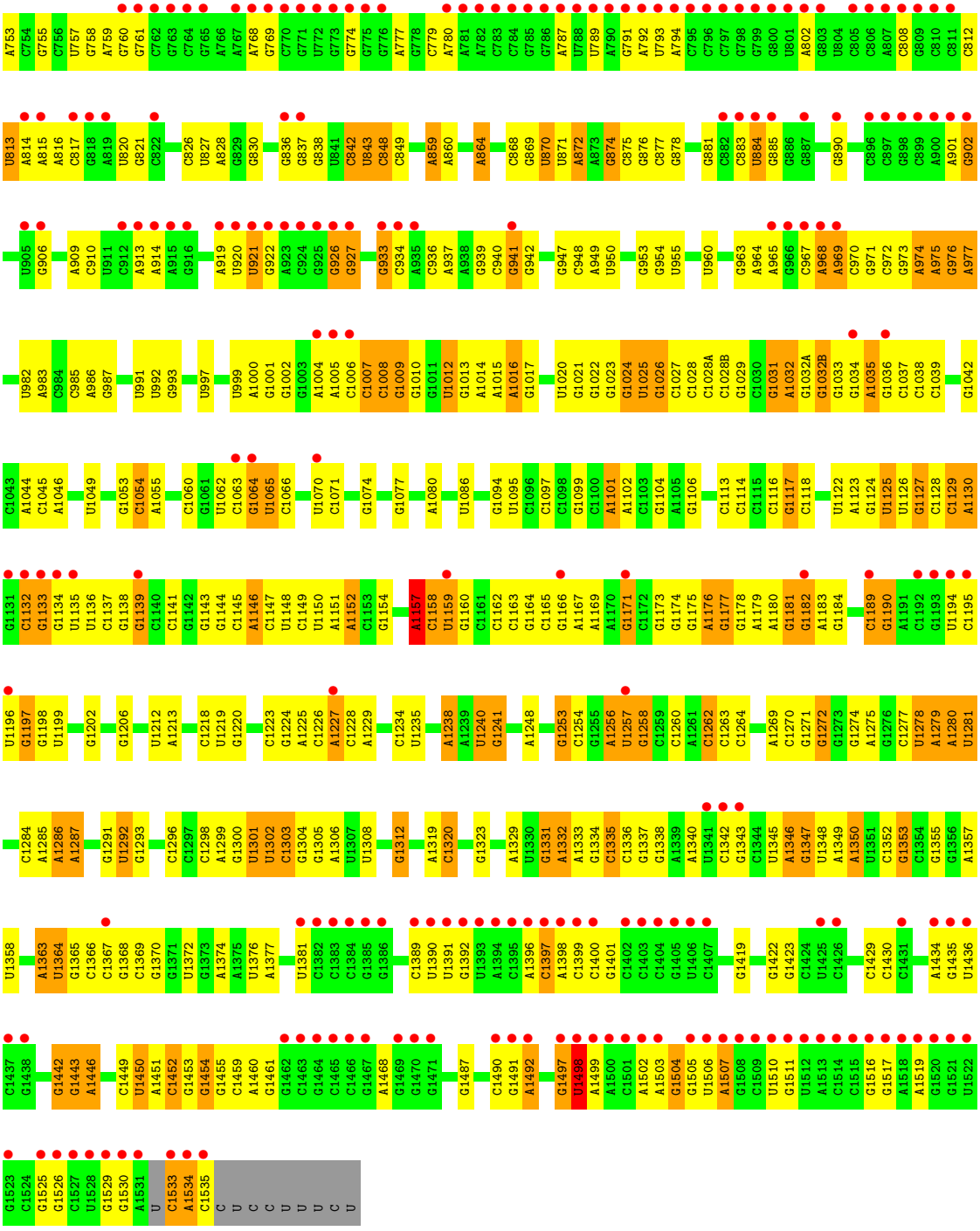
3 Residue-property plots (i)

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

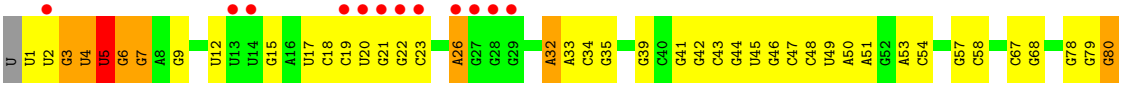
Chain 13:

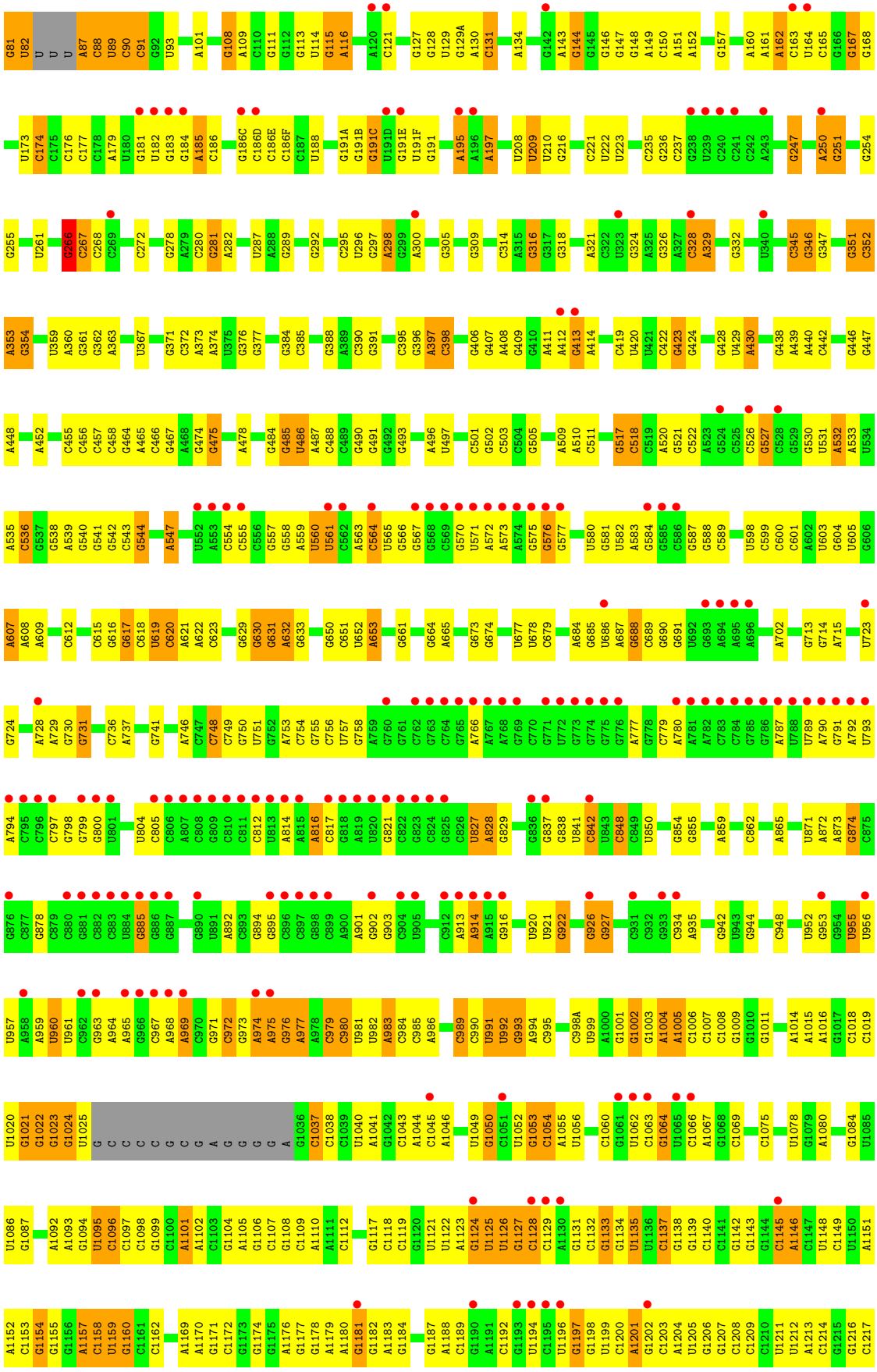


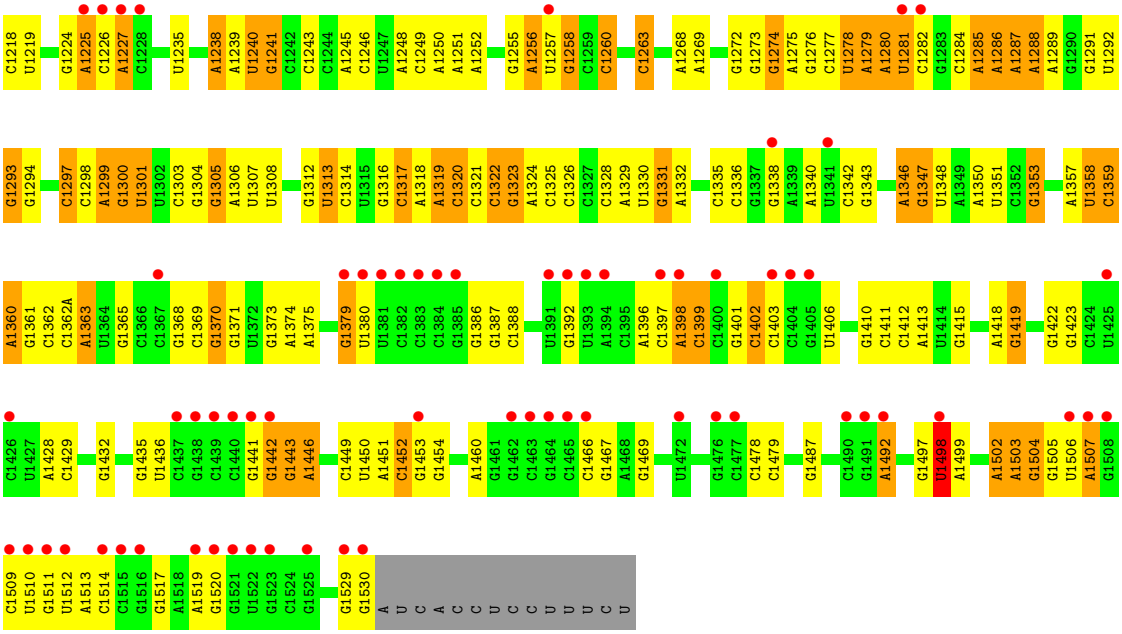


• Molecule 1: 16S ribosomal RNA

Chain 1G:

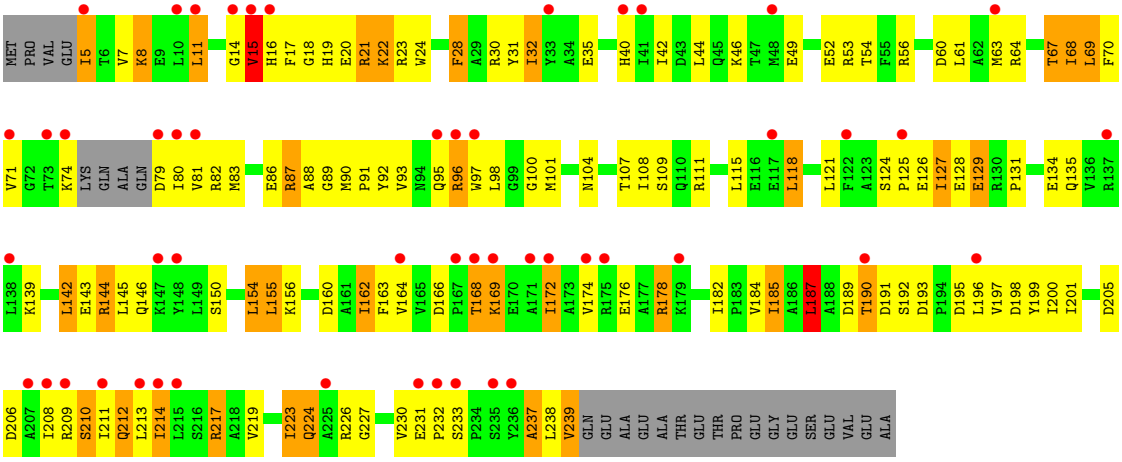






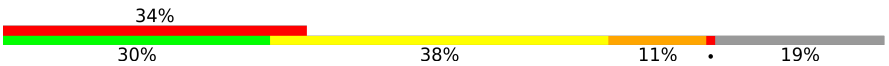
• Molecule 2: 30S ribosomal protein S2

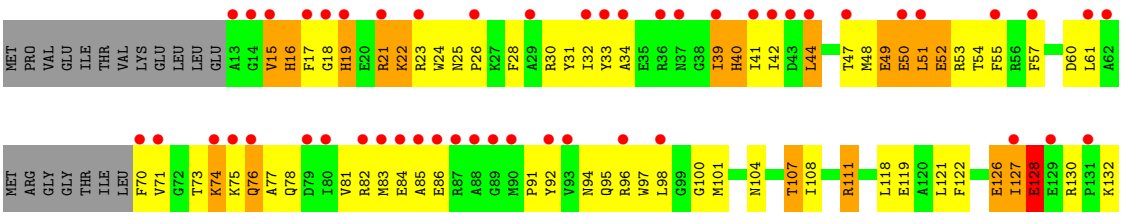
Chain 1E:

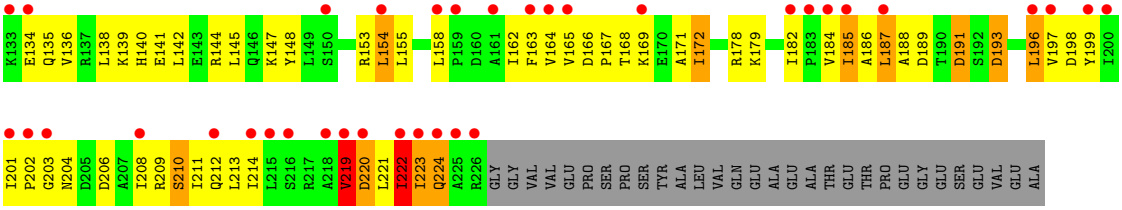


• Molecule 2: 30S ribosomal protein S2

Chain 12:

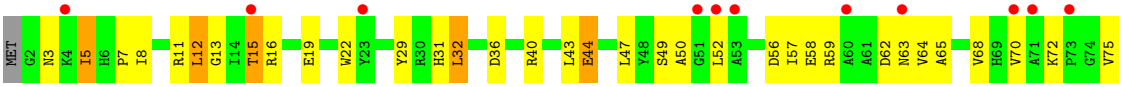


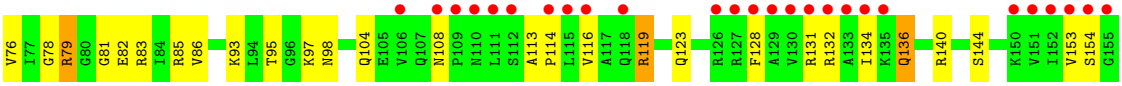


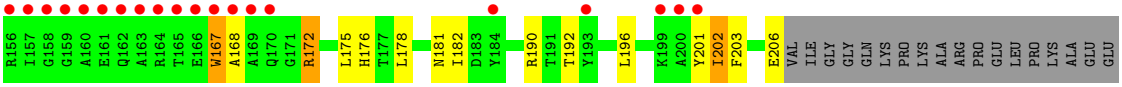


• Molecule 3: 30S ribosomal protein S3

Chain 2E:

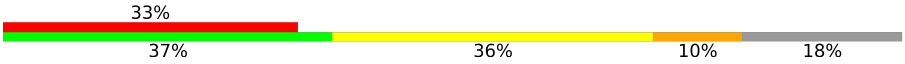


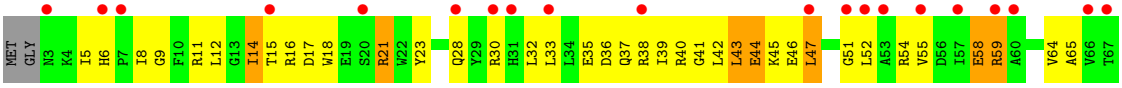


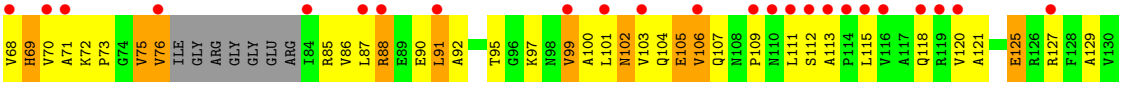


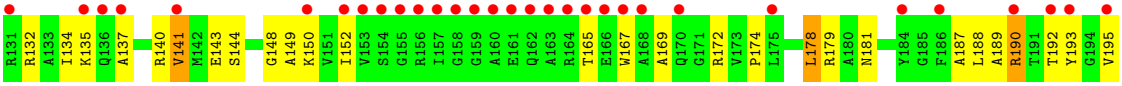
• Molecule 3: 30S ribosomal protein S3

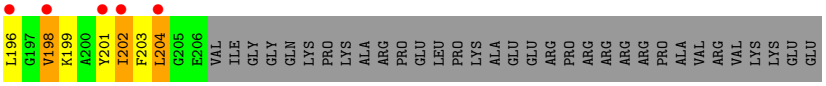
Chain 22:





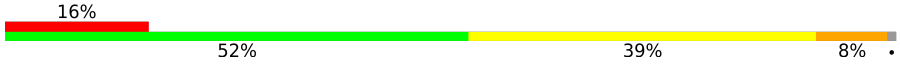


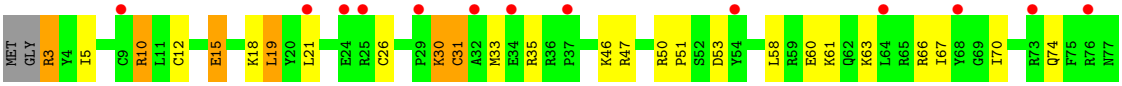


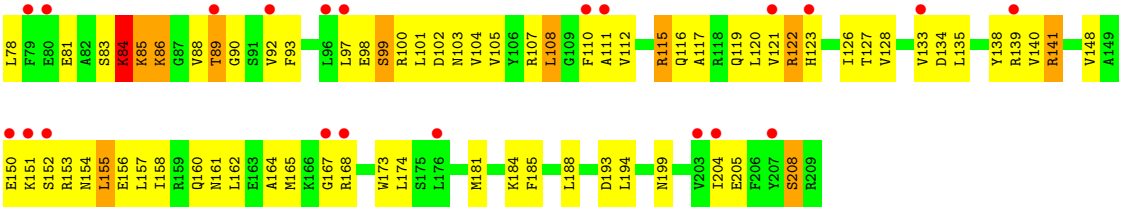


• Molecule 4: 30S ribosomal protein S4

Chain 3E:

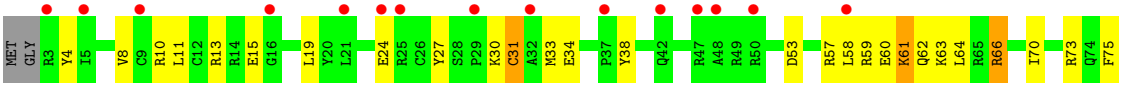


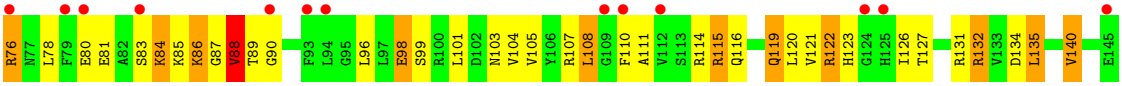


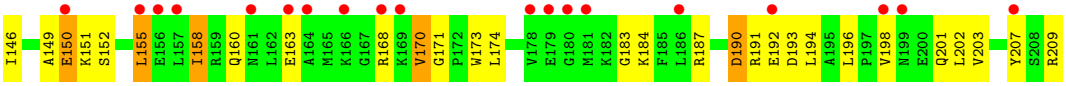


• Molecule 4: 30S ribosomal protein S4

Chain 32:

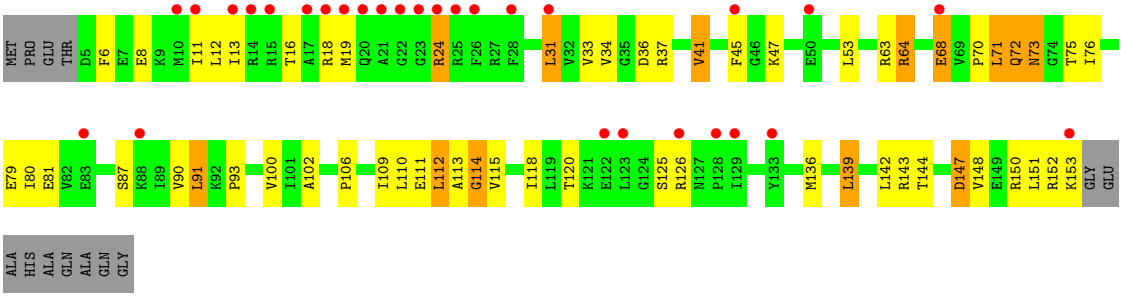






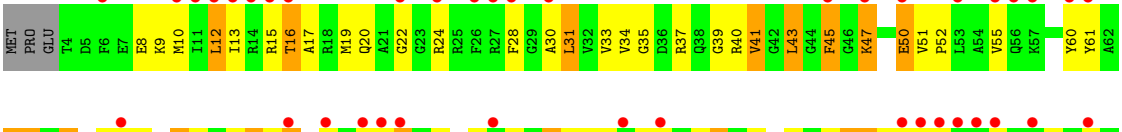
• Molecule 5: 30S ribosomal protein S5

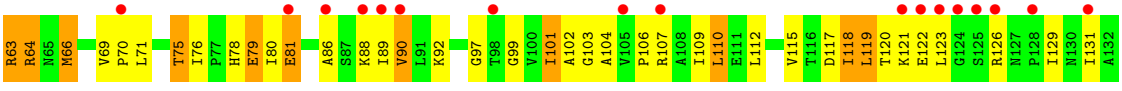
Chain 4E:



• Molecule 5: 30S ribosomal protein S5

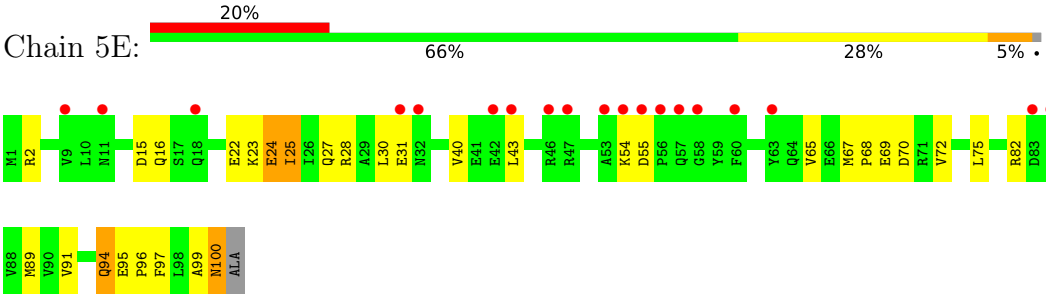
Chain 42:





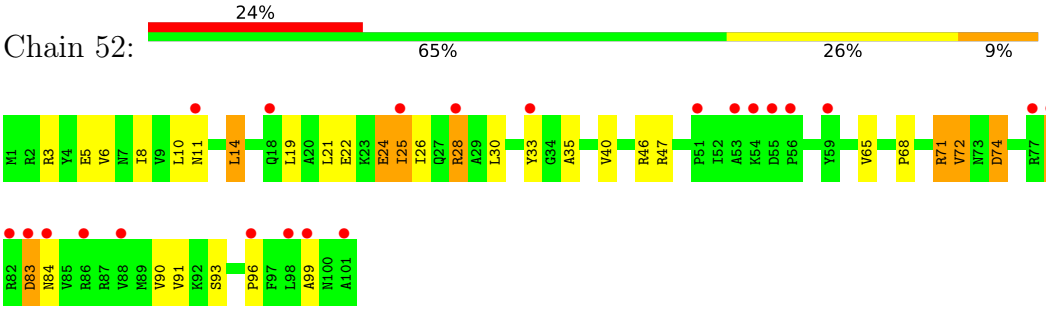
• Molecule 6: 30S ribosomal protein S6

Chain 5E:



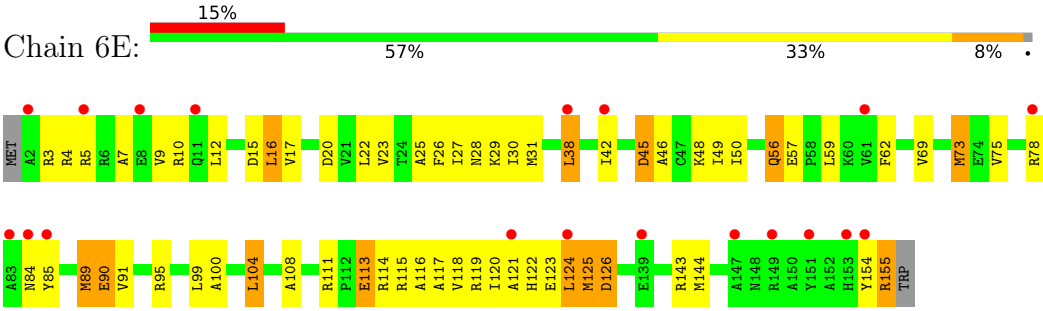
• Molecule 6: 30S ribosomal protein S6

Chain 52:



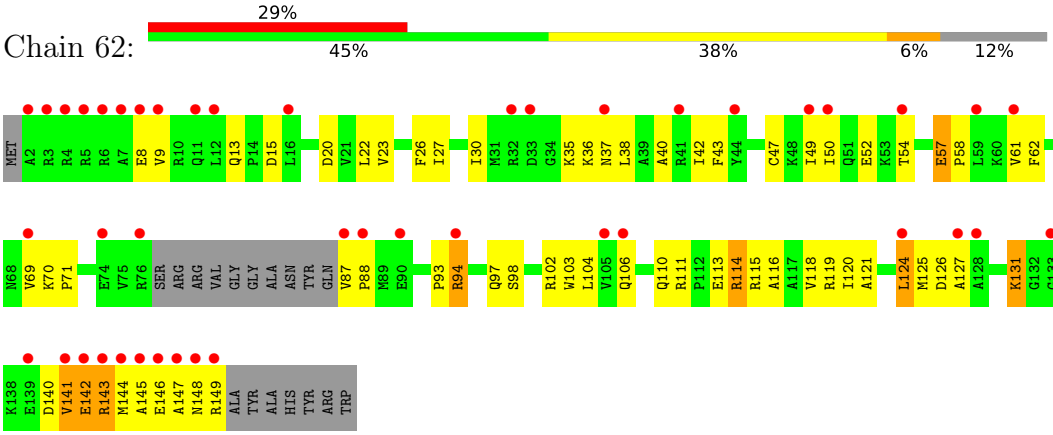
• Molecule 7: 30S ribosomal protein S7

Chain 6E:



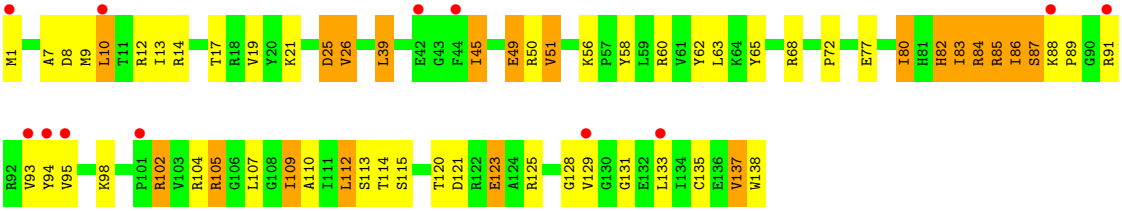
• Molecule 7: 30S ribosomal protein S7

Chain 62:



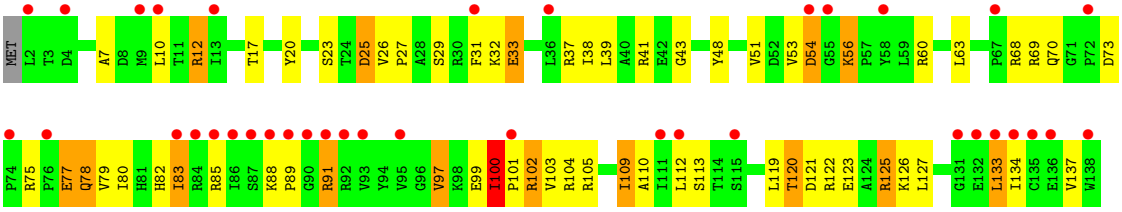
• Molecule 8: 30S ribosomal protein S8

Chain 7E:



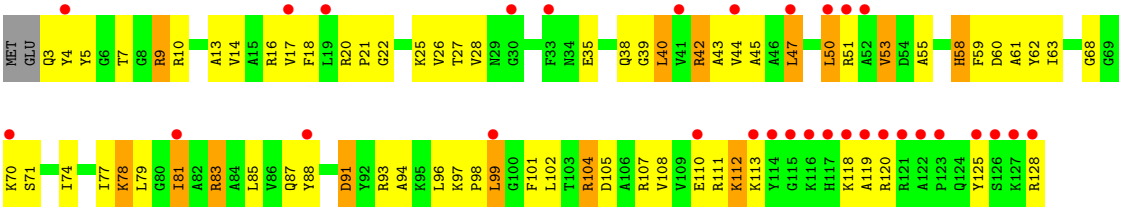
• Molecule 8: 30S ribosomal protein S8

Chain 72:



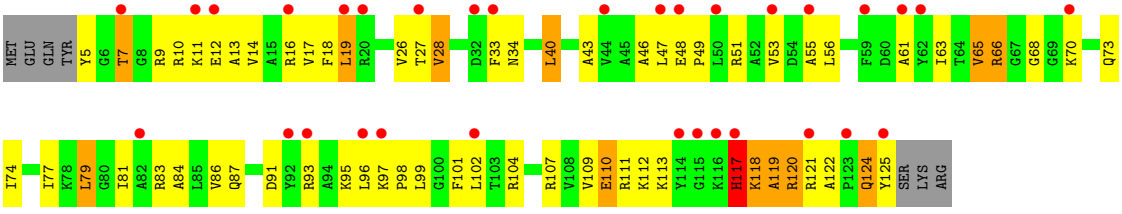
• Molecule 9: 30S ribosomal protein S9

Chain 8E:



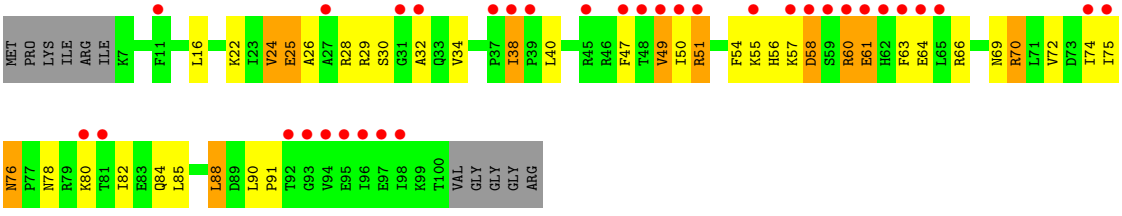
• Molecule 9: 30S ribosomal protein S9

Chain 82:



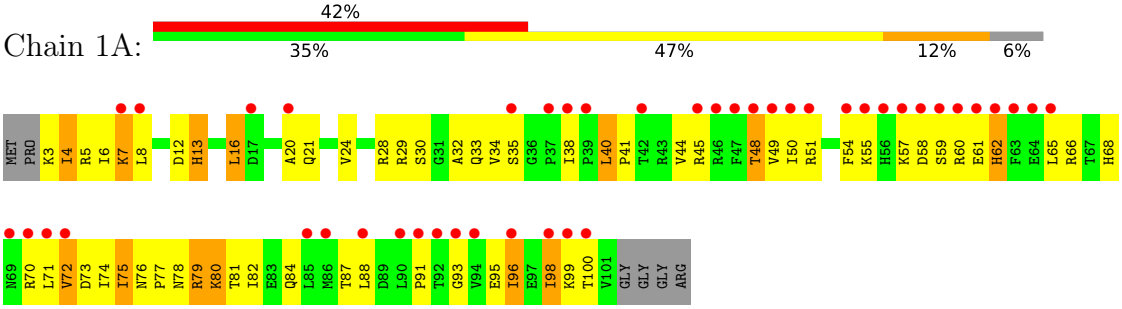
• Molecule 10: 30S ribosomal protein S10

Chain 1I:



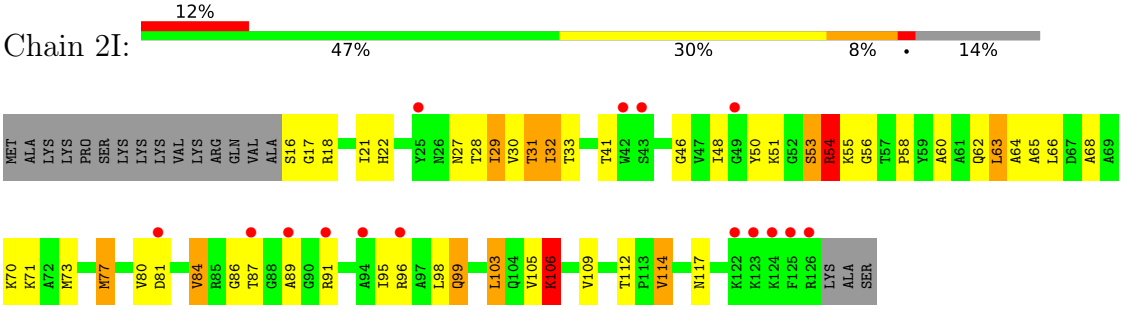
• Molecule 10: 30S ribosomal protein S10

Chain 1A:



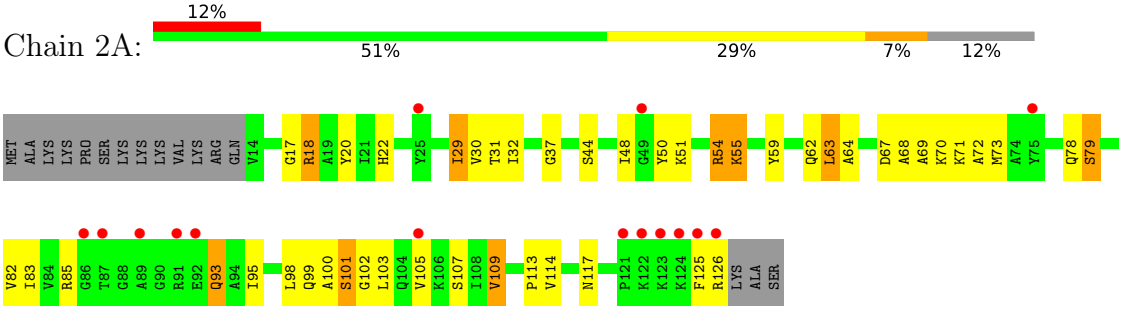
• Molecule 11: 30S ribosomal protein S11

Chain 2I:



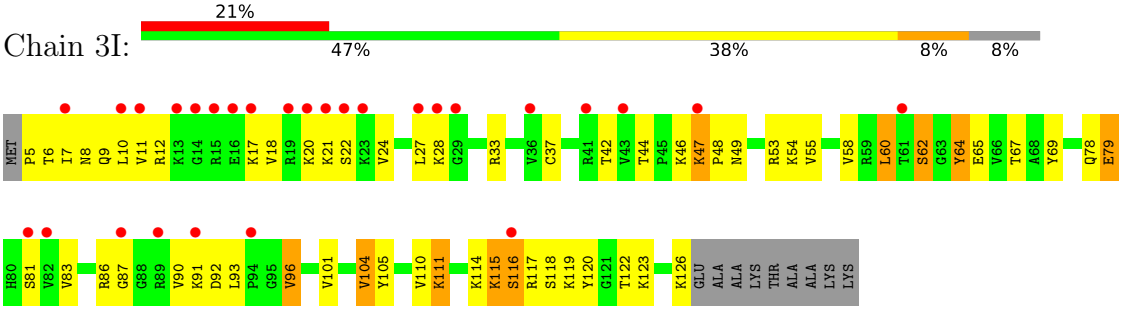
• Molecule 11: 30S ribosomal protein S11

Chain 2A:



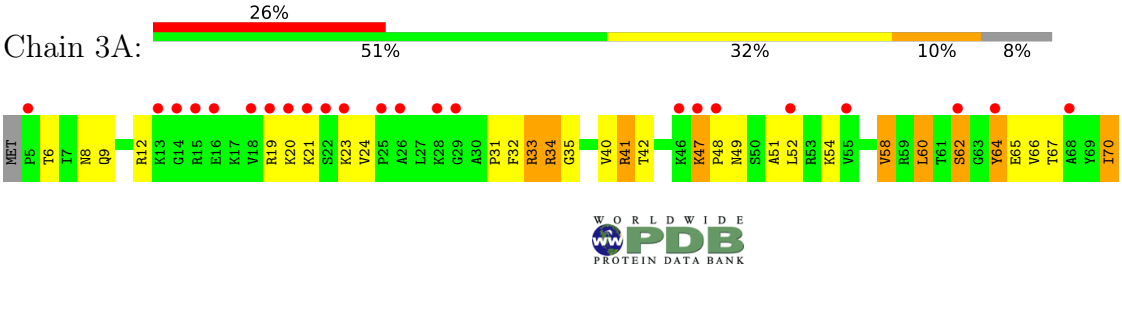
• Molecule 12: 30S ribosomal protein S12

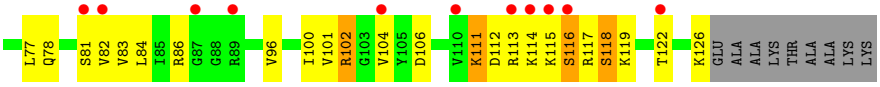
Chain 3I:



• Molecule 12: 30S ribosomal protein S12

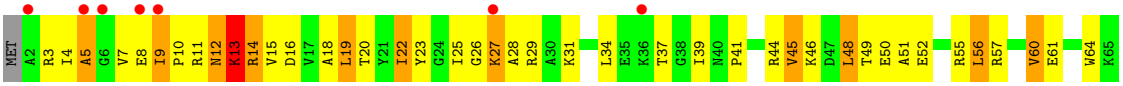
Chain 3A:





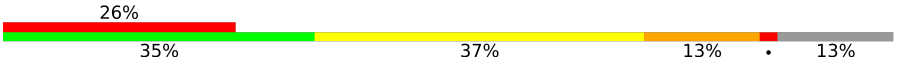
• Molecule 13: 30S ribosomal protein S13

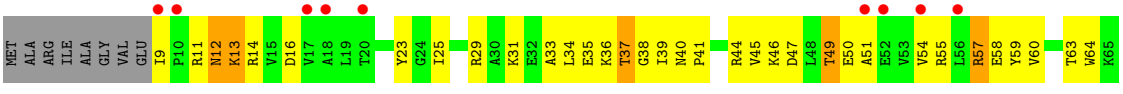
Chain 4I:

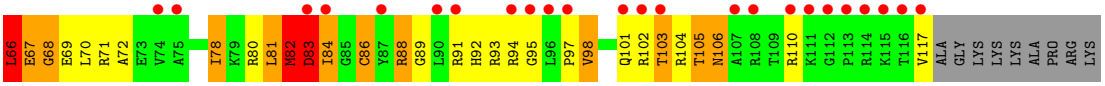


• Molecule 13: 30S ribosomal protein S13

Chain 4A:

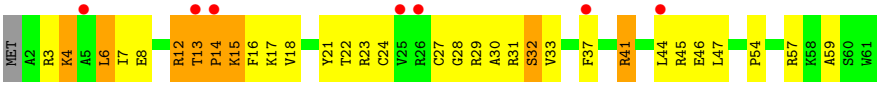






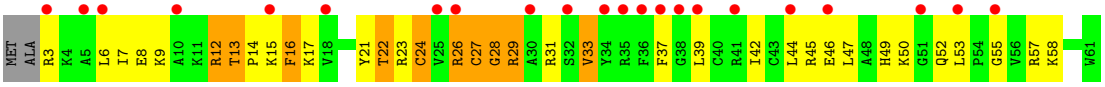
• Molecule 14: 30S ribosomal protein S14 type Z

Chain 5I:



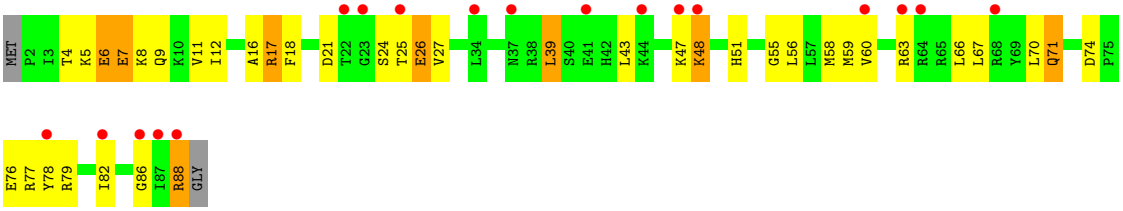
• Molecule 14: 30S ribosomal protein S14 type Z

Chain 5A:



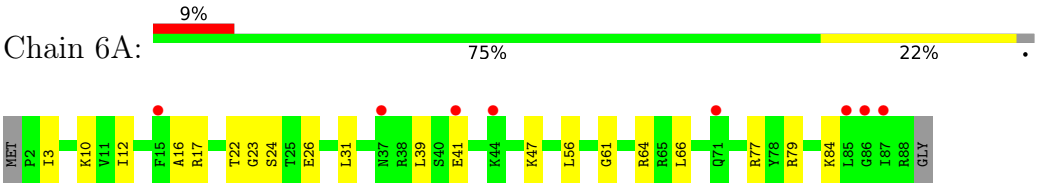
• Molecule 15: 30S ribosomal protein S15

Chain 6I:



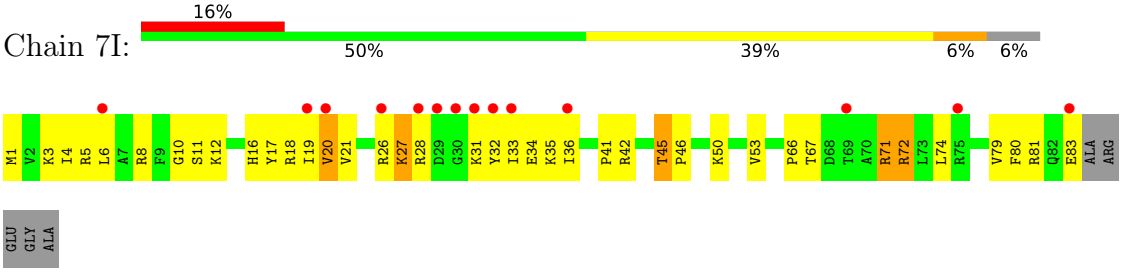
• Molecule 15: 30S ribosomal protein S15

Chain 6A:



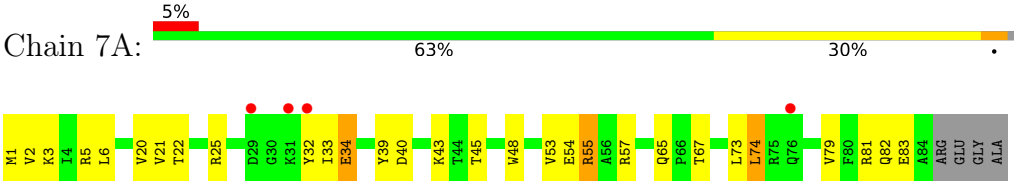
• Molecule 16: 30S ribosomal protein S16

Chain 7I:



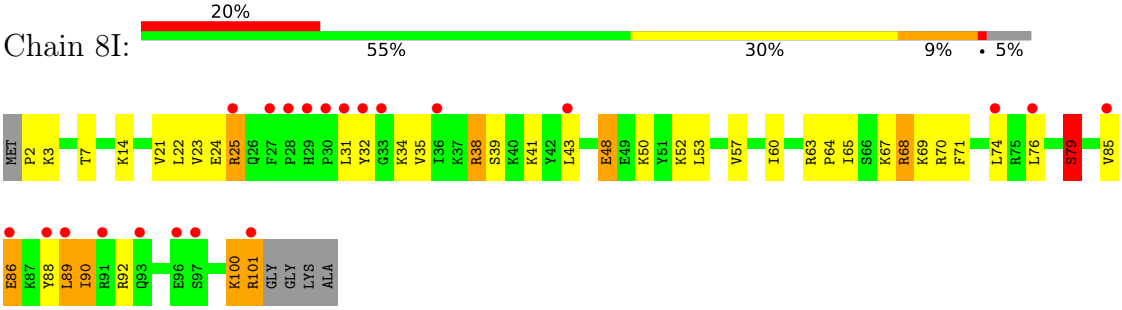
• Molecule 16: 30S ribosomal protein S16

Chain 7A:



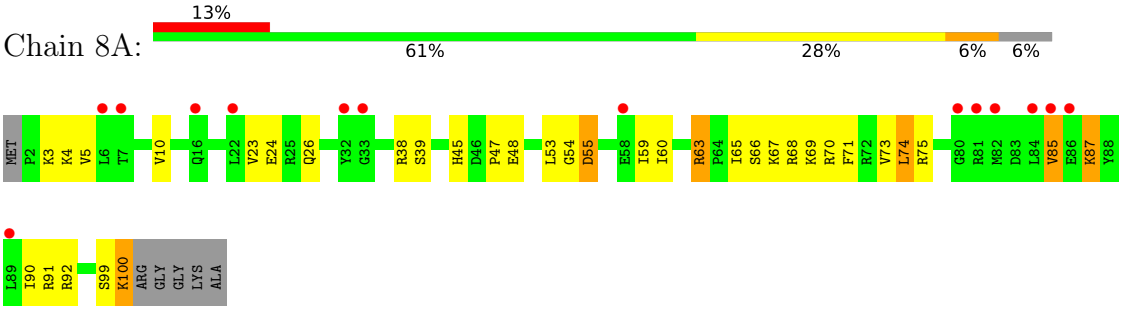
• Molecule 17: 30S ribosomal protein S17

Chain 8I:



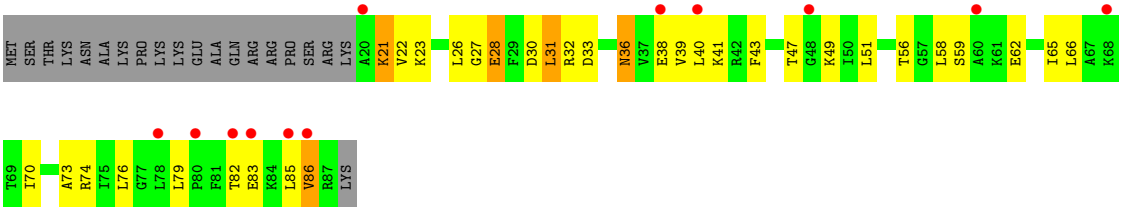
• Molecule 17: 30S ribosomal protein S17

Chain 8A:



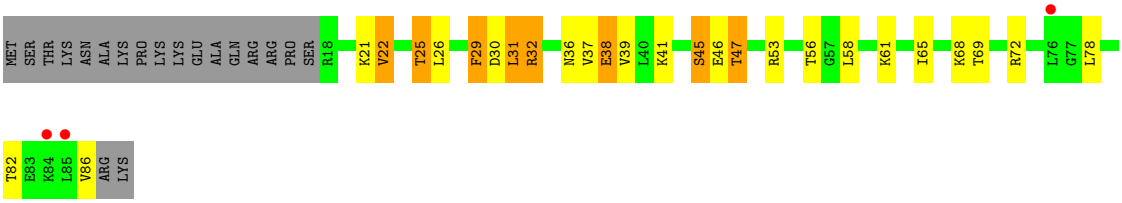
• Molecule 18: 30S ribosomal protein S18

Chain 9I:



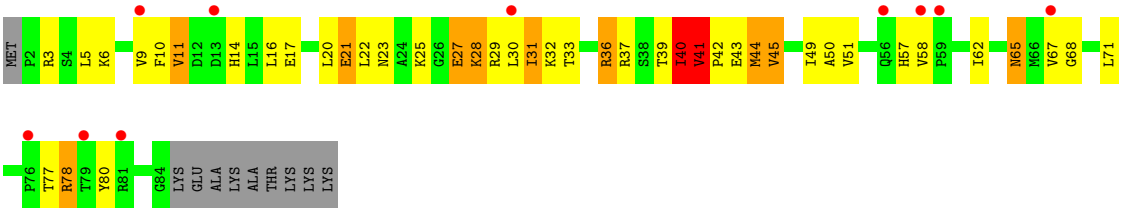
• Molecule 18: 30S ribosomal protein S18

Chain 9A:



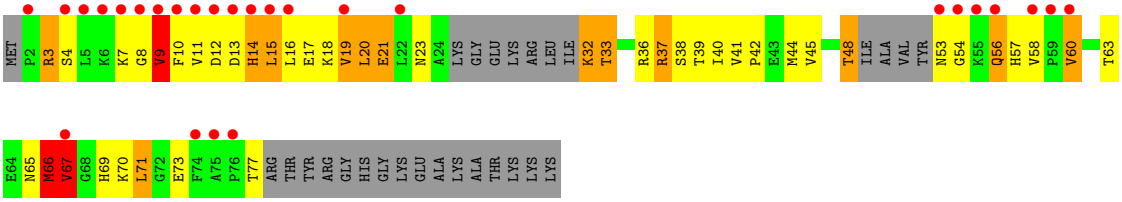
• Molecule 19: 30S ribosomal protein S19

Chain AI:



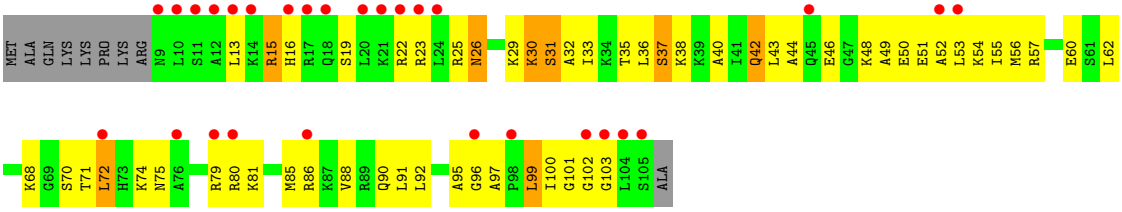
• Molecule 19: 30S ribosomal protein S19

Chain AA:



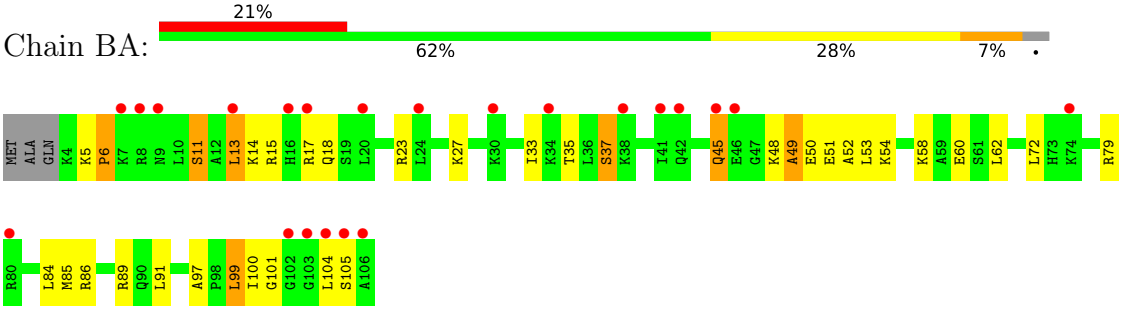
• Molecule 20: 30S ribosomal protein S20

Chain BI:



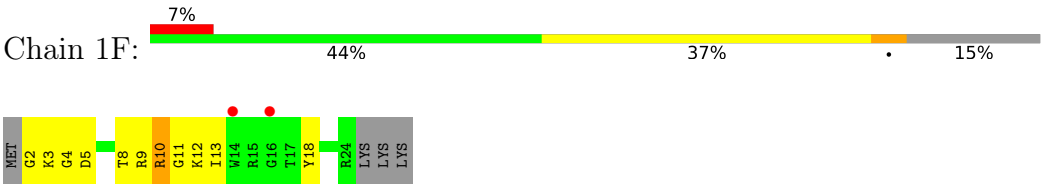
• Molecule 20: 30S ribosomal protein S20

Chain BA:



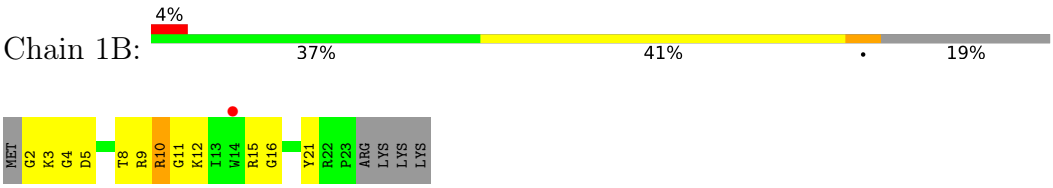
• Molecule 21: 30S ribosomal protein Thx

Chain 1F:



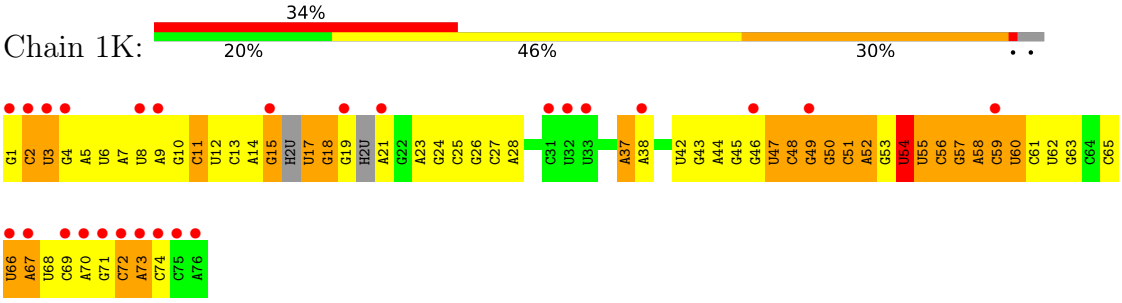
• Molecule 21: 30S ribosomal protein Thx

Chain 1B:



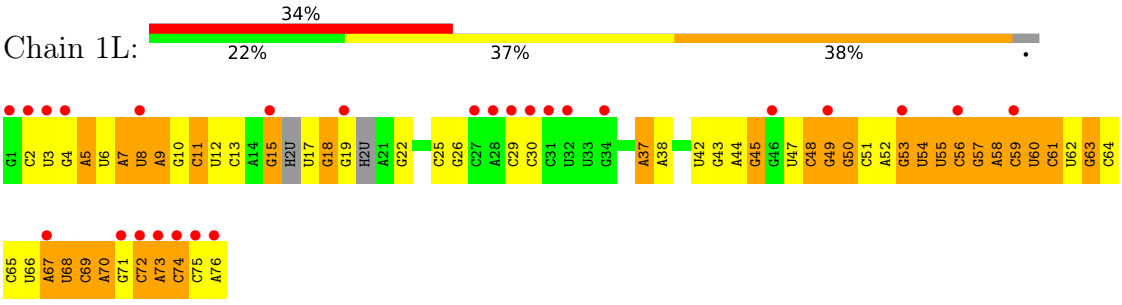
• Molecule 22: tRNAThr

Chain 1K:



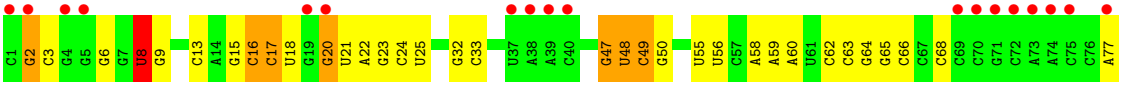
• Molecule 22: tRNAThr

Chain 1L:



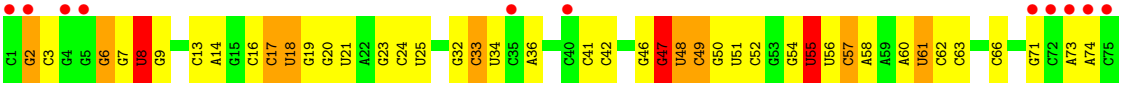
• Molecule 23: tRNAfMet

Chain 2K:



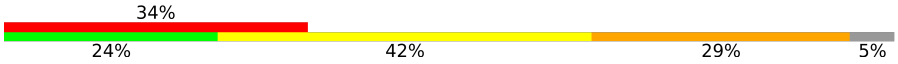
• Molecule 23: tRNAfMet

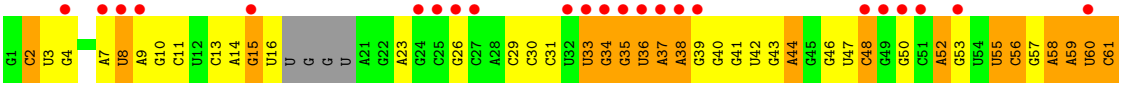
Chain 2L:

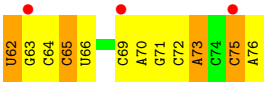


• Molecule 24: tRNAThr

Chain 3K:

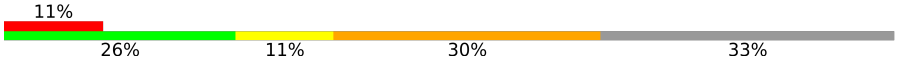


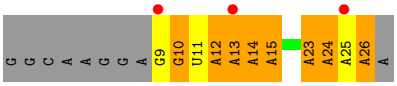




• Molecule 25: RNA (27-MER)

Chain 4K:



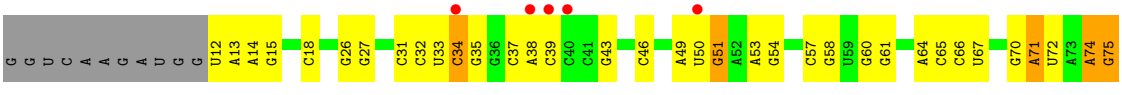


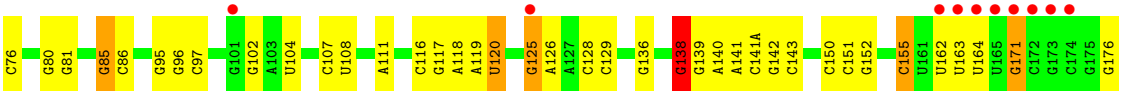
• Molecule 25: RNA (27-MER)

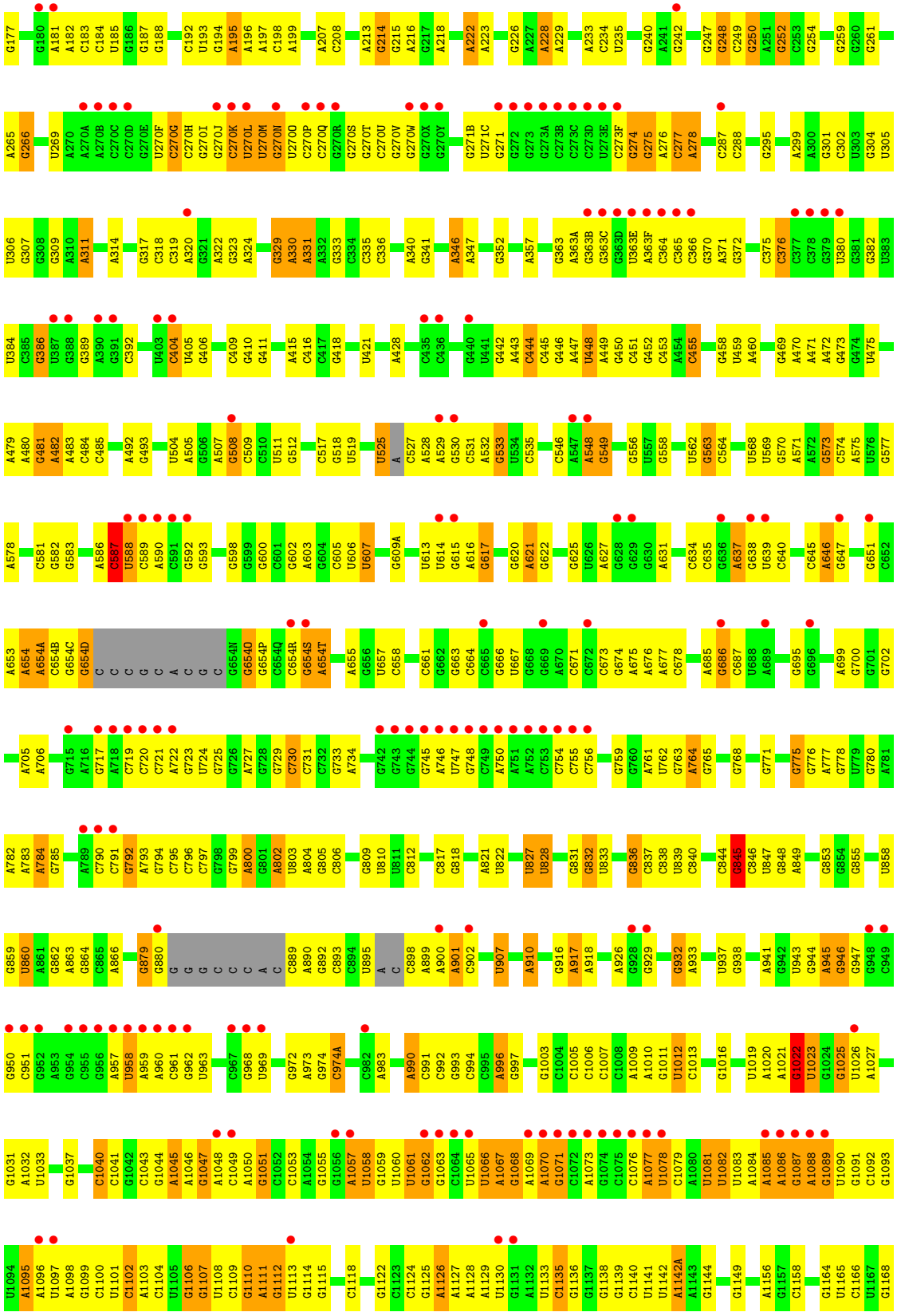
Chain 4L:

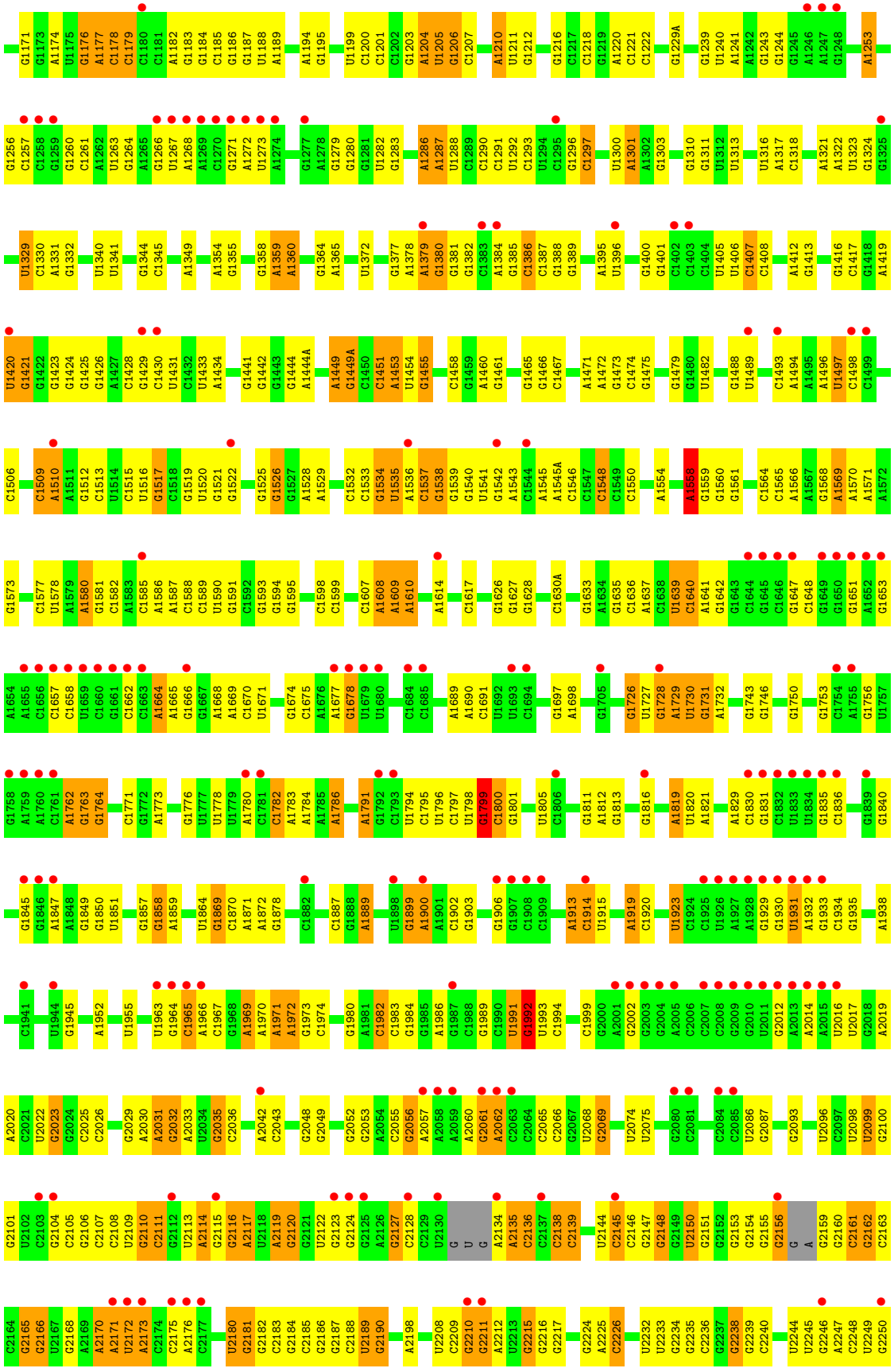
• Molecule 26: 23S ribosomal RNA

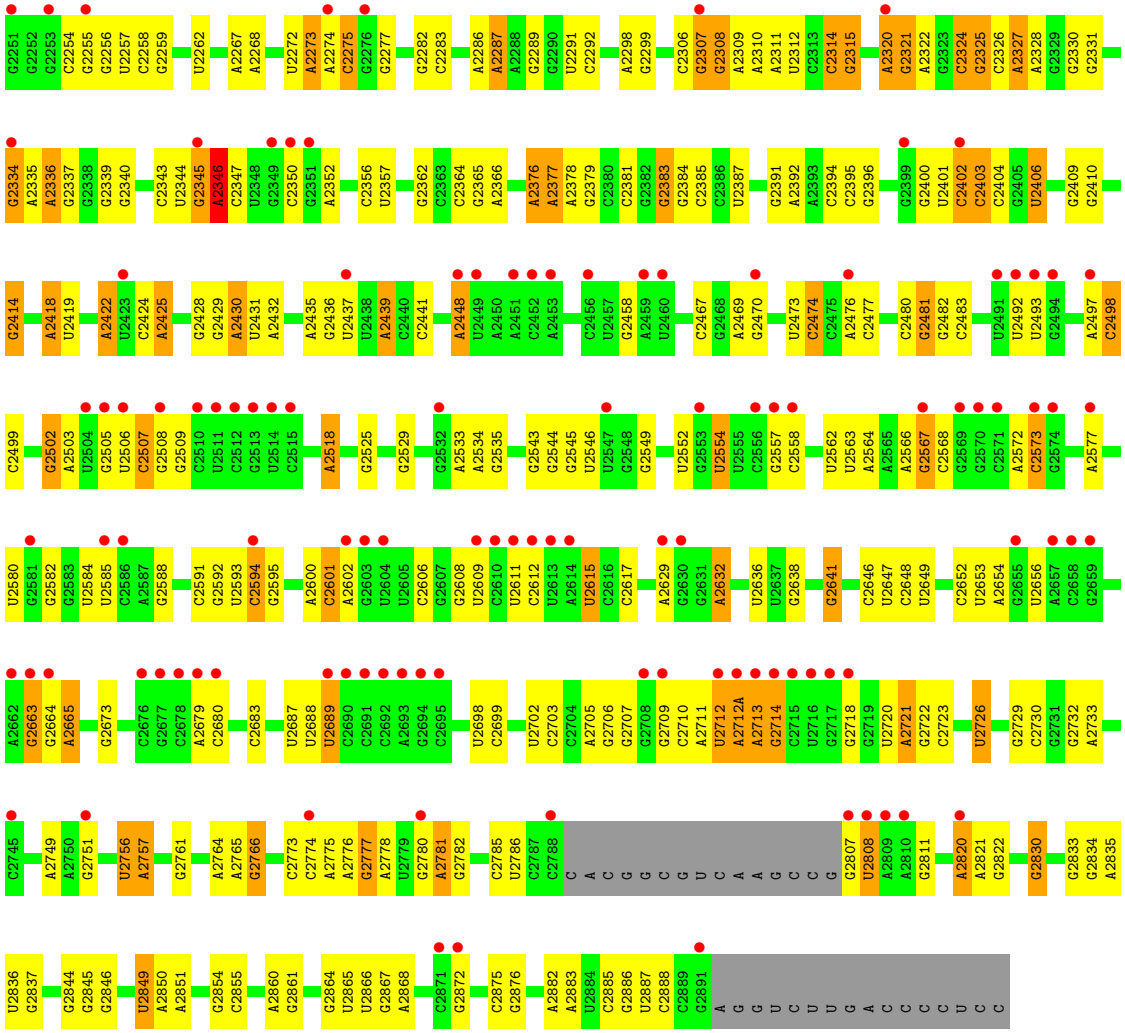
Chain 1H:





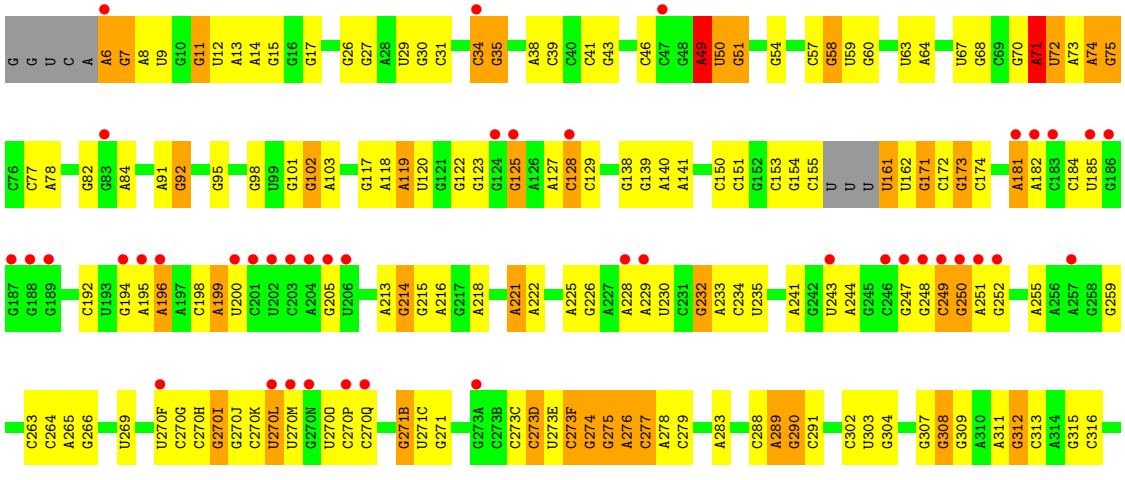


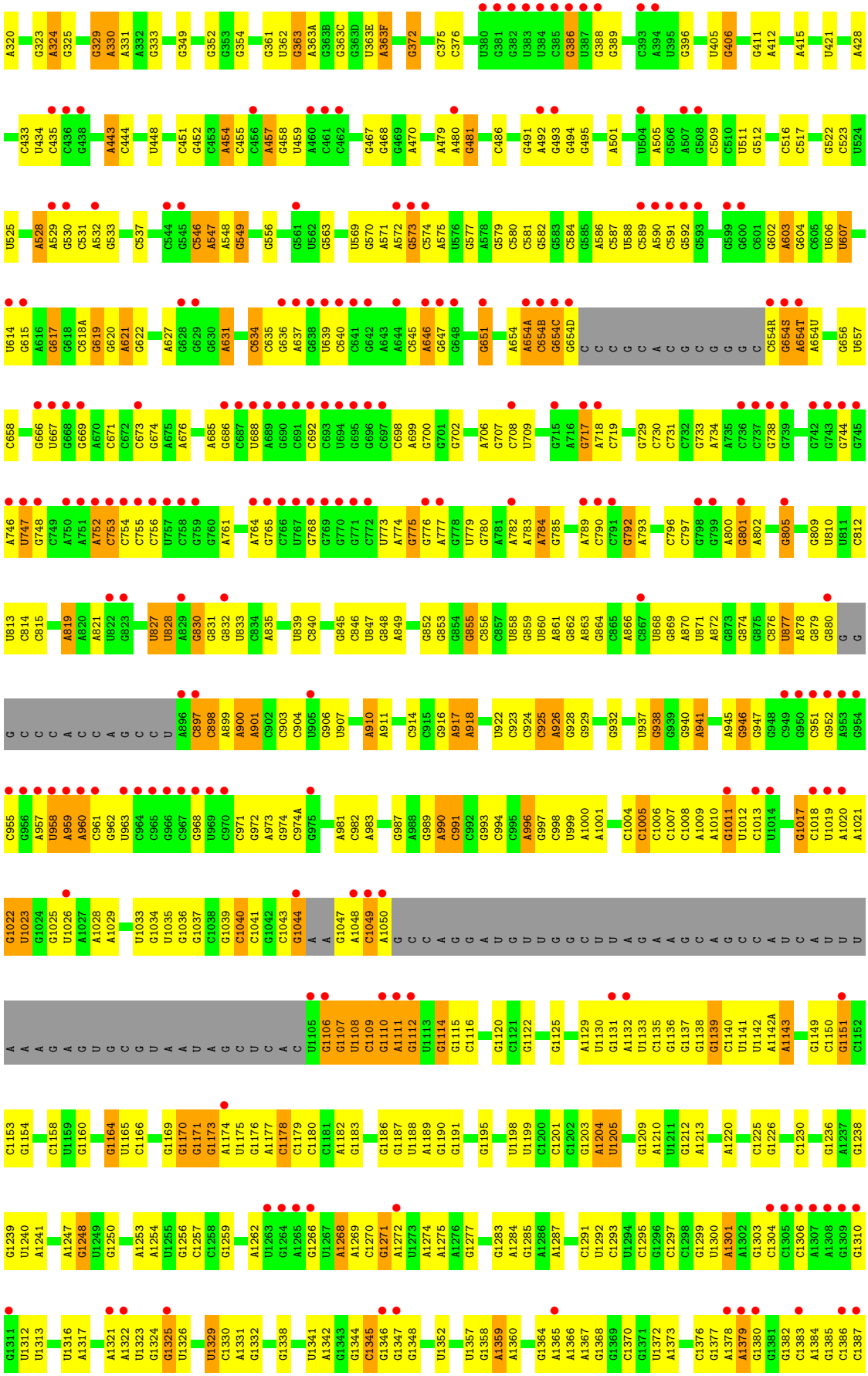


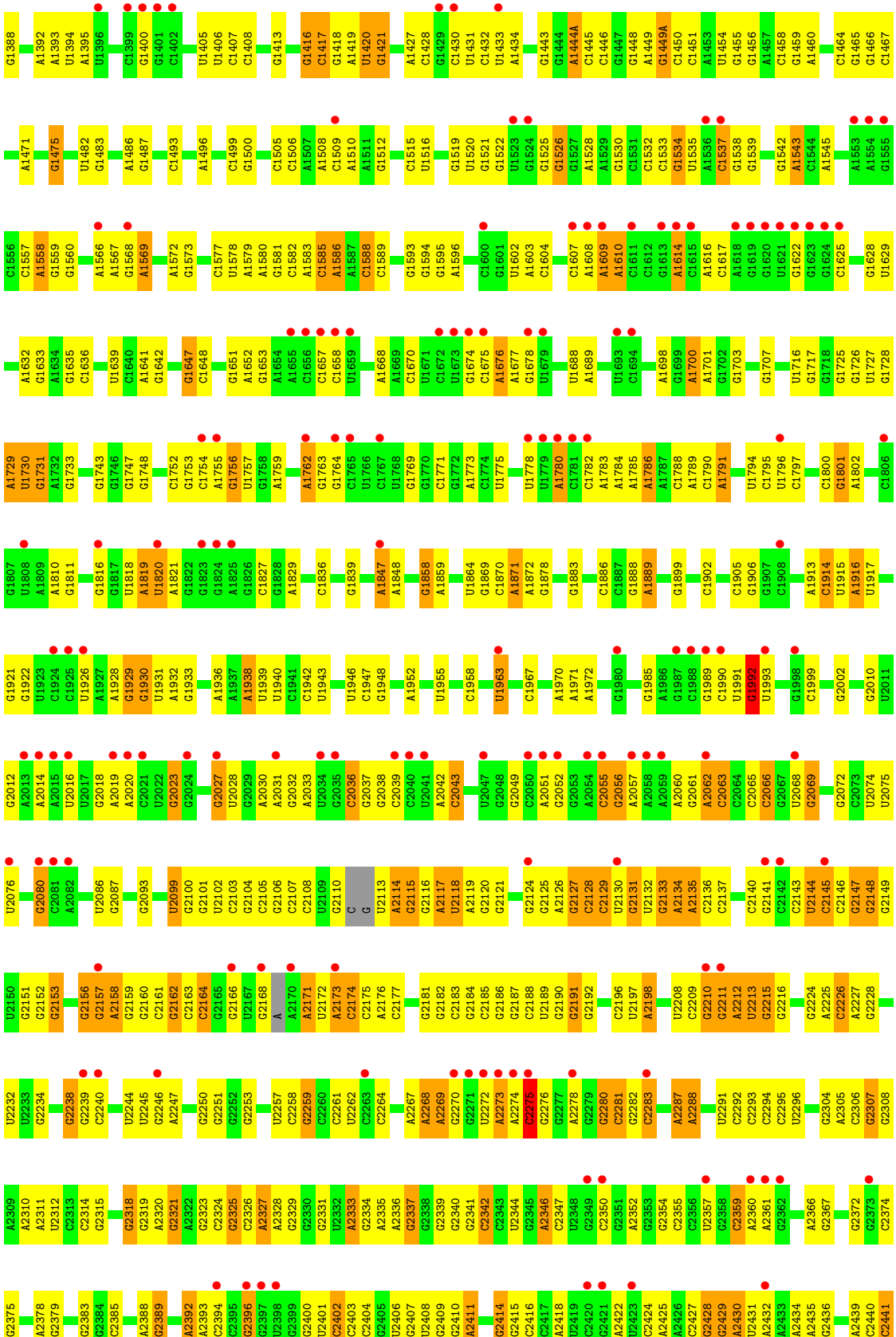


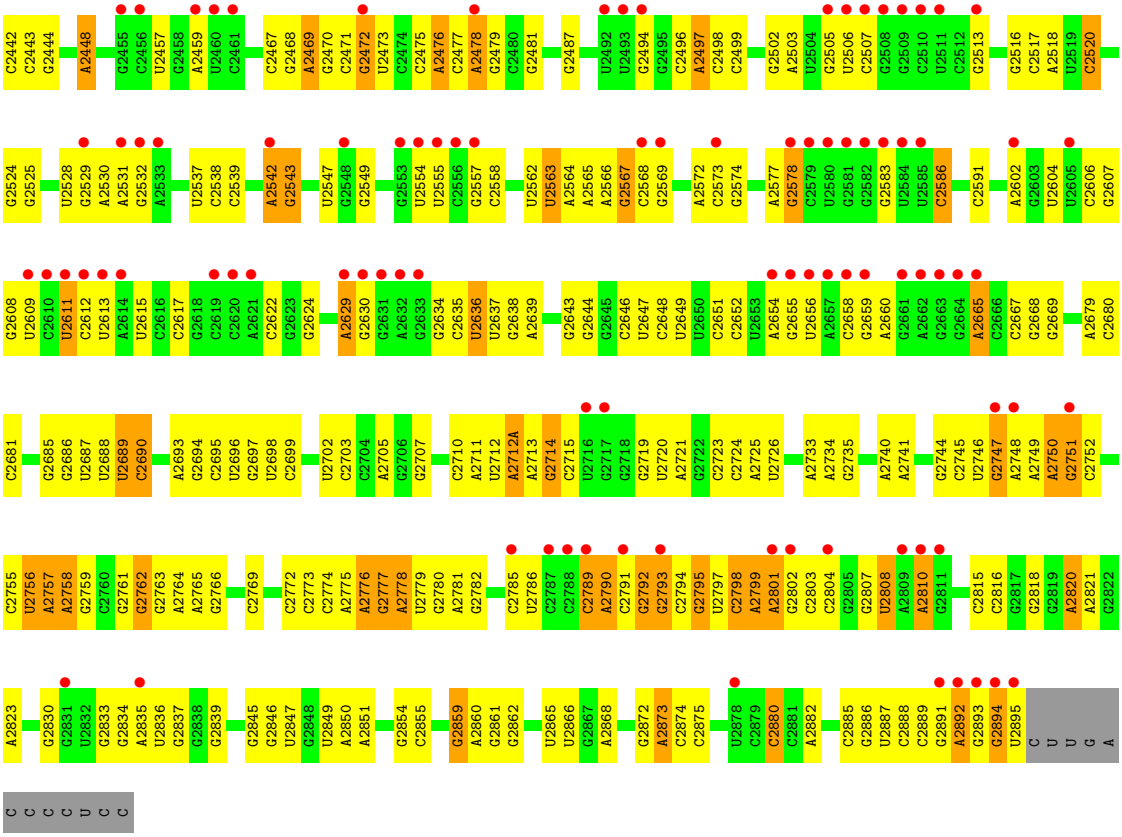
• Molecule 26: 23S ribosomal RNA

Chain 14:



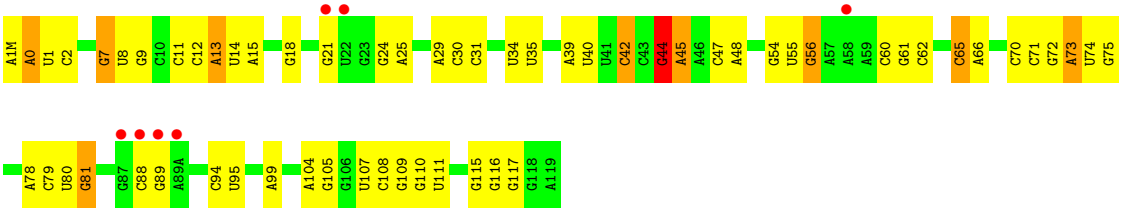






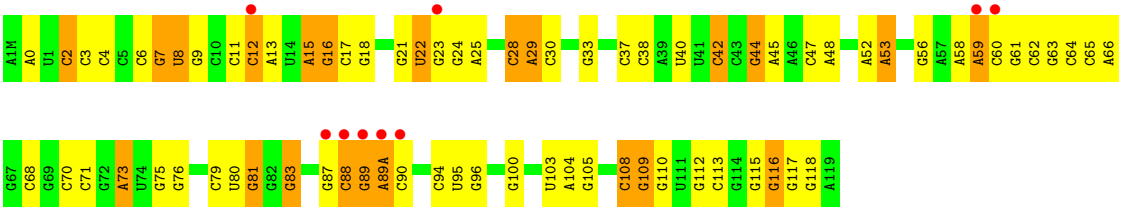
• Molecule 27: 5S ribosomal RNA

Chain 16:



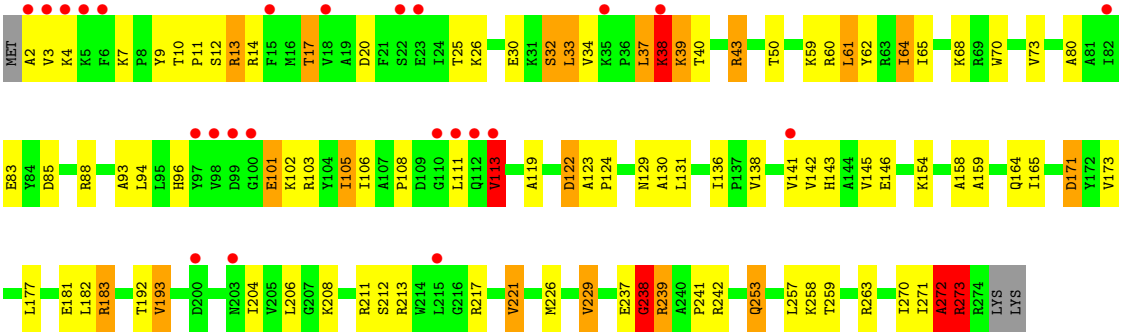
• Molecule 27: 5S ribosomal RNA

Chain 1J:



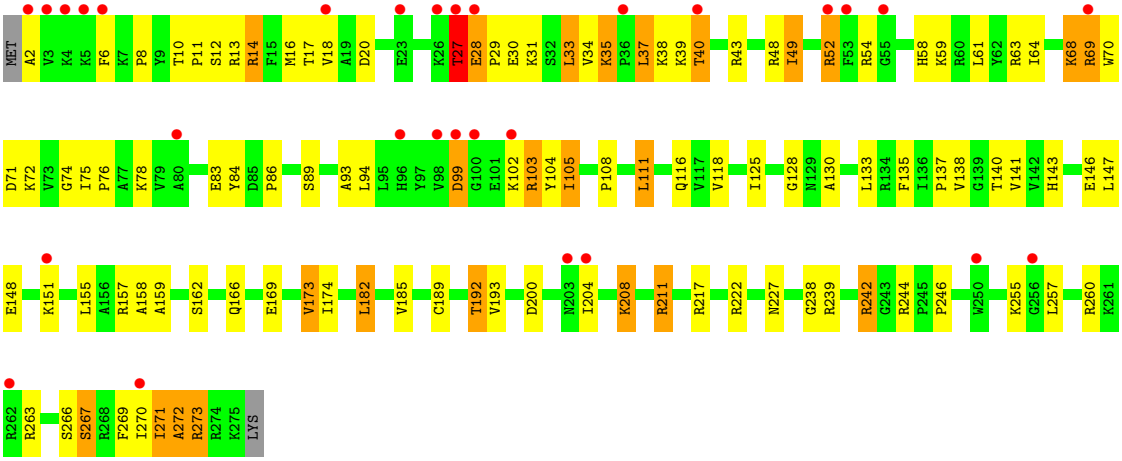
• Molecule 28: 50S ribosomal protein L2

Chain 11:



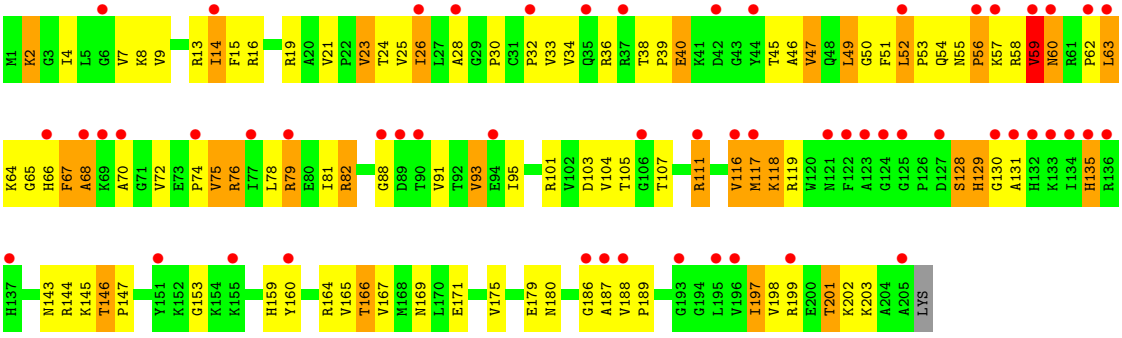
• Molecule 28: 50S ribosomal protein L2

Chain 19:



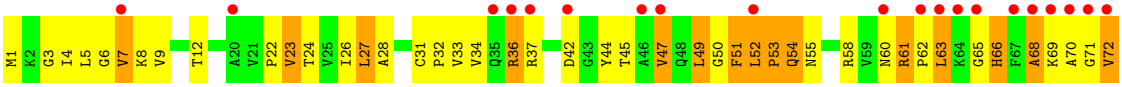
• Molecule 29: 50S ribosomal protein L3

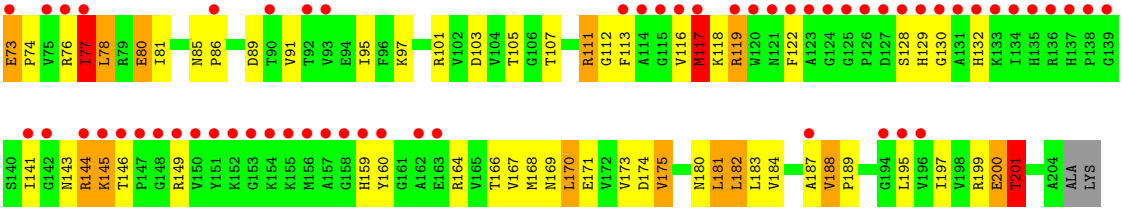
Chain 21:



• Molecule 29: 50S ribosomal protein L3

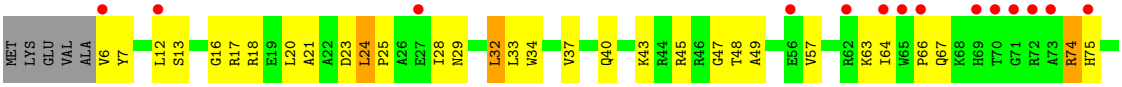
Chain 29:

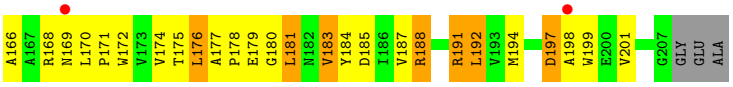




• Molecule 30: 50S ribosomal protein L4

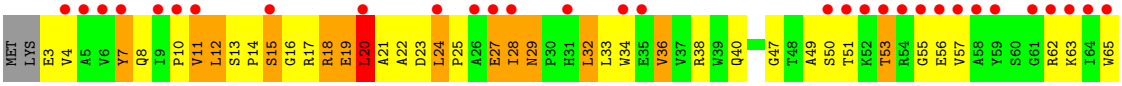
Chain 31:

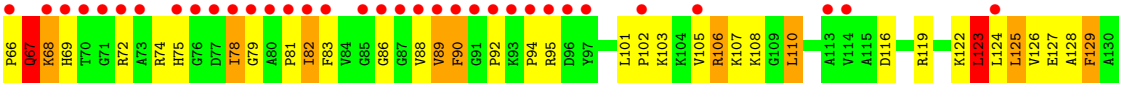


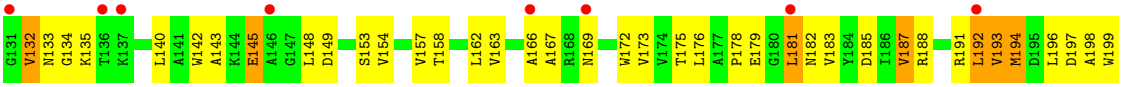


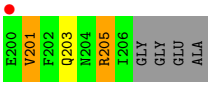
• Molecule 30: 50S ribosomal protein L4

Chain 39:



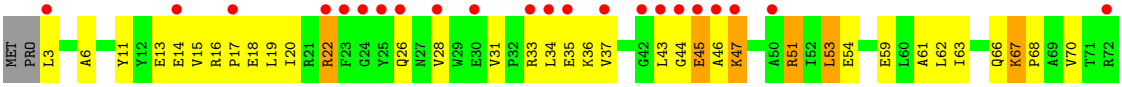


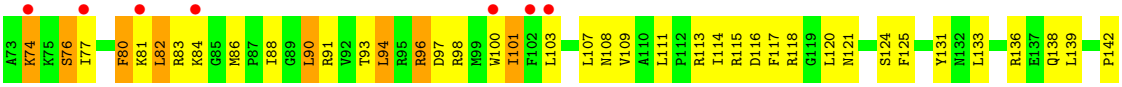


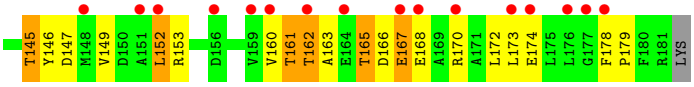


• Molecule 31: 50S ribosomal protein L5

Chain 41:

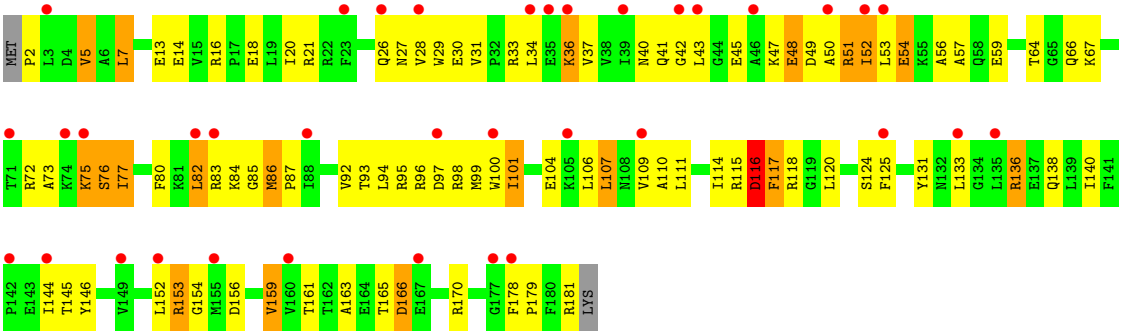






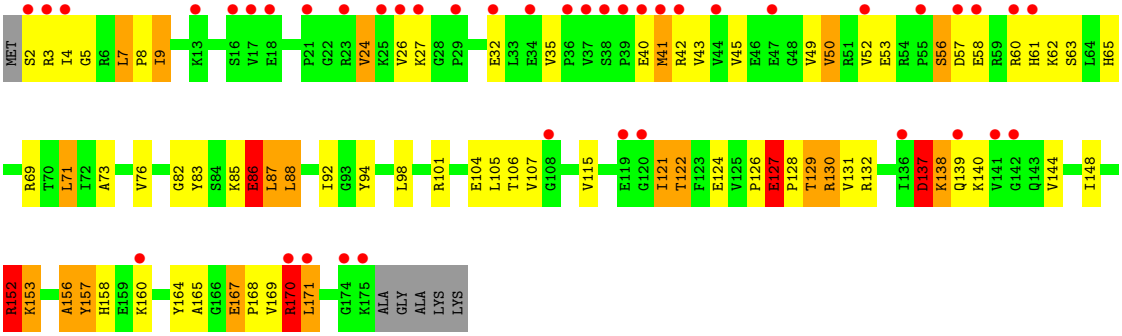
• Molecule 31: 50S ribosomal protein L5

Chain 49:



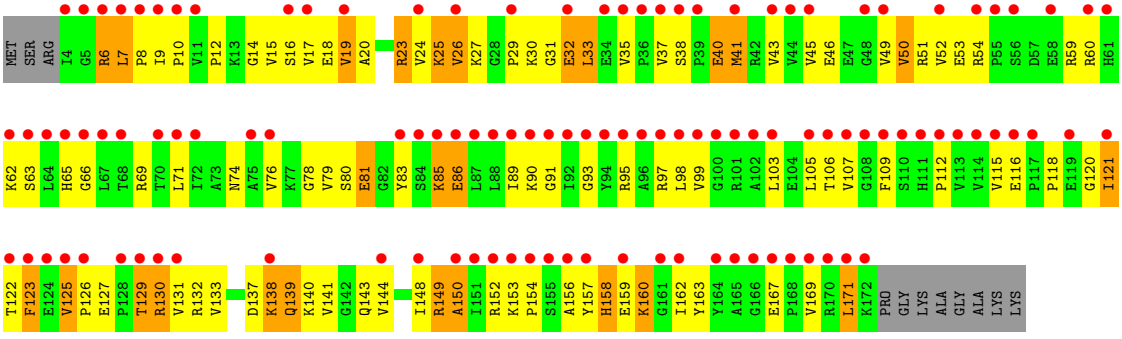
• Molecule 32: 50S ribosomal protein L6

Chain 51:



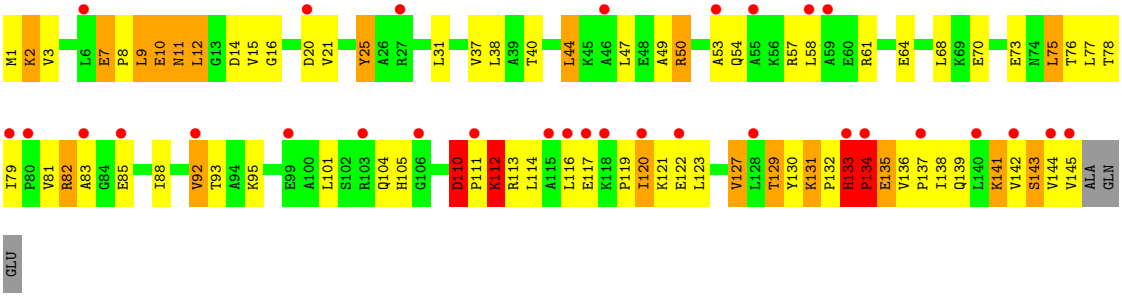
• Molecule 32: 50S ribosomal protein L6

Chain 59:



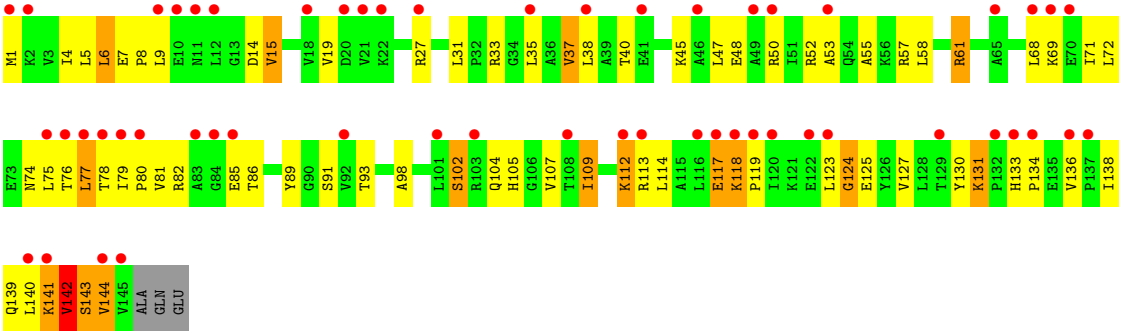
• Molecule 33: 50S ribosomal protein L9

Chain 61:



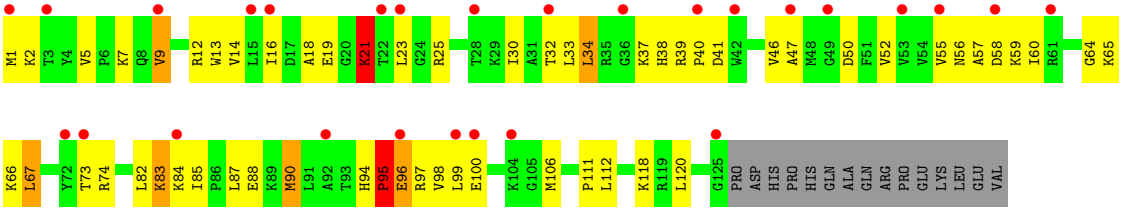
• Molecule 33: 50S ribosomal protein L9

Chain 69:



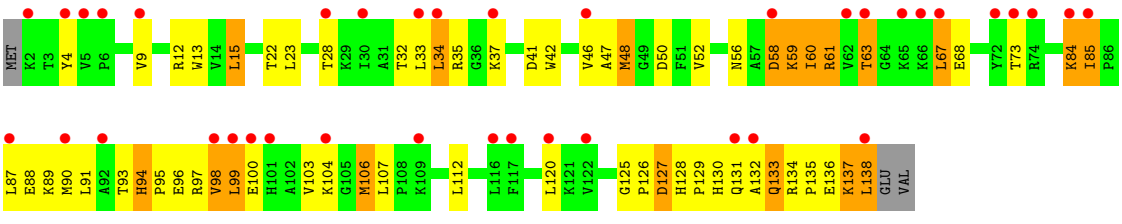
• Molecule 34: 50S ribosomal protein L13

Chain 58:



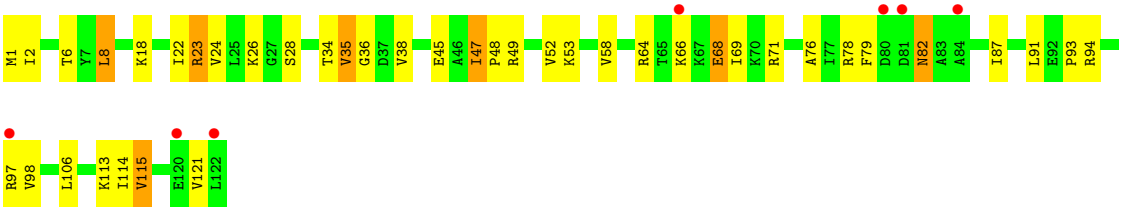
• Molecule 34: 50S ribosomal protein L13

Chain 15:



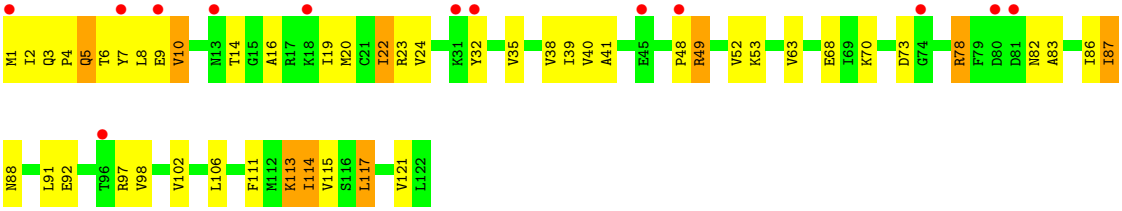
• Molecule 35: 50S ribosomal protein L14

Chain 68:



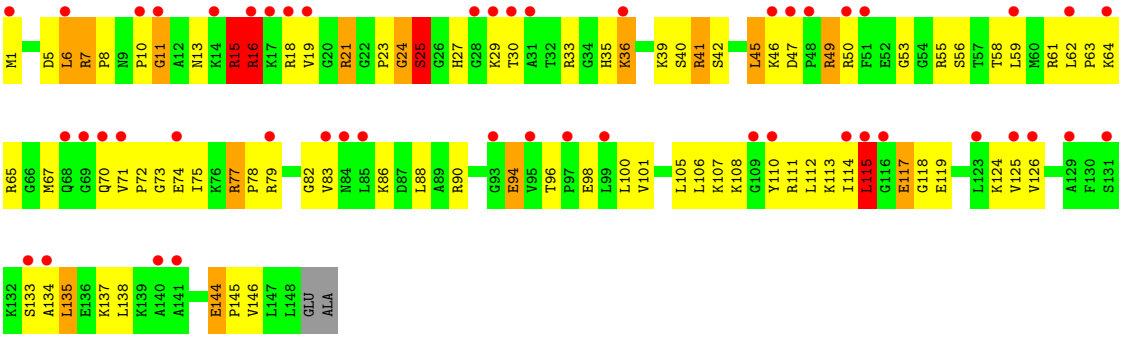
• Molecule 35: 50S ribosomal protein L14

Chain 25:



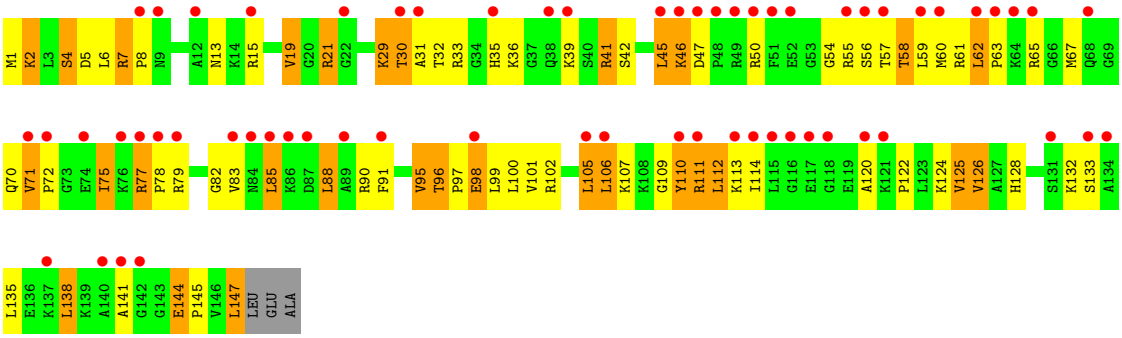
• Molecule 36: 50S ribosomal protein L15

Chain 78:



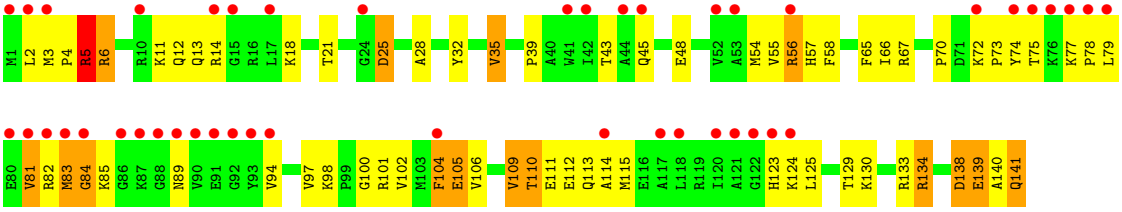
• Molecule 36: 50S ribosomal protein L15

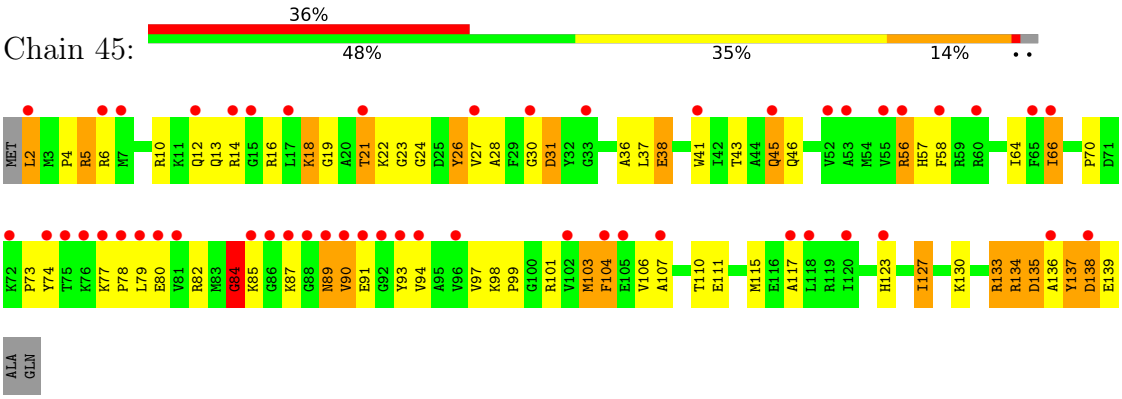
Chain 35:



• Molecule 37: 50S ribosomal protein L16

Chain 88:



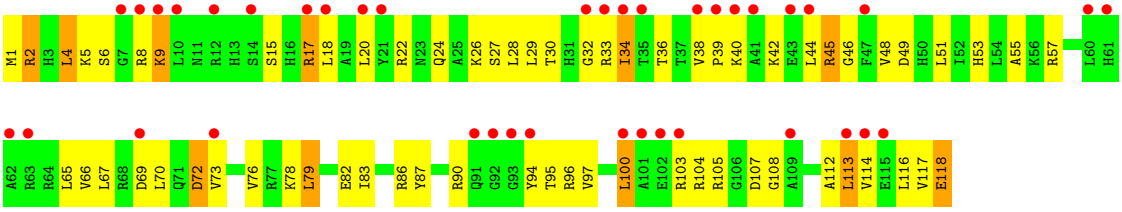


• Molecule 37: 50S ribosomal protein L16

Chain 45:

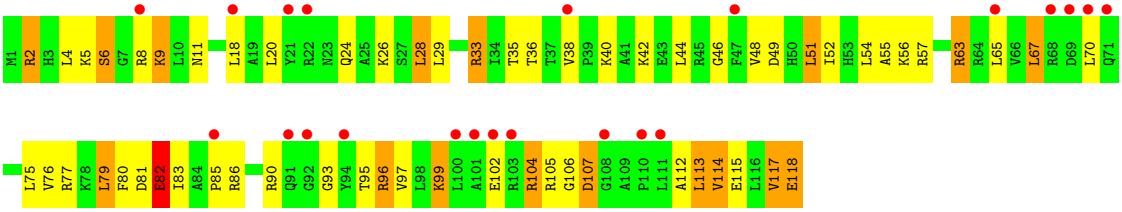
• Molecule 38: 50S ribosomal protein L17

Chain 98:



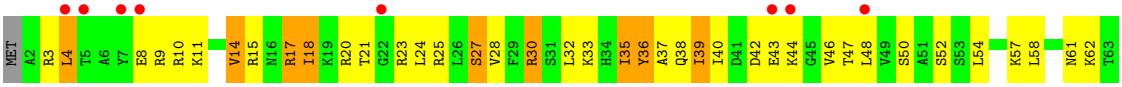
• Molecule 38: 50S ribosomal protein L17

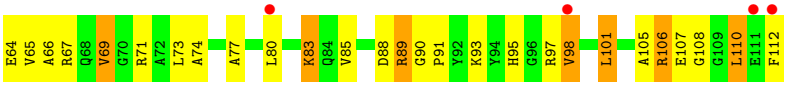
Chain 55:



• Molecule 39: 50S ribosomal protein L18

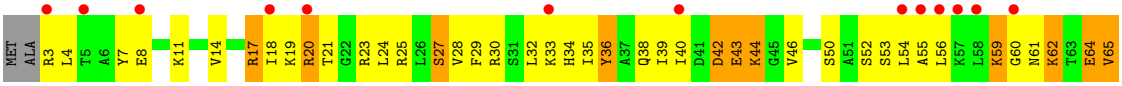
Chain A8:

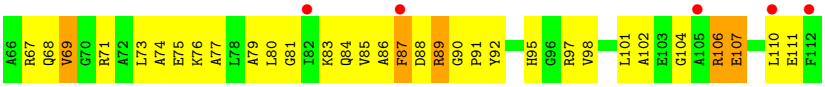




• Molecule 39: 50S ribosomal protein L18

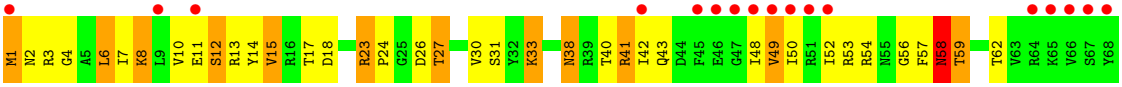
Chain 65:

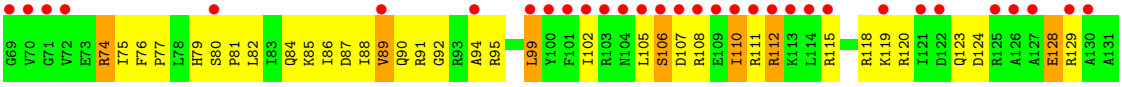


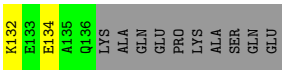


• Molecule 40: 50S ribosomal protein L19

Chain B8:

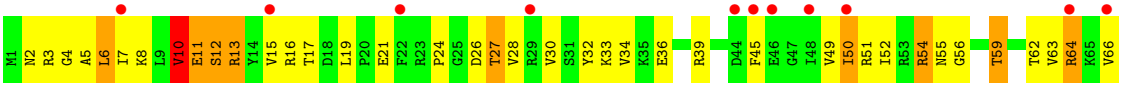


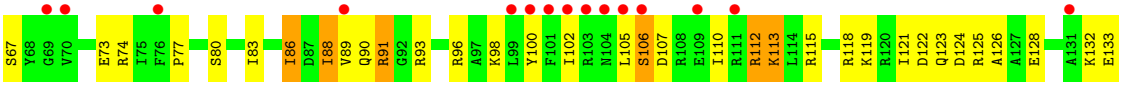


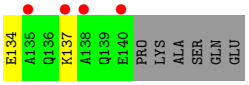


• Molecule 40: 50S ribosomal protein L19

Chain 75:

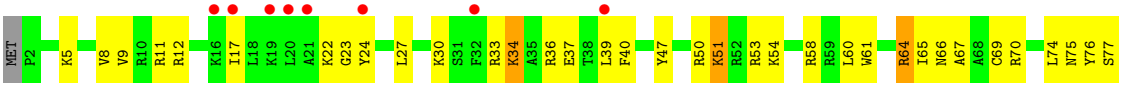


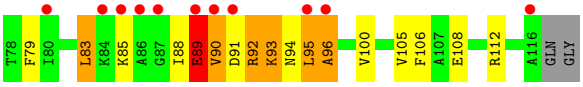




• Molecule 41: 50S ribosomal protein L20

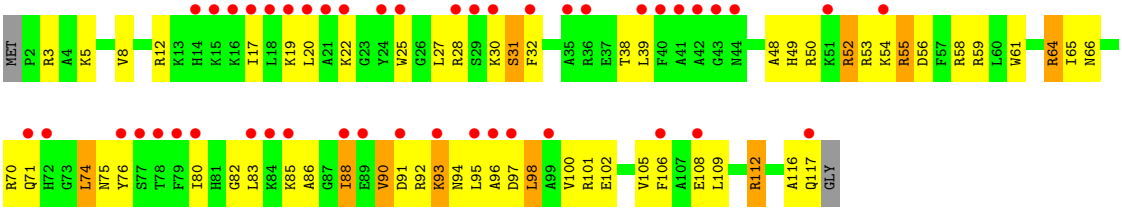
Chain C8:





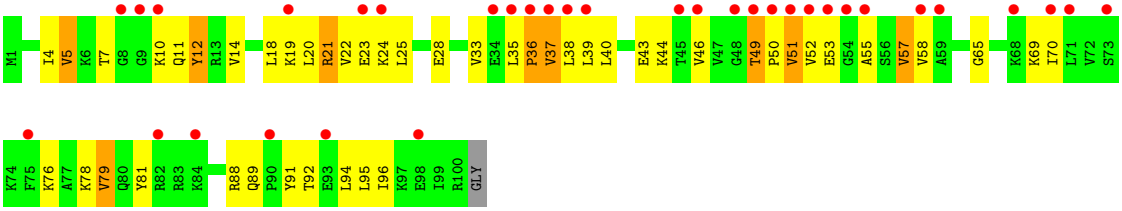
• Molecule 41: 50S ribosomal protein L20

Chain 85:



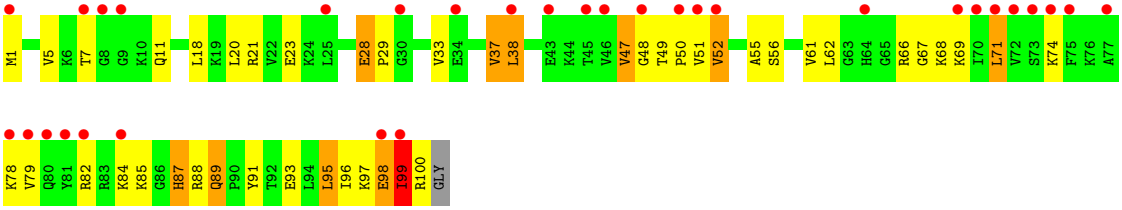
• Molecule 42: 50S ribosomal protein L21

Chain D8:



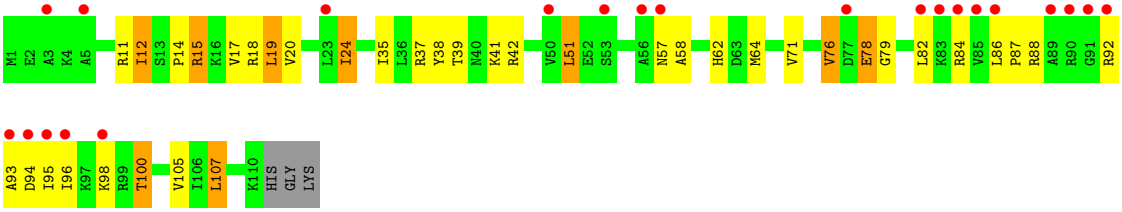
• Molecule 42: 50S ribosomal protein L21

Chain 95:



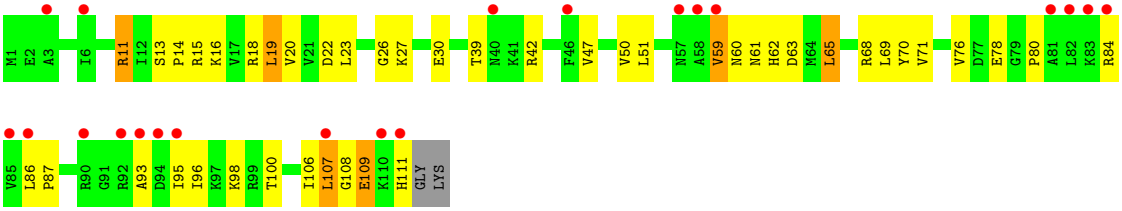
• Molecule 43: 50S ribosomal protein L22

Chain E8:



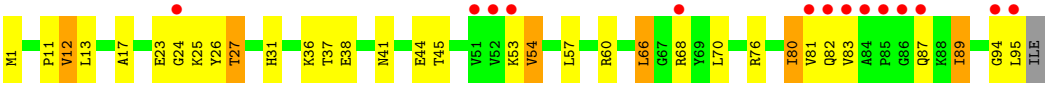
• Molecule 43: 50S ribosomal protein L22

Chain A5:



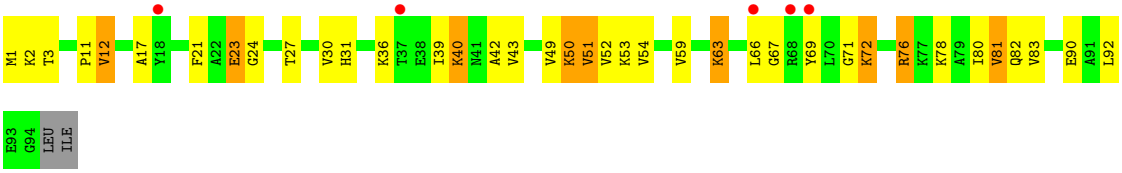
• Molecule 44: 50S ribosomal protein L23

Chain F8:



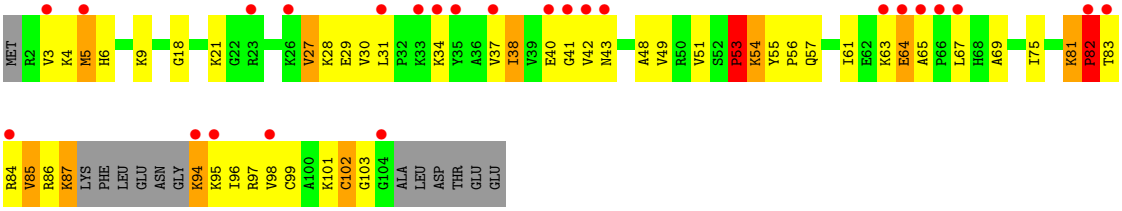
• Molecule 44: 50S ribosomal protein L23

Chain B5:



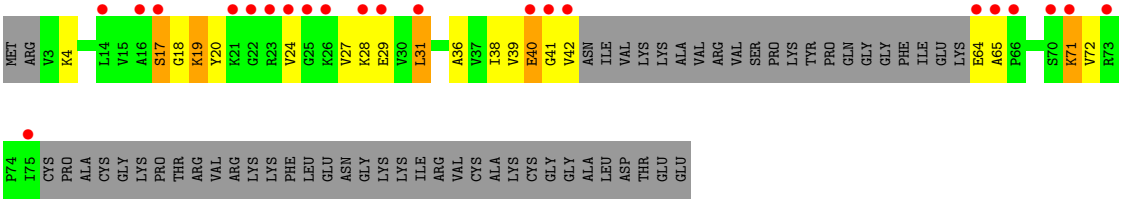
• Molecule 45: 50S ribosomal protein L24

Chain G8:



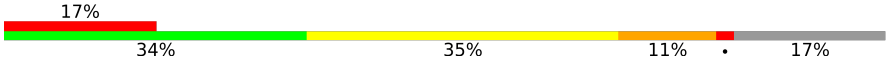
• Molecule 45: 50S ribosomal protein L24

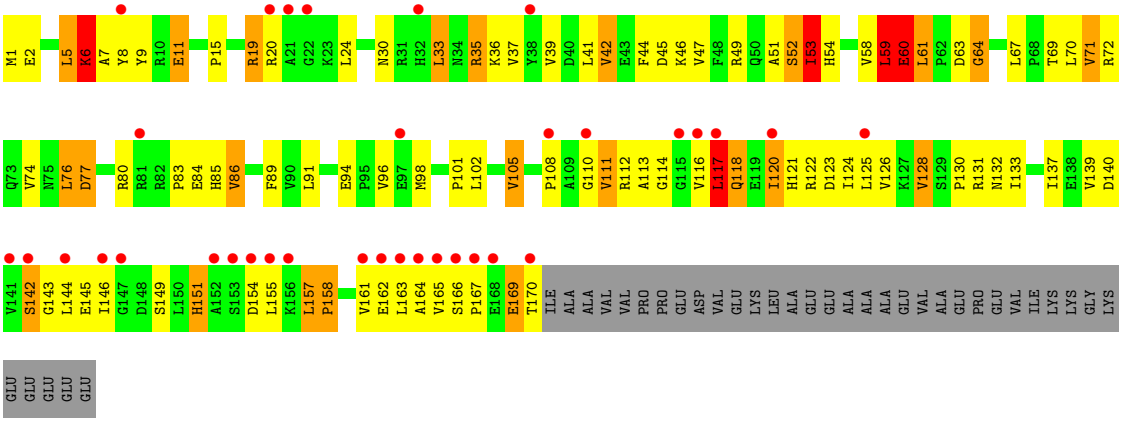
Chain C5:



• Molecule 46: 50S ribosomal protein L25

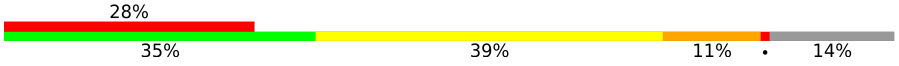
Chain H8:

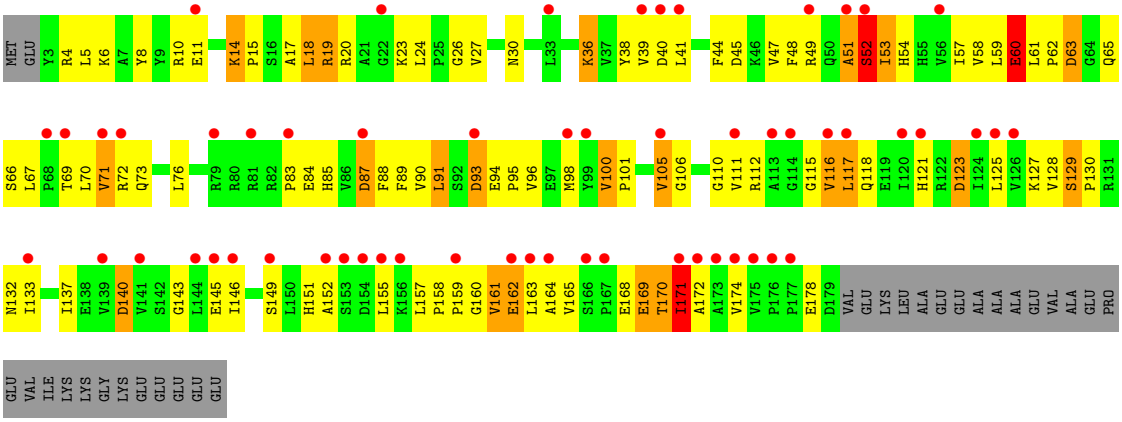




• Molecule 46: 50S ribosomal protein L25

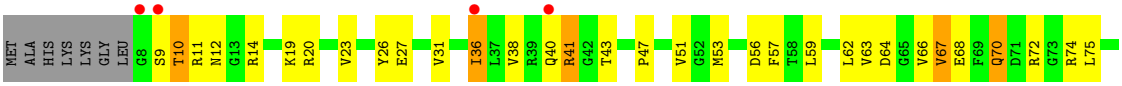
Chain D5:

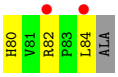




• Molecule 47: 50S ribosomal protein L27

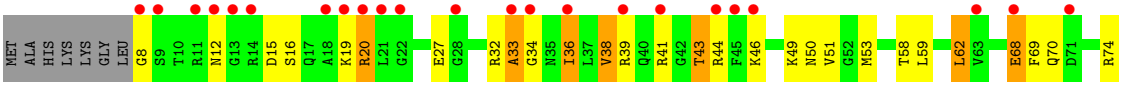
Chain I8:

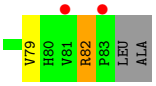




• Molecule 47: 50S ribosomal protein L27

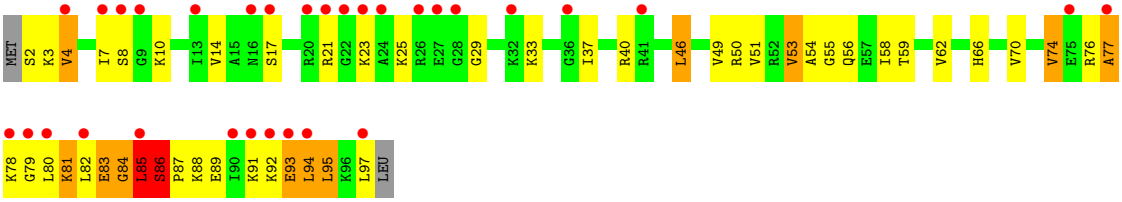
Chain E5:





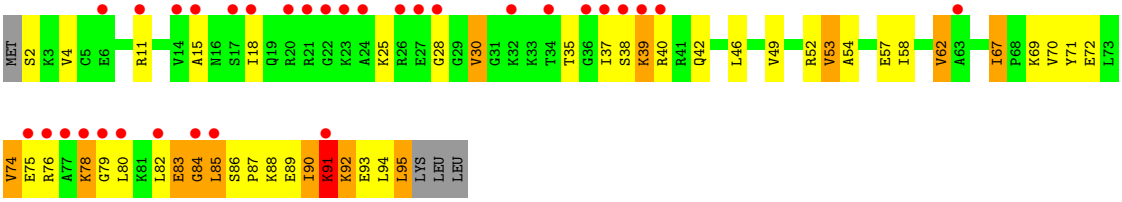
• Molecule 48: 50S ribosomal protein L28

Chain J8:



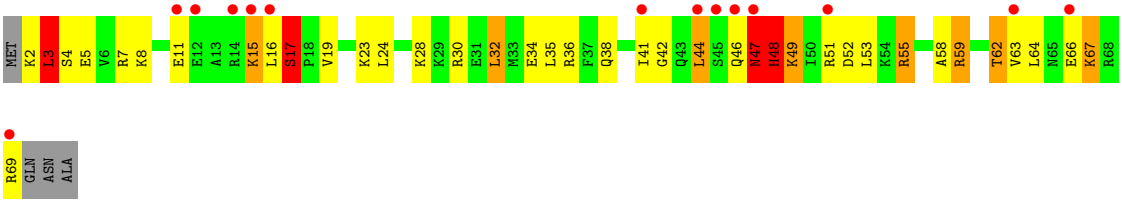
• Molecule 48: 50S ribosomal protein L28

Chain F5:



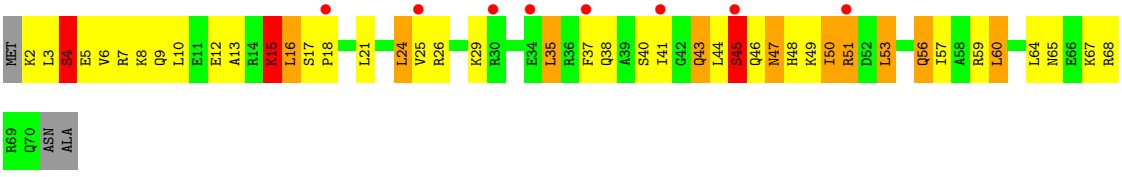
• Molecule 49: 50S ribosomal protein L29

Chain K8:



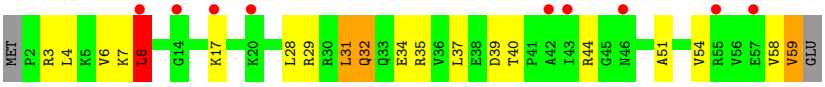
• Molecule 49: 50S ribosomal protein L29

Chain G5:



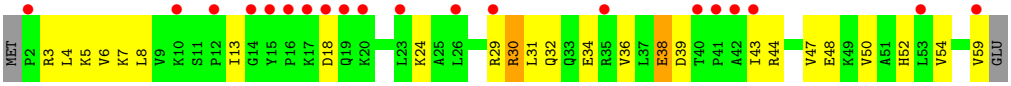
• Molecule 50: 50S ribosomal protein L30

Chain L8:



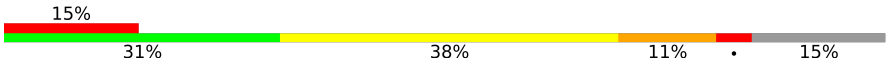
• Molecule 50: 50S ribosomal protein L30

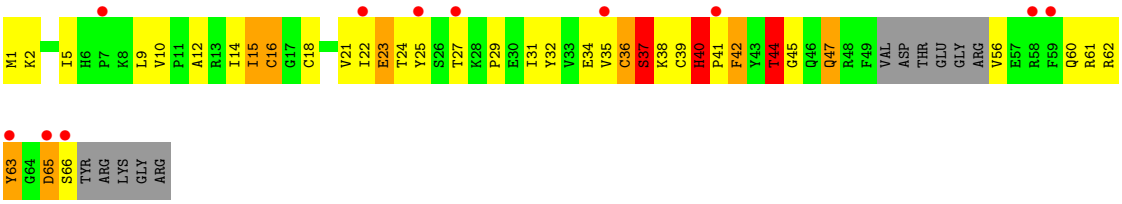
Chain H5:



• Molecule 51: 50S ribosomal protein L31

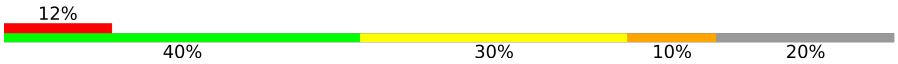
Chain M8:

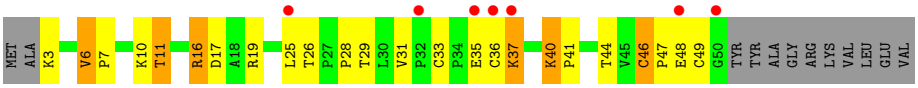




• Molecule 52: 50S ribosomal protein L32

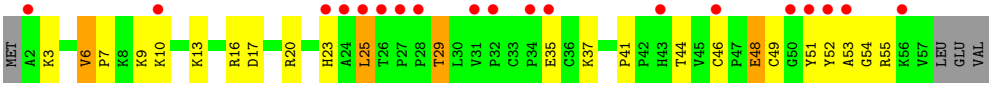
Chain N8:





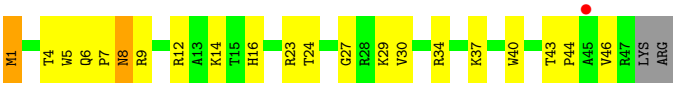
• Molecule 52: 50S ribosomal protein L32

Chain J5:



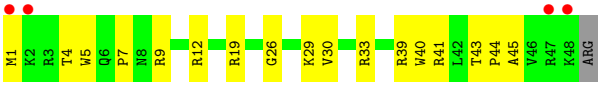
• Molecule 53: 50S ribosomal protein L34

Chain P8:

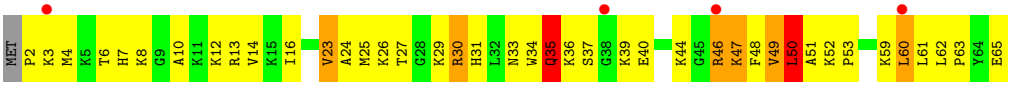


• Molecule 53: 50S ribosomal protein L34

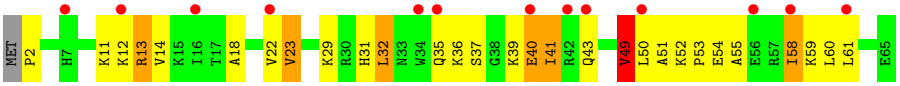
Chain L5:



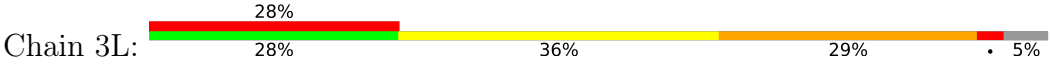
• Molecule 54: 50S ribosomal protein L35

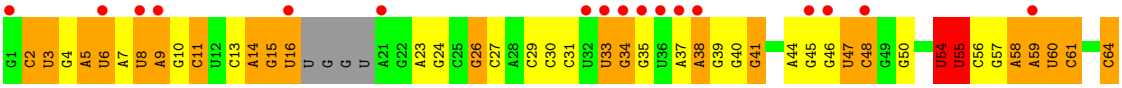


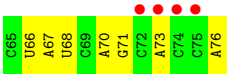
• Molecule 54: 50S ribosomal protein L35



• Molecule 55: tRNAThr







4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	209.41Å 449.24Å 618.40Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	224.62 – 2.96 224.62 – 2.96	Depositor EDS
% Data completeness (in resolution range)	100.0 (224.62-2.96) 94.4 (224.62-2.96)	Depositor EDS
R_{merge}	0.29	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	0.76 (at 2.96Å)	Xtriage
Refinement program	PHENIX 1.12_2829	Depositor
R, R_{free}	0.196 , 0.252 0.198 , 0.248	Depositor DCC
R_{free} test set	2000 reflections (0.17%)	wwPDB-VP
Wilson B-factor (Å^2)	82.0	Xtriage
Anisotropy	0.292	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 142.3	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.90	EDS
Total number of atoms	294252	wwPDB-VP
Average B, all atoms (Å^2)	97.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.41% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: MG, 4SU, H2U, 7MG, OMC, 5MU, ZN, PSU, SF4, AET

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	0.40	0/36095	0.65	7/56332 (0.0%)
1	1G	0.37	0/35850	0.60	4/55949 (0.0%)
2	12	0.41	0/1727	0.69	2/2326 (0.1%)
2	1E	0.38	0/1908	0.66	1/2573 (0.0%)
3	22	0.36	0/1569	0.63	0/2116
3	2E	0.38	0/1629	0.59	0/2195
4	32	0.40	1/1728 (0.1%)	0.62	0/2313
4	3E	0.42	0/1728	0.66	0/2313
5	42	0.37	0/1156	0.58	0/1557
5	4E	0.39	0/1158	0.61	0/1559
6	52	0.36	0/855	0.55	0/1154
6	5E	0.39	0/850	0.61	0/1147
7	62	0.35	0/1122	0.64	2/1500 (0.1%)
7	6E	0.38	0/1259	0.59	0/1686
8	72	0.33	0/1127	0.59	0/1517
8	7E	0.36	0/1135	0.66	0/1527
9	82	0.36	0/971	0.68	1/1304 (0.1%)
9	8E	0.38	0/1019	0.70	0/1367
10	1A	0.38	0/814	0.60	0/1095
10	1I	0.46	0/762	0.73	0/1027
11	2A	0.33	0/850	0.60	1/1150 (0.1%)
11	2I	0.41	0/838	0.71	1/1133 (0.1%)
12	3A	0.43	0/972	0.76	2/1301 (0.2%)
12	3I	0.55	0/972	0.86	0/1301
13	4A	0.41	0/889	0.73	0/1192
13	4I	0.46	0/952	0.75	0/1277
14	5A	0.37	0/495	0.70	0/657
14	5I	0.41	0/500	0.77	2/664 (0.3%)
15	6A	0.33	0/740	0.54	0/987
15	6I	0.42	0/740	0.59	0/987
16	7A	0.38	0/721	0.66	0/970
16	7I	0.40	0/716	0.67	0/963

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
17	8A	0.38	0/836	0.60	0/1117
17	8I	0.39	0/847	0.70	1/1131 (0.1%)
18	9A	0.39	0/559	0.59	0/746
18	9I	0.38	0/554	0.61	0/739
19	AA	0.51	0/520	0.86	1/700 (0.1%)
19	AI	0.39	0/680	0.81	2/915 (0.2%)
20	BA	0.36	0/781	0.59	0/1033
20	BI	0.35	0/748	0.61	0/986
21	1B	0.30	0/192	0.60	0/252
21	1F	0.36	0/203	0.61	0/266
22	1K	0.45	0/1675	0.65	0/2608
22	1L	0.40	0/1675	0.56	0/2608
23	2K	0.45	1/1721 (0.1%)	0.64	0/2682
23	2L	0.41	1/1721 (0.1%)	0.62	0/2682
24	3K	0.40	0/1716	0.59	0/2668
25	4K	0.49	0/440	0.67	0/684
25	4L	0.52	0/341	0.99	1/529 (0.2%)
26	14	0.47	0/67828	0.71	11/105880 (0.0%)
26	1H	0.54	0/68741	0.76	16/107295 (0.0%)
27	16	0.43	0/2928	0.74	1/4568 (0.0%)
27	1J	0.41	0/2928	0.68	0/4568
28	11	0.60	0/2170	0.92	5/2926 (0.2%)
28	19	0.58	0/2175	0.90	4/2933 (0.1%)
29	21	0.56	2/1589 (0.1%)	0.97	3/2145 (0.1%)
29	29	0.48	0/1596	0.90	4/2153 (0.2%)
30	31	0.55	0/1620	0.81	0/2194
30	39	0.46	0/1637	0.84	6/2218 (0.3%)
31	41	0.41	0/1481	0.74	0/1994
31	49	0.40	0/1483	0.72	1/1997 (0.1%)
32	51	0.47	0/1354	0.95	10/1833 (0.5%)
32	59	0.50	0/1320	0.77	1/1787 (0.1%)
33	61	0.41	0/1146	0.79	4/1551 (0.3%)
33	69	0.39	0/1146	0.72	1/1551 (0.1%)
34	15	0.52	1/1123 (0.1%)	0.73	0/1515
34	58	0.46	0/1017	0.82	3/1369 (0.2%)
35	25	0.42	0/942	0.67	0/1269
35	68	0.47	0/942	0.72	0/1269
36	35	0.51	0/1139	0.94	4/1514 (0.3%)
36	78	0.57	0/1144	1.10	5/1521 (0.3%)
37	45	0.47	0/1120	0.86	1/1498 (0.1%)
37	88	0.57	0/1138	0.90	3/1523 (0.2%)
38	55	0.49	0/981	0.78	0/1312
38	98	0.47	0/981	0.81	0/1312

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
39	65	0.43	0/886	0.81	2/1180 (0.2%)
39	A8	0.51	0/891	0.84	0/1187
40	75	0.45	0/1178	0.80	2/1573 (0.1%)
40	B8	0.50	0/1142	0.85	2/1526 (0.1%)
41	85	0.45	0/977	0.70	0/1301
41	C8	0.53	0/968	0.75	0/1289
42	95	0.43	0/781	0.85	4/1048 (0.4%)
42	D8	0.45	0/785	0.81	0/1052
43	A5	0.50	0/897	0.75	0/1204
43	E8	0.53	0/886	0.71	0/1189
44	B5	0.51	0/749	0.80	2/1007 (0.2%)
44	F8	0.57	0/764	0.84	0/1025
45	C5	0.49	0/401	0.80	0/535
45	G8	0.55	0/745	1.00	3/993 (0.3%)
46	D5	0.41	0/1443	0.72	0/1960
46	H8	0.42	0/1395	0.82	3/1890 (0.2%)
47	E5	0.50	0/611	0.83	0/814
47	I8	0.58	0/619	0.92	0/825
48	F5	0.52	0/744	0.87	2/989 (0.2%)
48	J8	0.59	0/754	0.95	3/1003 (0.3%)
49	G5	0.51	0/578	0.82	2/766 (0.3%)
49	K8	0.60	0/577	1.04	2/763 (0.3%)
50	H5	0.40	0/464	0.63	0/623
50	L8	0.49	0/464	0.79	2/623 (0.3%)
51	M8	0.49	0/485	0.93	0/652
52	J5	0.55	0/448	0.86	1/606 (0.2%)
52	N8	0.61	0/381	0.88	0/516
53	L5	0.54	0/414	0.81	2/547 (0.4%)
53	P8	0.71	0/409	0.91	0/540
54	M5	0.59	0/524	0.95	2/691 (0.3%)
54	Q8	0.60	0/524	1.09	2/691 (0.3%)
55	3L	0.39	0/1672	0.63	0/2600
All	All	0.47	6/315281 (0.0%)	0.71	147/472388 (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	6
2	1E	0	3

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Mol	Chain	#Chirality outliers	#Planarity outliers
3	22	0	2
4	32	0	2
5	4E	0	1
9	82	0	1
9	8E	0	2
10	1A	0	1
11	2I	0	3
12	3A	0	1
12	3I	0	3
13	4A	0	4
13	4I	0	2
14	5A	0	3
16	7A	0	1
19	AA	0	7
20	BA	0	3
20	BI	0	1
28	11	0	4
28	19	0	2
29	21	0	6
29	29	0	6
30	31	0	3
30	39	0	5
31	49	0	2
32	51	0	4
32	59	0	2
33	61	0	5
33	69	0	3
34	58	0	2
36	35	0	3
36	78	0	5
37	45	0	5
37	88	0	2
38	98	0	1
39	65	0	1
39	A8	0	1
40	75	0	2
40	B8	0	3
41	85	0	2
41	C8	0	4
42	95	0	2
42	D8	0	2
44	B5	0	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
45	G8	0	3
46	D5	0	6
46	H8	0	5
48	F5	0	4
48	J8	0	3
49	G5	0	4
49	K8	0	4
51	M8	0	4
54	M5	0	3
54	Q8	0	3
All	All	0	163

The worst 5 of 6 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
34	15	94	HIS	C-O	-11.07	1.18	1.23
23	2K	8	4SU	O3'-P	5.84	1.62	1.56
23	2L	8	4SU	O3'-P	5.38	1.61	1.56
29	21	135	HIS	CE1-NE2	5.36	1.38	1.32
4	32	87	GLY	C-N	5.14	1.36	1.33

The worst 5 of 147 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
36	78	15	ARG	CA-C-N	9.49	139.66	121.54
36	78	15	ARG	C-N-CA	9.49	139.66	121.54
45	G8	81	LYS	CA-C-N	9.27	149.26	127.00
45	G8	81	LYS	C-N-CA	9.27	149.26	127.00
29	29	23	VAL	N-CA-C	9.26	119.90	112.12

There are no chirality outliers.

5 of 163 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	1E	11	LEU	Peptide
2	1E	15	VAL	Peptide
2	1E	237	ALA	Peptide
5	4E	114	GLY	Peptide
9	8E	4	TYR	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	16276	651	0
1	1G	32028	0	16165	612	0
2	12	1696	0	1730	106	0
2	1E	1874	0	1926	86	0
3	22	1546	0	1608	82	0
3	2E	1605	0	1668	41	0
4	32	1698	0	1761	88	1
4	3E	1698	0	1760	70	0
5	42	1141	0	1199	61	0
5	4E	1142	0	1204	36	0
6	52	842	0	857	19	0
6	5E	837	0	852	20	1
7	62	1110	0	1163	52	0
7	6E	1242	0	1286	45	0
8	72	1107	0	1165	37	0
8	7E	1115	0	1177	46	0
9	82	953	0	983	55	0
9	8E	1000	0	1031	60	0
10	1A	801	0	849	53	0
10	1I	749	0	767	42	0
11	2A	835	0	847	30	0
11	2I	823	0	832	32	0
12	3A	956	0	1046	32	0
12	3I	956	0	1046	36	0
13	4A	879	0	935	49	0
13	4I	942	0	997	58	0
14	5A	486	0	526	23	0
14	5I	491	0	529	27	0
15	6A	729	0	768	12	0
15	6I	729	0	768	30	0
16	7A	705	0	725	19	0
16	7I	700	0	720	28	0
17	8A	823	0	891	33	0
17	8I	834	0	904	33	0
18	9A	554	0	609	16	0
18	9I	549	0	607	26	0
19	AA	510	0	507	33	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
19	AI	665	0	686	37	0
20	BA	778	0	863	27	0
20	BI	746	0	843	47	0
21	1B	188	0	195	16	0
21	1F	199	0	208	10	0
22	1K	1593	0	813	49	0
22	1L	1593	0	813	48	0
23	2K	1646	0	844	19	0
23	2L	1646	0	842	32	0
24	3K	1537	0	779	46	0
25	4K	391	0	197	7	0
25	4L	303	0	154	15	0
26	14	60561	0	30527	995	0
26	1H	61381	0	30944	1095	0
27	16	2617	0	1328	45	0
27	1J	2617	0	1328	70	0
28	11	2120	0	2197	61	0
28	19	2125	0	2199	73	0
29	21	1556	0	1612	76	0
29	29	1563	0	1629	85	0
30	31	1585	0	1632	76	0
30	39	1602	0	1649	88	0
31	41	1457	0	1514	71	0
31	49	1459	0	1507	62	0
32	51	1328	0	1396	47	0
32	59	1295	0	1366	82	0
33	61	1131	0	1218	49	0
33	69	1131	0	1218	47	0
34	15	1096	0	1168	55	0
34	58	995	0	1077	39	0
35	25	932	0	996	34	0
35	68	932	0	996	22	0
36	35	1122	0	1206	73	0
36	78	1127	0	1208	67	0
37	45	1099	0	1154	70	0
37	88	1117	0	1168	55	0
38	55	967	0	1033	45	0
38	98	967	0	1033	40	0
39	65	876	0	938	72	0
39	A8	881	0	943	46	0
40	75	1164	0	1221	61	0
40	B8	1128	0	1183	60	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
41	85	959	0	1019	62	0
41	C8	950	0	1011	49	0
42	95	770	0	838	34	0
42	D8	774	0	849	30	0
43	A5	886	0	948	25	0
43	E8	876	0	941	26	0
44	B5	735	0	785	21	0
44	F8	750	0	814	20	0
45	C5	396	0	444	18	0
45	G8	734	0	821	38	0
46	D5	1411	0	1436	73	0
46	H8	1365	0	1391	64	0
47	E5	603	0	620	23	0
47	I8	611	0	631	28	0
48	F5	737	0	813	34	0
48	J8	747	0	817	37	0
49	G5	576	0	625	33	0
49	K8	575	0	634	34	0
50	H5	459	0	512	19	0
50	L8	459	0	512	10	0
51	M8	475	0	465	33	0
52	J5	434	0	454	22	0
52	N8	369	0	388	23	0
53	L5	406	0	438	10	0
53	P8	401	0	436	12	0
54	M5	516	0	582	22	0
54	Q8	516	0	582	40	0
55	3L	1538	0	781	38	0
56	11	1	0	0	0	0
56	13	205	0	0	0	0
56	14	435	0	0	0	0
56	16	15	0	0	0	0
56	19	1	0	0	0	0
56	1B	1	0	0	0	0
56	1G	155	0	0	0	0
56	1H	622	0	0	0	0
56	1J	6	0	0	0	0
56	1K	1	0	0	0	0
56	21	4	0	0	0	0
56	25	1	0	0	0	0
56	29	3	0	0	0	0
56	2A	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
56	2I	1	0	0	0	0
56	2K	2	0	0	0	0
56	2L	2	0	0	0	0
56	31	2	0	0	0	0
56	35	3	0	0	0	0
56	39	1	0	0	0	0
56	3E	1	0	0	0	0
56	41	1	0	0	0	0
56	42	1	0	0	0	0
56	45	2	0	0	0	0
56	4A	1	0	0	0	0
56	4L	1	0	0	0	0
56	55	1	0	0	0	0
56	5E	1	0	0	0	0
56	5I	2	0	0	0	0
56	68	2	0	0	0	0
56	78	2	0	0	0	0
56	85	1	0	0	0	0
56	88	3	0	0	0	0
56	8I	1	0	0	0	0
56	98	1	0	0	0	0
56	9A	1	0	0	0	0
56	BA	2	0	0	0	0
56	BI	2	0	0	0	0
56	D8	1	0	0	0	0
56	E5	1	0	0	0	0
56	I8	2	0	0	0	0
56	P8	1	0	0	0	0
56	Q8	1	0	0	0	0
57	32	8	0	0	1	0
57	3E	8	0	0	1	0
58	5A	1	0	0	0	0
58	5I	1	0	0	0	0
59	11	11	0	0	0	0
59	13	339	0	0	42	0
59	14	730	0	0	89	0
59	15	1	0	0	0	0
59	16	19	0	0	0	0
59	19	10	0	0	1	0
59	1A	1	0	0	0	0
59	1E	1	0	0	1	0
59	1F	2	0	0	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
59	1G	289	0	0	25	0
59	1H	1047	0	0	184	0
59	1I	3	0	0	1	0
59	1K	1	0	0	0	0
59	21	8	0	0	0	0
59	25	6	0	0	0	0
59	29	2	0	0	0	0
59	2L	6	0	0	0	0
59	31	7	0	0	0	0
59	32	2	0	0	0	0
59	35	6	0	0	0	0
59	39	5	0	0	0	0
59	3E	2	0	0	0	0
59	3I	1	0	0	0	0
59	42	1	0	0	0	0
59	45	4	0	0	0	0
59	4E	2	0	0	0	0
59	4I	2	0	0	1	0
59	4K	2	0	0	0	0
59	4L	3	0	0	1	0
59	52	4	0	0	0	0
59	58	3	0	0	0	0
59	5I	1	0	0	0	0
59	6E	1	0	0	0	0
59	6I	1	0	0	0	0
59	75	1	0	0	0	0
59	78	6	0	0	0	0
59	7A	4	0	0	1	0
59	7I	3	0	0	0	0
59	8E	2	0	0	0	0
59	95	1	0	0	0	0
59	9A	2	0	0	1	0
59	B5	3	0	0	0	0
59	BA	2	0	0	0	0
59	D8	1	0	0	0	0
59	E8	1	0	0	0	0
59	G8	1	0	0	0	0
59	H5	3	0	0	1	0
59	I8	2	0	0	1	0
59	J8	1	0	0	0	0
59	L8	4	0	0	0	0
59	M5	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
59	P8	1	0	0	0	0
59	Q8	2	0	0	1	0
All	All	294252	0	195096	6898	1

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 15.

The worst 5 of 6898 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:810:U:OP1	59:1H:3720:HOH:O	1.68	1.09
29:29:54:GLN:HA	29:29:74:PRO:HA	1.35	1.08
26:14:1604:C:OP2	59:14:3509:HOH:O	1.71	1.07
37:45:27:VAL:HB	37:45:28:ALA:HA	1.32	1.07
26:14:2113:U:H3'	26:14:2114:A:H4'	1.34	1.06

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

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:5E:15:ASP:OD2	4:32:27:TYR:OH[4_555]	2.19	0.01

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
2	12	203/256 (79%)	161 (79%)	41 (20%)	1 (0%)	24 49
2	1E	227/256 (89%)	175 (77%)	49 (22%)	3 (1%)	9 26
3	22	193/239 (81%)	161 (83%)	31 (16%)	1 (0%)	24 49
3	2E	203/239 (85%)	181 (89%)	21 (10%)	1 (0%)	24 49

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
4	32	205/209 (98%)	186 (91%)	19 (9%)	0	100 100
4	3E	205/209 (98%)	175 (85%)	29 (14%)	1 (0%)	24 49
5	42	148/162 (91%)	136 (92%)	12 (8%)	0	100 100
5	4E	147/162 (91%)	140 (95%)	7 (5%)	0	100 100
6	52	99/101 (98%)	93 (94%)	6 (6%)	0	100 100
6	5E	98/101 (97%)	91 (93%)	7 (7%)	0	100 100
7	62	134/156 (86%)	127 (95%)	7 (5%)	0	100 100
7	6E	152/156 (97%)	142 (93%)	10 (7%)	0	100 100
8	72	135/138 (98%)	118 (87%)	16 (12%)	1 (1%)	18 40
8	7E	136/138 (99%)	123 (90%)	11 (8%)	2 (2%)	8 23
9	82	119/128 (93%)	103 (87%)	14 (12%)	2 (2%)	7 20
9	8E	124/128 (97%)	102 (82%)	22 (18%)	0	100 100
10	1A	97/105 (92%)	83 (86%)	14 (14%)	0	100 100
10	1I	92/105 (88%)	80 (87%)	12 (13%)	0	100 100
11	2A	111/129 (86%)	96 (86%)	14 (13%)	1 (1%)	14 34
11	2I	109/129 (84%)	94 (86%)	14 (13%)	1 (1%)	14 34
12	3A	120/132 (91%)	100 (83%)	19 (16%)	1 (1%)	16 37
12	3I	120/132 (91%)	104 (87%)	15 (12%)	1 (1%)	16 37
13	4A	107/126 (85%)	84 (78%)	17 (16%)	6 (6%)	1 2
13	4I	117/126 (93%)	86 (74%)	26 (22%)	5 (4%)	2 4
14	5A	57/61 (93%)	46 (81%)	10 (18%)	1 (2%)	6 19
14	5I	58/61 (95%)	50 (86%)	5 (9%)	3 (5%)	1 3
15	6A	85/89 (96%)	82 (96%)	3 (4%)	0	100 100
15	6I	85/89 (96%)	71 (84%)	14 (16%)	0	100 100
16	7A	82/88 (93%)	74 (90%)	7 (8%)	1 (1%)	10 28
16	7I	81/88 (92%)	72 (89%)	9 (11%)	0	100 100
17	8A	97/105 (92%)	91 (94%)	6 (6%)	0	100 100
17	8I	98/105 (93%)	87 (89%)	11 (11%)	0	100 100
18	9A	67/88 (76%)	65 (97%)	2 (3%)	0	100 100
18	9I	66/88 (75%)	62 (94%)	4 (6%)	0	100 100
19	AA	59/93 (63%)	43 (73%)	15 (25%)	1 (2%)	7 20

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
19	AI	81/93 (87%)	67 (83%)	13 (16%)	1 (1%)	10 28
20	BA	101/106 (95%)	83 (82%)	17 (17%)	1 (1%)	12 32
20	BI	95/106 (90%)	84 (88%)	11 (12%)	0	100 100
21	1B	20/27 (74%)	17 (85%)	2 (10%)	1 (5%)	1 3
21	1F	21/27 (78%)	19 (90%)	2 (10%)	0	100 100
28	11	271/276 (98%)	249 (92%)	17 (6%)	5 (2%)	6 19
28	19	272/276 (99%)	235 (86%)	36 (13%)	1 (0%)	30 53
29	21	203/206 (98%)	159 (78%)	39 (19%)	5 (2%)	4 13
29	29	202/206 (98%)	146 (72%)	48 (24%)	8 (4%)	2 5
30	31	200/210 (95%)	178 (89%)	22 (11%)	0	100 100
30	39	202/210 (96%)	163 (81%)	35 (17%)	4 (2%)	6 16
31	41	177/182 (97%)	153 (86%)	23 (13%)	1 (1%)	21 45
31	49	178/182 (98%)	149 (84%)	27 (15%)	2 (1%)	11 29
32	51	172/180 (96%)	132 (77%)	31 (18%)	9 (5%)	1 3
32	59	167/180 (93%)	125 (75%)	42 (25%)	0	100 100
33	61	143/148 (97%)	111 (78%)	28 (20%)	4 (3%)	4 11
33	69	143/148 (97%)	107 (75%)	34 (24%)	2 (1%)	9 24
34	15	135/140 (96%)	118 (87%)	16 (12%)	1 (1%)	18 40
34	58	123/140 (88%)	109 (89%)	13 (11%)	1 (1%)	16 37
35	25	120/122 (98%)	110 (92%)	10 (8%)	0	100 100
35	68	120/122 (98%)	112 (93%)	8 (7%)	0	100 100
36	35	145/150 (97%)	117 (81%)	26 (18%)	2 (1%)	9 24
36	78	146/150 (97%)	111 (76%)	30 (20%)	5 (3%)	3 7
37	45	136/141 (96%)	106 (78%)	29 (21%)	1 (1%)	18 40
37	88	139/141 (99%)	120 (86%)	15 (11%)	4 (3%)	3 10
38	55	116/118 (98%)	104 (90%)	10 (9%)	2 (2%)	7 20
38	98	116/118 (98%)	102 (88%)	14 (12%)	0	100 100
39	65	108/112 (96%)	84 (78%)	23 (21%)	1 (1%)	14 34
39	A8	109/112 (97%)	85 (78%)	24 (22%)	0	100 100
40	75	138/146 (94%)	120 (87%)	16 (12%)	2 (1%)	9 24
40	B8	134/146 (92%)	112 (84%)	21 (16%)	1 (1%)	18 40

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
41	85	114/118 (97%)	99 (87%)	15 (13%)	0	100 100
41	C8	113/118 (96%)	97 (86%)	14 (12%)	2 (2%)	6 19
42	95	98/101 (97%)	79 (81%)	16 (16%)	3 (3%)	3 8
42	D8	98/101 (97%)	85 (87%)	13 (13%)	0	100 100
43	A5	109/113 (96%)	102 (94%)	7 (6%)	0	100 100
43	E8	108/113 (96%)	100 (93%)	8 (7%)	0	100 100
44	B5	92/96 (96%)	77 (84%)	14 (15%)	1 (1%)	11 29
44	F8	93/96 (97%)	88 (95%)	5 (5%)	0	100 100
45	C5	48/110 (44%)	39 (81%)	8 (17%)	1 (2%)	5 16
45	G8	93/110 (84%)	64 (69%)	25 (27%)	4 (4%)	2 4
46	D5	175/206 (85%)	123 (70%)	45 (26%)	7 (4%)	2 5
46	H8	168/206 (82%)	127 (76%)	35 (21%)	6 (4%)	2 6
47	E5	74/85 (87%)	64 (86%)	8 (11%)	2 (3%)	4 11
47	I8	75/85 (88%)	66 (88%)	9 (12%)	0	100 100
48	F5	92/98 (94%)	78 (85%)	12 (13%)	2 (2%)	5 15
48	J8	94/98 (96%)	79 (84%)	13 (14%)	2 (2%)	5 16
49	G5	67/72 (93%)	60 (90%)	6 (9%)	1 (2%)	8 23
49	K8	66/72 (92%)	58 (88%)	7 (11%)	1 (2%)	8 23
50	H5	56/60 (93%)	52 (93%)	4 (7%)	0	100 100
50	L8	56/60 (93%)	50 (89%)	6 (11%)	0	100 100
51	M8	56/71 (79%)	35 (62%)	19 (34%)	2 (4%)	2 6
52	J5	54/60 (90%)	45 (83%)	9 (17%)	0	100 100
52	N8	46/60 (77%)	37 (80%)	9 (20%)	0	100 100
53	L5	46/49 (94%)	44 (96%)	2 (4%)	0	100 100
53	P8	45/49 (92%)	42 (93%)	2 (4%)	1 (2%)	5 15
54	M5	62/65 (95%)	54 (87%)	8 (13%)	0	100 100
54	Q8	62/65 (95%)	47 (76%)	12 (19%)	3 (5%)	2 3
All	All	10929/11875 (92%)	9262 (85%)	1532 (14%)	135 (1%)	10 28

5 of 135 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
13	4I	12	ASN

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Mol	Chain	Res	Type
28	11	239	ARG
33	61	134	PRO
34	58	96	GLU
36	78	36	LYS

5.3.2 Protein sidechains (i)

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%)	136 (76%)	43 (24%)	1	1
2	1E	200/220 (91%)	144 (72%)	56 (28%)	0	0
3	22	154/188 (82%)	113 (73%)	41 (27%)	0	1
3	2E	159/188 (85%)	126 (79%)	33 (21%)	1	3
4	32	180/181 (99%)	149 (83%)	31 (17%)	2	5
4	3E	180/181 (99%)	148 (82%)	32 (18%)	2	4
5	42	114/123 (93%)	88 (77%)	26 (23%)	1	2
5	4E	115/123 (94%)	92 (80%)	23 (20%)	1	3
6	52	90/90 (100%)	74 (82%)	16 (18%)	2	4
6	5E	90/90 (100%)	75 (83%)	15 (17%)	2	6
7	62	114/127 (90%)	92 (81%)	22 (19%)	1	3
7	6E	125/127 (98%)	99 (79%)	26 (21%)	1	3
8	72	118/119 (99%)	85 (72%)	33 (28%)	0	0
8	7E	119/119 (100%)	92 (77%)	27 (23%)	1	2
9	82	92/99 (93%)	70 (76%)	22 (24%)	1	1
9	8E	97/99 (98%)	75 (77%)	22 (23%)	1	2
10	1A	89/92 (97%)	66 (74%)	23 (26%)	0	1
10	1I	81/92 (88%)	66 (82%)	15 (18%)	1	4
11	2A	85/99 (86%)	70 (82%)	15 (18%)	2	5
11	2I	84/99 (85%)	64 (76%)	20 (24%)	1	1

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
12	3A	103/109 (94%)	73 (71%)	30 (29%)	0 0
12	3I	103/109 (94%)	80 (78%)	23 (22%)	1 2
13	4A	90/101 (89%)	66 (73%)	24 (27%)	0 0
13	4I	94/101 (93%)	72 (77%)	22 (23%)	1 2
14	5A	49/50 (98%)	33 (67%)	16 (33%)	0 0
14	5I	49/50 (98%)	38 (78%)	11 (22%)	1 2
15	6A	79/80 (99%)	72 (91%)	7 (9%)	9 24
15	6I	79/80 (99%)	65 (82%)	14 (18%)	2 4
16	7A	72/74 (97%)	63 (88%)	9 (12%)	4 13
16	7I	72/74 (97%)	55 (76%)	17 (24%)	1 1
17	8A	94/97 (97%)	81 (86%)	13 (14%)	3 10
17	8I	95/97 (98%)	75 (79%)	20 (21%)	1 2
18	9A	58/77 (75%)	43 (74%)	15 (26%)	0 1
18	9I	58/77 (75%)	51 (88%)	7 (12%)	5 14
19	AA	56/80 (70%)	43 (77%)	13 (23%)	1 2
19	AI	72/80 (90%)	51 (71%)	21 (29%)	0 0
20	BA	76/82 (93%)	67 (88%)	9 (12%)	5 15
20	BI	75/82 (92%)	62 (83%)	13 (17%)	2 5
21	1B	17/22 (77%)	16 (94%)	1 (6%)	18 41
21	1F	18/22 (82%)	16 (89%)	2 (11%)	6 17
28	11	214/218 (98%)	173 (81%)	41 (19%)	1 3
28	19	214/218 (98%)	164 (77%)	50 (23%)	1 2
29	21	162/166 (98%)	128 (79%)	34 (21%)	1 2
29	29	165/166 (99%)	132 (80%)	33 (20%)	1 3
30	31	161/166 (97%)	131 (81%)	30 (19%)	1 4
30	39	163/166 (98%)	118 (72%)	45 (28%)	0 0
31	41	153/156 (98%)	119 (78%)	34 (22%)	1 2
31	49	152/156 (97%)	120 (79%)	32 (21%)	1 2
32	51	143/148 (97%)	112 (78%)	31 (22%)	1 2
32	59	140/148 (95%)	98 (70%)	42 (30%)	0 0
33	61	122/124 (98%)	86 (70%)	36 (30%)	0 0

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
33	69	122/124 (98%)	93 (76%)	29 (24%)	1	1
34	15	116/119 (98%)	87 (75%)	29 (25%)	0	1
34	58	105/119 (88%)	83 (79%)	22 (21%)	1	2
35	25	100/100 (100%)	82 (82%)	18 (18%)	2	4
35	68	100/100 (100%)	80 (80%)	20 (20%)	1	3
36	35	114/116 (98%)	75 (66%)	39 (34%)	0	0
36	78	114/116 (98%)	77 (68%)	37 (32%)	0	0
37	45	109/111 (98%)	87 (80%)	22 (20%)	1	3
37	88	110/111 (99%)	94 (86%)	16 (14%)	3	9
38	55	101/101 (100%)	73 (72%)	28 (28%)	0	0
38	98	101/101 (100%)	73 (72%)	28 (28%)	0	0
39	65	87/88 (99%)	60 (69%)	27 (31%)	0	0
39	A8	87/88 (99%)	58 (67%)	29 (33%)	0	0
40	75	122/127 (96%)	95 (78%)	27 (22%)	1	2
40	B8	118/127 (93%)	82 (70%)	36 (30%)	0	0
41	85	93/94 (99%)	76 (82%)	17 (18%)	2	4
41	C8	92/94 (98%)	76 (83%)	16 (17%)	2	5
42	95	81/82 (99%)	62 (76%)	19 (24%)	1	1
42	D8	82/82 (100%)	57 (70%)	25 (30%)	0	0
43	A5	91/92 (99%)	71 (78%)	20 (22%)	1	2
43	E8	90/92 (98%)	74 (82%)	16 (18%)	2	4
44	B5	74/78 (95%)	59 (80%)	15 (20%)	1	3
44	F8	77/78 (99%)	63 (82%)	14 (18%)	2	4
45	C5	43/91 (47%)	35 (81%)	8 (19%)	1	4
45	G8	79/91 (87%)	62 (78%)	17 (22%)	1	2
46	D5	156/179 (87%)	125 (80%)	31 (20%)	1	3
46	H8	151/179 (84%)	104 (69%)	47 (31%)	0	0
47	E5	61/67 (91%)	48 (79%)	13 (21%)	1	2
47	I8	62/67 (92%)	53 (86%)	9 (14%)	3	9
48	F5	79/83 (95%)	59 (75%)	20 (25%)	0	1
48	J8	79/83 (95%)	62 (78%)	17 (22%)	1	2

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
49	G5	63/67 (94%)	41 (65%)	22 (35%)	0 0
49	K8	64/67 (96%)	41 (64%)	23 (36%)	0 0
50	H5	50/52 (96%)	44 (88%)	6 (12%)	5 14
50	L8	50/52 (96%)	42 (84%)	8 (16%)	2 8
51	M8	52/63 (82%)	37 (71%)	15 (29%)	0 0
52	J5	48/52 (92%)	40 (83%)	8 (17%)	2 6
52	N8	43/52 (83%)	32 (74%)	11 (26%)	0 1
53	L5	38/42 (90%)	33 (87%)	5 (13%)	4 12
53	P8	38/42 (90%)	31 (82%)	7 (18%)	1 4
54	M5	54/55 (98%)	44 (82%)	10 (18%)	1 4
54	Q8	54/55 (98%)	48 (89%)	6 (11%)	6 17
All	All	9213/9831 (94%)	7145 (78%)	2068 (22%)	1 2

5 of 2068 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
40	75	30	VAL
42	95	89	GLN
40	75	27	THR
40	B8	1	MET
39	A8	30	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 54 such sidechains are listed below:

Mol	Chain	Res	Type
3	22	3	ASN
6	52	100	ASN
44	B5	41	ASN
3	22	6	HIS
4	32	45	GLN

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	13	1499/1522 (98%)	328 (21%)	36 (2%)
1	1G	1488/1522 (97%)	315 (21%)	31 (2%)

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Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
22	1K	72/76 (94%)	39 (54%)	5 (6%)
22	1L	71/76 (93%)	40 (56%)	1 (1%)
23	2K	76/77 (98%)	18 (23%)	1 (1%)
23	2L	76/77 (98%)	18 (23%)	3 (3%)
24	3K	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%)	635 (22%)	35 (1%)
26	1H	2841/2917 (97%)	582 (20%)	45 (1%)
27	16	121/122 (99%)	17 (14%)	1 (0%)
27	1J	121/122 (99%)	33 (27%)	1 (0%)
55	3L	69/76 (90%)	31 (44%)	3 (4%)
All	All	9339/9634 (96%)	2108 (22%)	170 (1%)

5 of 2108 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	13	2	U
1	13	4	U
1	13	5	U
1	13	6	G
1	13	7	G

5 of 170 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	1G	1145	C
26	14	960	A
1	1G	1359	C
55	3L	58	A
26	14	1534	G

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

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

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

RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
22	5MU	1K	54	22	19,22,23	4.30	5 (26%)	27,32,35	3.49	13 (48%)
22	AET	1K	37	22	32,35,36	2.55	6 (18%)	43,51,54	2.23	12 (27%)
23	5MU	2K	55	23	19,22,23	3.92	5 (26%)	27,32,35	3.26	9 (33%)
22	PSU	1L	55	22	18,21,22	1.39	1 (5%)	21,30,33	1.87	5 (23%)
23	7MG	2K	47	23	23,26,27	3.02	9 (39%)	27,39,42	2.75	9 (33%)
22	H2U	1K	17	22	18,21,22	2.33	4 (22%)	19,30,33	1.57	3 (15%)
22	H2U	1L	17	22	18,21,22	2.52	4 (22%)	19,30,33	1.62	4 (21%)
23	4SU	2L	8	23	18,21,22	1.86	3 (16%)	25,30,33	2.44	7 (28%)
22	AET	1L	37	22	32,35,36	2.51	6 (18%)	43,51,54	2.19	18 (41%)
23	4SU	2K	8	23	18,21,22	1.90	4 (22%)	25,30,33	3.01	8 (32%)
23	OMC	2L	33	23	19,22,23	1.70	3 (15%)	25,31,34	0.83	0
23	PSU	2L	56	23	18,21,22	1.23	2 (11%)	21,30,33	1.58	2 (9%)
55	PSU	3L	55	55	18,21,22	1.27	2 (11%)	21,30,33	1.92	5 (23%)
23	7MG	2L	47	23	23,26,27	3.01	7 (30%)	27,39,42	2.88	9 (33%)
22	PSU	1K	55	22	18,21,22	1.37	2 (11%)	21,30,33	1.92	3 (14%)
23	5MU	2L	55	23	19,22,23	4.00	5 (26%)	27,32,35	3.40	10 (37%)
23	OMC	2K	33	23	19,22,23	1.80	3 (15%)	25,31,34	1.26	4 (16%)
23	PSU	2K	56	23	18,21,22	1.29	2 (11%)	21,30,33	2.12	4 (19%)
55	5MU	3L	54	55	19,22,23	3.97	5 (26%)	27,32,35	3.29	9 (33%)
22	5MU	1L	54	22	19,22,23	4.18	5 (26%)	27,32,35	3.25	10 (37%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	5MU	1K	54	22	-	0/7/25/26	0/2/2/2
22	AET	1K	37	22	-	10/27/45/46	0/3/3/3
23	5MU	2K	55	23	-	0/7/25/26	0/2/2/2
22	PSU	1L	55	22	-	2/7/25/26	0/2/2/2
23	7MG	2K	47	23	-	2/7/37/38	0/3/3/3
22	H2U	1K	17	22	-	4/7/38/39	0/2/2/2
22	H2U	1L	17	22	-	5/7/38/39	0/2/2/2
23	4SU	2L	8	23	-	2/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	AET	1L	37	22	-	5/27/45/46	0/3/3/3
23	4SU	2K	8	23	-	2/7/25/26	0/2/2/2
23	OMC	2L	33	23	-	0/9/27/28	0/2/2/2
23	PSU	2L	56	23	-	0/7/25/26	0/2/2/2
55	PSU	3L	55	55	-	2/7/25/26	0/2/2/2
23	7MG	2L	47	23	-	0/7/37/38	0/3/3/3
22	PSU	1K	55	22	-	2/7/25/26	0/2/2/2
23	5MU	2L	55	23	-	2/7/25/26	0/2/2/2
23	OMC	2K	33	23	-	1/9/27/28	0/2/2/2
23	PSU	2K	56	23	-	0/7/25/26	0/2/2/2
55	5MU	3L	54	55	-	2/7/25/26	0/2/2/2
22	5MU	1L	54	22	-	0/7/25/26	0/2/2/2

The worst 5 of 83 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	1K	54	5MU	C2-N1	14.60	1.61	1.38
22	1L	54	5MU	C2-N1	13.77	1.60	1.38
23	2L	55	5MU	C2-N1	13.02	1.58	1.38
23	2K	55	5MU	C2-N1	12.72	1.58	1.38
55	3L	54	5MU	C2-N1	12.47	1.58	1.38

The worst 5 of 144 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	2L	55	5MU	C5-C4-N3	10.91	124.81	115.32
55	3L	54	5MU	C5-C4-N3	10.61	124.55	115.32
22	1K	54	5MU	C5-C4-N3	10.52	124.46	115.32
22	1L	54	5MU	C5-C4-N3	10.46	124.41	115.32
23	2K	55	5MU	C5-C4-N3	9.57	123.64	115.32

There are no chirality outliers.

5 of 41 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
55	3L	54	5MU	C4'-C5'-O5'-P
22	1K	17	H2U	O4'-C1'-N1-C2
22	1K	17	H2U	O4'-C1'-N1-C6
22	1K	17	H2U	C2'-C1'-N1-C6
22	1L	17	H2U	O4'-C1'-N1-C2

There are no ring outliers.

12 monomers are involved in 23 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
22	1K	54	5MU	2	0
22	1K	37	AET	4	0
23	2K	47	7MG	3	0
23	2L	8	4SU	1	0
22	1L	37	AET	3	0
23	2K	8	4SU	1	0
23	2L	33	OMC	2	0
55	3L	55	PSU	2	0
23	2L	47	7MG	1	0
23	2L	55	5MU	2	0
55	3L	54	5MU	3	0
22	1L	54	5MU	1	0

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

Of 1498 ligands modelled in this entry, 1496 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	$\#\|Z\| > 2$
57	SF4	3E	302	4	0,12,12	-	-	-		
57	SF4	32	301	4	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
57	SF4	3E	302	4	-	-	0/6/5/5
57	SF4	32	301	4	-	-	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 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
57	3E	302	SF4	1	0
57	32	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
55	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	5.87
1	3K	48:C	O3'	49:G	P	5.53
1	1H	1053:C	O3'	1054:A	P	3.55

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} 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%)	1.00	303 (20%)	3	2	60, 99, 150, 173	0
1	1G	1490/1522 (97%)	0.89	254 (17%)	4	3	69, 111, 148, 171	0
2	12	207/256 (80%)	2.04	86 (41%)	0	0	116, 138, 149, 156	0
2	1E	231/256 (90%)	1.40	51 (22%)	2	2	107, 131, 148, 156	0
3	22	197/239 (82%)	2.26	80 (40%)	0	0	114, 131, 144, 153	0
3	2E	205/239 (85%)	1.68	57 (27%)	1	1	82, 106, 127, 136	0
4	32	207/209 (99%)	1.34	47 (22%)	2	2	91, 110, 129, 137	0
4	3E	207/209 (99%)	1.06	34 (16%)	4	4	82, 105, 125, 132	0
5	42	150/162 (92%)	1.70	46 (30%)	1	1	99, 117, 132, 142	0
5	4E	149/162 (91%)	1.29	29 (19%)	3	3	83, 100, 118, 125	0
6	52	101/101 (100%)	1.38	24 (23%)	2	2	87, 104, 119, 131	0
6	5E	100/101 (99%)	1.22	20 (20%)	3	3	88, 105, 119, 128	0
7	62	138/156 (88%)	1.74	46 (33%)	1	1	110, 120, 130, 136	0
7	6E	154/156 (98%)	1.75	23 (14%)	5	5	101, 116, 137, 150	0
8	72	137/138 (99%)	1.42	37 (27%)	1	1	97, 119, 130, 138	0
8	7E	138/138 (100%)	0.73	12 (8%)	16	14	91, 108, 122, 128	0
9	82	121/128 (94%)	1.48	32 (26%)	1	1	105, 135, 143, 150	0
9	8E	126/128 (98%)	1.64	31 (24%)	2	1	86, 127, 142, 150	0
10	1A	99/105 (94%)	2.15	44 (44%)	0	0	112, 135, 147, 153	0
10	1I	94/105 (89%)	1.68	34 (36%)	1	1	77, 120, 141, 143	0
11	2A	113/129 (87%)	1.15	15 (13%)	7	7	83, 108, 122, 131	0
11	2I	111/129 (86%)	1.32	15 (13%)	7	6	76, 105, 125, 137	0
12	3A	122/132 (92%)	1.78	34 (27%)	1	1	81, 99, 118, 132	0
12	3I	122/132 (92%)	1.37	28 (22%)	2	2	64, 77, 108, 126	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
13	4A	109/126 (86%)	1.73	33 (30%) 1 1	111, 131, 145, 152	0
13	4I	119/126 (94%)	1.10	21 (17%) 4 3	87, 116, 130, 141	0
14	5A	59/61 (96%)	2.21	22 (37%) 1 1	120, 129, 138, 142	0
14	5I	60/61 (98%)	0.79	7 (11%) 9 8	82, 95, 116, 123	0
15	6A	87/89 (97%)	0.74	8 (9%) 14 13	86, 108, 123, 126	0
15	6I	87/89 (97%)	1.10	18 (20%) 2 2	81, 100, 119, 128	0
16	7A	84/88 (95%)	0.86	4 (4%) 35 30	91, 101, 125, 143	0
16	7I	83/88 (94%)	1.23	14 (16%) 4 4	96, 110, 130, 143	0
17	8A	99/105 (94%)	0.95	14 (14%) 6 6	93, 107, 122, 127	0
17	8I	100/105 (95%)	1.26	21 (21%) 2 2	89, 105, 116, 119	0
18	9A	69/88 (78%)	0.62	3 (4%) 40 32	94, 110, 130, 139	0
18	9I	68/88 (77%)	1.05	12 (17%) 4 3	88, 106, 123, 131	0
19	AA	65/93 (69%)	1.98	27 (41%) 0 0	122, 140, 150, 156	0
19	AI	83/93 (89%)	0.99	10 (12%) 9 8	93, 112, 138, 145	0
20	BA	103/106 (97%)	1.22	22 (21%) 2 2	89, 110, 132, 136	0
20	BI	97/106 (91%)	1.48	28 (28%) 1 1	105, 116, 134, 137	0
21	1B	22/27 (81%)	0.48	1 (4%) 38 31	109, 122, 128, 128	0
21	1F	23/27 (85%)	0.36	2 (8%) 16 14	94, 102, 111, 117	0
22	1K	70/76 (92%)	2.60	26 (37%) 1 1	79, 151, 170, 173	0
22	1L	70/76 (92%)	2.40	26 (37%) 1 1	111, 158, 174, 179	0
23	2K	72/77 (93%)	1.58	18 (25%) 2 1	67, 93, 126, 137	0
23	2L	72/77 (93%)	0.92	12 (16%) 4 4	75, 104, 139, 145	0
24	3K	72/76 (94%)	2.06	26 (36%) 1 1	70, 157, 167, 169	0
25	4K	18/27 (66%)	0.72	3 (16%) 4 4	69, 124, 164, 170	0
25	4L	14/27 (51%)	0.42	0 100 100	87, 122, 152, 154	0
26	14	2811/2917 (96%)	0.79	483 (17%) 4 3	52, 85, 154, 176	0
26	1H	2850/2917 (97%)	0.64	443 (15%) 5 5	41, 73, 157, 180	0
27	16	122/122 (100%)	0.35	7 (5%) 29 24	67, 90, 108, 164	0
27	1J	122/122 (100%)	0.48	9 (7%) 20 18	85, 110, 127, 162	0
28	11	273/276 (98%)	0.44	24 (8%) 15 14	45, 67, 87, 99	0
28	19	274/276 (99%)	0.66	29 (10%) 11 10	50, 73, 91, 110	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2		OWAB(Å^2)	Q<0.9
29	21	205/206 (99%)	1.27	56 (27%)	1	1	51, 88, 122, 131	0
29	29	204/206 (99%)	2.26	79 (38%)	1	0	58, 97, 127, 140	0
30	31	202/210 (96%)	1.21	33 (16%)	4	4	47, 80, 115, 131	0
30	39	204/210 (97%)	1.96	74 (36%)	1	1	57, 102, 138, 149	0
31	41	179/182 (98%)	1.58	45 (25%)	1	1	84, 104, 132, 151	0
31	49	180/182 (98%)	1.21	36 (20%)	3	3	103, 122, 144, 154	0
32	51	174/180 (96%)	1.33	42 (24%)	2	2	83, 101, 117, 136	0
32	59	169/180 (93%)	3.44	114 (67%)	0	0	129, 156, 164, 168	0
33	61	145/148 (97%)	1.30	31 (21%)	2	2	79, 121, 132, 139	0
33	69	145/148 (97%)	1.83	54 (37%)	1	1	84, 117, 137, 143	0
34	15	137/140 (97%)	1.58	38 (27%)	1	1	80, 106, 131, 138	0
34	58	125/140 (89%)	1.29	27 (21%)	2	2	69, 89, 105, 131	0
35	25	122/122 (100%)	0.85	13 (10%)	11	10	68, 89, 105, 119	0
35	68	122/122 (100%)	0.41	7 (5%)	29	24	60, 78, 97, 105	0
36	35	147/150 (98%)	2.21	62 (42%)	0	0	59, 99, 130, 139	0
36	78	148/150 (98%)	1.55	49 (33%)	1	1	52, 83, 109, 121	0
37	45	138/141 (97%)	1.95	51 (36%)	1	1	72, 100, 121, 133	0
37	88	141/141 (100%)	2.30	45 (31%)	1	1	56, 80, 102, 129	0
38	55	118/118 (100%)	1.00	22 (18%)	3	3	64, 84, 99, 110	0
38	98	118/118 (100%)	1.57	39 (33%)	1	1	63, 83, 102, 115	0
39	65	110/112 (98%)	1.00	18 (16%)	4	4	86, 106, 125, 130	0
39	A8	111/112 (99%)	0.87	12 (10%)	11	10	77, 88, 106, 113	0
40	75	140/146 (95%)	1.34	30 (21%)	2	2	82, 98, 145, 155	0
40	B8	136/146 (93%)	2.04	49 (36%)	1	1	73, 92, 131, 146	0
41	85	116/118 (98%)	1.76	46 (39%)	1	0	68, 93, 128, 140	0
41	C8	115/118 (97%)	0.88	19 (16%)	4	4	56, 79, 108, 116	0
42	95	100/101 (99%)	1.72	32 (32%)	1	1	66, 114, 131, 136	0
42	D8	100/101 (99%)	1.60	34 (34%)	1	1	55, 101, 120, 127	0
43	A5	111/113 (98%)	1.16	21 (18%)	3	3	66, 78, 103, 131	0
43	E8	110/113 (97%)	1.57	22 (20%)	3	3	59, 74, 98, 108	0
44	B5	94/96 (97%)	0.51	5 (5%)	32	27	72, 84, 105, 116	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
44	F8	95/96 (98%)	0.66	14 (14%) 6 5	57, 70, 101, 112	0
45	C5	52/110 (47%)	2.02	22 (42%) 0 0	93, 103, 119, 123	0
45	G8	97/110 (88%)	1.35	25 (25%) 1 1	76, 96, 127, 133	0
46	D5	177/206 (85%)	1.72	57 (32%) 1 1	106, 131, 162, 166	0
46	H8	170/206 (82%)	1.33	34 (20%) 3 3	81, 116, 154, 162	0
47	E5	76/85 (89%)	1.49	25 (32%) 1 1	66, 87, 102, 110	0
47	I8	77/85 (90%)	0.60	6 (7%) 19 17	57, 72, 96, 104	0
48	F5	94/98 (95%)	1.80	32 (34%) 1 1	63, 83, 121, 129	0
48	J8	96/98 (97%)	1.48	31 (32%) 1 1	53, 75, 123, 138	0
49	G5	69/72 (95%)	0.94	8 (11%) 9 8	85, 106, 126, 142	0
49	K8	68/72 (94%)	1.06	14 (20%) 2 2	63, 84, 103, 121	0
50	H5	58/60 (96%)	1.68	20 (34%) 1 1	77, 98, 120, 127	0
50	L8	58/60 (96%)	1.19	9 (15%) 5 5	60, 81, 108, 113	0
51	M8	60/71 (84%)	1.37	11 (18%) 3 3	105, 135, 148, 152	0
52	J5	56/60 (93%)	1.71	19 (33%) 1 1	60, 85, 127, 136	0
52	N8	48/60 (80%)	0.84	7 (14%) 6 5	51, 87, 121, 128	0
53	L5	48/49 (97%)	0.12	4 (8%) 17 15	52, 61, 95, 104	0
53	P8	47/49 (95%)	-0.10	1 (2%) 63 55	47, 52, 71, 89	0
54	M5	64/65 (98%)	1.05	13 (20%) 3 2	68, 81, 95, 115	0
54	Q8	64/65 (98%)	0.41	4 (6%) 26 22	56, 69, 83, 95	0
55	3L	70/76 (92%)	1.67	21 (30%) 1 1	80, 150, 162, 164	0
All	All	20486/21509 (95%)	1.14	4337 (21%) 2 2	41, 98, 147, 180	0

The worst 5 of 4337 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
22	1L	76	A	19.5
32	59	151	ILE	19.2
7	6E	81	GLY	19.1
3	22	158	GLY	16.8
37	88	80	GLU	16.2

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

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} 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	H2U	1K	17	20/21	0.33	0.15	153,168,175,178	0
55	PSU	3L	55	20/21	0.46	0.14	140,146,152,152	0
55	5MU	3L	54	21/22	0.52	0.12	136,142,145,152	0
22	5MU	1L	54	21/22	0.55	0.21	122,128,134,140	0
22	H2U	1L	17	20/21	0.64	0.14	153,166,172,174	0
22	PSU	1L	55	20/21	0.69	0.14	122,134,145,147	0
22	5MU	1K	54	21/22	0.74	0.16	100,111,121,127	0
23	7MG	2L	47	24/25	0.75	0.14	113,120,131,141	0
23	5MU	2L	55	21/22	0.75	0.10	116,121,123,124	0
23	5MU	2K	55	21/22	0.79	0.13	99,109,114,119	0
23	PSU	2L	56	20/21	0.79	0.09	108,116,121,124	0
22	PSU	1K	55	20/21	0.83	0.13	104,115,130,130	0
23	7MG	2K	47	24/25	0.83	0.14	94,102,111,114	0
22	AET	1L	37	33/34	0.85	0.25	94,112,119,124	0
23	PSU	2K	56	20/21	0.86	0.10	96,104,114,115	0
23	4SU	2L	8	20/21	0.88	0.10	99,111,114,120	0
23	4SU	2K	8	20/21	0.89	0.13	85,93,98,99	0
22	AET	1K	37	33/34	0.89	0.23	69,82,106,115	0
23	OMC	2K	33	21/22	0.93	0.16	71,78,80,88	0
23	OMC	2L	33	21/22	0.94	0.10	93,95,98,101	0

6.3 Carbohydrates (i)

There are no oligosaccharides in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} 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
56	MG	13	1686	1/1	-0.09	0.58	129,129,129,129	0
56	MG	13	1685	1/1	0.20	0.36	114,114,114,114	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	13	1608	1/1	0.24	0.29	111,111,111,111	0
56	MG	1G	1646	1/1	0.24	0.42	116,116,116,116	0
56	MG	14	3029	1/1	0.27	0.42	96,96,96,96	0
56	MG	1J	201	1/1	0.28	0.43	95,95,95,95	0
56	MG	1H	3304	1/1	0.29	0.32	106,106,106,106	0
56	MG	13	1659	1/1	0.30	0.37	115,115,115,115	0
56	MG	13	1665	1/1	0.31	0.42	117,117,117,117	0
56	MG	16	211	1/1	0.34	0.39	79,79,79,79	0
56	MG	1H	3303	1/1	0.34	0.52	106,106,106,106	0
56	MG	1H	3198	1/1	0.36	0.47	108,108,108,108	0
56	MG	14	3280	1/1	0.37	0.46	89,89,89,89	0
56	MG	14	3285	1/1	0.39	0.52	95,95,95,95	0
56	MG	13	1741	1/1	0.40	0.43	99,99,99,99	0
56	MG	16	210	1/1	0.40	0.47	101,101,101,101	0
56	MG	1H	3328	1/1	0.41	0.47	86,86,86,86	0
56	MG	13	1618	1/1	0.41	0.40	97,97,97,97	0
56	MG	1H	3026	1/1	0.43	0.47	92,92,92,92	0
56	MG	14	3245	1/1	0.44	0.45	104,104,104,104	0
56	MG	1H	3386	1/1	0.44	0.42	96,96,96,96	0
56	MG	1G	1666	1/1	0.45	0.27	122,122,122,122	0
56	MG	1G	1642	1/1	0.45	0.37	110,110,110,110	0
56	MG	13	1690	1/1	0.45	0.28	118,118,118,118	0
56	MG	14	3298	1/1	0.46	0.41	100,100,100,100	0
56	MG	1G	1651	1/1	0.46	0.27	107,107,107,107	0
56	MG	1J	205	1/1	0.46	0.19	118,118,118,118	0
56	MG	14	3286	1/1	0.47	0.37	93,93,93,93	0
56	MG	14	3218	1/1	0.47	0.17	104,104,104,104	0
56	MG	1H	3153	1/1	0.48	0.42	92,92,92,92	0
56	MG	1H	3165	1/1	0.48	0.56	98,98,98,98	0
56	MG	14	3222	1/1	0.49	0.17	94,94,94,94	0
56	MG	1H	3345	1/1	0.49	0.37	87,87,87,87	0
56	MG	14	3077	1/1	0.49	0.49	87,87,87,87	0
56	MG	13	1711	1/1	0.49	0.30	114,114,114,114	0
56	MG	1H	3101	1/1	0.50	0.45	91,91,91,91	0
56	MG	14	3210	1/1	0.51	0.43	100,100,100,100	0
56	MG	1H	3177	1/1	0.52	0.38	79,79,79,79	0
56	MG	1G	1607	1/1	0.52	0.36	104,104,104,104	0
56	MG	1G	1696	1/1	0.52	0.28	103,103,103,103	0
56	MG	13	1657	1/1	0.52	0.36	101,101,101,101	0
56	MG	1H	3302	1/1	0.52	0.31	98,98,98,98	0
56	MG	1G	1656	1/1	0.54	0.20	99,99,99,99	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	13	1682	1/1	0.54	0.34	116,116,116,116	0
56	MG	14	3211	1/1	0.54	0.32	111,111,111,111	0
56	MG	14	3071	1/1	0.54	0.39	83,83,83,83	0
56	MG	13	1738	1/1	0.55	0.39	96,96,96,96	0
56	MG	1G	1658	1/1	0.55	0.29	108,108,108,108	0
56	MG	13	1689	1/1	0.55	0.23	105,105,105,105	0
56	MG	14	3171	1/1	0.55	0.34	89,89,89,89	0
56	MG	1J	202	1/1	0.55	0.30	92,92,92,92	0
56	MG	1G	1655	1/1	0.55	0.26	121,121,121,121	0
56	MG	88	201	1/1	0.56	0.49	79,79,79,79	0
56	MG	14	3126	1/1	0.56	0.33	102,102,102,102	0
56	MG	1H	3337	1/1	0.56	0.35	99,99,99,99	0
56	MG	14	3065	1/1	0.57	0.33	90,90,90,90	0
56	MG	14	3216	1/1	0.57	0.40	91,91,91,91	0
56	MG	1H	3081	1/1	0.57	0.35	91,91,91,91	0
56	MG	13	1634	1/1	0.57	0.34	118,118,118,118	0
56	MG	1G	1605	1/1	0.58	0.21	105,105,105,105	0
56	MG	13	1669	1/1	0.58	0.32	109,109,109,109	0
56	MG	1H	3258	1/1	0.58	0.36	115,115,115,115	0
56	MG	1G	1691	1/1	0.58	0.28	106,106,106,106	0
56	MG	13	1671	1/1	0.59	0.37	99,99,99,99	0
56	MG	1H	3199	1/1	0.59	0.17	116,116,116,116	0
56	MG	14	3246	1/1	0.59	0.37	86,86,86,86	0
56	MG	14	3179	1/1	0.59	0.20	83,83,83,83	0
56	MG	14	3183	1/1	0.59	0.19	96,96,96,96	0
56	MG	1H	3108	1/1	0.60	0.33	87,87,87,87	0
56	MG	1H	3292	1/1	0.60	0.27	108,108,108,108	0
56	MG	5I	101	1/1	0.60	0.26	85,85,85,85	0
56	MG	13	1619	1/1	0.61	0.35	95,95,95,95	0
56	MG	1H	3175	1/1	0.61	0.24	103,103,103,103	0
56	MG	14	3262	1/1	0.61	0.39	87,87,87,87	0
56	MG	1H	3080	1/1	0.61	0.40	80,80,80,80	0
56	MG	14	3162	1/1	0.61	0.32	89,89,89,89	0
56	MG	35	201	1/1	0.61	0.30	84,84,84,84	0
56	MG	1H	3405	1/1	0.62	0.47	80,80,80,80	0
56	MG	13	1706	1/1	0.62	0.16	111,111,111,111	0
56	MG	1G	1626	1/1	0.62	0.45	102,102,102,102	0
56	MG	13	1684	1/1	0.62	0.42	99,99,99,99	0
56	MG	14	3069	1/1	0.62	0.34	85,85,85,85	0
56	MG	1H	3227	1/1	0.62	0.48	99,99,99,99	0
56	MG	1G	1673	1/1	0.62	0.31	104,104,104,104	0
56	MG	14	3045	1/1	0.63	0.31	91,91,91,91	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	14	3217	1/1	0.63	0.31	96,96,96,96	0
56	MG	16	201	1/1	0.63	0.32	79,79,79,79	0
56	MG	13	1735	1/1	0.63	0.35	85,85,85,85	0
56	MG	1H	3294	1/1	0.63	0.18	112,112,112,112	0
56	MG	1H	3036	1/1	0.64	0.26	73,73,73,73	0
56	MG	14	3080	1/1	0.64	0.36	86,86,86,86	0
56	MG	13	1674	1/1	0.64	0.31	101,101,101,101	0
56	MG	13	1650	1/1	0.64	0.30	100,100,100,100	0
56	MG	1G	1653	1/1	0.65	0.33	112,112,112,112	0
56	MG	1H	3305	1/1	0.65	0.35	100,100,100,100	0
56	MG	14	3137	1/1	0.65	0.33	90,90,90,90	0
56	MG	4A	201	1/1	0.65	0.27	116,116,116,116	0
56	MG	4L	401	1/1	0.65	0.22	99,99,99,99	0
56	MG	1H	3333	1/1	0.65	0.34	96,96,96,96	0
56	MG	1H	3054	1/1	0.66	0.46	78,78,78,78	0
56	MG	1H	3279	1/1	0.66	0.28	93,93,93,93	0
56	MG	1H	3406	1/1	0.66	0.37	91,91,91,91	0
56	MG	13	1667	1/1	0.66	0.28	86,86,86,86	0
56	MG	1G	1654	1/1	0.66	0.24	98,98,98,98	0
56	MG	1G	1615	1/1	0.66	0.40	87,87,87,87	0
56	MG	14	3193	1/1	0.66	0.38	88,88,88,88	0
56	MG	1H	3374	1/1	0.66	0.31	101,101,101,101	0
56	MG	14	3225	1/1	0.67	0.18	111,111,111,111	0
56	MG	16	207	1/1	0.67	0.30	110,110,110,110	0
56	MG	16	209	1/1	0.67	0.42	81,81,81,81	0
56	MG	13	1721	1/1	0.67	0.32	74,74,74,74	0
56	MG	13	1615	1/1	0.67	0.23	103,103,103,103	0
56	MG	13	1622	1/1	0.67	0.30	72,72,72,72	0
56	MG	1G	1700	1/1	0.67	0.23	113,113,113,113	0
56	MG	13	1656	1/1	0.67	0.22	91,91,91,91	0
56	MG	1H	3421	1/1	0.67	0.43	92,92,92,92	0
56	MG	1H	3178	1/1	0.67	0.24	91,91,91,91	0
56	MG	14	3164	1/1	0.67	0.29	105,105,105,105	0
56	MG	14	3224	1/1	0.67	0.27	101,101,101,101	0
56	MG	13	1716	1/1	0.68	0.23	94,94,94,94	0
56	MG	13	1623	1/1	0.68	0.29	106,106,106,106	0
56	MG	14	3042	1/1	0.68	0.41	82,82,82,82	0
56	MG	14	3124	1/1	0.68	0.36	82,82,82,82	0
56	MG	1H	3041	1/1	0.68	0.41	65,65,65,65	0
56	MG	1H	3162	1/1	0.68	0.32	70,70,70,70	0
56	MG	14	3154	1/1	0.68	0.40	87,87,87,87	0
56	MG	1H	3272	1/1	0.68	0.30	85,85,85,85	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	1G	1622	1/1	0.69	0.35	87,87,87,87	0
56	MG	14	3219	1/1	0.69	0.20	100,100,100,100	0
56	MG	1G	1694	1/1	0.69	0.29	102,102,102,102	0
56	MG	13	1683	1/1	0.69	0.32	99,99,99,99	0
56	MG	13	1718	1/1	0.69	0.23	105,105,105,105	0
56	MG	13	1714	1/1	0.69	0.24	114,114,114,114	0
56	MG	1G	1609	1/1	0.69	0.30	96,96,96,96	0
56	MG	13	1727	1/1	0.69	0.16	103,103,103,103	0
56	MG	14	3261	1/1	0.70	0.34	93,93,93,93	0
56	MG	1G	1687	1/1	0.70	0.27	96,96,96,96	0
56	MG	14	3268	1/1	0.70	0.40	83,83,83,83	0
56	MG	1G	1624	1/1	0.70	0.28	109,109,109,109	0
56	MG	1H	3129	1/1	0.70	0.42	77,77,77,77	0
56	MG	13	1621	1/1	0.70	0.30	74,74,74,74	0
56	MG	14	3209	1/1	0.70	0.23	97,97,97,97	0
56	MG	13	1666	1/1	0.70	0.41	92,92,92,92	0
56	MG	14	3238	1/1	0.70	0.39	85,85,85,85	0
56	MG	1H	3113	1/1	0.70	0.32	67,67,67,67	0
56	MG	1H	3379	1/1	0.70	0.33	85,85,85,85	0
56	MG	14	3259	1/1	0.71	0.33	87,87,87,87	0
56	MG	14	3260	1/1	0.71	0.30	91,91,91,91	0
56	MG	1G	1650	1/1	0.71	0.16	81,81,81,81	0
56	MG	1H	3179	1/1	0.71	0.23	93,93,93,93	0
56	MG	14	3055	1/1	0.71	0.23	89,89,89,89	0
56	MG	14	3276	1/1	0.71	0.39	92,92,92,92	0
56	MG	1G	1659	1/1	0.71	0.31	104,104,104,104	0
56	MG	13	1620	1/1	0.71	0.37	69,69,69,69	0
56	MG	42	201	1/1	0.71	0.33	103,103,103,103	0
56	MG	1H	3297	1/1	0.71	0.10	80,80,80,80	0
56	MG	14	3079	1/1	0.71	0.28	91,91,91,91	0
56	MG	1G	1674	1/1	0.71	0.23	106,106,106,106	0
56	MG	14	3081	1/1	0.71	0.28	114,114,114,114	0
56	MG	1H	3248	1/1	0.71	0.29	86,86,86,86	0
56	MG	35	203	1/1	0.71	0.44	81,81,81,81	0
56	MG	13	1694	1/1	0.72	0.22	96,96,96,96	0
56	MG	14	3004	1/1	0.72	0.31	73,73,73,73	0
56	MG	1H	3361	1/1	0.72	0.21	89,89,89,89	0
56	MG	14	3082	1/1	0.72	0.37	91,91,91,91	0
56	MG	14	3096	1/1	0.72	0.47	87,87,87,87	0
56	MG	14	3275	1/1	0.72	0.17	77,77,77,77	0
56	MG	14	3041	1/1	0.72	0.42	85,85,85,85	0
56	MG	1H	3252	1/1	0.72	0.25	102,102,102,102	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	1G	1692	1/1	0.72	0.36	87,87,87,87	0
56	MG	16	206	1/1	0.72	0.44	80,80,80,80	0
56	MG	13	1680	1/1	0.72	0.32	103,103,103,103	0
56	MG	1G	1665	1/1	0.72	0.29	107,107,107,107	0
56	MG	14	3230	1/1	0.72	0.14	90,90,90,90	0
56	MG	13	1678	1/1	0.72	0.21	97,97,97,97	0
56	MG	14	3074	1/1	0.72	0.22	84,84,84,84	0
56	MG	1H	3163	1/1	0.72	0.33	74,74,74,74	0
56	MG	1H	3090	1/1	0.73	0.30	73,73,73,73	0
56	MG	13	1737	1/1	0.73	0.23	79,79,79,79	0
56	MG	1H	3029	1/1	0.73	0.23	69,69,69,69	0
56	MG	1G	1608	1/1	0.73	0.26	108,108,108,108	0
56	MG	1H	3035	1/1	0.73	0.36	90,90,90,90	0
56	MG	1H	3205	1/1	0.73	0.43	94,94,94,94	0
56	MG	13	1663	1/1	0.73	0.20	105,105,105,105	0
56	MG	1H	3134	1/1	0.73	0.40	85,85,85,85	0
56	MG	14	3151	1/1	0.74	0.34	88,88,88,88	0
56	MG	1H	3193	1/1	0.74	0.17	89,89,89,89	0
56	MG	1H	3334	1/1	0.74	0.41	93,93,93,93	0
56	MG	13	1606	1/1	0.74	0.34	81,81,81,81	0
56	MG	1H	3230	1/1	0.74	0.21	96,96,96,96	0
56	MG	1H	3062	1/1	0.74	0.31	72,72,72,72	0
56	MG	14	3182	1/1	0.74	0.27	91,91,91,91	0
56	MG	14	3023	1/1	0.74	0.31	82,82,82,82	0
56	MG	14	3223	1/1	0.74	0.29	93,93,93,93	0
56	MG	14	3147	1/1	0.74	0.33	94,94,94,94	0
56	MG	14	3272	1/1	0.74	0.42	94,94,94,94	0
56	MG	1H	3253	1/1	0.75	0.31	72,72,72,72	0
56	MG	14	3111	1/1	0.75	0.31	78,78,78,78	0
56	MG	1H	3191	1/1	0.75	0.19	99,99,99,99	0
56	MG	1G	1701	1/1	0.75	0.53	94,94,94,94	0
56	MG	1H	3028	1/1	0.75	0.37	64,64,64,64	0
56	MG	1H	3340	1/1	0.75	0.36	83,83,83,83	0
56	MG	13	1739	1/1	0.75	0.24	74,74,74,74	0
56	MG	1H	3290	1/1	0.75	0.19	94,94,94,94	0
56	MG	13	1736	1/1	0.75	0.31	96,96,96,96	0
56	MG	1H	3202	1/1	0.75	0.39	84,84,84,84	0
56	MG	13	1668	1/1	0.75	0.44	101,101,101,101	0
56	MG	14	3266	1/1	0.75	0.36	85,85,85,85	0
56	MG	1G	1662	1/1	0.75	0.38	96,96,96,96	0
56	MG	1G	1663	1/1	0.75	0.24	100,100,100,100	0
56	MG	1G	1664	1/1	0.75	0.18	106,106,106,106	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	1H	3221	1/1	0.75	0.19	89,89,89,89	0
56	MG	14	3197	1/1	0.75	0.29	91,91,91,91	0
56	MG	1G	1616	1/1	0.75	0.15	100,100,100,100	0
56	MG	5I	102	1/1	0.75	0.19	100,100,100,100	0
56	MG	1H	3023	1/1	0.75	0.33	72,72,72,72	0
56	MG	1G	1678	1/1	0.75	0.33	86,86,86,86	0
56	MG	1H	3061	1/1	0.75	0.27	66,66,66,66	0
56	MG	1G	1628	1/1	0.75	0.33	89,89,89,89	0
56	MG	13	1658	1/1	0.75	0.27	96,96,96,96	0
56	MG	1G	1644	1/1	0.75	0.18	100,100,100,100	0
56	MG	16	204	1/1	0.76	0.26	77,77,77,77	0
56	MG	16	205	1/1	0.76	0.33	70,70,70,70	0
56	MG	1H	3312	1/1	0.76	0.11	100,100,100,100	0
56	MG	1H	3368	1/1	0.76	0.33	106,106,106,106	0
56	MG	1G	1633	1/1	0.76	0.37	94,94,94,94	0
56	MG	14	3034	1/1	0.76	0.18	63,63,63,63	0
56	MG	1G	1671	1/1	0.76	0.19	92,92,92,92	0
56	MG	1H	3327	1/1	0.76	0.32	65,65,65,65	0
56	MG	13	1681	1/1	0.76	0.34	98,98,98,98	0
56	MG	14	3047	1/1	0.76	0.13	80,80,80,80	0
56	MG	1G	1675	1/1	0.76	0.23	92,92,92,92	0
56	MG	1H	3010	1/1	0.76	0.29	70,70,70,70	0
56	MG	14	3269	1/1	0.76	0.27	80,80,80,80	0
56	MG	1G	1684	1/1	0.76	0.21	89,89,89,89	0
56	MG	14	3070	1/1	0.76	0.24	72,72,72,72	0
56	MG	14	3201	1/1	0.76	0.19	91,91,91,91	0
56	MG	1H	3396	1/1	0.76	0.13	71,71,71,71	0
56	MG	1G	1690	1/1	0.76	0.43	75,75,75,75	0
56	MG	D8	201	1/1	0.76	0.21	76,76,76,76	0
56	MG	14	3294	1/1	0.76	0.25	94,94,94,94	0
56	MG	1H	3401	1/1	0.76	0.45	77,77,77,77	0
56	MG	1H	3276	1/1	0.76	0.45	68,68,68,68	0
56	MG	13	1728	1/1	0.76	0.21	97,97,97,97	0
56	MG	13	1705	1/1	0.76	0.17	111,111,111,111	0
56	MG	1H	3422	1/1	0.76	0.25	90,90,90,90	0
56	MG	1H	3148	1/1	0.76	0.32	89,89,89,89	0
56	MG	14	3235	1/1	0.77	0.23	88,88,88,88	0
56	MG	1G	1621	1/1	0.77	0.28	89,89,89,89	0
56	MG	14	3170	1/1	0.77	0.26	105,105,105,105	0
56	MG	1H	3207	1/1	0.77	0.40	87,87,87,87	0
56	MG	1H	3291	1/1	0.77	0.22	97,97,97,97	0
56	MG	1G	1625	1/1	0.77	0.22	111,111,111,111	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	13	1717	1/1	0.77	0.29	98,98,98,98	0
56	MG	1H	3224	1/1	0.77	0.29	85,85,85,85	0
56	MG	13	1649	1/1	0.77	0.27	76,76,76,76	0
56	MG	14	3198	1/1	0.77	0.29	96,96,96,96	0
56	MG	14	3200	1/1	0.77	0.23	72,72,72,72	0
56	MG	1H	3299	1/1	0.77	0.35	87,87,87,87	0
56	MG	14	3095	1/1	0.77	0.28	92,92,92,92	0
56	MG	1H	3300	1/1	0.77	0.28	86,86,86,86	0
56	MG	1H	3301	1/1	0.77	0.33	95,95,95,95	0
56	MG	14	3281	1/1	0.77	0.20	89,89,89,89	0
56	MG	14	3117	1/1	0.77	0.29	79,79,79,79	0
56	MG	14	3123	1/1	0.77	0.16	86,86,86,86	0
56	MG	13	1628	1/1	0.77	0.31	79,79,79,79	0
56	MG	1G	1606	1/1	0.77	0.17	97,97,97,97	0
56	MG	1H	3418	1/1	0.77	0.21	90,90,90,90	0
56	MG	1H	3093	1/1	0.77	0.15	56,56,56,56	0
56	MG	1H	3346	1/1	0.77	0.30	91,91,91,91	0
56	MG	1H	3356	1/1	0.77	0.41	76,76,76,76	0
56	MG	1H	3358	1/1	0.77	0.34	83,83,83,83	0
56	MG	13	1707	1/1	0.78	0.09	108,108,108,108	0
56	MG	BA	202	1/1	0.78	0.34	113,113,113,113	0
56	MG	1H	3183	1/1	0.78	0.38	80,80,80,80	0
56	MG	13	1703	1/1	0.78	0.30	93,93,93,93	0
56	MG	14	3006	1/1	0.78	0.16	56,56,56,56	0
56	MG	1H	3114	1/1	0.78	0.31	90,90,90,90	0
56	MG	14	3178	1/1	0.78	0.13	85,85,85,85	0
56	MG	13	1720	1/1	0.78	0.15	97,97,97,97	0
56	MG	1H	3238	1/1	0.78	0.47	87,87,87,87	0
56	MG	1H	3382	1/1	0.78	0.39	73,73,73,73	0
56	MG	1H	3247	1/1	0.78	0.32	65,65,65,65	0
56	MG	14	3290	1/1	0.78	0.26	85,85,85,85	0
56	MG	13	1624	1/1	0.78	0.16	102,102,102,102	0
56	MG	1H	3143	1/1	0.78	0.18	78,78,78,78	0
56	MG	1H	3339	1/1	0.78	0.15	74,74,74,74	0
56	MG	14	3248	1/1	0.78	0.40	80,80,80,80	0
56	MG	1J	204	1/1	0.78	0.16	95,95,95,95	0
56	MG	1H	3204	1/1	0.78	0.34	92,92,92,92	0
56	MG	1J	206	1/1	0.78	0.32	68,68,68,68	0
56	MG	13	1664	1/1	0.78	0.34	91,91,91,91	0
56	MG	1H	3269	1/1	0.78	0.42	80,80,80,80	0
56	MG	14	3150	1/1	0.79	0.13	73,73,73,73	0
56	MG	13	1643	1/1	0.79	0.35	78,78,78,78	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	1H	3176	1/1	0.79	0.28	93,93,93,93	0
56	MG	13	1729	1/1	0.79	0.22	95,95,95,95	0
56	MG	3E	301	1/1	0.79	0.19	121,121,121,121	0
56	MG	1H	3261	1/1	0.79	0.31	92,92,92,92	0
56	MG	1H	3030	1/1	0.79	0.29	75,75,75,75	0
56	MG	13	1655	1/1	0.79	0.33	94,94,94,94	0
56	MG	1G	1652	1/1	0.79	0.32	87,87,87,87	0
56	MG	13	1696	1/1	0.79	0.36	104,104,104,104	0
56	MG	13	1644	1/1	0.79	0.31	89,89,89,89	0
56	MG	1H	3282	1/1	0.79	0.22	94,94,94,94	0
56	MG	1H	3363	1/1	0.79	0.11	83,83,83,83	0
56	MG	1H	3283	1/1	0.79	0.29	79,79,79,79	0
56	MG	1H	3322	1/1	0.79	0.13	94,94,94,94	0
56	MG	13	1632	1/1	0.79	0.41	86,86,86,86	0
56	MG	14	3131	1/1	0.79	0.37	78,78,78,78	0
56	MG	39	301	1/1	0.79	0.29	94,94,94,94	0
56	MG	1G	1699	1/1	0.79	0.38	90,90,90,90	0
56	MG	1H	3059	1/1	0.79	0.26	60,60,60,60	0
56	MG	1G	1634	1/1	0.80	0.24	89,89,89,89	0
56	MG	1G	1693	1/1	0.80	0.34	84,84,84,84	0
56	MG	1H	3187	1/1	0.80	0.33	75,75,75,75	0
56	MG	1H	3350	1/1	0.80	0.23	85,85,85,85	0
56	MG	1H	3190	1/1	0.80	0.27	80,80,80,80	0
56	MG	14	3233	1/1	0.80	0.15	72,72,72,72	0
56	MG	1G	1648	1/1	0.80	0.30	85,85,85,85	0
56	MG	1H	3233	1/1	0.80	0.14	85,85,85,85	0
56	MG	1G	1672	1/1	0.80	0.24	96,96,96,96	0
56	MG	13	1662	1/1	0.80	0.24	105,105,105,105	0
56	MG	14	3299	1/1	0.80	0.37	78,78,78,78	0
56	MG	14	3204	1/1	0.80	0.39	76,76,76,76	0
56	MG	1H	3271	1/1	0.80	0.32	93,93,93,93	0
56	MG	1H	3412	1/1	0.80	0.30	86,86,86,86	0
56	MG	1H	3417	1/1	0.80	0.29	93,93,93,93	0
56	MG	13	1673	1/1	0.80	0.45	88,88,88,88	0
56	MG	1H	3034	1/1	0.80	0.29	64,64,64,64	0
56	MG	13	1630	1/1	0.80	0.23	74,74,74,74	0
56	MG	1H	3425	1/1	0.80	0.46	101,101,101,101	0
56	MG	13	1710	1/1	0.81	0.21	103,103,103,103	0
56	MG	1H	3281	1/1	0.81	0.30	86,86,86,86	0
56	MG	1H	3214	1/1	0.81	0.39	93,93,93,93	0
56	MG	14	3251	1/1	0.81	0.28	77,77,77,77	0
56	MG	1H	3021	1/1	0.81	0.23	67,67,67,67	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	14	3076	1/1	0.81	0.28	78,78,78,78	0
56	MG	1G	1668	1/1	0.81	0.24	106,106,106,106	0
56	MG	1G	1669	1/1	0.81	0.27	85,85,85,85	0
56	MG	1H	3347	1/1	0.81	0.50	89,89,89,89	0
56	MG	1H	3195	1/1	0.81	0.21	84,84,84,84	0
56	MG	1H	3049	1/1	0.81	0.19	95,95,95,95	0
56	MG	1H	3265	1/1	0.81	0.20	72,72,72,72	0
56	MG	14	3009	1/1	0.81	0.26	78,78,78,78	0
56	MG	14	3208	1/1	0.81	0.15	89,89,89,89	0
56	MG	14	3019	1/1	0.81	0.13	70,70,70,70	0
56	MG	1H	3326	1/1	0.81	0.33	67,67,67,67	0
56	MG	14	3119	1/1	0.81	0.09	91,91,91,91	0
56	MG	1H	3424	1/1	0.81	0.20	65,65,65,65	0
56	MG	1H	3293	1/1	0.81	0.15	95,95,95,95	0
56	MG	1H	3174	1/1	0.81	0.39	86,86,86,86	0
56	MG	16	203	1/1	0.81	0.28	85,85,85,85	0
56	MG	1H	3186	1/1	0.81	0.31	97,97,97,97	0
56	MG	13	1651	1/1	0.81	0.30	91,91,91,91	0
56	MG	14	3049	1/1	0.81	0.10	89,89,89,89	0
56	MG	14	3051	1/1	0.81	0.21	75,75,75,75	0
56	MG	14	3228	1/1	0.81	0.13	79,79,79,79	0
56	MG	1H	3335	1/1	0.81	0.37	103,103,103,103	0
56	MG	14	3064	1/1	0.81	0.16	53,53,53,53	0
56	MG	14	3163	1/1	0.81	0.27	90,90,90,90	0
56	MG	1H	3160	1/1	0.81	0.13	66,66,66,66	0
56	MG	45	201	1/1	0.81	0.19	95,95,95,95	0
56	MG	1H	3016	1/1	0.82	0.33	66,66,66,66	0
56	MG	1H	3044	1/1	0.82	0.20	66,66,66,66	0
56	MG	1H	3459	1/1	0.82	0.18	102,102,102,102	0
56	MG	13	1609	1/1	0.82	0.14	83,83,83,83	0
56	MG	1H	3118	1/1	0.82	0.22	74,74,74,74	0
56	MG	1H	3385	1/1	0.82	0.35	75,75,75,75	0
56	MG	14	3273	1/1	0.82	0.20	70,70,70,70	0
56	MG	13	1638	1/1	0.82	0.30	85,85,85,85	0
56	MG	13	1726	1/1	0.82	0.13	99,99,99,99	0
56	MG	1H	3201	1/1	0.82	0.31	77,77,77,77	0
56	MG	BA	201	1/1	0.82	0.14	102,102,102,102	0
56	MG	14	3075	1/1	0.82	0.29	94,94,94,94	0
56	MG	1H	3404	1/1	0.82	0.45	80,80,80,80	0
56	MG	1H	3321	1/1	0.82	0.21	99,99,99,99	0
56	MG	1G	1641	1/1	0.82	0.21	95,95,95,95	0
56	MG	1H	3266	1/1	0.82	0.20	83,83,83,83	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	78	202	1/1	0.82	0.22	87,87,87,87	0
56	MG	14	3237	1/1	0.82	0.20	81,81,81,81	0
56	MG	1H	3407	1/1	0.82	0.28	81,81,81,81	0
56	MG	14	3239	1/1	0.82	0.14	53,53,53,53	0
56	MG	1H	3268	1/1	0.82	0.21	86,86,86,86	0
56	MG	1G	1604	1/1	0.82	0.34	87,87,87,87	0
56	MG	1H	3231	1/1	0.82	0.22	83,83,83,83	0
56	MG	1H	3168	1/1	0.82	0.14	84,84,84,84	0
56	MG	13	1604	1/1	0.82	0.21	77,77,77,77	0
56	MG	1H	3365	1/1	0.82	0.17	83,83,83,83	0
56	MG	1G	1722	1/1	0.83	0.22	111,111,111,111	0
56	MG	1H	3083	1/1	0.83	0.27	82,82,82,82	0
56	MG	2K	102	1/1	0.83	0.35	81,81,81,81	0
56	MG	14	3068	1/1	0.83	0.13	78,78,78,78	0
56	MG	14	3143	1/1	0.83	0.40	86,86,86,86	0
56	MG	14	3213	1/1	0.83	0.27	87,87,87,87	0
56	MG	14	3146	1/1	0.83	0.28	83,83,83,83	0
56	MG	13	1763	1/1	0.83	0.10	131,131,131,131	0
56	MG	16	208	1/1	0.83	0.11	95,95,95,95	0
56	MG	1H	3338	1/1	0.83	0.37	83,83,83,83	0
56	MG	14	3220	1/1	0.83	0.17	95,95,95,95	0
56	MG	14	3152	1/1	0.83	0.23	77,77,77,77	0
56	MG	1H	3310	1/1	0.83	0.27	82,82,82,82	0
56	MG	1H	3147	1/1	0.83	0.30	83,83,83,83	0
56	MG	21	302	1/1	0.83	0.16	76,76,76,76	0
56	MG	1G	1689	1/1	0.83	0.33	81,81,81,81	0
56	MG	13	1764	1/1	0.83	0.15	128,128,128,128	0
56	MG	1G	1660	1/1	0.83	0.16	91,91,91,91	0
56	MG	14	3300	1/1	0.83	0.38	84,84,84,84	0
56	MG	14	3421	1/1	0.83	0.25	72,72,72,72	0
56	MG	1H	3423	1/1	0.83	0.16	74,74,74,74	0
56	MG	14	3035	1/1	0.83	0.20	67,67,67,67	0
56	MG	14	3083	1/1	0.83	0.21	73,73,73,73	0
56	MG	13	1642	1/1	0.83	0.34	66,66,66,66	0
56	MG	13	1731	1/1	0.83	0.26	75,75,75,75	0
56	MG	1H	3226	1/1	0.83	0.25	77,77,77,77	0
56	MG	1H	3354	1/1	0.83	0.20	81,81,81,81	0
56	MG	13	1734	1/1	0.83	0.41	87,87,87,87	0
56	MG	BI	202	1/1	0.83	0.13	122,122,122,122	0
56	MG	1G	1635	1/1	0.84	0.19	106,106,106,106	0
56	MG	1G	1639	1/1	0.84	0.18	113,113,113,113	0
56	MG	1H	3280	1/1	0.84	0.29	90,90,90,90	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	14	3252	1/1	0.84	0.25	76,76,76,76	0
56	MG	1H	3235	1/1	0.84	0.13	66,66,66,66	0
56	MG	14	3090	1/1	0.84	0.25	59,59,59,59	0
56	MG	1H	3415	1/1	0.84	0.28	77,77,77,77	0
56	MG	13	1654	1/1	0.84	0.34	86,86,86,86	0
56	MG	14	3264	1/1	0.84	0.29	82,82,82,82	0
56	MG	1G	1647	1/1	0.84	0.34	92,92,92,92	0
56	MG	1G	1679	1/1	0.84	0.22	74,74,74,74	0
56	MG	1G	1681	1/1	0.84	0.32	89,89,89,89	0
56	MG	1H	3102	1/1	0.84	0.34	63,63,63,63	0
56	MG	1H	3206	1/1	0.84	0.18	73,73,73,73	0
56	MG	1H	3103	1/1	0.84	0.31	64,64,64,64	0
56	MG	1H	3210	1/1	0.84	0.24	68,68,68,68	0
56	MG	1H	3332	1/1	0.84	0.13	83,83,83,83	0
56	MG	1H	3171	1/1	0.84	0.31	90,90,90,90	0
56	MG	14	3283	1/1	0.84	0.37	84,84,84,84	0
56	MG	14	3284	1/1	0.84	0.18	77,77,77,77	0
56	MG	1H	3172	1/1	0.84	0.35	96,96,96,96	0
56	MG	13	1725	1/1	0.84	0.14	101,101,101,101	0
56	MG	14	3287	1/1	0.84	0.31	86,86,86,86	0
56	MG	16	202	1/1	0.84	0.28	77,77,77,77	0
56	MG	1H	3084	1/1	0.84	0.22	72,72,72,72	0
56	MG	13	1672	1/1	0.84	0.08	80,80,80,80	0
56	MG	14	3153	1/1	0.84	0.09	90,90,90,90	0
56	MG	1H	3228	1/1	0.84	0.29	85,85,85,85	0
56	MG	14	3321	1/1	0.84	0.12	131,131,131,131	0
56	MG	14	3226	1/1	0.84	0.28	60,60,60,60	0
56	MG	1H	3397	1/1	0.84	0.27	60,60,60,60	0
56	MG	1G	1738	1/1	0.84	0.13	105,105,105,105	0
56	MG	1H	3229	1/1	0.84	0.25	83,83,83,83	0
56	MG	14	3165	1/1	0.84	0.27	83,83,83,83	0
56	MG	14	3166	1/1	0.84	0.17	88,88,88,88	0
56	MG	1H	3155	1/1	0.84	0.22	73,73,73,73	0
56	MG	13	1627	1/1	0.84	0.25	93,93,93,93	0
56	MG	14	3244	1/1	0.84	0.23	67,67,67,67	0
56	MG	1H	3119	1/1	0.84	0.29	76,76,76,76	0
56	MG	14	3001	1/1	0.85	0.30	76,76,76,76	0
56	MG	1H	3157	1/1	0.85	0.32	78,78,78,78	0
56	MG	1G	1637	1/1	0.85	0.14	121,121,121,121	0
56	MG	1H	3086	1/1	0.85	0.19	83,83,83,83	0
56	MG	1H	3055	1/1	0.85	0.19	69,69,69,69	0
56	MG	13	1712	1/1	0.85	0.08	106,106,106,106	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	14	3101	1/1	0.85	0.34	79,79,79,79	0
56	MG	13	1723	1/1	0.85	0.20	98,98,98,98	0
56	MG	14	3030	1/1	0.85	0.19	78,78,78,78	0
56	MG	1H	3409	1/1	0.85	0.37	75,75,75,75	0
56	MG	1H	3037	1/1	0.85	0.21	57,57,57,57	0
56	MG	1H	3413	1/1	0.85	0.24	81,81,81,81	0
56	MG	1H	3307	1/1	0.85	0.21	89,89,89,89	0
56	MG	14	3277	1/1	0.85	0.35	90,90,90,90	0
56	MG	14	3279	1/1	0.85	0.41	96,96,96,96	0
56	MG	14	3215	1/1	0.85	0.24	94,94,94,94	0
56	MG	14	3129	1/1	0.85	0.40	84,84,84,84	0
56	MG	1H	3188	1/1	0.85	0.07	90,90,90,90	0
56	MG	1H	3237	1/1	0.85	0.11	72,72,72,72	0
56	MG	1H	3208	1/1	0.85	0.28	86,86,86,86	0
56	MG	14	3145	1/1	0.85	0.30	88,88,88,88	0
56	MG	1H	3240	1/1	0.85	0.24	64,64,64,64	0
56	MG	14	3288	1/1	0.85	0.35	94,94,94,94	0
56	MG	1H	3145	1/1	0.85	0.43	91,91,91,91	0
56	MG	1H	3367	1/1	0.85	0.12	97,97,97,97	0
56	MG	14	3295	1/1	0.85	0.28	91,91,91,91	0
56	MG	13	1719	1/1	0.85	0.27	106,106,106,106	0
56	MG	14	3066	1/1	0.85	0.26	67,67,67,67	0
56	MG	1G	1617	1/1	0.85	0.14	92,92,92,92	0
56	MG	1H	3249	1/1	0.85	0.15	70,70,70,70	0
56	MG	14	3330	1/1	0.85	0.12	82,82,82,82	0
56	MG	1G	1661	1/1	0.85	0.31	94,94,94,94	0
56	MG	13	1747	1/1	0.85	0.17	93,93,93,93	0
56	MG	14	3073	1/1	0.85	0.19	72,72,72,72	0
56	MG	1J	203	1/1	0.85	0.12	98,98,98,98	0
56	MG	1H	3222	1/1	0.85	0.28	78,78,78,78	0
56	MG	1H	3255	1/1	0.85	0.29	75,75,75,75	0
56	MG	14	3169	1/1	0.85	0.58	73,73,73,73	0
56	MG	1H	3256	1/1	0.85	0.27	85,85,85,85	0
56	MG	1H	3391	1/1	0.85	0.24	61,61,61,61	0
56	MG	1H	3031	1/1	0.85	0.26	56,56,56,56	0
56	MG	13	1660	1/1	0.85	0.29	83,83,83,83	0
56	MG	1H	3184	1/1	0.86	0.52	79,79,79,79	0
56	MG	14	3102	1/1	0.86	0.18	67,67,67,67	0
56	MG	14	3053	1/1	0.86	0.14	72,72,72,72	0
56	MG	14	3173	1/1	0.86	0.19	77,77,77,77	0
56	MG	14	3112	1/1	0.86	0.22	83,83,83,83	0
56	MG	1H	3185	1/1	0.86	0.14	87,87,87,87	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	1H	3097	1/1	0.86	0.15	70,70,70,70	0
56	MG	1H	3009	1/1	0.86	0.23	66,66,66,66	0
56	MG	14	3191	1/1	0.86	0.16	84,84,84,84	0
56	MG	1H	3213	1/1	0.86	0.11	69,69,69,69	0
56	MG	1G	1631	1/1	0.86	0.20	85,85,85,85	0
56	MG	14	3291	1/1	0.86	0.28	86,86,86,86	0
56	MG	14	3293	1/1	0.86	0.27	81,81,81,81	0
56	MG	1H	3136	1/1	0.86	0.26	68,68,68,68	0
56	MG	1H	3139	1/1	0.86	0.31	79,79,79,79	0
56	MG	1H	3082	1/1	0.86	0.28	76,76,76,76	0
56	MG	1H	3025	1/1	0.86	0.15	49,49,49,49	0
56	MG	14	3022	1/1	0.86	0.26	78,78,78,78	0
56	MG	1H	3104	1/1	0.86	0.29	65,65,65,65	0
56	MG	1H	3550	1/1	0.86	0.12	70,70,70,70	0
56	MG	13	1693	1/1	0.86	0.12	82,82,82,82	0
56	MG	1H	3150	1/1	0.86	0.20	88,88,88,88	0
56	MG	1G	1697	1/1	0.86	0.15	106,106,106,106	0
56	MG	1H	3357	1/1	0.86	0.07	66,66,66,66	0
56	MG	13	1633	1/1	0.86	0.30	82,82,82,82	0
56	MG	14	3043	1/1	0.86	0.10	73,73,73,73	0
56	MG	14	3271	1/1	0.86	0.28	73,73,73,73	0
56	MG	14	3089	1/1	0.86	0.21	72,72,72,72	0
56	MG	1H	3065	1/1	0.86	0.18	69,69,69,69	0
56	MG	13	1605	1/1	0.86	0.09	86,86,86,86	0
56	MG	1H	3096	1/1	0.86	0.14	63,63,63,63	0
56	MG	85	201	1/1	0.86	0.50	75,75,75,75	0
56	MG	1G	1698	1/1	0.87	0.33	88,88,88,88	0
56	MG	1H	3131	1/1	0.87	0.29	65,65,65,65	0
56	MG	1H	3161	1/1	0.87	0.34	76,76,76,76	0
56	MG	1H	3018	1/1	0.87	0.28	49,49,49,49	0
56	MG	1H	3019	1/1	0.87	0.13	53,53,53,53	0
56	MG	1H	3020	1/1	0.87	0.15	56,56,56,56	0
56	MG	1G	1632	1/1	0.87	0.38	83,83,83,83	0
56	MG	14	3278	1/1	0.87	0.10	74,74,74,74	0
56	MG	1H	3003	1/1	0.87	0.29	56,56,56,56	0
56	MG	14	3148	1/1	0.87	0.18	84,84,84,84	0
56	MG	1H	3056	1/1	0.87	0.17	73,73,73,73	0
56	MG	1H	3275	1/1	0.87	0.08	70,70,70,70	0
56	MG	1H	3058	1/1	0.87	0.24	69,69,69,69	0
56	MG	1H	3353	1/1	0.87	0.24	77,77,77,77	0
56	MG	1H	3306	1/1	0.87	0.45	87,87,87,87	0
56	MG	1H	3246	1/1	0.87	0.14	81,81,81,81	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	1H	3218	1/1	0.87	0.24	70,70,70,70	0
56	MG	14	3227	1/1	0.87	0.38	75,75,75,75	0
56	MG	14	3011	1/1	0.87	0.09	70,70,70,70	0
56	MG	14	3292	1/1	0.87	0.23	88,88,88,88	0
56	MG	1G	1645	1/1	0.87	0.25	101,101,101,101	0
56	MG	1G	1602	1/1	0.87	0.17	83,83,83,83	0
56	MG	1H	3219	1/1	0.87	0.43	98,98,98,98	0
56	MG	1G	1683	1/1	0.87	0.42	87,87,87,87	0
56	MG	1H	3317	1/1	0.87	0.11	102,102,102,102	0
56	MG	13	1746	1/1	0.87	0.14	96,96,96,96	0
56	MG	14	3240	1/1	0.87	0.25	86,86,86,86	0
56	MG	1H	3364	1/1	0.87	0.19	87,87,87,87	0
56	MG	14	3099	1/1	0.87	0.11	66,66,66,66	0
56	MG	1H	3149	1/1	0.87	0.33	64,64,64,64	0
56	MG	1H	3285	1/1	0.87	0.60	85,85,85,85	0
56	MG	14	3184	1/1	0.87	0.30	85,85,85,85	0
56	MG	14	3190	1/1	0.87	0.29	81,81,81,81	0
56	MG	14	3108	1/1	0.87	0.10	81,81,81,81	0
56	MG	1H	3287	1/1	0.87	0.14	80,80,80,80	0
56	MG	1H	3116	1/1	0.87	0.26	71,71,71,71	0
56	MG	13	1687	1/1	0.87	0.34	82,82,82,82	0
56	MG	1H	3015	1/1	0.87	0.21	47,47,47,47	0
56	MG	13	1677	1/1	0.87	0.24	94,94,94,94	0
56	MG	14	3052	1/1	0.87	0.11	78,78,78,78	0
56	MG	14	3167	1/1	0.88	0.11	81,81,81,81	0
56	MG	1H	3076	1/1	0.88	0.17	88,88,88,88	0
56	MG	1H	3319	1/1	0.88	0.22	85,85,85,85	0
56	MG	1H	3274	1/1	0.88	0.26	79,79,79,79	0
56	MG	1H	3142	1/1	0.88	0.13	79,79,79,79	0
56	MG	98	201	1/1	0.88	0.26	56,56,56,56	0
56	MG	1H	3323	1/1	0.88	0.10	69,69,69,69	0
56	MG	14	3180	1/1	0.88	0.12	82,82,82,82	0
56	MG	13	1692	1/1	0.88	0.12	102,102,102,102	0
56	MG	1H	3232	1/1	0.88	0.20	82,82,82,82	0
56	MG	13	1724	1/1	0.88	0.12	97,97,97,97	0
56	MG	13	1614	1/1	0.88	0.14	69,69,69,69	0
56	MG	1H	3105	1/1	0.88	0.23	54,54,54,54	0
56	MG	14	3274	1/1	0.88	0.11	64,64,64,64	0
56	MG	13	1704	1/1	0.88	0.11	85,85,85,85	0
56	MG	14	3194	1/1	0.88	0.18	75,75,75,75	0
56	MG	1H	3024	1/1	0.88	0.22	54,54,54,54	0
56	MG	14	3097	1/1	0.88	0.10	76,76,76,76	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	1H	3244	1/1	0.88	0.08	70,70,70,70	0
56	MG	14	3017	1/1	0.88	0.17	77,77,77,77	0
56	MG	1H	3289	1/1	0.88	0.20	85,85,85,85	0
56	MG	14	3282	1/1	0.88	0.25	67,67,67,67	0
56	MG	14	3106	1/1	0.88	0.23	80,80,80,80	0
56	MG	1H	3245	1/1	0.88	0.24	57,57,57,57	0
56	MG	1H	3182	1/1	0.88	0.12	85,85,85,85	0
56	MG	1H	3341	1/1	0.88	0.11	80,80,80,80	0
56	MG	14	3114	1/1	0.88	0.29	60,60,60,60	0
56	MG	1H	3048	1/1	0.88	0.27	67,67,67,67	0
56	MG	1H	3211	1/1	0.88	0.25	80,80,80,80	0
56	MG	1H	3087	1/1	0.88	0.16	54,54,54,54	0
56	MG	1H	3156	1/1	0.88	0.37	69,69,69,69	0
56	MG	1G	1630	1/1	0.88	0.28	95,95,95,95	0
56	MG	1H	3217	1/1	0.88	0.22	87,87,87,87	0
56	MG	13	1670	1/1	0.88	0.15	84,84,84,84	0
56	MG	1H	3050	1/1	0.88	0.22	51,51,51,51	0
56	MG	14	3140	1/1	0.88	0.18	88,88,88,88	0
56	MG	1H	3469	1/1	0.88	0.14	93,93,93,93	0
56	MG	1G	1686	1/1	0.88	0.36	69,69,69,69	0
56	MG	1H	3120	1/1	0.88	0.24	75,75,75,75	0
56	MG	1H	3095	1/1	0.88	0.09	64,64,64,64	0
56	MG	1H	3264	1/1	0.88	0.25	74,74,74,74	0
56	MG	14	3057	1/1	0.88	0.20	78,78,78,78	0
56	MG	14	3061	1/1	0.88	0.09	74,74,74,74	0
56	MG	1H	3223	1/1	0.88	0.10	65,65,65,65	0
56	MG	1H	3068	1/1	0.88	0.23	65,65,65,65	0
56	MG	1H	3070	1/1	0.88	0.25	78,78,78,78	0
56	MG	1H	3366	1/1	0.88	0.24	89,89,89,89	0
56	MG	1H	3194	1/1	0.88	0.29	62,62,62,62	0
56	MG	1H	3098	1/1	0.88	0.28	66,66,66,66	0
56	MG	1H	3313	1/1	0.88	0.23	87,87,87,87	0
56	MG	1H	3376	1/1	0.88	0.20	113,113,113,113	0
56	MG	E5	101	1/1	0.88	0.09	67,67,67,67	0
56	MG	1H	3267	1/1	0.89	0.16	84,84,84,84	0
56	MG	13	1709	1/1	0.89	0.24	73,73,73,73	0
56	MG	13	1745	1/1	0.89	0.11	87,87,87,87	0
56	MG	1H	3270	1/1	0.89	0.44	87,87,87,87	0
56	MG	1H	3039	1/1	0.89	0.25	62,62,62,62	0
56	MG	1H	3309	1/1	0.89	0.13	76,76,76,76	0
56	MG	14	3087	1/1	0.89	0.22	60,60,60,60	0
56	MG	13	1691	1/1	0.89	0.21	94,94,94,94	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	14	3012	1/1	0.89	0.35	66,66,66,66	0
56	MG	1H	3001	1/1	0.89	0.26	55,55,55,55	0
56	MG	1H	3362	1/1	0.89	0.14	69,69,69,69	0
56	MG	1H	3047	1/1	0.89	0.26	60,60,60,60	0
56	MG	1G	1629	1/1	0.89	0.46	84,84,84,84	0
56	MG	13	1697	1/1	0.89	0.16	98,98,98,98	0
56	MG	1H	3547	1/1	0.89	0.13	85,85,85,85	0
56	MG	14	3033	1/1	0.89	0.30	86,86,86,86	0
56	MG	1H	3005	1/1	0.89	0.20	56,56,56,56	0
56	MG	13	1702	1/1	0.89	0.07	87,87,87,87	0
56	MG	14	3037	1/1	0.89	0.24	61,61,61,61	0
56	MG	14	3040	1/1	0.89	0.21	62,62,62,62	0
56	MG	1H	3152	1/1	0.89	0.12	75,75,75,75	0
56	MG	13	1679	1/1	0.89	0.16	83,83,83,83	0
56	MG	14	3122	1/1	0.89	0.16	55,55,55,55	0
56	MG	1G	1636	1/1	0.89	0.17	99,99,99,99	0
56	MG	1H	3011	1/1	0.89	0.08	46,46,46,46	0
56	MG	1H	3375	1/1	0.89	0.18	70,70,70,70	0
56	MG	1G	1688	1/1	0.89	0.16	89,89,89,89	0
56	MG	14	3130	1/1	0.89	0.14	65,65,65,65	0
56	MG	1H	3014	1/1	0.89	0.16	62,62,62,62	0
56	MG	1H	3057	1/1	0.89	0.24	52,52,52,52	0
56	MG	1H	3329	1/1	0.89	0.20	75,75,75,75	0
56	MG	1H	3220	1/1	0.89	0.34	79,79,79,79	0
56	MG	1H	3091	1/1	0.89	0.20	68,68,68,68	0
56	MG	14	3297	1/1	0.89	0.31	91,91,91,91	0
56	MG	1H	3254	1/1	0.89	0.23	68,68,68,68	0
56	MG	14	3063	1/1	0.89	0.16	80,80,80,80	0
56	MG	1H	3393	1/1	0.89	0.14	65,65,65,65	0
56	MG	1H	3123	1/1	0.89	0.21	70,70,70,70	0
56	MG	1H	3125	1/1	0.89	0.11	52,52,52,52	0
56	MG	14	3231	1/1	0.89	0.24	57,57,57,57	0
56	MG	14	3067	1/1	0.89	0.10	62,62,62,62	0
56	MG	13	1765	1/1	0.89	0.18	129,129,129,129	0
56	MG	1H	3259	1/1	0.89	0.12	69,69,69,69	0
56	MG	14	3156	1/1	0.89	0.31	68,68,68,68	0
56	MG	14	3159	1/1	0.89	0.26	66,66,66,66	0
56	MG	1H	3130	1/1	0.89	0.24	70,70,70,70	0
56	MG	14	3241	1/1	0.89	0.24	59,59,59,59	0
56	MG	1H	3196	1/1	0.89	0.12	68,68,68,68	0
56	MG	1H	3344	1/1	0.89	0.14	89,89,89,89	0
56	MG	13	1708	1/1	0.89	0.20	76,76,76,76	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	1H	3410	1/1	0.89	0.40	71,71,71,71	0
56	MG	13	1730	1/1	0.89	0.14	100,100,100,100	0
56	MG	14	3157	1/1	0.90	0.31	86,86,86,86	0
56	MG	1H	3071	1/1	0.90	0.07	71,71,71,71	0
56	MG	1H	3325	1/1	0.90	0.24	90,90,90,90	0
56	MG	14	3247	1/1	0.90	0.21	59,59,59,59	0
56	MG	1G	1729	1/1	0.90	0.11	113,113,113,113	0
56	MG	14	3072	1/1	0.90	0.08	69,69,69,69	0
56	MG	13	1647	1/1	0.90	0.09	97,97,97,97	0
56	MG	1G	1752	1/1	0.90	0.16	139,139,139,139	0
56	MG	13	1613	1/1	0.90	0.18	78,78,78,78	0
56	MG	13	1661	1/1	0.90	0.18	75,75,75,75	0
56	MG	13	1626	1/1	0.90	0.12	78,78,78,78	0
56	MG	14	3263	1/1	0.90	0.36	81,81,81,81	0
56	MG	1H	3419	1/1	0.90	0.13	77,77,77,77	0
56	MG	1B	101	1/1	0.90	0.17	92,92,92,92	0
56	MG	1H	3420	1/1	0.90	0.30	75,75,75,75	0
56	MG	1H	3043	1/1	0.90	0.21	48,48,48,48	0
56	MG	13	1793	1/1	0.90	0.14	114,114,114,114	0
56	MG	1H	3370	1/1	0.90	0.13	84,84,84,84	0
56	MG	1H	3372	1/1	0.90	0.24	71,71,71,71	0
56	MG	1G	1619	1/1	0.90	0.12	94,94,94,94	0
56	MG	14	3094	1/1	0.90	0.28	64,64,64,64	0
56	MG	1H	3241	1/1	0.90	0.18	93,93,93,93	0
56	MG	14	3192	1/1	0.90	0.07	77,77,77,77	0
56	MG	1G	1667	1/1	0.90	0.15	104,104,104,104	0
56	MG	14	3018	1/1	0.90	0.21	66,66,66,66	0
56	MG	1H	3426	1/1	0.90	0.31	80,80,80,80	0
56	MG	1H	3137	1/1	0.90	0.32	74,74,74,74	0
56	MG	1H	3466	1/1	0.90	0.08	115,115,115,115	0
56	MG	1H	3164	1/1	0.90	0.13	78,78,78,78	0
56	MG	1H	3192	1/1	0.90	0.17	75,75,75,75	0
56	MG	1H	3138	1/1	0.90	0.17	75,75,75,75	0
56	MG	1H	3618	1/1	0.90	0.20	104,104,104,104	0
56	MG	1G	1676	1/1	0.90	0.14	81,81,81,81	0
56	MG	1H	3383	1/1	0.90	0.25	58,58,58,58	0
56	MG	14	3038	1/1	0.90	0.20	63,63,63,63	0
56	MG	1H	3060	1/1	0.90	0.19	63,63,63,63	0
56	MG	1G	1680	1/1	0.90	0.25	69,69,69,69	0
56	MG	1H	3278	1/1	0.90	0.32	69,69,69,69	0
56	MG	1H	3112	1/1	0.90	0.13	57,57,57,57	0
56	MG	1H	3046	1/1	0.90	0.11	73,73,73,73	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	13	1645	1/1	0.90	0.19	74,74,74,74	0
56	MG	1H	3311	1/1	0.90	0.13	98,98,98,98	0
56	MG	14	3133	1/1	0.90	0.35	78,78,78,78	0
56	MG	1G	1638	1/1	0.90	0.22	93,93,93,93	0
56	MG	14	3138	1/1	0.90	0.15	71,71,71,71	0
56	MG	1H	3399	1/1	0.90	0.24	61,61,61,61	0
56	MG	14	3372	1/1	0.90	0.15	91,91,91,91	0
56	MG	1H	3115	1/1	0.90	0.13	69,69,69,69	0
56	MG	14	3054	1/1	0.90	0.09	48,48,48,48	0
56	MG	14	3229	1/1	0.90	0.23	92,92,92,92	0
56	MG	1H	3063	1/1	0.90	0.22	54,54,54,54	0
56	MG	1G	1643	1/1	0.90	0.25	92,92,92,92	0
56	MG	1H	3284	1/1	0.90	0.38	79,79,79,79	0
56	MG	16	212	1/1	0.90	0.49	65,65,65,65	0
56	MG	14	3236	1/1	0.90	0.16	69,69,69,69	0
56	MG	21	301	1/1	0.90	0.07	64,64,64,64	0
56	MG	13	1698	1/1	0.90	0.14	99,99,99,99	0
56	MG	68	201	1/1	0.90	0.13	84,84,84,84	0
56	MG	1H	3022	1/1	0.90	0.20	51,51,51,51	0
56	MG	13	1653	1/1	0.90	0.13	82,82,82,82	0
56	MG	1H	3180	1/1	0.91	0.32	88,88,88,88	0
56	MG	14	3158	1/1	0.91	0.25	80,80,80,80	0
56	MG	1H	3403	1/1	0.91	0.23	76,76,76,76	0
56	MG	14	3160	1/1	0.91	0.41	86,86,86,86	0
56	MG	1H	3296	1/1	0.91	0.08	68,68,68,68	0
56	MG	13	1795	1/1	0.91	0.09	100,100,100,100	0
56	MG	1H	3033	1/1	0.91	0.18	64,64,64,64	0
56	MG	14	3254	1/1	0.91	0.26	55,55,55,55	0
56	MG	14	3258	1/1	0.91	0.27	50,50,50,50	0
56	MG	13	1648	1/1	0.91	0.40	77,77,77,77	0
56	MG	2I	201	1/1	0.91	0.14	91,91,91,91	0
56	MG	2L	101	1/1	0.91	0.21	86,86,86,86	0
56	MG	1H	3349	1/1	0.91	0.28	74,74,74,74	0
56	MG	1H	3262	1/1	0.91	0.10	73,73,73,73	0
56	MG	1H	3351	1/1	0.91	0.08	68,68,68,68	0
56	MG	14	3265	1/1	0.91	0.21	83,83,83,83	0
56	MG	13	1629	1/1	0.91	0.19	71,71,71,71	0
56	MG	14	3267	1/1	0.91	0.14	77,77,77,77	0
56	MG	14	3084	1/1	0.91	0.17	77,77,77,77	0
56	MG	1H	3088	1/1	0.91	0.21	62,62,62,62	0
56	MG	14	3010	1/1	0.91	0.25	68,68,68,68	0
56	MG	13	1688	1/1	0.91	0.30	86,86,86,86	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	14	3092	1/1	0.91	0.20	79,79,79,79	0
56	MG	1H	3189	1/1	0.91	0.36	77,77,77,77	0
56	MG	13	1603	1/1	0.91	0.06	52,52,52,52	0
56	MG	1H	3121	1/1	0.91	0.23	67,67,67,67	0
56	MG	1H	3159	1/1	0.91	0.20	66,66,66,66	0
56	MG	1K	500	1/1	0.91	0.12	101,101,101,101	0
56	MG	1G	1623	1/1	0.91	0.15	86,86,86,86	0
56	MG	14	3195	1/1	0.91	0.13	84,84,84,84	0
56	MG	14	3026	1/1	0.91	0.17	65,65,65,65	0
56	MG	14	3105	1/1	0.91	0.17	64,64,64,64	0
56	MG	2K	101	1/1	0.91	0.23	69,69,69,69	0
56	MG	13	1713	1/1	0.91	0.13	82,82,82,82	0
56	MG	14	3110	1/1	0.91	0.38	85,85,85,85	0
56	MG	1H	3067	1/1	0.91	0.16	68,68,68,68	0
56	MG	1G	1677	1/1	0.91	0.09	94,94,94,94	0
56	MG	1H	3439	1/1	0.91	0.15	59,59,59,59	0
56	MG	13	1631	1/1	0.91	0.15	88,88,88,88	0
56	MG	13	1715	1/1	0.91	0.13	102,102,102,102	0
56	MG	14	3120	1/1	0.91	0.21	70,70,70,70	0
56	MG	1H	3166	1/1	0.91	0.14	87,87,87,87	0
56	MG	1H	3519	1/1	0.91	0.10	73,73,73,73	0
56	MG	1H	3239	1/1	0.91	0.13	78,78,78,78	0
56	MG	1H	3167	1/1	0.91	0.12	83,83,83,83	0
56	MG	14	3128	1/1	0.91	0.26	82,82,82,82	0
56	MG	1H	3135	1/1	0.91	0.22	59,59,59,59	0
56	MG	13	1616	1/1	0.91	0.12	79,79,79,79	0
56	MG	14	3301	1/1	0.91	0.14	85,85,85,85	0
56	MG	1H	3073	1/1	0.91	0.24	58,58,58,58	0
56	MG	1H	3380	1/1	0.91	0.28	66,66,66,66	0
56	MG	13	1774	1/1	0.91	0.12	87,87,87,87	0
56	MG	1H	3331	1/1	0.91	0.11	69,69,69,69	0
56	MG	1H	3286	1/1	0.91	0.23	68,68,68,68	0
56	MG	13	1779	1/1	0.91	0.15	106,106,106,106	0
56	MG	1H	3141	1/1	0.91	0.21	71,71,71,71	0
56	MG	1H	3392	1/1	0.91	0.27	54,54,54,54	0
56	MG	1H	3106	1/1	0.91	0.14	77,77,77,77	0
56	MG	13	1701	1/1	0.91	0.14	95,95,95,95	0
56	MG	29	301	1/1	0.91	0.07	78,78,78,78	0
56	MG	1H	3110	1/1	0.91	0.21	50,50,50,50	0
56	MG	11	301	1/1	0.91	0.30	47,47,47,47	0
56	MG	1G	1710	1/1	0.91	0.13	102,102,102,102	0
56	MG	1G	1712	1/1	0.91	0.07	132,132,132,132	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	1H	3215	1/1	0.91	0.10	61,61,61,61	0
56	MG	1H	3400	1/1	0.91	0.24	48,48,48,48	0
56	MG	13	1757	1/1	0.92	0.07	119,119,119,119	0
56	MG	1H	3053	1/1	0.92	0.07	53,53,53,53	0
56	MG	1H	3151	1/1	0.92	0.31	78,78,78,78	0
56	MG	1H	3170	1/1	0.92	0.18	73,73,73,73	0
56	MG	1H	3427	1/1	0.92	0.21	64,64,64,64	0
56	MG	1H	3434	1/1	0.92	0.07	86,86,86,86	0
56	MG	1G	1613	1/1	0.92	0.12	88,88,88,88	0
56	MG	14	3007	1/1	0.92	0.21	61,61,61,61	0
56	MG	14	3008	1/1	0.92	0.18	72,72,72,72	0
56	MG	14	3172	1/1	0.92	0.06	77,77,77,77	0
56	MG	1H	3387	1/1	0.92	0.35	71,71,71,71	0
56	MG	14	3174	1/1	0.92	0.07	81,81,81,81	0
56	MG	14	3177	1/1	0.92	0.12	92,92,92,92	0
56	MG	1H	3441	1/1	0.92	0.07	115,115,115,115	0
56	MG	1H	3445	1/1	0.92	0.22	90,90,90,90	0
56	MG	1H	3314	1/1	0.92	0.11	72,72,72,72	0
56	MG	1H	3209	1/1	0.92	0.28	80,80,80,80	0
56	MG	1H	3318	1/1	0.92	0.11	68,68,68,68	0
56	MG	1H	3471	1/1	0.92	0.12	91,91,91,91	0
56	MG	1H	3472	1/1	0.92	0.08	108,108,108,108	0
56	MG	1H	3394	1/1	0.92	0.20	67,67,67,67	0
56	MG	1H	3352	1/1	0.92	0.13	68,68,68,68	0
56	MG	14	3027	1/1	0.92	0.26	61,61,61,61	0
56	MG	1H	3288	1/1	0.92	0.13	79,79,79,79	0
56	MG	1H	3568	1/1	0.92	0.12	89,89,89,89	0
56	MG	14	3032	1/1	0.92	0.22	73,73,73,73	0
56	MG	1H	3608	1/1	0.92	0.07	110,110,110,110	0
56	MG	1H	3320	1/1	0.92	0.17	94,94,94,94	0
56	MG	1G	1682	1/1	0.92	0.13	79,79,79,79	0
56	MG	14	3203	1/1	0.92	0.20	83,83,83,83	0
56	MG	1H	3621	1/1	0.92	0.09	52,52,52,52	0
56	MG	14	3205	1/1	0.92	0.11	75,75,75,75	0
56	MG	1H	3069	1/1	0.92	0.22	80,80,80,80	0
56	MG	13	1652	1/1	0.92	0.12	75,75,75,75	0
56	MG	1H	3402	1/1	0.92	0.14	58,58,58,58	0
56	MG	1H	3236	1/1	0.92	0.10	80,80,80,80	0
56	MG	1H	3173	1/1	0.92	0.20	67,67,67,67	0
56	MG	13	1617	1/1	0.92	0.16	84,84,84,84	0
56	MG	1H	3012	1/1	0.92	0.08	40,40,40,40	0
56	MG	1G	1640	1/1	0.92	0.08	82,82,82,82	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	1H	3216	1/1	0.92	0.13	81,81,81,81	0
56	MG	13	1602	1/1	0.92	0.21	59,59,59,59	0
56	MG	14	3132	1/1	0.92	0.21	58,58,58,58	0
56	MG	14	3221	1/1	0.92	0.13	88,88,88,88	0
56	MG	1G	1695	1/1	0.92	0.44	96,96,96,96	0
56	MG	14	3135	1/1	0.92	0.12	90,90,90,90	0
56	MG	1H	3243	1/1	0.92	0.20	60,60,60,60	0
56	MG	14	3311	1/1	0.92	0.08	105,105,105,105	0
56	MG	14	3317	1/1	0.92	0.22	153,153,153,153	0
56	MG	14	3318	1/1	0.92	0.12	84,84,84,84	0
56	MG	1H	3042	1/1	0.92	0.10	79,79,79,79	0
56	MG	14	3056	1/1	0.92	0.13	80,80,80,80	0
56	MG	13	1743	1/1	0.92	0.09	91,91,91,91	0
56	MG	14	3400	1/1	0.92	0.15	87,87,87,87	0
56	MG	1H	3414	1/1	0.92	0.14	68,68,68,68	0
56	MG	1H	3197	1/1	0.92	0.19	65,65,65,65	0
56	MG	1H	3416	1/1	0.92	0.21	75,75,75,75	0
56	MG	1G	1708	1/1	0.92	0.13	105,105,105,105	0
56	MG	31	301	1/1	0.92	0.05	67,67,67,67	0
56	MG	13	1625	1/1	0.92	0.19	75,75,75,75	0
56	MG	13	1785	1/1	0.92	0.13	105,105,105,105	0
56	MG	13	1636	1/1	0.92	0.14	85,85,85,85	0
56	MG	13	1637	1/1	0.92	0.09	67,67,67,67	0
56	MG	1G	1748	1/1	0.92	0.10	107,107,107,107	0
56	MG	1H	3203	1/1	0.92	0.10	70,70,70,70	0
56	MG	P8	101	1/1	0.92	0.21	68,68,68,68	0
56	MG	55	201	1/1	0.92	0.40	85,85,85,85	0
56	MG	1G	1601	1/1	0.92	0.08	71,71,71,71	0
56	MG	13	1748	1/1	0.92	0.10	122,122,122,122	0
56	MG	68	202	1/1	0.93	0.16	90,90,90,90	0
56	MG	13	1635	1/1	0.93	0.18	75,75,75,75	0
56	MG	1H	3355	1/1	0.93	0.12	62,62,62,62	0
56	MG	1H	3478	1/1	0.93	0.11	68,68,68,68	0
56	MG	1H	3109	1/1	0.93	0.21	44,44,44,44	0
56	MG	I8	101	1/1	0.93	0.41	83,83,83,83	0
56	MG	1H	3040	1/1	0.93	0.09	62,62,62,62	0
56	MG	14	3103	1/1	0.93	0.24	78,78,78,78	0
56	MG	14	3161	1/1	0.93	0.12	66,66,66,66	0
56	MG	14	3104	1/1	0.93	0.17	48,48,48,48	0
56	MG	2L	102	1/1	0.93	0.07	113,113,113,113	0
56	MG	Q8	101	1/1	0.93	0.28	68,68,68,68	0
56	MG	13	1612	1/1	0.93	0.12	71,71,71,71	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	1H	3200	1/1	0.93	0.05	79,79,79,79	0
56	MG	1G	1603	1/1	0.93	0.15	78,78,78,78	0
56	MG	1H	3580	1/1	0.93	0.16	77,77,77,77	0
56	MG	1H	3599	1/1	0.93	0.10	85,85,85,85	0
56	MG	14	3289	1/1	0.93	0.32	79,79,79,79	0
56	MG	14	3116	1/1	0.93	0.12	57,57,57,57	0
56	MG	1H	3124	1/1	0.93	0.14	52,52,52,52	0
56	MG	14	3118	1/1	0.93	0.06	66,66,66,66	0
56	MG	1H	3234	1/1	0.93	0.18	67,67,67,67	0
56	MG	BI	201	1/1	0.93	0.07	113,113,113,113	0
56	MG	14	3121	1/1	0.93	0.18	65,65,65,65	0
56	MG	1H	3158	1/1	0.93	0.30	81,81,81,81	0
56	MG	1H	3127	1/1	0.93	0.17	81,81,81,81	0
56	MG	1H	3342	1/1	0.93	0.17	75,75,75,75	0
56	MG	14	3242	1/1	0.93	0.19	66,66,66,66	0
56	MG	14	3243	1/1	0.93	0.13	52,52,52,52	0
56	MG	14	3306	1/1	0.93	0.09	66,66,66,66	0
56	MG	1H	3298	1/1	0.93	0.07	82,82,82,82	0
56	MG	14	3021	1/1	0.93	0.16	47,47,47,47	0
56	MG	1H	3257	1/1	0.93	0.09	82,82,82,82	0
56	MG	1H	3128	1/1	0.93	0.14	60,60,60,60	0
56	MG	1H	3428	1/1	0.93	0.24	57,57,57,57	0
56	MG	14	3352	1/1	0.93	0.14	90,90,90,90	0
56	MG	14	3367	1/1	0.93	0.13	86,86,86,86	0
56	MG	1H	3430	1/1	0.93	0.22	80,80,80,80	0
56	MG	14	3393	1/1	0.93	0.07	67,67,67,67	0
56	MG	1H	3373	1/1	0.93	0.28	84,84,84,84	0
56	MG	14	3405	1/1	0.93	0.08	108,108,108,108	0
56	MG	14	3420	1/1	0.93	0.06	86,86,86,86	0
56	MG	13	1740	1/1	0.93	0.34	76,76,76,76	0
56	MG	14	3424	1/1	0.93	0.07	94,94,94,94	0
56	MG	14	3136	1/1	0.93	0.17	58,58,58,58	0
56	MG	13	1639	1/1	0.93	0.19	76,76,76,76	0
56	MG	14	3199	1/1	0.93	0.09	67,67,67,67	0
56	MG	1H	3078	1/1	0.93	0.06	59,59,59,59	0
56	MG	1H	3451	1/1	0.93	0.21	85,85,85,85	0
56	MG	1H	3242	1/1	0.93	0.14	82,82,82,82	0
56	MG	1H	3132	1/1	0.93	0.20	46,46,46,46	0
56	MG	29	302	1/1	0.93	0.09	57,57,57,57	0
56	MG	29	303	1/1	0.93	0.16	64,64,64,64	0
56	MG	21	303	1/1	0.93	0.17	51,51,51,51	0
56	MG	1H	3107	1/1	0.93	0.12	63,63,63,63	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	41	201	1/1	0.93	0.12	69,69,69,69	0
56	MG	1H	3470	1/1	0.93	0.15	94,94,94,94	0
56	MG	14	3093	1/1	0.93	0.14	56,56,56,56	0
56	MG	14	3270	1/1	0.93	0.21	70,70,70,70	0
56	MG	14	3212	1/1	0.93	0.13	91,91,91,91	0
56	MG	1G	1685	1/1	0.94	0.26	76,76,76,76	0
56	MG	13	1640	1/1	0.94	0.07	65,65,65,65	0
56	MG	1H	3324	1/1	0.94	0.21	78,78,78,78	0
56	MG	88	203	1/1	0.94	0.36	79,79,79,79	0
56	MG	14	3098	1/1	0.94	0.10	67,67,67,67	0
56	MG	14	3175	1/1	0.94	0.12	70,70,70,70	0
56	MG	14	3176	1/1	0.94	0.09	73,73,73,73	0
56	MG	1H	3475	1/1	0.94	0.11	58,58,58,58	0
56	MG	1H	3260	1/1	0.94	0.10	69,69,69,69	0
56	MG	1H	3498	1/1	0.94	0.07	70,70,70,70	0
56	MG	14	3031	1/1	0.94	0.14	63,63,63,63	0
56	MG	14	3181	1/1	0.94	0.17	87,87,87,87	0
56	MG	13	1744	1/1	0.94	0.07	81,81,81,81	0
56	MG	1H	3384	1/1	0.94	0.21	49,49,49,49	0
56	MG	13	1762	1/1	0.94	0.05	128,128,128,128	0
56	MG	14	3185	1/1	0.94	0.30	78,78,78,78	0
56	MG	14	3186	1/1	0.94	0.11	77,77,77,77	0
56	MG	1G	1649	1/1	0.94	0.12	90,90,90,90	0
56	MG	14	3109	1/1	0.94	0.10	69,69,69,69	0
56	MG	14	3036	1/1	0.94	0.07	71,71,71,71	0
56	MG	1H	3085	1/1	0.94	0.20	46,46,46,46	0
56	MG	1H	3575	1/1	0.94	0.10	63,63,63,63	0
56	MG	1H	3579	1/1	0.94	0.10	81,81,81,81	0
56	MG	1H	3126	1/1	0.94	0.17	54,54,54,54	0
56	MG	1H	3581	1/1	0.94	0.08	87,87,87,87	0
56	MG	1H	3583	1/1	0.94	0.08	52,52,52,52	0
56	MG	1H	3032	1/1	0.94	0.10	57,57,57,57	0
56	MG	14	3046	1/1	0.94	0.06	56,56,56,56	0
56	MG	1G	1657	1/1	0.94	0.12	117,117,117,117	0
56	MG	14	3048	1/1	0.94	0.07	66,66,66,66	0
56	MG	1H	3308	1/1	0.94	0.10	78,78,78,78	0
56	MG	14	3206	1/1	0.94	0.21	87,87,87,87	0
56	MG	14	3050	1/1	0.94	0.08	62,62,62,62	0
56	MG	14	3125	1/1	0.94	0.11	84,84,84,84	0
56	MG	1G	1718	1/1	0.94	0.05	140,140,140,140	0
56	MG	1G	1721	1/1	0.94	0.18	143,143,143,143	0
56	MG	1G	1611	1/1	0.94	0.15	86,86,86,86	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	1G	1725	1/1	0.94	0.09	111,111,111,111	0
56	MG	13	1789	1/1	0.94	0.08	63,63,63,63	0
56	MG	14	3296	1/1	0.94	0.12	68,68,68,68	0
56	MG	1G	1734	1/1	0.94	0.10	94,94,94,94	0
56	MG	13	1675	1/1	0.94	0.19	80,80,80,80	0
56	MG	14	3060	1/1	0.94	0.12	64,64,64,64	0
56	MG	1G	1741	1/1	0.94	0.13	98,98,98,98	0
56	MG	1G	1742	1/1	0.94	0.14	131,131,131,131	0
56	MG	14	3305	1/1	0.94	0.10	60,60,60,60	0
56	MG	1H	3089	1/1	0.94	0.14	62,62,62,62	0
56	MG	1H	3072	1/1	0.94	0.14	86,86,86,86	0
56	MG	13	1722	1/1	0.94	0.07	99,99,99,99	0
56	MG	14	3144	1/1	0.94	0.18	65,65,65,65	0
56	MG	2A	201	1/1	0.94	0.14	85,85,85,85	0
56	MG	1G	1620	1/1	0.94	0.09	83,83,83,83	0
56	MG	1H	3074	1/1	0.94	0.14	57,57,57,57	0
56	MG	14	3365	1/1	0.94	0.09	89,89,89,89	0
56	MG	1H	3316	1/1	0.94	0.08	106,106,106,106	0
56	MG	14	3149	1/1	0.94	0.12	74,74,74,74	0
56	MG	14	3388	1/1	0.94	0.14	87,87,87,87	0
56	MG	14	3391	1/1	0.94	0.10	106,106,106,106	0
56	MG	13	1732	1/1	0.94	0.13	65,65,65,65	0
56	MG	1H	3077	1/1	0.94	0.06	62,62,62,62	0
56	MG	14	3402	1/1	0.94	0.09	94,94,94,94	0
56	MG	1H	3343	1/1	0.94	0.09	76,76,76,76	0
56	MG	14	3234	1/1	0.94	0.11	60,60,60,60	0
56	MG	5E	201	1/1	0.94	0.17	79,79,79,79	0
56	MG	13	1766	1/1	0.94	0.08	70,70,70,70	0
56	MG	1H	3456	1/1	0.94	0.11	100,100,100,100	0
56	MG	1H	3100	1/1	0.94	0.05	69,69,69,69	0
56	MG	1H	3460	1/1	0.94	0.13	94,94,94,94	0
56	MG	1H	3463	1/1	0.94	0.07	101,101,101,101	0
56	MG	1H	3464	1/1	0.94	0.07	71,71,71,71	0
56	MG	1H	3465	1/1	0.94	0.07	111,111,111,111	0
56	MG	19	301	1/1	0.94	0.06	53,53,53,53	0
56	MG	1H	3051	1/1	0.94	0.05	46,46,46,46	0
56	MG	1H	3468	1/1	0.94	0.06	92,92,92,92	0
56	MG	14	3013	1/1	0.94	0.14	50,50,50,50	0
56	MG	14	3014	1/1	0.94	0.09	50,50,50,50	0
56	MG	1H	3348	1/1	0.94	0.06	87,87,87,87	0
56	MG	1H	3377	1/1	0.94	0.17	49,49,49,49	0
56	MG	14	3250	1/1	0.94	0.16	66,66,66,66	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	14	3168	1/1	0.94	0.10	65,65,65,65	0
56	MG	78	201	1/1	0.94	0.10	62,62,62,62	0
56	MG	14	3253	1/1	0.94	0.19	59,59,59,59	0
56	MG	1H	3094	1/1	0.95	0.14	48,48,48,48	0
56	MG	1H	3529	1/1	0.95	0.07	49,49,49,49	0
56	MG	1G	1746	1/1	0.95	0.16	95,95,95,95	0
56	MG	1G	1747	1/1	0.95	0.07	95,95,95,95	0
56	MG	14	3058	1/1	0.95	0.15	78,78,78,78	0
56	MG	13	1801	1/1	0.95	0.11	113,113,113,113	0
56	MG	1H	3075	1/1	0.95	0.16	72,72,72,72	0
56	MG	14	3134	1/1	0.95	0.24	81,81,81,81	0
56	MG	1H	3562	1/1	0.95	0.08	97,97,97,97	0
56	MG	14	3207	1/1	0.95	0.16	67,67,67,67	0
56	MG	1H	3565	1/1	0.95	0.08	110,110,110,110	0
56	MG	13	1805	1/1	0.95	0.06	115,115,115,115	0
56	MG	1H	3169	1/1	0.95	0.12	56,56,56,56	0
56	MG	14	3139	1/1	0.95	0.08	69,69,69,69	0
56	MG	1G	1610	1/1	0.95	0.10	83,83,83,83	0
56	MG	14	3142	1/1	0.95	0.26	70,70,70,70	0
56	MG	1H	3144	1/1	0.95	0.22	57,57,57,57	0
56	MG	1H	3251	1/1	0.95	0.06	66,66,66,66	0
56	MG	1G	1614	1/1	0.95	0.12	71,71,71,71	0
56	MG	13	1601	1/1	0.95	0.15	58,58,58,58	0
56	MG	1H	3381	1/1	0.95	0.15	97,97,97,97	0
56	MG	1H	3597	1/1	0.95	0.07	92,92,92,92	0
56	MG	1H	3122	1/1	0.95	0.08	49,49,49,49	0
56	MG	1H	3603	1/1	0.95	0.08	121,121,121,121	0
56	MG	1H	3225	1/1	0.95	0.16	76,76,76,76	0
56	MG	1H	3616	1/1	0.95	0.25	73,73,73,73	0
56	MG	1H	3315	1/1	0.95	0.07	101,101,101,101	0
56	MG	1H	3004	1/1	0.95	0.08	35,35,35,35	0
56	MG	14	3155	1/1	0.95	0.10	65,65,65,65	0
56	MG	13	1676	1/1	0.95	0.10	68,68,68,68	0
56	MG	1H	3006	1/1	0.95	0.14	52,52,52,52	0
56	MG	1H	3008	1/1	0.95	0.16	47,47,47,47	0
56	MG	14	3304	1/1	0.95	0.05	103,103,103,103	0
56	MG	14	3015	1/1	0.95	0.08	51,51,51,51	0
56	MG	13	1751	1/1	0.95	0.06	106,106,106,106	0
56	MG	14	3307	1/1	0.95	0.13	89,89,89,89	0
56	MG	14	3308	1/1	0.95	0.09	80,80,80,80	0
56	MG	1H	3437	1/1	0.95	0.06	90,90,90,90	0
56	MG	14	3315	1/1	0.95	0.06	93,93,93,93	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	1H	3045	1/1	0.95	0.19	75,75,75,75	0
56	MG	1H	3154	1/1	0.95	0.09	74,74,74,74	0
56	MG	13	1755	1/1	0.95	0.07	94,94,94,94	0
56	MG	14	3322	1/1	0.95	0.06	123,123,123,123	0
56	MG	13	1646	1/1	0.95	0.12	58,58,58,58	0
56	MG	14	3343	1/1	0.95	0.08	54,54,54,54	0
56	MG	14	3345	1/1	0.95	0.14	89,89,89,89	0
56	MG	14	3025	1/1	0.95	0.09	46,46,46,46	0
56	MG	1H	3295	1/1	0.95	0.19	65,65,65,65	0
56	MG	8I	201	1/1	0.95	0.19	98,98,98,98	0
56	MG	1H	3359	1/1	0.95	0.12	58,58,58,58	0
56	MG	14	3385	1/1	0.95	0.15	84,84,84,84	0
56	MG	16	213	1/1	0.95	0.06	98,98,98,98	0
56	MG	1H	3013	1/1	0.95	0.16	42,42,42,42	0
56	MG	1H	3133	1/1	0.95	0.14	67,67,67,67	0
56	MG	14	3395	1/1	0.95	0.06	89,89,89,89	0
56	MG	13	1788	1/1	0.95	0.14	123,123,123,123	0
56	MG	1H	3330	1/1	0.95	0.11	70,70,70,70	0
56	MG	14	3403	1/1	0.95	0.07	101,101,101,101	0
56	MG	1H	3212	1/1	0.95	0.46	91,91,91,91	0
56	MG	14	3408	1/1	0.95	0.06	91,91,91,91	0
56	MG	14	3410	1/1	0.95	0.07	81,81,81,81	0
56	MG	14	3416	1/1	0.95	0.06	98,98,98,98	0
56	MG	14	3417	1/1	0.95	0.08	80,80,80,80	0
56	MG	14	3249	1/1	0.95	0.16	54,54,54,54	0
56	MG	31	302	1/1	0.95	0.26	76,76,76,76	0
56	MG	13	1699	1/1	0.95	0.07	94,94,94,94	0
56	MG	14	3427	1/1	0.95	0.09	104,104,104,104	0
56	MG	14	3429	1/1	0.95	0.06	91,91,91,91	0
56	MG	14	3434	1/1	0.95	0.08	61,61,61,61	0
56	MG	1H	3408	1/1	0.95	0.30	60,60,60,60	0
56	MG	13	1607	1/1	0.95	0.33	78,78,78,78	0
56	MG	1G	1704	1/1	0.95	0.07	85,85,85,85	0
56	MG	14	3256	1/1	0.95	0.12	75,75,75,75	0
56	MG	14	3257	1/1	0.95	0.12	62,62,62,62	0
56	MG	1H	3092	1/1	0.95	0.16	62,62,62,62	0
56	MG	1H	3473	1/1	0.95	0.05	112,112,112,112	0
56	MG	14	3044	1/1	0.95	0.06	71,71,71,71	0
56	MG	1H	3411	1/1	0.95	0.10	71,71,71,71	0
56	MG	1G	1713	1/1	0.95	0.05	119,119,119,119	0
56	MG	1H	3477	1/1	0.95	0.11	90,90,90,90	0
56	MG	1H	3369	1/1	0.95	0.07	95,95,95,95	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	1H	3479	1/1	0.95	0.05	107,107,107,107	0
56	MG	1H	3480	1/1	0.95	0.08	113,113,113,113	0
56	MG	1H	3489	1/1	0.95	0.07	53,53,53,53	0
56	MG	13	1695	1/1	0.95	0.11	86,86,86,86	0
56	MG	1H	3506	1/1	0.95	0.09	58,58,58,58	0
56	MG	13	1610	1/1	0.96	0.06	56,56,56,56	0
56	MG	1H	3590	1/1	0.96	0.09	107,107,107,107	0
56	MG	1H	3591	1/1	0.96	0.06	70,70,70,70	0
56	MG	1H	3388	1/1	0.96	0.22	54,54,54,54	0
56	MG	14	3002	1/1	0.96	0.09	49,49,49,49	0
56	MG	13	1780	1/1	0.96	0.10	106,106,106,106	0
56	MG	14	3005	1/1	0.96	0.15	58,58,58,58	0
56	MG	1H	3601	1/1	0.96	0.06	84,84,84,84	0
56	MG	1H	3429	1/1	0.96	0.14	63,63,63,63	0
56	MG	14	3214	1/1	0.96	0.04	90,90,90,90	0
56	MG	1H	3064	1/1	0.96	0.07	59,59,59,59	0
56	MG	1H	3431	1/1	0.96	0.10	54,54,54,54	0
56	MG	13	1800	1/1	0.96	0.06	118,118,118,118	0
56	MG	1H	3436	1/1	0.96	0.10	98,98,98,98	0
56	MG	1H	3066	1/1	0.96	0.09	66,66,66,66	0
56	MG	1H	3002	1/1	0.96	0.13	40,40,40,40	0
56	MG	1G	1612	1/1	0.96	0.10	79,79,79,79	0
56	MG	1H	3481	1/1	0.96	0.08	122,122,122,122	0
56	MG	14	3078	1/1	0.96	0.05	54,54,54,54	0
56	MG	14	3016	1/1	0.96	0.13	51,51,51,51	0
56	MG	1H	3482	1/1	0.96	0.26	142,142,142,142	0
56	MG	1H	3484	1/1	0.96	0.06	45,45,45,45	0
56	MG	1H	3487	1/1	0.96	0.08	50,50,50,50	0
56	MG	14	3020	1/1	0.96	0.10	55,55,55,55	0
56	MG	1G	1702	1/1	0.96	0.06	101,101,101,101	0
56	MG	14	3085	1/1	0.96	0.15	62,62,62,62	0
56	MG	14	3086	1/1	0.96	0.10	59,59,59,59	0
56	MG	14	3313	1/1	0.96	0.06	82,82,82,82	0
56	MG	14	3232	1/1	0.96	0.14	66,66,66,66	0
56	MG	1H	3488	1/1	0.96	0.07	53,53,53,53	0
56	MG	14	3088	1/1	0.96	0.13	61,61,61,61	0
56	MG	14	3319	1/1	0.96	0.05	104,104,104,104	0
56	MG	14	3320	1/1	0.96	0.22	120,120,120,120	0
56	MG	1G	1706	1/1	0.96	0.10	95,95,95,95	0
56	MG	14	3024	1/1	0.96	0.12	57,57,57,57	0
56	MG	1H	3440	1/1	0.96	0.06	59,59,59,59	0
56	MG	1G	1709	1/1	0.96	0.11	108,108,108,108	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	1H	3491	1/1	0.96	0.08	57,57,57,57	0
56	MG	14	3028	1/1	0.96	0.05	53,53,53,53	0
56	MG	14	3364	1/1	0.96	0.10	108,108,108,108	0
56	MG	1G	1711	1/1	0.96	0.08	109,109,109,109	0
56	MG	14	3366	1/1	0.96	0.06	87,87,87,87	0
56	MG	13	1742	1/1	0.96	0.29	92,92,92,92	0
56	MG	14	3371	1/1	0.96	0.06	84,84,84,84	0
56	MG	1H	3505	1/1	0.96	0.08	51,51,51,51	0
56	MG	14	3382	1/1	0.96	0.05	88,88,88,88	0
56	MG	1G	1716	1/1	0.96	0.09	109,109,109,109	0
56	MG	14	3100	1/1	0.96	0.16	65,65,65,65	0
56	MG	1H	3398	1/1	0.96	0.11	47,47,47,47	0
56	MG	1H	3516	1/1	0.96	0.10	59,59,59,59	0
56	MG	1H	3446	1/1	0.96	0.07	87,87,87,87	0
56	MG	1H	3450	1/1	0.96	0.16	84,84,84,84	0
56	MG	13	1802	1/1	0.96	0.12	114,114,114,114	0
56	MG	1G	1670	1/1	0.96	0.08	99,99,99,99	0
56	MG	14	3404	1/1	0.96	0.14	85,85,85,85	0
56	MG	14	3107	1/1	0.96	0.07	68,68,68,68	0
56	MG	14	3039	1/1	0.96	0.08	61,61,61,61	0
56	MG	1G	1735	1/1	0.96	0.06	112,112,112,112	0
56	MG	13	1804	1/1	0.96	0.17	137,137,137,137	0
56	MG	1H	3554	1/1	0.96	0.23	108,108,108,108	0
56	MG	1H	3558	1/1	0.96	0.12	100,100,100,100	0
56	MG	14	3113	1/1	0.96	0.15	69,69,69,69	0
56	MG	1G	1745	1/1	0.96	0.18	124,124,124,124	0
56	MG	14	3115	1/1	0.96	0.09	57,57,57,57	0
56	MG	13	1750	1/1	0.96	0.12	122,122,122,122	0
56	MG	14	3432	1/1	0.96	0.09	91,91,91,91	0
56	MG	14	3433	1/1	0.96	0.07	87,87,87,87	0
56	MG	14	3187	1/1	0.96	0.14	62,62,62,62	0
56	MG	14	3435	1/1	0.96	0.09	121,121,121,121	0
56	MG	14	3188	1/1	0.96	0.08	68,68,68,68	0
56	MG	14	3189	1/1	0.96	0.09	63,63,63,63	0
56	MG	1H	3263	1/1	0.96	0.10	64,64,64,64	0
56	MG	1H	3017	1/1	0.96	0.10	51,51,51,51	0
56	MG	1H	3571	1/1	0.96	0.13	58,58,58,58	0
56	MG	1G	1753	1/1	0.96	0.04	109,109,109,109	0
56	MG	1G	1754	1/1	0.96	0.12	104,104,104,104	0
56	MG	1G	1755	1/1	0.96	0.08	119,119,119,119	0
56	MG	14	3196	1/1	0.96	0.06	78,78,78,78	0
56	MG	1H	3574	1/1	0.96	0.07	53,53,53,53	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	1H	3111	1/1	0.96	0.17	54,54,54,54	0
56	MG	25	201	1/1	0.96	0.06	123,123,123,123	0
56	MG	1H	3578	1/1	0.96	0.08	65,65,65,65	0
56	MG	9A	101	1/1	0.96	0.10	115,115,115,115	0
56	MG	1H	3250	1/1	0.96	0.08	67,67,67,67	0
56	MG	45	202	1/1	0.96	0.27	84,84,84,84	0
56	MG	14	3202	1/1	0.96	0.16	71,71,71,71	0
56	MG	13	1611	1/1	0.96	0.18	65,65,65,65	0
56	MG	1H	3181	1/1	0.96	0.09	71,71,71,71	0
56	MG	13	1761	1/1	0.97	0.05	110,110,110,110	0
56	MG	1H	3336	1/1	0.97	0.21	81,81,81,81	0
56	MG	13	1753	1/1	0.97	0.06	121,121,121,121	0
56	MG	1H	3277	1/1	0.97	0.06	66,66,66,66	0
56	MG	1H	3360	1/1	0.97	0.10	50,50,50,50	0
56	MG	1H	3443	1/1	0.97	0.13	74,74,74,74	0
56	MG	14	3303	1/1	0.97	0.06	69,69,69,69	0
56	MG	1H	3496	1/1	0.97	0.08	66,66,66,66	0
56	MG	1H	3444	1/1	0.97	0.06	78,78,78,78	0
56	MG	13	1754	1/1	0.97	0.07	108,108,108,108	0
56	MG	13	1781	1/1	0.97	0.07	97,97,97,97	0
56	MG	1H	3512	1/1	0.97	0.12	65,65,65,65	0
56	MG	14	3309	1/1	0.97	0.10	87,87,87,87	0
56	MG	1H	3513	1/1	0.97	0.24	83,83,83,83	0
56	MG	14	3312	1/1	0.97	0.05	99,99,99,99	0
56	MG	1H	3447	1/1	0.97	0.07	65,65,65,65	0
56	MG	1H	3448	1/1	0.97	0.09	96,96,96,96	0
56	MG	1H	3521	1/1	0.97	0.06	66,66,66,66	0
56	MG	14	3091	1/1	0.97	0.20	57,57,57,57	0
56	MG	1H	3524	1/1	0.97	0.07	56,56,56,56	0
56	MG	1H	3526	1/1	0.97	0.06	57,57,57,57	0
56	MG	1H	3527	1/1	0.97	0.12	50,50,50,50	0
56	MG	13	1784	1/1	0.97	0.10	104,104,104,104	0
56	MG	14	3323	1/1	0.97	0.13	100,100,100,100	0
56	MG	14	3324	1/1	0.97	0.05	50,50,50,50	0
56	MG	1G	1707	1/1	0.97	0.05	92,92,92,92	0
56	MG	14	3333	1/1	0.97	0.06	80,80,80,80	0
56	MG	14	3335	1/1	0.97	0.06	57,57,57,57	0
56	MG	14	3339	1/1	0.97	0.06	61,61,61,61	0
56	MG	14	3340	1/1	0.97	0.05	57,57,57,57	0
56	MG	1H	3535	1/1	0.97	0.05	80,80,80,80	0
56	MG	1H	3543	1/1	0.97	0.07	59,59,59,59	0
56	MG	1H	3146	1/1	0.97	0.05	71,71,71,71	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	14	3358	1/1	0.97	0.06	80,80,80,80	0
56	MG	14	3360	1/1	0.97	0.10	69,69,69,69	0
56	MG	14	3362	1/1	0.97	0.07	96,96,96,96	0
56	MG	14	3363	1/1	0.97	0.05	98,98,98,98	0
56	MG	1H	3453	1/1	0.97	0.06	94,94,94,94	0
56	MG	1H	3389	1/1	0.97	0.15	52,52,52,52	0
56	MG	88	202	1/1	0.97	0.38	69,69,69,69	0
56	MG	1G	1715	1/1	0.97	0.11	119,119,119,119	0
56	MG	14	3368	1/1	0.97	0.05	101,101,101,101	0
56	MG	1H	3457	1/1	0.97	0.09	99,99,99,99	0
56	MG	1G	1717	1/1	0.97	0.05	129,129,129,129	0
56	MG	14	3373	1/1	0.97	0.16	117,117,117,117	0
56	MG	14	3374	1/1	0.97	0.05	55,55,55,55	0
56	MG	14	3376	1/1	0.97	0.05	75,75,75,75	0
56	MG	14	3378	1/1	0.97	0.13	69,69,69,69	0
56	MG	1H	3561	1/1	0.97	0.08	78,78,78,78	0
56	MG	14	3383	1/1	0.97	0.08	62,62,62,62	0
56	MG	14	3384	1/1	0.97	0.11	81,81,81,81	0
56	MG	1G	1720	1/1	0.97	0.12	112,112,112,112	0
56	MG	13	1733	1/1	0.97	0.28	64,64,64,64	0
56	MG	13	1641	1/1	0.97	0.07	55,55,55,55	0
56	MG	14	3392	1/1	0.97	0.08	62,62,62,62	0
56	MG	1H	3462	1/1	0.97	0.06	95,95,95,95	0
56	MG	1G	1727	1/1	0.97	0.14	108,108,108,108	0
56	MG	1H	3079	1/1	0.97	0.04	59,59,59,59	0
56	MG	1H	3573	1/1	0.97	0.08	51,51,51,51	0
56	MG	13	1760	1/1	0.97	0.21	127,127,127,127	0
56	MG	1H	3395	1/1	0.97	0.05	54,54,54,54	0
56	MG	1G	1739	1/1	0.97	0.09	107,107,107,107	0
56	MG	14	3407	1/1	0.97	0.07	84,84,84,84	0
56	MG	1G	1740	1/1	0.97	0.14	93,93,93,93	0
56	MG	13	1792	1/1	0.97	0.10	73,73,73,73	0
56	MG	14	3411	1/1	0.97	0.04	109,109,109,109	0
56	MG	14	3412	1/1	0.97	0.06	102,102,102,102	0
56	MG	1H	3467	1/1	0.97	0.07	102,102,102,102	0
56	MG	1G	1744	1/1	0.97	0.12	101,101,101,101	0
56	MG	1H	3007	1/1	0.97	0.04	60,60,60,60	0
56	MG	1H	3371	1/1	0.97	0.11	72,72,72,72	0
56	MG	14	3422	1/1	0.97	0.14	72,72,72,72	0
56	MG	1H	3099	1/1	0.97	0.12	55,55,55,55	0
56	MG	14	3425	1/1	0.97	0.10	95,95,95,95	0
56	MG	1H	3587	1/1	0.97	0.06	51,51,51,51	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	1G	1751	1/1	0.97	0.05	95,95,95,95	0
56	MG	1H	3052	1/1	0.97	0.07	41,41,41,41	0
56	MG	14	3127	1/1	0.97	0.13	61,61,61,61	0
56	MG	13	1767	1/1	0.97	0.06	61,61,61,61	0
56	MG	1H	3592	1/1	0.97	0.07	96,96,96,96	0
56	MG	1H	3593	1/1	0.97	0.10	61,61,61,61	0
56	MG	14	3059	1/1	0.97	0.14	41,41,41,41	0
56	MG	1H	3595	1/1	0.97	0.04	99,99,99,99	0
56	MG	13	1794	1/1	0.97	0.08	79,79,79,79	0
56	MG	14	3062	1/1	0.97	0.07	59,59,59,59	0
56	MG	1H	3474	1/1	0.97	0.06	83,83,83,83	0
56	MG	13	1770	1/1	0.97	0.05	89,89,89,89	0
56	MG	1G	1618	1/1	0.97	0.12	74,74,74,74	0
56	MG	1H	3476	1/1	0.97	0.06	92,92,92,92	0
56	MG	13	1796	1/1	0.97	0.07	79,79,79,79	0
56	MG	1H	3611	1/1	0.97	0.08	88,88,88,88	0
56	MG	14	3141	1/1	0.97	0.29	74,74,74,74	0
56	MG	1H	3614	1/1	0.97	0.28	97,97,97,97	0
56	MG	35	202	1/1	0.97	0.09	79,79,79,79	0
56	MG	1H	3378	1/1	0.97	0.16	56,56,56,56	0
56	MG	1H	3432	1/1	0.97	0.18	83,83,83,83	0
56	MG	1H	3433	1/1	0.97	0.06	51,51,51,51	0
56	MG	14	3003	1/1	0.97	0.16	47,47,47,47	0
56	MG	1H	3140	1/1	0.97	0.33	78,78,78,78	0
56	MG	1G	1627	1/1	0.97	0.10	88,88,88,88	0
56	MG	14	3332	1/1	0.98	0.04	57,57,57,57	0
56	MG	1H	3540	1/1	0.98	0.06	85,85,85,85	0
56	MG	14	3255	1/1	0.98	0.09	72,72,72,72	0
56	MG	1H	3542	1/1	0.98	0.12	68,68,68,68	0
56	MG	13	1768	1/1	0.98	0.14	92,92,92,92	0
56	MG	14	3342	1/1	0.98	0.06	51,51,51,51	0
56	MG	1H	3485	1/1	0.98	0.06	55,55,55,55	0
56	MG	1H	3486	1/1	0.98	0.05	45,45,45,45	0
56	MG	14	3347	1/1	0.98	0.04	53,53,53,53	0
56	MG	13	1791	1/1	0.98	0.07	85,85,85,85	0
56	MG	14	3353	1/1	0.98	0.05	64,64,64,64	0
56	MG	14	3354	1/1	0.98	0.04	68,68,68,68	0
56	MG	1H	3555	1/1	0.98	0.20	85,85,85,85	0
56	MG	1H	3556	1/1	0.98	0.04	58,58,58,58	0
56	MG	1H	3557	1/1	0.98	0.04	59,59,59,59	0
56	MG	13	1803	1/1	0.98	0.04	97,97,97,97	0
56	MG	1H	3560	1/1	0.98	0.09	84,84,84,84	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	1H	3273	1/1	0.98	0.04	73,73,73,73	0
56	MG	1H	3490	1/1	0.98	0.05	63,63,63,63	0
56	MG	1H	3564	1/1	0.98	0.09	95,95,95,95	0
56	MG	16	214	1/1	0.98	0.06	82,82,82,82	0
56	MG	14	3369	1/1	0.98	0.10	87,87,87,87	0
56	MG	1H	3117	1/1	0.98	0.09	59,59,59,59	0
56	MG	1H	3493	1/1	0.98	0.06	48,48,48,48	0
56	MG	1H	3570	1/1	0.98	0.04	54,54,54,54	0
56	MG	13	1769	1/1	0.98	0.08	82,82,82,82	0
56	MG	14	3375	1/1	0.98	0.05	75,75,75,75	0
56	MG	1H	3572	1/1	0.98	0.04	73,73,73,73	0
56	MG	13	1700	1/1	0.98	0.05	90,90,90,90	0
56	MG	14	3380	1/1	0.98	0.06	92,92,92,92	0
56	MG	1H	3501	1/1	0.98	0.05	57,57,57,57	0
56	MG	1H	3502	1/1	0.98	0.05	49,49,49,49	0
56	MG	1H	3577	1/1	0.98	0.04	49,49,49,49	0
56	MG	13	1783	1/1	0.98	0.07	77,77,77,77	0
56	MG	14	3386	1/1	0.98	0.04	54,54,54,54	0
56	MG	1G	1703	1/1	0.98	0.09	87,87,87,87	0
56	MG	14	3390	1/1	0.98	0.09	66,66,66,66	0
56	MG	13	1773	1/1	0.98	0.10	96,96,96,96	0
56	MG	1H	3511	1/1	0.98	0.07	42,42,42,42	0
56	MG	13	1758	1/1	0.98	0.04	111,111,111,111	0
56	MG	14	3394	1/1	0.98	0.05	98,98,98,98	0
56	MG	1H	3582	1/1	0.98	0.05	56,56,56,56	0
56	MG	14	3396	1/1	0.98	0.04	54,54,54,54	0
56	MG	14	3398	1/1	0.98	0.04	81,81,81,81	0
56	MG	1H	3454	1/1	0.98	0.05	93,93,93,93	0
56	MG	1H	3585	1/1	0.98	0.05	95,95,95,95	0
56	MG	1H	3435	1/1	0.98	0.10	68,68,68,68	0
56	MG	I8	102	1/1	0.98	0.08	66,66,66,66	0
56	MG	1H	3588	1/1	0.98	0.06	52,52,52,52	0
56	MG	14	3406	1/1	0.98	0.07	60,60,60,60	0
56	MG	1G	1714	1/1	0.98	0.11	123,123,123,123	0
56	MG	1H	3589	1/1	0.98	0.07	60,60,60,60	0
56	MG	1H	3038	1/1	0.98	0.20	44,44,44,44	0
56	MG	1H	3520	1/1	0.98	0.05	54,54,54,54	0
56	MG	1H	3458	1/1	0.98	0.10	85,85,85,85	0
56	MG	14	3414	1/1	0.98	0.12	86,86,86,86	0
56	MG	14	3415	1/1	0.98	0.12	101,101,101,101	0
56	MG	1G	1719	1/1	0.98	0.07	112,112,112,112	0
56	MG	1H	3522	1/1	0.98	0.11	59,59,59,59	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	14	3419	1/1	0.98	0.05	84,84,84,84	0
56	MG	1H	3523	1/1	0.98	0.14	82,82,82,82	0
56	MG	13	1798	1/1	0.98	0.13	80,80,80,80	0
56	MG	1H	3525	1/1	0.98	0.05	58,58,58,58	0
56	MG	1G	1726	1/1	0.98	0.14	86,86,86,86	0
56	MG	1H	3600	1/1	0.98	0.06	84,84,84,84	0
56	MG	14	3426	1/1	0.98	0.05	108,108,108,108	0
56	MG	14	3302	1/1	0.98	0.04	56,56,56,56	0
56	MG	14	3428	1/1	0.98	0.05	81,81,81,81	0
56	MG	1G	1728	1/1	0.98	0.16	96,96,96,96	0
56	MG	14	3430	1/1	0.98	0.05	90,90,90,90	0
56	MG	14	3431	1/1	0.98	0.09	104,104,104,104	0
56	MG	1H	3438	1/1	0.98	0.07	94,94,94,94	0
56	MG	1G	1731	1/1	0.98	0.07	99,99,99,99	0
56	MG	1G	1732	1/1	0.98	0.10	102,102,102,102	0
56	MG	1H	3602	1/1	0.98	0.04	88,88,88,88	0
56	MG	1H	3461	1/1	0.98	0.03	102,102,102,102	0
56	MG	1G	1737	1/1	0.98	0.21	127,127,127,127	0
56	MG	13	1799	1/1	0.98	0.04	93,93,93,93	0
56	MG	1H	3610	1/1	0.98	0.17	106,106,106,106	0
56	MG	1H	3533	1/1	0.98	0.04	46,46,46,46	0
56	MG	14	3314	1/1	0.98	0.22	126,126,126,126	0
56	MG	1H	3613	1/1	0.98	0.12	78,78,78,78	0
56	MG	14	3316	1/1	0.98	0.21	79,79,79,79	0
56	MG	1H	3534	1/1	0.98	0.04	51,51,51,51	0
56	MG	1G	1743	1/1	0.98	0.16	122,122,122,122	0
56	MG	1H	3615	1/1	0.98	0.10	108,108,108,108	0
56	MG	13	1776	1/1	0.98	0.11	93,93,93,93	0
56	MG	1H	3617	1/1	0.98	0.28	127,127,127,127	0
56	MG	1H	3538	1/1	0.98	0.05	46,46,46,46	0
56	MG	1H	3620	1/1	0.98	0.06	73,73,73,73	0
56	MG	1G	1749	1/1	0.98	0.12	114,114,114,114	0
56	MG	14	3327	1/1	0.98	0.04	63,63,63,63	0
56	MG	14	3329	1/1	0.98	0.04	57,57,57,57	0
56	MG	1G	1750	1/1	0.98	0.10	109,109,109,109	0
56	MG	14	3331	1/1	0.98	0.15	82,82,82,82	0
58	ZN	5A	101	1/1	0.98	0.04	125,125,125,125	0
56	MG	1H	3536	1/1	0.99	0.04	62,62,62,62	0
56	MG	14	3361	1/1	0.99	0.02	80,80,80,80	0
56	MG	1H	3537	1/1	0.99	0.04	52,52,52,52	0
56	MG	1H	3452	1/1	0.99	0.02	81,81,81,81	0
56	MG	1H	3539	1/1	0.99	0.07	76,76,76,76	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	1H	3497	1/1	0.99	0.07	40,40,40,40	0
56	MG	1H	3594	1/1	0.99	0.15	95,95,95,95	0
56	MG	1H	3541	1/1	0.99	0.03	75,75,75,75	0
56	MG	1H	3596	1/1	0.99	0.05	75,75,75,75	0
56	MG	1G	1723	1/1	0.99	0.05	72,72,72,72	0
56	MG	14	3370	1/1	0.99	0.05	70,70,70,70	0
56	MG	13	1786	1/1	0.99	0.03	65,65,65,65	0
56	MG	1H	3598	1/1	0.99	0.08	105,105,105,105	0
56	MG	1H	3499	1/1	0.99	0.07	49,49,49,49	0
56	MG	1H	3546	1/1	0.99	0.10	60,60,60,60	0
56	MG	1H	3027	1/1	0.99	0.07	40,40,40,40	0
56	MG	1G	1730	1/1	0.99	0.03	72,72,72,72	0
56	MG	14	3377	1/1	0.99	0.04	51,51,51,51	0
56	MG	1H	3549	1/1	0.99	0.03	61,61,61,61	0
56	MG	14	3379	1/1	0.99	0.03	66,66,66,66	0
56	MG	1H	3455	1/1	0.99	0.03	92,92,92,92	0
56	MG	14	3381	1/1	0.99	0.09	89,89,89,89	0
56	MG	1G	1733	1/1	0.99	0.17	121,121,121,121	0
56	MG	1H	3604	1/1	0.99	0.10	118,118,118,118	0
56	MG	1H	3605	1/1	0.99	0.05	90,90,90,90	0
56	MG	1G	1736	1/1	0.99	0.12	111,111,111,111	0
56	MG	1H	3606	1/1	0.99	0.04	85,85,85,85	0
56	MG	14	3387	1/1	0.99	0.06	61,61,61,61	0
56	MG	1H	3551	1/1	0.99	0.04	53,53,53,53	0
56	MG	14	3389	1/1	0.99	0.05	54,54,54,54	0
56	MG	1H	3552	1/1	0.99	0.11	78,78,78,78	0
56	MG	1H	3553	1/1	0.99	0.05	62,62,62,62	0
56	MG	1H	3612	1/1	0.99	0.12	62,62,62,62	0
56	MG	1H	3504	1/1	0.99	0.04	56,56,56,56	0
56	MG	13	1787	1/1	0.99	0.15	109,109,109,109	0
56	MG	13	1752	1/1	0.99	0.08	86,86,86,86	0
56	MG	1H	3507	1/1	0.99	0.16	65,65,65,65	0
56	MG	14	3397	1/1	0.99	0.10	70,70,70,70	0
56	MG	1H	3508	1/1	0.99	0.09	74,74,74,74	0
56	MG	14	3399	1/1	0.99	0.07	47,47,47,47	0
56	MG	1H	3559	1/1	0.99	0.06	73,73,73,73	0
56	MG	14	3401	1/1	0.99	0.04	85,85,85,85	0
56	MG	1H	3619	1/1	0.99	0.04	55,55,55,55	0
56	MG	1H	3509	1/1	0.99	0.07	77,77,77,77	0
56	MG	14	3310	1/1	0.99	0.04	53,53,53,53	0
56	MG	1H	3510	1/1	0.99	0.11	54,54,54,54	0
56	MG	1H	3622	1/1	0.99	0.03	76,76,76,76	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	1H	3390	1/1	0.99	0.10	53,53,53,53	0
56	MG	1H	3563	1/1	0.99	0.03	81,81,81,81	0
56	MG	14	3409	1/1	0.99	0.05	80,80,80,80	0
56	MG	13	1777	1/1	0.99	0.07	69,69,69,69	0
56	MG	13	1790	1/1	0.99	0.06	59,59,59,59	0
56	MG	1H	3566	1/1	0.99	0.03	93,93,93,93	0
56	MG	14	3413	1/1	0.99	0.04	93,93,93,93	0
56	MG	1H	3567	1/1	0.99	0.03	51,51,51,51	0
56	MG	1H	3514	1/1	0.99	0.05	84,84,84,84	0
56	MG	1H	3569	1/1	0.99	0.04	73,73,73,73	0
56	MG	13	1778	1/1	0.99	0.03	79,79,79,79	0
56	MG	14	3418	1/1	0.99	0.10	99,99,99,99	0
56	MG	1H	3442	1/1	0.99	0.07	73,73,73,73	0
56	MG	13	1749	1/1	0.99	0.05	92,92,92,92	0
56	MG	13	1771	1/1	0.99	0.14	81,81,81,81	0
56	MG	14	3325	1/1	0.99	0.11	63,63,63,63	0
56	MG	14	3423	1/1	0.99	0.12	95,95,95,95	0
56	MG	14	3326	1/1	0.99	0.04	53,53,53,53	0
56	MG	13	1772	1/1	0.99	0.07	93,93,93,93	0
56	MG	14	3328	1/1	0.99	0.05	58,58,58,58	0
56	MG	13	1782	1/1	0.99	0.05	81,81,81,81	0
56	MG	16	215	1/1	0.99	0.11	71,71,71,71	0
56	MG	1H	3576	1/1	0.99	0.08	68,68,68,68	0
56	MG	13	1759	1/1	0.99	0.04	105,105,105,105	0
56	MG	13	1797	1/1	0.99	0.19	105,105,105,105	0
56	MG	14	3334	1/1	0.99	0.03	51,51,51,51	0
56	MG	1H	3449	1/1	0.99	0.04	88,88,88,88	0
56	MG	14	3336	1/1	0.99	0.03	60,60,60,60	0
56	MG	14	3337	1/1	0.99	0.05	53,53,53,53	0
56	MG	14	3338	1/1	0.99	0.03	51,51,51,51	0
56	MG	1G	1705	1/1	0.99	0.11	84,84,84,84	0
56	MG	13	1756	1/1	0.99	0.03	95,95,95,95	0
56	MG	14	3341	1/1	0.99	0.05	46,46,46,46	0
56	MG	1H	3492	1/1	0.99	0.03	54,54,54,54	0
56	MG	1H	3531	1/1	0.99	0.12	66,66,66,66	0
56	MG	14	3344	1/1	0.99	0.06	66,66,66,66	0
56	MG	1H	3532	1/1	0.99	0.12	85,85,85,85	0
56	MG	14	3346	1/1	0.99	0.10	60,60,60,60	0
56	MG	1H	3584	1/1	0.99	0.06	58,58,58,58	0
56	MG	14	3348	1/1	0.99	0.04	59,59,59,59	0
56	MG	14	3349	1/1	0.99	0.05	60,60,60,60	0
56	MG	14	3351	1/1	0.99	0.08	76,76,76,76	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	13	1775	1/1	0.99	0.06	68,68,68,68	0
56	MG	1H	3586	1/1	0.99	0.04	53,53,53,53	0
56	MG	1H	3494	1/1	0.99	0.04	40,40,40,40	0
56	MG	14	3355	1/1	0.99	0.11	75,75,75,75	0
56	MG	14	3356	1/1	0.99	0.16	81,81,81,81	0
56	MG	14	3357	1/1	0.99	0.06	67,67,67,67	0
56	MG	1H	3495	1/1	0.99	0.03	48,48,48,48	0
57	SF4	3E	302	8/8	0.99	0.04	85,90,93,95	0
57	SF4	32	301	8/8	0.99	0.04	95,103,111,112	0
58	ZN	5I	103	1/1	0.99	0.06	97,97,97,97	0
56	MG	14	3359	1/1	0.99	0.16	105,105,105,105	0
56	MG	1H	3503	1/1	1.00	0.07	55,55,55,55	0
56	MG	1G	1724	1/1	1.00	0.04	75,75,75,75	0
56	MG	14	3350	1/1	1.00	0.07	45,45,45,45	0
56	MG	21	304	1/1	1.00	0.02	54,54,54,54	0
56	MG	1H	3548	1/1	1.00	0.02	50,50,50,50	0
56	MG	1H	3530	1/1	1.00	0.03	54,54,54,54	0
56	MG	1H	3517	1/1	1.00	0.04	54,54,54,54	0
56	MG	1H	3518	1/1	1.00	0.02	51,51,51,51	0
56	MG	1H	3607	1/1	1.00	0.04	61,61,61,61	0
56	MG	1H	3483	1/1	1.00	0.07	63,63,63,63	0
56	MG	1H	3609	1/1	1.00	0.12	90,90,90,90	0
56	MG	1H	3500	1/1	1.00	0.09	43,43,43,43	0
56	MG	1H	3515	1/1	1.00	0.02	41,41,41,41	0
56	MG	1H	3544	1/1	1.00	0.08	57,57,57,57	0
56	MG	1H	3545	1/1	1.00	0.04	63,63,63,63	0
56	MG	1H	3528	1/1	1.00	0.04	49,49,49,49	0

6.5 Other polymers (i)

There are no such residues in this entry.