



# wwPDB X-ray Structure Validation Summary Report ⓘ

May 21, 2020 – 04:58 am BST

PDB ID : 6GSJ  
Title : Structure of T. thermophilus 70S ribosome complex with mRNA, tRNA<sup>fMet</sup> and cognate tRNA<sup>Thr</sup> 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](mailto:validation@mail.wwpdb.org)

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

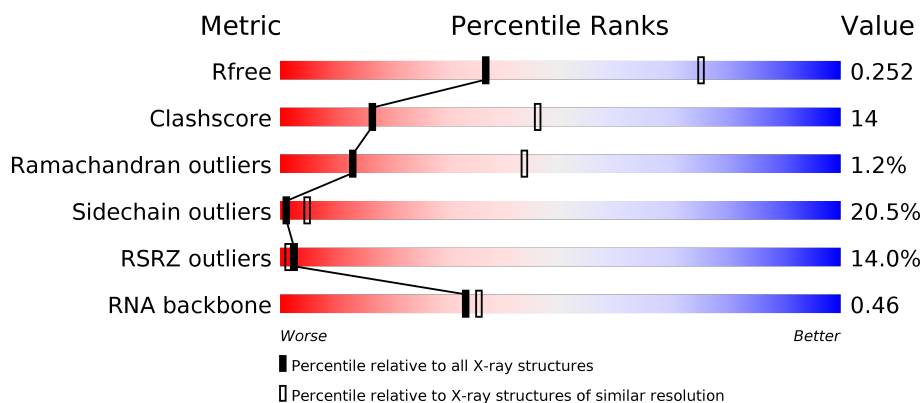
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 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))
$R_{free}$	130704	3104 (3.00-2.92)
Clashscore	141614	3462 (3.00-2.92)
Ramachandran outliers	138981	3340 (3.00-2.92)
Sidechain outliers	138945	3343 (3.00-2.92)
RSRZ outliers	127900	2986 (3.00-2.92)
RNA backbone	3102	1065 (3.22-2.70)

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

Mol	Chain	Length	Quality of chain
1	13	1522	<div> <div>11%</div> <div> <div>41%</div> <div>40%</div> <div>15%</div> <div>..</div> </div> </div>
1	1G	1522	<div> <div>2%</div> <div> <div>46%</div> <div>37%</div> <div>12%</div> <div>..</div> </div> </div>
2	12	256	<div> <div>2%</div> <div> <div>30%</div> <div>38%</div> <div>12%</div> <div>19%</div> </div> </div>
2	1E	256	<div> <div>11%</div> <div> <div>41%</div> <div>36%</div> <div>13%</div> <div>10%</div> </div> </div>

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

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Mol	Chain	Length	Quality of chain
15	6I	89	
16	7A	88	
16	7I	88	
17	8A	105	
17	8I	105	
18	9A	88	
18	9I	88	
19	AA	93	
19	AI	93	
20	BA	106	
20	BI	106	
21	1B	27	
21	1F	27	
22	1K	76	
22	1L	76	
23	2K	77	
23	2L	77	
24	3K	76	
25	4K	27	
25	4L	27	
26	14	2917	
26	1H	2917	
27	16	122	
27	1J	122	
28	11	276	

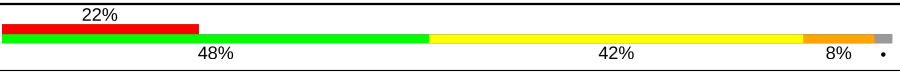
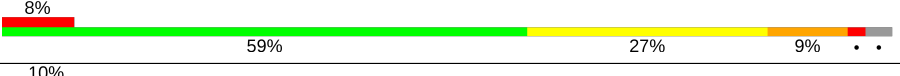



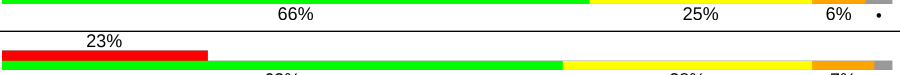
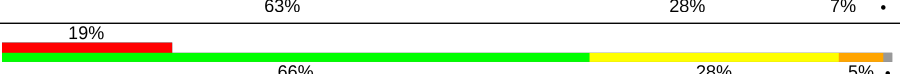
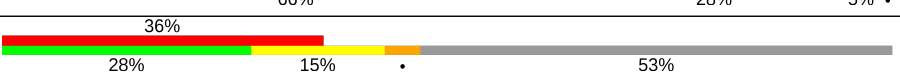
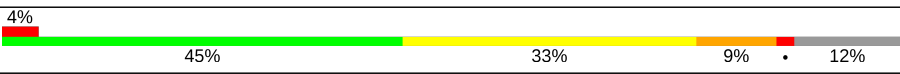
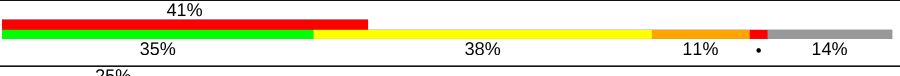
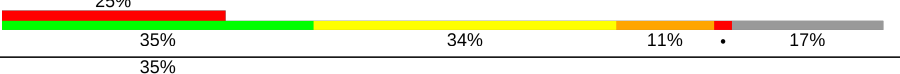


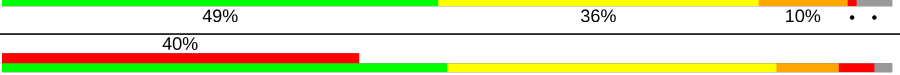
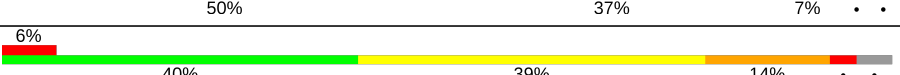
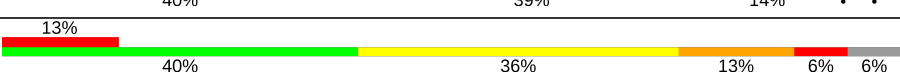

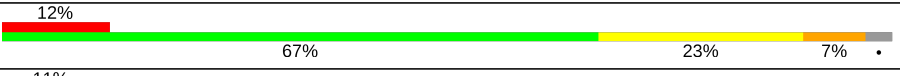
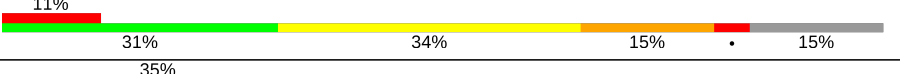



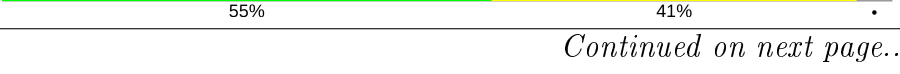


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Mol	Chain	Length	Quality of chain
28	19	276	
29	21	206	
29	29	206	
30	31	210	
30	39	210	
31	41	182	
31	49	182	
32	51	180	
32	59	180	
33	61	148	
33	69	148	
34	15	140	
34	58	140	
35	25	122	
35	68	122	
36	35	150	
36	78	150	
37	45	141	
37	88	141	
38	55	118	
38	98	118	
39	65	112	
39	A8	112	
40	75	146	
40	B8	146	

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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	1665	-	-	-	X
56	MG	13	1685	-	-	-	X
56	MG	13	1686	-	-	-	X
56	MG	13	1689	-	-	-	X
56	MG	13	1696	-	-	-	X
56	MG	13	1706	-	-	-	X
56	MG	13	1710	-	-	-	X
56	MG	13	1712	-	-	-	X
56	MG	13	1725	-	-	-	X
56	MG	13	1763	-	-	-	X
56	MG	13	1764	-	-	-	X
56	MG	14	3178	-	-	-	X
56	MG	14	3179	-	-	-	X
56	MG	14	3191	-	-	-	X
56	MG	14	3245	-	-	-	X
56	MG	14	3262	-	-	-	X
56	MG	1G	1647	-	-	-	X
56	MG	1G	1667	-	-	-	X
56	MG	1G	1722	-	-	-	X
56	MG	1H	3046	-	-	-	X
56	MG	1H	3165	-	-	-	X
56	MG	1H	3196	-	-	-	X
56	MG	1H	3205	-	-	-	X
56	MG	1H	3219	-	-	-	X
56	MG	1H	3259	-	-	-	X
56	MG	1H	3264	-	-	-	X
56	MG	1H	3300	-	-	-	X
56	MG	1H	3332	-	-	-	X
56	MG	1H	3333	-	-	-	X
56	MG	1H	3370	-	-	-	X
56	MG	21	302	-	-	-	X
56	MG	78	202	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
56	MG	BA	202	-	-	-	X



## 2 Entry composition

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	S	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 (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
56	98	1	Total	Mg	0	0
			1	1		
56	45	2	Total	Mg	0	0
			2	2		
56	55	1	Total	Mg	0	0
			1	1		
56	BA	2	Total	Mg	0	0
			2	2		
56	P8	1	Total	Mg	0	0
			1	1		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
56	85	1	Total 1	Mg 1	0	0
56	2I	1	Total 1	Mg 1	0	0
56	13	205	Total 205	Mg 205	0	0
56	1J	6	Total 6	Mg 6	0	0
56	5I	2	Total 2	Mg 2	0	0
56	35	3	Total 3	Mg 3	0	0
56	BI	2	Total 2	Mg 2	0	0
56	4L	1	Total 1	Mg 1	0	0
56	16	15	Total 15	Mg 15	0	0
56	42	1	Total 1	Mg 1	0	0
56	25	1	Total 1	Mg 1	0	0
56	21	4	Total 4	Mg 4	0	0
56	31	2	Total 2	Mg 2	0	0
56	Q8	1	Total 1	Mg 1	0	0
56	8I	1	Total 1	Mg 1	0	0
56	9A	1	Total 1	Mg 1	0	0
56	I8	2	Total 2	Mg 2	0	0
56	D8	1	Total 1	Mg 1	0	0
56	68	2	Total 2	Mg 2	0	0
56	29	3	Total 3	Mg 3	0	0
56	2K	2	Total 2	Mg 2	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
56	4A	1	Total 1	Mg 1	0	0
56	39	1	Total 1	Mg 1	0	0
56	1G	155	Total 155	Mg 155	0	0
56	11	1	Total 1	Mg 1	0	0
56	1H	622	Total 622	Mg 622	0	0
56	E5	1	Total 1	Mg 1	0	0
56	88	3	Total 3	Mg 3	0	0
56	5E	1	Total 1	Mg 1	0	0
56	14	435	Total 435	Mg 435	0	0
56	78	2	Total 2	Mg 2	0	0
56	3E	1	Total 1	Mg 1	0	0
56	19	1	Total 1	Mg 1	0	0
56	2A	1	Total 1	Mg 1	0	0
56	1K	1	Total 1	Mg 1	0	0
56	41	1	Total 1	Mg 1	0	0
56	1B	1	Total 1	Mg 1	0	0
56	2L	2	Total 2	Mg 2	0	0

- Molecule 57 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe<sub>4</sub>S<sub>4</sub>).



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

- Molecule 58 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

- Molecule 59 is water.

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

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

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

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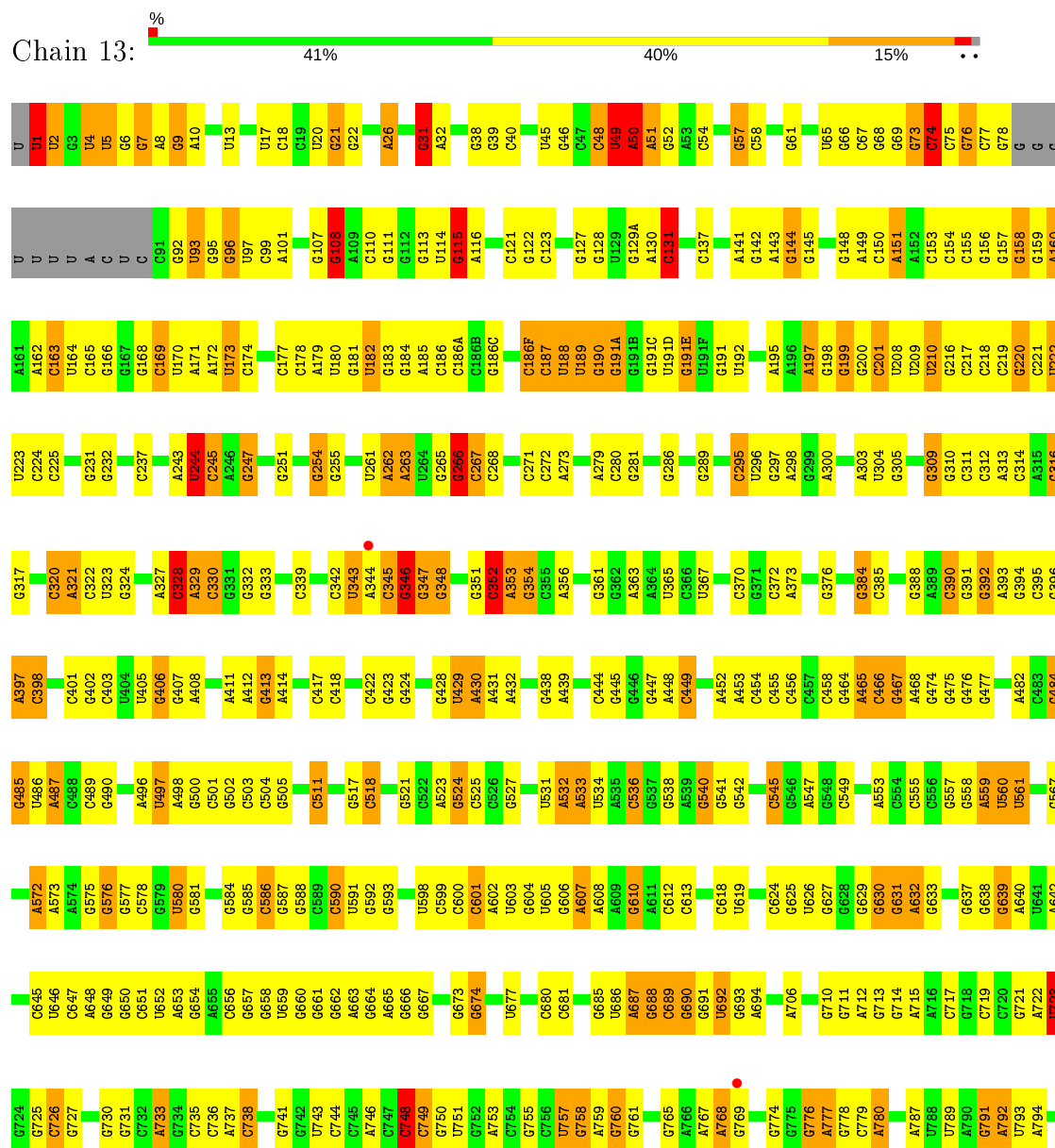
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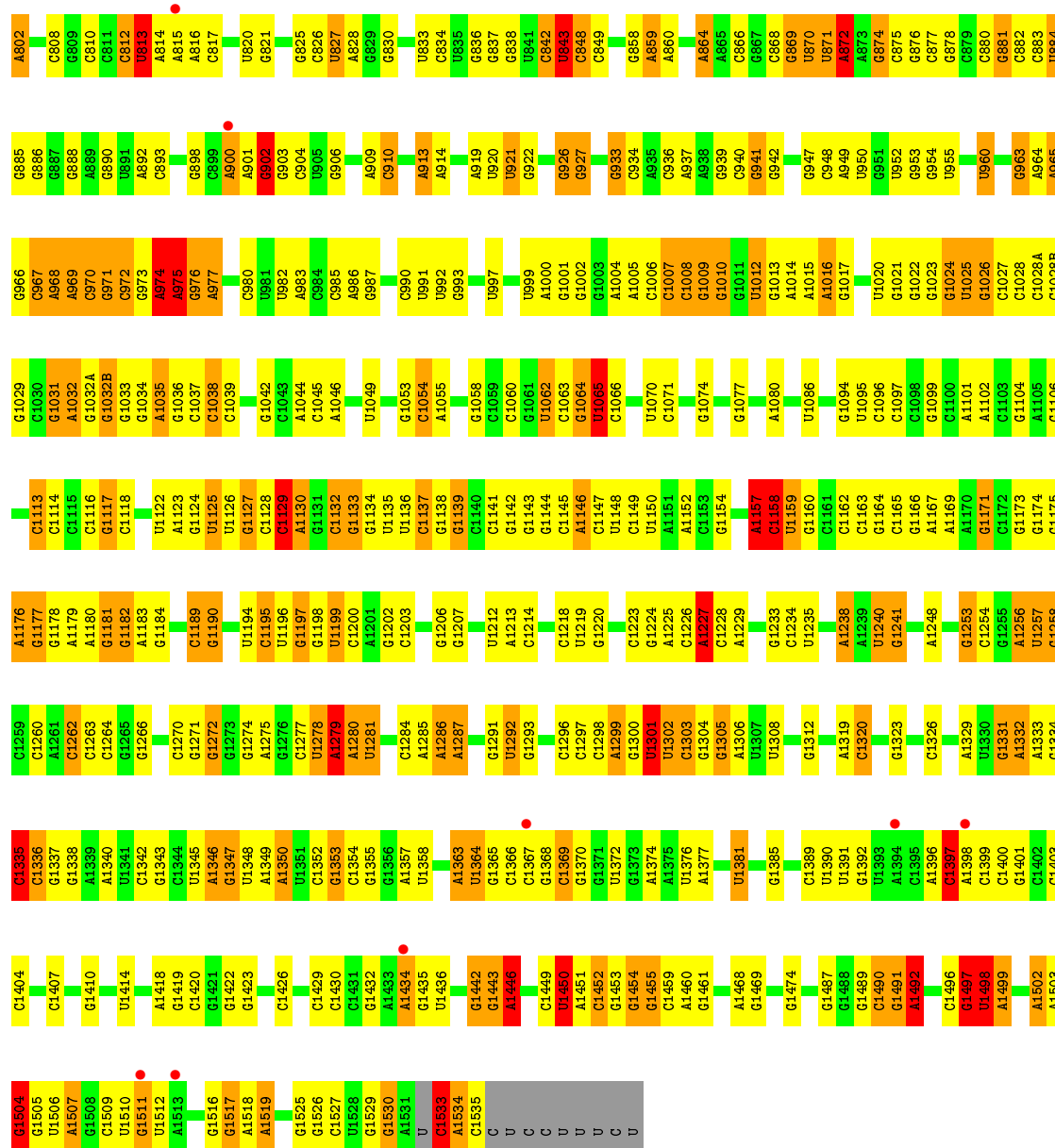
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
59	45	4	Total 4	O 4	0	0
59	75	1	Total 1	O 1	0	0
59	95	1	Total 1	O 1	0	0
59	B5	3	Total 3	O 3	0	0
59	H5	3	Total 3	O 3	0	0
59	M5	2	Total 2	O 2	0	0

### 3 Residue-property plots

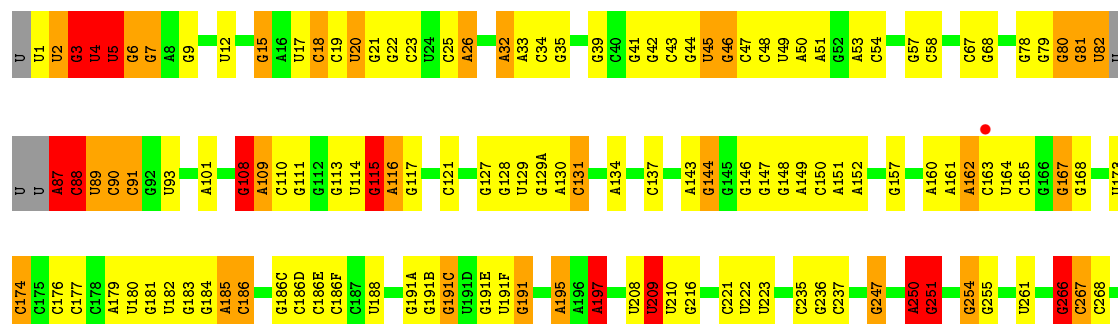
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are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

- Molecule 1: 16S ribosomal RNA





• Molecule 1: 16S ribosomal RNA



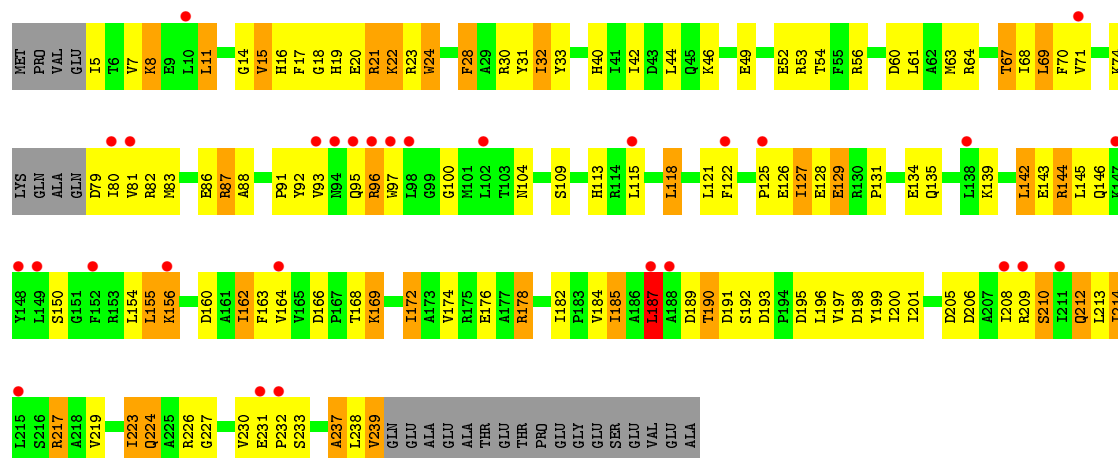
A1432	G1432	A1350	A1285	C1208	C1141	C1069	G1010	C948	C842	A746	U619	G541	C457	U367	C272
G1435	A1287	C1209	A1286	C1210	G1142	C1075	G1011	A949	U643	A747	C620	G542	C458	G371	G278
U1436	A1288	U1211	G1144	U1212	G1143	U1078	A1014	G951	C848	C747	A621	G543	G464	A372	A279
A1357	A1289	A1213	C1145	C1214	A1146	A1079	A1015	U952	U850	C749	C623	G544	A465	A373	G280
U1358	G1290	G1215	C1147	G1216	G1017	A1080	A1016	G953	G854	G750	A547	G545	C466	A374	G281
C1359	G1291	G1217	U1148	C1217	C1018	G1081	G1017	U955	G855	U751	G629	G546	A468	G376	A282
G1443	U1292	G1218	U1149	C1218	C1019	G1082	A1018	U956	A859	G752	G630	C554	G475	G377	U287
A1446	G1294	C1219	U1150	U1219	U1020	U1085	U1021	U957	A859	C754	A632	C555	G476	G378	A288
U1449	G1297	G1224	A1151	U1219	G1022	U1086	G1022	U958	C862	G755	G633	C556	A478	G379	G289
U1450	C1298	A1225	C1152	U1219	G1023	U1087	G1023	U959	A865	G756	G650	C557	G479	C385	C290
A1451	A1299	A1226	G1153	U1219	G1024	U1087	G1024	U961	A865	U757	G651	C558	G480	C391	C291
G1452	G1300	C1226	G1155	U1219	U1025	A1092	U1025	G962	U871	G758	U652	C559	C483	C392	G292
G1454	U1301	A1227	A1156	U1219	G	A1093	G	G963	A872	A766	A653	C562	G484	A389	C295
A1460	C1303	U1235	A1157	U1235	C	U1094	C	A964	A873	A777	G661	C563	G485	G391	U296
C1466	G1304	U1235	U1159	U1235	C	U1095	C	A965	A874	A778	U664	C564	A487	C395	C297
G1467	A1306	A1238	G1160	U1238	C	C1097	C	A967	G879	C779	A665	C565	C489	G396	A298
A1468	U1307	A1239	C1161	U1239	G	U1098	G	A969	G879	A780	G669	C566	G490	G397	A300
G1469	U1308	U1240	C1162	U1240	C	G1099	C	A970	G885	C784	U669	C567	G492	C398	G305
A1473	G1312	C1241	A1169	U1241	A	A1101	A	G971	G890	A787	G673	U571	U494	G406	G309
C1478	U1313	C1242	G1170	U1242	G	A1102	G	G972	U891	A787	G674	A572	A495	G407	A408
C1479	C1314	C1243	G1171	U1243	G	G1103	G	G973	U891	A787	U677	A573	A496	A408	C314
C1484	U1315	C1244	G1172	U1244	G	A1104	G	A974	A892	A790	U678	C575	U497	G410	A315
U1485	G1316	U1245	G1173	U1245	G	A1105	G	A975	C893	G791	U679	C576	A498	A411	G316
G1486	C1317	U1246	G1174	U1246	A	G1106	A	A976	G894	A792	C679	C577	G499	A412	G317
G1487	G1318	U1247	G1175	U1247	G1036	C1107	G1036	A977	G895	A793	U680	C578	G502	G413	G318
A1492	A1319	C1248	G1176	U1248	C1037	U1108	C1037	A978	G898	A794	U684	U580	C504	A414	G319
C1496	C1320	A1250	G1177	U1249	C1038	C1109	C1038	C979	A901	C797	G685	G581	G505	C419	C320
U1498	C1321	A1251	G1178	U1250	C1039	A1110	C1039	U981	A902	G798	U686	U582	A509	U420	A321
A1502	G1322	A1252	A1180	U1251	G1042	C1112	G1042	A983	G903	G800	A687	U583	A510	G421	G324
G1503	C1323	U1256	G1181	U1256	C1043	G1117	C1043	C984	A909	U804	C689	G587	C511	G422	A325
U1504	A1324	U1257	G1182	U1257	C1044	C1118	A1044	C985	A913	C810	G690	G588	G517	G423	G326
G1505	C1325	G1258	A1183	U1258	C1045	C1119	A1045	A986	A914	C811	G691	C589	C518	G424	A327
A1507	G1326	C1259	G1184	U1259	C1046	G1120	A1046	U991	A915	C812	U697	U598	C519	G425	C328
C1509	C1327	U1260	G1187	U1260	C1050	U1121	G1050	U992	G916	C813	A702	C599	A520	U427	A329
U1510	G1328	C1263	C1189	U1263	C1051	A1123	C1051	U993	G916	U813	G713	G600	G521	U428	G332
A1511	A1330	A1268	C1192	U1268	C1052	U1125	U1052	U994	U920	A814	C601	C522	G526	U429	C345
U1512	C1331	A1269	G1193	A1269	C1053	U1126	G1053	A994	G922	A815	A602	C527	G527	G438	G346
A1513	G1332	G1272	U1194	U1272	C1054	C1127	C1054	U995	U921	C816	U603	C528	G528	A439	G347
C1514	C1333	U1273	C1195	U1273	A1055	C1128	A1055	U996	G926	C817	G604	G604	G529	A440	G351
G1517	A1334	G1274	U1197	U1274	C1056	C1129	U1056	G988A	G927	A818	U605	G606	G530	A442	C352
A1518	C1335	A1275	G1198	U1275	C1057	A1130	G1057	U999	U927	U820	G607	C531	G531	C449	A353
A1519	U1340	G1276	U1199	U1276	C1058	G1131	G1058	A1000	C932	A821	A608	U531	U531	G446	G354
C1514	C1341	C1277	C1200	U1277	C1059	C1132	C1059	G1001	G933	G821	G447	A532	A532	G447	U359
G1520	G1342	U1278	A1201	U1278	C1060	G1133	G1061	G1002	C934	U827	A609	U533	U533	A448	A360
	C1343	A1279	G1202	U1279	C1061	G1134	U1061	G1003	A935	A828	C612	C534	C534	C449	G361
	G1344	A1280	C1203	U1280	C1062	U1135	U1062	A1005	G829	G829	C615	C535	C535	G452	G362
	A1346	U1281	A1204	U1281	C1063	C1137	G1064	C1006	G942	G837	G616	G537	G537	A452	A363
	G1347	C1282	U1205	U1282	C1064	G1138	U1065	C1007	U943	G838	C455	G538	G538	C455	C366
	U1348	G1283	G1206	U1283	C1065	G1139	U1066	C1008	G944	U841	C456	G540	G540	C456	
	A1349	C1284	G1207	U1284	C1066	C1140	U1066	G1009							



• Molecule 2: 30S ribosomal protein S2



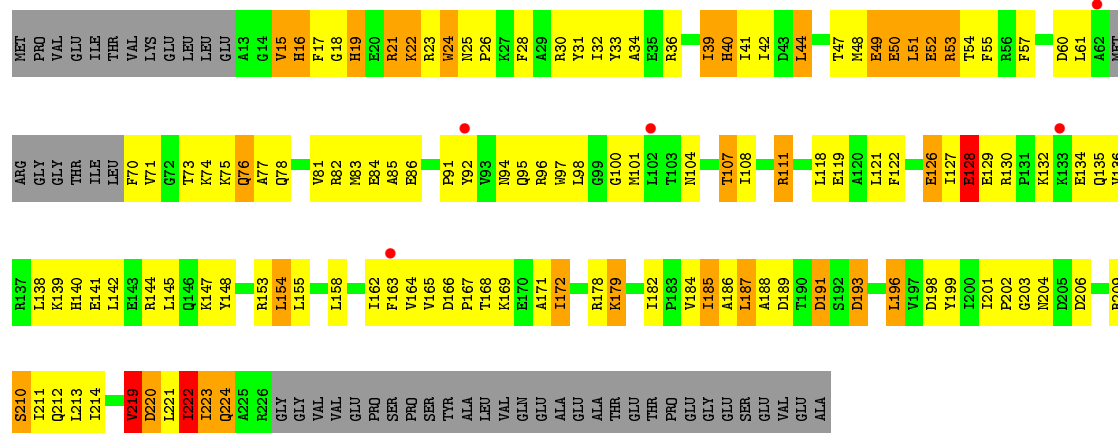
Chain 1E:



• Molecule 2: 30S ribosomal protein S2



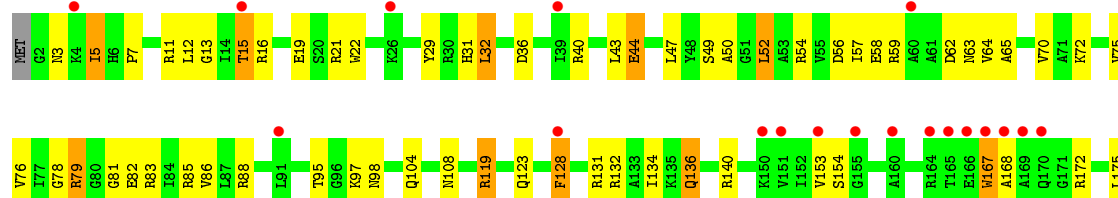
Chain 12:



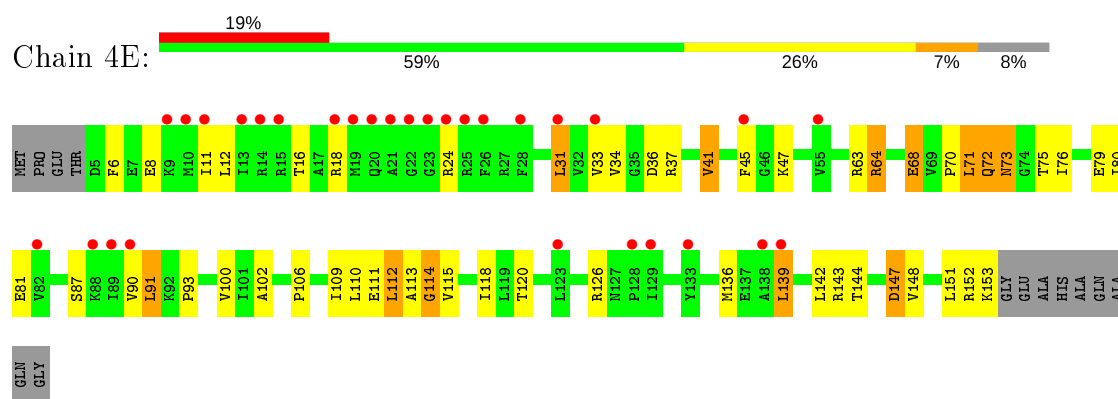
• Molecule 3: 30S ribosomal protein S3



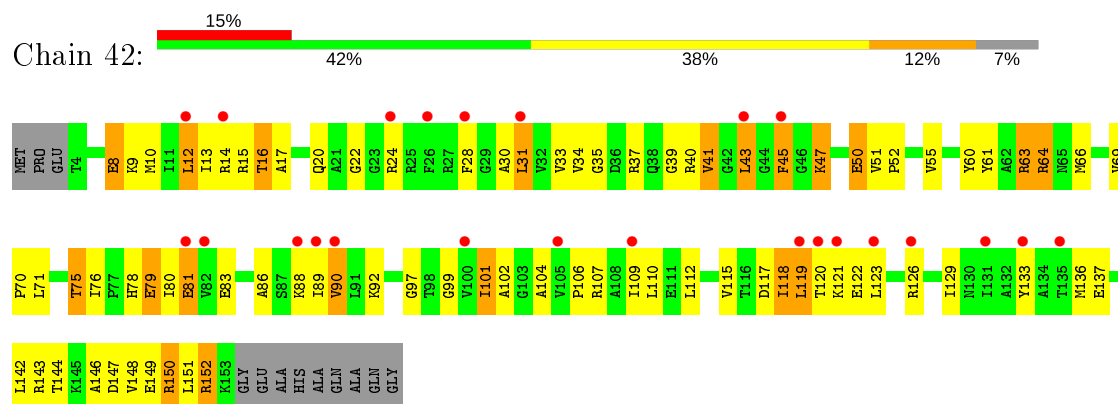
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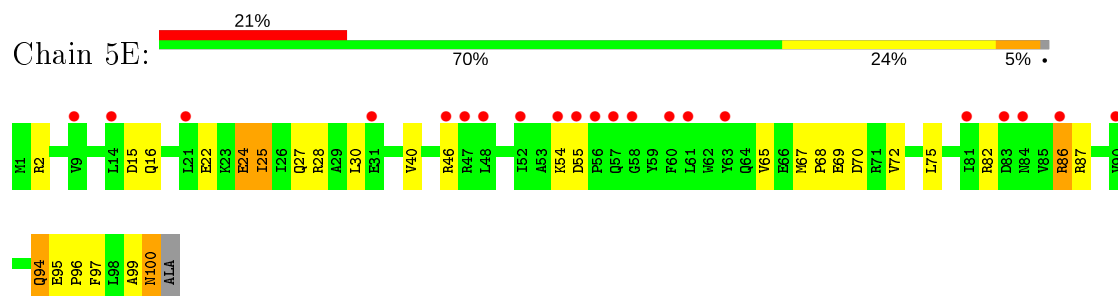




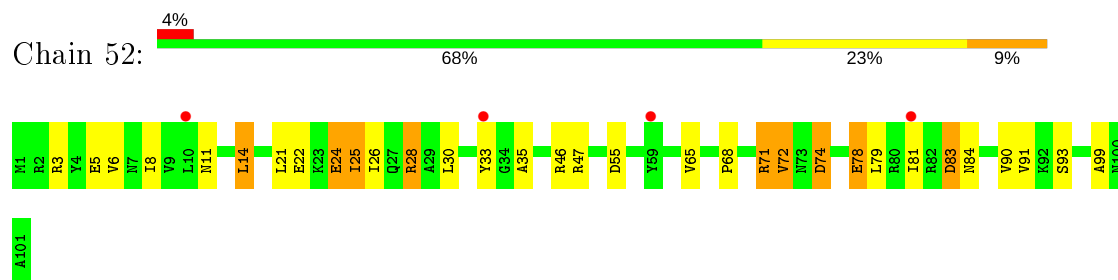
- Molecule 5: 30S ribosomal protein S5



- Molecule 6: 30S ribosomal protein S6

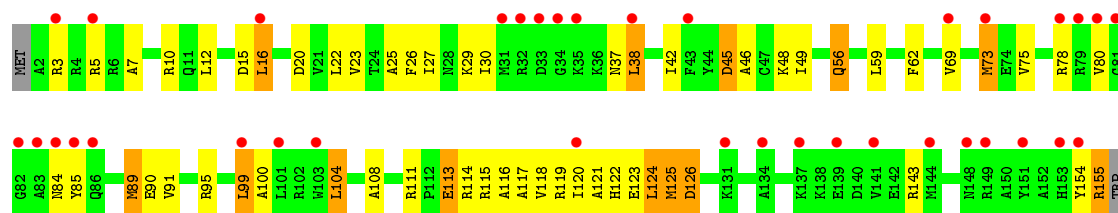


- Molecule 6: 30S ribosomal protein S6

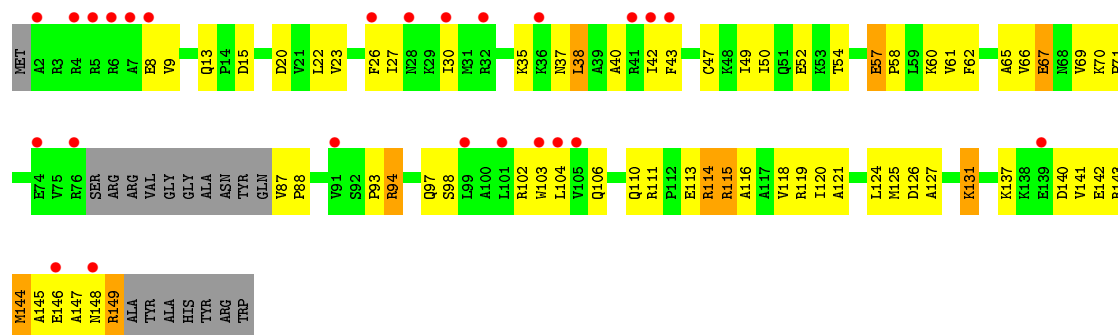


- Molecule 7: 30S ribosomal protein S7

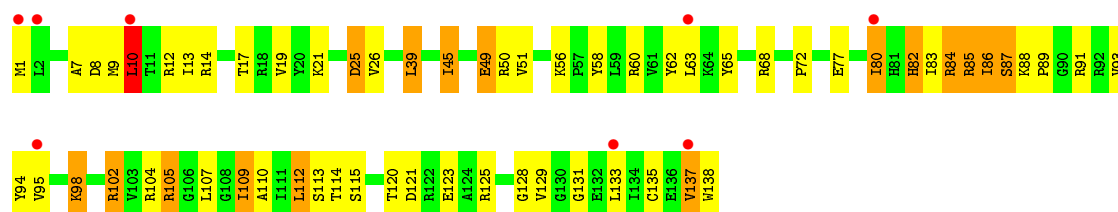




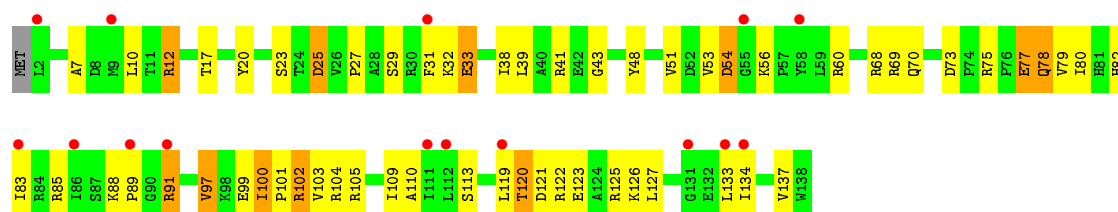
• Molecule 7: 30S ribosomal protein S7



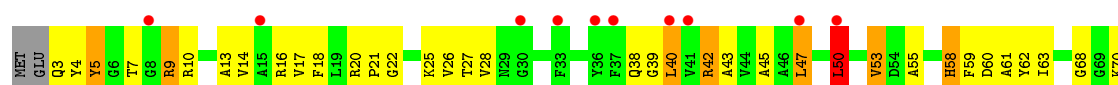
• Molecule 8: 30S ribosomal protein S8



• Molecule 8: 30S ribosomal protein S8



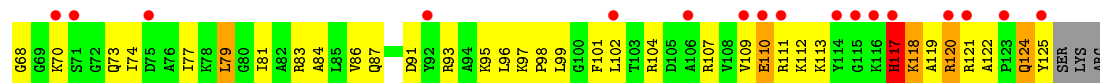
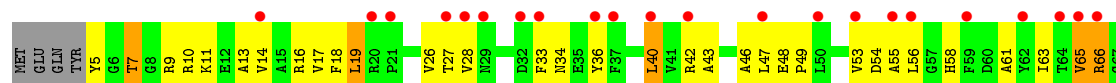
• Molecule 9: 30S ribosomal protein S9



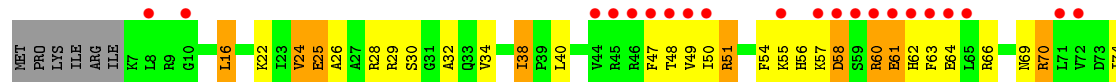




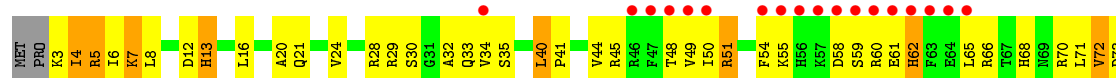
• Molecule 9: 30S ribosomal protein S9



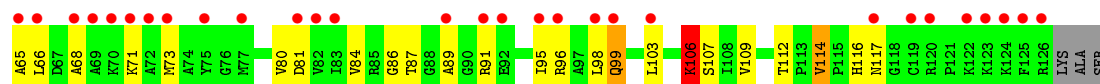
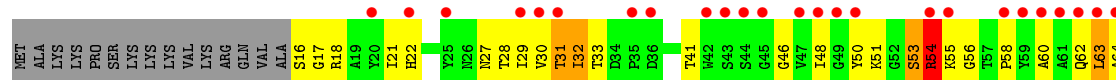
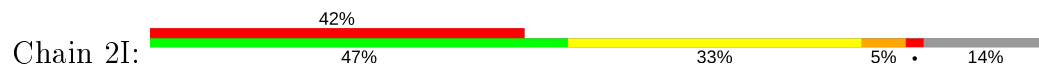
• Molecule 10: 30S ribosomal protein S10



• Molecule 10: 30S ribosomal protein S10

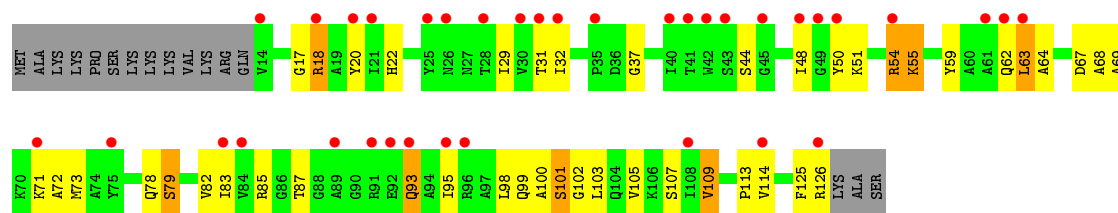


• Molecule 11: 30S ribosomal protein S11

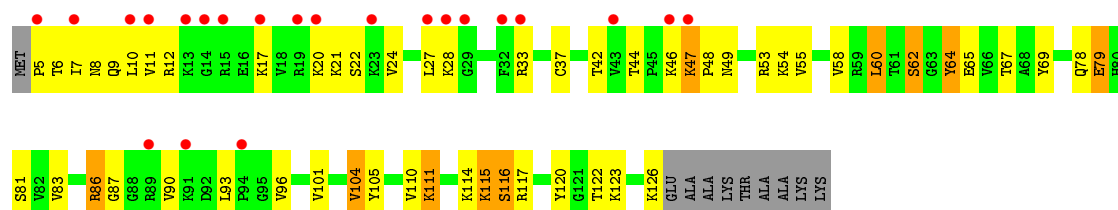


• Molecule 11: 30S ribosomal protein S11

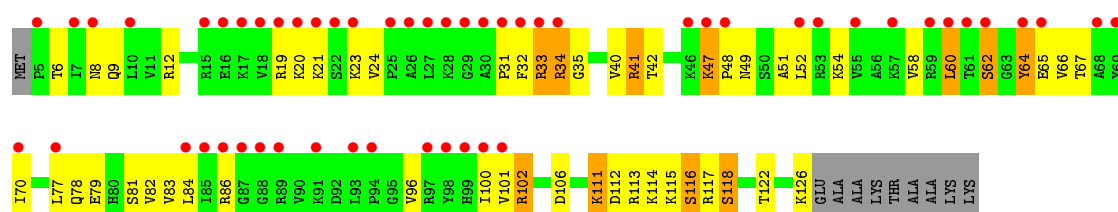
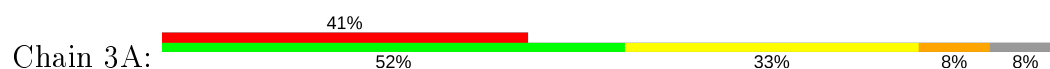




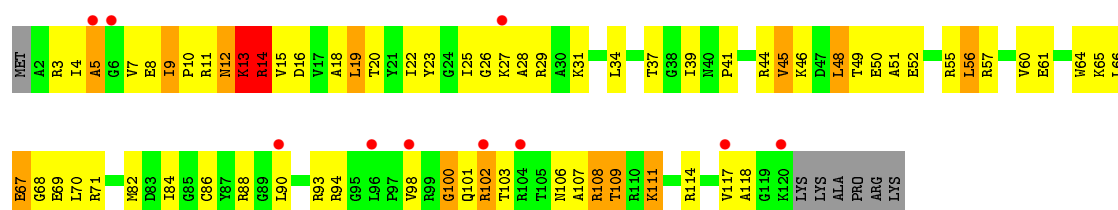
• Molecule 12: 30S ribosomal protein S12



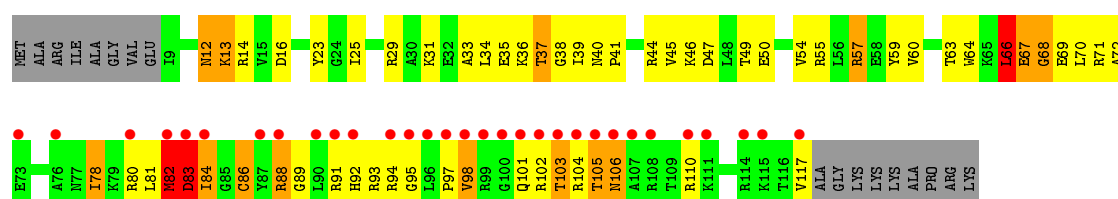
• Molecule 12: 30S ribosomal protein S12



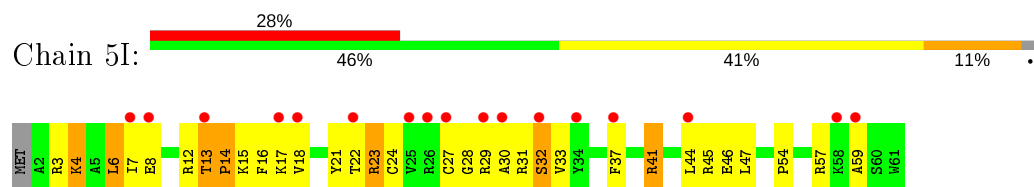
• Molecule 13: 30S ribosomal protein S13



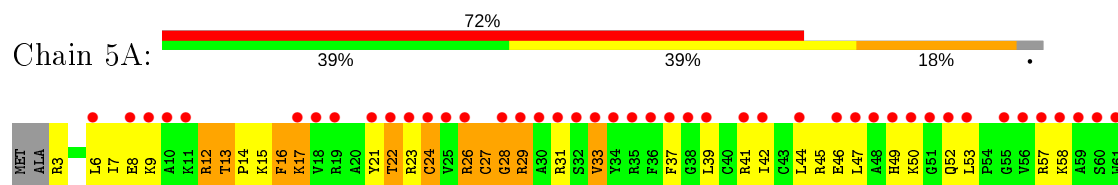
• Molecule 13: 30S ribosomal protein S13



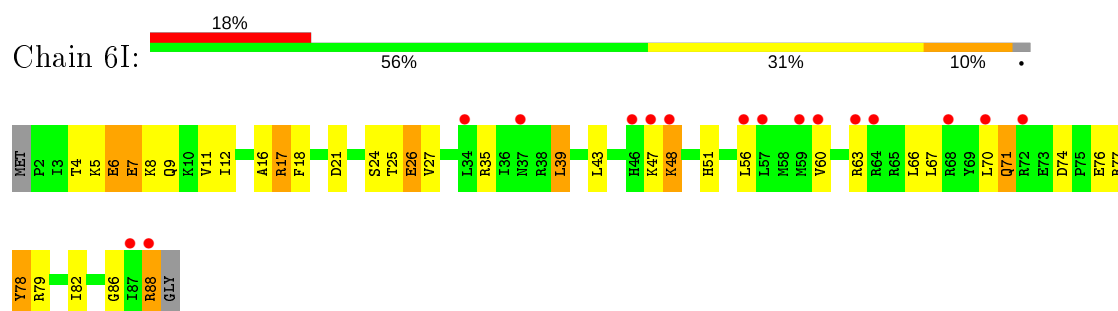
- Molecule 14: 30S ribosomal protein S14 type Z



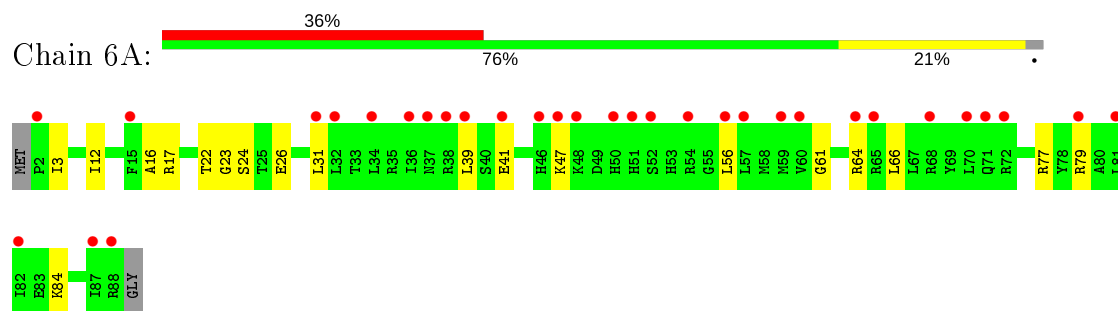
- Molecule 14: 30S ribosomal protein S14 type Z



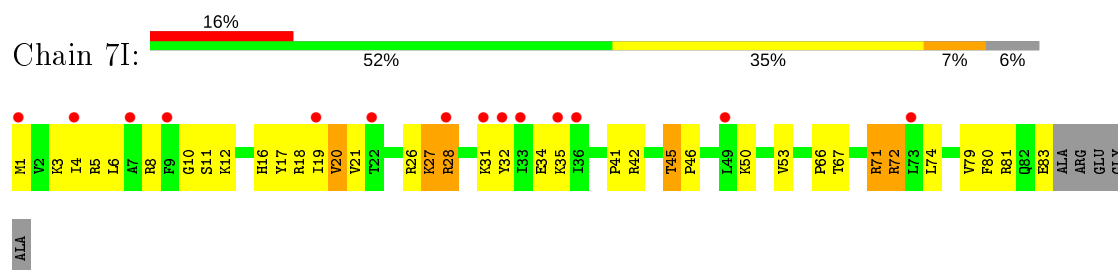
- Molecule 15: 30S ribosomal protein S15



- Molecule 15: 30S ribosomal protein S15



- Molecule 16: 30S ribosomal protein S16

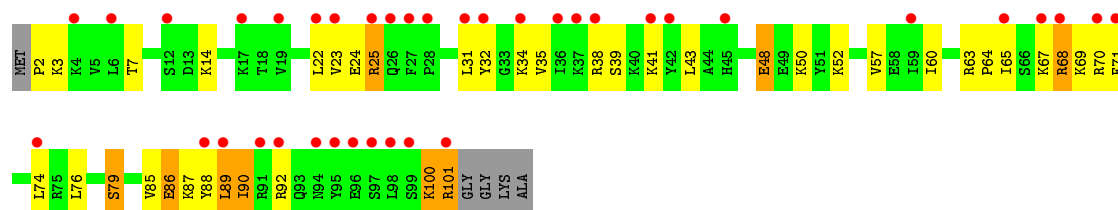


- Molecule 16: 30S ribosomal protein S16

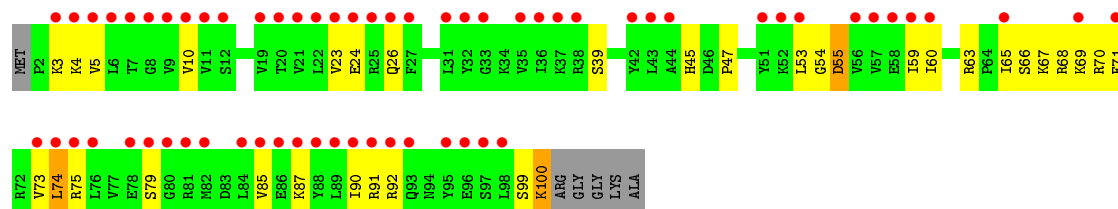




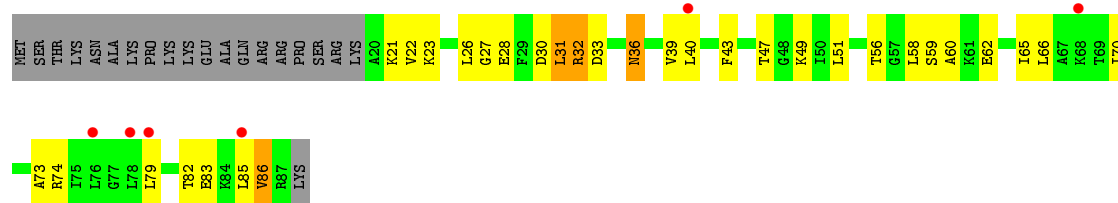
- Molecule 17: 30S ribosomal protein S17



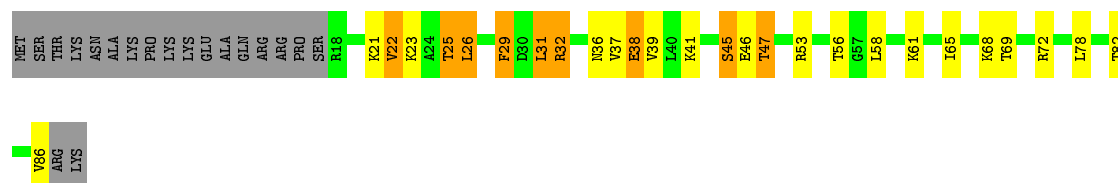
- Molecule 17: 30S ribosomal protein S17



- Molecule 18: 30S ribosomal protein S18

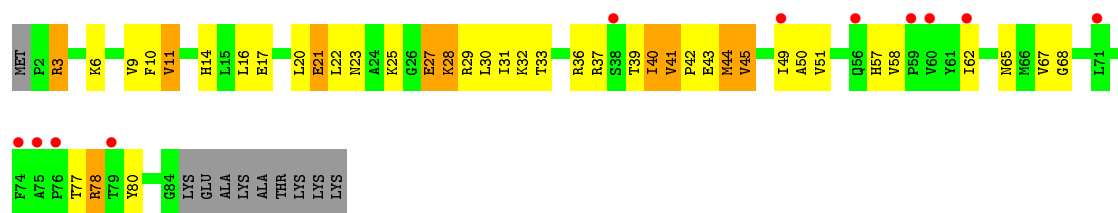


- Molecule 18: 30S ribosomal protein S18

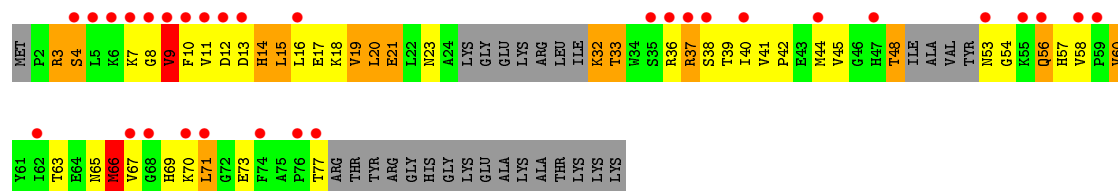
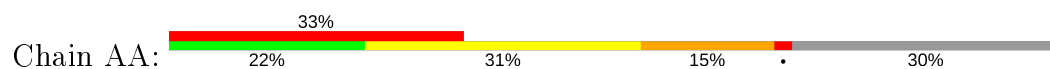


- Molecule 19: 30S ribosomal protein S19

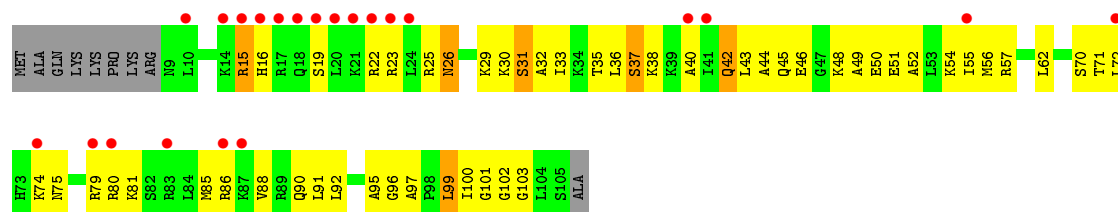
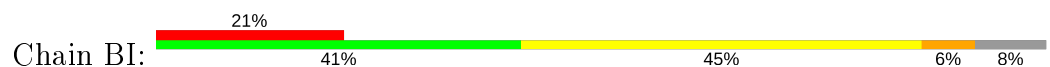




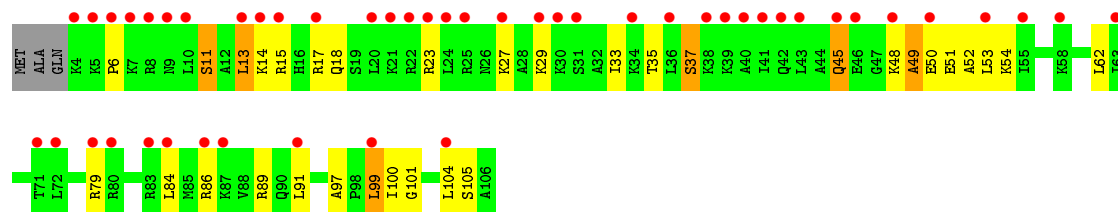
• Molecule 19: 30S ribosomal protein S19



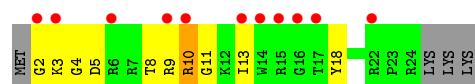
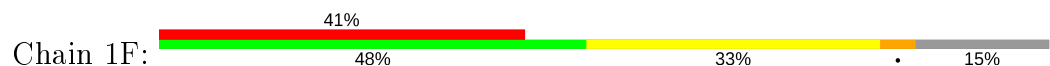
• Molecule 20: 30S ribosomal protein S20



• Molecule 20: 30S ribosomal protein S20

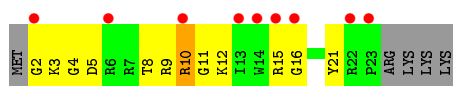


• Molecule 21: 30S ribosomal protein Thx

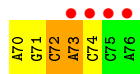
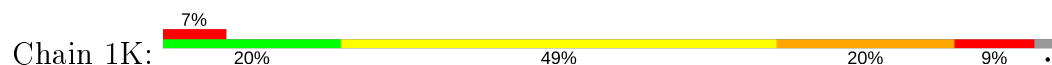


• Molecule 21: 30S ribosomal protein Thx

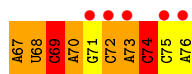
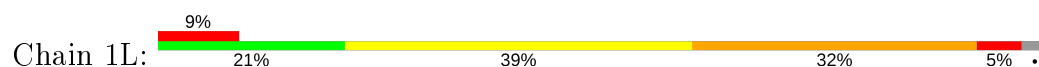




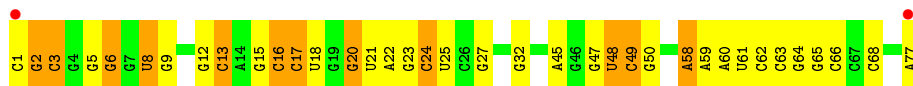
• Molecule 22: tRNA<sup>Thr</sup>



• Molecule 22: tRNA<sup>Thr</sup>



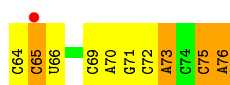
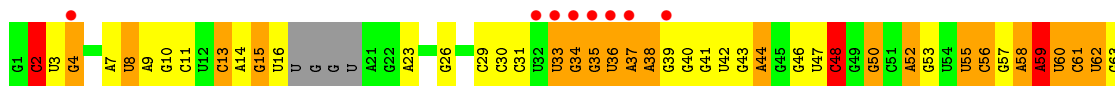
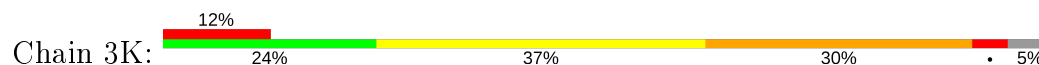
• Molecule 23: tRNA<sup>Met</sup>



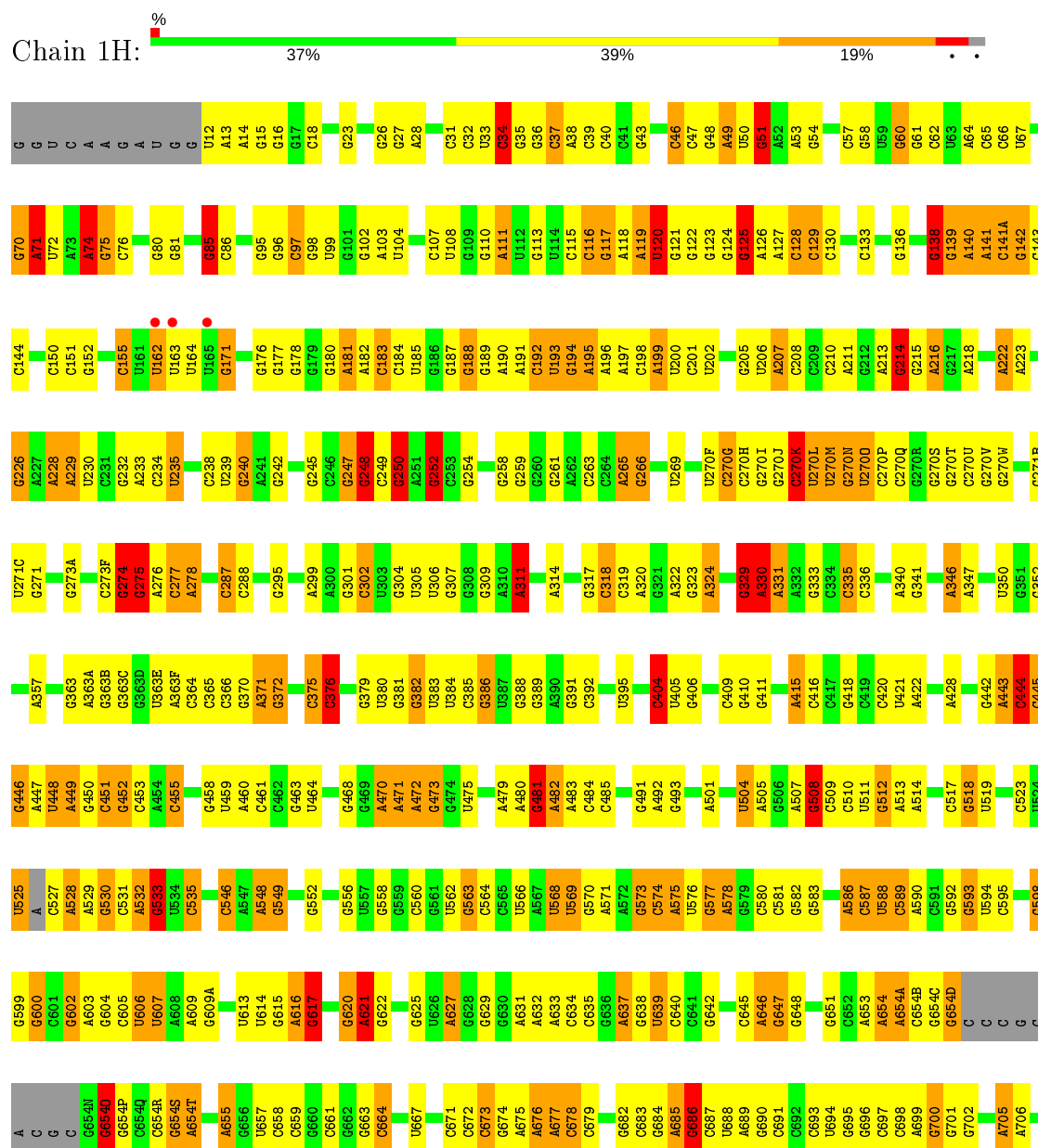
• Molecule 23: tRNA<sup>Met</sup>



• Molecule 24: tRNA<sup>Thr</sup>



• Molecule 25: RNA (27-MER)



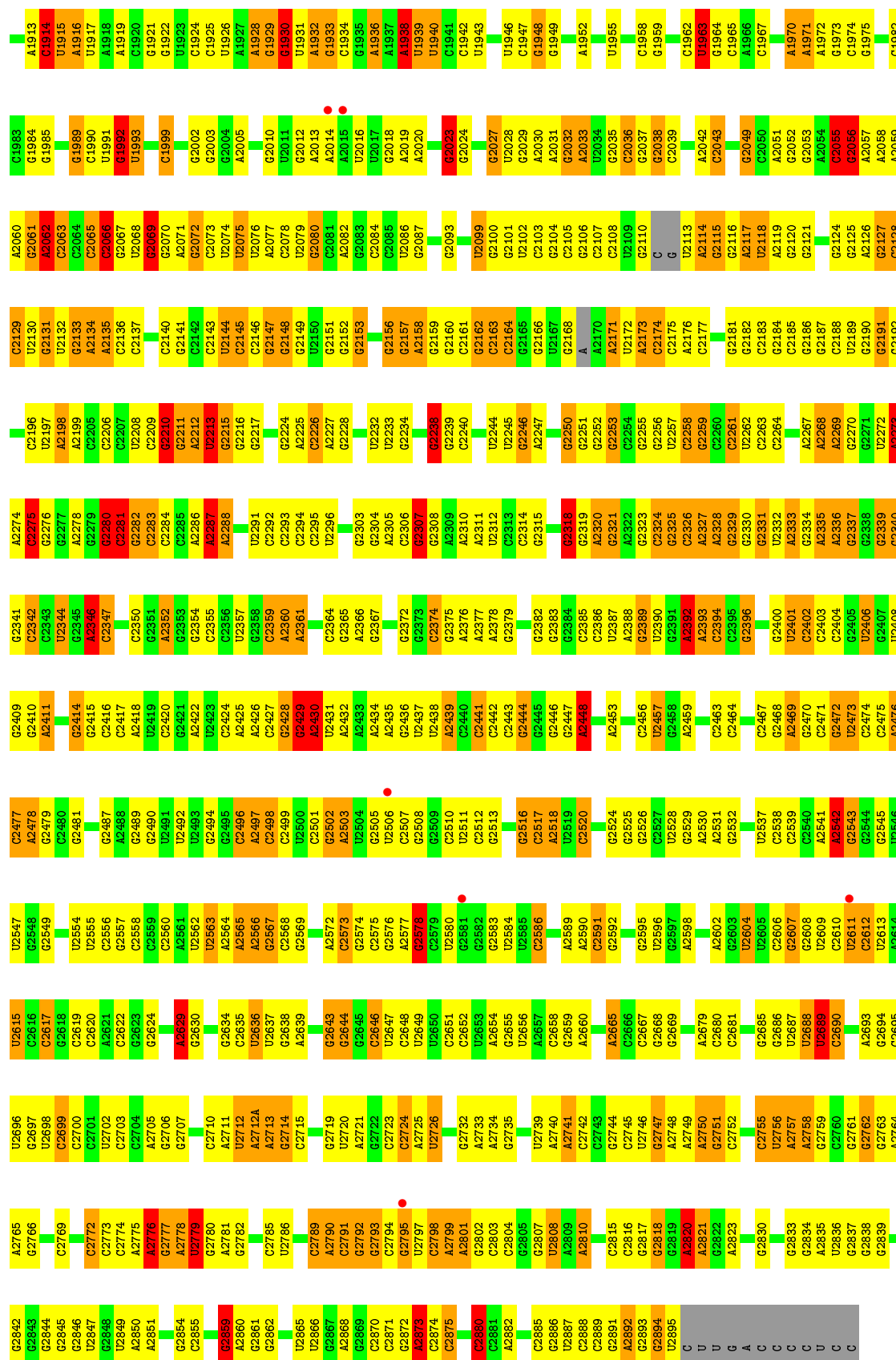
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G1561	C1564	C1565	A1566	U1567	A1568	A1569	A1570	A1571	A1572	C1573	C1574		G1577	U1578	A1579	A1580		G1581	C1582	A1583	A1585	A1586	A1587	C1588	C1589	U1590	G1591	C1592	G1593	A1594	G1595	A1596	C1597	C1598	C1599	C1600	G1601	U1602	A1603	G1604	C1605	G1606	U1607	A1608	A1609	A1610	C1611		A1614	C1615	A1616	C1617	A1618	C1619	G1620	U1621	G1622	A1623	G1624	G1625	G1626	G1627	G1628	G1629	G1630																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																														
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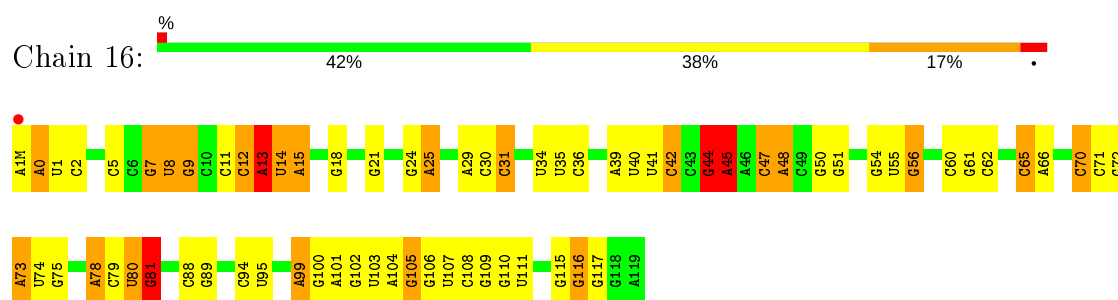




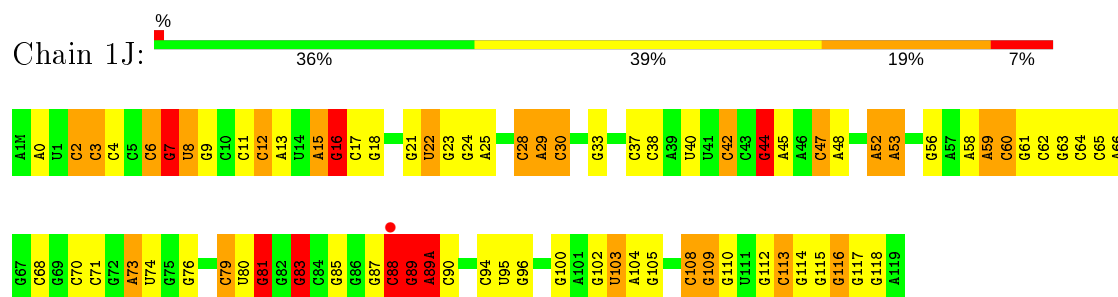
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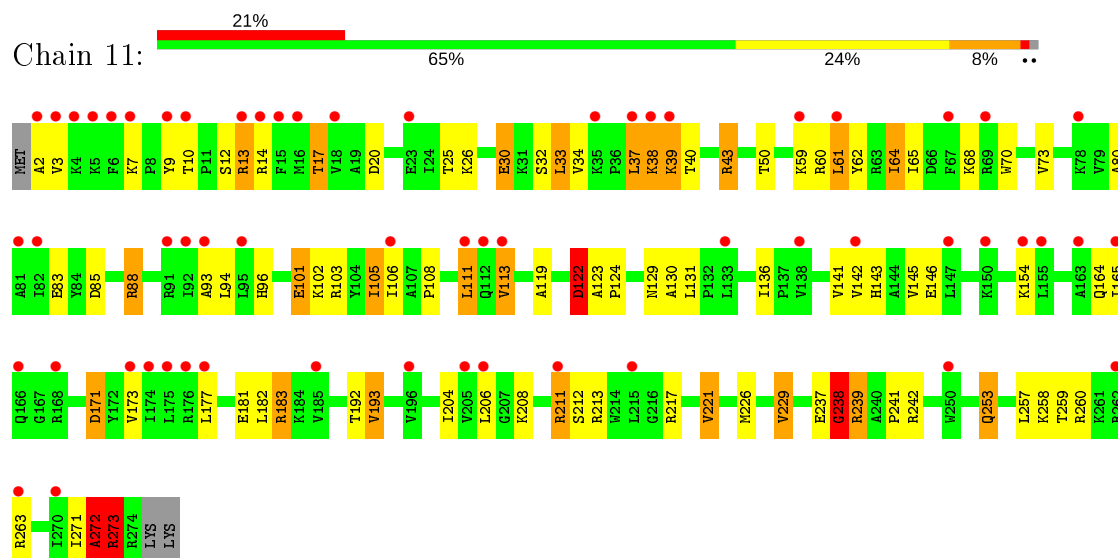
- Molecule 27: 5S ribosomal RNA



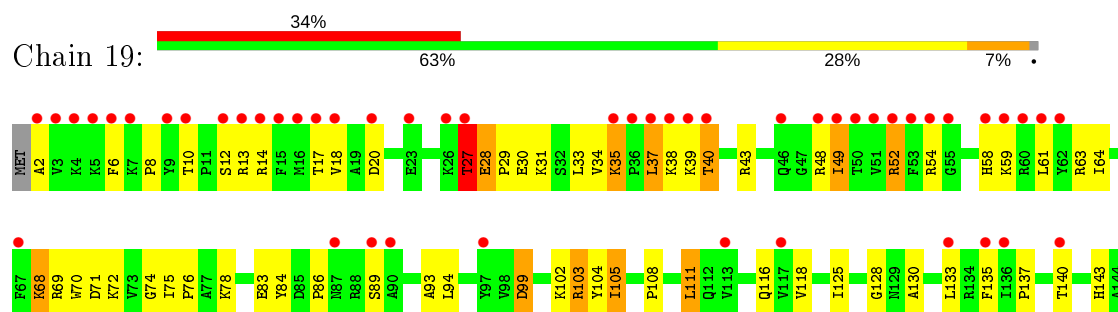
- Molecule 27: 5S ribosomal RNA

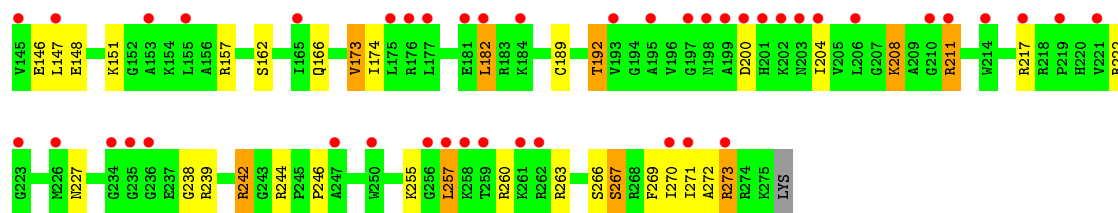


- Molecule 28: 50S ribosomal protein L2

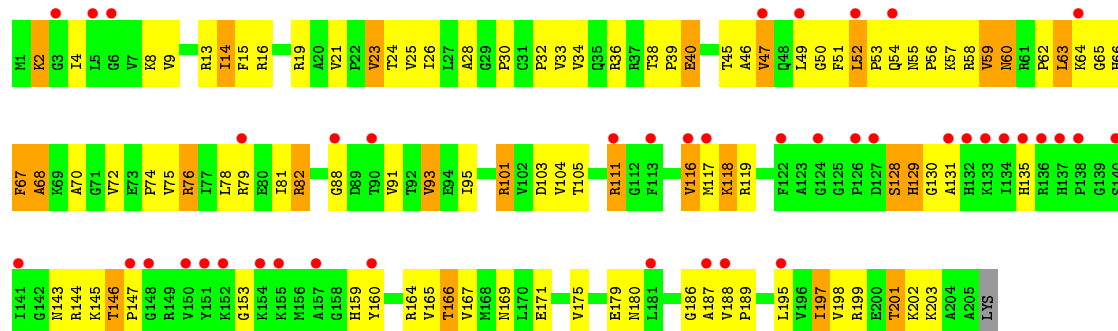


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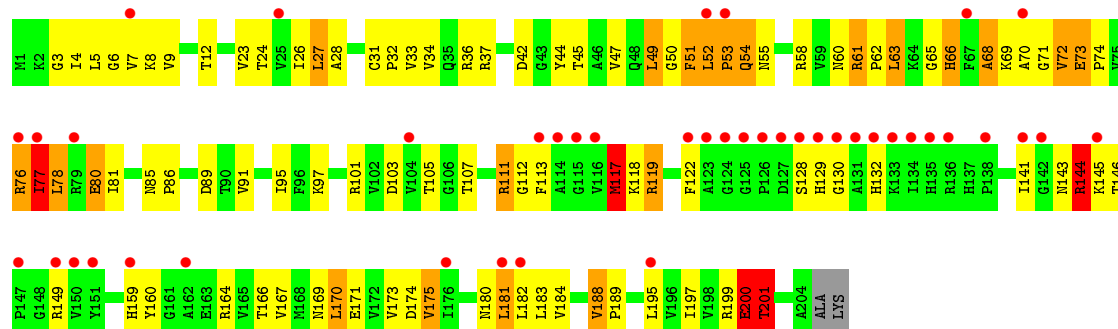




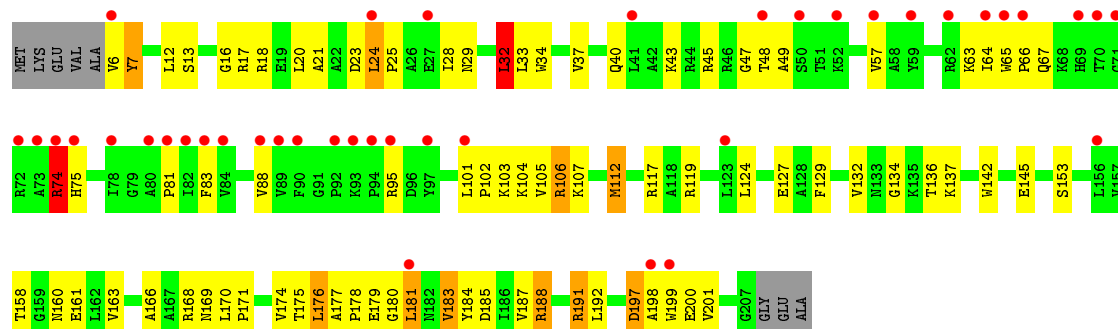
• Molecule 29: 50S ribosomal protein L3



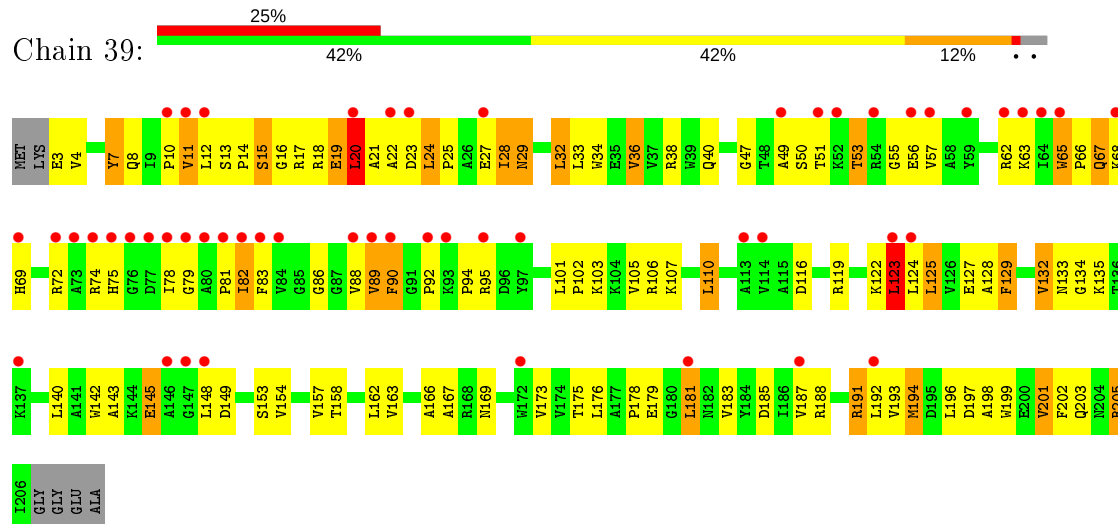
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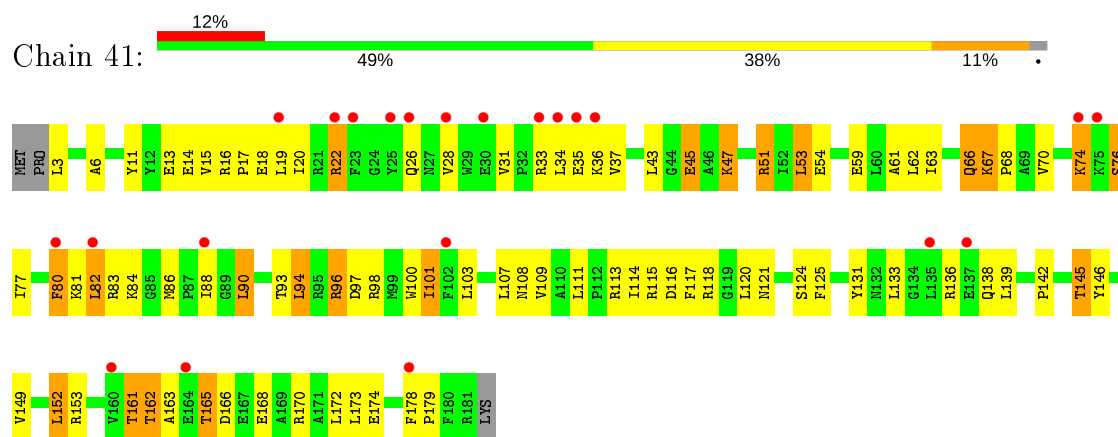
• Molecule 30: 50S ribosomal protein L4



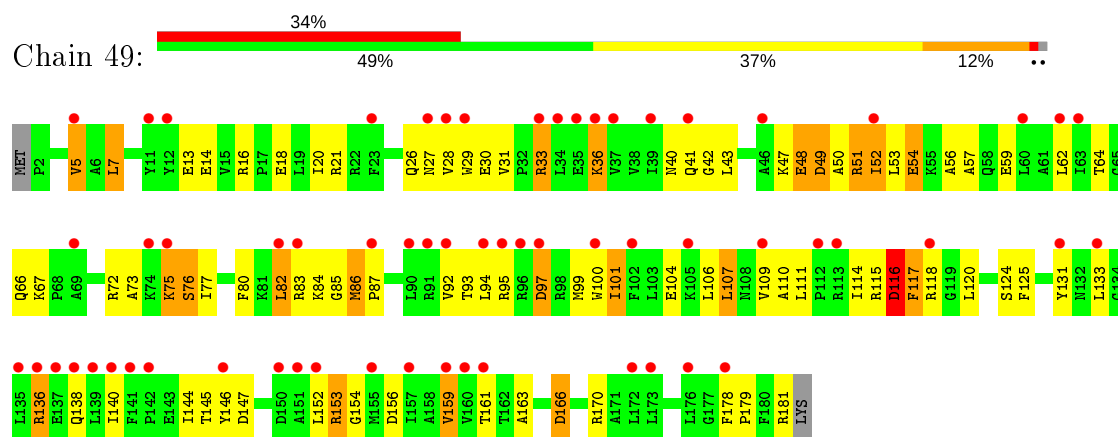
- Molecule 30: 50S ribosomal protein L4



- Molecule 31: 50S ribosomal protein L5

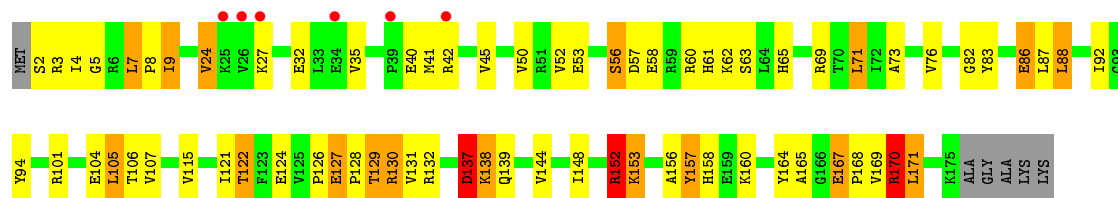


- Molecule 31: 50S ribosomal protein L5

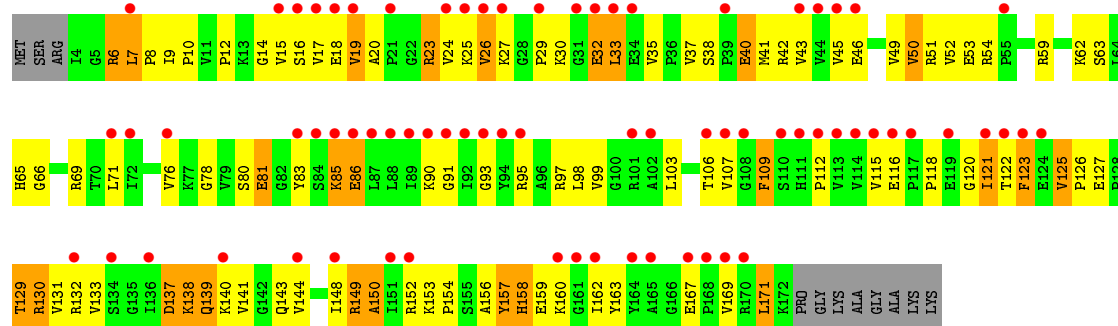
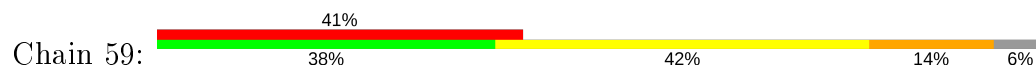


- Molecule 32: 50S ribosomal protein L6

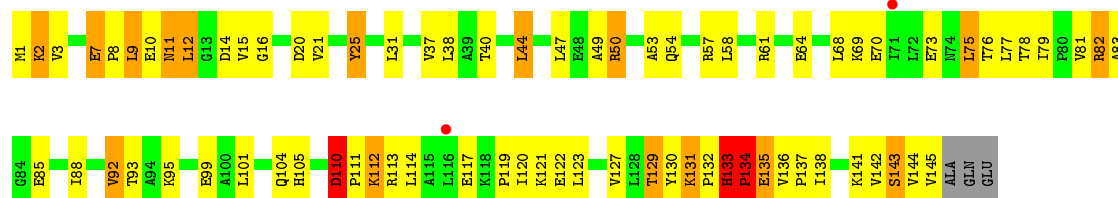




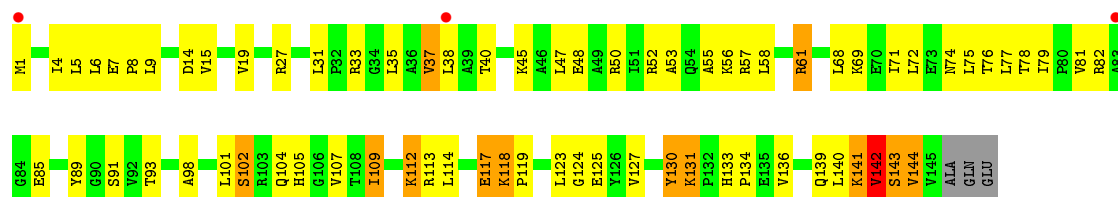
• Molecule 32: 50S ribosomal protein L6



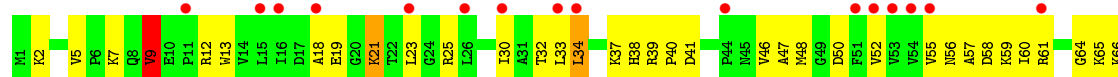
• Molecule 33: 50S ribosomal protein L9



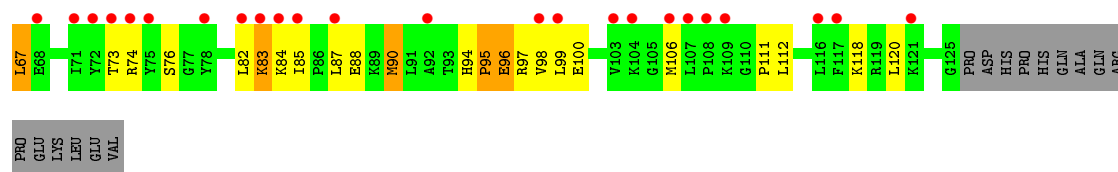
• Molecule 33: 50S ribosomal protein L9



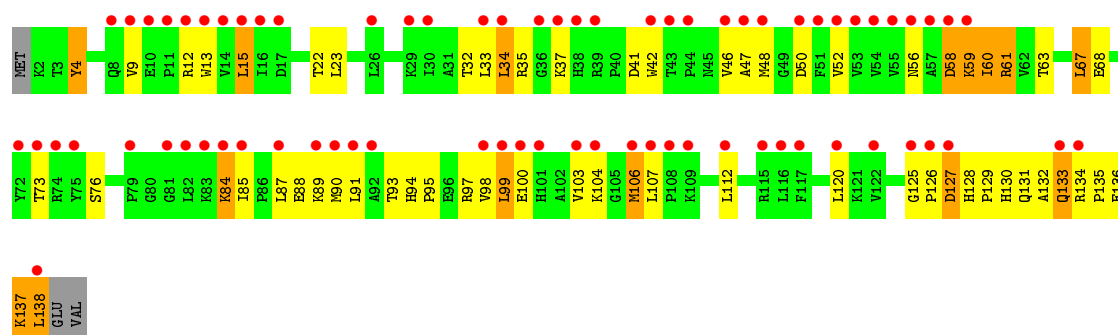
• Molecule 34: 50S ribosomal protein L13



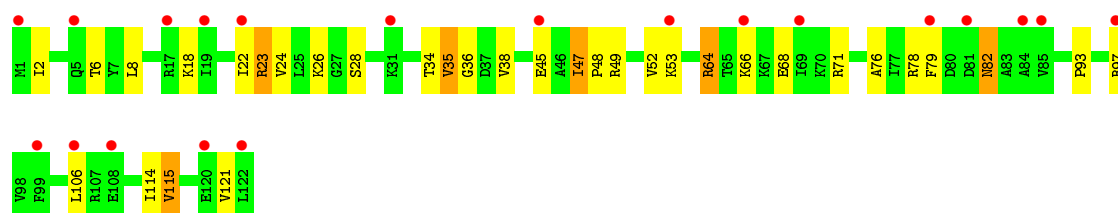
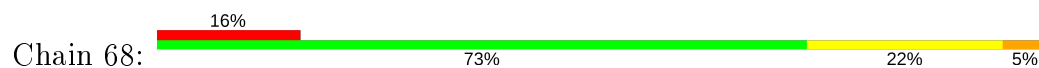




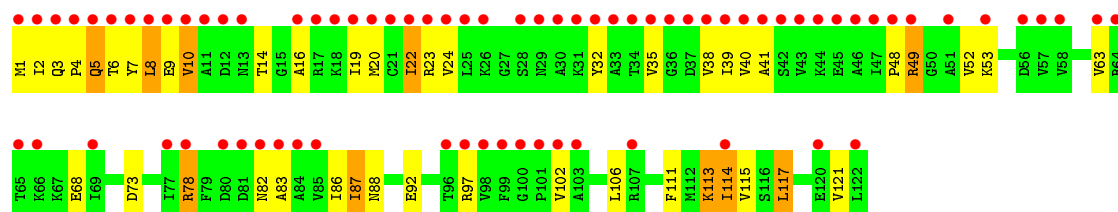
• Molecule 34: 50S ribosomal protein L13



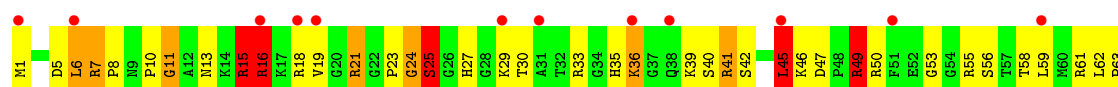
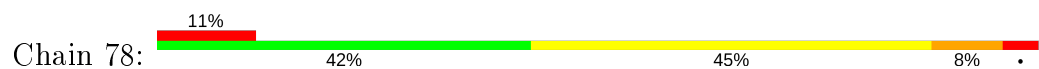
• Molecule 35: 50S ribosomal protein L14

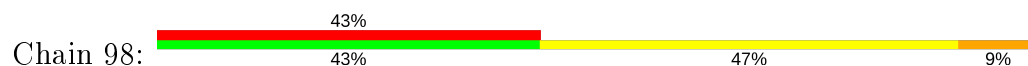


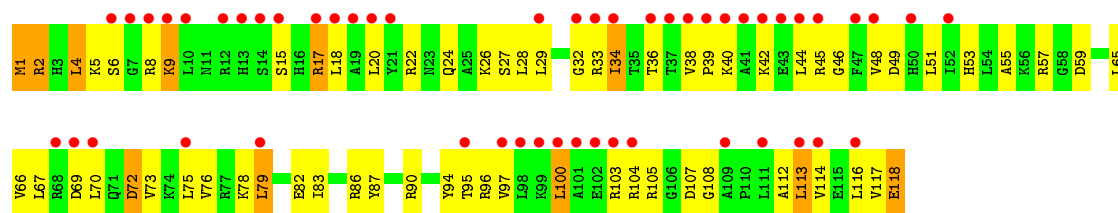
• Molecule 35: 50S ribosomal protein L14



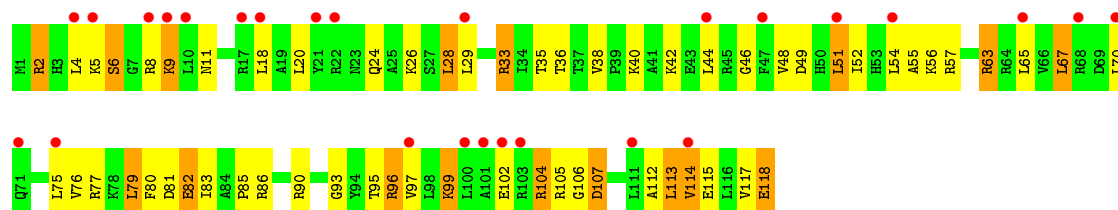
• Molecule 36: 50S ribosomal protein L15



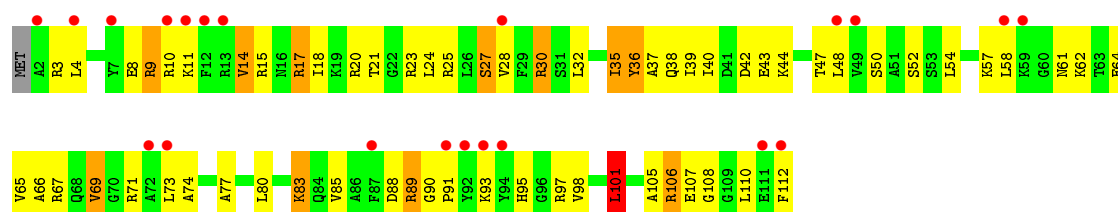




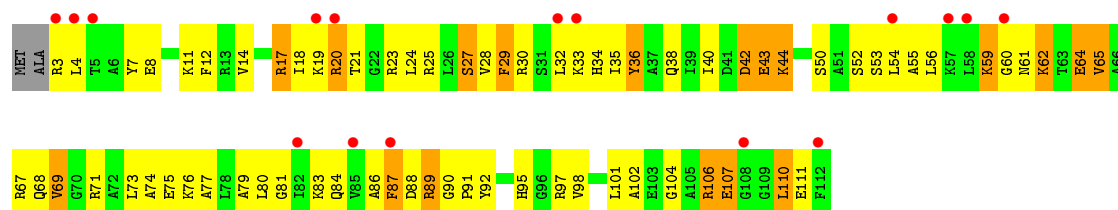
• Molecule 38: 50S ribosomal protein L17



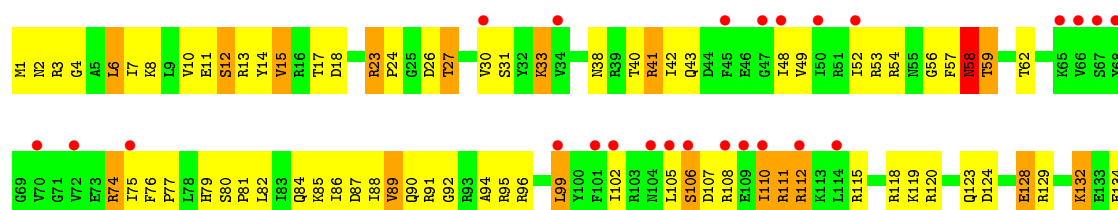
• Molecule 39: 50S ribosomal protein L18



• Molecule 39: 50S ribosomal protein L18

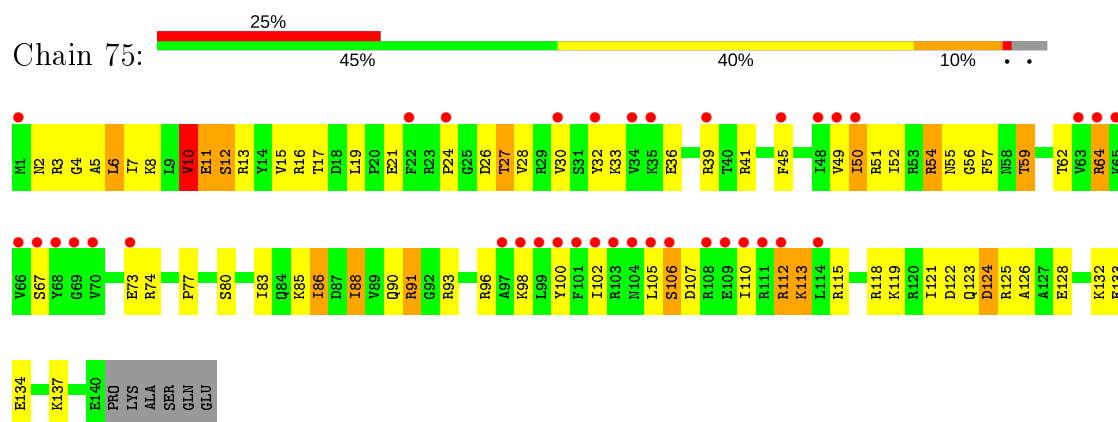


• Molecule 40: 50S ribosomal protein L19

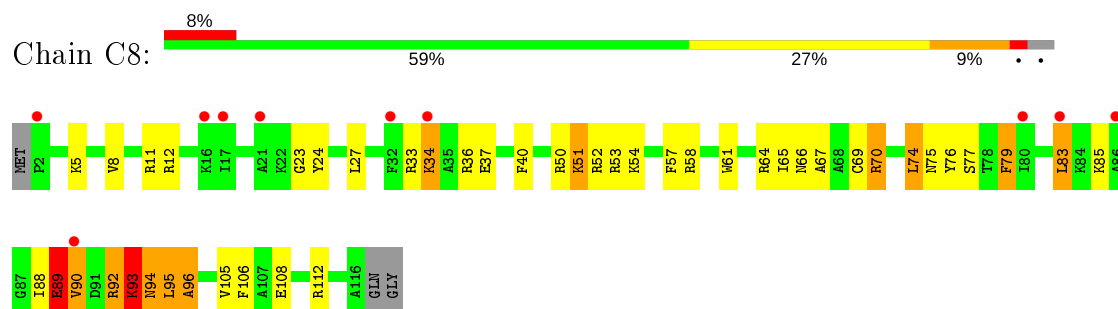


A135  
Q136  
LYS  
ALA  
GLN  
GLU  
PRO  
LYS  
ALA  
SER  
GLN  
GLU

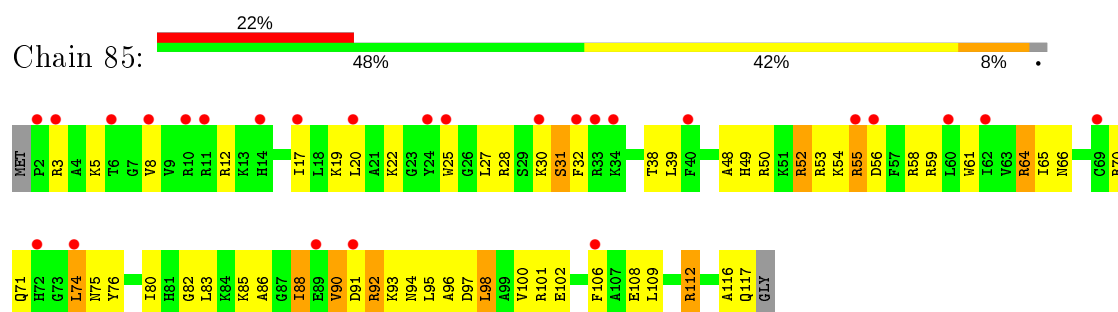
- Molecule 40: 50S ribosomal protein L19



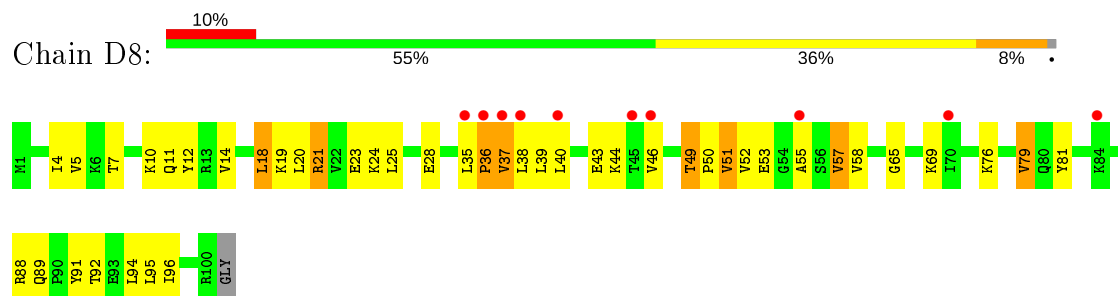
- Molecule 41: 50S ribosomal protein L20



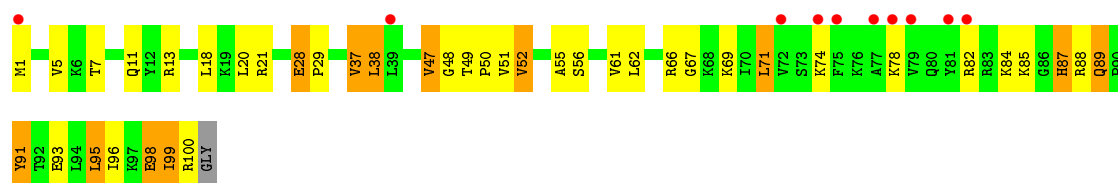
- Molecule 41: 50S ribosomal protein L20



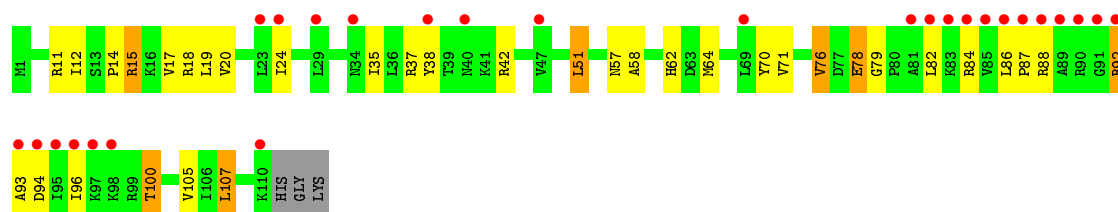
- Molecule 42: 50S ribosomal protein L21



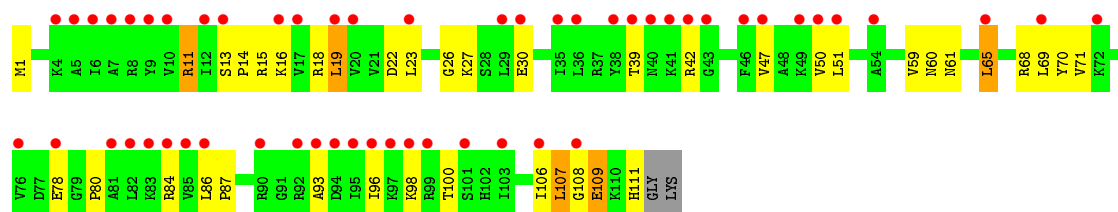
- Molecule 42: 50S ribosomal protein L21



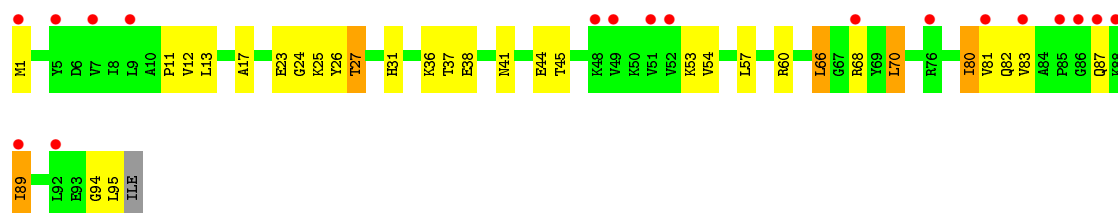
• Molecule 43: 50S ribosomal protein L22



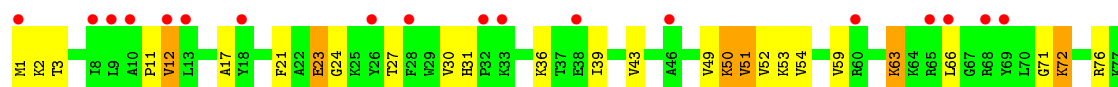
• Molecule 43: 50S ribosomal protein L22

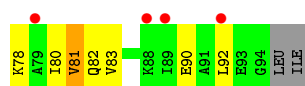


• Molecule 44: 50S ribosomal protein L23

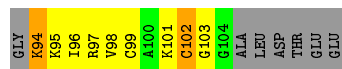
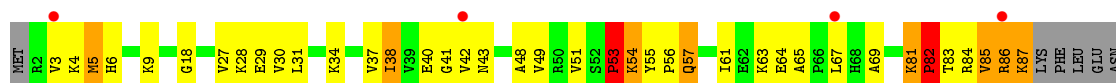


• Molecule 44: 50S ribosomal protein L23

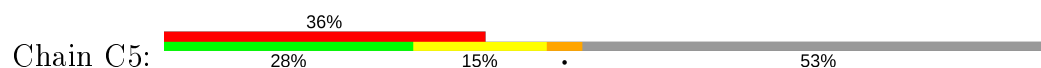




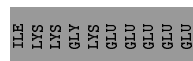
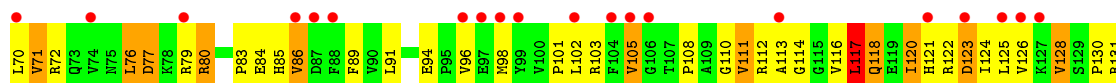
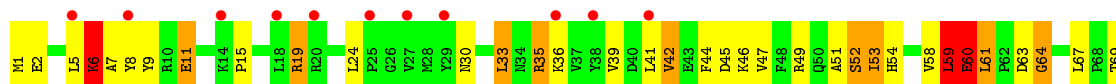
- Molecule 45: 50S ribosomal protein L24



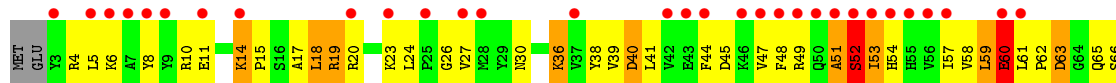
- Molecule 45: 50S ribosomal protein L24

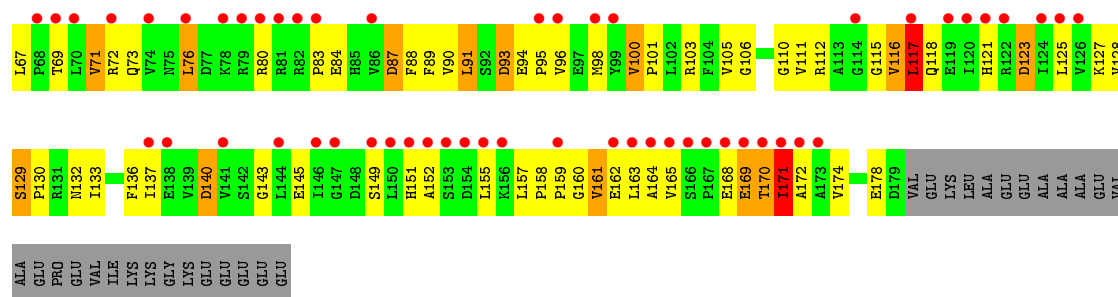


- Molecule 46: 50S ribosomal protein L25

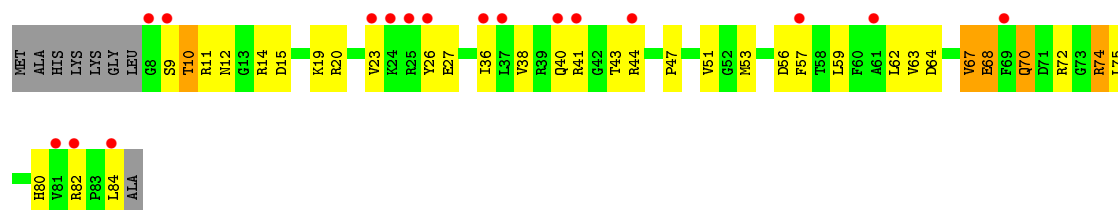


- Molecule 46: 50S ribosomal protein L25

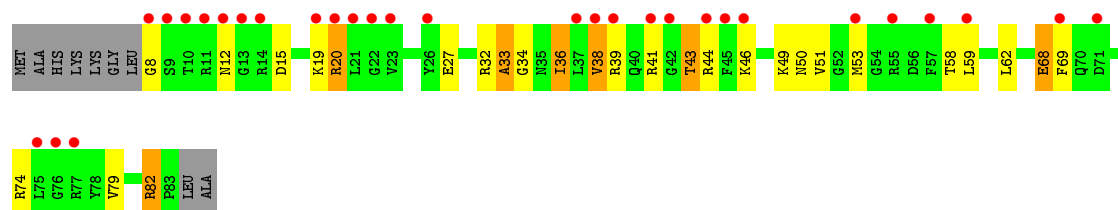




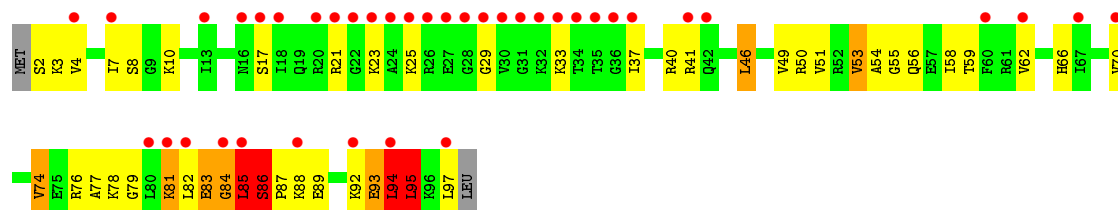
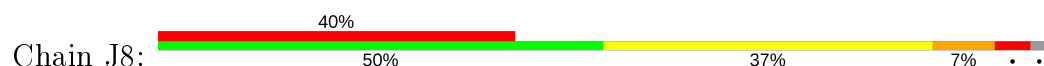
- Molecule 47: 50S ribosomal protein L27



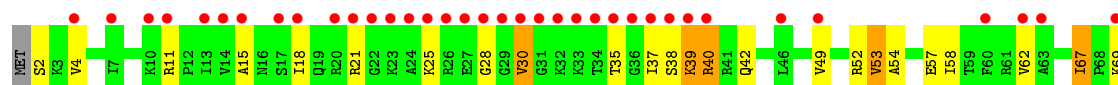
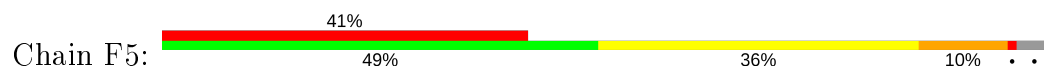
- Molecule 47: 50S ribosomal protein L27

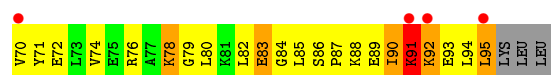


- Molecule 48: 50S ribosomal protein L28

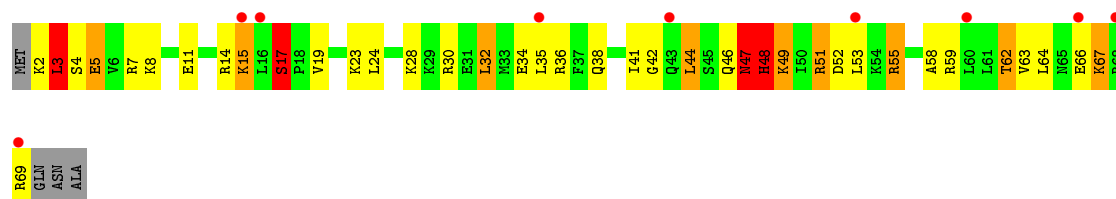
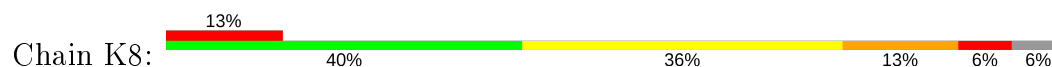


- Molecule 48: 50S ribosomal protein L28

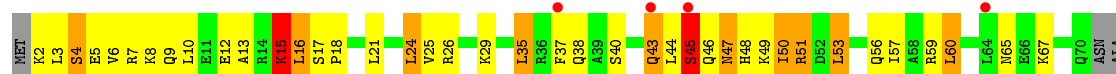
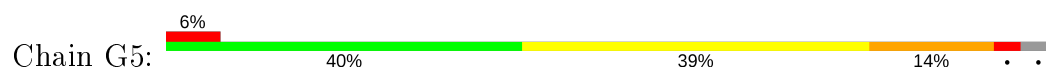




- Molecule 49: 50S ribosomal protein L29



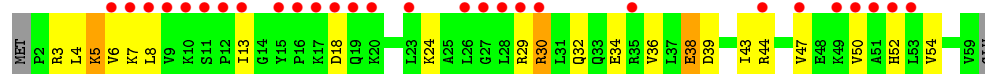
- Molecule 49: 50S ribosomal protein L29



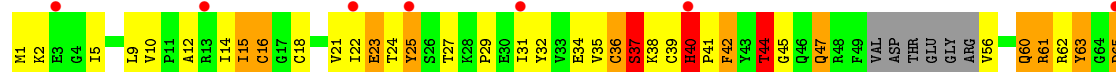
- Molecule 50: 50S ribosomal protein L30



- Molecule 50: 50S ribosomal protein L30



- Molecule 51: 50S ribosomal protein L31



- Molecule 52: 50S ribosomal protein L32



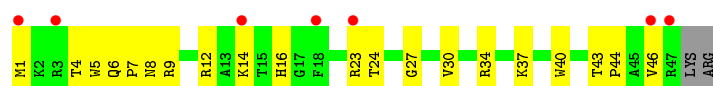




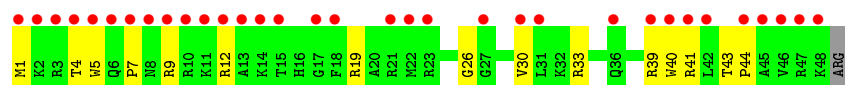
- Molecule 52: 50S ribosomal protein L32



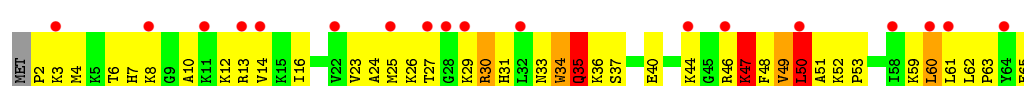
- Molecule 53: 50S ribosomal protein L34



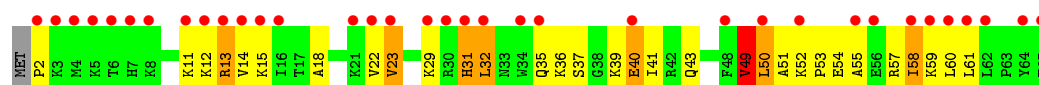
- Molecule 53: 50S ribosomal protein L34



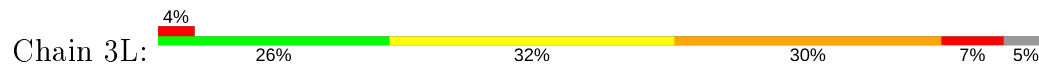
- Molecule 54: 50S ribosomal protein L35



- Molecule 54: 50S ribosomal protein L35



- Molecule 55: tRNA<sup>Thr</sup>



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	209.41Å 449.24Å 618.40Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	224.62 – 2.96 309.20 – 2.96	Depositor EDS
% Data completeness (in resolution range)	100.0 (224.62-2.96) 94.4 (309.20-2.96)	Depositor EDS
$R_{merge}$	0.29	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	0.76 (at 2.96Å)	Xtriage
Refinement program	PHENIX 1.12_2829	Depositor
R, $R_{free}$	0.196 , 0.252 0.196 , 0.252	Depositor DCC
$R_{free}$ test set	2000 reflections (0.17%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	82.0	Xtriage
Anisotropy	0.292	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.26 , 59.2	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.89	EDS
Total number of atoms	294252	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	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.*

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

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

## 5 Model quality ⓘ

### 5.1 Standard geometry ⓘ

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z  > 5$	RMSZ	$\# Z  > 5$
1	13	0.73	2/36095 (0.0%)	1.34	310/56332 (0.6%)
1	1G	0.66	4/35850 (0.0%)	1.24	189/55949 (0.3%)
2	12	0.46	0/1727	0.62	1/2326 (0.0%)
2	1E	0.42	0/1908	0.63	1/2573 (0.0%)
3	22	0.43	0/1569	0.62	1/2116 (0.0%)
3	2E	0.44	0/1629	0.62	1/2195 (0.0%)
4	32	0.45	0/1728	0.62	0/2313
4	3E	0.47	0/1728	0.65	0/2313
5	42	0.44	0/1156	0.61	0/1557
5	4E	0.45	0/1158	0.63	0/1559
6	52	0.44	0/855	0.58	0/1154
6	5E	0.46	0/850	0.61	0/1147
7	62	0.41	0/1122	0.57	0/1500
7	6E	0.44	0/1259	0.56	0/1686
8	72	0.38	0/1127	0.59	0/1517
8	7E	0.41	0/1135	0.65	1/1527 (0.1%)
9	82	0.42	0/971	0.63	0/1304
9	8E	0.44	0/1019	0.65	1/1367 (0.1%)
10	1A	0.41	0/814	0.56	0/1095
10	1I	0.45	0/762	0.66	1/1027 (0.1%)
11	2A	0.39	0/850	0.59	0/1150
11	2I	0.45	0/838	0.65	0/1133
12	3A	0.46	0/972	0.71	0/1301
12	3I	0.60	0/972	0.79	1/1301 (0.1%)
13	4A	0.43	0/889	0.66	0/1192
13	4I	0.52	0/952	0.64	0/1277
14	5A	0.45	0/495	0.66	0/657
14	5I	0.47	0/500	0.73	1/664 (0.2%)
15	6A	0.40	0/740	0.54	0/987
15	6I	0.44	0/740	0.59	0/987
16	7A	0.45	0/721	0.64	0/970
16	7I	0.44	0/716	0.67	0/963

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
17	8A	0.47	0/836	0.59	0/1117
17	8I	0.46	0/847	0.65	0/1131
18	9A	0.46	0/559	0.68	1/746 (0.1%)
18	9I	0.44	0/554	0.61	0/739
19	AA	0.53	0/520	0.78	0/700
19	AI	0.45	0/680	0.70	0/915
20	BA	0.39	0/781	0.58	0/1033
20	BI	0.39	0/748	0.59	0/986
21	1B	0.35	0/192	0.57	0/252
21	1F	0.41	0/203	0.63	0/266
22	1K	0.77	1/1675 (0.1%)	1.36	20/2608 (0.8%)
22	1L	0.71	0/1675	1.23	9/2608 (0.3%)
23	2K	0.77	1/1721 (0.1%)	1.37	16/2682 (0.6%)
23	2L	0.69	0/1721	1.30	10/2682 (0.4%)
24	3K	0.72	1/1716 (0.1%)	1.32	20/2668 (0.7%)
25	4K	0.88	0/440	1.28	2/684 (0.3%)
25	4L	0.84	0/341	1.57	9/529 (1.7%)
26	14	0.87	52/67828 (0.1%)	1.53	1188/105880 (1.1%)
26	1H	1.01	119/68741 (0.2%)	1.69	1859/107295 (1.7%)
27	16	0.77	0/2928	1.53	51/4568 (1.1%)
27	1J	0.73	1/2928 (0.0%)	1.44	41/4568 (0.9%)
28	11	0.63	0/2170	0.83	2/2926 (0.1%)
28	19	0.61	0/2175	0.82	2/2933 (0.1%)
29	21	0.55	0/1589	0.84	1/2145 (0.0%)
29	29	0.54	1/1596 (0.1%)	0.78	1/2153 (0.0%)
30	31	0.62	1/1620 (0.1%)	0.80	4/2194 (0.2%)
30	39	0.52	1/1637 (0.1%)	0.74	0/2218
31	41	0.50	1/1481 (0.1%)	0.73	1/1994 (0.1%)
31	49	0.45	0/1483	0.67	0/1997
32	51	0.50	0/1354	0.82	4/1833 (0.2%)
32	59	0.48	0/1320	0.70	1/1787 (0.1%)
33	61	0.44	0/1146	0.71	2/1551 (0.1%)
33	69	0.42	0/1146	0.65	0/1551
34	15	0.44	0/1123	0.66	0/1515
34	58	0.49	0/1017	0.78	2/1369 (0.1%)
35	25	0.49	0/942	0.70	1/1269 (0.1%)
35	68	0.54	0/942	0.71	0/1269
36	35	0.53	0/1139	0.86	3/1514 (0.2%)
36	78	0.58	0/1144	0.98	5/1521 (0.3%)
37	45	0.50	0/1120	0.78	0/1498
37	88	0.62	0/1138	0.85	0/1523
38	55	0.49	0/981	0.79	0/1312
38	98	0.48	0/981	0.78	1/1312 (0.1%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
39	65	0.47	0/886	0.74	1/1180 (0.1%)
39	A8	0.54	0/891	0.83	2/1187 (0.2%)
40	75	0.51	0/1178	0.73	1/1573 (0.1%)
40	B8	0.54	0/1142	0.75	1/1526 (0.1%)
41	85	0.51	0/977	0.68	0/1301
41	C8	0.57	0/968	0.76	1/1289 (0.1%)
42	95	0.47	0/781	0.77	0/1048
42	D8	0.52	0/785	0.77	1/1052 (0.1%)
43	A5	0.53	0/897	0.73	0/1204
43	E8	0.58	0/886	0.71	0/1189
44	B5	0.57	0/749	0.71	0/1007
44	F8	0.61	0/764	0.83	1/1025 (0.1%)
45	C5	0.56	0/401	0.74	0/535
45	G8	0.60	0/745	0.84	2/993 (0.2%)
46	D5	0.45	0/1443	0.70	2/1960 (0.1%)
46	H8	0.46	0/1395	0.80	2/1890 (0.1%)
47	E5	0.54	0/611	0.76	0/814
47	I8	0.68	1/619 (0.2%)	0.82	2/825 (0.2%)
48	F5	0.58	0/744	0.82	0/989
48	J8	0.66	0/754	0.92	3/1003 (0.3%)
49	G5	0.54	0/578	0.70	0/766
49	K8	0.63	0/577	0.93	2/763 (0.3%)
50	H5	0.46	0/464	0.63	0/623
50	L8	0.55	0/464	0.69	0/623
51	M8	0.56	0/485	0.77	0/652
52	J5	0.61	0/448	0.86	1/606 (0.2%)
52	N8	0.61	0/381	0.81	0/516
53	L5	0.55	0/414	0.73	0/547
53	P8	0.72	0/409	0.87	0/540
54	M5	0.62	0/524	0.88	1/691 (0.1%)
54	Q8	0.61	0/524	0.95	1/691 (0.1%)
55	3L	0.73	0/1672	1.37	22/2600 (0.8%)
All	All	0.77	186/315281 (0.1%)	1.34	3810/472388 (0.8%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
2	12	0	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 186 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	1H	774	A	N9-C4	-13.04	1.30	1.37
26	1H	676	A	N9-C4	-11.33	1.31	1.37
26	1H	2430	A	N9-C4	-10.69	1.31	1.37
26	1H	945	A	N9-C4	-10.48	1.31	1.37
26	1H	783	A	N9-C4	-10.03	1.31	1.37

The worst 5 of 3810 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	1H	1899	G	N3-C4-N9	-22.84	112.30	126.00
26	1H	2430	A	N1-C6-N6	20.05	130.63	118.60
26	1H	2430	A	C2-N3-C4	-19.74	100.73	110.60
26	1H	783	A	C2-N3-C4	-18.96	101.12	110.60
26	1H	676	A	C2-N3-C4	-18.87	101.17	110.60

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 ⓘ

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	648	0
1	1G	32028	0	16165	605	0
2	12	1696	0	1730	102	0
2	1E	1874	0	1926	85	0
3	22	1546	0	1608	79	0
3	2E	1605	0	1668	37	0
4	32	1698	0	1761	87	1
4	3E	1698	0	1760	71	0
5	42	1141	0	1199	58	0
5	4E	1142	0	1204	34	0
6	52	842	0	857	18	0
6	5E	837	0	852	19	1
7	62	1110	0	1163	51	0
7	6E	1242	0	1286	41	0
8	72	1107	0	1165	37	0
8	7E	1115	0	1177	46	0
9	82	953	0	983	56	0
9	8E	1000	0	1031	58	0
10	1A	801	0	849	51	0
10	1I	749	0	767	45	0
11	2A	835	0	847	29	0
11	2I	823	0	832	30	0
12	3A	956	0	1046	32	0
12	3I	956	0	1046	33	0
13	4A	879	0	935	48	0
13	4I	942	0	997	56	0
14	5A	486	0	526	22	0
14	5I	491	0	529	27	0
15	6A	729	0	768	12	0
15	6I	729	0	768	28	0
16	7A	705	0	725	19	0
16	7I	700	0	720	28	0
17	8A	823	0	891	32	0
17	8I	834	0	904	33	0
18	9A	554	0	609	15	0
18	9I	549	0	607	25	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	36	0
20	BA	778	0	863	26	0
20	BI	746	0	843	46	0
21	1B	188	0	195	14	0
21	1F	199	0	208	8	0
22	1K	1593	0	813	50	0
22	1L	1593	0	813	48	0
23	2K	1646	0	844	19	0
23	2L	1646	0	842	31	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	996	0
26	1H	61381	0	30944	1089	0
27	16	2617	0	1328	45	0
27	1J	2617	0	1328	68	0
28	11	2120	0	2197	58	0
28	19	2125	0	2199	67	0
29	21	1556	0	1612	74	0
29	29	1563	0	1629	82	0
30	31	1585	0	1632	70	0
30	39	1602	0	1649	84	0
31	41	1457	0	1514	64	0
31	49	1459	0	1507	54	0
32	51	1328	0	1396	46	0
32	59	1295	0	1366	78	0
33	61	1131	0	1218	49	0
33	69	1131	0	1218	46	0
34	15	1096	0	1168	51	0
34	58	995	0	1077	36	0
35	25	932	0	996	32	0
35	68	932	0	996	21	0
36	35	1122	0	1206	71	0
36	78	1127	0	1208	64	0
37	45	1099	0	1154	67	0
37	88	1117	0	1168	51	0
38	55	967	0	1033	45	0
38	98	967	0	1033	41	0
39	65	876	0	938	71	0
39	A8	881	0	943	43	0
40	75	1164	0	1221	59	0
40	B8	1128	0	1183	57	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
41	85	959	0	1019	61	0
41	C8	950	0	1011	43	0
42	95	770	0	838	32	0
42	D8	774	0	849	29	0
43	A5	886	0	948	23	0
43	E8	876	0	941	24	0
44	B5	735	0	785	19	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	71	0
46	H8	1365	0	1391	61	0
47	E5	603	0	620	22	0
47	I8	611	0	631	26	0
48	F5	737	0	813	32	0
48	J8	747	0	817	35	0
49	G5	576	0	625	31	0
49	K8	575	0	634	33	0
50	H5	459	0	512	18	0
50	L8	459	0	512	9	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	10	0
54	M5	516	0	582	22	0
54	Q8	516	0	582	37	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	6738	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 14.

The worst 5 of 6738 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%)	29	64
2	1E	227/256 (89%)	175 (77%)	49 (22%)	3 (1%)	12	41
3	22	193/239 (81%)	161 (83%)	31 (16%)	1 (0%)	29	64
3	2E	203/239 (85%)	181 (89%)	21 (10%)	1 (0%)	29	64

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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%)	29	64
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%)	22	56
8	7E	136/138 (99%)	123 (90%)	11 (8%)	2 (2%)	10	38
9	82	119/128 (93%)	103 (87%)	14 (12%)	2 (2%)	9	34
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%)	17	51
11	2I	109/129 (84%)	94 (86%)	14 (13%)	1 (1%)	17	51
12	3A	120/132 (91%)	100 (83%)	19 (16%)	1 (1%)	19	53
12	3I	120/132 (91%)	104 (87%)	15 (12%)	1 (1%)	19	53
13	4A	107/126 (85%)	84 (78%)	17 (16%)	6 (6%)	2	8
13	4I	117/126 (93%)	86 (74%)	26 (22%)	5 (4%)	2	12
14	5A	57/61 (93%)	46 (81%)	10 (18%)	1 (2%)	8	33
14	5I	58/61 (95%)	50 (86%)	5 (9%)	3 (5%)	2	9
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%)	13	43
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%)	9	34

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
19	AI	81/93 (87%)	67 (83%)	13 (16%)	1 (1%)	13	43
20	BA	101/106 (95%)	83 (82%)	17 (17%)	1 (1%)	15	48
20	BI	95/106 (90%)	84 (88%)	11 (12%)	0	100	100
21	1B	20/27 (74%)	17 (85%)	2 (10%)	1 (5%)	2	10
21	1F	21/27 (78%)	19 (90%)	2 (10%)	0	100	100
28	11	271/276 (98%)	249 (92%)	17 (6%)	5 (2%)	8	33
28	19	272/276 (99%)	235 (86%)	36 (13%)	1 (0%)	34	69
29	21	203/206 (98%)	159 (78%)	39 (19%)	5 (2%)	5	25
29	29	202/206 (98%)	146 (72%)	48 (24%)	8 (4%)	3	14
30	31	200/210 (95%)	178 (89%)	22 (11%)	0	100	100
30	39	202/210 (96%)	163 (81%)	35 (17%)	4 (2%)	7	30
31	41	177/182 (97%)	153 (86%)	23 (13%)	1 (1%)	25	60
31	49	178/182 (98%)	149 (84%)	27 (15%)	2 (1%)	14	46
32	51	172/180 (96%)	132 (77%)	31 (18%)	9 (5%)	2	9
32	59	167/180 (93%)	125 (75%)	42 (25%)	0	100	100
33	61	143/148 (97%)	111 (78%)	28 (20%)	4 (3%)	5	22
33	69	143/148 (97%)	107 (75%)	34 (24%)	2 (1%)	11	39
34	15	135/140 (96%)	118 (87%)	16 (12%)	1 (1%)	22	56
34	58	123/140 (88%)	109 (89%)	13 (11%)	1 (1%)	19	53
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%)	11	39
36	78	146/150 (97%)	111 (76%)	30 (20%)	5 (3%)	3	17
37	45	136/141 (96%)	106 (78%)	29 (21%)	1 (1%)	22	56
37	88	139/141 (99%)	120 (86%)	15 (11%)	4 (3%)	4	21
38	55	116/118 (98%)	104 (90%)	10 (9%)	2 (2%)	9	34
38	98	116/118 (98%)	102 (88%)	14 (12%)	0	100	100
39	65	108/112 (96%)	84 (78%)	23 (21%)	1 (1%)	17	51
39	A8	109/112 (97%)	85 (78%)	24 (22%)	0	100	100
40	75	138/146 (94%)	120 (87%)	16 (12%)	2 (1%)	11	39
40	B8	134/146 (92%)	112 (84%)	21 (16%)	1 (1%)	22	56

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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%)	8	33
42	95	98/101 (97%)	79 (81%)	16 (16%)	3 (3%)	4	19
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%)	14	46
44	F8	93/96 (97%)	88 (95%)	5 (5%)	0	100	100
45	C5	48/110 (44%)	39 (81%)	8 (17%)	1 (2%)	7	29
45	G8	93/110 (84%)	64 (69%)	25 (27%)	4 (4%)	2	12
46	D5	175/206 (85%)	123 (70%)	45 (26%)	7 (4%)	3	14
46	H8	168/206 (82%)	127 (76%)	35 (21%)	6 (4%)	3	16
47	E5	74/85 (87%)	64 (86%)	8 (11%)	2 (3%)	5	23
47	I8	75/85 (88%)	66 (88%)	9 (12%)	0	100	100
48	F5	92/98 (94%)	78 (85%)	12 (13%)	2 (2%)	6	28
48	J8	94/98 (96%)	79 (84%)	13 (14%)	2 (2%)	7	29
49	G5	67/72 (93%)	60 (90%)	6 (9%)	1 (2%)	10	38
49	K8	66/72 (92%)	58 (88%)	7 (11%)	1 (2%)	10	38
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%)	3	16
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%)	6	28
54	M5	62/65 (95%)	54 (87%)	8 (13%)	0	100	100
54	Q8	62/65 (95%)	47 (76%)	12 (19%)	3 (5%)	2	11
All	All	10929/11875 (92%)	9262 (85%)	1532 (14%)	135 (1%)	13	43

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 ⓘ

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%)	135 (75%)	44 (25%)	0	2
2	1E	200/220 (91%)	152 (76%)	48 (24%)	0	2
3	22	154/188 (82%)	120 (78%)	34 (22%)	1	3
3	2E	159/188 (85%)	128 (80%)	31 (20%)	1	6
4	32	180/181 (99%)	152 (84%)	28 (16%)	2	11
4	3E	180/181 (99%)	148 (82%)	32 (18%)	2	8
5	42	114/123 (93%)	86 (75%)	28 (25%)	0	2
5	4E	115/123 (94%)	95 (83%)	20 (17%)	2	8
6	52	90/90 (100%)	76 (84%)	14 (16%)	2	11
6	5E	90/90 (100%)	78 (87%)	12 (13%)	4	15
7	62	114/127 (90%)	90 (79%)	24 (21%)	1	4
7	6E	125/127 (98%)	103 (82%)	22 (18%)	2	8
8	72	118/119 (99%)	95 (80%)	23 (20%)	1	6
8	7E	119/119 (100%)	95 (80%)	24 (20%)	1	5
9	82	92/99 (93%)	69 (75%)	23 (25%)	0	2
9	8E	97/99 (98%)	77 (79%)	20 (21%)	1	4
10	1A	89/92 (97%)	69 (78%)	20 (22%)	1	3
10	1I	81/92 (88%)	68 (84%)	13 (16%)	2	10
11	2A	85/99 (86%)	72 (85%)	13 (15%)	2	11
11	2I	84/99 (85%)	68 (81%)	16 (19%)	1	6

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
12	3A	103/109 (94%)	75 (73%)	28 (27%)	0	1
12	3I	103/109 (94%)	83 (81%)	20 (19%)	1	6
13	4A	90/101 (89%)	70 (78%)	20 (22%)	1	3
13	4I	94/101 (93%)	72 (77%)	22 (23%)	1	3
14	5A	49/50 (98%)	31 (63%)	18 (37%)	0	0
14	5I	49/50 (98%)	38 (78%)	11 (22%)	1	3
15	6A	79/80 (99%)	73 (92%)	6 (8%)	13	39
15	6I	79/80 (99%)	64 (81%)	15 (19%)	1	6
16	7A	72/74 (97%)	63 (88%)	9 (12%)	4	17
16	7I	72/74 (97%)	56 (78%)	16 (22%)	1	3
17	8A	94/97 (97%)	85 (90%)	9 (10%)	8	28
17	8I	95/97 (98%)	77 (81%)	18 (19%)	1	7
18	9A	58/77 (75%)	42 (72%)	16 (28%)	0	1
18	9I	58/77 (75%)	52 (90%)	6 (10%)	7	25
19	AA	56/80 (70%)	43 (77%)	13 (23%)	1	3
19	AI	72/80 (90%)	56 (78%)	16 (22%)	1	3
20	BA	76/82 (93%)	69 (91%)	7 (9%)	9	30
20	BI	75/82 (92%)	65 (87%)	10 (13%)	4	15
21	1B	17/22 (77%)	16 (94%)	1 (6%)	19	50
21	1F	18/22 (82%)	17 (94%)	1 (6%)	21	53
28	11	214/218 (98%)	172 (80%)	42 (20%)	1	6
28	19	214/218 (98%)	173 (81%)	41 (19%)	1	6
29	21	162/166 (98%)	132 (82%)	30 (18%)	1	7
29	29	165/166 (99%)	138 (84%)	27 (16%)	2	9
30	31	161/166 (97%)	131 (81%)	30 (19%)	1	7
30	39	163/166 (98%)	124 (76%)	39 (24%)	0	2
31	41	153/156 (98%)	121 (79%)	32 (21%)	1	4
31	49	152/156 (97%)	117 (77%)	35 (23%)	1	3
32	51	143/148 (97%)	120 (84%)	23 (16%)	2	10
32	59	140/148 (95%)	101 (72%)	39 (28%)	0	1
33	61	122/124 (98%)	91 (75%)	31 (25%)	0	2

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
33	69	122/124 (98%)	95 (78%)	27 (22%)	1	3
34	15	116/119 (98%)	88 (76%)	28 (24%)	0	2
34	58	105/119 (88%)	83 (79%)	22 (21%)	1	4
35	25	100/100 (100%)	85 (85%)	15 (15%)	3	12
35	68	100/100 (100%)	88 (88%)	12 (12%)	5	19
36	35	114/116 (98%)	80 (70%)	34 (30%)	0	1
36	78	114/116 (98%)	77 (68%)	37 (32%)	0	1
37	45	109/111 (98%)	85 (78%)	24 (22%)	1	4
37	88	110/111 (99%)	96 (87%)	14 (13%)	4	17
38	55	101/101 (100%)	75 (74%)	26 (26%)	0	2
38	98	101/101 (100%)	74 (73%)	27 (27%)	0	2
39	65	87/88 (99%)	60 (69%)	27 (31%)	0	1
39	A8	87/88 (99%)	63 (72%)	24 (28%)	0	1
40	75	122/127 (96%)	95 (78%)	27 (22%)	1	3
40	B8	118/127 (93%)	82 (70%)	36 (30%)	0	1
41	85	93/94 (99%)	77 (83%)	16 (17%)	2	8
41	C8	92/94 (98%)	77 (84%)	15 (16%)	2	9
42	95	81/82 (99%)	64 (79%)	17 (21%)	1	4
42	D8	82/82 (100%)	62 (76%)	20 (24%)	0	2
43	A5	91/92 (99%)	74 (81%)	17 (19%)	1	7
43	E8	90/92 (98%)	79 (88%)	11 (12%)	5	19
44	B5	74/78 (95%)	60 (81%)	14 (19%)	1	7
44	F8	77/78 (99%)	66 (86%)	11 (14%)	3	13
45	C5	43/91 (47%)	35 (81%)	8 (19%)	1	7
45	G8	79/91 (87%)	64 (81%)	15 (19%)	1	6
46	D5	156/179 (87%)	124 (80%)	32 (20%)	1	5
46	H8	151/179 (84%)	108 (72%)	43 (28%)	0	1
47	E5	61/67 (91%)	51 (84%)	10 (16%)	2	9
47	I8	62/67 (92%)	55 (89%)	7 (11%)	6	21
48	F5	79/83 (95%)	62 (78%)	17 (22%)	1	4
48	J8	79/83 (95%)	64 (81%)	15 (19%)	1	6

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
49	G5	63/67 (94%)	45 (71%)	18 (29%)	0	1
49	K8	64/67 (96%)	41 (64%)	23 (36%)	0	1
50	H5	50/52 (96%)	45 (90%)	5 (10%)	7	26
50	L8	50/52 (96%)	42 (84%)	8 (16%)	2	10
51	M8	52/63 (82%)	34 (65%)	18 (35%)	0	1
52	J5	48/52 (92%)	37 (77%)	11 (23%)	1	3
52	N8	43/52 (83%)	32 (74%)	11 (26%)	0	2
53	L5	38/42 (90%)	34 (90%)	4 (10%)	7	24
53	P8	38/42 (90%)	32 (84%)	6 (16%)	2	10
54	M5	54/55 (98%)	42 (78%)	12 (22%)	1	3
54	Q8	54/55 (98%)	48 (89%)	6 (11%)	6	22
All	All	9213/9831 (94%)	7323 (80%)	1890 (20%)	1	5

5 of 1890 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
47	I8	84	LEU
5	42	43	LEU
43	A5	23	LEU
49	K8	32	LEU
2	12	61	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 20 such sidechains are listed below:

Mol	Chain	Res	Type
3	22	6	HIS
4	32	119	GLN
37	45	123	HIS
51	M8	60	GLN
2	12	212	GLN

### 5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	13	1499/1522 (98%)	326 (21%)	36 (2%)
1	1G	1488/1522 (97%)	314 (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%)	630 (22%)	35 (1%)
26	1H	2841/2917 (97%)	579 (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%)	2097 (22%)	170 (1%)

5 of 2097 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
26	1H	1608	A
1	1G	80	G
26	14	2174	C
26	1H	1858	G
26	1H	2422	A

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

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
55	PSU	3L	55	55	17,21,22	1.14	2 (11%)	20,30,33	3.33	8 (40%)
22	AET	1K	37	22	25,35,36	2.70	4 (16%)	26,51,54	2.04	3 (11%)
23	OMC	2K	33	23	15,22,23	2.19	4 (26%)	17,31,34	1.73	4 (23%)
23	PSU	2L	56	23	17,21,22	1.05	1 (5%)	20,30,33	3.45	5 (25%)
22	5MU	1L	54	22	15,22,23	2.27	3 (20%)	16,32,35	1.78	2 (12%)
23	5MU	2K	55	23	15,22,23	2.19	3 (20%)	16,32,35	1.83	2 (12%)
22	H2U	1L	17	22	18,21,22	2.46	4 (22%)	21,30,33	1.83	5 (23%)
23	7MG	2K	47	23	22,26,27	3.36	7 (31%)	28,39,42	2.46	10 (35%)
55	5MU	3L	54	55	15,22,23	2.22	3 (20%)	16,32,35	1.84	2 (12%)
23	7MG	2L	47	23	22,26,27	3.49	7 (31%)	28,39,42	2.54	11 (39%)
23	PSU	2K	56	23	17,21,22	1.12	1 (5%)	20,30,33	2.92	6 (30%)
23	4SU	2K	8	23	14,21,22	3.26	2 (14%)	15,30,33	0.86	1 (6%)
22	AET	1L	37	22	25,35,36	2.67	4 (16%)	26,51,54	1.91	7 (26%)
22	H2U	1K	17	22	18,21,22	2.27	4 (22%)	21,30,33	1.87	4 (19%)
22	PSU	1L	55	22	17,21,22	1.08	1 (5%)	20,30,33	3.58	7 (35%)
23	OMC	2L	33	23	15,22,23	2.20	4 (26%)	17,31,34	1.33	2 (11%)
22	PSU	1K	55	22	17,21,22	1.09	1 (5%)	20,30,33	3.15	6 (30%)
23	5MU	2L	55	23	15,22,23	2.19	3 (20%)	16,32,35	1.70	2 (12%)
23	4SU	2L	8	23	14,21,22	3.22	2 (14%)	15,30,33	1.32	1 (6%)
22	5MU	1K	54	22	15,22,23	2.30	3 (20%)	16,32,35	1.95	3 (18%)

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
55	PSU	3L	55	55	-	0/7/25/26	0/2/2/2
22	AET	1K	37	22	-	9/19/45/46	0/3/3/3
23	OMC	2K	33	23	-	1/7/27/28	0/2/2/2
23	PSU	2L	56	23	-	0/7/25/26	0/2/2/2
22	5MU	1L	54	22	-	0/5/25/26	0/2/2/2
23	5MU	2K	55	23	-	0/5/25/26	0/2/2/2
22	H2U	1L	17	22	-	5/7/38/39	0/2/2/2
23	7MG	2K	47	23	-	3/7/37/38	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
55	5MU	3L	54	55	-	2/5/25/26	0/2/2/2
23	7MG	2L	47	23	-	0/7/37/38	0/3/3/3
23	PSU	2K	56	23	-	0/7/25/26	0/2/2/2
23	4SU	2K	8	23	-	2/5/25/26	0/2/2/2
22	AET	1L	37	22	-	3/19/45/46	0/3/3/3
22	H2U	1K	17	22	-	4/7/38/39	0/2/2/2
22	PSU	1L	55	22	-	2/7/25/26	0/2/2/2
23	OMC	2L	33	23	-	0/7/27/28	0/2/2/2
22	PSU	1K	55	22	-	2/7/25/26	0/2/2/2
23	5MU	2L	55	23	-	2/5/25/26	0/2/2/2
23	4SU	2L	8	23	-	2/5/25/26	0/2/2/2
22	5MU	1K	54	22	-	0/5/25/26	0/2/2/2

The worst 5 of 63 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	2L	47	7MG	C4-N3	11.13	1.48	1.34
23	2K	47	7MG	C4-N3	10.78	1.48	1.34
22	1K	37	AET	C10-N6	10.38	1.51	1.37
22	1L	37	AET	C10-N6	10.14	1.51	1.37
23	2K	8	4SU	C5-C4	9.42	1.49	1.38

The worst 5 of 91 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	2L	56	PSU	N1-C2-N3	-12.04	118.86	128.43
55	3L	55	PSU	N1-C2-N3	-10.76	119.87	128.43
22	1L	55	PSU	N1-C2-N3	-10.64	119.97	128.43
22	1K	55	PSU	N1-C2-N3	-10.30	120.24	128.43
23	2K	56	PSU	N1-C2-N3	-9.60	120.80	128.43

There are no chirality outliers.

5 of 37 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
22	1K	37	AET	C5-C6-N6-CM6
22	1K	37	AET	N1-C6-N6-CM6
22	1K	37	AET	C14-C12-N11-C10
22	1K	37	AET	C13-C12-C14-O14
22	1K	37	AET	C13-C12-C14-C15

There are no ring outliers.

12 monomers are involved in 24 short contacts:

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

## 5.5 Carbohydrates [i](#)

There are no carbohydrates 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	0.00	-	-		
57	SF4	32	301	4	0,12,12	0.00	-	-		

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



Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
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
26	1H	1
24	3K	1
55	3L	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	3L	48:C	O3'	49:G	P	5.87
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<sup>th</sup> percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	13	1500/1522 (98%)	0.02	10 (0%) 87 76	60, 99, 150, 173	0
1	1G	1490/1522 (97%)	-0.07	8 (0%) 91 81	69, 111, 148, 171	0
2	12	207/256 (80%)	0.13	5 (2%) 59 42	116, 138, 149, 156	0
2	1E	231/256 (90%)	0.64	29 (12%) 3 2	107, 131, 148, 156	0
3	22	197/239 (82%)	0.56	26 (13%) 3 2	114, 131, 144, 153	0
3	2E	205/239 (85%)	0.70	25 (12%) 4 2	82, 106, 127, 136	0
4	32	207/209 (99%)	1.31	60 (28%) 0 0	91, 110, 129, 137	0
4	3E	207/209 (99%)	1.14	44 (21%) 0 0	82, 105, 125, 132	0
5	42	150/162 (92%)	0.69	24 (16%) 1 1	99, 117, 132, 142	0
5	4E	149/162 (91%)	1.12	30 (20%) 1 0	83, 100, 118, 125	0
6	52	101/101 (100%)	0.38	4 (3%) 38 25	87, 104, 119, 131	0
6	5E	100/101 (99%)	0.94	21 (21%) 1 0	88, 105, 119, 128	0
7	62	138/156 (88%)	0.84	25 (18%) 1 1	110, 120, 130, 136	0
7	6E	154/156 (98%)	1.34	36 (23%) 0 0	101, 116, 137, 150	0
8	72	137/138 (99%)	0.63	15 (10%) 5 3	97, 119, 130, 138	0
8	7E	138/138 (100%)	0.33	8 (5%) 23 14	91, 108, 122, 128	0
9	82	121/128 (94%)	1.51	39 (32%) 0 0	105, 135, 143, 150	0
9	8E	126/128 (98%)	0.95	30 (23%) 0 0	86, 127, 142, 150	0
10	1A	99/105 (94%)	0.90	21 (21%) 0 0	112, 135, 147, 153	0
10	1I	94/105 (89%)	1.02	25 (26%) 0 0	77, 120, 141, 143	0
11	2A	113/129 (87%)	1.55	36 (31%) 0 0	83, 108, 122, 131	0
11	2I	111/129 (86%)	2.10	54 (48%) 0 0	76, 105, 125, 137	0
12	3A	122/132 (92%)	1.97	54 (44%) 0 0	81, 99, 118, 132	0
12	3I	122/132 (92%)	0.81	22 (18%) 1 1	64, 77, 108, 126	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
13	4A	109/126 (86%)	1.11	31 (28%) 0 0	111, 131, 145, 152	0
13	4I	119/126 (94%)	0.46	10 (8%) 11 6	87, 116, 130, 141	0
14	5A	59/61 (96%)	3.96	44 (74%) 0 0	120, 129, 138, 142	0
14	5I	60/61 (98%)	1.31	17 (28%) 0 0	82, 95, 116, 123	0
15	6A	87/89 (97%)	1.41	32 (36%) 0 0	86, 108, 123, 126	0
15	6I	87/89 (97%)	0.94	16 (18%) 1 1	81, 100, 119, 128	0
16	7A	84/88 (95%)	0.40	2 (2%) 59 42	91, 101, 125, 143	0
16	7I	83/88 (94%)	0.90	14 (16%) 1 1	96, 110, 130, 143	0
17	8A	99/105 (94%)	2.78	63 (63%) 0 0	93, 107, 122, 127	0
17	8I	100/105 (95%)	1.71	38 (38%) 0 0	89, 105, 116, 119	0
18	9A	69/88 (78%)	-0.00	0 100 100	94, 110, 130, 139	0
18	9I	68/88 (77%)	0.52	6 (8%) 10 5	88, 106, 123, 131	0
19	AA	65/93 (69%)	2.25	31 (47%) 0 0	122, 140, 150, 156	0
19	AI	83/93 (89%)	0.66	11 (13%) 3 2	93, 112, 138, 145	0
20	BA	103/106 (97%)	1.98	48 (46%) 0 0	89, 110, 132, 136	0
20	BI	97/106 (91%)	1.01	22 (22%) 0 0	105, 116, 134, 137	0
21	1B	22/27 (81%)	2.07	9 (40%) 0 0	109, 122, 128, 128	0
21	1F	23/27 (85%)	2.23	11 (47%) 0 0	94, 102, 111, 117	0
22	1K	70/76 (92%)	0.16	5 (7%) 16 9	79, 151, 170, 173	0
22	1L	70/76 (92%)	0.29	7 (10%) 7 4	111, 158, 174, 179	0
23	2K	72/77 (93%)	0.21	2 (2%) 53 36	67, 93, 126, 137	0
23	2L	72/77 (93%)	-0.20	0 100 100	75, 104, 139, 145	0
24	3K	72/76 (94%)	0.41	9 (12%) 3 2	70, 157, 167, 169	0
25	4K	18/27 (66%)	2.13	7 (38%) 0 0	69, 124, 164, 170	0
25	4L	14/27 (51%)	0.68	2 (14%) 2 1	87, 122, 152, 154	0
26	14	2811/2917 (96%)	0.16	27 (0%) 82 68	52, 85, 154, 176	0
26	1H	2850/2917 (97%)	0.19	22 (0%) 86 73	41, 73, 157, 180	0
27	16	122/122 (100%)	-0.24	1 (0%) 86 73	67, 90, 108, 164	0
27	1J	122/122 (100%)	-0.21	1 (0%) 86 73	85, 110, 127, 162	0
28	11	273/276 (98%)	1.24	59 (21%) 0 0	45, 67, 87, 99	0
28	19	274/276 (99%)	1.65	94 (34%) 0 0	50, 73, 91, 110	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å <sup>2</sup> )	Q<0.9
29	21	205/206 (99%)	1.17	42 (20%)	1	0	51, 88, 122, 131	0
29	29	204/206 (99%)	1.07	43 (21%)	1	0	58, 97, 127, 140	0
30	31	202/210 (96%)	1.11	40 (19%)	1	0	47, 80, 115, 131	0
30	39	204/210 (97%)	1.18	52 (25%)	0	0	57, 102, 138, 149	0
31	41	179/182 (98%)	0.58	22 (12%)	4	2	84, 104, 132, 151	0
31	49	180/182 (98%)	1.78	62 (34%)	0	0	103, 122, 144, 154	0
32	51	174/180 (96%)	0.30	6 (3%)	45	29	83, 101, 117, 136	0
32	59	169/180 (93%)	2.33	73 (43%)	0	0	129, 156, 164, 168	0
33	61	145/148 (97%)	0.02	2 (1%)	75	59	79, 121, 132, 139	0
33	69	145/148 (97%)	0.05	3 (2%)	63	46	84, 117, 137, 143	0
34	15	137/140 (97%)	2.19	72 (52%)	0	0	80, 106, 131, 138	0
34	58	125/140 (89%)	1.51	40 (32%)	0	0	69, 89, 105, 131	0
35	25	122/122 (100%)	2.55	76 (62%)	0	0	68, 89, 105, 119	0
35	68	122/122 (100%)	1.21	20 (16%)	1	1	60, 78, 97, 105	0
36	35	147/150 (98%)	1.67	54 (36%)	0	0	59, 99, 130, 139	0
36	78	148/150 (98%)	0.67	16 (10%)	5	3	52, 83, 109, 121	0
37	45	138/141 (97%)	2.41	69 (50%)	0	0	72, 100, 121, 133	0
37	88	141/141 (100%)	1.55	42 (29%)	0	0	56, 80, 102, 129	0
38	55	118/118 (100%)	1.17	26 (22%)	0	0	64, 84, 99, 110	0
38	98	118/118 (100%)	1.74	51 (43%)	0	0	63, 83, 102, 115	0
39	65	110/112 (98%)	0.78	16 (14%)	2	1	86, 106, 125, 130	0
39	A8	111/112 (99%)	1.03	21 (18%)	1	0	77, 88, 106, 113	0
40	75	140/146 (95%)	1.29	37 (26%)	0	0	82, 98, 145, 155	0
40	B8	136/146 (93%)	0.91	25 (18%)	1	1	73, 92, 131, 146	0
41	85	116/118 (98%)	1.22	26 (22%)	0	0	68, 93, 128, 140	0
41	C8	115/118 (97%)	0.71	10 (8%)	10	6	56, 79, 108, 116	0
42	95	100/101 (99%)	0.58	10 (10%)	7	4	66, 114, 131, 136	0
42	D8	100/101 (99%)	0.80	10 (10%)	7	4	55, 101, 120, 127	0
43	A5	111/113 (98%)	2.19	54 (48%)	0	0	66, 78, 103, 131	0
43	E8	110/113 (97%)	1.35	27 (24%)	0	0	59, 74, 98, 108	0
44	B5	94/96 (97%)	1.36	22 (23%)	0	0	72, 84, 105, 116	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
44	F8	95/96 (98%)	0.97	18 (18%) 1 0	57, 70, 101, 112	0
45	C5	52/110 (47%)	3.37	40 (76%) 0 0	93, 103, 119, 123	0
45	G8	97/110 (88%)	0.57	4 (4%) 37 24	76, 96, 127, 133	0
46	D5	177/206 (85%)	2.26	84 (47%) 0 0	106, 131, 162, 166	0
46	H8	170/206 (82%)	1.48	52 (30%) 0 0	81, 116, 154, 162	0
47	E5	76/85 (89%)	1.84	30 (39%) 0 0	66, 87, 102, 110	0
47	I8	77/85 (90%)	1.21	17 (22%) 0 0	57, 72, 96, 104	0
48	F5	94/98 (95%)	1.90	40 (42%) 0 0	63, 83, 121, 129	0
48	J8	96/98 (97%)	1.87	39 (40%) 0 0	53, 75, 123, 138	0
49	G5	69/72 (95%)	0.71	4 (5%) 23 14	85, 106, 126, 142	0
49	K8	68/72 (94%)	1.03	9 (13%) 3 2	63, 84, 103, 121	0
50	H5	58/60 (96%)	2.18	28 (48%) 0 0	77, 98, 120, 127	0
50	L8	58/60 (96%)	0.68	7 (12%) 4 2	60, 81, 108, 113	0
51	M8	60/71 (84%)	0.63	8 (13%) 3 2	105, 135, 148, 152	0
52	J5	56/60 (93%)	1.47	21 (37%) 0 0	60, 85, 127, 136	0
52	N8	48/60 (80%)	1.26	12 (25%) 0 0	51, 87, 121, 128	0
53	L5	48/49 (97%)	3.07	33 (68%) 0 0	52, 61, 95, 104	0
53	P8	47/49 (95%)	1.00	7 (14%) 2 1	47, 52, 71, 89	0
54	M5	64/65 (98%)	2.36	35 (54%) 0 0	68, 81, 95, 115	0
54	Q8	64/65 (98%)	1.36	18 (28%) 0 0	56, 69, 83, 95	0
55	3L	70/76 (92%)	-0.03	3 (4%) 35 22	80, 150, 162, 164	0
All	All	20486/21509 (95%)	0.71	2870 (14%) 2 1	41, 98, 147, 180	0

The worst 5 of 2870 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
32	59	151	ILE	16.1
32	59	112	PRO	14.6
32	59	111	HIS	14.3
12	3A	64	TYR	13.4
32	59	114	VAL	13.1

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

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
22	H2U	1L	17	20/21	0.46	0.39	153,166,172,174	0
22	H2U	1K	17	20/21	0.54	0.26	153,168,175,178	0
55	PSU	3L	55	20/21	0.87	0.11	140,146,152,152	0
22	PSU	1L	55	20/21	0.90	0.10	122,134,145,147	0
23	4SU	2L	8	20/21	0.90	0.12	99,111,114,120	0
55	5MU	3L	54	21/22	0.91	0.09	136,142,145,152	0
23	7MG	2L	47	24/25	0.92	0.13	113,120,131,141	0
22	5MU	1L	54	21/22	0.92	0.11	122,128,134,140	0
23	PSU	2L	56	20/21	0.93	0.10	108,116,121,124	0
22	5MU	1K	54	21/22	0.93	0.15	100,111,121,127	0
23	7MG	2K	47	24/25	0.94	0.15	94,102,111,114	0
23	4SU	2K	8	20/21	0.94	0.14	85,93,98,99	0
22	PSU	1K	55	20/21	0.95	0.11	104,115,130,130	0
23	PSU	2K	56	20/21	0.95	0.10	96,104,114,115	0
23	5MU	2K	55	21/22	0.95	0.15	99,109,114,119	0
23	OMC	2K	33	21/22	0.96	0.30	71,78,80,88	0
22	AET	1L	37	33/34	0.96	0.23	94,112,119,124	0
23	OMC	2L	33	21/22	0.96	0.16	93,95,98,101	0
22	AET	1K	37	33/34	0.97	0.24	69,82,106,115	0
23	5MU	2L	55	21/22	0.98	0.10	116,121,123,124	0

## 6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 6.4 Ligands ⓘ

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
56	MG	1G	1666	1/1	0.12	0.09	122,122,122,122	0
56	MG	1G	1663	1/1	0.13	0.34	100,100,100,100	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	14	3245	1/1	0.40	0.42	104,104,104,104	0
56	MG	13	1726	1/1	0.41	0.27	99,99,99,99	0
56	MG	1H	3448	1/1	0.43	0.20	96,96,96,96	0
56	MG	68	201	1/1	0.44	0.19	84,84,84,84	0
56	MG	1H	3430	1/1	0.44	0.34	80,80,80,80	0
56	MG	13	1763	1/1	0.44	0.56	131,131,131,131	0
56	MG	1H	3345	1/1	0.47	0.26	87,87,87,87	0
56	MG	13	1674	1/1	0.48	0.17	101,101,101,101	0
56	MG	1H	3340	1/1	0.48	0.33	83,83,83,83	0
56	MG	14	3216	1/1	0.48	0.18	91,91,91,91	0
56	MG	14	3053	1/1	0.49	0.20	72,72,72,72	0
56	MG	13	1606	1/1	0.51	0.19	81,81,81,81	0
56	MG	13	1711	1/1	0.51	0.26	114,114,114,114	0
56	MG	13	1682	1/1	0.51	0.29	116,116,116,116	0
56	MG	BA	202	1/1	0.51	3.85	113,113,113,113	0
56	MG	13	1662	1/1	0.53	0.29	105,105,105,105	0
56	MG	68	202	1/1	0.53	0.19	90,90,90,90	0
56	MG	14	3179	1/1	0.54	0.43	83,83,83,83	0
56	MG	1H	3294	1/1	0.55	0.16	112,112,112,112	0
56	MG	35	201	1/1	0.55	0.20	84,84,84,84	0
56	MG	14	3211	1/1	0.56	0.26	111,111,111,111	0
56	MG	14	3178	1/1	0.56	0.40	85,85,85,85	0
56	MG	1G	1674	1/1	0.56	0.16	106,106,106,106	0
56	MG	1H	3301	1/1	0.56	0.19	95,95,95,95	0
56	MG	16	209	1/1	0.57	0.22	81,81,81,81	0
56	MG	14	3193	1/1	0.57	0.20	88,88,88,88	0
56	MG	14	3201	1/1	0.57	0.38	91,91,91,91	0
56	MG	14	3427	1/1	0.58	0.08	104,104,104,104	0
56	MG	1H	3608	1/1	0.58	0.08	110,110,110,110	0
56	MG	1H	3481	1/1	0.58	0.13	122,122,122,122	0
56	MG	1H	3176	1/1	0.59	0.27	93,93,93,93	0
56	MG	1H	3445	1/1	0.59	0.34	90,90,90,90	0
56	MG	1H	3523	1/1	0.60	0.18	82,82,82,82	0
56	MG	1H	3241	1/1	0.60	0.21	93,93,93,93	0
56	MG	1J	205	1/1	0.60	0.17	118,118,118,118	0
56	MG	1G	1661	1/1	0.60	0.18	94,94,94,94	0
56	MG	1H	3172	1/1	0.61	0.40	96,96,96,96	0
56	MG	13	1706	1/1	0.61	1.38	111,111,111,111	0
56	MG	1H	3186	1/1	0.61	0.28	97,97,97,97	0
56	MG	1H	3093	1/1	0.61	0.20	56,56,56,56	0
56	MG	1H	3463	1/1	0.61	0.07	101,101,101,101	0
56	MG	1H	3177	1/1	0.62	0.36	79,79,79,79	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	1H	3193	1/1	0.62	0.31	89,89,89,89	0
56	MG	14	3424	1/1	0.62	0.09	94,94,94,94	0
56	MG	13	1631	1/1	0.62	0.08	88,88,88,88	0
56	MG	14	3029	1/1	0.62	0.20	96,96,96,96	0
56	MG	1H	3138	1/1	0.62	0.23	75,75,75,75	0
56	MG	1H	3139	1/1	0.63	0.24	79,79,79,79	0
56	MG	16	213	1/1	0.63	0.09	98,98,98,98	0
56	MG	1G	1643	1/1	0.63	0.26	92,92,92,92	0
56	MG	55	201	1/1	0.64	0.31	85,85,85,85	0
56	MG	1G	1630	1/1	0.64	0.18	95,95,95,95	0
56	MG	1H	3337	1/1	0.64	0.14	99,99,99,99	0
56	MG	13	1667	1/1	0.65	0.22	86,86,86,86	0
56	MG	1H	3021	1/1	0.65	0.29	67,67,67,67	0
56	MG	14	3292	1/1	0.65	0.19	88,88,88,88	0
56	MG	1H	3479	1/1	0.65	0.12	107,107,107,107	0
56	MG	1H	3328	1/1	0.65	0.27	86,86,86,86	0
56	MG	13	1804	1/1	0.65	0.14	137,137,137,137	0
56	MG	13	1608	1/1	0.66	0.12	111,111,111,111	0
56	MG	14	3278	1/1	0.66	0.23	74,74,74,74	0
56	MG	1G	1672	1/1	0.66	0.36	96,96,96,96	0
56	MG	13	1764	1/1	0.66	0.52	128,128,128,128	0
56	MG	5I	101	1/1	0.67	0.29	85,85,85,85	0
56	MG	1H	3292	1/1	0.67	0.19	108,108,108,108	0
56	MG	13	1619	1/1	0.67	0.11	95,95,95,95	0
56	MG	1G	1675	1/1	0.67	0.20	92,92,92,92	0
56	MG	1H	3227	1/1	0.67	0.21	99,99,99,99	0
56	MG	14	3047	1/1	0.67	0.26	80,80,80,80	0
56	MG	1G	1651	1/1	0.68	0.22	107,107,107,107	0
56	MG	1G	1715	1/1	0.68	0.07	119,119,119,119	0
56	MG	1H	3053	1/1	0.68	0.17	53,53,53,53	0
56	MG	1H	3307	1/1	0.68	0.31	89,89,89,89	0
56	MG	1G	1665	1/1	0.68	0.17	107,107,107,107	0
56	MG	1H	3333	1/1	0.68	0.51	96,96,96,96	0
56	MG	13	1741	1/1	0.68	0.27	99,99,99,99	0
56	MG	14	3235	1/1	0.68	0.19	88,88,88,88	0
56	MG	1H	3205	1/1	0.68	0.49	94,94,94,94	0
56	MG	14	3183	1/1	0.68	0.21	96,96,96,96	0
56	MG	16	211	1/1	0.68	0.31	79,79,79,79	0
56	MG	1H	3248	1/1	0.69	0.19	86,86,86,86	0
56	MG	14	3286	1/1	0.69	0.29	93,93,93,93	0
56	MG	13	1670	1/1	0.69	0.11	84,84,84,84	0
56	MG	13	1737	1/1	0.69	0.20	79,79,79,79	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	1G	1654	1/1	0.69	0.14	98,98,98,98	0
56	MG	1H	3465	1/1	0.69	0.11	111,111,111,111	0
56	MG	16	206	1/1	0.70	0.21	80,80,80,80	0
56	MG	25	201	1/1	0.70	0.04	123,123,123,123	0
56	MG	1H	3264	1/1	0.70	0.87	74,74,74,74	0
56	MG	13	1788	1/1	0.70	0.08	123,123,123,123	0
56	MG	16	207	1/1	0.70	0.25	110,110,110,110	0
56	MG	1H	3482	1/1	0.70	0.07	142,142,142,142	0
56	MG	1G	1604	1/1	0.70	0.21	87,87,87,87	0
56	MG	1H	3332	1/1	0.70	0.79	83,83,83,83	0
56	MG	1H	3266	1/1	0.70	0.28	83,83,83,83	0
56	MG	1H	3070	1/1	0.71	0.15	78,78,78,78	0
56	MG	1H	3459	1/1	0.71	0.35	102,102,102,102	0
56	MG	1H	3265	1/1	0.71	0.19	72,72,72,72	0
56	MG	13	1686	1/1	0.71	0.60	129,129,129,129	0
56	MG	14	3229	1/1	0.71	0.36	92,92,92,92	0
56	MG	1H	3252	1/1	0.71	0.10	102,102,102,102	0
56	MG	1H	3268	1/1	0.71	0.18	86,86,86,86	0
56	MG	14	3023	1/1	0.71	0.22	82,82,82,82	0
56	MG	1H	3426	1/1	0.72	0.29	80,80,80,80	0
56	MG	1G	1722	1/1	0.72	0.51	111,111,111,111	0
56	MG	1H	3293	1/1	0.72	0.31	95,95,95,95	0
56	MG	1H	3575	1/1	0.72	0.10	63,63,63,63	0
56	MG	1H	3185	1/1	0.72	0.21	87,87,87,87	0
56	MG	13	1696	1/1	0.72	2.85	104,104,104,104	0
56	MG	1G	1667	1/1	0.72	0.65	104,104,104,104	0
56	MG	1H	3419	1/1	0.72	0.21	77,77,77,77	0
56	MG	13	1689	1/1	0.72	0.64	105,105,105,105	0
56	MG	14	3277	1/1	0.72	0.22	90,90,90,90	0
56	MG	1H	3283	1/1	0.72	0.24	79,79,79,79	0
56	MG	13	1712	1/1	0.73	1.39	106,106,106,106	0
56	MG	1H	3269	1/1	0.73	0.28	80,80,80,80	0
56	MG	1G	1696	1/1	0.73	0.29	103,103,103,103	0
56	MG	13	1727	1/1	0.73	0.19	103,103,103,103	0
56	MG	14	3318	1/1	0.73	0.14	84,84,84,84	0
56	MG	14	3206	1/1	0.73	0.27	87,87,87,87	0
56	MG	13	1690	1/1	0.73	0.12	118,118,118,118	0
56	MG	1H	3055	1/1	0.73	0.12	69,69,69,69	0
56	MG	13	1748	1/1	0.73	0.08	122,122,122,122	0
56	MG	1H	3441	1/1	0.74	0.10	115,115,115,115	0
56	MG	1H	3219	1/1	0.74	0.46	98,98,98,98	0
56	MG	14	3312	1/1	0.74	0.08	99,99,99,99	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	13	1673	1/1	0.74	0.27	88,88,88,88	0
56	MG	1H	3235	1/1	0.74	0.24	66,66,66,66	0
56	MG	1H	3386	1/1	0.74	0.37	96,96,96,96	0
56	MG	14	3300	1/1	0.74	0.21	84,84,84,84	0
56	MG	14	3073	1/1	0.74	0.15	72,72,72,72	0
56	MG	13	1622	1/1	0.74	0.30	72,72,72,72	0
56	MG	1H	3180	1/1	0.74	0.38	88,88,88,88	0
56	MG	14	3215	1/1	0.74	0.26	94,94,94,94	0
56	MG	13	1607	1/1	0.74	0.20	78,78,78,78	0
56	MG	13	1685	1/1	0.74	0.48	114,114,114,114	0
56	MG	1G	1642	1/1	0.74	0.21	110,110,110,110	0
56	MG	1H	3564	1/1	0.74	0.18	95,95,95,95	0
56	MG	14	3154	1/1	0.74	0.27	87,87,87,87	0
56	MG	14	3262	1/1	0.74	0.43	87,87,87,87	0
56	MG	1H	3270	1/1	0.74	0.28	87,87,87,87	0
56	MG	1G	1605	1/1	0.74	0.16	105,105,105,105	0
56	MG	1H	3054	1/1	0.74	0.29	78,78,78,78	0
56	MG	14	3168	1/1	0.75	0.30	65,65,65,65	0
56	MG	1G	1752	1/1	0.75	0.06	139,139,139,139	0
56	MG	14	3041	1/1	0.75	0.26	85,85,85,85	0
56	MG	21	301	1/1	0.75	0.14	64,64,64,64	0
56	MG	14	3051	1/1	0.75	0.14	75,75,75,75	0
56	MG	31	301	1/1	0.75	0.09	67,67,67,67	0
56	MG	1G	1626	1/1	0.75	0.28	102,102,102,102	0
56	MG	1H	3568	1/1	0.75	0.10	89,89,89,89	0
56	MG	1G	1656	1/1	0.75	0.15	99,99,99,99	0
56	MG	14	3224	1/1	0.75	0.29	101,101,101,101	0
56	MG	1H	3520	1/1	0.75	0.14	54,54,54,54	0
56	MG	14	3435	1/1	0.75	0.08	121,121,121,121	0
56	MG	78	202	1/1	0.75	1.41	87,87,87,87	0
56	MG	1G	1718	1/1	0.76	0.17	140,140,140,140	0
56	MG	35	202	1/1	0.76	0.26	79,79,79,79	0
56	MG	1H	3599	1/1	0.76	0.11	85,85,85,85	0
56	MG	2L	102	1/1	0.76	0.06	113,113,113,113	0
56	MG	1H	3228	1/1	0.76	0.32	85,85,85,85	0
56	MG	1H	3046	1/1	0.76	0.67	73,73,73,73	0
56	MG	1G	1639	1/1	0.76	0.21	113,113,113,113	0
56	MG	13	1710	1/1	0.76	2.00	103,103,103,103	0
56	MG	13	1734	1/1	0.76	0.23	87,87,87,87	0
56	MG	1H	3238	1/1	0.76	0.39	87,87,87,87	0
56	MG	14	3191	1/1	0.76	0.66	84,84,84,84	0
56	MG	1H	3213	1/1	0.76	0.15	69,69,69,69	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	14	3184	1/1	0.76	0.12	85,85,85,85	0
56	MG	14	3315	1/1	0.76	0.10	93,93,93,93	0
56	MG	14	3217	1/1	0.76	0.12	96,96,96,96	0
56	MG	1G	1734	1/1	0.77	0.12	94,94,94,94	0
56	MG	1H	3562	1/1	0.77	0.10	97,97,97,97	0
56	MG	1H	3162	1/1	0.77	0.26	70,70,70,70	0
56	MG	1H	3597	1/1	0.77	0.10	92,92,92,92	0
56	MG	1G	1646	1/1	0.77	0.23	116,116,116,116	0
56	MG	1G	1627	1/1	0.77	0.09	88,88,88,88	0
56	MG	14	3205	1/1	0.77	0.27	75,75,75,75	0
56	MG	1H	3096	1/1	0.77	0.24	63,63,63,63	0
56	MG	13	1666	1/1	0.77	0.13	92,92,92,92	0
56	MG	1H	3434	1/1	0.77	0.17	86,86,86,86	0
56	MG	1H	3300	1/1	0.77	0.52	86,86,86,86	0
56	MG	14	3319	1/1	0.77	0.07	104,104,104,104	0
56	MG	1H	3456	1/1	0.77	0.08	100,100,100,100	0
56	MG	1H	3370	1/1	0.77	1.53	84,84,84,84	0
56	MG	14	3330	1/1	0.77	0.16	82,82,82,82	0
56	MG	1H	3165	1/1	0.77	0.42	98,98,98,98	0
56	MG	1H	3595	1/1	0.77	0.07	99,99,99,99	0
56	MG	1H	3202	1/1	0.77	0.30	84,84,84,84	0
56	MG	1H	3316	1/1	0.77	0.18	106,106,106,106	0
56	MG	14	3210	1/1	0.77	0.33	100,100,100,100	0
56	MG	14	3275	1/1	0.77	0.31	77,77,77,77	0
56	MG	1G	1695	1/1	0.77	0.23	96,96,96,96	0
56	MG	14	3065	1/1	0.77	0.22	90,90,90,90	0
56	MG	1G	1739	1/1	0.78	0.09	107,107,107,107	0
56	MG	14	3385	1/1	0.78	0.16	84,84,84,84	0
56	MG	1G	1647	1/1	0.78	0.44	92,92,92,92	0
56	MG	1H	3142	1/1	0.78	0.23	79,79,79,79	0
56	MG	1G	1738	1/1	0.78	0.33	105,105,105,105	0
56	MG	14	3276	1/1	0.78	0.24	92,92,92,92	0
56	MG	4L	401	1/1	0.78	0.23	99,99,99,99	0
56	MG	14	3012	1/1	0.78	0.24	66,66,66,66	0
56	MG	14	3157	1/1	0.78	0.19	86,86,86,86	0
56	MG	14	3071	1/1	0.78	0.18	83,83,83,83	0
56	MG	1H	3062	1/1	0.78	0.18	72,72,72,72	0
56	MG	21	302	1/1	0.78	1.24	76,76,76,76	0
56	MG	13	1665	1/1	0.78	0.42	117,117,117,117	0
56	MG	1H	3462	1/1	0.78	0.08	95,95,95,95	0
56	MG	1G	1685	1/1	0.78	0.22	76,76,76,76	0
56	MG	1H	3259	1/1	0.79	0.50	69,69,69,69	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	14	3391	1/1	0.79	0.08	106,106,106,106	0
56	MG	1H	3223	1/1	0.79	0.37	65,65,65,65	0
56	MG	14	3317	1/1	0.79	0.12	153,153,153,153	0
56	MG	1G	1716	1/1	0.79	0.10	109,109,109,109	0
56	MG	1G	1673	1/1	0.79	0.23	104,104,104,104	0
56	MG	1H	3016	1/1	0.79	0.27	66,66,66,66	0
56	MG	1H	3473	1/1	0.79	0.12	112,112,112,112	0
56	MG	14	3068	1/1	0.79	0.21	78,78,78,78	0
56	MG	1G	1609	1/1	0.79	0.12	96,96,96,96	0
56	MG	1H	3579	1/1	0.79	0.09	81,81,81,81	0
56	MG	1G	1659	1/1	0.79	0.36	104,104,104,104	0
56	MG	13	1757	1/1	0.79	0.11	119,119,119,119	0
56	MG	13	1725	1/1	0.79	0.80	101,101,101,101	0
56	MG	14	3162	1/1	0.79	0.14	89,89,89,89	0
56	MG	1H	3196	1/1	0.79	0.43	68,68,68,68	0
56	MG	1H	3487	1/1	0.79	0.09	50,50,50,50	0
56	MG	1H	3189	1/1	0.79	0.18	77,77,77,77	0
56	MG	14	3320	1/1	0.80	0.17	120,120,120,120	0
56	MG	1H	3284	1/1	0.80	0.30	79,79,79,79	0
56	MG	1H	3236	1/1	0.80	0.25	80,80,80,80	0
56	MG	35	203	1/1	0.80	0.30	81,81,81,81	0
56	MG	1H	3291	1/1	0.80	0.09	97,97,97,97	0
56	MG	1J	202	1/1	0.80	0.07	92,92,92,92	0
56	MG	13	1721	1/1	0.80	0.21	74,74,74,74	0
56	MG	1H	3281	1/1	0.80	0.24	86,86,86,86	0
56	MG	14	3129	1/1	0.80	0.22	84,84,84,84	0
56	MG	1G	1669	1/1	0.80	0.22	85,85,85,85	0
56	MG	1H	3229	1/1	0.80	0.13	83,83,83,83	0
56	MG	13	1789	1/1	0.80	0.08	63,63,63,63	0
56	MG	1G	1701	1/1	0.80	0.36	94,94,94,94	0
56	MG	13	1680	1/1	0.81	0.30	103,103,103,103	0
56	MG	1H	3298	1/1	0.81	0.28	82,82,82,82	0
56	MG	14	3421	1/1	0.81	0.30	72,72,72,72	0
56	MG	1H	3362	1/1	0.81	0.22	69,69,69,69	0
56	MG	1G	1748	1/1	0.81	0.07	107,107,107,107	0
56	MG	1H	3209	1/1	0.81	0.23	80,80,80,80	0
56	MG	1G	1743	1/1	0.81	0.07	122,122,122,122	0
56	MG	1H	3210	1/1	0.81	0.22	68,68,68,68	0
56	MG	1H	3121	1/1	0.81	0.24	67,67,67,67	0
56	MG	14	3420	1/1	0.81	0.07	86,86,86,86	0
56	MG	13	1729	1/1	0.81	0.11	95,95,95,95	0
56	MG	1H	3614	1/1	0.81	0.26	97,97,97,97	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	14	3160	1/1	0.81	0.47	86,86,86,86	0
56	MG	13	1805	1/1	0.81	0.06	115,115,115,115	0
56	MG	14	3006	1/1	0.81	0.18	56,56,56,56	0
56	MG	14	3405	1/1	0.81	0.12	108,108,108,108	0
56	MG	14	3432	1/1	0.81	0.12	91,91,91,91	0
56	MG	1H	3036	1/1	0.81	0.09	73,73,73,73	0
56	MG	1H	3422	1/1	0.81	0.27	90,90,90,90	0
56	MG	14	3001	1/1	0.81	0.17	76,76,76,76	0
56	MG	1G	1699	1/1	0.81	0.14	90,90,90,90	0
56	MG	1H	3591	1/1	0.81	0.08	70,70,70,70	0
56	MG	1H	3526	1/1	0.81	0.12	57,57,57,57	0
56	MG	13	1801	1/1	0.81	0.12	113,113,113,113	0
56	MG	1G	1708	1/1	0.81	0.16	105,105,105,105	0
56	MG	1H	3356	1/1	0.81	0.41	76,76,76,76	0
56	MG	1H	3146	1/1	0.81	0.14	71,71,71,71	0
56	MG	14	3124	1/1	0.81	0.34	82,82,82,82	0
56	MG	14	3043	1/1	0.81	0.59	73,73,73,73	0
56	MG	1H	3457	1/1	0.82	0.11	99,99,99,99	0
56	MG	13	1702	1/1	0.82	1.01	87,87,87,87	0
56	MG	1H	3297	1/1	0.82	0.28	80,80,80,80	0
56	MG	13	1656	1/1	0.82	0.23	91,91,91,91	0
56	MG	14	3110	1/1	0.82	0.40	85,85,85,85	0
56	MG	1H	3396	1/1	0.82	0.12	71,71,71,71	0
56	MG	14	3273	1/1	0.82	0.23	70,70,70,70	0
56	MG	1H	3028	1/1	0.82	0.17	64,64,64,64	0
56	MG	1H	3455	1/1	0.82	0.07	92,92,92,92	0
56	MG	14	3434	1/1	0.82	0.06	61,61,61,61	0
56	MG	1H	3153	1/1	0.82	0.49	92,92,92,92	0
56	MG	1H	3312	1/1	0.82	0.23	100,100,100,100	0
56	MG	13	1659	1/1	0.82	0.49	115,115,115,115	0
56	MG	1H	3034	1/1	0.82	0.19	64,64,64,64	0
56	MG	1H	3435	1/1	0.82	0.11	68,68,68,68	0
56	MG	1H	3247	1/1	0.82	0.32	65,65,65,65	0
56	MG	14	3171	1/1	0.82	0.30	89,89,89,89	0
56	MG	1H	3071	1/1	0.82	0.23	71,71,71,71	0
56	MG	14	3239	1/1	0.82	0.15	53,53,53,53	0
56	MG	13	1779	1/1	0.82	0.31	106,106,106,106	0
56	MG	1H	3065	1/1	0.82	0.14	69,69,69,69	0
56	MG	1H	3141	1/1	0.82	0.20	71,71,71,71	0
56	MG	1H	3148	1/1	0.82	0.23	89,89,89,89	0
56	MG	14	3082	1/1	0.82	0.25	91,91,91,91	0
56	MG	1H	3188	1/1	0.82	0.24	90,90,90,90	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	1H	3137	1/1	0.82	0.33	74,74,74,74	0
56	MG	13	1684	1/1	0.82	0.53	99,99,99,99	0
56	MG	14	3018	1/1	0.82	0.13	66,66,66,66	0
56	MG	13	1675	1/1	0.82	0.33	80,80,80,80	0
56	MG	14	3143	1/1	0.83	0.41	86,86,86,86	0
56	MG	14	3156	1/1	0.83	0.12	68,68,68,68	0
56	MG	1H	3271	1/1	0.83	0.17	93,93,93,93	0
56	MG	13	1753	1/1	0.83	0.07	121,121,121,121	0
56	MG	1H	3421	1/1	0.83	0.43	92,92,92,92	0
56	MG	1H	3033	1/1	0.83	0.21	64,64,64,64	0
56	MG	1H	3437	1/1	0.83	0.07	90,90,90,90	0
56	MG	14	3200	1/1	0.83	0.40	72,72,72,72	0
56	MG	1H	3425	1/1	0.83	0.33	101,101,101,101	0
56	MG	14	3240	1/1	0.83	0.31	86,86,86,86	0
56	MG	1H	3039	1/1	0.83	0.22	62,62,62,62	0
56	MG	14	3064	1/1	0.83	0.44	53,53,53,53	0
56	MG	14	3002	1/1	0.83	0.09	49,49,49,49	0
56	MG	1H	3347	1/1	0.83	0.73	89,89,89,89	0
56	MG	13	1714	1/1	0.83	0.20	114,114,114,114	0
56	MG	14	3140	1/1	0.83	0.11	88,88,88,88	0
56	MG	1H	3044	1/1	0.83	0.08	66,66,66,66	0
56	MG	1H	3361	1/1	0.83	0.08	89,89,89,89	0
56	MG	1G	1664	1/1	0.83	0.20	106,106,106,106	0
56	MG	1H	3206	1/1	0.83	0.64	73,73,73,73	0
56	MG	1H	3311	1/1	0.83	0.36	98,98,98,98	0
56	MG	1H	3278	1/1	0.83	0.18	69,69,69,69	0
56	MG	1H	3275	1/1	0.83	0.18	70,70,70,70	0
56	MG	1H	3280	1/1	0.83	0.25	90,90,90,90	0
56	MG	1G	1693	1/1	0.83	0.20	84,84,84,84	0
56	MG	14	3299	1/1	0.83	0.30	78,78,78,78	0
56	MG	14	3429	1/1	0.83	0.08	91,91,91,91	0
56	MG	14	3285	1/1	0.83	0.37	95,95,95,95	0
56	MG	13	1613	1/1	0.83	0.12	78,78,78,78	0
56	MG	14	3365	1/1	0.83	0.10	89,89,89,89	0
56	MG	1H	3104	1/1	0.83	0.25	65,65,65,65	0
56	MG	1H	3194	1/1	0.83	0.27	62,62,62,62	0
56	MG	1H	3276	1/1	0.83	2.11	68,68,68,68	0
56	MG	14	3102	1/1	0.83	0.21	67,67,67,67	0
56	MG	14	3130	1/1	0.83	0.19	65,65,65,65	0
56	MG	1H	3080	1/1	0.83	0.30	80,80,80,80	0
56	MG	1H	3341	1/1	0.83	0.96	80,80,80,80	0
56	MG	29	301	1/1	0.83	0.17	78,78,78,78	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	1G	1652	1/1	0.84	0.24	87,87,87,87	0
56	MG	13	1621	1/1	0.84	0.30	74,74,74,74	0
56	MG	14	3298	1/1	0.84	0.31	100,100,100,100	0
56	MG	1H	3470	1/1	0.84	0.16	94,94,94,94	0
56	MG	14	3369	1/1	0.84	0.14	87,87,87,87	0
56	MG	13	1678	1/1	0.84	0.22	97,97,97,97	0
56	MG	1H	3201	1/1	0.84	0.32	77,77,77,77	0
56	MG	14	3077	1/1	0.84	0.43	87,87,87,87	0
56	MG	14	3400	1/1	0.84	0.10	87,87,87,87	0
56	MG	14	3309	1/1	0.84	0.11	87,87,87,87	0
56	MG	1H	3029	1/1	0.84	0.14	69,69,69,69	0
56	MG	1G	1631	1/1	0.84	0.21	85,85,85,85	0
56	MG	14	3343	1/1	0.84	0.12	54,54,54,54	0
56	MG	1H	3418	1/1	0.84	0.17	90,90,90,90	0
56	MG	1G	1710	1/1	0.84	0.13	102,102,102,102	0
56	MG	14	3166	1/1	0.84	0.62	88,88,88,88	0
56	MG	13	1774	1/1	0.84	0.10	87,87,87,87	0
56	MG	14	3218	1/1	0.84	0.37	104,104,104,104	0
56	MG	88	202	1/1	0.84	0.43	69,69,69,69	0
56	MG	1H	3136	1/1	0.84	0.29	68,68,68,68	0
56	MG	1H	3063	1/1	0.84	0.12	54,54,54,54	0
56	MG	1H	3195	1/1	0.84	0.67	84,84,84,84	0
56	MG	1H	3336	1/1	0.84	0.17	81,81,81,81	0
56	MG	14	3281	1/1	0.84	0.17	89,89,89,89	0
56	MG	1H	3056	1/1	0.84	0.11	73,73,73,73	0
56	MG	1H	3097	1/1	0.84	0.31	70,70,70,70	0
56	MG	1H	3590	1/1	0.84	0.06	107,107,107,107	0
56	MG	1G	1727	1/1	0.84	0.09	108,108,108,108	0
56	MG	13	1792	1/1	0.84	0.15	73,73,73,73	0
56	MG	1H	3610	1/1	0.84	0.15	106,106,106,106	0
56	MG	13	1605	1/1	0.84	0.14	86,86,86,86	0
56	MG	1H	3329	1/1	0.84	0.19	75,75,75,75	0
56	MG	1H	3404	1/1	0.84	0.25	80,80,80,80	0
56	MG	1H	3603	1/1	0.84	0.07	121,121,121,121	0
56	MG	1H	3489	1/1	0.84	0.12	53,53,53,53	0
56	MG	1H	3031	1/1	0.84	0.16	56,56,56,56	0
56	MG	1H	3334	1/1	0.84	0.47	93,93,93,93	0
56	MG	1H	3387	1/1	0.85	0.35	71,71,71,71	0
56	MG	14	3030	1/1	0.85	0.18	78,78,78,78	0
56	MG	1G	1729	1/1	0.85	0.24	113,113,113,113	0
56	MG	1H	3484	1/1	0.85	0.10	45,45,45,45	0
56	MG	1H	3222	1/1	0.85	0.40	78,78,78,78	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	13	1653	1/1	0.85	0.11	82,82,82,82	0
56	MG	1H	3183	1/1	0.85	0.27	80,80,80,80	0
56	MG	1H	3237	1/1	0.85	0.19	72,72,72,72	0
56	MG	1H	3335	1/1	0.85	0.13	103,103,103,103	0
56	MG	1G	1725	1/1	0.85	0.05	111,111,111,111	0
56	MG	1H	3025	1/1	0.85	0.18	49,49,49,49	0
56	MG	1H	3187	1/1	0.85	0.27	75,75,75,75	0
56	MG	14	3287	1/1	0.85	0.42	86,86,86,86	0
56	MG	14	3323	1/1	0.85	0.18	100,100,100,100	0
56	MG	1H	3198	1/1	0.85	0.44	108,108,108,108	0
56	MG	1G	1698	1/1	0.85	0.23	88,88,88,88	0
56	MG	1G	1603	1/1	0.85	0.10	78,78,78,78	0
56	MG	13	1603	1/1	0.85	0.12	52,52,52,52	0
56	MG	1H	3191	1/1	0.85	0.21	99,99,99,99	0
56	MG	13	1639	1/1	0.85	0.18	76,76,76,76	0
56	MG	39	301	1/1	0.85	0.17	94,94,94,94	0
56	MG	31	302	1/1	0.85	0.28	76,76,76,76	0
56	MG	1G	1641	1/1	0.85	0.09	95,95,95,95	0
56	MG	D8	201	1/1	0.85	0.46	76,76,76,76	0
56	MG	1H	3547	1/1	0.85	0.11	85,85,85,85	0
56	MG	1G	1658	1/1	0.85	0.21	108,108,108,108	0
56	MG	1H	3578	1/1	0.85	0.09	65,65,65,65	0
56	MG	1H	3317	1/1	0.85	0.13	102,102,102,102	0
56	MG	1H	3041	1/1	0.85	0.16	65,65,65,65	0
56	MG	2K	102	1/1	0.85	0.30	81,81,81,81	0
56	MG	14	3072	1/1	0.85	0.37	69,69,69,69	0
56	MG	1H	3466	1/1	0.85	0.16	115,115,115,115	0
56	MG	14	3268	1/1	0.85	0.21	83,83,83,83	0
56	MG	1H	3621	1/1	0.85	0.12	52,52,52,52	0
56	MG	14	3225	1/1	0.85	0.43	111,111,111,111	0
56	MG	1H	3218	1/1	0.85	0.28	70,70,70,70	0
56	MG	85	201	1/1	0.85	0.33	75,75,75,75	0
56	MG	14	3230	1/1	0.85	0.20	90,90,90,90	0
56	MG	1H	3010	1/1	0.85	0.23	70,70,70,70	0
56	MG	1H	3424	1/1	0.85	0.21	65,65,65,65	0
56	MG	1G	1638	1/1	0.86	0.18	93,93,93,93	0
56	MG	78	201	1/1	0.86	0.27	62,62,62,62	0
56	MG	1H	3060	1/1	0.86	0.25	63,63,63,63	0
56	MG	14	3084	1/1	0.86	0.10	77,77,77,77	0
56	MG	1H	3447	1/1	0.86	0.10	65,65,65,65	0
56	MG	1H	3145	1/1	0.86	0.45	91,91,91,91	0
56	MG	1G	1726	1/1	0.86	0.17	86,86,86,86	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	1H	3522	1/1	0.86	0.10	59,59,59,59	0
56	MG	14	3158	1/1	0.86	0.29	80,80,80,80	0
56	MG	14	3291	1/1	0.86	0.41	86,86,86,86	0
56	MG	88	203	1/1	0.86	0.68	79,79,79,79	0
56	MG	1G	1616	1/1	0.86	0.43	100,100,100,100	0
56	MG	1G	1702	1/1	0.86	0.30	101,101,101,101	0
56	MG	1G	1683	1/1	0.86	0.28	87,87,87,87	0
56	MG	1H	3461	1/1	0.86	0.08	102,102,102,102	0
56	MG	14	3294	1/1	0.86	0.28	94,94,94,94	0
56	MG	14	3057	1/1	0.86	0.16	78,78,78,78	0
56	MG	14	3297	1/1	0.86	0.28	91,91,91,91	0
56	MG	14	3209	1/1	0.86	0.19	97,97,97,97	0
56	MG	1H	3417	1/1	0.86	0.17	93,93,93,93	0
56	MG	14	3360	1/1	0.86	0.10	69,69,69,69	0
56	MG	14	3402	1/1	0.86	0.11	94,94,94,94	0
56	MG	1H	3095	1/1	0.86	0.21	64,64,64,64	0
56	MG	1G	1637	1/1	0.86	0.08	121,121,121,121	0
56	MG	1H	3342	1/1	0.86	1.77	75,75,75,75	0
56	MG	14	3290	1/1	0.86	0.34	85,85,85,85	0
56	MG	1G	1721	1/1	0.86	0.08	143,143,143,143	0
56	MG	13	1697	1/1	0.86	1.59	98,98,98,98	0
56	MG	1G	1745	1/1	0.86	0.08	124,124,124,124	0
56	MG	1H	3207	1/1	0.86	0.41	87,87,87,87	0
56	MG	1H	3049	1/1	0.86	0.10	95,95,95,95	0
56	MG	1H	3073	1/1	0.86	0.28	58,58,58,58	0
56	MG	1H	3100	1/1	0.86	0.16	69,69,69,69	0
56	MG	13	1668	1/1	0.86	0.39	101,101,101,101	0
56	MG	14	3045	1/1	0.86	0.24	91,91,91,91	0
56	MG	13	1663	1/1	0.87	0.17	105,105,105,105	0
56	MG	1H	3083	1/1	0.87	0.24	82,82,82,82	0
56	MG	13	1705	1/1	0.87	1.02	111,111,111,111	0
56	MG	1H	3040	1/1	0.87	0.20	62,62,62,62	0
56	MG	14	3054	1/1	0.87	0.18	48,48,48,48	0
56	MG	14	3280	1/1	0.87	0.30	89,89,89,89	0
56	MG	1H	3444	1/1	0.87	0.10	78,78,78,78	0
56	MG	14	3367	1/1	0.87	0.14	86,86,86,86	0
56	MG	14	3372	1/1	0.87	0.25	91,91,91,91	0
56	MG	14	3197	1/1	0.87	0.22	91,91,91,91	0
56	MG	14	3092	1/1	0.87	0.14	79,79,79,79	0
56	MG	1H	3598	1/1	0.87	0.10	105,105,105,105	0
56	MG	1G	1720	1/1	0.87	0.23	112,112,112,112	0
56	MG	1H	3498	1/1	0.87	0.08	70,70,70,70	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	14	3079	1/1	0.87	0.11	91,91,91,91	0
56	MG	13	1747	1/1	0.87	0.29	93,93,93,93	0
56	MG	1H	3304	1/1	0.87	0.21	106,106,106,106	0
56	MG	1H	3174	1/1	0.87	0.27	86,86,86,86	0
56	MG	14	3213	1/1	0.87	0.34	87,87,87,87	0
56	MG	1G	1746	1/1	0.87	0.18	95,95,95,95	0
56	MG	1H	3436	1/1	0.87	0.14	98,98,98,98	0
56	MG	1H	3324	1/1	0.87	0.27	78,78,78,78	0
56	MG	13	1610	1/1	0.87	0.10	56,56,56,56	0
56	MG	1G	1671	1/1	0.87	0.15	92,92,92,92	0
56	MG	1H	3554	1/1	0.87	0.19	108,108,108,108	0
56	MG	1H	3472	1/1	0.87	0.11	108,108,108,108	0
56	MG	1K	500	1/1	0.87	0.14	101,101,101,101	0
56	MG	1H	3308	1/1	0.87	0.48	78,78,78,78	0
56	MG	1G	1687	1/1	0.87	0.25	96,96,96,96	0
56	MG	1H	3550	1/1	0.87	0.18	70,70,70,70	0
56	MG	1H	3358	1/1	0.87	0.57	83,83,83,83	0
56	MG	13	1707	1/1	0.87	0.84	108,108,108,108	0
56	MG	14	3208	1/1	0.87	0.68	89,89,89,89	0
56	MG	1H	3231	1/1	0.87	0.11	83,83,83,83	0
56	MG	1G	1625	1/1	0.87	0.17	111,111,111,111	0
56	MG	P8	101	1/1	0.87	0.24	68,68,68,68	0
56	MG	14	3368	1/1	0.87	0.07	101,101,101,101	0
56	MG	1G	1735	1/1	0.87	0.06	112,112,112,112	0
56	MG	14	3125	1/1	0.87	0.18	84,84,84,84	0
56	MG	14	3046	1/1	0.87	0.09	56,56,56,56	0
56	MG	14	3306	1/1	0.87	0.18	66,66,66,66	0
56	MG	1H	3134	1/1	0.87	0.44	85,85,85,85	0
56	MG	1H	3019	1/1	0.87	0.14	53,53,53,53	0
56	MG	16	214	1/1	0.87	0.09	82,82,82,82	0
56	MG	14	3099	1/1	0.87	0.13	66,66,66,66	0
56	MG	1H	3574	1/1	0.87	0.11	53,53,53,53	0
56	MG	13	1724	1/1	0.87	0.11	97,97,97,97	0
56	MG	1H	3469	1/1	0.87	0.32	93,93,93,93	0
56	MG	1H	3573	1/1	0.87	0.07	51,51,51,51	0
56	MG	14	3052	1/1	0.87	0.27	78,78,78,78	0
56	MG	14	3009	1/1	0.88	0.20	78,78,78,78	0
56	MG	14	3025	1/1	0.88	0.12	46,46,46,46	0
56	MG	1H	3416	1/1	0.88	0.30	75,75,75,75	0
56	MG	14	3034	1/1	0.88	0.14	63,63,63,63	0
56	MG	1H	3233	1/1	0.88	0.13	85,85,85,85	0
56	MG	14	3373	1/1	0.88	0.09	117,117,117,117	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	1H	3408	1/1	0.88	0.37	60,60,60,60	0
56	MG	1H	3047	1/1	0.88	0.13	60,60,60,60	0
56	MG	42	201	1/1	0.88	0.30	103,103,103,103	0
56	MG	13	1693	1/1	0.88	0.15	82,82,82,82	0
56	MG	1H	3127	1/1	0.88	0.21	81,81,81,81	0
56	MG	1H	3453	1/1	0.88	0.07	94,94,94,94	0
56	MG	14	3176	1/1	0.88	0.24	73,73,73,73	0
56	MG	1H	3023	1/1	0.88	0.34	72,72,72,72	0
56	MG	16	202	1/1	0.88	0.11	77,77,77,77	0
56	MG	14	3310	1/1	0.88	0.11	53,53,53,53	0
56	MG	13	1614	1/1	0.88	0.13	69,69,69,69	0
56	MG	13	1648	1/1	0.88	0.36	77,77,77,77	0
56	MG	14	3411	1/1	0.88	0.07	109,109,109,109	0
56	MG	14	3279	1/1	0.88	0.47	96,96,96,96	0
56	MG	1H	3212	1/1	0.88	0.28	91,91,91,91	0
56	MG	1H	3420	1/1	0.88	0.39	75,75,75,75	0
56	MG	1H	3439	1/1	0.88	0.14	59,59,59,59	0
56	MG	1G	1621	1/1	0.88	0.32	89,89,89,89	0
56	MG	13	1799	1/1	0.88	0.10	93,93,93,93	0
56	MG	14	3403	1/1	0.88	0.11	101,101,101,101	0
56	MG	1H	3343	1/1	0.88	0.15	76,76,76,76	0
56	MG	14	3100	1/1	0.88	0.18	65,65,65,65	0
56	MG	14	3433	1/1	0.88	0.11	87,87,87,87	0
56	MG	14	3096	1/1	0.88	0.31	87,87,87,87	0
56	MG	1H	3151	1/1	0.88	0.25	78,78,78,78	0
56	MG	1H	3410	1/1	0.88	0.47	71,71,71,71	0
56	MG	1H	3290	1/1	0.88	0.40	94,94,94,94	0
56	MG	1H	3026	1/1	0.88	0.25	92,92,92,92	0
56	MG	1H	3192	1/1	0.88	0.28	75,75,75,75	0
56	MG	1H	3516	1/1	0.88	0.09	59,59,59,59	0
56	MG	1G	1619	1/1	0.88	0.18	94,94,94,94	0
56	MG	14	3080	1/1	0.88	0.16	86,86,86,86	0
56	MG	13	1765	1/1	0.88	0.45	129,129,129,129	0
56	MG	13	1669	1/1	0.88	0.22	109,109,109,109	0
56	MG	14	3186	1/1	0.88	0.20	77,77,77,77	0
56	MG	1H	3267	1/1	0.88	0.31	84,84,84,84	0
56	MG	1H	3239	1/1	0.88	0.31	78,78,78,78	0
56	MG	1J	206	1/1	0.88	0.27	68,68,68,68	0
56	MG	14	3135	1/1	0.88	0.11	90,90,90,90	0
56	MG	1H	3272	1/1	0.88	0.15	85,85,85,85	0
56	MG	1G	1712	1/1	0.88	0.08	132,132,132,132	0
56	MG	14	3322	1/1	0.88	0.17	123,123,123,123	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	1H	3090	1/1	0.88	0.19	73,73,73,73	0
56	MG	14	3284	1/1	0.88	0.23	77,77,77,77	0
56	MG	1G	1601	1/1	0.88	0.11	71,71,71,71	0
56	MG	14	3011	1/1	0.88	0.52	70,70,70,70	0
56	MG	1H	3058	1/1	0.88	0.16	69,69,69,69	0
56	MG	1H	3256	1/1	0.88	0.18	85,85,85,85	0
56	MG	1H	3012	1/1	0.88	0.08	40,40,40,40	0
56	MG	14	3190	1/1	0.89	0.23	81,81,81,81	0
56	MG	1H	3075	1/1	0.89	0.21	72,72,72,72	0
56	MG	14	3024	1/1	0.89	0.10	57,57,57,57	0
56	MG	14	3134	1/1	0.89	0.24	81,81,81,81	0
56	MG	1G	1690	1/1	0.89	0.23	75,75,75,75	0
56	MG	14	3321	1/1	0.89	0.14	131,131,131,131	0
56	MG	13	1773	1/1	0.89	0.07	96,96,96,96	0
56	MG	1H	3086	1/1	0.89	0.11	83,83,83,83	0
56	MG	14	3026	1/1	0.89	0.12	65,65,65,65	0
56	MG	13	1671	1/1	0.89	0.44	99,99,99,99	0
56	MG	13	1768	1/1	0.89	0.10	92,92,92,92	0
56	MG	1H	3067	1/1	0.89	0.18	68,68,68,68	0
56	MG	1H	3407	1/1	0.89	0.33	81,81,81,81	0
56	MG	14	3283	1/1	0.89	0.29	84,84,84,84	0
56	MG	1H	3323	1/1	0.89	0.45	69,69,69,69	0
56	MG	14	3008	1/1	0.89	0.33	72,72,72,72	0
56	MG	1H	3092	1/1	0.89	0.21	62,62,62,62	0
56	MG	1H	3374	1/1	0.89	0.26	101,101,101,101	0
56	MG	1H	3582	1/1	0.89	0.06	56,56,56,56	0
56	MG	1H	3313	1/1	0.89	0.65	87,87,87,87	0
56	MG	14	3101	1/1	0.89	0.24	79,79,79,79	0
56	MG	14	3342	1/1	0.89	0.13	51,51,51,51	0
56	MG	13	1688	1/1	0.89	0.29	86,86,86,86	0
56	MG	14	3340	1/1	0.89	0.10	57,57,57,57	0
56	MG	13	1793	1/1	0.89	0.15	114,114,114,114	0
56	MG	1H	3450	1/1	0.89	0.17	84,84,84,84	0
56	MG	1H	3261	1/1	0.89	0.16	92,92,92,92	0
56	MG	1G	1655	1/1	0.89	0.09	121,121,121,121	0
56	MG	13	1629	1/1	0.89	0.12	71,71,71,71	0
56	MG	13	1698	1/1	0.89	2.42	99,99,99,99	0
56	MG	1H	3318	1/1	0.89	0.68	68,68,68,68	0
56	MG	14	3304	1/1	0.89	0.23	103,103,103,103	0
56	MG	1G	1753	1/1	0.89	0.12	109,109,109,109	0
56	MG	1G	1703	1/1	0.89	0.13	87,87,87,87	0
56	MG	8I	201	1/1	0.89	0.58	98,98,98,98	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	1H	3107	1/1	0.89	0.22	63,63,63,63	0
56	MG	1G	1697	1/1	0.89	0.21	106,106,106,106	0
56	MG	1H	3594	1/1	0.89	0.17	95,95,95,95	0
56	MG	1H	3179	1/1	0.89	0.26	93,93,93,93	0
56	MG	1H	3030	1/1	0.89	0.25	75,75,75,75	0
56	MG	1H	3296	1/1	0.89	0.77	68,68,68,68	0
56	MG	1G	1635	1/1	0.89	0.22	106,106,106,106	0
56	MG	14	3067	1/1	0.89	0.13	62,62,62,62	0
56	MG	13	1784	1/1	0.89	0.10	104,104,104,104	0
56	MG	1H	3001	1/1	0.89	0.18	55,55,55,55	0
56	MG	1H	3182	1/1	0.89	0.27	85,85,85,85	0
56	MG	1H	3244	1/1	0.89	0.19	70,70,70,70	0
56	MG	13	1746	1/1	0.89	0.25	96,96,96,96	0
56	MG	1H	3216	1/1	0.89	0.57	81,81,81,81	0
56	MG	13	1723	1/1	0.89	0.22	98,98,98,98	0
56	MG	1H	3288	1/1	0.89	0.79	79,79,79,79	0
56	MG	14	3074	1/1	0.89	0.09	84,84,84,84	0
56	MG	13	1683	1/1	0.89	0.21	99,99,99,99	0
56	MG	13	1766	1/1	0.89	0.14	70,70,70,70	0
56	MG	1G	1650	1/1	0.89	0.09	81,81,81,81	0
56	MG	14	3366	1/1	0.89	0.14	87,87,87,87	0
56	MG	13	1703	1/1	0.89	0.11	93,93,93,93	0
56	MG	16	210	1/1	0.89	0.36	101,101,101,101	0
56	MG	1H	3217	1/1	0.89	0.20	87,87,87,87	0
56	MG	13	1609	1/1	0.89	0.15	83,83,83,83	0
56	MG	14	3410	1/1	0.89	0.12	81,81,81,81	0
56	MG	1H	3414	1/1	0.89	0.15	68,68,68,68	0
56	MG	14	3423	1/1	0.90	0.11	95,95,95,95	0
56	MG	14	3027	1/1	0.90	0.15	61,61,61,61	0
56	MG	14	3272	1/1	0.90	0.34	94,94,94,94	0
56	MG	13	1758	1/1	0.90	0.24	111,111,111,111	0
56	MG	14	3214	1/1	0.90	0.59	90,90,90,90	0
56	MG	13	1704	1/1	0.90	0.17	85,85,85,85	0
56	MG	1H	3565	1/1	0.90	0.08	110,110,110,110	0
56	MG	1H	3140	1/1	0.90	0.30	78,78,78,78	0
56	MG	13	1802	1/1	0.90	0.07	114,114,114,114	0
56	MG	1H	3113	1/1	0.90	0.41	67,67,67,67	0
56	MG	1H	3078	1/1	0.90	0.30	59,59,59,59	0
56	MG	14	3270	1/1	0.90	0.20	70,70,70,70	0
56	MG	1H	3214	1/1	0.90	0.40	93,93,93,93	0
56	MG	13	1694	1/1	0.90	0.12	96,96,96,96	0
56	MG	14	3155	1/1	0.90	0.23	65,65,65,65	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	13	1636	1/1	0.90	0.19	85,85,85,85	0
56	MG	1H	3020	1/1	0.90	0.10	56,56,56,56	0
56	MG	1H	3043	1/1	0.90	0.12	48,48,48,48	0
56	MG	14	3219	1/1	0.90	0.14	100,100,100,100	0
56	MG	14	3264	1/1	0.90	0.29	82,82,82,82	0
56	MG	1H	3087	1/1	0.90	0.17	54,54,54,54	0
56	MG	1G	1657	1/1	0.90	0.20	117,117,117,117	0
56	MG	14	3380	1/1	0.90	0.14	92,92,92,92	0
56	MG	13	1762	1/1	0.90	0.21	128,128,128,128	0
56	MG	1G	1706	1/1	0.90	0.12	95,95,95,95	0
56	MG	1G	1742	1/1	0.90	0.09	131,131,131,131	0
56	MG	14	3388	1/1	0.90	0.18	87,87,87,87	0
56	MG	13	1767	1/1	0.90	0.14	61,61,61,61	0
56	MG	1G	1714	1/1	0.90	0.05	123,123,123,123	0
56	MG	14	3128	1/1	0.90	0.26	82,82,82,82	0
56	MG	13	1642	1/1	0.90	0.20	66,66,66,66	0
56	MG	14	3364	1/1	0.90	0.10	108,108,108,108	0
56	MG	1G	1633	1/1	0.90	0.31	94,94,94,94	0
56	MG	14	3307	1/1	0.90	0.12	89,89,89,89	0
56	MG	14	3393	1/1	0.90	0.13	67,67,67,67	0
56	MG	1H	3079	1/1	0.90	0.27	59,59,59,59	0
56	MG	1H	3589	1/1	0.90	0.14	60,60,60,60	0
56	MG	13	1728	1/1	0.90	0.26	97,97,97,97	0
56	MG	1H	3373	1/1	0.90	0.17	84,84,84,84	0
56	MG	1H	3204	1/1	0.90	0.34	92,92,92,92	0
56	MG	1H	3032	1/1	0.90	0.45	57,57,57,57	0
56	MG	1H	3382	1/1	0.90	0.22	73,73,73,73	0
56	MG	14	3149	1/1	0.90	0.15	74,74,74,74	0
56	MG	1G	1624	1/1	0.90	0.25	109,109,109,109	0
56	MG	13	1736	1/1	0.90	0.35	96,96,96,96	0
56	MG	14	3267	1/1	0.90	0.34	77,77,77,77	0
56	MG	1H	3468	1/1	0.90	0.18	92,92,92,92	0
56	MG	14	3308	1/1	0.90	0.13	80,80,80,80	0
56	MG	13	1624	1/1	0.90	0.10	102,102,102,102	0
56	MG	1H	3477	1/1	0.90	0.29	90,90,90,90	0
56	MG	1H	3581	1/1	0.90	0.12	87,87,87,87	0
56	MG	14	3324	1/1	0.90	0.13	50,50,50,50	0
56	MG	13	1709	1/1	0.90	0.24	73,73,73,73	0
56	MG	1G	1606	1/1	0.90	0.12	97,97,97,97	0
56	MG	1H	3009	1/1	0.90	0.20	66,66,66,66	0
56	MG	1H	3168	1/1	0.90	0.09	84,84,84,84	0
56	MG	14	3352	1/1	0.90	0.21	90,90,90,90	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	1G	1617	1/1	0.90	0.05	92,92,92,92	0
56	MG	14	3289	1/1	0.90	0.13	79,79,79,79	0
56	MG	14	3035	1/1	0.91	0.16	67,67,67,67	0
56	MG	16	205	1/1	0.91	0.17	70,70,70,70	0
56	MG	14	3126	1/1	0.91	0.24	102,102,102,102	0
56	MG	1H	3084	1/1	0.91	0.22	72,72,72,72	0
56	MG	1H	3173	1/1	0.91	0.14	67,67,67,67	0
56	MG	1G	1707	1/1	0.91	0.08	92,92,92,92	0
56	MG	1H	3082	1/1	0.91	0.15	76,76,76,76	0
56	MG	14	3311	1/1	0.91	0.10	105,105,105,105	0
56	MG	1H	3536	1/1	0.91	0.10	62,62,62,62	0
56	MG	1H	3592	1/1	0.91	0.09	96,96,96,96	0
56	MG	1G	1648	1/1	0.91	0.24	85,85,85,85	0
56	MG	1H	3351	1/1	0.91	0.26	68,68,68,68	0
56	MG	13	1630	1/1	0.91	0.12	74,74,74,74	0
56	MG	1G	1613	1/1	0.91	0.09	88,88,88,88	0
56	MG	1H	3543	1/1	0.91	0.14	59,59,59,59	0
56	MG	13	1672	1/1	0.91	0.14	80,80,80,80	0
56	MG	13	1660	1/1	0.91	0.11	83,83,83,83	0
56	MG	1H	3413	1/1	0.91	0.19	81,81,81,81	0
56	MG	1H	3412	1/1	0.91	0.17	86,86,86,86	0
56	MG	1H	3116	1/1	0.91	0.28	71,71,71,71	0
56	MG	14	3038	1/1	0.91	0.13	63,63,63,63	0
56	MG	1H	3101	1/1	0.91	0.38	91,91,91,91	0
56	MG	14	3266	1/1	0.91	0.26	85,85,85,85	0
56	MG	1H	3077	1/1	0.91	0.45	62,62,62,62	0
56	MG	13	1745	1/1	0.91	0.20	87,87,87,87	0
56	MG	1H	3163	1/1	0.91	0.28	74,74,74,74	0
56	MG	1H	3076	1/1	0.91	0.16	88,88,88,88	0
56	MG	14	3055	1/1	0.91	0.27	89,89,89,89	0
56	MG	45	201	1/1	0.91	0.06	95,95,95,95	0
56	MG	1H	3452	1/1	0.91	0.04	81,81,81,81	0
56	MG	13	1658	1/1	0.91	0.19	96,96,96,96	0
56	MG	1H	3309	1/1	0.91	0.47	76,76,76,76	0
56	MG	14	3042	1/1	0.91	0.34	82,82,82,82	0
56	MG	14	3419	1/1	0.91	0.06	84,84,84,84	0
56	MG	1G	1732	1/1	0.91	0.08	102,102,102,102	0
56	MG	1G	1747	1/1	0.91	0.12	95,95,95,95	0
56	MG	13	1720	1/1	0.91	0.13	97,97,97,97	0
56	MG	13	1749	1/1	0.91	0.06	92,92,92,92	0
56	MG	1H	3618	1/1	0.91	0.36	104,104,104,104	0
56	MG	1H	3279	1/1	0.91	0.15	93,93,93,93	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	14	3133	1/1	0.91	0.28	78,78,78,78	0
56	MG	1H	3285	1/1	0.91	1.01	85,85,85,85	0
56	MG	1H	3535	1/1	0.91	0.09	80,80,80,80	0
56	MG	14	3418	1/1	0.91	0.12	99,99,99,99	0
56	MG	14	3010	1/1	0.91	0.16	68,68,68,68	0
56	MG	1H	3580	1/1	0.91	0.33	77,77,77,77	0
56	MG	14	3173	1/1	0.91	0.11	77,77,77,77	0
56	MG	1H	3471	1/1	0.91	0.36	91,91,91,91	0
56	MG	1H	3230	1/1	0.91	0.18	96,96,96,96	0
56	MG	1H	3170	1/1	0.91	0.17	73,73,73,73	0
56	MG	14	3222	1/1	0.91	0.33	94,94,94,94	0
56	MG	13	1657	1/1	0.91	0.22	101,101,101,101	0
56	MG	1H	3364	1/1	0.91	0.12	87,87,87,87	0
56	MG	1G	1705	1/1	0.91	0.10	84,84,84,84	0
56	MG	41	201	1/1	0.91	0.12	69,69,69,69	0
56	MG	13	1681	1/1	0.91	0.12	98,98,98,98	0
56	MG	14	3220	1/1	0.91	0.13	95,95,95,95	0
56	MG	1G	1728	1/1	0.91	0.11	96,96,96,96	0
56	MG	1H	3409	1/1	0.91	0.53	75,75,75,75	0
56	MG	1H	3354	1/1	0.91	0.09	81,81,81,81	0
56	MG	1H	3158	1/1	0.91	0.17	81,81,81,81	0
56	MG	14	3118	1/1	0.91	0.07	66,66,66,66	0
56	MG	14	3353	1/1	0.91	0.08	64,64,64,64	0
56	MG	9A	101	1/1	0.91	0.07	115,115,115,115	0
56	MG	13	1769	1/1	0.91	0.11	82,82,82,82	0
56	MG	13	1625	1/1	0.91	0.25	75,75,75,75	0
56	MG	14	3039	1/1	0.91	0.15	61,61,61,61	0
56	MG	88	201	1/1	0.91	0.26	79,79,79,79	0
56	MG	1H	3415	1/1	0.91	0.31	77,77,77,77	0
56	MG	14	3032	1/1	0.91	0.15	73,73,73,73	0
56	MG	1H	3068	1/1	0.91	0.21	65,65,65,65	0
56	MG	1G	1717	1/1	0.91	0.07	129,129,129,129	0
56	MG	1H	3220	1/1	0.91	0.29	79,79,79,79	0
56	MG	1H	3367	1/1	0.91	0.15	97,97,97,97	0
56	MG	1H	3315	1/1	0.91	0.26	101,101,101,101	0
56	MG	1H	3200	1/1	0.91	0.18	79,79,79,79	0
56	MG	1H	3476	1/1	0.91	0.08	92,92,92,92	0
56	MG	4A	201	1/1	0.91	0.10	116,116,116,116	0
56	MG	1H	3143	1/1	0.92	0.23	78,78,78,78	0
56	MG	14	3044	1/1	0.92	0.09	71,71,71,71	0
56	MG	14	3139	1/1	0.92	0.18	69,69,69,69	0
56	MG	1G	1694	1/1	0.92	0.15	102,102,102,102	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	1H	3310	1/1	0.92	0.15	82,82,82,82	0
56	MG	14	3170	1/1	0.92	0.23	105,105,105,105	0
56	MG	1G	1660	1/1	0.92	0.15	91,91,91,91	0
56	MG	1H	3534	1/1	0.92	0.11	51,51,51,51	0
56	MG	1H	3103	1/1	0.92	0.39	64,64,64,64	0
56	MG	1H	3376	1/1	0.92	0.26	113,113,113,113	0
56	MG	1H	3488	1/1	0.92	0.18	53,53,53,53	0
56	MG	14	3019	1/1	0.92	0.14	70,70,70,70	0
56	MG	14	3141	1/1	0.92	0.32	74,74,74,74	0
56	MG	14	3003	1/1	0.92	0.13	47,47,47,47	0
56	MG	13	1743	1/1	0.92	0.20	91,91,91,91	0
56	MG	13	1787	1/1	0.92	0.18	109,109,109,109	0
56	MG	1H	3131	1/1	0.92	0.26	65,65,65,65	0
56	MG	14	3172	1/1	0.92	0.18	77,77,77,77	0
56	MG	1H	3558	1/1	0.92	0.09	100,100,100,100	0
56	MG	14	3288	1/1	0.92	0.32	94,94,94,94	0
56	MG	1H	3144	1/1	0.92	0.16	57,57,57,57	0
56	MG	14	3358	1/1	0.92	0.07	80,80,80,80	0
56	MG	14	3345	1/1	0.92	0.10	89,89,89,89	0
56	MG	1H	3393	1/1	0.92	0.12	65,65,65,65	0
56	MG	1H	3052	1/1	0.92	0.10	41,41,41,41	0
56	MG	14	3070	1/1	0.92	0.14	72,72,72,72	0
56	MG	14	3332	1/1	0.92	0.09	57,57,57,57	0
56	MG	1H	3326	1/1	0.92	0.18	67,67,67,67	0
56	MG	13	1687	1/1	0.92	0.26	82,82,82,82	0
56	MG	1H	3319	1/1	0.92	0.15	85,85,85,85	0
56	MG	1H	3221	1/1	0.92	0.34	89,89,89,89	0
56	MG	1H	3287	1/1	0.92	0.79	80,80,80,80	0
56	MG	1H	3339	1/1	0.92	0.27	74,74,74,74	0
56	MG	1G	1628	1/1	0.92	0.31	89,89,89,89	0
56	MG	1H	3493	1/1	0.92	0.15	48,48,48,48	0
56	MG	1H	3401	1/1	0.92	0.34	77,77,77,77	0
56	MG	14	3349	1/1	0.92	0.09	60,60,60,60	0
56	MG	13	1735	1/1	0.92	0.33	85,85,85,85	0
56	MG	1G	1634	1/1	0.92	0.15	89,89,89,89	0
56	MG	13	1640	1/1	0.92	0.16	65,65,65,65	0
56	MG	1G	1731	1/1	0.92	0.08	99,99,99,99	0
56	MG	14	3425	1/1	0.92	0.17	95,95,95,95	0
56	MG	14	3036	1/1	0.92	0.34	71,71,71,71	0
56	MG	14	3145	1/1	0.92	0.21	88,88,88,88	0
56	MG	1G	1608	1/1	0.92	0.17	108,108,108,108	0
56	MG	14	3007	1/1	0.92	0.10	61,61,61,61	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	14	3161	1/1	0.92	0.20	66,66,66,66	0
56	MG	14	3256	1/1	0.92	0.13	75,75,75,75	0
56	MG	1H	3405	1/1	0.92	0.24	80,80,80,80	0
56	MG	1G	1679	1/1	0.92	0.16	74,74,74,74	0
56	MG	1H	3593	1/1	0.92	0.21	61,61,61,61	0
56	MG	14	3132	1/1	0.92	0.19	58,58,58,58	0
56	MG	14	3004	1/1	0.92	0.12	73,73,73,73	0
56	MG	1H	3059	1/1	0.92	0.17	60,60,60,60	0
56	MG	1H	3098	1/1	0.92	0.18	66,66,66,66	0
56	MG	1H	3557	1/1	0.92	0.09	59,59,59,59	0
56	MG	1G	1755	1/1	0.92	0.05	119,119,119,119	0
56	MG	1B	101	1/1	0.92	0.17	92,92,92,92	0
56	MG	1H	3184	1/1	0.92	0.30	79,79,79,79	0
56	MG	14	3221	1/1	0.92	0.10	88,88,88,88	0
56	MG	13	1664	1/1	0.92	0.41	91,91,91,91	0
56	MG	2A	201	1/1	0.92	0.11	85,85,85,85	0
56	MG	14	3164	1/1	0.92	0.36	105,105,105,105	0
56	MG	14	3263	1/1	0.92	0.41	81,81,81,81	0
56	MG	1H	3480	1/1	0.92	0.08	113,113,113,113	0
56	MG	1H	3366	1/1	0.92	0.08	89,89,89,89	0
56	MG	1G	1607	1/1	0.92	0.19	104,104,104,104	0
56	MG	14	3261	1/1	0.92	0.40	93,93,93,93	0
56	MG	1H	3570	1/1	0.92	0.11	54,54,54,54	0
56	MG	14	3212	1/1	0.92	0.43	91,91,91,91	0
56	MG	1H	3352	1/1	0.92	0.69	68,68,68,68	0
56	MG	14	3185	1/1	0.92	0.31	78,78,78,78	0
56	MG	1H	3157	1/1	0.92	0.24	78,78,78,78	0
56	MG	1H	3066	1/1	0.92	0.20	66,66,66,66	0
56	MG	14	3362	1/1	0.92	0.08	96,96,96,96	0
56	MG	14	3056	1/1	0.92	0.09	80,80,80,80	0
56	MG	1H	3616	1/1	0.92	0.35	73,73,73,73	0
56	MG	1H	3620	1/1	0.92	0.05	73,73,73,73	0
56	MG	1H	3105	1/1	0.92	0.15	54,54,54,54	0
56	MG	13	1634	1/1	0.93	0.19	118,118,118,118	0
56	MG	1G	1751	1/1	0.93	0.13	95,95,95,95	0
56	MG	14	3066	1/1	0.93	0.24	67,67,67,67	0
56	MG	13	1643	1/1	0.93	0.29	78,78,78,78	0
56	MG	1G	1733	1/1	0.93	0.09	121,121,121,121	0
56	MG	1H	3156	1/1	0.93	0.40	69,69,69,69	0
56	MG	14	3354	1/1	0.93	0.06	68,68,68,68	0
56	MG	1G	1615	1/1	0.93	0.32	87,87,87,87	0
56	MG	13	1708	1/1	0.93	0.22	76,76,76,76	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	1G	1713	1/1	0.93	0.08	119,119,119,119	0
56	MG	1G	1681	1/1	0.93	0.22	89,89,89,89	0
56	MG	1H	3506	1/1	0.93	0.15	58,58,58,58	0
56	MG	1H	3327	1/1	0.93	0.30	65,65,65,65	0
56	MG	14	3151	1/1	0.93	0.34	88,88,88,88	0
56	MG	1H	3011	1/1	0.93	0.12	46,46,46,46	0
56	MG	1H	3302	1/1	0.93	0.07	98,98,98,98	0
56	MG	14	3313	1/1	0.93	0.05	82,82,82,82	0
56	MG	1G	1662	1/1	0.93	0.30	96,96,96,96	0
56	MG	14	3033	1/1	0.93	0.13	86,86,86,86	0
56	MG	13	1750	1/1	0.93	0.09	122,122,122,122	0
56	MG	1H	3199	1/1	0.93	0.08	116,116,116,116	0
56	MG	14	3339	1/1	0.93	0.08	61,61,61,61	0
56	MG	1H	3556	1/1	0.93	0.11	58,58,58,58	0
56	MG	1H	3513	1/1	0.93	0.23	83,83,83,83	0
56	MG	1G	1610	1/1	0.93	0.22	83,83,83,83	0
56	MG	13	1677	1/1	0.93	0.26	94,94,94,94	0
56	MG	13	1795	1/1	0.93	0.15	100,100,100,100	0
56	MG	1H	3380	1/1	0.93	0.26	66,66,66,66	0
56	MG	13	1646	1/1	0.93	0.19	58,58,58,58	0
56	MG	1H	3501	1/1	0.93	0.12	57,57,57,57	0
56	MG	1H	3371	1/1	0.93	0.76	72,72,72,72	0
56	MG	1H	3478	1/1	0.93	0.17	68,68,68,68	0
56	MG	13	1800	1/1	0.93	0.20	118,118,118,118	0
56	MG	1H	3467	1/1	0.93	0.14	102,102,102,102	0
56	MG	1H	3540	1/1	0.93	0.05	85,85,85,85	0
56	MG	1H	3601	1/1	0.93	0.09	84,84,84,84	0
56	MG	14	3379	1/1	0.93	0.06	66,66,66,66	0
56	MG	1H	3091	1/1	0.93	0.20	68,68,68,68	0
56	MG	1H	3061	1/1	0.93	0.20	66,66,66,66	0
56	MG	13	1612	1/1	0.93	0.16	71,71,71,71	0
56	MG	1H	3338	1/1	0.93	0.16	83,83,83,83	0
56	MG	1H	3521	1/1	0.93	0.13	66,66,66,66	0
56	MG	13	1616	1/1	0.93	0.38	79,79,79,79	0
56	MG	1H	3561	1/1	0.93	0.12	78,78,78,78	0
56	MG	1H	3048	1/1	0.93	0.27	67,67,67,67	0
56	MG	1G	1730	1/1	0.93	0.08	72,72,72,72	0
56	MG	13	1713	1/1	0.93	0.22	82,82,82,82	0
56	MG	1H	3529	1/1	0.93	0.12	49,49,49,49	0
56	MG	14	3406	1/1	0.93	0.07	60,60,60,60	0
56	MG	1H	3519	1/1	0.93	0.25	73,73,73,73	0
56	MG	14	3346	1/1	0.93	0.07	60,60,60,60	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	13	1739	1/1	0.93	0.26	74,74,74,74	0
56	MG	14	3223	1/1	0.93	0.08	93,93,93,93	0
56	MG	1H	3003	1/1	0.93	0.17	56,56,56,56	0
56	MG	14	3265	1/1	0.93	0.16	83,83,83,83	0
56	MG	14	3195	1/1	0.93	0.14	84,84,84,84	0
56	MG	1H	3368	1/1	0.93	0.22	106,106,106,106	0
56	MG	1J	201	1/1	0.93	0.30	95,95,95,95	0
56	MG	1H	3363	1/1	0.93	0.22	83,83,83,83	0
56	MG	1G	1691	1/1	0.93	0.33	106,106,106,106	0
56	MG	13	1780	1/1	0.93	0.07	106,106,106,106	0
56	MG	1H	3169	1/1	0.93	0.22	56,56,56,56	0
56	MG	1J	203	1/1	0.93	0.10	98,98,98,98	0
56	MG	1H	3133	1/1	0.93	0.20	67,67,67,67	0
56	MG	13	1620	1/1	0.93	0.40	69,69,69,69	0
56	MG	14	3378	1/1	0.93	0.11	69,69,69,69	0
56	MG	14	3020	1/1	0.93	0.27	55,55,55,55	0
56	MG	1H	3583	1/1	0.93	0.17	52,52,52,52	0
56	MG	14	3383	1/1	0.93	0.09	62,62,62,62	0
56	MG	1H	3505	1/1	0.93	0.12	51,51,51,51	0
56	MG	1H	3496	1/1	0.93	0.12	66,66,66,66	0
56	MG	1H	3129	1/1	0.93	0.23	77,77,77,77	0
56	MG	1H	3355	1/1	0.93	0.36	62,62,62,62	0
56	MG	14	3192	1/1	0.93	0.09	77,77,77,77	0
56	MG	1H	3154	1/1	0.93	0.17	74,74,74,74	0
56	MG	1H	3622	1/1	0.93	0.09	76,76,76,76	0
56	MG	14	3251	1/1	0.93	0.24	77,77,77,77	0
56	MG	1H	3460	1/1	0.93	0.16	94,94,94,94	0
56	MG	14	3083	1/1	0.93	0.15	73,73,73,73	0
56	MG	1H	3508	1/1	0.93	0.15	74,74,74,74	0
56	MG	1H	3064	1/1	0.93	0.08	59,59,59,59	0
56	MG	13	1654	1/1	0.93	0.32	86,86,86,86	0
56	MG	13	1760	1/1	0.93	0.15	127,127,127,127	0
56	MG	1H	3171	1/1	0.94	0.24	90,90,90,90	0
56	MG	1H	3262	1/1	0.94	0.65	73,73,73,73	0
56	MG	14	3404	1/1	0.94	0.16	85,85,85,85	0
56	MG	13	1740	1/1	0.94	0.47	76,76,76,76	0
56	MG	1H	3161	1/1	0.94	0.23	76,76,76,76	0
56	MG	13	1655	1/1	0.94	0.25	94,94,94,94	0
56	MG	14	3058	1/1	0.94	0.10	78,78,78,78	0
56	MG	1J	204	1/1	0.94	0.12	95,95,95,95	0
56	MG	1H	3502	1/1	0.94	0.15	49,49,49,49	0
56	MG	1H	3512	1/1	0.94	0.13	65,65,65,65	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	1H	3577	1/1	0.94	0.10	49,49,49,49	0
56	MG	1H	3399	1/1	0.94	0.31	61,61,61,61	0
56	MG	13	1618	1/1	0.94	0.12	97,97,97,97	0
56	MG	14	3016	1/1	0.94	0.17	51,51,51,51	0
56	MG	16	212	1/1	0.94	0.37	65,65,65,65	0
56	MG	13	1615	1/1	0.94	0.23	103,103,103,103	0
56	MG	14	3398	1/1	0.94	0.09	81,81,81,81	0
56	MG	1G	1754	1/1	0.94	0.08	104,104,104,104	0
56	MG	13	1661	1/1	0.94	0.20	75,75,75,75	0
56	MG	13	1803	1/1	0.94	0.06	97,97,97,97	0
56	MG	14	3169	1/1	0.94	1.10	73,73,73,73	0
56	MG	1H	3432	1/1	0.94	0.14	83,83,83,83	0
56	MG	1H	3423	1/1	0.94	0.33	74,74,74,74	0
56	MG	14	3390	1/1	0.94	0.12	66,66,66,66	0
56	MG	14	3159	1/1	0.94	0.20	66,66,66,66	0
56	MG	13	1717	1/1	0.94	0.18	98,98,98,98	0
56	MG	1H	3406	1/1	0.94	0.29	91,91,91,91	0
56	MG	14	3236	1/1	0.94	0.20	69,69,69,69	0
56	MG	1H	3587	1/1	0.94	0.13	51,51,51,51	0
56	MG	1H	3586	1/1	0.94	0.08	53,53,53,53	0
56	MG	1H	3108	1/1	0.94	0.29	87,87,87,87	0
56	MG	14	3382	1/1	0.94	0.06	88,88,88,88	0
56	MG	1H	3527	1/1	0.94	0.17	50,50,50,50	0
56	MG	Q8	101	1/1	0.94	0.19	68,68,68,68	0
56	MG	14	3207	1/1	0.94	0.18	67,67,67,67	0
56	MG	1H	3322	1/1	0.94	0.09	94,94,94,94	0
56	MG	14	3022	1/1	0.94	0.10	78,78,78,78	0
56	MG	14	3359	1/1	0.94	0.09	105,105,105,105	0
56	MG	14	3153	1/1	0.94	0.18	90,90,90,90	0
56	MG	14	3031	1/1	0.94	0.18	63,63,63,63	0
56	MG	1G	1689	1/1	0.94	0.31	81,81,81,81	0
56	MG	1H	3560	1/1	0.94	0.12	84,84,84,84	0
56	MG	1H	3286	1/1	0.94	1.15	68,68,68,68	0
56	MG	1H	3245	1/1	0.94	0.23	57,57,57,57	0
56	MG	1H	3491	1/1	0.94	0.16	57,57,57,57	0
56	MG	1H	3106	1/1	0.94	0.17	77,77,77,77	0
56	MG	14	3422	1/1	0.94	0.14	72,72,72,72	0
56	MG	1G	1614	1/1	0.94	0.12	71,71,71,71	0
56	MG	14	3333	1/1	0.94	0.10	80,80,80,80	0
56	MG	1H	3381	1/1	0.94	0.06	97,97,97,97	0
56	MG	14	3408	1/1	0.94	0.14	91,91,91,91	0
56	MG	1H	3585	1/1	0.94	0.19	95,95,95,95	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	1H	3613	1/1	0.94	0.09	78,78,78,78	0
56	MG	14	3175	1/1	0.94	0.11	70,70,70,70	0
56	MG	1H	3074	1/1	0.94	0.10	57,57,57,57	0
56	MG	14	3413	1/1	0.94	0.04	93,93,93,93	0
56	MG	1H	3037	1/1	0.94	0.14	57,57,57,57	0
56	MG	3E	301	1/1	0.94	0.11	121,121,121,121	0
56	MG	1G	1719	1/1	0.94	0.11	112,112,112,112	0
56	MG	13	1679	1/1	0.94	0.36	83,83,83,83	0
56	MG	1H	3584	1/1	0.94	0.06	58,58,58,58	0
56	MG	14	3021	1/1	0.94	0.19	47,47,47,47	0
56	MG	1H	3454	1/1	0.94	0.14	93,93,93,93	0
56	MG	1H	3257	1/1	0.94	0.27	82,82,82,82	0
56	MG	1G	1668	1/1	0.94	0.30	106,106,106,106	0
56	MG	1H	3615	1/1	0.94	0.06	108,108,108,108	0
56	MG	1H	3559	1/1	0.94	0.10	73,73,73,73	0
56	MG	1G	1700	1/1	0.94	0.28	113,113,113,113	0
56	MG	1H	3431	1/1	0.94	0.13	54,54,54,54	0
56	MG	14	3363	1/1	0.94	0.04	98,98,98,98	0
56	MG	1H	3022	1/1	0.94	0.16	51,51,51,51	0
56	MG	1H	3369	1/1	0.94	0.81	95,95,95,95	0
56	MG	1H	3017	1/1	0.94	0.18	51,51,51,51	0
56	MG	14	3431	1/1	0.94	0.12	104,104,104,104	0
56	MG	1H	3015	1/1	0.94	0.20	47,47,47,47	0
56	MG	13	1602	1/1	0.94	0.18	59,59,59,59	0
56	MG	1H	3538	1/1	0.94	0.10	46,46,46,46	0
56	MG	13	1633	1/1	0.94	0.23	82,82,82,82	0
56	MG	1H	3150	1/1	0.94	0.17	88,88,88,88	0
56	MG	16	208	1/1	0.94	0.30	95,95,95,95	0
56	MG	14	3146	1/1	0.94	0.27	83,83,83,83	0
56	MG	13	1781	1/1	0.94	0.07	97,97,97,97	0
56	MG	14	3412	1/1	0.94	0.04	102,102,102,102	0
56	MG	1G	1622	1/1	0.94	0.23	87,87,87,87	0
56	MG	14	3204	1/1	0.94	0.24	76,76,76,76	0
56	MG	1H	3357	1/1	0.94	0.30	66,66,66,66	0
56	MG	13	1732	1/1	0.94	0.15	65,65,65,65	0
56	MG	13	1754	1/1	0.94	0.25	108,108,108,108	0
56	MG	1G	1629	1/1	0.94	0.36	84,84,84,84	0
56	MG	1H	3225	1/1	0.94	0.16	76,76,76,76	0
56	MG	1H	3008	1/1	0.94	0.11	47,47,47,47	0
56	MG	1H	3274	1/1	0.94	0.29	79,79,79,79	0
56	MG	1H	3125	1/1	0.94	0.16	52,52,52,52	0
56	MG	13	1604	1/1	0.94	0.08	77,77,77,77	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	14	3237	1/1	0.94	0.28	81,81,81,81	0
56	MG	14	3241	1/1	0.94	0.18	59,59,59,59	0
56	MG	14	3417	1/1	0.94	0.12	80,80,80,80	0
56	MG	1H	3018	1/1	0.94	0.17	49,49,49,49	0
56	MG	1H	3400	1/1	0.94	0.29	48,48,48,48	0
56	MG	14	3123	1/1	0.94	0.19	86,86,86,86	0
56	MG	1H	3224	1/1	0.94	0.32	85,85,85,85	0
56	MG	14	3050	1/1	0.94	0.09	62,62,62,62	0
56	MG	14	3341	1/1	0.94	0.11	46,46,46,46	0
56	MG	1H	3013	1/1	0.94	0.19	42,42,42,42	0
56	MG	I8	101	1/1	0.94	0.20	83,83,83,83	0
56	MG	1H	3042	1/1	0.94	0.35	79,79,79,79	0
56	MG	13	1715	1/1	0.94	0.28	102,102,102,102	0
56	MG	1H	3344	1/1	0.94	0.22	89,89,89,89	0
56	MG	1H	3226	1/1	0.94	0.13	77,77,77,77	0
56	MG	1H	3365	1/1	0.94	0.18	83,83,83,83	0
56	MG	14	3314	1/1	0.94	0.12	126,126,126,126	0
56	MG	1G	1692	1/1	0.94	0.35	87,87,87,87	0
56	MG	1H	3532	1/1	0.94	0.14	85,85,85,85	0
56	MG	14	3048	1/1	0.95	0.29	66,66,66,66	0
56	MG	16	203	1/1	0.95	0.12	85,85,85,85	0
56	MG	13	1796	1/1	0.95	0.08	79,79,79,79	0
56	MG	1H	3475	1/1	0.95	0.19	58,58,58,58	0
56	MG	14	3107	1/1	0.95	0.19	68,68,68,68	0
56	MG	14	3335	1/1	0.95	0.12	57,57,57,57	0
56	MG	14	3108	1/1	0.95	0.16	81,81,81,81	0
56	MG	1G	1688	1/1	0.95	0.19	89,89,89,89	0
56	MG	29	303	1/1	0.95	0.17	64,64,64,64	0
56	MG	14	3049	1/1	0.95	0.10	89,89,89,89	0
56	MG	1H	3159	1/1	0.95	0.21	66,66,66,66	0
56	MG	13	1738	1/1	0.95	0.21	96,96,96,96	0
56	MG	1H	3181	1/1	0.95	0.67	71,71,71,71	0
56	MG	1H	3600	1/1	0.95	0.10	84,84,84,84	0
56	MG	14	3232	1/1	0.95	0.17	66,66,66,66	0
56	MG	1G	1744	1/1	0.95	0.17	101,101,101,101	0
56	MG	1H	3563	1/1	0.95	0.06	81,81,81,81	0
56	MG	14	3334	1/1	0.95	0.07	51,51,51,51	0
56	MG	1H	3443	1/1	0.95	0.18	74,74,74,74	0
56	MG	1G	1686	1/1	0.95	0.32	69,69,69,69	0
56	MG	13	1733	1/1	0.95	0.11	64,64,64,64	0
56	MG	1G	1623	1/1	0.95	0.18	86,86,86,86	0
56	MG	13	1649	1/1	0.95	0.23	76,76,76,76	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	14	3387	1/1	0.95	0.11	61,61,61,61	0
56	MG	14	3177	1/1	0.95	0.14	92,92,92,92	0
56	MG	14	3015	1/1	0.95	0.06	51,51,51,51	0
56	MG	1G	1711	1/1	0.95	0.11	109,109,109,109	0
56	MG	1H	3348	1/1	0.95	0.18	87,87,87,87	0
56	MG	14	3174	1/1	0.95	0.25	81,81,81,81	0
56	MG	1H	3149	1/1	0.95	0.24	64,64,64,64	0
56	MG	14	3089	1/1	0.95	0.20	72,72,72,72	0
56	MG	14	3136	1/1	0.95	0.24	58,58,58,58	0
56	MG	13	1791	1/1	0.95	0.09	85,85,85,85	0
56	MG	13	1638	1/1	0.95	0.34	85,85,85,85	0
56	MG	1G	1636	1/1	0.95	0.26	99,99,99,99	0
56	MG	21	303	1/1	0.95	0.23	51,51,51,51	0
56	MG	14	3148	1/1	0.95	0.30	84,84,84,84	0
56	MG	14	3248	1/1	0.95	0.20	80,80,80,80	0
56	MG	14	3014	1/1	0.95	0.08	50,50,50,50	0
56	MG	1H	3474	1/1	0.95	0.05	83,83,83,83	0
56	MG	13	1755	1/1	0.95	0.06	94,94,94,94	0
56	MG	1H	3255	1/1	0.95	0.22	75,75,75,75	0
56	MG	1H	3152	1/1	0.95	0.26	75,75,75,75	0
56	MG	1H	3411	1/1	0.95	0.17	71,71,71,71	0
56	MG	1H	3619	1/1	0.95	0.08	55,55,55,55	0
56	MG	13	1632	1/1	0.95	0.30	86,86,86,86	0
56	MG	1H	3325	1/1	0.95	0.09	90,90,90,90	0
56	MG	1H	3511	1/1	0.95	0.13	42,42,42,42	0
56	MG	13	1775	1/1	0.95	0.05	68,68,68,68	0
56	MG	1H	3375	1/1	0.95	0.17	70,70,70,70	0
56	MG	1H	3115	1/1	0.95	0.12	69,69,69,69	0
56	MG	13	1701	1/1	0.95	0.88	95,95,95,95	0
56	MG	1H	3253	1/1	0.95	0.21	72,72,72,72	0
56	MG	13	1647	1/1	0.95	0.13	97,97,97,97	0
56	MG	13	1719	1/1	0.95	0.14	106,106,106,106	0
56	MG	1H	3234	1/1	0.95	0.12	67,67,67,67	0
56	MG	1H	3088	1/1	0.95	0.10	62,62,62,62	0
56	MG	1H	3069	1/1	0.95	0.21	80,80,80,80	0
56	MG	1H	3485	1/1	0.95	0.11	55,55,55,55	0
56	MG	1H	3007	1/1	0.95	0.07	60,60,60,60	0
56	MG	14	3356	1/1	0.95	0.13	81,81,81,81	0
56	MG	16	201	1/1	0.95	0.29	79,79,79,79	0
56	MG	1H	3243	1/1	0.95	0.20	60,60,60,60	0
56	MG	14	3227	1/1	0.95	0.12	75,75,75,75	0
56	MG	14	3269	1/1	0.95	0.21	80,80,80,80	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	1H	3504	1/1	0.95	0.10	56,56,56,56	0
56	MG	1G	1749	1/1	0.95	0.08	114,114,114,114	0
56	MG	1H	3433	1/1	0.95	0.15	51,51,51,51	0
56	MG	1G	1644	1/1	0.95	0.17	100,100,100,100	0
56	MG	14	3182	1/1	0.95	0.10	91,91,91,91	0
56	MG	E5	101	1/1	0.95	0.18	67,67,67,67	0
56	MG	1G	1602	1/1	0.95	0.11	83,83,83,83	0
56	MG	13	1731	1/1	0.95	0.30	75,75,75,75	0
56	MG	14	3395	1/1	0.95	0.10	89,89,89,89	0
56	MG	13	1652	1/1	0.95	0.16	75,75,75,75	0
56	MG	14	3196	1/1	0.95	0.13	78,78,78,78	0
56	MG	1H	3208	1/1	0.95	0.29	86,86,86,86	0
56	MG	14	3428	1/1	0.95	0.08	81,81,81,81	0
56	MG	13	1626	1/1	0.95	0.05	78,78,78,78	0
56	MG	1H	3321	1/1	0.95	0.07	99,99,99,99	0
56	MG	1G	1618	1/1	0.95	0.11	74,74,74,74	0
56	MG	13	1785	1/1	0.95	0.25	105,105,105,105	0
56	MG	14	3131	1/1	0.95	0.38	78,78,78,78	0
56	MG	13	1771	1/1	0.95	0.14	81,81,81,81	0
56	MG	1H	3314	1/1	0.95	0.12	72,72,72,72	0
56	MG	1H	3006	1/1	0.95	0.18	52,52,52,52	0
56	MG	14	3111	1/1	0.95	0.24	78,78,78,78	0
56	MG	2L	101	1/1	0.95	0.23	86,86,86,86	0
56	MG	13	1628	1/1	0.95	0.18	79,79,79,79	0
56	MG	1H	3242	1/1	0.95	0.26	82,82,82,82	0
56	MG	13	1635	1/1	0.95	0.23	75,75,75,75	0
56	MG	1G	1704	1/1	0.95	0.07	85,85,85,85	0
56	MG	14	3331	1/1	0.95	0.19	82,82,82,82	0
56	MG	1H	3588	1/1	0.95	0.15	52,52,52,52	0
56	MG	1H	3388	1/1	0.95	0.26	54,54,54,54	0
56	MG	14	3150	1/1	0.95	0.12	73,73,73,73	0
56	MG	14	3370	1/1	0.95	0.07	70,70,70,70	0
56	MG	1H	3576	1/1	0.95	0.06	68,68,68,68	0
58	ZN	5A	101	1/1	0.95	0.09	125,125,125,125	0
56	MG	13	1772	1/1	0.95	0.09	93,93,93,93	0
56	MG	14	3105	1/1	0.95	0.18	64,64,64,64	0
56	MG	1H	3258	1/1	0.95	0.27	115,115,115,115	0
56	MG	1H	3246	1/1	0.95	0.21	81,81,81,81	0
56	MG	11	301	1/1	0.95	0.30	47,47,47,47	0
56	MG	14	3325	1/1	0.95	0.17	63,63,63,63	0
56	MG	14	3407	1/1	0.95	0.14	84,84,84,84	0
56	MG	1H	3464	1/1	0.95	0.11	71,71,71,71	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	14	3301	1/1	0.95	0.19	85,85,85,85	0
56	MG	1H	3135	1/1	0.95	0.30	59,59,59,59	0
56	MG	13	1751	1/1	0.95	0.28	106,106,106,106	0
56	MG	1H	3611	1/1	0.95	0.12	88,88,88,88	0
56	MG	1H	3072	1/1	0.95	0.09	86,86,86,86	0
56	MG	1H	3552	1/1	0.95	0.12	78,78,78,78	0
56	MG	1H	3553	1/1	0.95	0.07	62,62,62,62	0
56	MG	1H	3035	1/1	0.95	0.27	90,90,90,90	0
56	MG	1H	3606	1/1	0.95	0.12	85,85,85,85	0
56	MG	1H	3147	1/1	0.95	0.26	83,83,83,83	0
56	MG	BI	201	1/1	0.95	0.10	113,113,113,113	0
56	MG	1H	3024	1/1	0.95	0.13	54,54,54,54	0
56	MG	1H	3190	1/1	0.95	0.15	80,80,80,80	0
56	MG	1H	3081	1/1	0.95	0.25	91,91,91,91	0
56	MG	13	1722	1/1	0.95	0.26	99,99,99,99	0
56	MG	13	1676	1/1	0.95	0.13	68,68,68,68	0
56	MG	13	1617	1/1	0.96	0.08	84,84,84,84	0
56	MG	13	1770	1/1	0.96	0.10	89,89,89,89	0
56	MG	1G	1740	1/1	0.96	0.17	93,93,93,93	0
56	MG	1H	3057	1/1	0.96	0.21	52,52,52,52	0
56	MG	13	1761	1/1	0.96	0.09	110,110,110,110	0
56	MG	14	3040	1/1	0.96	0.16	62,62,62,62	0
56	MG	1G	1737	1/1	0.96	0.13	127,127,127,127	0
56	MG	1H	3402	1/1	0.96	0.14	58,58,58,58	0
56	MG	16	204	1/1	0.96	0.24	77,77,77,77	0
56	MG	1H	3203	1/1	0.96	0.09	70,70,70,70	0
56	MG	1H	3123	1/1	0.96	0.16	70,70,70,70	0
56	MG	13	1786	1/1	0.96	0.06	65,65,65,65	0
56	MG	1G	1750	1/1	0.96	0.06	109,109,109,109	0
56	MG	14	3260	1/1	0.96	0.29	91,91,91,91	0
56	MG	13	1695	1/1	0.96	0.15	86,86,86,86	0
56	MG	14	3327	1/1	0.96	0.09	63,63,63,63	0
56	MG	1H	3566	1/1	0.96	0.08	93,93,93,93	0
56	MG	14	3238	1/1	0.96	0.27	85,85,85,85	0
56	MG	13	1744	1/1	0.96	0.17	81,81,81,81	0
56	MG	14	3060	1/1	0.96	0.10	64,64,64,64	0
56	MG	14	3187	1/1	0.96	0.18	62,62,62,62	0
56	MG	1H	3545	1/1	0.96	0.04	63,63,63,63	0
56	MG	14	3415	1/1	0.96	0.09	101,101,101,101	0
56	MG	13	1782	1/1	0.96	0.09	81,81,81,81	0
56	MG	1G	1680	1/1	0.96	0.26	69,69,69,69	0
56	MG	14	3085	1/1	0.96	0.27	62,62,62,62	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	14	3106	1/1	0.96	0.26	80,80,80,80	0
56	MG	14	3389	1/1	0.96	0.09	54,54,54,54	0
56	MG	14	3167	1/1	0.96	0.15	81,81,81,81	0
56	MG	14	3271	1/1	0.96	0.22	73,73,73,73	0
56	MG	1H	3509	1/1	0.96	0.09	77,77,77,77	0
56	MG	1H	3051	1/1	0.96	0.10	46,46,46,46	0
56	MG	1H	3175	1/1	0.96	0.10	103,103,103,103	0
56	MG	14	3414	1/1	0.96	0.11	86,86,86,86	0
56	MG	1H	3094	1/1	0.96	0.11	48,48,48,48	0
56	MG	13	1776	1/1	0.96	0.10	93,93,93,93	0
56	MG	1H	3045	1/1	0.96	0.15	75,75,75,75	0
56	MG	1H	3495	1/1	0.96	0.08	48,48,48,48	0
56	MG	14	3282	1/1	0.96	0.23	67,67,67,67	0
56	MG	1G	1611	1/1	0.96	0.15	86,86,86,86	0
56	MG	5I	102	1/1	0.96	0.33	100,100,100,100	0
56	MG	5E	201	1/1	0.96	0.15	79,79,79,79	0
56	MG	13	1797	1/1	0.96	0.13	105,105,105,105	0
56	MG	1H	3320	1/1	0.96	0.11	94,94,94,94	0
56	MG	14	3392	1/1	0.96	0.07	62,62,62,62	0
56	MG	14	3069	1/1	0.96	0.31	85,85,85,85	0
56	MG	14	3037	1/1	0.96	0.13	61,61,61,61	0
56	MG	1H	3440	1/1	0.96	0.14	59,59,59,59	0
56	MG	14	3180	1/1	0.96	0.29	82,82,82,82	0
56	MG	14	3142	1/1	0.96	0.14	70,70,70,70	0
56	MG	14	3416	1/1	0.96	0.09	98,98,98,98	0
56	MG	1H	3350	1/1	0.96	0.15	85,85,85,85	0
56	MG	14	3295	1/1	0.96	0.24	91,91,91,91	0
56	MG	1H	3390	1/1	0.96	0.20	53,53,53,53	0
56	MG	1H	3451	1/1	0.96	0.34	85,85,85,85	0
56	MG	14	3361	1/1	0.96	0.07	80,80,80,80	0
56	MG	14	3328	1/1	0.96	0.08	58,58,58,58	0
56	MG	1H	3114	1/1	0.96	0.42	90,90,90,90	0
56	MG	1H	3346	1/1	0.96	0.24	91,91,91,91	0
56	MG	1G	1724	1/1	0.96	0.08	75,75,75,75	0
56	MG	1H	3494	1/1	0.96	0.12	40,40,40,40	0
56	MG	14	3005	1/1	0.96	0.16	58,58,58,58	0
56	MG	1H	3112	1/1	0.96	0.15	57,57,57,57	0
56	MG	45	202	1/1	0.96	0.23	84,84,84,84	0
56	MG	14	3371	1/1	0.96	0.13	84,84,84,84	0
56	MG	BA	201	1/1	0.96	0.07	102,102,102,102	0
56	MG	1H	3299	1/1	0.96	0.25	87,87,87,87	0
56	MG	14	3109	1/1	0.96	0.20	69,69,69,69	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	1G	1676	1/1	0.96	0.14	81,81,81,81	0
56	MG	1H	3544	1/1	0.96	0.16	57,57,57,57	0
56	MG	1H	3273	1/1	0.96	0.08	73,73,73,73	0
56	MG	14	3386	1/1	0.96	0.12	54,54,54,54	0
56	MG	14	3430	1/1	0.96	0.10	90,90,90,90	0
56	MG	1H	3507	1/1	0.96	0.18	65,65,65,65	0
56	MG	1H	3397	1/1	0.96	0.34	60,60,60,60	0
56	MG	1H	3178	1/1	0.96	0.14	91,91,91,91	0
56	MG	14	3116	1/1	0.96	0.19	57,57,57,57	0
56	MG	14	3258	1/1	0.96	0.27	50,50,50,50	0
56	MG	1H	3394	1/1	0.96	0.31	67,67,67,67	0
56	MG	1H	3541	1/1	0.96	0.07	75,75,75,75	0
56	MG	1H	3602	1/1	0.96	0.06	88,88,88,88	0
56	MG	14	3376	1/1	0.96	0.09	75,75,75,75	0
56	MG	1H	3085	1/1	0.96	0.18	46,46,46,46	0
56	MG	1H	3392	1/1	0.96	0.25	54,54,54,54	0
56	MG	14	3231	1/1	0.96	0.23	57,57,57,57	0
56	MG	1H	3306	1/1	0.96	0.28	87,87,87,87	0
56	MG	14	3017	1/1	0.96	0.19	77,77,77,77	0
56	MG	1H	3377	1/1	0.96	0.24	49,49,49,49	0
56	MG	14	3246	1/1	0.96	0.32	86,86,86,86	0
56	MG	1H	3119	1/1	0.96	0.37	76,76,76,76	0
56	MG	14	3329	1/1	0.96	0.10	57,57,57,57	0
56	MG	18	102	1/1	0.96	0.05	66,66,66,66	0
56	MG	1H	3089	1/1	0.96	0.14	62,62,62,62	0
56	MG	13	1798	1/1	0.96	0.22	80,80,80,80	0
56	MG	1H	3130	1/1	0.96	0.25	70,70,70,70	0
56	MG	14	3243	1/1	0.96	0.11	52,52,52,52	0
56	MG	1H	3211	1/1	0.96	0.19	80,80,80,80	0
56	MG	1G	1684	1/1	0.96	0.07	89,89,89,89	0
56	MG	14	3061	1/1	0.96	0.09	74,74,74,74	0
56	MG	1G	1632	1/1	0.96	0.27	83,83,83,83	0
56	MG	13	1691	1/1	0.96	0.28	94,94,94,94	0
56	MG	1H	3438	1/1	0.96	0.07	94,94,94,94	0
56	MG	1H	3215	1/1	0.96	0.40	61,61,61,61	0
56	MG	1H	3349	1/1	0.96	1.26	74,74,74,74	0
56	MG	1H	3111	1/1	0.96	0.20	54,54,54,54	0
56	MG	14	3152	1/1	0.96	0.10	77,77,77,77	0
56	MG	1H	3232	1/1	0.96	0.30	82,82,82,82	0
56	MG	14	3254	1/1	0.96	0.32	55,55,55,55	0
56	MG	14	3122	1/1	0.96	0.25	55,55,55,55	0
56	MG	14	3203	1/1	0.96	0.65	83,83,83,83	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	1H	3539	1/1	0.96	0.06	76,76,76,76	0
56	MG	14	3374	1/1	0.96	0.15	55,55,55,55	0
56	MG	1G	1741	1/1	0.96	0.12	98,98,98,98	0
56	MG	1H	3427	1/1	0.96	0.25	64,64,64,64	0
56	MG	13	1644	1/1	0.96	0.26	89,89,89,89	0
56	MG	1H	3330	1/1	0.96	0.43	70,70,70,70	0
56	MG	13	1794	1/1	0.96	0.09	79,79,79,79	0
56	MG	14	3397	1/1	0.96	0.18	70,70,70,70	0
56	MG	1H	3391	1/1	0.96	0.24	61,61,61,61	0
56	MG	14	3357	1/1	0.97	0.10	67,67,67,67	0
56	MG	1H	3486	1/1	0.97	0.14	45,45,45,45	0
56	MG	14	3401	1/1	0.97	0.06	85,85,85,85	0
56	MG	13	1611	1/1	0.97	0.20	65,65,65,65	0
56	MG	14	3095	1/1	0.97	0.28	92,92,92,92	0
56	MG	14	3199	1/1	0.97	0.29	67,67,67,67	0
56	MG	1H	3027	1/1	0.97	0.18	40,40,40,40	0
56	MG	14	3381	1/1	0.97	0.12	89,89,89,89	0
56	MG	14	3274	1/1	0.97	0.27	64,64,64,64	0
56	MG	1H	3525	1/1	0.97	0.13	58,58,58,58	0
56	MG	14	3093	1/1	0.97	0.17	56,56,56,56	0
56	MG	1H	3353	1/1	0.97	0.15	77,77,77,77	0
56	MG	1H	3609	1/1	0.97	0.07	90,90,90,90	0
56	MG	1G	1649	1/1	0.97	0.14	90,90,90,90	0
56	MG	14	3384	1/1	0.97	0.14	81,81,81,81	0
56	MG	14	3063	1/1	0.97	0.12	80,80,80,80	0
56	MG	14	3103	1/1	0.97	0.29	78,78,78,78	0
56	MG	1H	3050	1/1	0.97	0.18	51,51,51,51	0
56	MG	19	301	1/1	0.97	0.12	53,53,53,53	0
56	MG	1H	3331	1/1	0.97	0.55	69,69,69,69	0
56	MG	14	3293	1/1	0.97	0.23	81,81,81,81	0
56	MG	14	3163	1/1	0.97	0.33	90,90,90,90	0
56	MG	14	3090	1/1	0.97	0.25	59,59,59,59	0
56	MG	1H	3002	1/1	0.97	0.12	40,40,40,40	0
56	MG	13	1692	1/1	0.97	0.27	102,102,102,102	0
56	MG	14	3426	1/1	0.97	0.06	108,108,108,108	0
56	MG	1H	3164	1/1	0.97	0.18	78,78,78,78	0
56	MG	14	3086	1/1	0.97	0.20	59,59,59,59	0
56	MG	14	3119	1/1	0.97	0.14	91,91,91,91	0
56	MG	1H	3303	1/1	0.97	0.33	106,106,106,106	0
56	MG	14	3305	1/1	0.97	0.13	60,60,60,60	0
56	MG	1H	3117	1/1	0.97	0.17	59,59,59,59	0
56	MG	14	3165	1/1	0.97	0.30	83,83,83,83	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	1H	3005	1/1	0.97	0.23	56,56,56,56	0
56	MG	14	3097	1/1	0.97	0.08	76,76,76,76	0
56	MG	14	3259	1/1	0.97	0.36	87,87,87,87	0
56	MG	14	3338	1/1	0.97	0.08	51,51,51,51	0
56	MG	14	3375	1/1	0.97	0.09	75,75,75,75	0
56	MG	14	3059	1/1	0.97	0.16	41,41,41,41	0
56	MG	1H	3458	1/1	0.97	0.21	85,85,85,85	0
56	MG	1G	1640	1/1	0.97	0.11	82,82,82,82	0
56	MG	13	1752	1/1	0.97	0.07	86,86,86,86	0
56	MG	14	3344	1/1	0.97	0.10	66,66,66,66	0
56	MG	1H	3295	1/1	0.97	0.18	65,65,65,65	0
56	MG	1H	3263	1/1	0.97	0.20	64,64,64,64	0
56	MG	14	3316	1/1	0.97	0.30	79,79,79,79	0
56	MG	13	1777	1/1	0.97	0.12	69,69,69,69	0
56	MG	14	3233	1/1	0.97	0.20	72,72,72,72	0
56	MG	14	3228	1/1	0.97	0.11	79,79,79,79	0
56	MG	14	3138	1/1	0.97	0.11	71,71,71,71	0
56	MG	14	3098	1/1	0.97	0.17	67,67,67,67	0
56	MG	14	3120	1/1	0.97	0.23	70,70,70,70	0
56	MG	14	3296	1/1	0.97	0.18	68,68,68,68	0
56	MG	14	3087	1/1	0.97	0.28	60,60,60,60	0
56	MG	1H	3497	1/1	0.97	0.12	40,40,40,40	0
56	MG	1H	3517	1/1	0.97	0.10	54,54,54,54	0
56	MG	14	3242	1/1	0.97	0.22	66,66,66,66	0
56	MG	14	3117	1/1	0.97	0.31	79,79,79,79	0
56	MG	1H	3449	1/1	0.97	0.07	88,88,88,88	0
56	MG	14	3326	1/1	0.97	0.10	53,53,53,53	0
56	MG	1H	3546	1/1	0.97	0.15	60,60,60,60	0
56	MG	14	3144	1/1	0.97	0.13	65,65,65,65	0
56	MG	1H	3492	1/1	0.97	0.08	54,54,54,54	0
56	MG	14	3351	1/1	0.97	0.10	76,76,76,76	0
56	MG	14	3347	1/1	0.97	0.10	53,53,53,53	0
56	MG	1H	3551	1/1	0.97	0.07	53,53,53,53	0
56	MG	1H	3514	1/1	0.97	0.13	84,84,84,84	0
56	MG	14	3226	1/1	0.97	0.31	60,60,60,60	0
56	MG	1H	3383	1/1	0.97	0.14	58,58,58,58	0
56	MG	1H	3533	1/1	0.97	0.07	46,46,46,46	0
56	MG	1H	3442	1/1	0.97	0.12	73,73,73,73	0
56	MG	1H	3160	1/1	0.97	0.15	66,66,66,66	0
56	MG	1H	3500	1/1	0.97	0.14	43,43,43,43	0
56	MG	14	3189	1/1	0.97	0.14	63,63,63,63	0
56	MG	14	3302	1/1	0.97	0.12	56,56,56,56	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	14	3088	1/1	0.97	0.18	61,61,61,61	0
56	MG	1G	1736	1/1	0.97	0.09	111,111,111,111	0
56	MG	1H	3572	1/1	0.97	0.08	73,73,73,73	0
56	MG	1H	3571	1/1	0.97	0.11	58,58,58,58	0
56	MG	14	3252	1/1	0.97	0.28	76,76,76,76	0
56	MG	13	1623	1/1	0.97	0.17	106,106,106,106	0
56	MG	1H	3385	1/1	0.97	0.23	75,75,75,75	0
56	MG	1H	3120	1/1	0.97	0.29	75,75,75,75	0
56	MG	14	3181	1/1	0.97	0.08	87,87,87,87	0
56	MG	BI	202	1/1	0.97	0.15	122,122,122,122	0
56	MG	1G	1645	1/1	0.97	0.14	101,101,101,101	0
56	MG	13	1645	1/1	0.97	0.14	74,74,74,74	0
56	MG	1G	1709	1/1	0.97	0.08	108,108,108,108	0
56	MG	1H	3549	1/1	0.97	0.08	61,61,61,61	0
56	MG	14	3409	1/1	0.97	0.06	80,80,80,80	0
56	MG	1H	3004	1/1	0.97	0.15	35,35,35,35	0
56	MG	14	3112	1/1	0.97	0.20	83,83,83,83	0
56	MG	1H	3260	1/1	0.97	0.28	69,69,69,69	0
56	MG	14	3113	1/1	0.98	0.17	69,69,69,69	0
56	MG	1H	3503	1/1	0.98	0.11	55,55,55,55	0
56	MG	1H	3395	1/1	0.98	0.11	54,54,54,54	0
56	MG	1H	3524	1/1	0.98	0.17	56,56,56,56	0
56	MG	14	3062	1/1	0.98	0.10	59,59,59,59	0
56	MG	14	3377	1/1	0.98	0.09	51,51,51,51	0
56	MG	14	3303	1/1	0.98	0.11	69,69,69,69	0
56	MG	14	3114	1/1	0.98	0.24	60,60,60,60	0
56	MG	14	3147	1/1	0.98	0.31	94,94,94,94	0
56	MG	1G	1620	1/1	0.98	0.11	83,83,83,83	0
56	MG	1H	3305	1/1	0.98	0.45	100,100,100,100	0
56	MG	1H	3128	1/1	0.98	0.20	60,60,60,60	0
56	MG	1H	3398	1/1	0.98	0.17	47,47,47,47	0
56	MG	14	3078	1/1	0.98	0.10	54,54,54,54	0
56	MG	1H	3124	1/1	0.98	0.20	52,52,52,52	0
56	MG	14	3137	1/1	0.98	0.36	90,90,90,90	0
56	MG	1H	3126	1/1	0.98	0.22	54,54,54,54	0
56	MG	14	3348	1/1	0.98	0.12	59,59,59,59	0
56	MG	1H	3099	1/1	0.98	0.09	55,55,55,55	0
56	MG	1G	1612	1/1	0.98	0.10	79,79,79,79	0
56	MG	14	3076	1/1	0.98	0.36	78,78,78,78	0
56	MG	14	3028	1/1	0.98	0.18	53,53,53,53	0
56	MG	1H	3110	1/1	0.98	0.18	50,50,50,50	0
56	MG	13	1778	1/1	0.98	0.06	79,79,79,79	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	1H	3612	1/1	0.98	0.08	62,62,62,62	0
56	MG	2I	304	1/1	0.98	0.08	54,54,54,54	0
56	MG	1H	3604	1/1	0.98	0.07	118,118,118,118	0
56	MG	13	1718	1/1	0.98	0.12	105,105,105,105	0
56	MG	1H	3403	1/1	0.98	0.20	76,76,76,76	0
56	MG	13	1759	1/1	0.98	0.04	105,105,105,105	0
56	MG	14	3094	1/1	0.98	0.18	64,64,64,64	0
56	MG	13	1730	1/1	0.98	0.12	100,100,100,100	0
56	MG	13	1637	1/1	0.98	0.14	67,67,67,67	0
56	MG	1H	3384	1/1	0.98	0.29	49,49,49,49	0
56	MG	1H	3289	1/1	0.98	0.10	85,85,85,85	0
56	MG	1H	3166	1/1	0.98	0.17	87,87,87,87	0
56	MG	13	1742	1/1	0.98	0.52	92,92,92,92	0
56	MG	1H	3167	1/1	0.98	0.24	83,83,83,83	0
56	MG	1G	1678	1/1	0.98	0.31	86,86,86,86	0
56	MG	14	3350	1/1	0.98	0.14	45,45,45,45	0
56	MG	1H	3531	1/1	0.98	0.11	66,66,66,66	0
56	MG	14	3194	1/1	0.98	0.17	75,75,75,75	0
56	MG	14	3255	1/1	0.98	0.14	72,72,72,72	0
56	MG	14	3355	1/1	0.98	0.07	75,75,75,75	0
56	MG	14	3394	1/1	0.98	0.02	98,98,98,98	0
56	MG	29	302	1/1	0.98	0.15	57,57,57,57	0
56	MG	1H	3607	1/1	0.98	0.06	61,61,61,61	0
56	MG	1G	1682	1/1	0.98	0.16	79,79,79,79	0
56	MG	13	1627	1/1	0.98	0.20	93,93,93,93	0
56	MG	14	3075	1/1	0.98	0.18	94,94,94,94	0
56	MG	1H	3250	1/1	0.98	0.42	67,67,67,67	0
56	MG	14	3121	1/1	0.98	0.20	65,65,65,65	0
56	MG	14	3250	1/1	0.98	0.26	66,66,66,66	0
56	MG	1H	3605	1/1	0.98	0.09	90,90,90,90	0
56	MG	1H	3359	1/1	0.98	0.18	58,58,58,58	0
56	MG	1H	3499	1/1	0.98	0.13	49,49,49,49	0
56	MG	13	1601	1/1	0.98	0.10	58,58,58,58	0
56	MG	14	3396	1/1	0.98	0.11	54,54,54,54	0
56	MG	1H	3429	1/1	0.98	0.17	63,63,63,63	0
56	MG	14	3247	1/1	0.98	0.22	59,59,59,59	0
56	MG	1G	1723	1/1	0.98	0.08	72,72,72,72	0
56	MG	14	3399	1/1	0.98	0.06	47,47,47,47	0
56	MG	13	1650	1/1	0.98	0.36	100,100,100,100	0
56	MG	14	3013	1/1	0.98	0.15	50,50,50,50	0
56	MG	2I	201	1/1	0.98	0.12	91,91,91,91	0
56	MG	14	3104	1/1	0.98	0.34	48,48,48,48	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	1H	3102	1/1	0.98	0.33	63,63,63,63	0
56	MG	1H	3617	1/1	0.98	0.24	127,127,127,127	0
56	MG	1H	3038	1/1	0.98	0.16	44,44,44,44	0
56	MG	1H	3014	1/1	0.98	0.19	62,62,62,62	0
56	MG	1H	3537	1/1	0.98	0.08	52,52,52,52	0
56	MG	1H	3555	1/1	0.98	0.22	85,85,85,85	0
56	MG	1H	3118	1/1	0.98	0.26	74,74,74,74	0
56	MG	1H	3379	1/1	0.98	0.32	85,85,85,85	0
56	MG	13	1716	1/1	0.98	0.10	94,94,94,94	0
56	MG	1H	3569	1/1	0.98	0.11	73,73,73,73	0
56	MG	1H	3378	1/1	0.98	0.18	56,56,56,56	0
56	MG	14	3337	1/1	0.98	0.05	53,53,53,53	0
56	MG	1G	1670	1/1	0.98	0.27	99,99,99,99	0
56	MG	1H	3249	1/1	0.98	0.13	70,70,70,70	0
56	MG	1H	3446	1/1	0.98	0.10	87,87,87,87	0
56	MG	1G	1677	1/1	0.98	0.09	94,94,94,94	0
56	MG	1H	3155	1/1	0.98	0.29	73,73,73,73	0
56	MG	1H	3490	1/1	0.98	0.14	63,63,63,63	0
56	MG	1H	3109	1/1	0.98	0.26	44,44,44,44	0
56	MG	1H	3530	1/1	0.98	0.08	54,54,54,54	0
56	MG	1H	3596	1/1	0.98	0.11	75,75,75,75	0
56	MG	14	3198	1/1	0.99	0.30	96,96,96,96	0
56	MG	14	3336	1/1	0.99	0.08	60,60,60,60	0
56	MG	13	1756	1/1	0.99	0.04	95,95,95,95	0
56	MG	1H	3254	1/1	0.99	0.24	68,68,68,68	0
56	MG	1H	3277	1/1	0.99	0.11	66,66,66,66	0
56	MG	1H	3240	1/1	0.99	0.27	64,64,64,64	0
56	MG	1H	3567	1/1	0.99	0.13	51,51,51,51	0
56	MG	14	3091	1/1	0.99	0.23	57,57,57,57	0
56	MG	14	3234	1/1	0.99	0.18	60,60,60,60	0
58	ZN	5I	103	1/1	0.99	0.16	97,97,97,97	0
56	MG	1H	3360	1/1	0.99	0.17	50,50,50,50	0
56	MG	1H	3428	1/1	0.99	0.25	57,57,57,57	0
57	SF4	3E	302	8/8	0.99	0.21	85,90,93,95	0
56	MG	14	3257	1/1	0.99	0.21	62,62,62,62	0
56	MG	1H	3548	1/1	0.99	0.08	50,50,50,50	0
56	MG	1H	3372	1/1	0.99	0.12	71,71,71,71	0
56	MG	1H	3542	1/1	0.99	0.20	68,68,68,68	0
56	MG	1H	3515	1/1	0.99	0.10	41,41,41,41	0
56	MG	13	1641	1/1	0.99	0.17	55,55,55,55	0
56	MG	1H	3518	1/1	0.99	0.08	51,51,51,51	0
56	MG	1H	3389	1/1	0.99	0.23	52,52,52,52	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	13	1790	1/1	0.99	0.07	59,59,59,59	0
56	MG	1G	1653	1/1	0.99	0.33	112,112,112,112	0
56	MG	13	1699	1/1	0.99	0.47	94,94,94,94	0
56	MG	14	3188	1/1	0.99	0.13	68,68,68,68	0
56	MG	16	215	1/1	0.99	0.09	71,71,71,71	0
56	MG	98	201	1/1	0.99	0.28	56,56,56,56	0
56	MG	1H	3251	1/1	0.99	0.32	66,66,66,66	0
56	MG	13	1700	1/1	0.99	0.19	90,90,90,90	0
56	MG	1H	3197	1/1	0.99	0.21	65,65,65,65	0
56	MG	1H	3528	1/1	0.99	0.08	49,49,49,49	0
56	MG	14	3127	1/1	0.99	0.11	61,61,61,61	0
56	MG	1H	3122	1/1	0.99	0.18	49,49,49,49	0
56	MG	14	3249	1/1	0.99	0.27	54,54,54,54	0
56	MG	14	3202	1/1	0.99	0.17	71,71,71,71	0
56	MG	1H	3282	1/1	0.99	0.05	94,94,94,94	0
56	MG	14	3253	1/1	0.99	0.33	59,59,59,59	0
56	MG	14	3115	1/1	0.99	0.16	57,57,57,57	0
56	MG	13	1783	1/1	0.99	0.14	77,77,77,77	0
56	MG	14	3081	1/1	0.99	0.21	114,114,114,114	0
57	SF4	32	301	8/8	0.99	0.19	95,103,111,112	0
56	MG	14	3244	1/1	0.99	0.25	67,67,67,67	0
56	MG	1H	3132	1/1	0.99	0.24	46,46,46,46	0
56	MG	2K	101	1/1	0.99	0.30	69,69,69,69	0
56	MG	1H	3510	1/1	0.99	0.19	54,54,54,54	0
56	MG	1H	3483	1/1	0.99	0.13	63,63,63,63	0
56	MG	13	1651	1/1	1.00	0.32	91,91,91,91	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.