



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 5, 2026 – 07:45 PM UTC

PDB ID : 5EL5 / pdb_00005el5
Title : Structure of T. thermophilus 70S ribosome complex with mRNA and tRNA^{Lys} in the A-site with a U-U mismatch in the second position
Authors : Rozov, A.; Demeshkina, N.; Khusainov, I.; Yusupov, M.; Yusupova, G.
Deposited on : 2015-11-04
Resolution : 3.15 Å(reported)

This is a wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

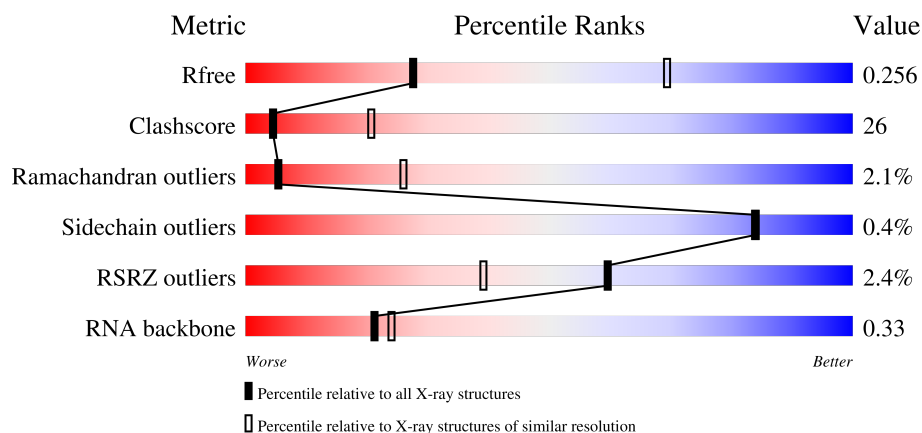
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.15 Å.

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



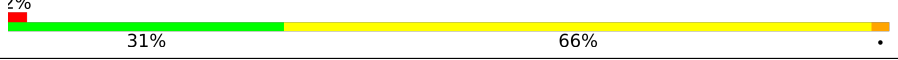
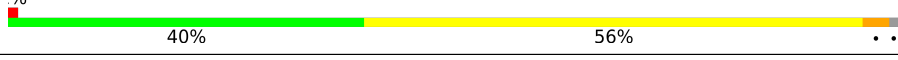
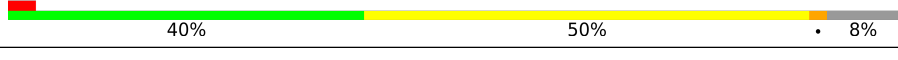
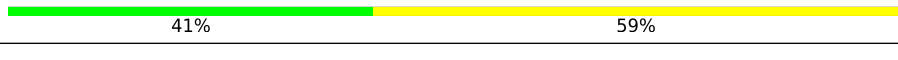
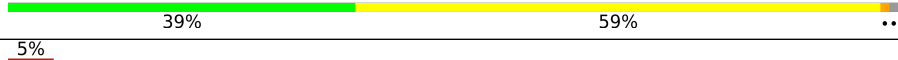
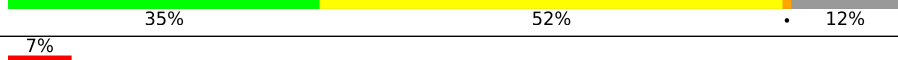
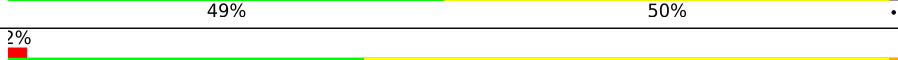
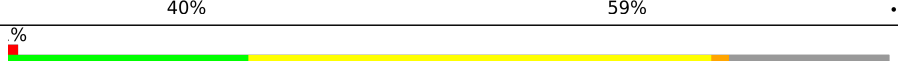
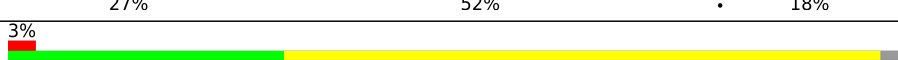
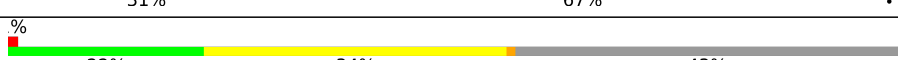
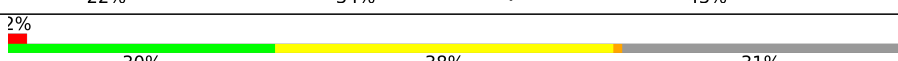
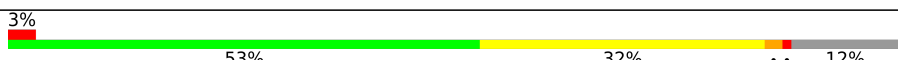
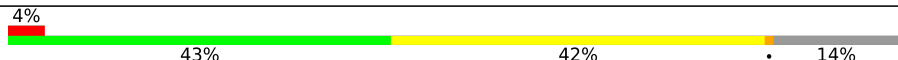
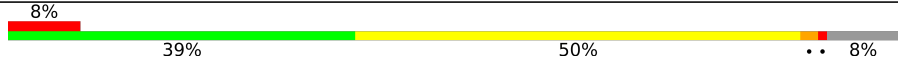
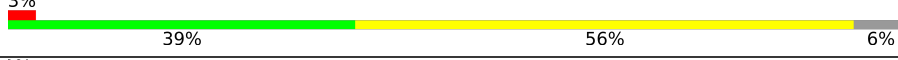
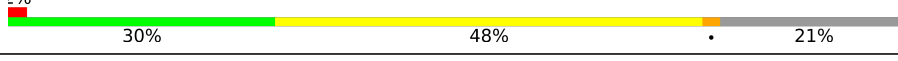
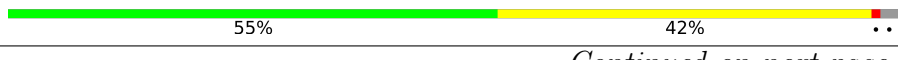
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	2361 (3.20-3.12)
Clashscore	190562	2486 (3.20-3.12)
Ramachandran outliers	187476	2405 (3.20-3.12)
Sidechain outliers	187428	2404 (3.20-3.12)
RSRZ outliers	180081	2361 (3.20-3.12)
RNA backbone	3983	1113 (3.42-2.90)

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

Mol	Chain	Length	Quality of chain
1	13	1522	3% 29% 50% 18% ..
1	1G	1522	2% 24% 53% 22% .
2	12	256	27% 50% . 20%
2	1E	256	34% 54% . 10%

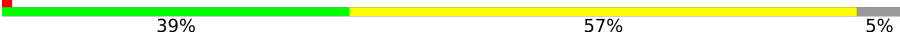
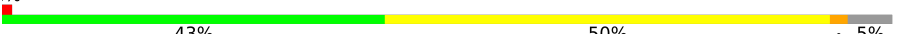
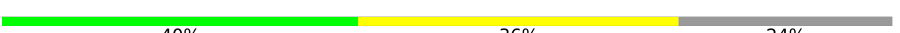
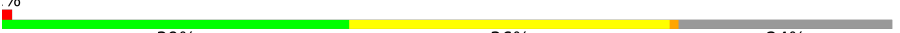
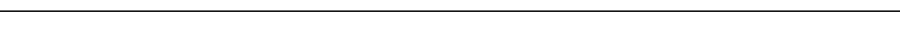
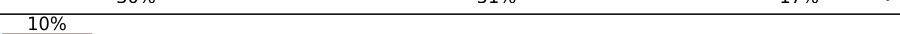
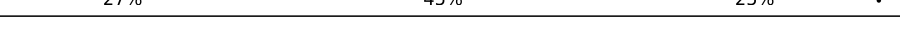
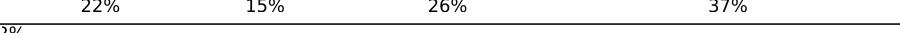
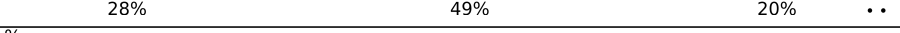
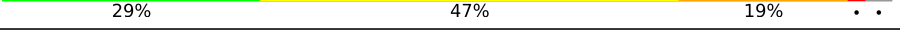
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Mol	Chain	Length	Quality of chain
3	22	239	
3	2E	239	
4	32	209	
4	3E	209	
5	42	162	
5	4E	162	
6	52	101	
6	5E	101	
7	62	156	
7	6E	156	
8	72	138	
8	7E	138	
9	82	128	
9	8E	128	
10	1A	105	
10	1I	105	
11	2A	129	
11	2I	129	
12	3A	132	
12	3I	132	
13	4A	126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

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Mol	Chain	Length	Quality of chain
15	6I	89	
16	7A	88	
16	7I	88	
17	8A	105	
17	8I	105	
18	9A	88	
18	9I	88	
19	AA	93	
19	AI	93	
20	BA	106	
20	BI	106	
21	1B	27	
21	1F	27	
22	1K	76	
23	2K	77	
23	2L	77	
24	3K	76	
25	4K	27	
25	4L	27	
26	14	2912	
26	1H	2912	
27	16	122	
27	1J	122	
28	7I	229	
29	11	276	

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

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

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Mol	Chain	Length	Quality of chain
55	M5	65	
55	Q8	65	
56	1L	76	
57	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
58	MG	13	1648	-	-	-	X
58	MG	14	3089	-	-	-	X
58	MG	14	3188	-	-	-	X
58	MG	14	3247	-	-	-	X
58	MG	14	3260	-	-	-	X
58	MG	14	3294	-	-	-	X
58	MG	1H	3141	-	-	-	X
58	MG	1H	3235	-	-	-	X
58	MG	1H	3289	-	-	-	X
59	SF4	32	302	-	-	X	-

2 Entry composition

There are 61 unique types of molecules in this entry. The entry contains 292607 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	1493	Total	C	N	O	P	0	0	0
			32097	14286	5951	10367	1493			
1	1G	1496	Total	C	N	O	P	0	0	0
			32152	14311	5953	10392	1496			

- 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	206	Total	C	N	O	S	0	0	0
			1695	1082	305	304	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	194	Total	C	N	O	S	0	0	0
			1529	967	296	265	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
			1696	1062	338	289	7			
4	32	208	Total	C	N	O	S	0	0	0
			1702	1066	339	290	7			

- Molecule 5 is a protein called 30S ribosomal protein S5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	4E	149	Total	C	N	O	S	0	0	0
			1142	722	216	200	4			
5	42	149	Total	C	N	O	S	0	0	0
			1136	716	216	200	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	151	Total	C	N	O	S	0	0	0
			1229	763	247	213	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	105	Total	C	N	O		0	0	0
			820	523	158	139				

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	1I	72	Total	C	N	O	S	0	0	0
			593	373	115	104	1			

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
10	1A	60	Total	C	N	O	0	0	0
			474	298	91	85			

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
11	2I	111	Total	C	N	O	0	0	0
			823	512	154	154			
11	2A	113	Total	C	N	O	0	0	0
			835	520	156	156			

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
12	3I	122	Total	C	N	O	0	0	0
			956	603	193	159			
12	3A	121	Total	C	N	O	0	0	0
			947	597	191	158			

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
13	4I	119	Total	C	N	O	0	0	0
			942	582	194	164			
13	4A	111	Total	C	N	O	0	0	0
			893	552	183	156			

- 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	0	0	0
			491	312	104	71			
14	5A	48	Total	C	N	O	0	0	0
			388	245	82	57			

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
16	7I	80	Total	C	N	O	S	0	0	0
			671	427	132	111	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	67	Total	C	N	O	0	0	0
			544	349	104	91			
18	9A	67	Total	C	N	O	0	0	0
			544	349	104	91			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
19	AI	81	Total	C	N	O	S	0	0	0
			654	417	122	113	2			
19	AA	36	Total	C	N	O	S	0	0	0
			283	182	49	51	1			

- 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	98	Total	C	N	O	S	0	0	0
			757	467	161	127	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	23	Total	C	N	O	0	0	0
			204	126	49	29			

- Molecule 22 is a RNA chain called tRNA^{Lys}.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
22	1K	69	Total	C	N	O	P	S	0	0	0
			1477	662	257	488	69	1			

- Molecule 23 is a RNA chain called tRNA^{fMet}.

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

- Molecule 24 is a RNA chain called tRNA^{Lys}.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
24	3K	76	Total	C	N	O	P	0	0	0
			1611	721	281	534	75			

- Molecule 25 is a RNA chain called mRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
25	4K	20	Total	C	N	O	P	0	0	0
			439	197	91	131	20			
25	4L	17	Total	C	N	O	P	0	0	0
			373	167	76	113	17			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
26	1H	2830	Total	C	N	O	P	0	0	0
			60960	27129	11403	19598	2830			
26	14	2861	Total	C	N	O	P	0	0	0
			61630	27429	11535	19806	2860			

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 L1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
28	71	135	Total	C	N	O	S	0	0	0
			1050	662	197	190	1			

- Molecule 29 is a protein called 50S ribosomal protein L2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
29	11	273	Total	C	N	O	S	0	0	0
			2120	1338	421	358	3			
29	19	273	Total	C	N	O	S	0	0	0
			2120	1338	421	358	3			

- Molecule 30 is a protein called 50S ribosomal protein L3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
30	21	203	Total	C	N	O	S	0	0	0
			1558	985	298	269	6			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
30	29	203	Total	C	N	O	S	0	0	0
			1558	985	298	269	6			

- Molecule 31 is a protein called 50S ribosomal protein L4.

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

- Molecule 32 is a protein called 50S ribosomal protein L5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
32	41	179	Total	C	N	O	S	0	0	0
			1457	931	265	257	4			
32	49	179	Total	C	N	O	S	0	0	0
			1457	931	265	257	4			

- Molecule 33 is a protein called 50S ribosomal protein L6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
33	51	171	Total	C	N	O	S	0	0	0
			1312	832	246	233	1			
33	59	69	Total	C	N	O		0	0	0
			539	339	109	91				

- Molecule 34 is a protein called 50S ribosomal protein L9.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
34	61	145	Total	C	N	O	S	0	0	0
			1131	723	200	207	1			
34	69	145	Total	C	N	O	S	0	0	0
			1131	723	200	207	1			

- Molecule 35 is a protein called 50S ribosomal protein L13.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
35	58	138	Total	C	N	O	S	0	0	0
			1104	712	206	182	4			
35	15	137	Total	C	N	O	S	0	0	0
			1096	707	205	181	3			

- Molecule 36 is a protein called 50S ribosomal protein L14.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
36	68	122	Total	C	N	O	S	0	0	0
			932	588	171	169	4			
36	25	122	Total	C	N	O	S	0	0	0
			932	588	171	169	4			

- Molecule 37 is a protein called 50S ribosomal protein L15.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
37	78	147	Total	C	N	O	S	0	0	0
			1122	698	229	192	3			
37	35	148	Total	C	N	O	S	0	0	0
			1130	704	230	193	3			

- Molecule 38 is a protein called 50S ribosomal protein L16.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
38	88	141	Total	C	N	O	S	0	0	0
			1113	709	210	187	7			
38	45	138	Total	C	N	O	S	0	0	0
			1099	702	208	183	6			

- Molecule 39 is a protein called 50S ribosomal protein L17.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
39	98	118	Total	C	N	O	S	0	0	0
			967	604	203	159	1			
39	55	118	Total	C	N	O	S	0	0	0
			967	604	203	159	1			

- Molecule 40 is a protein called 50S ribosomal protein L18.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
40	A8	111	Total	C	N	O	0	0	0
			881	556	176	149			
40	65	110	Total	C	N	O	0	0	0
			876	553	175	148			

- Molecule 41 is a protein called 50S ribosomal protein L19.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
41	B8	135	Total	C	N	O	S	0	0	0
			1123	699	230	193	1			
41	75	136	Total	C	N	O		0	0	0
			1133	705	233	195				

- Molecule 42 is a protein called 50S ribosomal protein L20.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
42	C8	115	Total	C	N	O	S	0	0	0
			950	603	199	147	1			
42	85	116	Total	C	N	O	S	0	0	0
			959	608	201	149	1			

- Molecule 43 is a protein called 50S ribosomal protein L21.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
43	D8	101	Total	C	N	O	S	0	0	0
			778	501	142	134	1			
43	95	99	Total	C	N	O		0	0	0
			766	494	140	132				

- Molecule 44 is a protein called 50S ribosomal protein L22.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
44	E8	110	Total	C	N	O	S	0	0	0
			876	552	171	151	2			
44	A5	110	Total	C	N	O	S	0	0	0
			876	552	171	151	2			

- Molecule 45 is a protein called 50S ribosomal protein L23.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
45	F8	95	Total	C	N	O	0	0	0
			740	480	134	126			
45	B5	94	Total	C	N	O	0	0	0
			735	477	133	125			

- Molecule 46 is a protein called 50S ribosomal protein L24.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
46	G8	104	Total	C	N	O	S	0	0	0
			788	507	149	127	5			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
46	C5	105	Total	C	N	O	S	0	0	0
			799	513	153	128	5			

- Molecule 47 is a protein called 50S ribosomal protein L25.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
47	H8	148	Total	C	N	O	S	0	0	0
			1218	779	220	217	2			
47	D5	130	Total	C	N	O	S	0	0	0
			1064	685	191	186	2			

- Molecule 48 is a protein called 50S ribosomal protein L27.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
48	I8	76	Total	C	N	O	S	0	0	0
			606	376	128	101	1			
48	E5	78	Total	C	N	O	S	0	0	0
			616	381	130	104	1			

- Molecule 49 is a protein called 50S ribosomal protein L28.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
49	J8	94	Total	C	N	O	S	0	0	0
			737	463	146	127	1			
49	F5	94	Total	C	N	O	S	0	0	0
			737	463	146	127	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
50	K8	68	Total	C	N	O	S	0	0	0
			568	352	115	100	1			
50	G5	67	Total	C	N	O	S	0	0	0
			563	349	114	99	1			

- Molecule 51 is a protein called 50S ribosomal protein L30.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
51	L8	58	Total	C	N	O	0	0	0
			459	293	89	77			
51	H5	58	Total	C	N	O	0	0	0
			459	293	89	77			

- Molecule 52 is a protein called 50S ribosomal protein L31.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
52	M8	47	Total	C	N	O	S	0	0	0
			366	234	61	66	5			

- Molecule 53 is a protein called 50S ribosomal protein L32.

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

- Molecule 54 is a protein called 50S ribosomal protein L34.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
54	P8	47	Total	C	N	O	S	0	0	0
			401	246	99	54	2			
54	L5	45	Total	C	N	O	S	0	0	0
			391	240	97	52	2			

- Molecule 55 is a protein called 50S ribosomal protein L35.

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

- Molecule 56 is a RNA chain called tRNA^{Lys}.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
56	1L	74	Total	C	N	O	P	0	0	0
			1570	702	271	523	74			

- Molecule 57 is a RNA chain called tRNA^{Lys}.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
57	3L	76	Total	C	N	O	P	0	0	0
			1611	721	281	534	75			

- Molecule 58 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

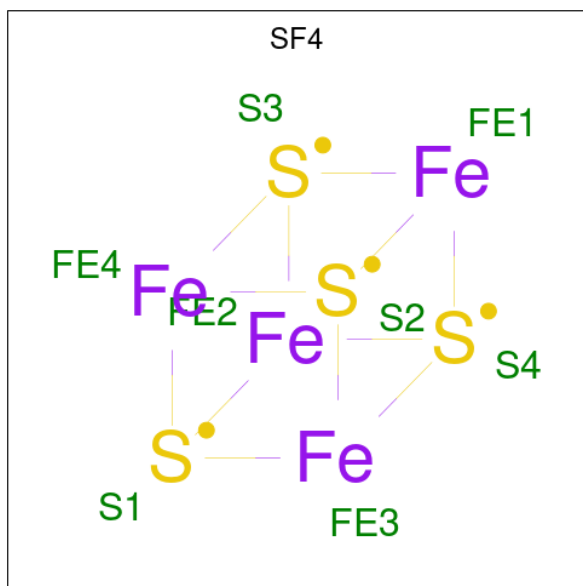
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
58	13	141	Total Mg 141 141	0	0
58	5E	2	Total Mg 2 2	0	0
58	3I	1	Total Mg 1 1	0	0
58	5I	1	Total Mg 1 1	0	0
58	2K	3	Total Mg 3 3	0	0
58	1H	488	Total Mg 488 488	0	0
58	16	12	Total Mg 12 12	0	0
58	11	1	Total Mg 1 1	0	0
58	21	2	Total Mg 2 2	0	0
58	41	1	Total Mg 1 1	0	0
58	78	1	Total Mg 1 1	0	0
58	88	1	Total Mg 1 1	0	0
58	C8	1	Total Mg 1 1	0	0
58	I8	1	Total Mg 1 1	0	0
58	J8	2	Total Mg 2 2	0	0
58	P8	1	Total Mg 1 1	0	0
58	Q8	1	Total Mg 1 1	0	0
58	1G	78	Total Mg 78 78	0	0
58	32	1	Total Mg 1 1	0	0
58	7A	1	Total Mg 1 1	0	0
58	2L	3	Total Mg 3 3	0	0
58	14	420	Total Mg 420 420	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
58	1J	6	Total 6	Mg 6	0	0
58	29	3	Total 3	Mg 3	0	0
58	35	1	Total 1	Mg 1	0	0
58	45	3	Total 3	Mg 3	0	0
58	55	1	Total 1	Mg 1	0	0
58	85	2	Total 2	Mg 2	0	0
58	C5	1	Total 1	Mg 1	0	0
58	E5	1	Total 1	Mg 1	0	0
58	L5	1	Total 1	Mg 1	0	0

- Molecule 59 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe₄S₄).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
59	3E	1	Total 8	Fe 4	S 4	0	0
59	32	1	Total 8	Fe 4	S 4	0	0

- Molecule 60 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
60	5I	1	Total 1	Zn 1	0	0
60	G8	1	Total 1	Zn 1	0	0
60	5A	1	Total 1	Zn 1	0	0
60	C5	1	Total 1	Zn 1	0	0

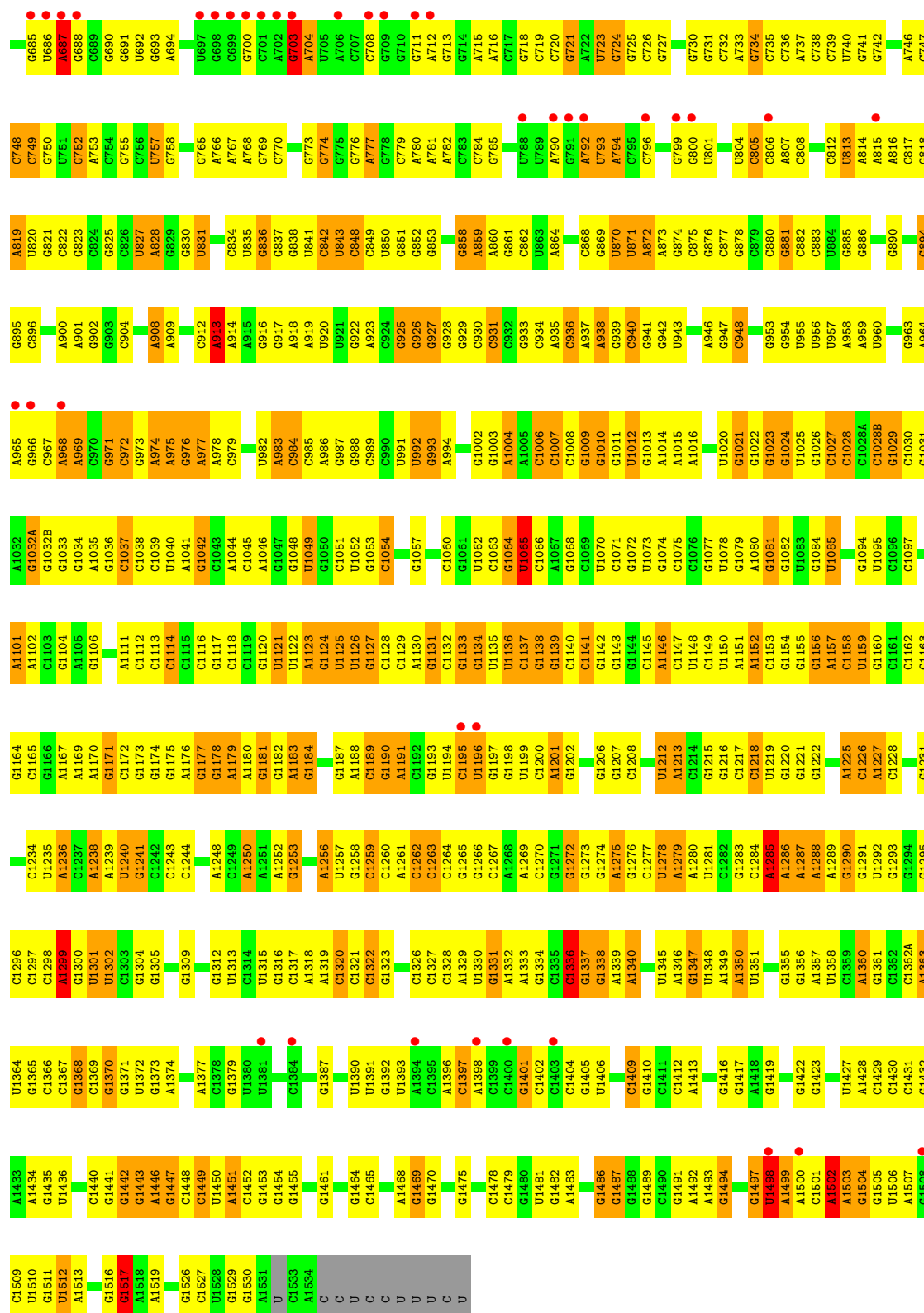
- Molecule 61 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
61	13	148	Total 148	O 148	0	0
61	3E	2	Total 2	O 2	0	0
61	3I	2	Total 2	O 2	0	0
61	5I	1	Total 1	O 1	0	0
61	6I	1	Total 1	O 1	0	0
61	1K	1	Total 1	O 1	0	0
61	4K	6	Total 6	O 6	0	0
61	1H	670	Total 670	O 670	0	0
61	16	18	Total 18	O 18	0	0
61	11	9	Total 9	O 9	0	0
61	21	5	Total 5	O 5	0	0
61	31	6	Total 6	O 6	0	0
61	58	2	Total 2	O 2	0	0
61	78	3	Total 3	O 3	0	0
61	B8	1	Total 1	O 1	0	0

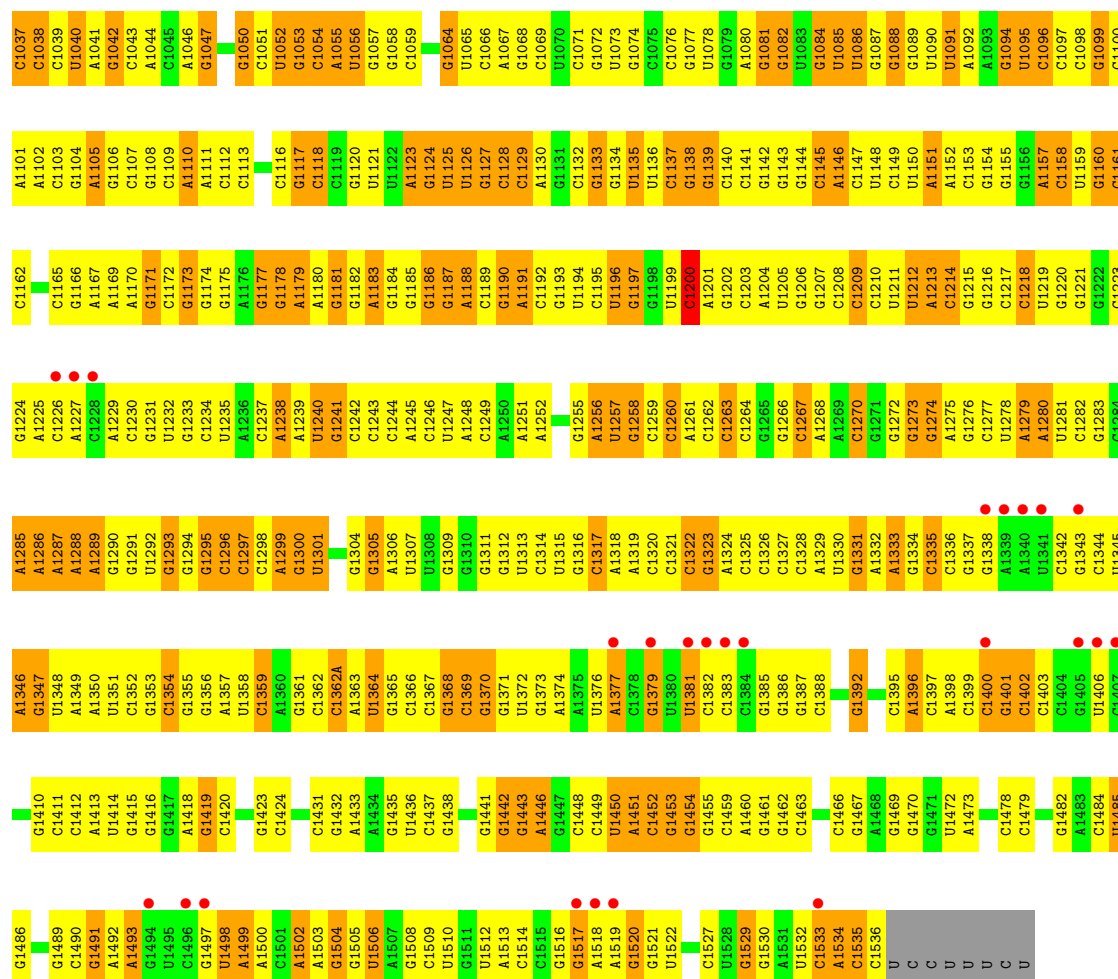
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
61	D8	1	Total 1	O 1	0	0
61	E8	1	Total 1	O 1	0	0
61	G8	1	Total 1	O 1	0	0
61	I8	1	Total 1	O 1	0	0
61	Q8	1	Total 1	O 1	0	0
61	1G	44	Total 44	O 44	0	0
61	5A	3	Total 3	O 3	0	0
61	BA	1	Total 1	O 1	0	0
61	14	411	Total 411	O 411	0	0
61	1J	11	Total 11	O 11	0	0
61	19	4	Total 4	O 4	0	0
61	29	3	Total 3	O 3	0	0
61	39	8	Total 8	O 8	0	0
61	35	2	Total 2	O 2	0	0
61	55	1	Total 1	O 1	0	0
61	E5	1	Total 1	O 1	0	0
61	F5	2	Total 2	O 2	0	0
61	L5	1	Total 1	O 1	0	0
61	M5	2	Total 2	O 2	0	0

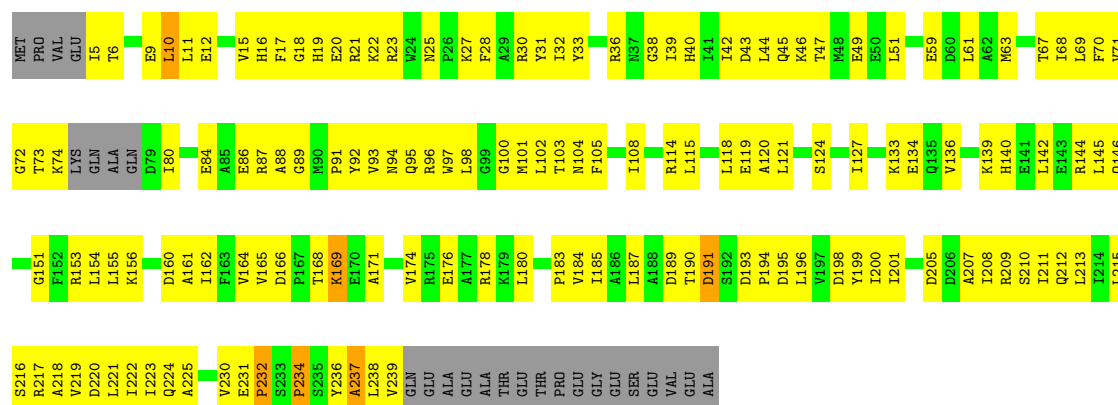






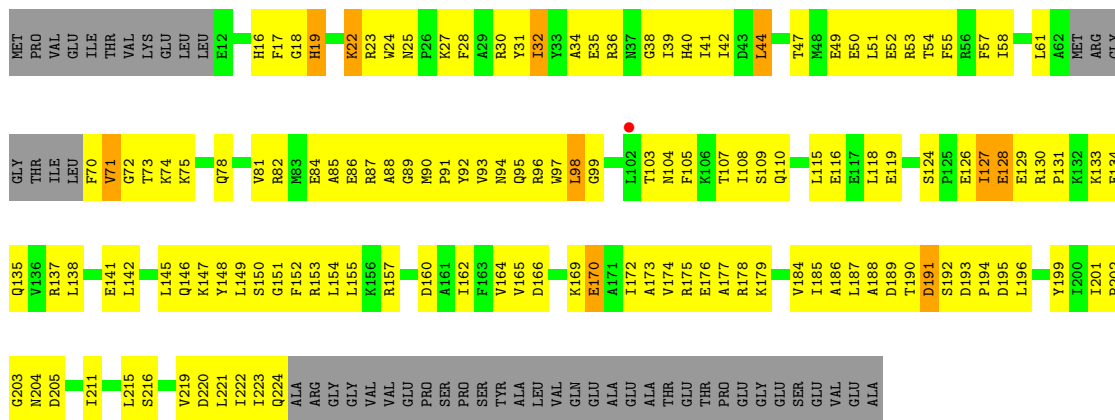
• Molecule 2: 30S ribosomal protein S2

Chain 1E: 34% 54% 10%

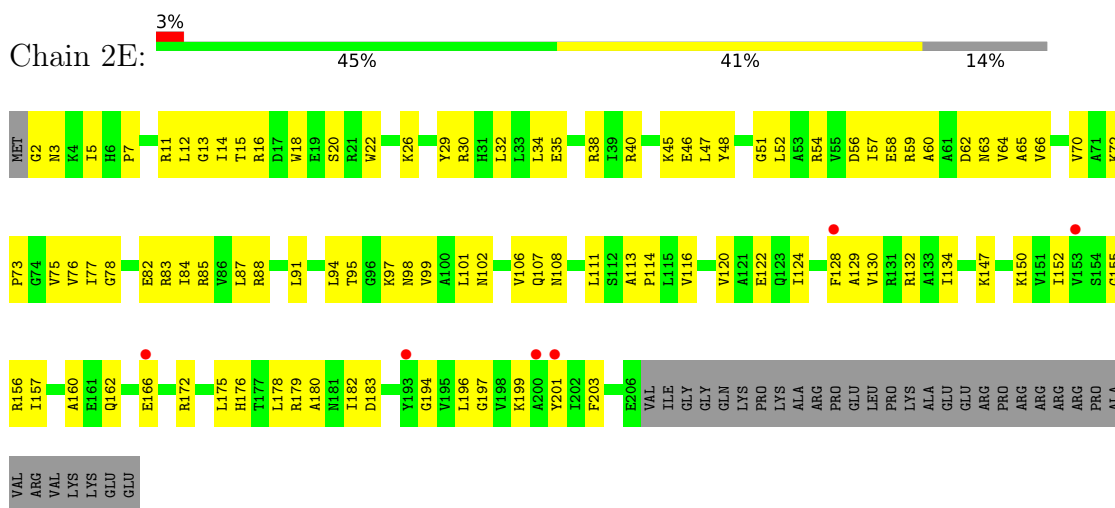


• Molecule 2: 30S ribosomal protein S2

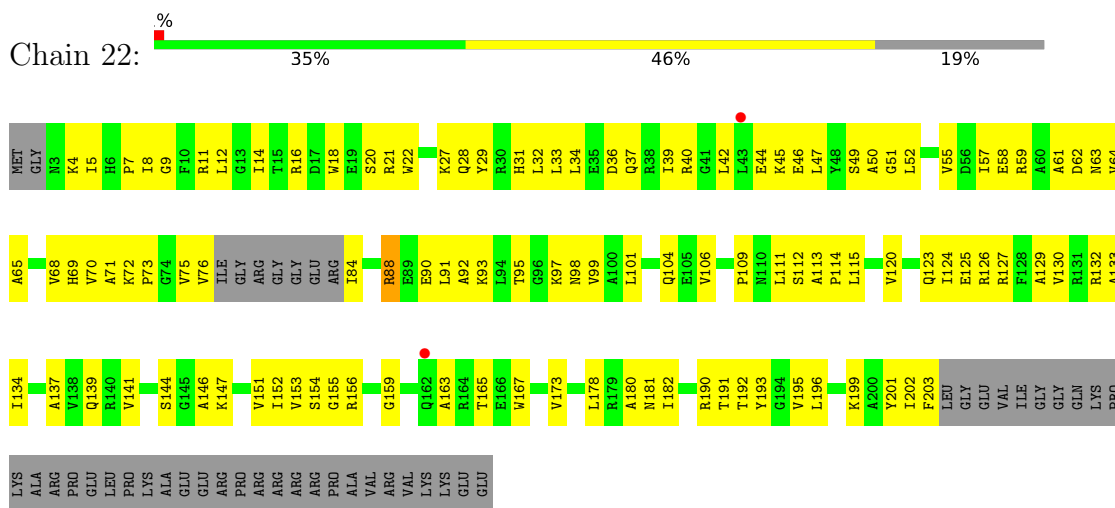
Chain 12: 27% 50% 20%



- Molecule 3: 30S ribosomal protein S3

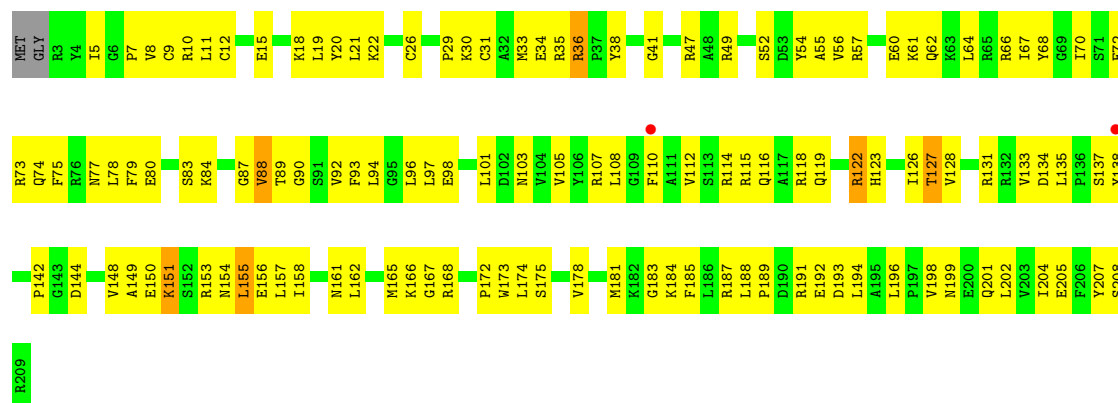


- Molecule 3: 30S ribosomal protein S3

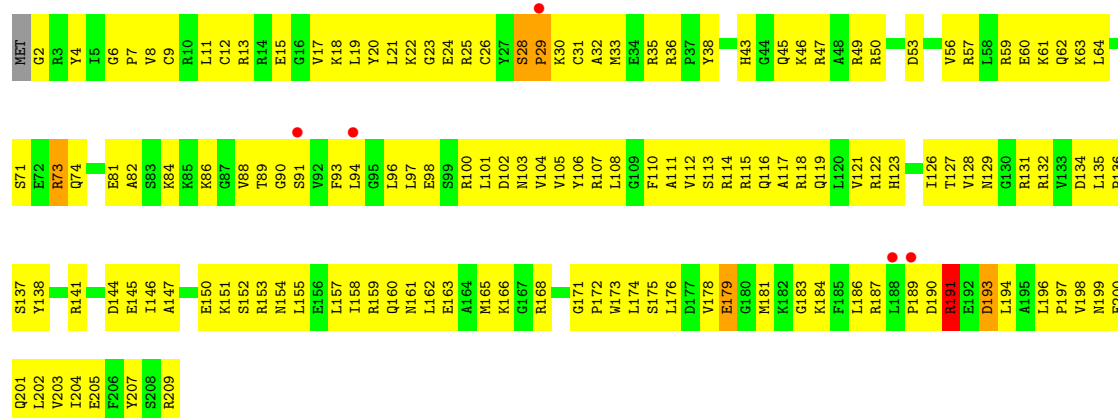


- Molecule 4: 30S ribosomal protein S4





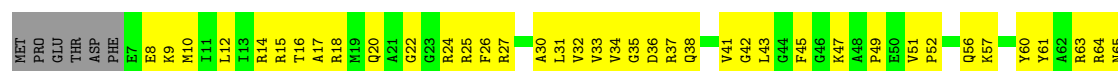
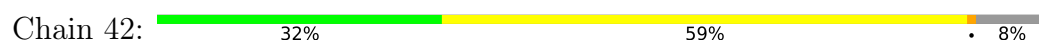
• Molecule 4: 30S ribosomal protein S4

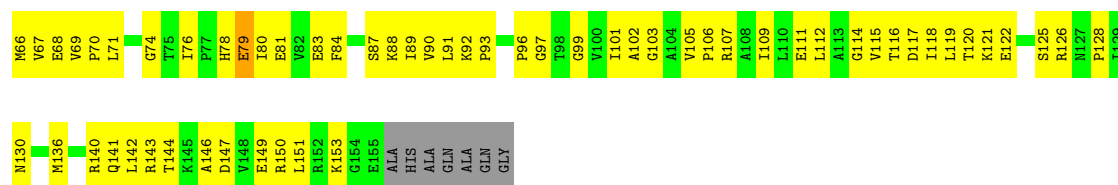


• Molecule 5: 30S ribosomal protein S5



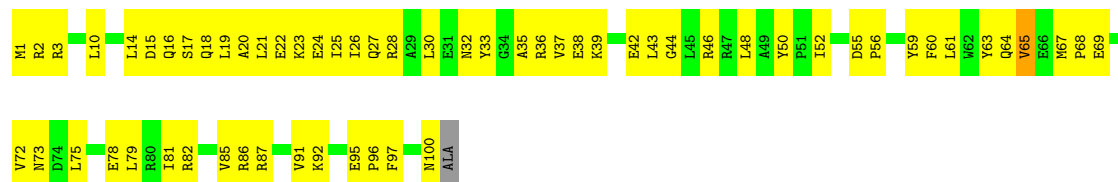
• Molecule 5: 30S ribosomal protein S5





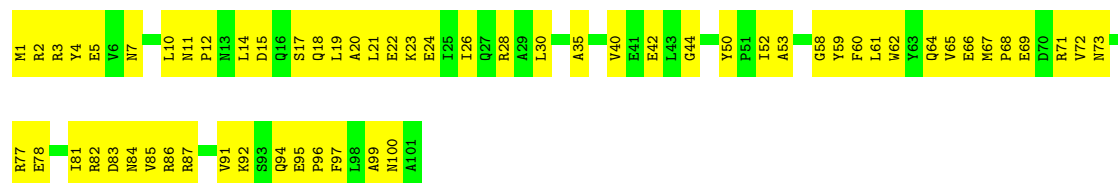
• Molecule 6: 30S ribosomal protein S6

Chain 5E: 39% 59% ..



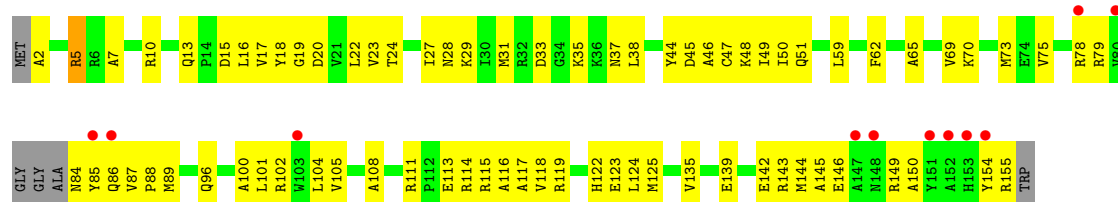
• Molecule 6: 30S ribosomal protein S6

Chain 52: 41% 59%



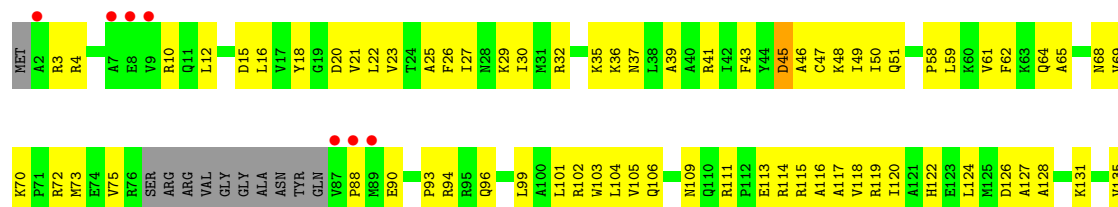
• Molecule 7: 30S ribosomal protein S7

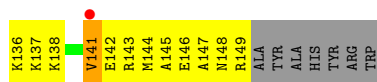
Chain 6E: 7% 49% 47% ..



• Molecule 7: 30S ribosomal protein S7

Chain 62: 5% 35% 52% 12%

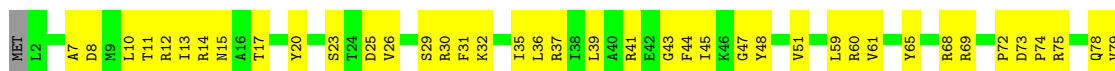




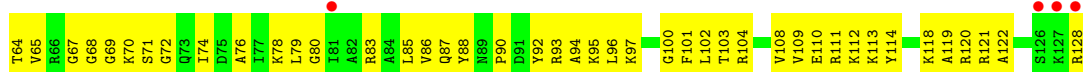
• Molecule 8: 30S ribosomal protein S8



• Molecule 8: 30S ribosomal protein S8



• Molecule 9: 30S ribosomal protein S9

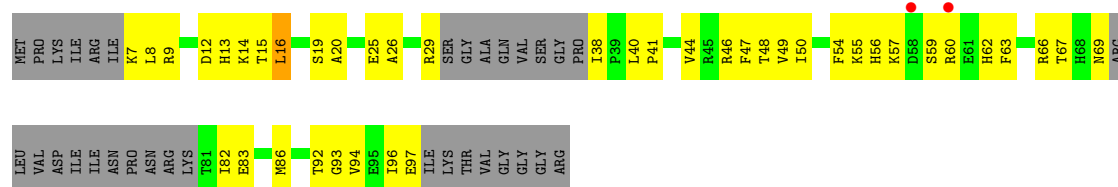


• Molecule 9: 30S ribosomal protein S9

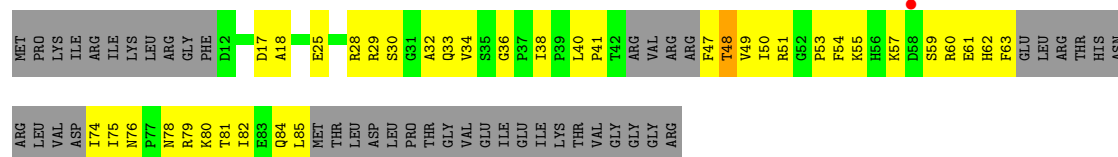
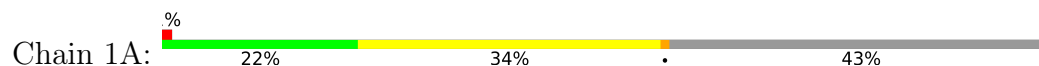


• Molecule 10: 30S ribosomal protein S10

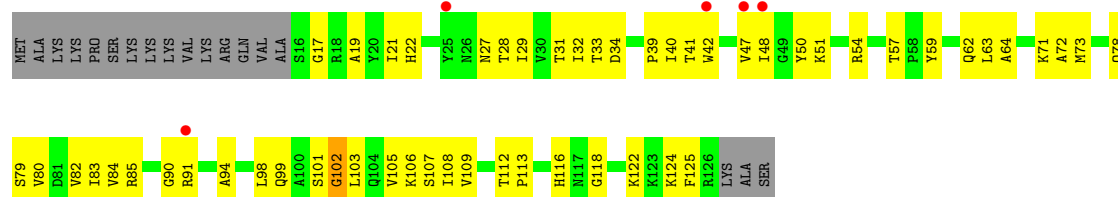
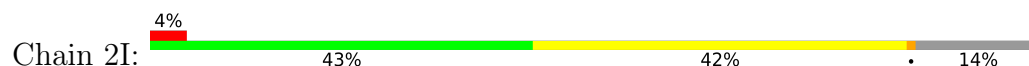




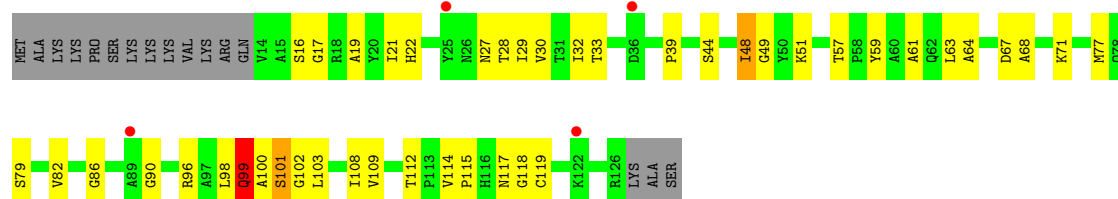
• Molecule 10: 30S ribosomal protein S10



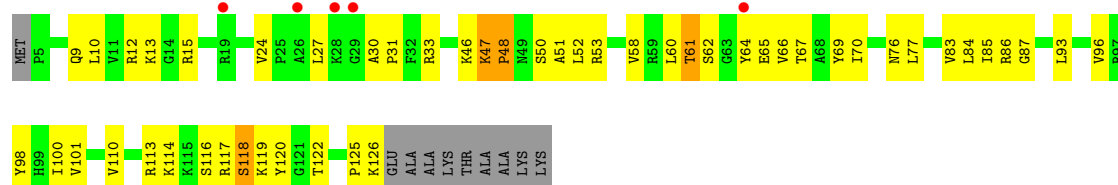
• Molecule 11: 30S ribosomal protein S11



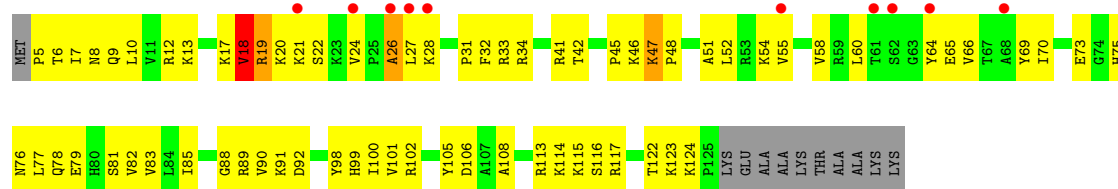
• Molecule 11: 30S ribosomal protein S11



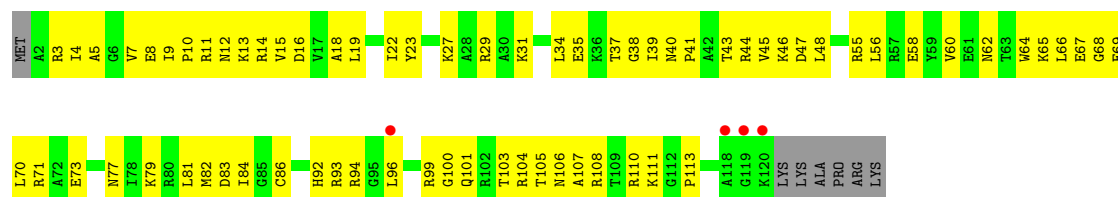
• Molecule 12: 30S ribosomal protein S12



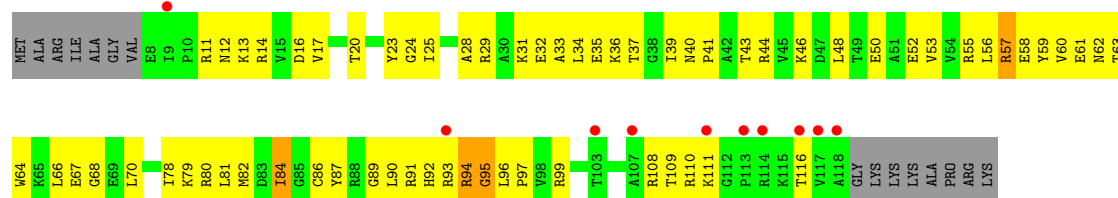
• Molecule 12: 30S ribosomal protein S12



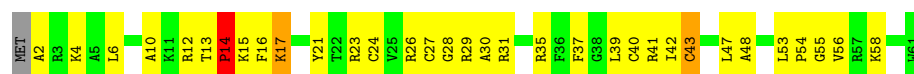
• Molecule 13: 30S ribosomal protein S13



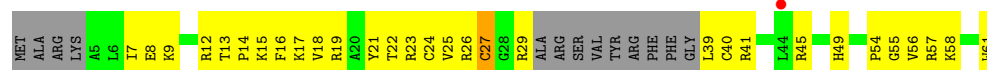
• Molecule 13: 30S ribosomal protein S13



• Molecule 14: 30S ribosomal protein S14 type Z

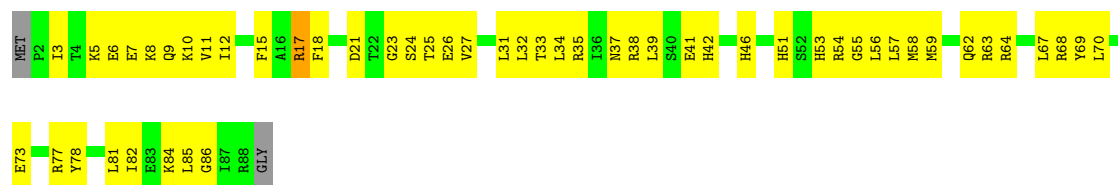


• Molecule 14: 30S ribosomal protein S14 type Z



• Molecule 15: 30S ribosomal protein S15

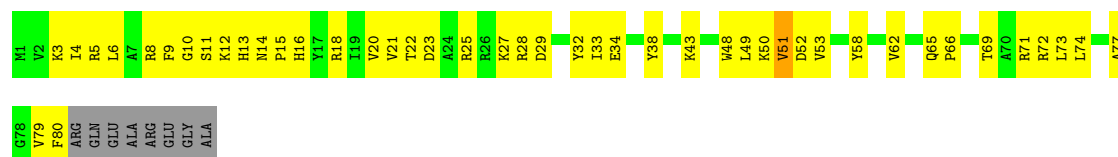




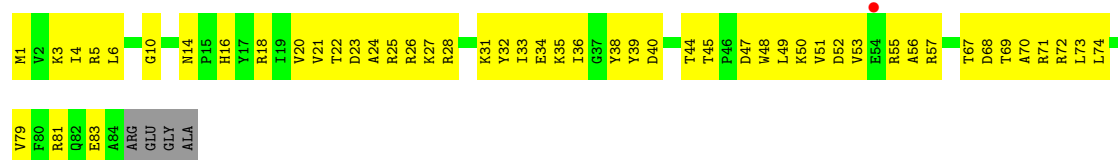
- Molecule 15: 30S ribosomal protein S15



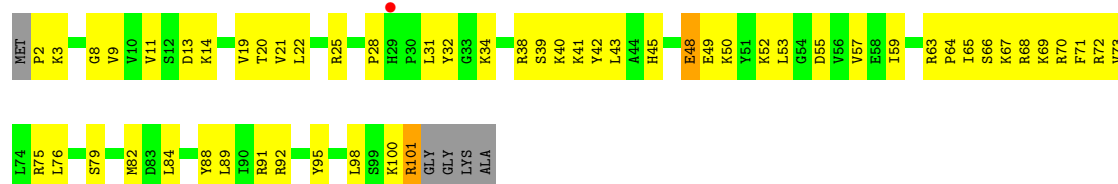
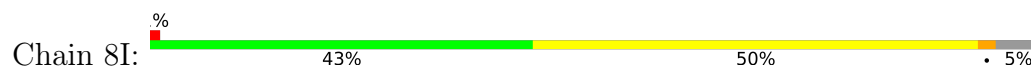
- Molecule 16: 30S ribosomal protein S16



- Molecule 16: 30S ribosomal protein S16



- Molecule 17: 30S ribosomal protein S17

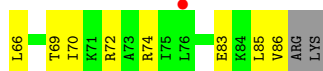


- Molecule 17: 30S ribosomal protein S17

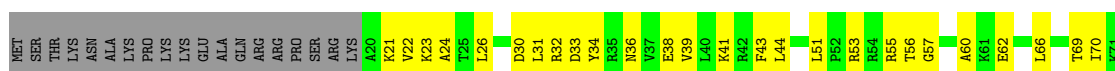




- Molecule 18: 30S ribosomal protein S18



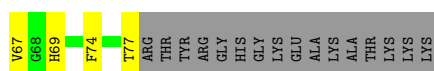
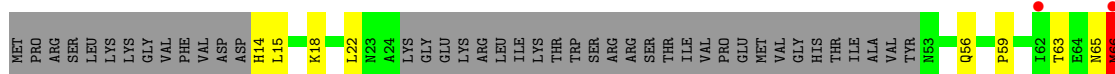
- Molecule 18: 30S ribosomal protein S18



- Molecule 19: 30S ribosomal protein S19

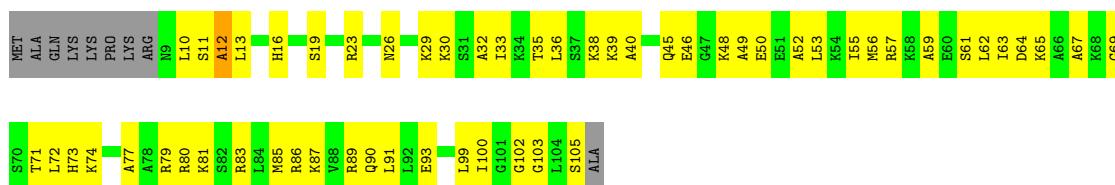


- Molecule 19: 30S ribosomal protein S19

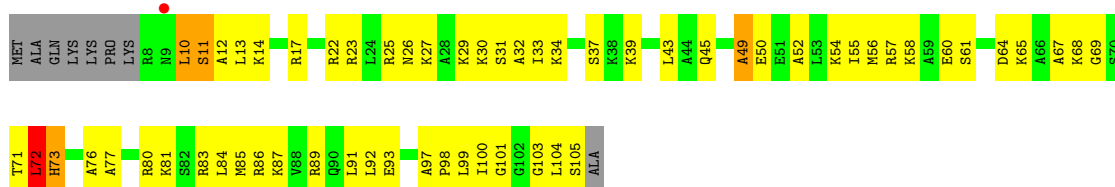


- Molecule 20: 30S ribosomal protein S20





- Molecule 20: 30S ribosomal protein S20



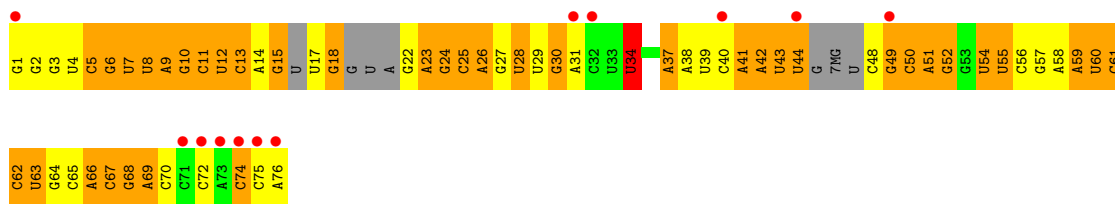
- Molecule 21: 30S ribosomal protein Thx



- Molecule 21: 30S ribosomal protein Thx



- Molecule 22: tRNA^{Lys}

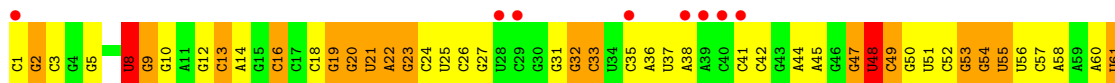


- Molecule 23: tRNA^{fMet}

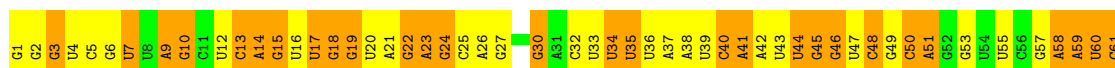




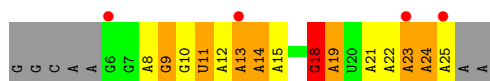
• Molecule 23: tRNA^fMet



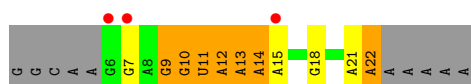
• Molecule 24: tRNA^{Lys}



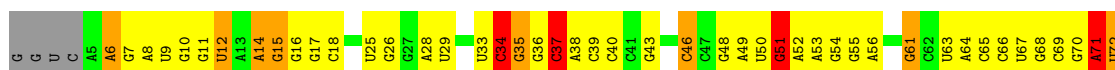
• Molecule 25: mRNA



• Molecule 25: mRNA

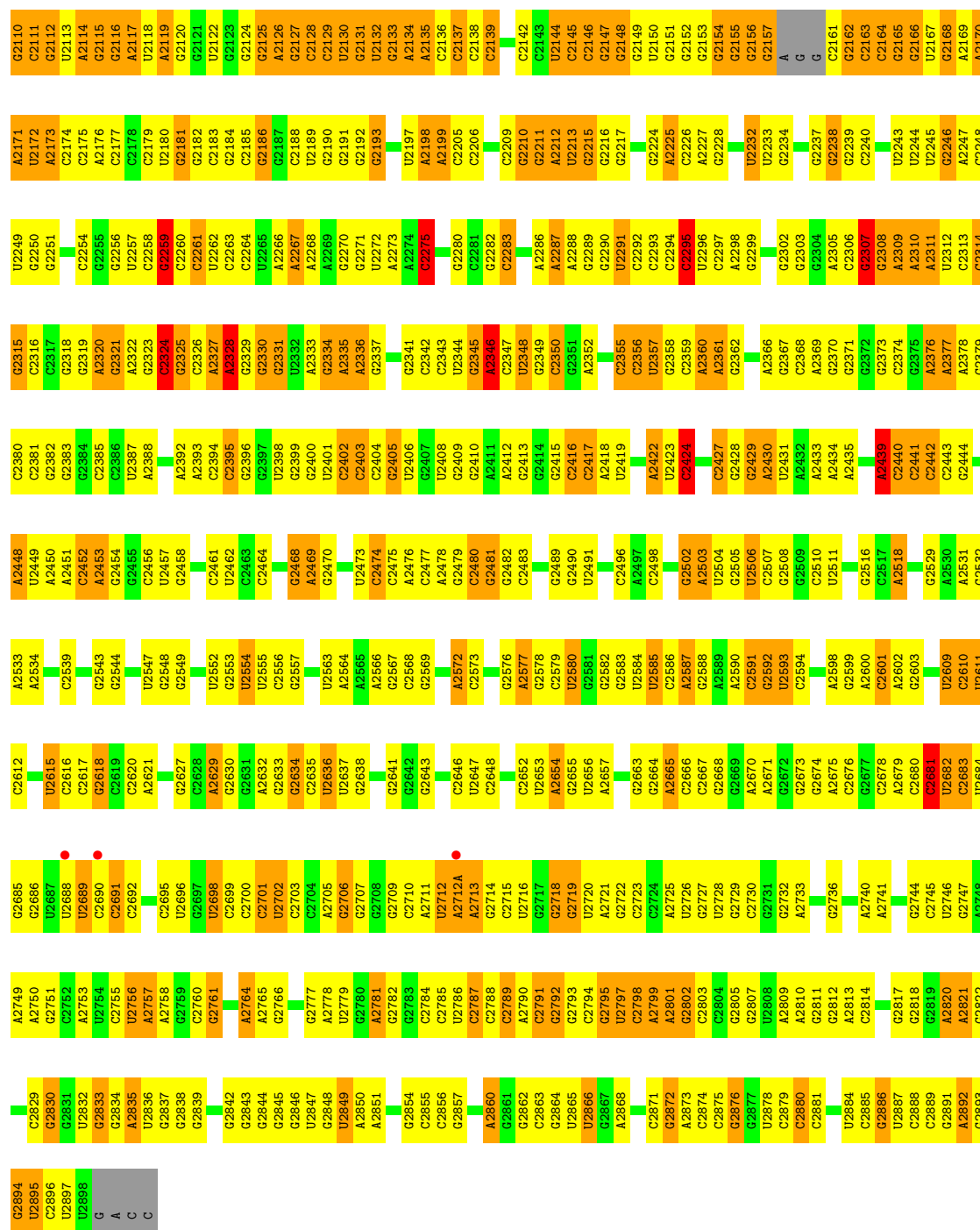


• Molecule 26: 23S ribosomal RNA

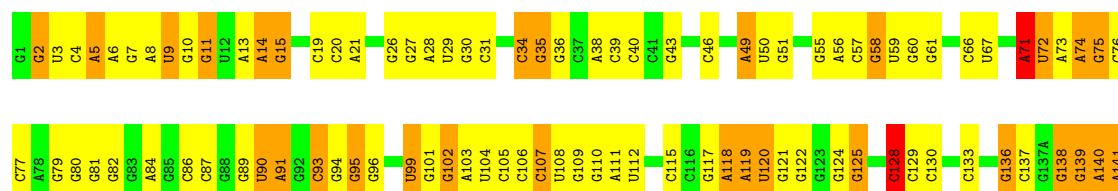




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C2043	A1978	A1901	U1805	G1731	C1588	U1522	C1458	A1392	G1328	G1259	G1193	A1126
C2044	C1979	C1806	A1654	A1732	C1589	U1523	C1459	A1393	C1329	G1260	G1194	A1127
C2045	G1980	G1903	C1656	G1733	U1590	G1524	A1460	U1394	U1329	C1261	G1195	A1128
G2046	A1981	G1904	C1657	C1735	G1591	G1525	A1461	U1395	A1331	A1262	G1196	A1129
U2047	C1982	C1905	C1658	G1736	C1592	G1526	G1462	U1396	G1332	U1263	G1197	U1130
G2048	C1983	G1906	U1659	G1743	G1593	A1527	C1463	U1397	C1333	G1264	U1133	U1133
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C2050	G1985	G1910	C1661	G1747	G1595	A1529	G1465	C1399	U1335	G1266	C1201	C1136
A2051	G1986	U1911	C1662	G1748	U1600	U1530	G1466	C1400	U1336	U1267	C1202	G1137
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G2053	A1913	G1815	A1664	G1750	C1600	G1534	G1468	C1402	G1338	A1269	U1205	G1139
G2054	G1816	G1750	A1665	C1751	C1601	U1535	A1469	C1403	G1339	G1270	G1206	C1140
C2055	G1817	C1752	A1666	G1753	U1602	U1536	A1470	C1404	U1340	G1271	C1207	U1141
G2056	U1818	G1754	C1670	A1755	A1603	G1537	A1471	U1405	U1341	A1272	U1208	U1142
A2057	U1819	C1755	C1671	G1756	G1604	G1538	A1472	U1406	A1342	U1273	G1209	A1142A
C2058	U1820	C1757	C1672	A1757	C1605	G1539	G1473	C1407	G1343	A1274	C1210	G1143
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G2062	A1829	A1760	C1675	C1761	A1609	U1543	A1477	G1419	G1347	G1280	G1218	G1154
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C2064	G1831	C1762	C1677	A1763	C1615	A1545	G1479	G1418	U1352	A1282	A1220	A1156
G2065	C1832	U1763	U1678	G1764	A1616	A1546	G1480	G1419	A1353	A1283	C1222	G1157
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C2068	C1835	C1767	C1682	C1767	G1619	C1549	G1484	G1422	G1356	A1286	G1227	G1160
G2069	G1836	U1768	C1683	G1768	G1620	U1550	A1485	G1423	G1357	A1287	A1227	C1161
G2070	C1837	C1769	C1684	G1769	G1621	C1551	A1486	G1424	U1357	G1288	G1228	G1162
U2074	G1843	U1770	C1685	G1770	U1622	G1552	G1487	G1425	G1358	U1289	G1229	G1163
U2075	C1844	G1771	C1686	G1771	G1623	A1553	G1488	G1426	A1359	C1291	G1229A	G1164
U2076	G1845	G1772	C1687	G1772	G1624	U1554	U1489	A1427	G1360	U1292	C1230	U1165
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C2081	G1847	U1774	C1689	U1774	C1626	G1556	G1492	G1429	G1364	U1294	G1232	U1167
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G2087	G1857	U1777	U1692	U1777	U1629	G1559	A1495	C1432	G1369	G1297	G1235	G1170
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G2095	C1870	A1783	G1696	A1783	A1634	G1563	C1499	G1436	A1302	G1303	G1239	U1175
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C2097	G1878	A1786	C1699	A1786	A1637	A1566	C1504	A1439	G1373	G1306	A1242	C1178
G2098	C1879	G1787	G1703	G1787	C1638	A1567	U1508	G1441	C1376	G1307	G1243	C1179
U2099	G1883	C1788	G1704	C1788	U1639	G1568	A1509	G1442	G1377	G1310	G1244	C1180
G2100	A1884	A1789	G1705	A1789	C1640	A1569	A1510	G1443	A1378	G1311	G1245	G1181
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G2108	G1897	G1799	G1650	G1799	A1642	C1581	C1518	C1451	C1386	G1322	G1256	A1189
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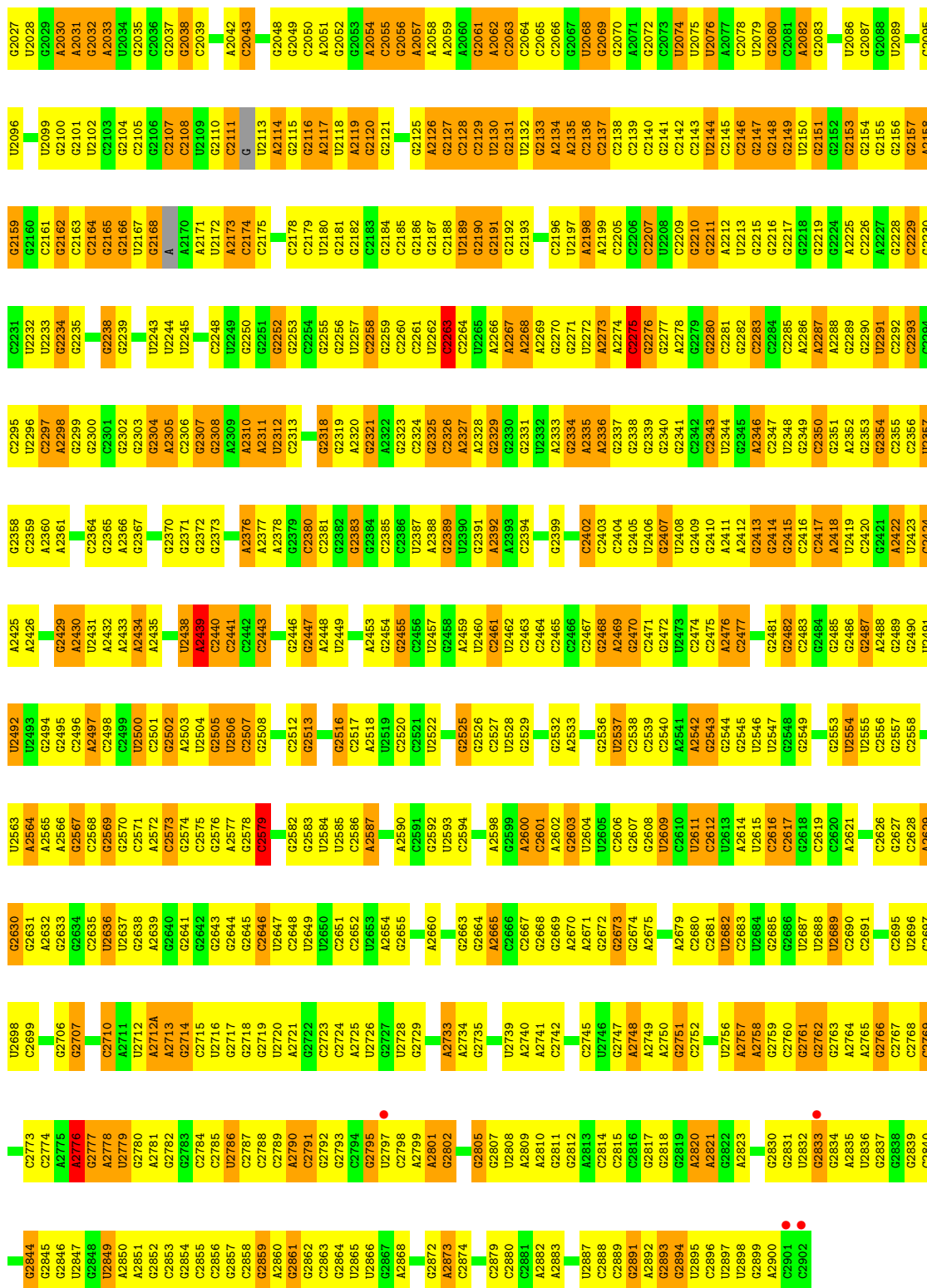


• Molecule 26: 23S ribosomal RNA



A983	G920	G859	G795	G730	G654R	G609A	G545	G473	G403	A324	G270V	G219	C141A
G986	G921	U860	G796	G731	G654S	C610	C946	G474	C404	G329	G270Y	G220	G142
G987	U922	A861	G732	G732	A654T		A547	G475	C405	A330	G270Y	A221	C143
A988	G923	G862	G733	G733	A654U	U614	A548	U475	C406	A331	G270Z	A222	G145
G989	G924	A863	G734	G734	G656	A616	G549	A479	C409	A332	C271A	G224	G146
A990	G925	G864	A735	A735	U657	A617	G550	A480	C410		G271B	A225	
A991	A926	C965	A802	G736	C658	G618	U553	G481	G411		U271C	G226	A149
G992	G928	A866		G737	G659	C618A	U554	A482	C412		G271C	A227	C150
G993	G929	U868	G805	G738	C660	G619	U555	A483	C413		G271C	G228	C151
G994	U930	U869	C806	G739	G661	G620	U556	A484	C414		G271C	A229	G152
C995	G931	G869	U807	G740	G662	A621	G558	C485			G271A	G273	C153
A996	G932	A870	G808	G741	G663	G622	G559	C486			G271B		G154
A997	A933	U871	G809	G742	G664	G623	C560		U421		C273C	A233	G155
G997		A872	U810	G743	C665	G624	U562	G493	A422		G273D	C234	
G998	U937	G873	U811	G744	C666	G625	G561	G494	A423		U273E	U285	U
G999	G938	G874	G812	G745	G668	G626	U562	G495	A424		G273F	C236	U
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A1001	G940	C976	C814	U747	A670	G628	C565	A502	C426		G275	G240	U162
G1002	A941	U877	C815	G748	A671	G629	C566	A503	C427		G276	A241	G171
G1003	G942	A878	C816	G749	C671	G630	U566	U504	U428		C277	G242	G172
C1004	U943	C817	C817	A750	C672	A631	U567	U505	A429		G278	C172	G173
C1005	G944	G818	U818	A751	C673	A632	U568	A506			G279	U243	G174
C1006	A945	A819	A752	A752	C674	G633	U569	G506				G174	C174
C1007	G946	G	A820	C753	A675	A633	G570	A507	A432			A282	G175
C1008	G947	G	A821	C754	A676	C634	A571	A508	C433			G247	G176
A1009	G948	C	U822	C755	A677	C635	A572	C509	U434			G248	G177
A1010	G949	C	G823		C678	G636	G573	C510	C435			G249	G178
G1011	G950	C	A824	A761	G682	A637	C574	U511	G436			G250	G179
G1012	C951	A	C825	U762	G683	G638	A575	A512	G438			G251	G180
C1013	G952	C	U826	G763	G683	U639	G576	A513				G252	A181
U1014	A953	C	U827	A764	G684	C640	G577	A514	U441			G253	A182
G1015	G954	A	U828	G765	A685	C641	A578	A515	C442			G254	C183
G1016	C955	G	A829	C766	G686	G642	G579	A516	A443			A285	C184
G1017	G956	C	G831	U767	C687		C580	C517	C444			G259	U185
C1018	A957	C	G832	G768	U688	G647	G582	U519	C445			G260	G186
U1019	U958	U	G833	G769	A689	A648	G583	G520	C446			G261	G187
A1020	A959	A896	H833	G770	G690	G647		G521	A447			A282	G188
A1021	A960	C897	C834	G771	C691	G648		G522	G450			C283	G189
G1022	C961	G898	A835		C692	G649		C523	C451			A285	A190
U1023	G962	A900	G836	A774	G693	G650		U524	C452			G266	C192
G1024	U963		C837	G775	G698	G651		U525	C375			G267	U193
G1025	A1026	A901	C838	G776	A699			A526	C376			G268	G194
U1026	G966	C902	U839	A777	G700	A654A		C527	G382			U269	A195
A1027	C967	C903	C840	G778	G704	C654B		A528	U383			C270C	A196
A1028	G968	C904	A841	U779		G654C		G529	U384			G270E	C198
A1029	U969	U905	G842	G780	G704	G654D		C530	A310			U270F	A199
				A781				A532	G385			G270G	G205
U1033	G971	U907	C846	A782	C708	C		G533	A311			G270G	U206
G1034	G972	A783	U847	A783	U709	C		U534	A314			C270K	C210
U1035	A973	A909	G848	A784	C	C		C535	G315			U270L	A211
G1036	G974	A910	A849	G785	A717	G		A536	G316			U270M	G212
					A718	C		C537	G317			G270N	A213
C1040	C974A	C912	C850	U787	A722	A		G539	G318			U270O	G214
G1041	G975	U913	U851	G788	G723	C		A466	C392			U270P	G215
C1042	G976	C914	G853	A789	U724	G		G467	U395			G270Q	A216
G1043	G977	C915	G854	C790	G725	G		C468	G396				
G978	G978	G916	G855	G791	G726	G		C469					
A980	A980	A917	C856	G792	G726	G		A470	G399				
A981	A981	A918	C857	A793	G729	C		A471	G400				
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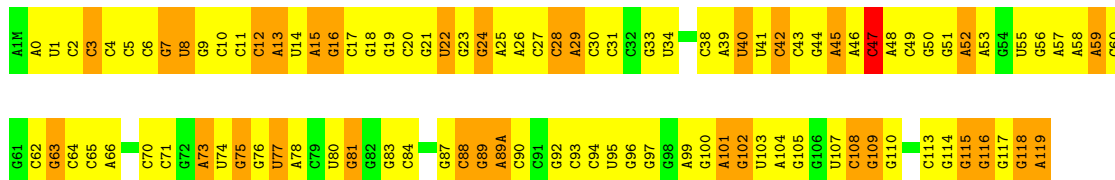
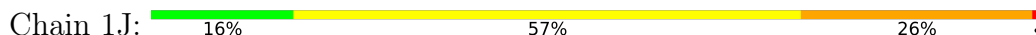
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U1963	G1899	G1817	G1666	C1591	C1531	C1463	C1399	G1327	G1249	G1176	C1309	A1049
G1964	A1900	C1752	G1667	C1592	C1532	C1464	G1400	C1328	G1250	A1177	C1109	A1050
G1965	A1901	G1753	A1668	G1593	C1533	G1465	U1329	U1325	G1251	G1178	A1111	G1051
A1966	C1902	U1820	A1669	G1594	G1534	G1403	C1403	C1330	G1252	C1179	G1112	C1052
A1967	G1903	A1821	C1670	U1595	U1535	C1404	C1404	A1331	A1263	C1180	U1113	C1053
G1968	G1904	G1756	U1671	A1596	A1536	U1405	U1405	G1332	A1264	C1181	G1114	A1054
A1969	G1905	U1757	G1758	A1597	C1537	U1406	U1406	G1337	U1255	A1182	G1115	G1055
A1970	G1906	G1758	C1598	C1598	G1538	C1407	C1408	G1338	G1256	G1183	G1116	G1056
A1971	A1970	A1759	A1602	U1602	G1540	C1474	A1412	G1339	A1262	C1185	G1117	A1057
A1972	G1910	A1762	A1603	U1603	C1541	C1475	A1413	U1340	U1265	G1186	G1122	G1058
G1973	U1911	G1763	C1604	C1604	G1542	A1477	G1413	U1341	G1264	G1187	G1125	U1060
C1974	A1912	G1764	U1679	A1543	A1543	G1478	G1416	A1342	A1265	U1188	A1126	U1061
G1975	C1832	G1680	G1681	C1544	U1480	G1479	G1417	U1342	G1266	A1189	A1127	G1062
A1981	U1913	U1834	C1684	A1545	U1481	G1480	G1418	C1346	G1271	G1190	A1128	G1063
C1982	A1915	G1765	C1685	A1546	U1482	A1419	G1419	G1347	G1272	G1191	A1129	C
G1983	U1917	G1770	G1686	C1547	A1486	U1420	U1420	G1348	A1273	G1192	A1130	U
G1984	A1918	C1771	G1687	C1548	G1487	G1421	G1421	A1349	G1272	G1193	U1131	U
G1985	A1919	G1772	U1688	C1549	G1488	G1422	G1422	U1352	A1275	G1194	G1131	A
G1986	C1920	A1616	A1689	C1550	U1489	G1423	G1423	U1357	G1275	G1195	G1135	G
G1989	G1921	C1774	A1689	C1551	G1490	G1424	G1424	U1358	A1275	G1196	C1135	A1069
G1990	G1922	U1775	U1692	G1552	G1491	G1425	G1425	U1198	A1278	U1199	G1136	A1070
U1991	U1923	G1776	U1693	A1553	G1492	G1426	G1426	U1199	G1279	G1200	G1137	G1071
G1992	C1924	U1777	C1625	A1554	C1493	A1427	A1427	G1355	G1279	G1201	G1138	C1072
U1993	G1925	U1778	C1694	G1555	C1493	G1428	G1428	G1356	G1279	G1202	G1139	A1073
G1994	U1926	U1779	G1695	C1556	A1496	G1429	G1429	U1357	U1282	C1202	C1140	G1074
A1995	U1926	A1770	G1696	C1557	U1497	G1430	G1430	A1359	G1283	G1203	G1141	C1075
G1996	A1927	G1781	G1697	C1558	C1498	U1431	U1431	C1363	A1284	A1204	U1142	C1076
A1997	A1928	C1782	A1698	C1559	C1499	G1432	G1432	G1364	G1285	U1205	A1142A	A
G1998	G1930	A1783	C1699	G1560	G1500	U1433	U1433	G1365	A1286	U1205	A1143	U
U1999	U1931	A1784	A1700	G1561	U1503	G1434	G1434	G1366	A1287	A1210	G1144	C
G2000	A1932	G1785	A1701	C1562	C1504	G1435	G1435	A1367	U1288	G1211	C1145	U
A2001	G1933	A1786	G1702	G1563	C1505	G1436	G1436	G1368	C1289	G1212	G1145	A
G2002	C1934	A1787	G1703	C1564	C1505	G1437	G1437	G1369	G1290	A1213	U	U
G2003	G1935	C1788	G1704	C1565	C1506	U1438	U1438	C1370	G1291	G1218	G1149	U
A2004	A1936	A1789	G1705	A1566	A1507	A1439	A1439	G1371	U1292	G1219	C1150	A
G2005	A1937	C1790	C1706	C1566	A1508	G1440	G1440	U1372	C1293	G1219	G1151	A1085
C2006	U1938	G1791	C1710	A1567	C1509	G1441	G1441	A1373	G1296	A1220	C1152	A1086
C2007	U1939	A1641	C1711	G1568	C1510	G1442	G1442	G1374	G1297	C1221	C1153	G1087
U1940	C1940	G1642	C1712	A1569	A1511	G1443	G1443	C1375	G1298	C1222	G1154	A1088
C1941	C1941	G1643	C1713	A1570	G1512	G1444	G1444	C1376	G1299	G1223	A1155	G1089
C1942	C1942	C1644	C1714	A1571	G1513	A1444A	A1444A	G1377	U1300	C1225	G1157	U1090
A2013	U1943	G1645	C1715	A1572	U1514	C1445	C1445	A1378	G1299	G1225	C1158	G1091
U1944	C1880	C1646	C1574	C1515	C1446	G1447	G1447	A1379	A1302	G1229A	U1159	C1092
G1945	U1945	G1647	C1575	U1516	G1448	G1448	G1448	G1380	G1303	C1230	G1160	U
U1946	U1946	C1648	U1576	U1517	G1517	G1448	G1448	G1381	G1303	G1231	C1161	A
C1982	C1882	C1800	G1728	C1577	C1518	A1449	A1449	A1384	G1309	G1236	G1162	U
U2016	G1883	G1801	A1729	U1578	G1519	G1449A	G1449A	A1385	G1310	A1237	G1163	A1098
U2017	A1884	A1802	A1652	U1579	U1520	C1450	C1450	G1386	G1310	G1238	G1164	G1099
G2018	A1885	G1730	G1653	A1580	G1521	C1451	C1451	C1387	U1316	G1239	U1165	G1099
A2019	G1950	A1803	G1732	G1581	G1522	A1453	A1453	C1387	A1317	G1239	C1166	C1100
U1951	C1887	C1804	C1733	C1582	U1524	G1454	G1454	G1388	U1240	A1241	G1167	U1101
C2021	A1952	U1805	C1734	C1583	G1524	G1455	G1455	G1389	G1319	A1241	C1168	C1102
U1953	A1953	C1806	C1735	C1585	G1525	G1456	G1456	U1390	C1320	A1242	G1169	A1103
G2023	G1954	C1806	C1735	C1586	G1526	G1456	G1456	U1391	A1322	A1243	G1170	C1104
U1955	U1955	A1812	C1741	A1586	G1527	G1459	G1459	A1392	A1322	G1243	G1171	U1105
C2025	G2025	C1742	U1659	A1587	G1528	A1460	A1460	A1392	A1322	G1243	G1171	C1105
C2026	C1958	G1743	C1660	C1588	A1528	A1460	A1460	A1393	G1322	A1246	G1173	G1106



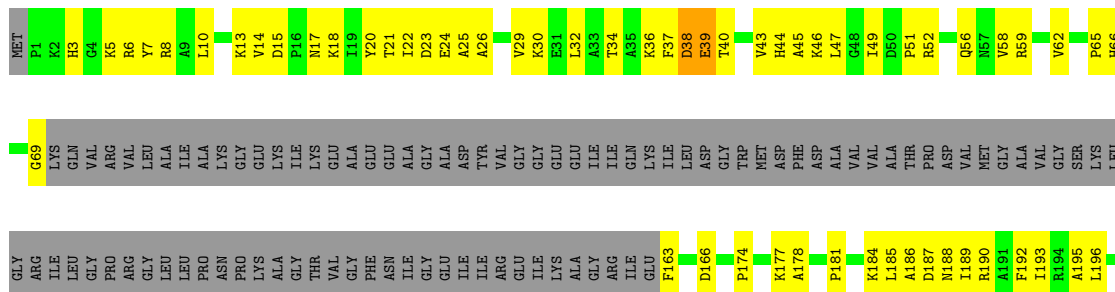
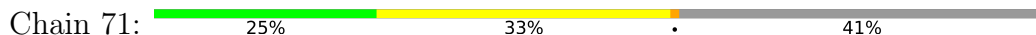
• Molecule 27: 5S ribosomal RNA

Chain 16: 31% 53% 13%

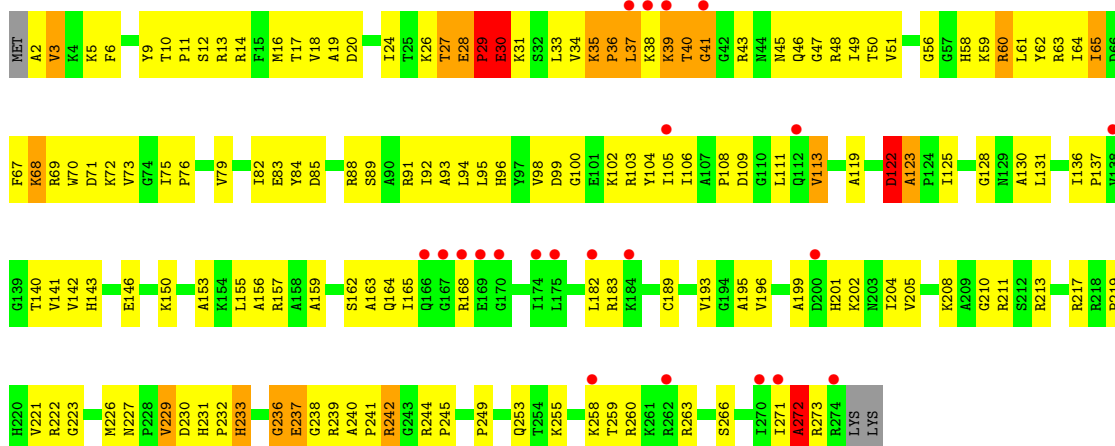
- Molecule 27: 5S ribosomal RNA



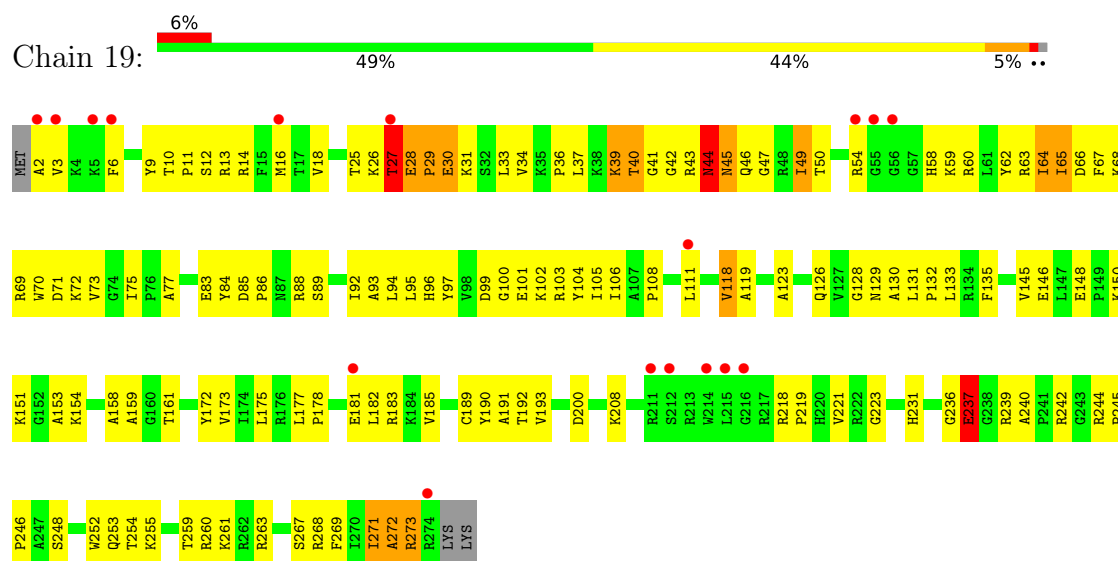
- Molecule 28: 50S ribosomal protein L1



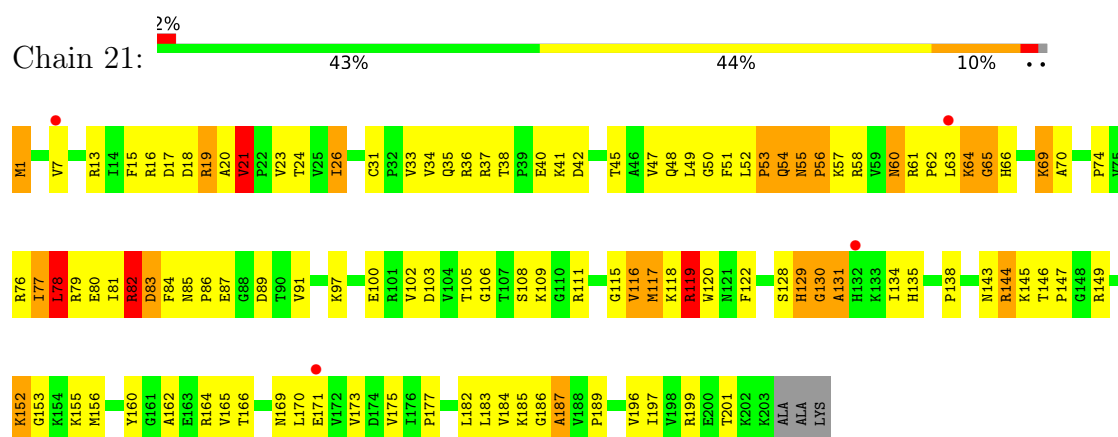
- Molecule 29: 50S ribosomal protein L2



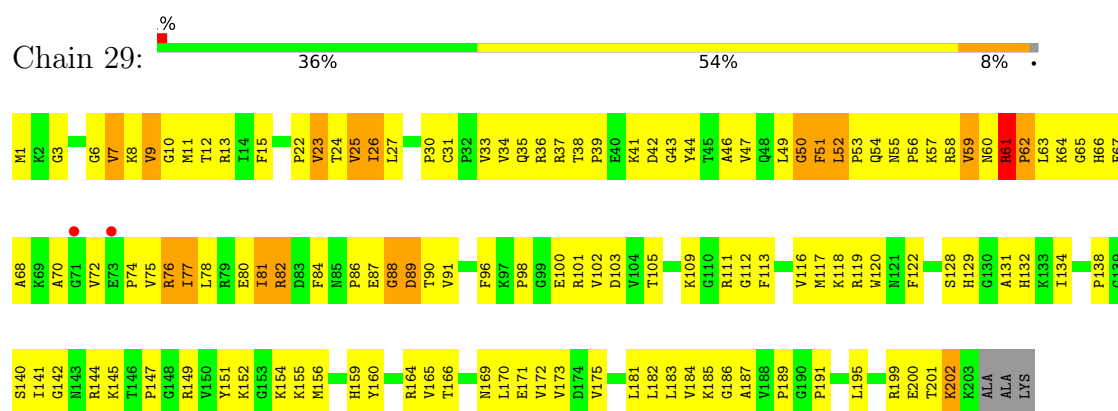
• Molecule 29: 50S ribosomal protein L2



• Molecule 30: 50S ribosomal protein L3



• Molecule 30: 50S ribosomal protein L3

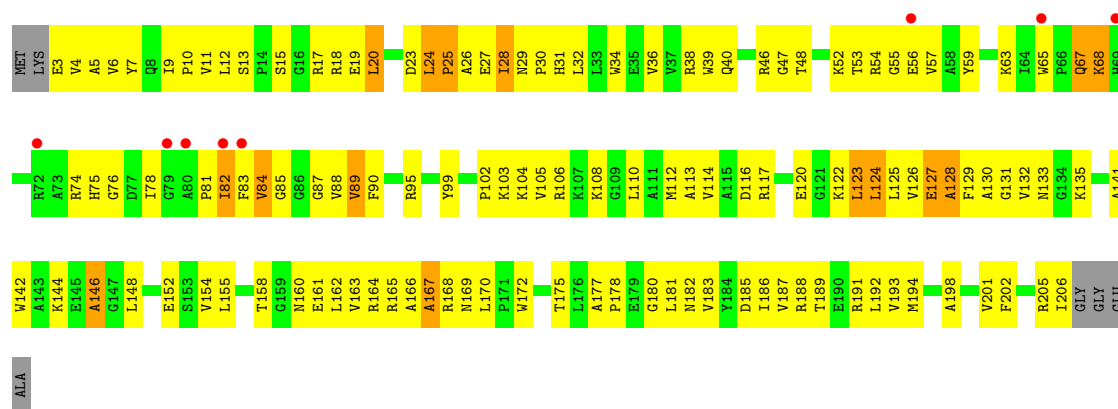


• Molecule 31: 50S ribosomal protein L4

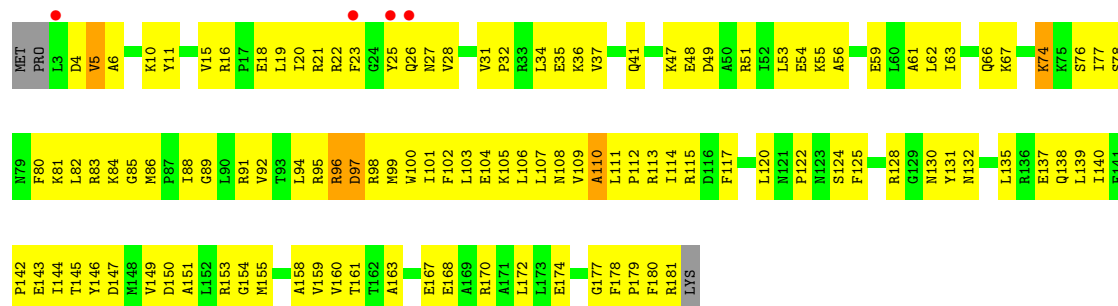




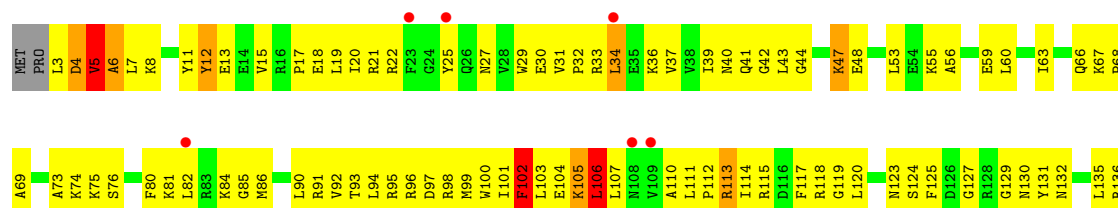
• Molecule 31: 50S ribosomal protein L4



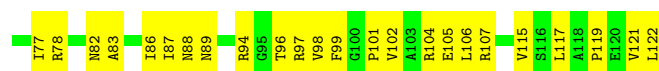
• Molecule 32: 50S ribosomal protein L5



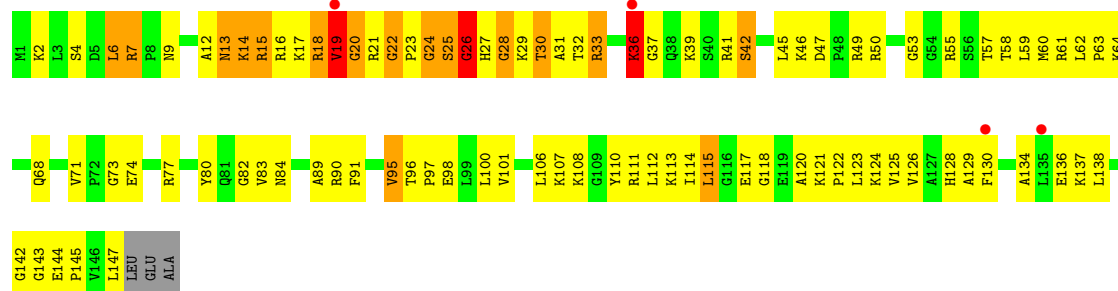
• Molecule 32: 50S ribosomal protein L5



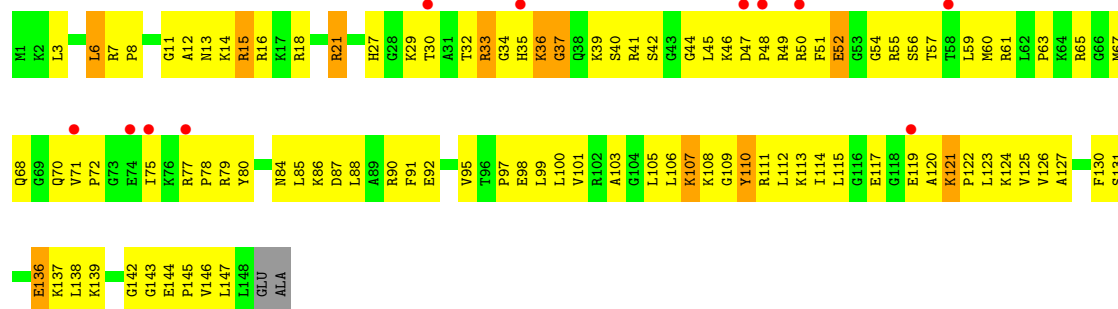




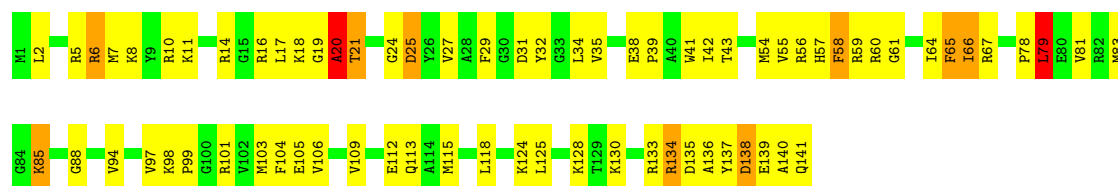
• Molecule 37: 50S ribosomal protein L15



• Molecule 37: 50S ribosomal protein L15

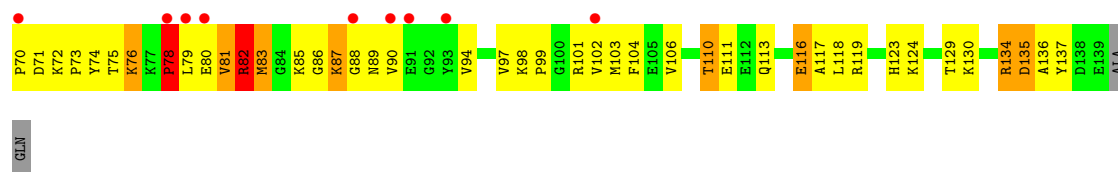


• Molecule 38: 50S ribosomal protein L16



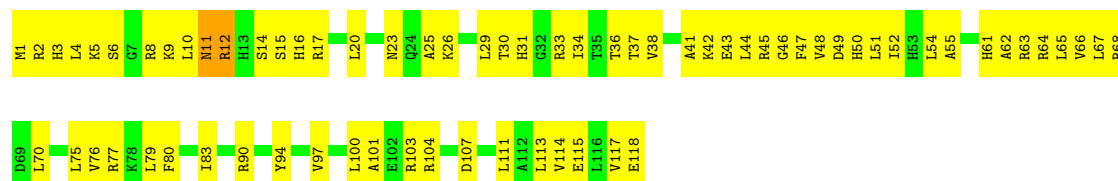
• Molecule 38: 50S ribosomal protein L16





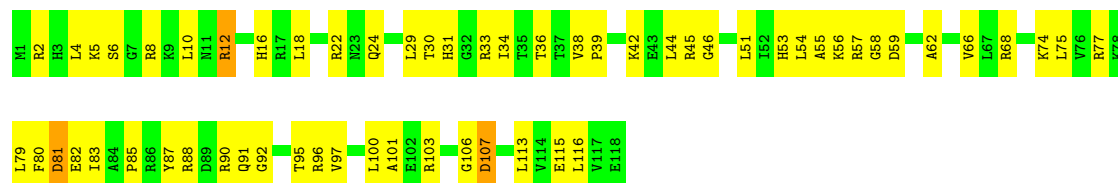
- Molecule 39: 50S ribosomal protein L17

Chain 98: 41% 58%



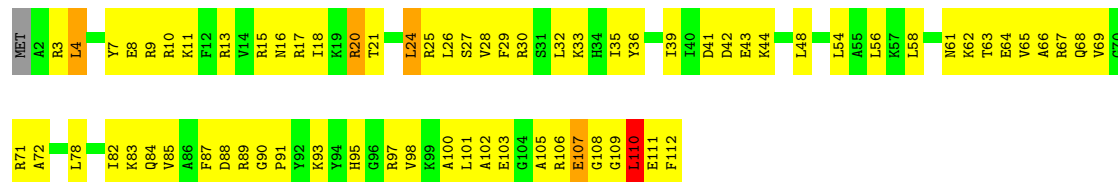
- Molecule 39: 50S ribosomal protein L17

Chain 55: 50% 47%



- Molecule 40: 50S ribosomal protein L18

Chain A8: 36% 59%



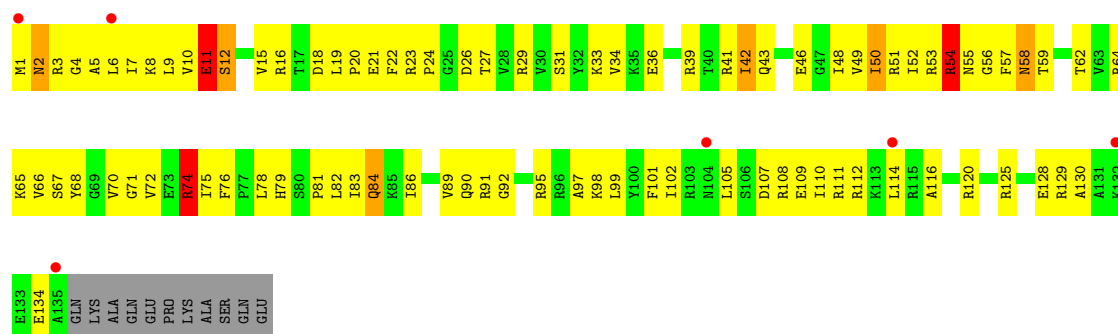
- Molecule 40: 50S ribosomal protein L18

Chain 65: 36% 60%

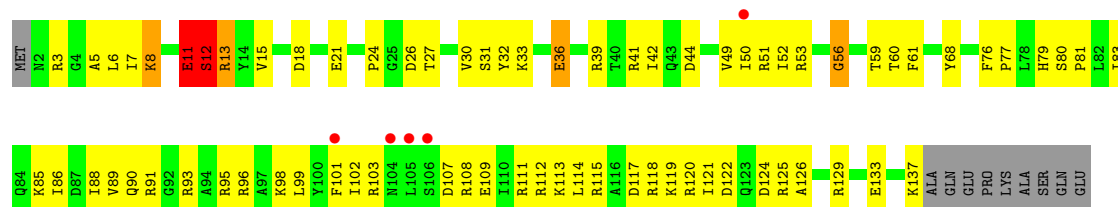
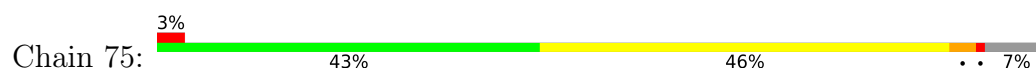


- Molecule 41: 50S ribosomal protein L19

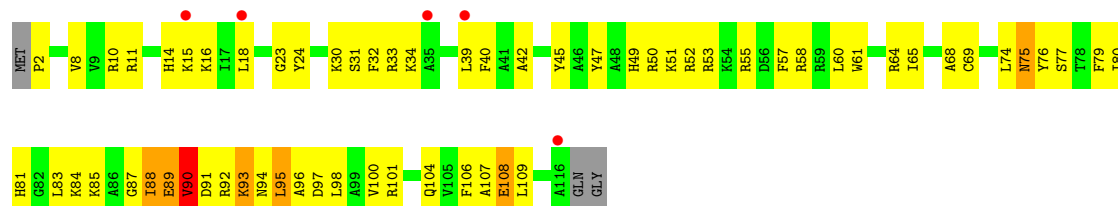
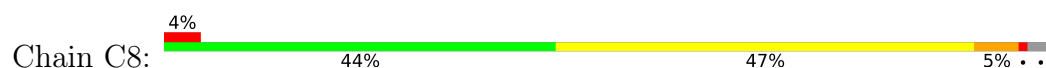
Chain B8: 4% 32% 55% 8%



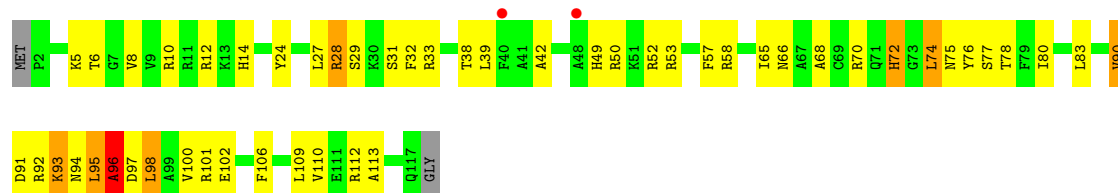
• Molecule 41: 50S ribosomal protein L19



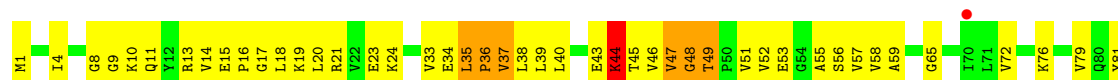
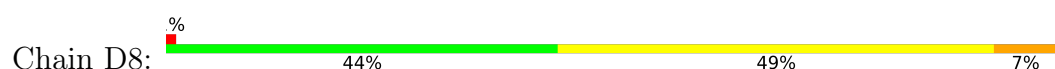
• Molecule 42: 50S ribosomal protein L20

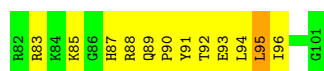


• Molecule 42: 50S ribosomal protein L20

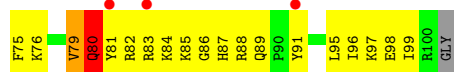


• Molecule 43: 50S ribosomal protein L21

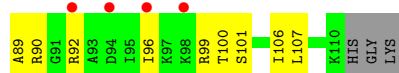
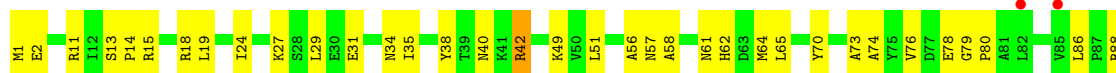




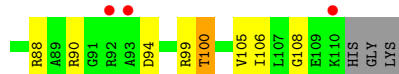
- Molecule 43: 50S ribosomal protein L21



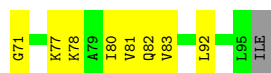
- Molecule 44: 50S ribosomal protein L22



- Molecule 44: 50S ribosomal protein L22

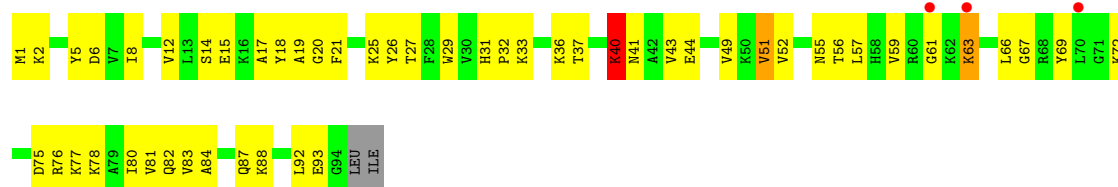


- Molecule 45: 50S ribosomal protein L23

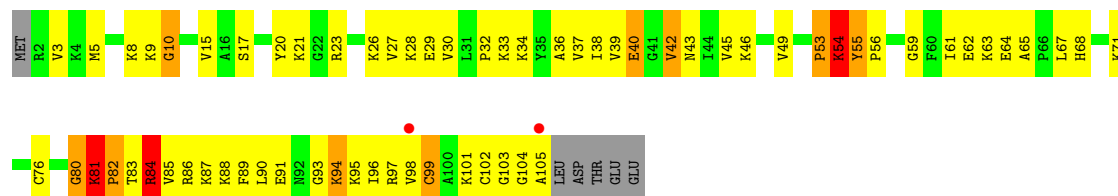


- Molecule 45: 50S ribosomal protein L23

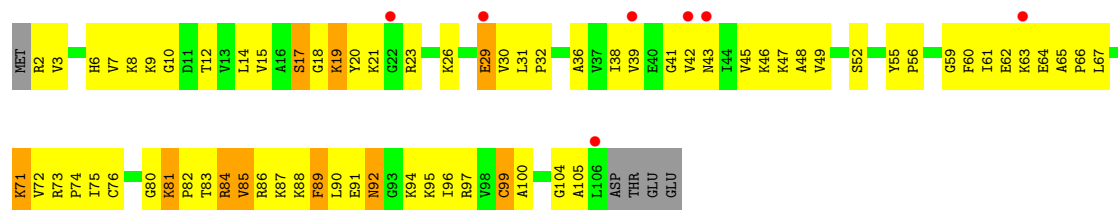




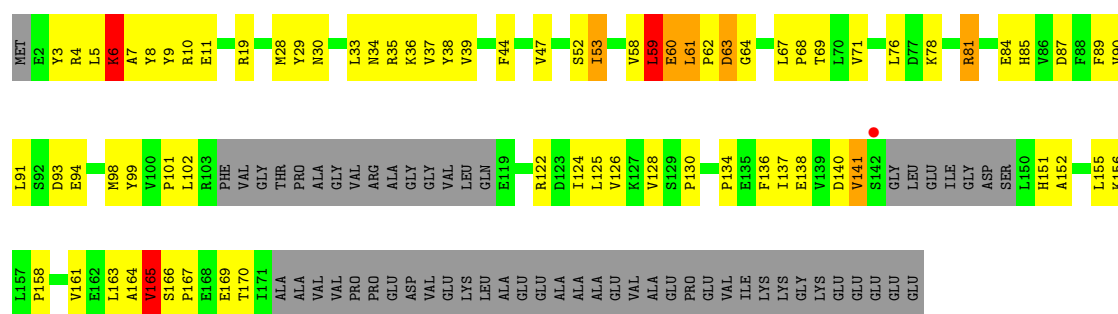
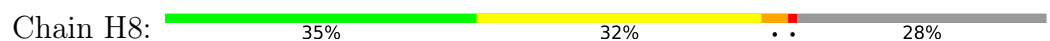
• Molecule 46: 50S ribosomal protein L24



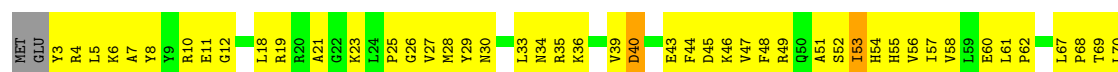
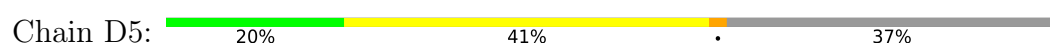
• Molecule 46: 50S ribosomal protein L24

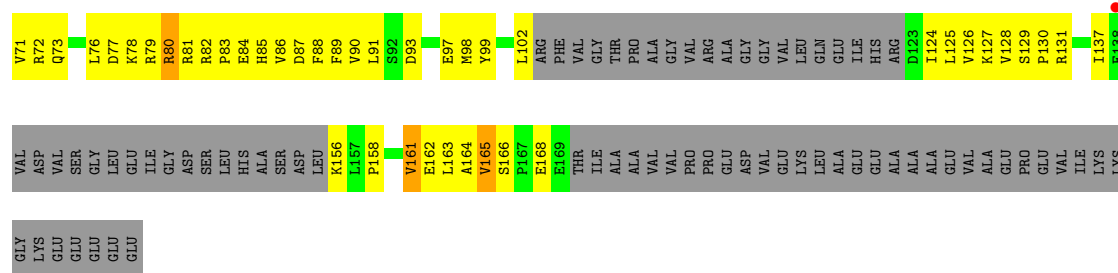


• Molecule 47: 50S ribosomal protein L25

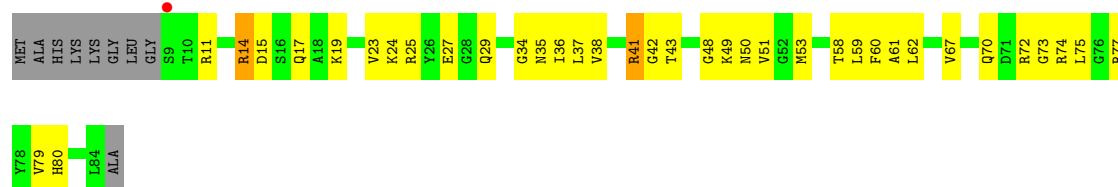


• Molecule 47: 50S ribosomal protein L25





- Molecule 48: 50S ribosomal protein L27



- Molecule 48: 50S ribosomal protein L27

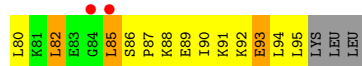


- Molecule 49: 50S ribosomal protein L28

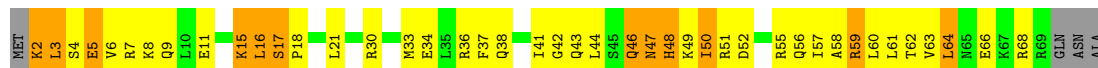


- Molecule 49: 50S ribosomal protein L28

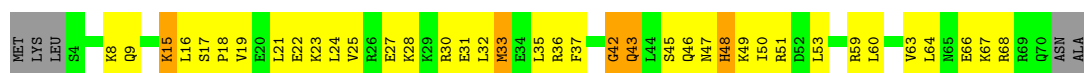




- Molecule 50: 50S ribosomal protein L29



- Molecule 50: 50S ribosomal protein L29



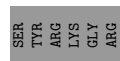
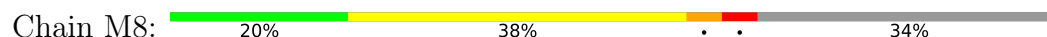
- Molecule 51: 50S ribosomal protein L30



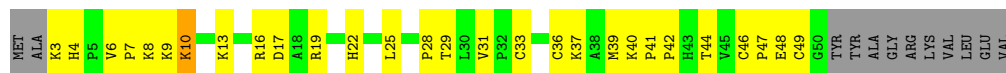
- Molecule 51: 50S ribosomal protein L30



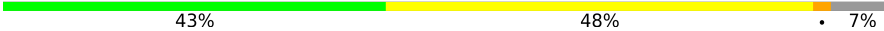
- Molecule 52: 50S ribosomal protein L31



- Molecule 53: 50S ribosomal protein L32



- Molecule 53: 50S ribosomal protein L32

Chain J5:  43% 48% 7%



- Molecule 54: 50S ribosomal protein L34

Chain P8:  2% 53% 37% 6%



- Molecule 54: 50S ribosomal protein L34

Chain L5:  4% 53% 39% 8%



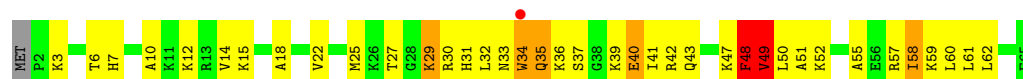
- Molecule 55: 50S ribosomal protein L35

Chain Q8:  2% 35% 51% 11%



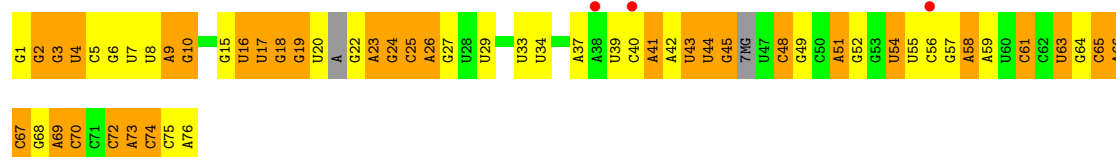
- Molecule 55: 50S ribosomal protein L35

Chain M5:  2% 40% 48% 8%



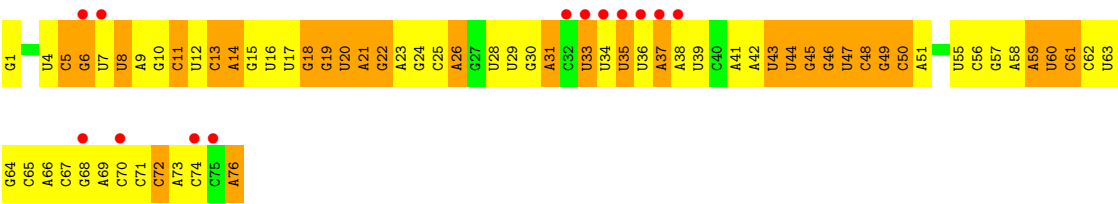
- Molecule 56: tRNA^{Lys}

Chain 1L:  4% 22% 34% 41%



- Molecule 57: tRNA^{Lys}

Chain 3L:  17% 12% 50% 38%



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	208.40Å 447.10Å 616.90Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	152.44 – 3.15 152.44 – 3.15	Depositor EDS
% Data completeness (in resolution range)	100.0 (152.44-3.15) 92.0 (152.44-3.15)	Depositor EDS
R_{merge}	0.23	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.84 (at 3.13Å)	Xtriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.198 , 0.254 0.196 , 0.256	Depositor DCC
R_{free} test set	2000 reflections (0.20%)	wwPDB-VP
Wilson B-factor (Å ²)	107.7	Xtriage
Anisotropy	0.223	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.26 , 55.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.44$, $\langle L^2 \rangle = 0.27$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	292607	wwPDB-VP
Average B, all atoms (Å ²)	131.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.47% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, U8U, OMC, G7M, MG, 4SU, T6A, PSU, SF4, 5MU

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	0/35927	0.98	35/56065 (0.1%)
1	1G	0.62	0/35987	0.86	6/56159 (0.0%)
2	12	0.50	0/1726	0.84	2/2324 (0.1%)
2	1E	0.59	0/1908	0.84	0/2573
3	22	0.49	1/1552 (0.1%)	0.76	0/2093
3	2E	0.72	0/1629	0.91	0/2195
4	32	0.69	1/1732 (0.1%)	0.95	1/2318 (0.0%)
4	3E	0.80	1/1726 (0.1%)	0.94	1/2310 (0.0%)
5	42	0.64	1/1151 (0.1%)	0.82	0/1549
5	4E	0.81	1/1158 (0.1%)	0.99	0/1559
6	52	0.68	0/855	0.89	0/1154
6	5E	0.76	0/850	0.98	1/1147 (0.1%)
7	62	0.63	0/1122	0.86	1/1500 (0.1%)
7	6E	0.60	0/1245	0.75	0/1666
8	72	0.53	0/1127	0.80	2/1517 (0.1%)
8	7E	0.93	4/1135 (0.4%)	0.99	2/1527 (0.1%)
9	82	0.62	1/835 (0.1%)	0.85	0/1120
9	8E	0.60	0/1019	0.86	0/1367
10	1A	0.60	0/482	0.78	0/647
10	1I	0.71	0/602	0.87	0/806
11	2A	0.69	2/850 (0.2%)	0.84	0/1150
11	2I	0.72	0/838	0.98	0/1133
12	3A	0.69	0/963	1.02	2/1290 (0.2%)
12	3I	0.98	0/972	1.29	7/1301 (0.5%)
13	4A	0.63	0/903	0.95	1/1211 (0.1%)
13	4I	0.71	0/952	0.94	0/1277
14	5A	0.58	0/393	0.94	0/521
14	5I	0.79	0/500	1.06	1/664 (0.2%)
15	6A	0.74	2/740 (0.3%)	0.88	0/987
15	6I	0.80	1/740 (0.1%)	0.91	0/987
16	7A	0.74	0/721	0.93	0/970
16	7I	0.72	0/687	0.95	0/925

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
17	8A	0.60	0/836	0.81	0/1117
17	8I	0.82	3/847 (0.4%)	0.99	0/1131
18	9A	0.70	0/549	0.89	0/732
18	9I	0.69	0/549	0.92	0/732
19	AA	0.67	0/288	1.03	1/388 (0.3%)
19	AI	0.78	1/668 (0.1%)	1.05	0/899
20	BA	0.71	1/759 (0.1%)	0.96	2/1000 (0.2%)
20	BI	0.61	0/748	0.83	0/986
21	1B	0.56	0/208	0.87	0/272
21	1F	0.57	0/203	0.78	0/266
22	1K	0.63	0/1516	0.79	0/2350
23	2K	0.87	2/1721 (0.1%)	1.08	0/2682
23	2L	0.65	0/1721	0.89	1/2682 (0.0%)
24	3K	0.63	0/1799	0.81	0/2801
25	4K	0.88	0/494	1.01	1/767 (0.1%)
25	4L	0.73	0/420	0.87	0/654
26	14	0.83	4/69023 (0.0%)	1.10	146/107740 (0.1%)
26	1H	0.97	10/68273 (0.0%)	1.23	270/106575 (0.3%)
27	16	0.82	0/2928	1.18	7/4568 (0.2%)
27	1J	0.69	0/2928	1.02	2/4568 (0.0%)
28	7I	0.74	0/1073	0.89	0/1447
29	11	1.14	4/2170 (0.2%)	1.50	28/2926 (1.0%)
29	19	1.07	1/2170 (0.0%)	1.42	24/2926 (0.8%)
30	21	1.06	7/1591 (0.4%)	1.38	18/2146 (0.8%)
30	29	0.95	0/1591	1.26	5/2146 (0.2%)
31	31	1.04	2/1620 (0.1%)	1.25	6/2194 (0.3%)
31	39	0.87	2/1637 (0.1%)	1.23	3/2218 (0.1%)
32	41	0.80	0/1481	1.06	0/1994
32	49	0.64	1/1481 (0.1%)	1.03	9/1994 (0.5%)
33	51	0.91	0/1337	1.30	9/1809 (0.5%)
33	59	0.70	1/548 (0.2%)	0.99	0/738
34	61	0.70	0/1146	0.97	0/1551
34	69	0.67	0/1146	0.98	3/1551 (0.2%)
35	15	1.04	2/1123 (0.2%)	1.01	3/1515 (0.2%)
35	58	0.91	0/1131	1.15	7/1525 (0.5%)
36	25	0.88	0/942	1.11	2/1269 (0.2%)
36	68	0.95	0/942	1.21	2/1269 (0.2%)
37	35	1.11	3/1147 (0.3%)	1.33	8/1525 (0.5%)
37	78	1.11	1/1139 (0.1%)	1.53	16/1514 (1.1%)
38	45	0.98	3/1120 (0.3%)	1.16	4/1498 (0.3%)
38	88	1.15	3/1134 (0.3%)	1.37	8/1519 (0.5%)
39	55	0.93	0/981	1.14	1/1312 (0.1%)
39	98	0.87	0/981	1.20	7/1312 (0.5%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
40	65	0.71	0/886	1.11	0/1180
40	A8	0.92	0/891	1.25	4/1187 (0.3%)
41	75	0.98	5/1147 (0.4%)	1.19	7/1532 (0.5%)
41	B8	1.10	4/1137 (0.4%)	1.26	5/1519 (0.3%)
42	85	0.82	0/977	1.10	2/1301 (0.2%)
42	C8	0.98	0/968	1.17	0/1289
43	95	0.93	1/777 (0.1%)	1.14	5/1042 (0.5%)
43	D8	0.90	1/789 (0.1%)	1.21	4/1057 (0.4%)
44	A5	1.02	0/886	1.20	0/1189
44	E8	1.06	0/886	1.23	2/1189 (0.2%)
45	B5	1.00	0/749	1.14	3/1007 (0.3%)
45	F8	1.12	1/754 (0.1%)	1.48	5/1014 (0.5%)
46	C5	1.06	5/812 (0.6%)	1.28	0/1083
46	G8	1.27	5/801 (0.6%)	1.55	9/1069 (0.8%)
47	D5	0.89	4/1088 (0.4%)	0.93	0/1473
47	H8	0.75	1/1244 (0.1%)	1.06	1/1683 (0.1%)
48	E5	0.91	0/624	1.23	3/832 (0.4%)
48	I8	1.10	0/614	1.31	4/819 (0.5%)
49	F5	0.93	0/744	1.23	3/989 (0.3%)
49	J8	1.03	1/744 (0.1%)	1.32	1/989 (0.1%)
50	G5	0.80	0/565	1.09	1/748 (0.1%)
50	K8	1.08	0/570	1.65	9/755 (1.2%)
51	H5	0.76	0/464	0.94	0/623
51	L8	0.94	1/464 (0.2%)	1.14	1/623 (0.2%)
52	M8	0.82	0/375	1.36	4/507 (0.8%)
53	J5	0.87	0/448	1.16	1/606 (0.2%)
53	N8	1.00	0/381	1.28	2/516 (0.4%)
54	L5	1.05	0/399	1.23	0/526
54	P8	1.21	0/409	1.47	5/540 (0.9%)
55	M5	1.10	1/524 (0.2%)	1.44	7/691 (1.0%)
55	Q8	1.19	1/524 (0.2%)	1.61	5/691 (0.7%)
56	1L	0.46	0/1683	0.62	0/2615
57	3L	0.56	0/1777	0.74	0/2767
All	All	0.83	97/315237 (0.0%)	1.09	748/472471 (0.2%)

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

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Mol	Chain	#Chirality outliers	#Planarity outliers
2	1E	0	3
3	22	0	2
3	2E	0	2
4	32	0	4
4	3E	0	1
5	4E	0	1
7	6E	0	1
9	82	0	1
9	8E	0	1
11	2A	0	1
11	2I	0	1
12	3A	0	1
12	3I	0	5
13	4A	0	2
13	4I	0	3
14	5A	0	1
14	5I	0	1
15	6A	0	1
16	7I	0	1
17	8I	0	1
19	AA	0	1
19	AI	0	2
20	BA	0	4
20	BI	0	1
26	14	0	1
28	71	0	1
29	11	0	6
29	19	0	6
30	21	0	11
30	29	0	6
31	31	0	3
31	39	0	11
32	41	0	3
32	49	0	6
33	51	0	3
33	59	0	3
34	61	0	4
34	69	0	6
35	15	0	4
35	58	0	3
37	35	0	4
37	78	0	7

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Mol	Chain	#Chirality outliers	#Planarity outliers
38	45	0	7
38	88	0	3
40	A8	0	2
41	75	0	2
41	B8	0	4
42	85	0	5
42	C8	0	3
43	95	0	3
43	D8	0	4
44	A5	0	1
45	B5	0	2
45	F8	0	2
46	C5	0	1
46	G8	0	6
47	D5	0	1
47	H8	0	2
48	E5	0	1
49	F5	0	3
49	J8	0	2
50	G5	0	4
50	K8	0	4
52	M8	0	5
54	P8	0	1
55	M5	0	3
55	Q8	0	2
All	All	0	209

The worst 5 of 97 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
35	15	94	HIS	C-O	-19.69	1.14	1.23
37	35	121	LYS	C-N	18.44	1.76	1.33
47	D5	80	ARG	NE-CZ	-13.25	1.18	1.33
8	7E	102	ARG	CZ-NH2	-12.09	1.17	1.33
4	3E	36	ARG	C-N	-11.41	1.07	1.33

The worst 5 of 748 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
50	K8	17	SER	N-CA-C	20.37	126.47	108.13
45	F8	3	THR	CA-C-N	11.75	142.85	121.70
45	F8	3	THR	C-N-CA	11.75	142.85	121.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	49	6	ALA	N-CA-C	11.52	127.33	113.28
29	19	44	ASN	CA-C-N	11.42	142.25	121.70

There are no chirality outliers.

5 of 209 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	1E	169	LYS	Peptide
2	1E	234	PRO	Peptide
2	1E	9	GLU	Peptide
3	2E	128	PHE	Peptide
3	2E	166	GLU	Peptide

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	13	32097	0	16197	1110	0
1	1G	32152	0	16231	1236	2
2	12	1695	0	1729	136	0
2	1E	1874	0	1926	147	0
3	22	1529	0	1592	136	0
3	2E	1605	0	1668	87	0
4	32	1702	0	1764	163	0
4	3E	1696	0	1752	140	0
5	42	1136	0	1200	106	0
5	4E	1142	0	1204	90	0
6	52	842	0	857	51	0
6	5E	837	0	852	50	0
7	62	1110	0	1163	83	0
7	6E	1229	0	1274	78	0
8	72	1107	0	1165	75	0
8	7E	1115	0	1177	81	0
9	82	820	0	848	86	0
9	8E	1000	0	1031	98	0
10	1A	474	0	484	44	0
10	1I	593	0	610	48	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
11	2A	835	0	847	31	0
11	2I	823	0	833	52	0
12	3A	947	0	1033	81	0
12	3I	956	0	1046	50	0
13	4A	893	0	946	89	0
13	4I	942	0	997	71	0
14	5A	388	0	424	49	0
14	5I	491	0	530	38	0
15	6A	729	0	768	35	0
15	6I	729	0	768	54	0
16	7A	705	0	725	53	0
16	7I	671	0	693	60	0
17	8A	823	0	891	37	0
17	8I	834	0	904	55	0
18	9A	544	0	605	35	0
18	9I	544	0	605	34	0
19	AA	283	0	284	23	0
19	AI	654	0	675	56	0
20	BA	757	0	856	56	0
20	BI	746	0	843	58	0
21	1B	204	0	218	18	0
21	1F	199	0	208	10	0
22	1K	1477	0	758	63	0
23	2K	1646	0	844	42	0
23	2L	1646	0	844	58	0
24	3K	1611	0	817	93	0
25	4K	439	0	219	17	0
25	4L	373	0	185	10	0
26	14	61630	0	31047	1930	1
26	1H	60960	0	30668	1948	0
27	16	2617	0	1328	92	0
27	1J	2617	0	1328	135	0
28	7I	1050	0	1071	89	0
29	11	2120	0	2197	176	0
29	19	2120	0	2197	175	0
30	21	1558	0	1624	126	0
30	29	1558	0	1622	193	0
31	31	1585	0	1632	129	0
31	39	1602	0	1649	128	0
32	41	1457	0	1514	137	0
32	49	1457	0	1514	173	0
33	51	1312	0	1384	88	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
33	59	539	0	563	42	0
34	61	1131	0	1218	81	1
34	69	1131	0	1218	86	0
35	15	1096	0	1168	65	0
35	58	1104	0	1180	78	0
36	25	932	0	996	69	0
36	68	932	0	996	52	0
37	35	1130	0	1217	144	0
37	78	1122	0	1206	127	0
38	45	1099	0	1154	114	0
38	88	1113	0	1156	83	0
39	55	967	0	1033	59	0
39	98	967	0	1033	66	0
40	65	876	0	938	93	0
40	A8	881	0	943	87	0
41	75	1133	0	1190	82	0
41	B8	1123	0	1181	108	0
42	85	959	0	1019	74	0
42	C8	950	0	1011	85	0
43	95	766	0	837	83	0
43	D8	778	0	851	84	0
44	A5	876	0	941	41	0
44	E8	876	0	941	50	0
45	B5	735	0	785	56	0
45	F8	740	0	787	52	0
46	C5	799	0	888	80	0
46	G8	788	0	875	93	0
47	D5	1064	0	1082	93	0
47	H8	1218	0	1241	76	0
48	E5	616	0	633	50	0
48	I8	606	0	625	41	0
49	F5	737	0	813	63	0
49	J8	737	0	813	53	0
50	G5	563	0	612	35	0
50	K8	568	0	614	48	0
51	H5	459	0	512	19	0
51	L8	459	0	512	20	0
52	M8	366	0	370	50	0
53	J5	434	0	454	32	0
53	N8	369	0	388	46	0
54	L5	391	0	432	24	0
54	P8	401	0	436	19	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
55	M5	516	0	582	51	0
55	Q8	516	0	582	59	0
56	1L	1570	0	798	39	0
57	3L	1611	0	817	69	0
58	11	1	0	0	0	0
58	13	141	0	0	0	0
58	14	420	0	0	0	0
58	16	12	0	0	0	0
58	1G	78	0	0	0	0
58	1H	488	0	0	0	0
58	1J	6	0	0	0	0
58	21	2	0	0	0	0
58	29	3	0	0	0	0
58	2K	3	0	0	0	0
58	2L	3	0	0	0	0
58	32	1	0	0	0	0
58	35	1	0	0	0	0
58	3I	1	0	0	0	0
58	41	1	0	0	0	0
58	45	3	0	0	0	0
58	55	1	0	0	0	0
58	5E	2	0	0	0	0
58	5I	1	0	0	0	0
58	78	1	0	0	0	0
58	7A	1	0	0	0	0
58	85	2	0	0	0	0
58	88	1	0	0	0	0
58	C5	1	0	0	0	0
58	C8	1	0	0	0	0
58	E5	1	0	0	0	0
58	I8	1	0	0	0	0
58	J8	2	0	0	0	0
58	L5	1	0	0	0	0
58	P8	1	0	0	0	0
58	Q8	1	0	0	0	0
59	32	8	0	0	4	0
59	3E	8	0	0	0	0
60	5A	1	0	0	0	0
60	5I	1	0	0	0	0
60	C5	1	0	0	0	0
60	G8	1	0	0	0	0
61	11	9	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
61	13	148	0	0	21	0
61	14	411	0	0	57	0
61	16	18	0	0	4	0
61	19	4	0	0	2	0
61	1G	44	0	0	6	0
61	1H	670	0	0	78	0
61	1J	11	0	0	2	0
61	1K	1	0	0	0	0
61	21	5	0	0	2	0
61	29	3	0	0	0	0
61	31	6	0	0	0	0
61	35	2	0	0	0	0
61	39	8	0	0	0	0
61	3E	2	0	0	1	0
61	3I	2	0	0	0	0
61	4K	6	0	0	0	0
61	55	1	0	0	0	0
61	58	2	0	0	0	0
61	5A	3	0	0	2	0
61	5I	1	0	0	0	0
61	6I	1	0	0	0	0
61	78	3	0	0	1	0
61	B8	1	0	0	0	0
61	BA	1	0	0	0	0
61	D8	1	0	0	0	0
61	E5	1	0	0	0	0
61	E8	1	0	0	0	0
61	F5	2	0	0	0	0
61	G8	1	0	0	0	0
61	I8	1	0	0	0	0
61	L5	1	0	0	0	0
61	M5	2	0	0	0	0
61	Q8	1	0	0	0	0
All	All	292607	0	194506	12295	2

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 26.

The worst 5 of 12295 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)
46:G8:84:ARG:CB	46:G8:84:ARG:CG	1.75	1.63
46:G8:84:ARG:CG	46:G8:84:ARG:CD	1.76	1.61
29:19:246:PRO:N	29:19:255:LYS:HZ1	1.11	1.43
37:35:121:LYS:C	37:35:122:PRO:N	1.77	1.40
30:29:119:ARG:HH11	30:29:120:TRP:NE1	1.15	1.38

All (2) 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)
1:1G:82:U:O2'	26:14:271(C):U:O4[3_545]	1.99	0.21
34:61:89:TYR:O	1:1G:357:G:O2'[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	202/256 (79%)	170 (84%)	26 (13%)	6 (3%)	3	19
2	1E	227/256 (89%)	194 (86%)	28 (12%)	5 (2%)	5	25
3	22	190/239 (80%)	167 (88%)	22 (12%)	1 (0%)	24	55
3	2E	203/239 (85%)	183 (90%)	20 (10%)	0	100	100
4	32	206/209 (99%)	181 (88%)	22 (11%)	3 (2%)	8	33
4	3E	205/209 (98%)	189 (92%)	14 (7%)	2 (1%)	12	41
5	42	147/162 (91%)	136 (92%)	11 (8%)	0	100	100
5	4E	147/162 (91%)	137 (93%)	9 (6%)	1 (1%)	18	49
6	52	99/101 (98%)	94 (95%)	5 (5%)	0	100	100
6	5E	98/101 (97%)	92 (94%)	6 (6%)	0	100	100
7	62	134/156 (86%)	121 (90%)	13 (10%)	0	100	100
7	6E	147/156 (94%)	141 (96%)	6 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
8	72	135/138 (98%)	124 (92%)	10 (7%)	1 (1%)	18	49
8	7E	136/138 (99%)	125 (92%)	10 (7%)	1 (1%)	18	49
9	82	101/128 (79%)	88 (87%)	11 (11%)	2 (2%)	6	27
9	8E	124/128 (97%)	103 (83%)	20 (16%)	1 (1%)	16	46
10	1A	54/105 (51%)	46 (85%)	8 (15%)	0	100	100
10	1I	66/105 (63%)	58 (88%)	6 (9%)	2 (3%)	3	19
11	2A	111/129 (86%)	97 (87%)	12 (11%)	2 (2%)	6	29
11	2I	109/129 (84%)	94 (86%)	13 (12%)	2 (2%)	6	29
12	3A	119/132 (90%)	97 (82%)	17 (14%)	5 (4%)	2	13
12	3I	120/132 (91%)	103 (86%)	16 (13%)	1 (1%)	16	46
13	4A	109/126 (86%)	93 (85%)	15 (14%)	1 (1%)	14	43
13	4I	117/126 (93%)	97 (83%)	20 (17%)	0	100	100
14	5A	44/61 (72%)	37 (84%)	7 (16%)	0	100	100
14	5I	58/61 (95%)	48 (83%)	8 (14%)	2 (3%)	3	16
15	6A	85/89 (96%)	77 (91%)	8 (9%)	0	100	100
15	6I	85/89 (96%)	74 (87%)	11 (13%)	0	100	100
16	7A	82/88 (93%)	76 (93%)	6 (7%)	0	100	100
16	7I	78/88 (89%)	73 (94%)	5 (6%)	0	100	100
17	8A	97/105 (92%)	91 (94%)	6 (6%)	0	100	100
17	8I	98/105 (93%)	91 (93%)	7 (7%)	0	100	100
18	9A	65/88 (74%)	62 (95%)	3 (5%)	0	100	100
18	9I	65/88 (74%)	60 (92%)	4 (6%)	1 (2%)	8	33
19	AA	32/93 (34%)	25 (78%)	6 (19%)	1 (3%)	3	18
19	AI	79/93 (85%)	66 (84%)	11 (14%)	2 (2%)	4	22
20	BA	96/106 (91%)	81 (84%)	12 (12%)	3 (3%)	3	18
20	BI	95/106 (90%)	80 (84%)	15 (16%)	0	100	100
21	1B	21/27 (78%)	21 (100%)	0	0	100	100
21	1F	21/27 (78%)	20 (95%)	1 (5%)	0	100	100
28	71	131/229 (57%)	121 (92%)	9 (7%)	1 (1%)	16	46
29	11	271/276 (98%)	233 (86%)	26 (10%)	12 (4%)	2	12
29	19	271/276 (98%)	245 (90%)	19 (7%)	7 (3%)	4	21

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
30	21	201/206 (98%)	158 (79%)	34 (17%)	9 (4%)	2	12
30	29	201/206 (98%)	153 (76%)	37 (18%)	11 (6%)	1	9
31	31	200/210 (95%)	176 (88%)	22 (11%)	2 (1%)	12	41
31	39	202/210 (96%)	158 (78%)	36 (18%)	8 (4%)	2	14
32	41	177/182 (97%)	154 (87%)	18 (10%)	5 (3%)	4	20
32	49	177/182 (97%)	152 (86%)	23 (13%)	2 (1%)	11	39
33	51	169/180 (94%)	135 (80%)	20 (12%)	14 (8%)	0	3
33	59	63/180 (35%)	44 (70%)	13 (21%)	6 (10%)	0	2
34	61	143/148 (97%)	118 (82%)	24 (17%)	1 (1%)	18	49
34	69	143/148 (97%)	111 (78%)	27 (19%)	5 (4%)	3	16
35	15	135/140 (96%)	119 (88%)	13 (10%)	3 (2%)	5	25
35	58	136/140 (97%)	117 (86%)	15 (11%)	4 (3%)	3	20
36	25	120/122 (98%)	110 (92%)	9 (8%)	1 (1%)	16	46
36	68	120/122 (98%)	110 (92%)	10 (8%)	0	100	100
37	35	146/150 (97%)	111 (76%)	31 (21%)	4 (3%)	4	21
37	78	145/150 (97%)	116 (80%)	21 (14%)	8 (6%)	1	9
38	45	136/141 (96%)	109 (80%)	23 (17%)	4 (3%)	3	20
38	88	139/141 (99%)	115 (83%)	17 (12%)	7 (5%)	1	10
39	55	116/118 (98%)	109 (94%)	6 (5%)	1 (1%)	14	43
39	98	116/118 (98%)	93 (80%)	22 (19%)	1 (1%)	14	43
40	65	108/112 (96%)	87 (81%)	18 (17%)	3 (3%)	4	20
40	A8	109/112 (97%)	89 (82%)	19 (17%)	1 (1%)	14	43
41	75	134/146 (92%)	121 (90%)	13 (10%)	0	100	100
41	B8	133/146 (91%)	117 (88%)	14 (10%)	2 (2%)	8	33
42	85	114/118 (97%)	99 (87%)	13 (11%)	2 (2%)	6	29
42	C8	113/118 (96%)	104 (92%)	5 (4%)	4 (4%)	3	16
43	95	97/101 (96%)	77 (79%)	16 (16%)	4 (4%)	2	14
43	D8	99/101 (98%)	89 (90%)	7 (7%)	3 (3%)	3	19
44	A5	108/113 (96%)	100 (93%)	7 (6%)	1 (1%)	14	43
44	E8	108/113 (96%)	97 (90%)	11 (10%)	0	100	100
45	B5	92/96 (96%)	85 (92%)	5 (5%)	2 (2%)	5	25

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
45	F8	93/96 (97%)	82 (88%)	10 (11%)	1 (1%)	11	39
46	C5	103/110 (94%)	70 (68%)	26 (25%)	7 (7%)	1	6
46	G8	102/110 (93%)	80 (78%)	16 (16%)	6 (6%)	1	8
47	D5	124/206 (60%)	96 (77%)	25 (20%)	3 (2%)	4	23
47	H8	142/206 (69%)	112 (79%)	22 (16%)	8 (6%)	1	9
48	E5	76/85 (89%)	66 (87%)	8 (10%)	2 (3%)	4	21
48	I8	74/85 (87%)	68 (92%)	6 (8%)	0	100	100
49	F5	92/98 (94%)	83 (90%)	7 (8%)	2 (2%)	5	25
49	J8	92/98 (94%)	84 (91%)	6 (6%)	2 (2%)	5	25
50	G5	65/72 (90%)	61 (94%)	3 (5%)	1 (2%)	8	33
50	K8	66/72 (92%)	55 (83%)	7 (11%)	4 (6%)	1	7
51	H5	56/60 (93%)	53 (95%)	3 (5%)	0	100	100
51	L8	56/60 (93%)	53 (95%)	3 (5%)	0	100	100
52	M8	45/71 (63%)	28 (62%)	15 (33%)	2 (4%)	2	12
53	J5	54/60 (90%)	46 (85%)	8 (15%)	0	100	100
53	N8	46/60 (77%)	42 (91%)	4 (9%)	0	100	100
54	L5	43/49 (88%)	39 (91%)	4 (9%)	0	100	100
54	P8	45/49 (92%)	41 (91%)	3 (7%)	1 (2%)	5	25
55	M5	62/65 (95%)	52 (84%)	7 (11%)	3 (5%)	2	11
55	Q8	62/65 (95%)	48 (77%)	10 (16%)	4 (6%)	1	6
All	All	10778/12104 (89%)	9303 (86%)	1246 (12%)	229 (2%)	5	26

5 of 229 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
11	2I	91	ARG
18	9I	22	VAL
19	AI	67	VAL
29	11	28	GLU
29	11	40	THR

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	180/220 (82%)	179 (99%)	1 (1%)	78	81
2	1E	200/220 (91%)	200 (100%)	0	100	100
3	22	153/188 (81%)	153 (100%)	0	100	100
3	2E	159/188 (85%)	159 (100%)	0	100	100
4	32	180/181 (99%)	178 (99%)	2 (1%)	65	75
4	3E	179/181 (99%)	178 (99%)	1 (1%)	78	81
5	42	114/123 (93%)	114 (100%)	0	100	100
5	4E	115/123 (94%)	114 (99%)	1 (1%)	70	77
6	52	90/90 (100%)	90 (100%)	0	100	100
6	5E	90/90 (100%)	89 (99%)	1 (1%)	65	75
7	62	114/127 (90%)	113 (99%)	1 (1%)	70	77
7	6E	125/127 (98%)	125 (100%)	0	100	100
8	72	118/119 (99%)	118 (100%)	0	100	100
8	7E	119/119 (100%)	118 (99%)	1 (1%)	73	78
9	82	79/99 (80%)	78 (99%)	1 (1%)	61	73
9	8E	97/99 (98%)	97 (100%)	0	100	100
10	1A	52/92 (56%)	51 (98%)	1 (2%)	50	69
10	1I	65/92 (71%)	64 (98%)	1 (2%)	57	72
11	2A	85/99 (86%)	84 (99%)	1 (1%)	63	74
11	2I	84/99 (85%)	84 (100%)	0	100	100
12	3A	102/109 (94%)	102 (100%)	0	100	100
12	3I	103/109 (94%)	103 (100%)	0	100	100
13	4A	91/101 (90%)	91 (100%)	0	100	100
13	4I	94/101 (93%)	94 (100%)	0	100	100
14	5A	40/50 (80%)	40 (100%)	0	100	100
14	5I	49/50 (98%)	49 (100%)	0	100	100
15	6A	79/80 (99%)	78 (99%)	1 (1%)	61	73
15	6I	79/80 (99%)	79 (100%)	0	100	100
16	7A	72/74 (97%)	72 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
16	7I	69/74 (93%)	69 (100%)	0	100	100
17	8A	94/97 (97%)	94 (100%)	0	100	100
17	8I	95/97 (98%)	95 (100%)	0	100	100
18	9A	58/77 (75%)	58 (100%)	0	100	100
18	9I	58/77 (75%)	58 (100%)	0	100	100
19	AA	31/80 (39%)	31 (100%)	0	100	100
19	AI	71/80 (89%)	71 (100%)	0	100	100
20	BA	76/82 (93%)	76 (100%)	0	100	100
20	BI	75/82 (92%)	75 (100%)	0	100	100
21	1B	19/22 (86%)	18 (95%)	1 (5%)	20	49
21	1F	18/22 (82%)	18 (100%)	0	100	100
28	7I	111/181 (61%)	111 (100%)	0	100	100
29	11	214/218 (98%)	214 (100%)	0	100	100
29	19	214/218 (98%)	214 (100%)	0	100	100
30	21	165/166 (99%)	164 (99%)	1 (1%)	78	81
30	29	165/166 (99%)	165 (100%)	0	100	100
31	31	161/166 (97%)	161 (100%)	0	100	100
31	39	163/166 (98%)	163 (100%)	0	100	100
32	41	153/156 (98%)	153 (100%)	0	100	100
32	49	153/156 (98%)	152 (99%)	1 (1%)	76	80
33	51	142/148 (96%)	142 (100%)	0	100	100
33	59	56/148 (38%)	56 (100%)	0	100	100
34	61	122/124 (98%)	122 (100%)	0	100	100
34	69	122/124 (98%)	122 (100%)	0	100	100
35	15	116/119 (98%)	114 (98%)	2 (2%)	53	70
35	58	117/119 (98%)	117 (100%)	0	100	100
36	25	100/100 (100%)	100 (100%)	0	100	100
36	68	100/100 (100%)	100 (100%)	0	100	100
37	35	115/116 (99%)	115 (100%)	0	100	100
37	78	114/116 (98%)	114 (100%)	0	100	100
38	45	109/111 (98%)	106 (97%)	3 (3%)	38	63

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
38	88	109/111 (98%)	109 (100%)	0	100	100
39	55	101/101 (100%)	100 (99%)	1 (1%)	68	76
39	98	101/101 (100%)	101 (100%)	0	100	100
40	65	87/88 (99%)	87 (100%)	0	100	100
40	A8	87/88 (99%)	86 (99%)	1 (1%)	65	75
41	75	119/127 (94%)	115 (97%)	4 (3%)	32	60
41	B8	118/127 (93%)	115 (98%)	3 (2%)	42	65
42	85	93/94 (99%)	93 (100%)	0	100	100
42	C8	92/94 (98%)	91 (99%)	1 (1%)	65	75
43	95	81/82 (99%)	81 (100%)	0	100	100
43	D8	82/82 (100%)	81 (99%)	1 (1%)	63	74
44	A5	90/92 (98%)	88 (98%)	2 (2%)	45	67
44	E8	90/92 (98%)	90 (100%)	0	100	100
45	B5	74/78 (95%)	74 (100%)	0	100	100
45	F8	74/78 (95%)	74 (100%)	0	100	100
46	C5	85/91 (93%)	85 (100%)	0	100	100
46	G8	84/91 (92%)	84 (100%)	0	100	100
47	D5	118/179 (66%)	117 (99%)	1 (1%)	73	78
47	H8	137/179 (76%)	137 (100%)	0	100	100
48	E5	62/67 (92%)	62 (100%)	0	100	100
48	I8	61/67 (91%)	61 (100%)	0	100	100
49	F5	79/83 (95%)	79 (100%)	0	100	100
49	J8	79/83 (95%)	79 (100%)	0	100	100
50	G5	62/67 (92%)	62 (100%)	0	100	100
50	K8	62/67 (92%)	60 (97%)	2 (3%)	34	61
51	H5	50/52 (96%)	50 (100%)	0	100	100
51	L8	50/52 (96%)	50 (100%)	0	100	100
52	M8	42/63 (67%)	42 (100%)	0	100	100
53	J5	48/52 (92%)	47 (98%)	1 (2%)	47	67
53	N8	43/52 (83%)	43 (100%)	0	100	100
54	L5	38/42 (90%)	37 (97%)	1 (3%)	40	64

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
54	P8	38/42 (90%)	37 (97%)	1 (3%)	40 64
55	M5	54/55 (98%)	54 (100%)	0	100 100
55	Q8	54/55 (98%)	54 (100%)	0	100 100
All	All	9127/10012 (91%)	9087 (100%)	40 (0%)	84 84

5 of 40 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
38	45	110	THR
44	A5	39	THR
38	45	116	GLU
41	75	12	SER
47	D5	40	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 94 such sidechains are listed below:

Mol	Chain	Res	Type
9	82	58	HIS
30	29	55	ASN
11	2A	99	GLN
19	AA	65	ASN
31	39	133	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	13	1488/1522 (97%)	388 (26%)	35 (2%)
1	1G	1493/1522 (98%)	431 (28%)	39 (2%)
22	1K	65/76 (85%)	42 (64%)	2 (3%)
23	2K	76/77 (98%)	23 (30%)	2 (2%)
23	2L	76/77 (98%)	21 (27%)	2 (2%)
24	3K	75/76 (98%)	40 (53%)	4 (5%)
25	4K	18/27 (66%)	10 (55%)	2 (11%)
25	4L	16/27 (59%)	9 (56%)	1 (6%)
26	14	2852/2912 (97%)	792 (27%)	58 (2%)
26	1H	2824/2912 (96%)	739 (26%)	78 (2%)
27	16	121/122 (99%)	27 (22%)	1 (0%)
27	1J	121/122 (99%)	41 (33%)	2 (1%)
56	1L	71/76 (93%)	40 (56%)	5 (7%)

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Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
57	3L	75/76 (98%)	40 (53%)	1 (1%)
All	All	9371/9624 (97%)	2643 (28%)	232 (2%)

5 of 2643 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	13	2	U
1	13	5	U
1	13	6	G
1	13	8	A
1	13	9	G

5 of 232 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
26	1H	2481	G
26	14	2611	U
1	1G	889	A
26	14	2447	G
26	14	1420	U

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

19 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
56	PSU	1L	55	56	18,21,22	1.38	1 (5%)	21,30,33	1.98	4 (19%)
23	4SU	2K	8	23	18,21,22	1.93	3 (16%)	25,30,33	2.45	7 (28%)
23	PSU	2K	56	23	18,21,22	1.42	2 (11%)	21,30,33	2.67	5 (23%)
57	PSU	3L	39	57	18,21,22	1.15	1 (5%)	21,30,33	1.61	3 (14%)
23	4SU	2L	8	23	18,21,22	1.97	4 (22%)	25,30,33	2.91	7 (28%)
23	5MU	2K	55	23	19,22,23	4.02	5 (26%)	27,32,35	3.48	9 (33%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
23	OMC	2L	33	23	19,22,23	1.95	3 (15%)	25,31,34	1.56	4 (16%)
23	G7M	2K	47	23	23,26,27	2.56	7 (30%)	34,39,42	1.64	8 (23%)
23	5MU	2L	55	23	19,22,23	4.14	5 (26%)	27,32,35	3.17	11 (40%)
22	PSU	1K	55	22	18,21,22	1.28	1 (5%)	21,30,33	1.98	4 (19%)
22	5MU	1K	54	22	19,22,23	4.02	5 (26%)	27,32,35	2.89	9 (33%)
56	5MU	1L	54	56	19,22,23	3.87	5 (26%)	27,32,35	3.25	11 (40%)
22	PSU	1K	39	22	18,21,22	1.13	2 (11%)	21,30,33	1.92	5 (23%)
23	PSU	2L	56	23	18,21,22	1.32	2 (11%)	21,30,33	1.97	4 (19%)
22	U8U	1K	34	22,25	20,24,25	2.50	6 (30%)	22,34,37	1.38	4 (18%)
56	PSU	1L	39	56	18,21,22	1.16	2 (11%)	21,30,33	1.59	5 (23%)
23	G7M	2L	47	23	23,26,27	2.49	8 (34%)	34,39,42	1.83	10 (29%)
22	T6A	1K	37	22	31,34,35	2.31	12 (38%)	43,49,52	3.28	19 (44%)
23	OMC	2K	33	23	19,22,23	1.66	3 (15%)	25,31,34	1.40	3 (12%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
56	PSU	1L	55	56	-	1/7/25/26	0/2/2/2
23	4SU	2K	8	23	-	0/7/25/26	0/2/2/2
23	PSU	2K	56	23	-	0/7/25/26	0/2/2/2
57	PSU	3L	39	57	-	0/7/25/26	0/2/2/2
23	4SU	2L	8	23	-	0/7/25/26	0/2/2/2
23	5MU	2K	55	23	-	2/7/25/26	0/2/2/2
23	OMC	2L	33	23	-	2/9/27/28	0/2/2/2
23	G7M	2K	47	23	-	3/7/25/26	0/3/3/3
23	5MU	2L	55	23	-	0/7/25/26	0/2/2/2
22	PSU	1K	55	22	-	0/7/25/26	0/2/2/2
22	5MU	1K	54	22	-	2/7/25/26	0/2/2/2
56	5MU	1L	54	56	-	0/7/25/26	0/2/2/2
22	PSU	1K	39	22	-	0/7/25/26	0/2/2/2
23	PSU	2L	56	23	-	0/7/25/26	0/2/2/2
22	U8U	1K	34	22,25	-	3/10/28/29	0/2/2/2
56	PSU	1L	39	56	-	2/7/25/26	0/2/2/2
23	G7M	2L	47	23	-	2/7/25/26	0/3/3/3
22	T6A	1K	37	22	-	5/23/41/42	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
23	OMC	2K	33	23	-	2/9/27/28	0/2/2/2

The worst 5 of 77 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	2L	55	5MU	C2-N1	13.42	1.59	1.38
23	2K	55	5MU	C2-N1	13.26	1.59	1.38
22	1K	54	5MU	C2-N1	12.67	1.58	1.38
56	1L	54	5MU	C2-N1	12.26	1.57	1.38
23	2K	55	5MU	C2-N3	7.04	1.50	1.38

The worst 5 of 132 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
56	1L	54	5MU	C5-C4-N3	10.73	124.65	115.32
22	1K	37	T6A	N3-C2-N1	-10.12	113.27	128.58
23	2K	55	5MU	C5-C4-N3	9.41	123.50	115.32
23	2L	8	4SU	C4-N3-C2	-9.19	118.50	127.31
22	1K	54	5MU	C5-C4-N3	8.97	123.12	115.32

There are no chirality outliers.

5 of 24 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
22	1K	34	U8U	N-C-C5-C4
22	1K	34	U8U	N-C-C5-C6
22	1K	37	T6A	C13-C12-C14-O14
22	1K	37	T6A	C13-C12-C14-C15
23	2L	47	G7M	O4'-C4'-C5'-O5'

There are no ring outliers.

12 monomers are involved in 24 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
23	2K	8	4SU	1	0
23	2L	8	4SU	1	0
23	2K	55	5MU	3	0
23	2L	33	OMC	1	0
23	2K	47	G7M	2	0
23	2L	55	5MU	3	0
22	1K	55	PSU	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
56	1L	54	5MU	2	0
22	1K	34	U8U	3	0
23	2L	47	G7M	3	0
22	1K	37	T6A	1	0
23	2K	33	OMC	3	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 1188 ligands modelled in this entry, 1186 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	$\# Z > 2$
59	SF4	3E	301	4	0,12,12	-	-	-		
59	SF4	32	302	4	0,12,12	-	-	-		

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

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

1 monomer is involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
59	32	302	SF4	4	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
25	4K	1
37	35	1
38	45	1
5	4E	1
38	88	1
4	3E	1

The worst 5 of 6 chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	4K	24:A	O3'	25:A	P	4.44
1	35	121:LYS	C	122:PRO	N	1.77
1	45	124:LYS	C	125:LEU	N	1.15
1	4E	69:VAL	C	70:PRO	N	1.12
1	88	124:LYS	C	125:LEU	N	1.12

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	13	1493/1522 (98%)	-0.64	47 (3%) 51 31	83, 129, 202, 287	0
1	1G	1496/1522 (98%)	-0.60	37 (2%) 58 37	100, 152, 223, 279	0
2	12	206/256 (80%)	-0.03	1 (0%) 87 75	173, 206, 218, 228	0
2	1E	231/256 (90%)	-0.39	0 100 100	140, 173, 197, 207	0
3	22	194/239 (81%)	-0.27	2 (1%) 79 62	172, 196, 209, 214	0
3	2E	205/239 (85%)	-0.24	6 (2%) 53 34	115, 136, 165, 176	0
4	32	208/209 (99%)	-0.08	5 (2%) 59 39	129, 152, 173, 183	0
4	3E	207/209 (99%)	-0.19	2 (0%) 79 62	104, 131, 154, 164	0
5	42	149/162 (91%)	0.00	0 100 100	138, 160, 177, 190	0
5	4E	149/162 (91%)	-0.05	5 (3%) 48 28	104, 125, 147, 155	0
6	52	101/101 (100%)	-0.42	0 100 100	119, 135, 156, 163	0
6	5E	100/101 (99%)	-0.40	0 100 100	103, 129, 149, 159	0
7	62	138/156 (88%)	0.21	8 (5%) 29 16	150, 164, 173, 181	0
7	6E	151/156 (96%)	0.03	11 (7%) 21 12	134, 150, 170, 179	0
8	72	137/138 (99%)	-0.10	0 100 100	136, 164, 180, 190	0
8	7E	138/138 (100%)	-0.08	3 (2%) 62 41	112, 138, 152, 161	0
9	82	105/128 (82%)	-0.09	1 (0%) 79 62	149, 196, 209, 221	0
9	8E	126/128 (98%)	-0.18	4 (3%) 50 30	111, 170, 192, 200	0
10	1A	60/105 (57%)	-0.28	1 (1%) 69 48	166, 193, 204, 205	0
10	1I	72/105 (68%)	-0.09	2 (2%) 55 34	112, 150, 193, 204	0
11	2A	113/129 (87%)	0.27	4 (3%) 47 28	118, 143, 157, 167	0
11	2I	111/129 (86%)	0.13	5 (4%) 38 22	102, 136, 151, 164	0
12	3A	121/132 (91%)	0.44	10 (8%) 17 10	119, 142, 165, 179	0
12	3I	122/132 (92%)	-0.02	5 (4%) 41 24	91, 102, 126, 160	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
13	4A	111/126 (88%)	0.26	10 (9%) 15 9	162, 187, 202, 212	0
13	4I	119/126 (94%)	-0.23	4 (3%) 48 28	111, 146, 162, 173	0
14	5A	48/61 (78%)	0.05	1 (2%) 63 42	170, 191, 208, 218	0
14	5I	60/61 (98%)	-0.63	0 100 100	107, 124, 141, 155	0
15	6A	87/89 (97%)	-0.40	0 100 100	123, 148, 167, 174	0
15	6I	87/89 (97%)	-0.71	0 100 100	106, 127, 148, 153	0
16	7A	84/88 (95%)	-0.30	1 (1%) 76 57	120, 139, 161, 184	0
16	7I	80/88 (90%)	-0.22	0 100 100	127, 140, 169, 180	0
17	8A	99/105 (94%)	-0.52	0 100 100	121, 143, 156, 159	0
17	8I	100/105 (95%)	-0.64	1 (1%) 79 62	117, 136, 148, 154	0
18	9A	67/88 (76%)	-0.24	0 100 100	128, 145, 163, 171	0
18	9I	67/88 (76%)	-0.30	1 (1%) 72 52	115, 134, 159, 164	0
19	AA	36/93 (38%)	0.39	2 (5%) 30 17	191, 209, 217, 223	0
19	AI	81/93 (87%)	-0.43	0 100 100	125, 148, 173, 183	0
20	BA	98/106 (92%)	-0.64	1 (1%) 79 62	107, 139, 163, 176	0
20	BI	97/106 (91%)	-0.29	0 100 100	135, 152, 181, 193	0
21	1B	23/27 (85%)	-0.71	0 100 100	157, 179, 187, 189	0
21	1F	23/27 (85%)	-0.86	0 100 100	119, 134, 143, 145	0
22	1K	64/76 (84%)	1.04	12 (18%) 3 2	112, 226, 251, 253	0
23	2K	72/77 (93%)	-0.65	0 100 100	94, 125, 153, 169	0
23	2L	72/77 (93%)	0.55	8 (11%) 10 6	100, 151, 178, 198	0
24	3K	76/76 (100%)	-0.59	0 100 100	96, 189, 207, 218	0
25	4K	20/27 (74%)	0.65	4 (20%) 3 2	96, 156, 196, 199	0
25	4L	17/27 (62%)	0.93	3 (17%) 4 2	131, 170, 208, 211	0
26	14	2861/2912 (98%)	-0.79	44 (1%) 72 52	72, 111, 235, 276	0
26	1H	2830/2912 (97%)	-0.92	24 (0%) 82 66	65, 97, 204, 287	0
27	16	122/122 (100%)	-1.10	0 100 100	92, 117, 143, 228	0
27	1J	122/122 (100%)	-0.85	0 100 100	117, 155, 179, 225	0
28	7I	135/229 (58%)	-0.37	0 100 100	149, 167, 190, 202	0
29	11	273/276 (98%)	0.18	22 (8%) 18 10	65, 90, 111, 122	0
29	19	273/276 (98%)	0.13	17 (6%) 26 15	74, 100, 121, 136	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
30	21	203/206 (98%)	0.12	4 (1%) 65 44	73, 112, 157, 172	0
30	29	203/206 (98%)	-0.38	2 (0%) 79 62	79, 116, 162, 178	0
31	31	202/210 (96%)	-0.37	3 (1%) 72 52	70, 102, 136, 155	0
31	39	204/210 (97%)	-0.18	8 (3%) 43 25	83, 128, 181, 201	0
32	41	179/182 (98%)	-0.50	4 (2%) 62 41	107, 128, 164, 174	0
32	49	179/182 (98%)	0.22	10 (5%) 30 17	151, 171, 195, 204	0
33	51	171/180 (95%)	0.13	7 (4%) 41 24	102, 128, 146, 157	0
33	59	69/180 (38%)	0.44	7 (10%) 12 7	170, 198, 213, 220	0
34	61	145/148 (97%)	-0.17	2 (1%) 73 53	102, 163, 188, 199	0
34	69	145/148 (97%)	-0.27	9 (6%) 26 15	111, 152, 176, 189	0
35	15	137/140 (97%)	0.14	7 (5%) 33 19	106, 134, 162, 179	0
35	58	138/140 (98%)	0.12	9 (6%) 25 14	86, 112, 154, 172	0
36	25	122/122 (100%)	-0.09	0 100 100	92, 113, 132, 142	0
36	68	122/122 (100%)	0.07	2 (1%) 70 50	81, 98, 118, 131	0
37	35	148/150 (98%)	0.15	11 (7%) 20 12	84, 135, 174, 190	0
37	78	147/150 (98%)	-0.23	4 (2%) 56 35	72, 104, 136, 144	0
38	45	138/141 (97%)	0.07	13 (9%) 14 8	99, 131, 151, 168	0
38	88	141/141 (100%)	-0.38	0 100 100	76, 101, 123, 153	0
39	55	118/118 (100%)	-0.72	0 100 100	87, 102, 118, 138	0
39	98	118/118 (100%)	-0.46	0 100 100	87, 109, 131, 147	0
40	65	110/112 (98%)	-0.56	0 100 100	116, 145, 164, 172	0
40	A8	111/112 (99%)	-0.66	0 100 100	93, 112, 135, 144	0
41	75	136/146 (93%)	-0.28	5 (3%) 45 26	102, 120, 169, 198	0
41	B8	135/146 (92%)	0.10	6 (4%) 39 22	92, 116, 166, 185	0
42	85	116/118 (98%)	-0.05	2 (1%) 69 48	90, 121, 154, 166	0
42	C8	115/118 (97%)	0.10	5 (4%) 40 23	77, 102, 130, 141	0
43	95	99/101 (98%)	0.22	5 (5%) 33 19	91, 152, 166, 174	0
43	D8	101/101 (100%)	-0.30	1 (0%) 79 62	78, 124, 149, 160	0
44	A5	110/113 (97%)	0.11	5 (4%) 38 22	84, 96, 127, 133	0
44	E8	110/113 (97%)	0.09	6 (5%) 30 17	79, 95, 125, 140	0
45	B5	94/96 (97%)	-0.28	3 (3%) 50 30	94, 110, 134, 144	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
45	F8	95/96 (98%)	-0.34	0 100 100	78, 93, 120, 133	0
46	C5	105/110 (95%)	0.56	7 (6%) 24 13	110, 143, 175, 185	0
46	G8	104/110 (94%)	0.27	2 (1%) 66 45	88, 116, 148, 161	0
47	D5	130/206 (63%)	-0.38	1 (0%) 82 66	138, 163, 188, 194	0
47	H8	148/206 (71%)	-0.39	1 (0%) 84 69	106, 140, 195, 207	0
48	E5	78/85 (91%)	-0.08	4 (5%) 33 19	99, 116, 136, 149	0
48	I8	76/85 (89%)	-0.66	1 (1%) 75 55	79, 95, 111, 130	0
49	F5	94/98 (95%)	0.06	3 (3%) 50 30	86, 109, 144, 159	0
49	J8	94/98 (95%)	-0.31	1 (1%) 78 60	79, 96, 143, 153	0
50	G5	67/72 (93%)	-0.31	0 100 100	113, 134, 152, 171	0
50	K8	68/72 (94%)	-0.12	0 100 100	82, 105, 124, 151	0
51	H5	58/60 (96%)	-0.49	0 100 100	103, 128, 155, 180	0
51	L8	58/60 (96%)	-0.47	0 100 100	83, 104, 140, 152	0
52	M8	47/71 (66%)	-0.17	0 100 100	131, 172, 183, 188	0
53	J5	56/60 (93%)	-0.31	0 100 100	82, 108, 155, 165	0
53	N8	48/60 (80%)	-0.30	0 100 100	72, 108, 153, 164	0
54	L5	45/49 (91%)	-0.24	2 (4%) 39 22	75, 83, 95, 107	0
54	P8	47/49 (95%)	-0.50	1 (2%) 63 42	68, 74, 98, 108	0
55	M5	64/65 (98%)	-0.07	1 (1%) 70 50	90, 105, 123, 143	0
55	Q8	64/65 (98%)	-0.27	1 (1%) 70 50	80, 91, 108, 123	0
56	1L	71/76 (93%)	0.09	3 (4%) 40 23	140, 257, 274, 277	0
57	3L	75/76 (98%)	1.11	13 (17%) 4 2	107, 259, 277, 285	0
All	All	20395/21728 (93%)	-0.41	495 (2%) 59 39	65, 127, 204, 287	0

The worst 5 of 495 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
57	3L	34	U	15.7
57	3L	35	U	11.8
9	8E	126	SER	7.8
48	E5	7	LEU	7.3
9	8E	127	LYS	7.2

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

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
56	PSU	1L	55	20/21	0.61	0.08	176,201,207,207	0
22	PSU	1K	55	20/21	0.79	0.08	143,175,183,183	0
56	5MU	1L	54	21/22	0.80	0.07	184,194,212,217	0
23	PSU	2L	56	20/21	0.81	0.08	143,152,158,162	0
22	5MU	1K	54	21/22	0.85	0.07	155,171,185,188	0
23	5MU	2K	55	21/22	0.87	0.05	122,135,144,159	0
23	4SU	2L	8	20/21	0.88	0.09	131,155,165,169	0
56	PSU	1L	39	20/21	0.88	0.17	155,179,185,187	0
23	PSU	2K	56	20/21	0.88	0.05	122,127,139,140	0
57	PSU	3L	39	20/21	0.88	0.24	160,164,169,170	0
23	G7M	2L	47	24/25	0.89	0.08	161,169,178,179	0
23	4SU	2K	8	20/21	0.90	0.09	111,120,124,128	0
23	5MU	2L	55	21/22	0.90	0.07	146,159,164,166	0
23	G7M	2K	47	24/25	0.93	0.06	124,132,139,146	0
23	OMC	2L	33	21/22	0.93	0.15	132,140,144,151	0
22	T6A	1K	37	32/33	0.94	0.26	100,113,152,156	0
22	U8U	1K	34	23/24	0.95	0.15	116,123,130,131	0
23	OMC	2K	33	21/22	0.96	0.10	95,105,111,117	0
22	PSU	1K	39	20/21	0.96	0.15	98,124,139,139	0

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
58	MG	1G	1602	1/1	-0.02	0.33	133,133,133,133	0
58	MG	1G	1627	1/1	0.14	0.38	142,142,142,142	0
58	MG	14	3062	1/1	0.18	0.28	129,129,129,129	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
58	MG	1H	3327	1/1	0.19	0.33	120,120,120,120	0
58	MG	32	301	1/1	0.20	0.33	128,128,128,128	0
58	MG	14	3310	1/1	0.22	0.34	124,124,124,124	0
58	MG	14	3051	1/1	0.23	0.26	158,158,158,158	0
58	MG	1H	3264	1/1	0.24	0.29	122,122,122,122	0
58	MG	1H	3318	1/1	0.25	0.35	116,116,116,116	0
58	MG	1H	3272	1/1	0.26	0.29	118,118,118,118	0
58	MG	1H	3337	1/1	0.26	0.31	140,140,140,140	0
58	MG	13	1705	1/1	0.28	0.29	150,150,150,150	0
58	MG	14	3168	1/1	0.29	0.27	122,122,122,122	0
58	MG	1H	3343	1/1	0.29	0.18	137,137,137,137	0
58	MG	1H	3317	1/1	0.32	0.37	106,106,106,106	0
58	MG	14	3324	1/1	0.32	0.27	104,104,104,104	0
58	MG	1G	1642	1/1	0.33	0.32	114,114,114,114	0
58	MG	1H	3035	1/1	0.35	0.28	123,123,123,123	0
58	MG	13	1704	1/1	0.36	0.21	134,134,134,134	0
58	MG	14	3301	1/1	0.37	0.18	115,115,115,115	0
58	MG	2K	103	1/1	0.37	0.19	134,134,134,134	0
58	MG	1G	1669	1/1	0.37	0.20	151,151,151,151	0
58	MG	14	3303	1/1	0.38	0.33	115,115,115,115	0
58	MG	14	3293	1/1	0.39	0.36	109,109,109,109	0
58	MG	1H	3323	1/1	0.40	0.29	122,122,122,122	0
58	MG	C5	201	1/1	0.40	0.28	137,137,137,137	0
58	MG	14	3284	1/1	0.41	0.40	112,112,112,112	0
58	MG	13	1650	1/1	0.42	0.24	134,134,134,134	0
58	MG	1H	3033	1/1	0.43	0.23	109,109,109,109	0
58	MG	29	303	1/1	0.44	0.15	106,106,106,106	0
58	MG	1H	3257	1/1	0.44	0.37	97,97,97,97	0
58	MG	13	1652	1/1	0.45	0.20	138,138,138,138	0
58	MG	1H	3261	1/1	0.46	0.28	115,115,115,115	0
58	MG	14	3335	1/1	0.46	0.29	124,124,124,124	0
58	MG	1H	3313	1/1	0.47	0.29	114,114,114,114	0
58	MG	1H	3291	1/1	0.48	0.36	116,116,116,116	0
58	MG	13	1644	1/1	0.48	0.21	120,120,120,120	0
58	MG	1H	3322	1/1	0.48	0.27	121,121,121,121	0
58	MG	1H	3247	1/1	0.49	0.24	101,101,101,101	0
58	MG	1H	3187	1/1	0.50	0.26	105,105,105,105	0
58	MG	14	3089	1/1	0.50	0.43	104,104,104,104	0
58	MG	1G	1666	1/1	0.51	0.33	121,121,121,121	0
58	MG	1G	1635	1/1	0.51	0.34	111,111,111,111	0
58	MG	1H	3288	1/1	0.52	0.26	99,99,99,99	0
58	MG	14	3057	1/1	0.52	0.25	119,119,119,119	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
58	MG	14	3195	1/1	0.52	0.30	107,107,107,107	0
58	MG	14	3022	1/1	0.52	0.31	101,101,101,101	0
58	MG	1H	3314	1/1	0.53	0.20	107,107,107,107	0
58	MG	1G	1667	1/1	0.53	0.23	111,111,111,111	0
58	MG	13	1709	1/1	0.53	0.26	112,112,112,112	0
58	MG	1H	3350	1/1	0.53	0.33	113,113,113,113	0
58	MG	1H	3351	1/1	0.53	0.20	122,122,122,122	0
58	MG	14	3028	1/1	0.54	0.33	124,124,124,124	0
58	MG	1H	3161	1/1	0.54	0.24	115,115,115,115	0
58	MG	1H	3331	1/1	0.55	0.21	120,120,120,120	0
58	MG	13	1678	1/1	0.55	0.22	121,121,121,121	0
58	MG	1H	3230	1/1	0.55	0.20	104,104,104,104	0
58	MG	1G	1640	1/1	0.55	0.33	115,115,115,115	0
58	MG	14	3319	1/1	0.55	0.18	128,128,128,128	0
58	MG	13	1703	1/1	0.55	0.20	128,128,128,128	0
58	MG	14	3199	1/1	0.55	0.36	91,91,91,91	0
58	MG	13	1645	1/1	0.55	0.26	113,113,113,113	0
58	MG	14	3289	1/1	0.55	0.24	116,116,116,116	0
58	MG	1H	3330	1/1	0.56	0.23	105,105,105,105	0
58	MG	1H	3112	1/1	0.56	0.29	101,101,101,101	0
58	MG	14	3328	1/1	0.56	0.39	107,107,107,107	0
58	MG	1G	1643	1/1	0.56	0.36	102,102,102,102	0
58	MG	14	3058	1/1	0.56	0.23	107,107,107,107	0
58	MG	2K	102	1/1	0.56	0.29	109,109,109,109	0
58	MG	1H	3069	1/1	0.57	0.19	101,101,101,101	0
58	MG	1H	3070	1/1	0.57	0.28	100,100,100,100	0
58	MG	14	3255	1/1	0.57	0.29	105,105,105,105	0
58	MG	13	1675	1/1	0.57	0.21	149,149,149,149	0
58	MG	14	3286	1/1	0.57	0.34	117,117,117,117	0
58	MG	1H	3154	1/1	0.57	0.32	106,106,106,106	0
58	MG	1H	3256	1/1	0.57	0.29	104,104,104,104	0
58	MG	1G	1659	1/1	0.57	0.23	142,142,142,142	0
58	MG	14	3267	1/1	0.58	0.37	104,104,104,104	0
58	MG	1H	3286	1/1	0.58	0.34	109,109,109,109	0
58	MG	14	3018	1/1	0.58	0.25	111,111,111,111	0
58	MG	1H	3338	1/1	0.58	0.18	112,112,112,112	0
58	MG	1G	1611	1/1	0.58	0.29	129,129,129,129	0
58	MG	14	3068	1/1	0.58	0.37	108,108,108,108	0
58	MG	14	3260	1/1	0.58	0.42	115,115,115,115	0
58	MG	1H	3244	1/1	0.59	0.37	103,103,103,103	0
58	MG	14	3182	1/1	0.59	0.21	105,105,105,105	0
58	MG	1H	3309	1/1	0.59	0.22	126,126,126,126	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
58	MG	1H	3285	1/1	0.59	0.19	115,115,115,115	0
58	MG	14	3232	1/1	0.59	0.24	89,89,89,89	0
58	MG	14	3234	1/1	0.59	0.21	85,85,85,85	0
58	MG	2L	103	1/1	0.59	0.31	128,128,128,128	0
58	MG	14	3005	1/1	0.59	0.25	101,101,101,101	0
58	MG	1H	3016	1/1	0.59	0.26	105,105,105,105	0
58	MG	1H	3269	1/1	0.59	0.32	99,99,99,99	0
58	MG	14	3150	1/1	0.59	0.37	102,102,102,102	0
58	MG	1G	1616	1/1	0.60	0.26	118,118,118,118	0
58	MG	14	3223	1/1	0.60	0.16	116,116,116,116	0
58	MG	14	3033	1/1	0.60	0.30	95,95,95,95	0
58	MG	1H	3289	1/1	0.60	0.45	86,86,86,86	0
58	MG	14	3152	1/1	0.60	0.31	102,102,102,102	0
58	MG	1H	3282	1/1	0.60	0.24	106,106,106,106	0
58	MG	1H	3340	1/1	0.60	0.38	101,101,101,101	0
58	MG	14	3185	1/1	0.60	0.27	113,113,113,113	0
58	MG	14	3193	1/1	0.60	0.28	79,79,79,79	0
58	MG	1H	3212	1/1	0.60	0.27	93,93,93,93	0
58	MG	14	3316	1/1	0.61	0.25	111,111,111,111	0
58	MG	14	3026	1/1	0.61	0.20	115,115,115,115	0
58	MG	14	3322	1/1	0.61	0.30	117,117,117,117	0
58	MG	1H	3301	1/1	0.61	0.38	99,99,99,99	0
58	MG	14	3295	1/1	0.61	0.37	96,96,96,96	0
58	MG	1H	3328	1/1	0.61	0.28	119,119,119,119	0
58	MG	14	3339	1/1	0.61	0.31	120,120,120,120	0
58	MG	1G	1628	1/1	0.61	0.31	120,120,120,120	0
58	MG	1H	3105	1/1	0.61	0.34	86,86,86,86	0
58	MG	1H	3297	1/1	0.62	0.22	133,133,133,133	0
58	MG	1H	3320	1/1	0.62	0.28	107,107,107,107	0
58	MG	14	3233	1/1	0.62	0.29	108,108,108,108	0
58	MG	1H	3054	1/1	0.62	0.19	110,110,110,110	0
58	MG	14	3163	1/1	0.62	0.30	104,104,104,104	0
58	MG	1H	3198	1/1	0.62	0.28	119,119,119,119	0
58	MG	14	3258	1/1	0.63	0.24	93,93,93,93	0
58	MG	1H	3300	1/1	0.63	0.29	99,99,99,99	0
58	MG	13	1710	1/1	0.63	0.23	118,118,118,118	0
58	MG	13	1681	1/1	0.63	0.20	124,124,124,124	0
58	MG	13	1684	1/1	0.63	0.21	141,141,141,141	0
58	MG	1H	3146	1/1	0.63	0.27	103,103,103,103	0
58	MG	14	3170	1/1	0.63	0.22	119,119,119,119	0
58	MG	13	1637	1/1	0.63	0.23	123,123,123,123	0
58	MG	14	3245	1/1	0.63	0.22	97,97,97,97	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
58	MG	1H	3346	1/1	0.63	0.29	113,113,113,113	0
58	MG	14	3337	1/1	0.64	0.37	125,125,125,125	0
58	MG	14	3272	1/1	0.64	0.30	96,96,96,96	0
58	MG	14	3321	1/1	0.64	0.25	109,109,109,109	0
58	MG	13	1653	1/1	0.64	0.20	144,144,144,144	0
58	MG	1H	3319	1/1	0.65	0.29	102,102,102,102	0
58	MG	13	1694	1/1	0.65	0.25	114,114,114,114	0
58	MG	1H	3120	1/1	0.65	0.26	107,107,107,107	0
58	MG	1H	3290	1/1	0.65	0.32	103,103,103,103	0
58	MG	1G	1644	1/1	0.65	0.30	110,110,110,110	0
58	MG	1H	3220	1/1	0.65	0.21	115,115,115,115	0
58	MG	1G	1665	1/1	0.65	0.25	122,122,122,122	0
58	MG	1H	3060	1/1	0.66	0.29	111,111,111,111	0
58	MG	1H	3023	1/1	0.66	0.27	92,92,92,92	0
58	MG	14	3269	1/1	0.66	0.14	115,115,115,115	0
58	MG	14	3325	1/1	0.66	0.23	110,110,110,110	0
58	MG	14	3240	1/1	0.66	0.19	111,111,111,111	0
58	MG	14	3304	1/1	0.66	0.28	87,87,87,87	0
58	MG	14	3200	1/1	0.66	0.25	94,94,94,94	0
58	MG	14	3315	1/1	0.66	0.23	114,114,114,114	0
58	MG	13	1692	1/1	0.66	0.37	99,99,99,99	0
58	MG	1H	3176	1/1	0.66	0.30	110,110,110,110	0
58	MG	14	3192	1/1	0.67	0.27	104,104,104,104	0
58	MG	13	1625	1/1	0.67	0.36	102,102,102,102	0
58	MG	13	1670	1/1	0.67	0.19	119,119,119,119	0
58	MG	7A	101	1/1	0.67	0.27	104,104,104,104	0
58	MG	1H	3011	1/1	0.67	0.36	71,71,71,71	0
58	MG	1H	3268	1/1	0.67	0.30	104,104,104,104	0
58	MG	1H	3315	1/1	0.67	0.19	99,99,99,99	0
58	MG	1G	1645	1/1	0.67	0.31	122,122,122,122	0
58	MG	14	3024	1/1	0.67	0.37	106,106,106,106	0
58	MG	13	1702	1/1	0.67	0.30	114,114,114,114	0
58	MG	13	1690	1/1	0.67	0.35	113,113,113,113	0
58	MG	1H	3281	1/1	0.67	0.34	108,108,108,108	0
58	MG	1H	3206	1/1	0.67	0.28	100,100,100,100	0
58	MG	14	3165	1/1	0.68	0.29	102,102,102,102	0
58	MG	14	3331	1/1	0.68	0.32	108,108,108,108	0
58	MG	14	3101	1/1	0.68	0.21	108,108,108,108	0
58	MG	1H	3165	1/1	0.68	0.19	99,99,99,99	0
58	MG	14	3338	1/1	0.68	0.13	114,114,114,114	0
58	MG	14	3309	1/1	0.68	0.20	109,109,109,109	0
58	MG	14	3179	1/1	0.68	0.26	102,102,102,102	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
58	MG	14	3297	1/1	0.68	0.29	91,91,91,91	0
58	MG	1H	3062	1/1	0.69	0.19	103,103,103,103	0
58	MG	1H	3255	1/1	0.69	0.38	94,94,94,94	0
58	MG	14	3263	1/1	0.69	0.28	102,102,102,102	0
58	MG	14	3265	1/1	0.69	0.16	110,110,110,110	0
58	MG	14	3056	1/1	0.69	0.22	109,109,109,109	0
58	MG	1H	3262	1/1	0.69	0.25	100,100,100,100	0
58	MG	14	3271	1/1	0.69	0.20	101,101,101,101	0
58	MG	13	1606	1/1	0.69	0.20	119,119,119,119	0
58	MG	14	3059	1/1	0.69	0.24	92,92,92,92	0
58	MG	14	3215	1/1	0.69	0.31	89,89,89,89	0
58	MG	14	3318	1/1	0.69	0.24	102,102,102,102	0
58	MG	14	3257	1/1	0.69	0.17	143,143,143,143	0
58	MG	1H	3182	1/1	0.70	0.20	91,91,91,91	0
58	MG	1G	1630	1/1	0.70	0.23	120,120,120,120	0
58	MG	1H	3202	1/1	0.70	0.27	95,95,95,95	0
58	MG	1G	1652	1/1	0.70	0.27	110,110,110,110	0
58	MG	14	3129	1/1	0.70	0.25	84,84,84,84	0
58	MG	14	3290	1/1	0.70	0.19	113,113,113,113	0
58	MG	14	3143	1/1	0.70	0.26	110,110,110,110	0
58	MG	1H	3141	1/1	0.70	0.41	83,83,83,83	0
58	MG	1H	3341	1/1	0.70	0.16	110,110,110,110	0
58	MG	14	3153	1/1	0.70	0.24	102,102,102,102	0
58	MG	E5	101	1/1	0.70	0.39	100,100,100,100	0
58	MG	14	3262	1/1	0.71	0.26	109,109,109,109	0
58	MG	1H	3194	1/1	0.71	0.19	91,91,91,91	0
58	MG	14	3052	1/1	0.71	0.16	83,83,83,83	0
58	MG	1H	3347	1/1	0.71	0.12	102,102,102,102	0
58	MG	1H	3149	1/1	0.71	0.29	102,102,102,102	0
58	MG	14	3227	1/1	0.71	0.32	104,104,104,104	0
58	MG	13	1626	1/1	0.71	0.25	113,113,113,113	0
58	MG	14	3281	1/1	0.71	0.34	103,103,103,103	0
58	MG	16	208	1/1	0.71	0.13	111,111,111,111	0
58	MG	13	1698	1/1	0.71	0.21	96,96,96,96	0
58	MG	14	3239	1/1	0.71	0.30	90,90,90,90	0
58	MG	1H	3119	1/1	0.71	0.31	81,81,81,81	0
58	MG	14	3333	1/1	0.71	0.28	102,102,102,102	0
58	MG	13	1679	1/1	0.71	0.24	122,122,122,122	0
58	MG	13	1663	1/1	0.71	0.29	86,86,86,86	0
58	MG	14	3256	1/1	0.71	0.25	110,110,110,110	0
58	MG	14	3299	1/1	0.71	0.26	118,118,118,118	0
58	MG	14	3112	1/1	0.71	0.14	108,108,108,108	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
58	MG	1H	3342	1/1	0.71	0.24	105,105,105,105	0
58	MG	1H	3090	1/1	0.71	0.23	76,76,76,76	0
58	MG	14	3283	1/1	0.72	0.32	98,98,98,98	0
58	MG	14	3247	1/1	0.72	0.42	104,104,104,104	0
58	MG	1H	3082	1/1	0.72	0.22	79,79,79,79	0
58	MG	13	1740	1/1	0.72	0.22	107,107,107,107	0
58	MG	13	1680	1/1	0.72	0.25	125,125,125,125	0
58	MG	14	3202	1/1	0.72	0.21	79,79,79,79	0
58	MG	14	3294	1/1	0.72	0.45	100,100,100,100	0
58	MG	1H	3310	1/1	0.72	0.30	95,95,95,95	0
58	MG	1H	3208	1/1	0.72	0.37	99,99,99,99	0
58	MG	13	1708	1/1	0.72	0.32	102,102,102,102	0
58	MG	14	3300	1/1	0.72	0.15	118,118,118,118	0
58	MG	1H	3031	1/1	0.72	0.36	115,115,115,115	0
58	MG	1H	3008	1/1	0.72	0.28	99,99,99,99	0
58	MG	1G	1612	1/1	0.72	0.28	105,105,105,105	0
58	MG	1H	3034	1/1	0.72	0.21	145,145,145,145	0
58	MG	35	201	1/1	0.72	0.37	90,90,90,90	0
58	MG	1H	3296	1/1	0.72	0.33	86,86,86,86	0
58	MG	1H	3081	1/1	0.72	0.15	88,88,88,88	0
58	MG	13	1612	1/1	0.73	0.29	108,108,108,108	0
58	MG	1G	1604	1/1	0.73	0.21	119,119,119,119	0
58	MG	1H	3132	1/1	0.73	0.25	87,87,87,87	0
58	MG	14	3320	1/1	0.73	0.17	119,119,119,119	0
58	MG	1G	1647	1/1	0.73	0.25	101,101,101,101	0
58	MG	1H	3274	1/1	0.73	0.28	105,105,105,105	0
58	MG	1H	3235	1/1	0.73	0.43	112,112,112,112	0
58	MG	1H	3152	1/1	0.73	0.30	108,108,108,108	0
58	MG	14	3113	1/1	0.73	0.23	102,102,102,102	0
58	MG	14	3030	1/1	0.73	0.14	104,104,104,104	0
58	MG	14	3132	1/1	0.73	0.33	86,86,86,86	0
58	MG	14	3135	1/1	0.73	0.23	115,115,115,115	0
58	MG	1H	3263	1/1	0.73	0.34	92,92,92,92	0
58	MG	14	3045	1/1	0.73	0.23	89,89,89,89	0
58	MG	13	1647	1/1	0.73	0.23	108,108,108,108	0
58	MG	1J	201	1/1	0.73	0.29	100,100,100,100	0
58	MG	1H	3143	1/1	0.73	0.27	101,101,101,101	0
58	MG	1H	3339	1/1	0.73	0.35	104,104,104,104	0
58	MG	45	202	1/1	0.73	0.17	122,122,122,122	0
58	MG	14	3311	1/1	0.73	0.26	105,105,105,105	0
58	MG	78	201	1/1	0.73	0.27	92,92,92,92	0
58	MG	13	1621	1/1	0.74	0.26	99,99,99,99	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
58	MG	14	3241	1/1	0.74	0.20	115,115,115,115	0
58	MG	1G	1634	1/1	0.74	0.22	127,127,127,127	0
58	MG	1H	3086	1/1	0.74	0.33	89,89,89,89	0
58	MG	1H	3316	1/1	0.74	0.18	91,91,91,91	0
58	MG	1H	3210	1/1	0.74	0.25	101,101,101,101	0
58	MG	1H	3077	1/1	0.74	0.24	65,65,65,65	0
58	MG	14	3218	1/1	0.74	0.23	97,97,97,97	0
58	MG	13	1700	1/1	0.74	0.21	123,123,123,123	0
58	MG	1H	3348	1/1	0.74	0.26	111,111,111,111	0
58	MG	14	3117	1/1	0.74	0.26	91,91,91,91	0
58	MG	14	3001	1/1	0.74	0.36	97,97,97,97	0
58	MG	1H	3169	1/1	0.74	0.18	95,95,95,95	0
58	MG	1H	3173	1/1	0.74	0.23	108,108,108,108	0
58	MG	16	205	1/1	0.75	0.17	106,106,106,106	0
58	MG	1H	3324	1/1	0.75	0.18	97,97,97,97	0
58	MG	14	3231	1/1	0.75	0.21	107,107,107,107	0
58	MG	13	1673	1/1	0.75	0.34	106,106,106,106	0
58	MG	1G	1636	1/1	0.75	0.29	111,111,111,111	0
58	MG	1H	3229	1/1	0.75	0.30	89,89,89,89	0
58	MG	14	3235	1/1	0.75	0.18	102,102,102,102	0
58	MG	1G	1603	1/1	0.75	0.26	132,132,132,132	0
58	MG	13	1648	1/1	0.75	0.42	108,108,108,108	0
58	MG	14	3134	1/1	0.75	0.31	100,100,100,100	0
58	MG	13	1660	1/1	0.75	0.21	104,104,104,104	0
58	MG	1H	3333	1/1	0.75	0.24	93,93,93,93	0
58	MG	1H	3240	1/1	0.75	0.32	96,96,96,96	0
58	MG	13	1605	1/1	0.75	0.21	134,134,134,134	0
58	MG	14	3023	1/1	0.75	0.31	103,103,103,103	0
58	MG	13	1603	1/1	0.75	0.29	102,102,102,102	0
58	MG	1G	1664	1/1	0.76	0.21	122,122,122,122	0
58	MG	13	1662	1/1	0.76	0.15	116,116,116,116	0
58	MG	1H	3155	1/1	0.76	0.14	86,86,86,86	0
58	MG	14	3054	1/1	0.76	0.12	99,99,99,99	0
58	MG	1G	1605	1/1	0.76	0.20	125,125,125,125	0
58	MG	1H	3128	1/1	0.76	0.22	90,90,90,90	0
58	MG	14	3274	1/1	0.76	0.18	97,97,97,97	0
58	MG	14	3313	1/1	0.76	0.22	107,107,107,107	0
58	MG	14	3032	1/1	0.76	0.20	109,109,109,109	0
58	MG	1H	3205	1/1	0.76	0.39	114,114,114,114	0
58	MG	14	3317	1/1	0.77	0.18	122,122,122,122	0
58	MG	1H	3312	1/1	0.77	0.28	103,103,103,103	0
58	MG	1H	3030	1/1	0.77	0.34	85,85,85,85	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
58	MG	1G	1606	1/1	0.77	0.26	93,93,93,93	0
58	MG	1H	3036	1/1	0.77	0.14	118,118,118,118	0
58	MG	14	3146	1/1	0.77	0.24	77,77,77,77	0
58	MG	1H	3071	1/1	0.77	0.21	94,94,94,94	0
58	MG	1G	1614	1/1	0.77	0.17	127,127,127,127	0
58	MG	14	3261	1/1	0.77	0.17	101,101,101,101	0
58	MG	13	1634	1/1	0.77	0.27	104,104,104,104	0
58	MG	1G	1621	1/1	0.77	0.27	110,110,110,110	0
58	MG	1H	3116	1/1	0.77	0.32	88,88,88,88	0
58	MG	14	3302	1/1	0.77	0.37	95,95,95,95	0
58	MG	1G	1663	1/1	0.77	0.16	133,133,133,133	0
58	MG	16	209	1/1	0.77	0.14	106,106,106,106	0
58	MG	14	3174	1/1	0.77	0.26	98,98,98,98	0
58	MG	13	1707	1/1	0.77	0.33	114,114,114,114	0
58	MG	1G	1632	1/1	0.77	0.22	130,130,130,130	0
58	MG	14	3275	1/1	0.77	0.23	90,90,90,90	0
58	MG	13	1688	1/1	0.77	0.23	96,96,96,96	0
58	MG	1H	3332	1/1	0.77	0.34	93,93,93,93	0
58	MG	13	1685	1/1	0.78	0.26	107,107,107,107	0
58	MG	1H	3349	1/1	0.78	0.14	119,119,119,119	0
58	MG	13	1627	1/1	0.78	0.33	105,105,105,105	0
58	MG	1H	3295	1/1	0.78	0.22	110,110,110,110	0
58	MG	1H	3355	1/1	0.78	0.35	88,88,88,88	0
58	MG	1H	3005	1/1	0.78	0.25	79,79,79,79	0
58	MG	14	3031	1/1	0.78	0.21	89,89,89,89	0
58	MG	16	207	1/1	0.78	0.17	92,92,92,92	0
58	MG	13	1695	1/1	0.78	0.17	122,122,122,122	0
58	MG	14	3326	1/1	0.78	0.31	104,104,104,104	0
58	MG	1H	3175	1/1	0.78	0.17	92,92,92,92	0
58	MG	1H	3209	1/1	0.78	0.31	99,99,99,99	0
58	MG	J8	101	1/1	0.78	0.23	89,89,89,89	0
58	MG	14	3053	1/1	0.78	0.29	82,82,82,82	0
58	MG	14	3216	1/1	0.78	0.21	101,101,101,101	0
58	MG	14	3217	1/1	0.78	0.30	89,89,89,89	0
58	MG	14	3264	1/1	0.78	0.23	106,106,106,106	0
58	MG	1H	3150	1/1	0.78	0.30	63,63,63,63	0
58	MG	1J	204	1/1	0.78	0.13	119,119,119,119	0
58	MG	13	1646	1/1	0.78	0.18	129,129,129,129	0
58	MG	13	1699	1/1	0.78	0.29	97,97,97,97	0
58	MG	14	3156	1/1	0.78	0.32	88,88,88,88	0
58	MG	1H	3226	1/1	0.78	0.23	88,88,88,88	0
58	MG	1H	3102	1/1	0.78	0.31	73,73,73,73	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
58	MG	14	3298	1/1	0.79	0.29	104,104,104,104	0
58	MG	1H	3242	1/1	0.79	0.17	90,90,90,90	0
58	MG	14	3110	1/1	0.79	0.25	94,94,94,94	0
58	MG	1H	3049	1/1	0.79	0.23	82,82,82,82	0
58	MG	1G	1620	1/1	0.79	0.28	91,91,91,91	0
58	MG	1H	3167	1/1	0.79	0.34	96,96,96,96	0
58	MG	14	3277	1/1	0.79	0.23	111,111,111,111	0
58	MG	1H	3178	1/1	0.79	0.26	93,93,93,93	0
58	MG	1H	3486	1/1	0.79	0.28	106,106,106,106	0
58	MG	1H	3129	1/1	0.79	0.36	85,85,85,85	0
58	MG	2L	101	1/1	0.79	0.23	97,97,97,97	0
58	MG	14	3136	1/1	0.79	0.27	93,93,93,93	0
58	MG	1J	202	1/1	0.79	0.28	110,110,110,110	0
58	MG	1H	3336	1/1	0.79	0.17	93,93,93,93	0
58	MG	14	3292	1/1	0.79	0.32	83,83,83,83	0
58	MG	14	3188	1/1	0.79	0.42	93,93,93,93	0
58	MG	1H	3237	1/1	0.79	0.16	88,88,88,88	0
58	MG	13	1676	1/1	0.79	0.17	130,130,130,130	0
58	MG	14	3151	1/1	0.79	0.24	109,109,109,109	0
58	MG	13	1661	1/1	0.80	0.21	90,90,90,90	0
58	MG	1G	1633	1/1	0.80	0.08	137,137,137,137	0
58	MG	14	3105	1/1	0.80	0.29	110,110,110,110	0
58	MG	13	1671	1/1	0.80	0.12	107,107,107,107	0
58	MG	1H	3275	1/1	0.80	0.15	83,83,83,83	0
58	MG	13	1604	1/1	0.80	0.29	90,90,90,90	0
58	MG	14	3171	1/1	0.80	0.35	91,91,91,91	0
58	MG	1G	1638	1/1	0.80	0.33	102,102,102,102	0
58	MG	1H	3038	1/1	0.80	0.18	102,102,102,102	0
58	MG	1H	3024	1/1	0.80	0.19	99,99,99,99	0
58	MG	14	3183	1/1	0.80	0.26	89,89,89,89	0
58	MG	14	3238	1/1	0.80	0.36	83,83,83,83	0
58	MG	1H	3196	1/1	0.80	0.26	102,102,102,102	0
58	MG	14	3342	1/1	0.80	0.14	120,120,120,120	0
58	MG	13	1674	1/1	0.80	0.18	121,121,121,121	0
58	MG	13	1691	1/1	0.80	0.35	94,94,94,94	0
58	MG	1J	203	1/1	0.80	0.22	124,124,124,124	0
58	MG	1G	1622	1/1	0.80	0.24	103,103,103,103	0
58	MG	1H	3032	1/1	0.80	0.27	110,110,110,110	0
58	MG	1G	1656	1/1	0.80	0.20	102,102,102,102	0
58	MG	14	3287	1/1	0.80	0.20	101,101,101,101	0
58	MG	1H	3063	1/1	0.80	0.23	57,57,57,57	0
58	MG	13	1624	1/1	0.80	0.20	118,118,118,118	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
58	MG	14	3166	1/1	0.81	0.16	79,79,79,79	0
58	MG	13	1641	1/1	0.81	0.13	112,112,112,112	0
58	MG	14	3224	1/1	0.81	0.05	105,105,105,105	0
58	MG	1H	3219	1/1	0.81	0.17	120,120,120,120	0
58	MG	14	3327	1/1	0.81	0.23	83,83,83,83	0
58	MG	13	1635	1/1	0.81	0.27	111,111,111,111	0
58	MG	1G	1654	1/1	0.81	0.24	110,110,110,110	0
58	MG	14	3011	1/1	0.81	0.32	85,85,85,85	0
58	MG	1H	3222	1/1	0.81	0.19	94,94,94,94	0
58	MG	1H	3003	1/1	0.81	0.24	72,72,72,72	0
58	MG	13	1623	1/1	0.81	0.21	88,88,88,88	0
58	MG	13	1672	1/1	0.81	0.14	133,133,133,133	0
58	MG	1H	3207	1/1	0.81	0.24	93,93,93,93	0
58	MG	1H	3039	1/1	0.81	0.27	100,100,100,100	0
58	MG	14	3075	1/1	0.81	0.29	96,96,96,96	0
58	MG	14	3080	1/1	0.81	0.28	105,105,105,105	0
58	MG	14	3251	1/1	0.81	0.12	90,90,90,90	0
58	MG	1G	1641	1/1	0.81	0.21	131,131,131,131	0
58	MG	1H	3043	1/1	0.81	0.18	75,75,75,75	0
58	MG	14	3162	1/1	0.81	0.36	90,90,90,90	0
58	MG	85	202	1/1	0.81	0.47	100,100,100,100	0
58	MG	5E	201	1/1	0.81	0.12	107,107,107,107	0
58	MG	1H	3294	1/1	0.81	0.16	103,103,103,103	0
58	MG	13	1666	1/1	0.82	0.11	99,99,99,99	0
58	MG	14	3106	1/1	0.82	0.21	85,85,85,85	0
58	MG	14	3108	1/1	0.82	0.18	88,88,88,88	0
58	MG	1H	3051	1/1	0.82	0.18	90,90,90,90	0
58	MG	1H	3303	1/1	0.82	0.21	102,102,102,102	0
58	MG	1H	3277	1/1	0.82	0.09	122,122,122,122	0
58	MG	1H	3118	1/1	0.82	0.26	104,104,104,104	0
58	MG	1H	3066	1/1	0.82	0.29	86,86,86,86	0
58	MG	1H	3179	1/1	0.82	0.23	101,101,101,101	0
58	MG	14	3288	1/1	0.82	0.18	120,120,120,120	0
58	MG	14	3133	1/1	0.82	0.23	98,98,98,98	0
58	MG	5I	101	1/1	0.82	0.11	110,110,110,110	0
58	MG	14	3291	1/1	0.82	0.21	96,96,96,96	0
58	MG	14	3246	1/1	0.82	0.15	95,95,95,95	0
58	MG	1H	3057	1/1	0.82	0.20	75,75,75,75	0
58	MG	14	3191	1/1	0.82	0.26	93,93,93,93	0
58	MG	1H	3158	1/1	0.82	0.16	105,105,105,105	0
58	MG	1H	3093	1/1	0.82	0.35	88,88,88,88	0
58	MG	14	3144	1/1	0.82	0.16	112,112,112,112	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
58	MG	1H	3162	1/1	0.82	0.29	106,106,106,106	0
58	MG	14	3147	1/1	0.82	0.24	110,110,110,110	0
58	MG	14	3149	1/1	0.82	0.32	94,94,94,94	0
58	MG	14	3213	1/1	0.82	0.15	114,114,114,114	0
58	MG	13	1696	1/1	0.82	0.25	95,95,95,95	0
58	MG	1G	1660	1/1	0.82	0.20	111,111,111,111	0
58	MG	14	3308	1/1	0.82	0.41	104,104,104,104	0
58	MG	1H	3232	1/1	0.82	0.20	98,98,98,98	0
58	MG	1H	3072	1/1	0.82	0.15	120,120,120,120	0
58	MG	14	3029	1/1	0.82	0.22	90,90,90,90	0
58	MG	1H	3109	1/1	0.82	0.25	102,102,102,102	0
58	MG	1H	3231	1/1	0.83	0.25	85,85,85,85	0
58	MG	1H	3097	1/1	0.83	0.20	72,72,72,72	0
58	MG	14	3296	1/1	0.83	0.16	110,110,110,110	0
58	MG	1H	3280	1/1	0.83	0.13	114,114,114,114	0
58	MG	14	3098	1/1	0.83	0.20	86,86,86,86	0
58	MG	1H	3215	1/1	0.83	0.25	69,69,69,69	0
58	MG	1H	3166	1/1	0.83	0.28	95,95,95,95	0
58	MG	14	3148	1/1	0.83	0.27	94,94,94,94	0
58	MG	13	1687	1/1	0.83	0.42	100,100,100,100	0
58	MG	1G	1662	1/1	0.83	0.19	118,118,118,118	0
58	MG	14	3109	1/1	0.83	0.27	94,94,94,94	0
58	MG	1H	3321	1/1	0.83	0.23	84,84,84,84	0
58	MG	1H	3145	1/1	0.83	0.25	117,117,117,117	0
58	MG	14	3196	1/1	0.83	0.20	98,98,98,98	0
58	MG	14	3197	1/1	0.83	0.23	124,124,124,124	0
58	MG	14	3155	1/1	0.83	0.18	101,101,101,101	0
58	MG	1H	3073	1/1	0.83	0.33	84,84,84,84	0
58	MG	14	3161	1/1	0.83	0.21	80,80,80,80	0
58	MG	1H	3074	1/1	0.83	0.24	94,94,94,94	0
58	MG	1H	3250	1/1	0.83	0.13	94,94,94,94	0
58	MG	14	3061	1/1	0.83	0.15	102,102,102,102	0
58	MG	1H	3134	1/1	0.83	0.21	103,103,103,103	0
58	MG	1H	3292	1/1	0.83	0.17	82,82,82,82	0
58	MG	14	3201	1/1	0.84	0.31	91,91,91,91	0
58	MG	14	3016	1/1	0.84	0.40	68,68,68,68	0
58	MG	14	3065	1/1	0.84	0.20	80,80,80,80	0
58	MG	13	1668	1/1	0.84	0.12	117,117,117,117	0
58	MG	1H	3203	1/1	0.84	0.20	91,91,91,91	0
58	MG	14	3078	1/1	0.84	0.19	82,82,82,82	0
58	MG	1G	1658	1/1	0.84	0.20	99,99,99,99	0
58	MG	1H	3017	1/1	0.84	0.21	79,79,79,79	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
58	MG	14	3096	1/1	0.84	0.26	57,57,57,57	0
58	MG	14	3278	1/1	0.84	0.18	86,86,86,86	0
58	MG	14	3279	1/1	0.84	0.20	103,103,103,103	0
58	MG	13	1667	1/1	0.84	0.23	91,91,91,91	0
58	MG	1H	3117	1/1	0.84	0.14	75,75,75,75	0
58	MG	1H	3075	1/1	0.84	0.39	82,82,82,82	0
58	MG	1H	3076	1/1	0.84	0.25	78,78,78,78	0
58	MG	1H	3184	1/1	0.84	0.34	94,94,94,94	0
58	MG	16	203	1/1	0.84	0.13	112,112,112,112	0
58	MG	1H	3010	1/1	0.84	0.24	98,98,98,98	0
58	MG	14	3035	1/1	0.84	0.18	89,89,89,89	0
58	MG	14	3039	1/1	0.84	0.28	86,86,86,86	0
58	MG	14	3116	1/1	0.84	0.30	75,75,75,75	0
58	MG	1H	3148	1/1	0.84	0.20	92,92,92,92	0
58	MG	14	3049	1/1	0.84	0.28	74,74,74,74	0
58	MG	14	3130	1/1	0.84	0.18	93,93,93,93	0
58	MG	14	3250	1/1	0.84	0.20	79,79,79,79	0
58	MG	1H	3127	1/1	0.84	0.19	79,79,79,79	0
58	MG	13	1683	1/1	0.84	0.26	119,119,119,119	0
58	MG	1G	1623	1/1	0.84	0.23	100,100,100,100	0
58	MG	1G	1626	1/1	0.84	0.19	118,118,118,118	0
58	MG	1G	1648	1/1	0.84	0.24	128,128,128,128	0
58	MG	14	3004	1/1	0.84	0.29	76,76,76,76	0
58	MG	1G	1649	1/1	0.84	0.18	128,128,128,128	0
58	MG	1H	3344	1/1	0.84	0.20	81,81,81,81	0
58	MG	14	3013	1/1	0.84	0.19	98,98,98,98	0
58	MG	1H	3020	1/1	0.85	0.26	84,84,84,84	0
58	MG	14	3120	1/1	0.85	0.09	94,94,94,94	0
58	MG	13	1617	1/1	0.85	0.22	97,97,97,97	0
58	MG	13	1693	1/1	0.85	0.28	108,108,108,108	0
58	MG	14	3076	1/1	0.85	0.17	83,83,83,83	0
58	MG	14	3205	1/1	0.85	0.12	97,97,97,97	0
58	MG	1H	3236	1/1	0.85	0.19	89,89,89,89	0
58	MG	14	3167	1/1	0.85	0.15	105,105,105,105	0
58	MG	41	201	1/1	0.85	0.14	102,102,102,102	0
58	MG	1H	3048	1/1	0.85	0.21	80,80,80,80	0
58	MG	14	3015	1/1	0.85	0.32	82,82,82,82	0
58	MG	14	3220	1/1	0.85	0.20	97,97,97,97	0
58	MG	14	3332	1/1	0.85	0.23	98,98,98,98	0
58	MG	1H	3180	1/1	0.85	0.12	97,97,97,97	0
58	MG	14	3334	1/1	0.85	0.19	92,92,92,92	0
58	MG	14	3177	1/1	0.85	0.33	87,87,87,87	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
58	MG	13	1659	1/1	0.85	0.06	116,116,116,116	0
58	MG	14	3181	1/1	0.85	0.41	91,91,91,91	0
58	MG	14	3270	1/1	0.85	0.23	97,97,97,97	0
58	MG	14	3102	1/1	0.85	0.15	92,92,92,92	0
58	MG	1H	3137	1/1	0.85	0.22	93,93,93,93	0
58	MG	1H	3307	1/1	0.85	0.23	97,97,97,97	0
58	MG	1G	1646	1/1	0.85	0.14	126,126,126,126	0
58	MG	1G	1629	1/1	0.85	0.16	121,121,121,121	0
58	MG	14	3027	1/1	0.85	0.20	79,79,79,79	0
58	MG	13	1649	1/1	0.85	0.12	118,118,118,118	0
58	MG	14	3312	1/1	0.85	0.17	97,97,97,97	0
58	MG	55	201	1/1	0.85	0.31	96,96,96,96	0
58	MG	14	3280	1/1	0.85	0.29	98,98,98,98	0
58	MG	1H	3126	1/1	0.85	0.14	83,83,83,83	0
58	MG	1H	3253	1/1	0.85	0.25	84,84,84,84	0
58	MG	14	3021	1/1	0.86	0.20	73,73,73,73	0
58	MG	1H	3009	1/1	0.86	0.13	98,98,98,98	0
58	MG	1G	1625	1/1	0.86	0.12	136,136,136,136	0
58	MG	1H	3157	1/1	0.86	0.24	88,88,88,88	0
58	MG	1H	3100	1/1	0.86	0.36	82,82,82,82	0
58	MG	14	3111	1/1	0.86	0.25	82,82,82,82	0
58	MG	14	3158	1/1	0.86	0.20	92,92,92,92	0
58	MG	1H	3329	1/1	0.86	0.12	105,105,105,105	0
58	MG	1H	3243	1/1	0.86	0.10	96,96,96,96	0
58	MG	14	3206	1/1	0.86	0.09	88,88,88,88	0
58	MG	14	3330	1/1	0.86	0.27	104,104,104,104	0
58	MG	1H	3002	1/1	0.86	0.24	64,64,64,64	0
58	MG	1H	3224	1/1	0.86	0.18	76,76,76,76	0
58	MG	13	1677	1/1	0.86	0.49	113,113,113,113	0
58	MG	1H	3085	1/1	0.86	0.21	92,92,92,92	0
58	MG	13	1618	1/1	0.86	0.15	108,108,108,108	0
58	MG	1H	3089	1/1	0.86	0.20	83,83,83,83	0
58	MG	13	1620	1/1	0.86	0.21	117,117,117,117	0
58	MG	14	3041	1/1	0.86	0.20	80,80,80,80	0
58	MG	14	3084	1/1	0.86	0.19	92,92,92,92	0
58	MG	14	3230	1/1	0.86	0.10	122,122,122,122	0
58	MG	14	3042	1/1	0.86	0.15	74,74,74,74	0
58	MG	14	3273	1/1	0.86	0.15	110,110,110,110	0
58	MG	14	3138	1/1	0.86	0.12	96,96,96,96	0
58	MG	29	301	1/1	0.86	0.20	69,69,69,69	0
58	MG	14	3091	1/1	0.86	0.22	92,92,92,92	0
58	MG	14	3044	1/1	0.86	0.12	88,88,88,88	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
58	MG	45	201	1/1	0.86	0.28	101,101,101,101	0
58	MG	1H	3019	1/1	0.86	0.28	65,65,65,65	0
58	MG	1H	3305	1/1	0.86	0.27	96,96,96,96	0
58	MG	1H	3214	1/1	0.86	0.19	65,65,65,65	0
58	MG	14	3103	1/1	0.86	0.15	81,81,81,81	0
58	MG	14	3282	1/1	0.86	0.13	96,96,96,96	0
58	MG	14	3266	1/1	0.87	0.16	99,99,99,99	0
58	MG	16	201	1/1	0.87	0.10	114,114,114,114	0
58	MG	1H	3065	1/1	0.87	0.21	77,77,77,77	0
58	MG	14	3208	1/1	0.87	0.11	93,93,93,93	0
58	MG	1H	3110	1/1	0.87	0.16	83,83,83,83	0
58	MG	1H	3053	1/1	0.87	0.20	81,81,81,81	0
58	MG	13	1739	1/1	0.87	0.21	113,113,113,113	0
58	MG	1H	3177	1/1	0.87	0.37	93,93,93,93	0
58	MG	1H	3136	1/1	0.87	0.31	80,80,80,80	0
58	MG	1H	3156	1/1	0.87	0.11	121,121,121,121	0
58	MG	1H	3311	1/1	0.87	0.11	77,77,77,77	0
58	MG	14	3323	1/1	0.87	0.08	159,159,159,159	0
58	MG	14	3107	1/1	0.87	0.21	80,80,80,80	0
58	MG	J8	102	1/1	0.87	0.23	77,77,77,77	0
58	MG	Q8	101	1/1	0.87	0.28	89,89,89,89	0
58	MG	1H	3047	1/1	0.87	0.33	71,71,71,71	0
58	MG	1H	3213	1/1	0.87	0.13	81,81,81,81	0
58	MG	1H	3283	1/1	0.87	0.51	95,95,95,95	0
58	MG	14	3007	1/1	0.87	0.26	81,81,81,81	0
58	MG	14	3115	1/1	0.87	0.20	88,88,88,88	0
58	MG	14	3055	1/1	0.87	0.18	77,77,77,77	0
58	MG	1H	3139	1/1	0.87	0.13	75,75,75,75	0
58	MG	1H	3248	1/1	0.87	0.44	93,93,93,93	0
58	MG	14	3336	1/1	0.87	0.29	120,120,120,120	0
58	MG	14	3124	1/1	0.87	0.24	90,90,90,90	0
58	MG	1H	3037	1/1	0.87	0.19	87,87,87,87	0
58	MG	13	1657	1/1	0.87	0.14	103,103,103,103	0
58	MG	14	3341	1/1	0.87	0.14	105,105,105,105	0
58	MG	1H	3189	1/1	0.87	0.31	93,93,93,93	0
58	MG	1H	3163	1/1	0.87	0.31	84,84,84,84	0
58	MG	1G	1650	1/1	0.87	0.24	98,98,98,98	0
58	MG	14	3253	1/1	0.87	0.10	90,90,90,90	0
58	MG	1H	3083	1/1	0.87	0.14	74,74,74,74	0
58	MG	1J	205	1/1	0.87	0.19	122,122,122,122	0
58	MG	1J	206	1/1	0.87	0.11	130,130,130,130	0
58	MG	1H	3225	1/1	0.87	0.27	70,70,70,70	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
58	MG	14	3137	1/1	0.87	0.08	119,119,119,119	0
58	MG	2K	101	1/1	0.87	0.23	84,84,84,84	0
58	MG	1H	3199	1/1	0.87	0.27	87,87,87,87	0
58	MG	1H	3326	1/1	0.87	0.24	97,97,97,97	0
58	MG	1H	3107	1/1	0.87	0.20	95,95,95,95	0
58	MG	14	3085	1/1	0.87	0.20	85,85,85,85	0
58	MG	14	3088	1/1	0.87	0.22	78,78,78,78	0
58	MG	14	3204	1/1	0.87	0.20	73,73,73,73	0
58	MG	1H	3027	1/1	0.88	0.12	95,95,95,95	0
58	MG	1H	3056	1/1	0.88	0.13	89,89,89,89	0
58	MG	14	3066	1/1	0.88	0.17	95,95,95,95	0
58	MG	1G	1610	1/1	0.88	0.14	118,118,118,118	0
58	MG	1H	3298	1/1	0.88	0.29	95,95,95,95	0
58	MG	14	3019	1/1	0.88	0.19	87,87,87,87	0
58	MG	1H	3217	1/1	0.88	0.09	81,81,81,81	0
58	MG	1H	3200	1/1	0.88	0.21	79,79,79,79	0
58	MG	1H	3029	1/1	0.88	0.21	92,92,92,92	0
58	MG	1G	1618	1/1	0.88	0.15	131,131,131,131	0
58	MG	1G	1619	1/1	0.88	0.12	109,109,109,109	0
58	MG	1H	3304	1/1	0.88	0.26	94,94,94,94	0
58	MG	1H	3481	1/1	0.88	0.07	133,133,133,133	0
58	MG	14	3094	1/1	0.88	0.26	82,82,82,82	0
58	MG	14	3095	1/1	0.88	0.25	75,75,75,75	0
58	MG	1H	3121	1/1	0.88	0.25	93,93,93,93	0
58	MG	1H	3488	1/1	0.88	0.07	92,92,92,92	0
58	MG	1G	1624	1/1	0.88	0.20	92,92,92,92	0
58	MG	14	3157	1/1	0.88	0.10	81,81,81,81	0
58	MG	14	3228	1/1	0.88	0.14	96,96,96,96	0
58	MG	1H	3204	1/1	0.88	0.10	87,87,87,87	0
58	MG	1H	3124	1/1	0.88	0.19	77,77,77,77	0
58	MG	14	3104	1/1	0.88	0.21	78,78,78,78	0
58	MG	1H	3252	1/1	0.88	0.17	75,75,75,75	0
58	MG	13	1609	1/1	0.88	0.14	99,99,99,99	0
58	MG	1H	3334	1/1	0.88	0.15	77,77,77,77	0
58	MG	1H	3227	1/1	0.88	0.19	92,92,92,92	0
58	MG	1G	1631	1/1	0.88	0.28	97,97,97,97	0
58	MG	21	301	1/1	0.88	0.23	69,69,69,69	0
58	MG	1H	3021	1/1	0.88	0.19	86,86,86,86	0
58	MG	1H	3172	1/1	0.88	0.18	89,89,89,89	0
58	MG	1H	3260	1/1	0.88	0.35	95,95,95,95	0
58	MG	1H	3188	1/1	0.88	0.27	84,84,84,84	0
58	MG	14	3003	1/1	0.88	0.13	76,76,76,76	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
58	MG	1H	3006	1/1	0.88	0.17	71,71,71,71	0
58	MG	1H	3174	1/1	0.88	0.24	99,99,99,99	0
58	MG	14	3122	1/1	0.88	0.26	95,95,95,95	0
58	MG	14	3186	1/1	0.88	0.29	100,100,100,100	0
58	MG	14	3123	1/1	0.88	0.19	109,109,109,109	0
58	MG	13	1631	1/1	0.88	0.12	82,82,82,82	0
58	MG	14	3009	1/1	0.88	0.18	74,74,74,74	0
58	MG	14	3010	1/1	0.88	0.19	73,73,73,73	0
58	MG	1H	3267	1/1	0.88	0.14	85,85,85,85	0
58	MG	14	3259	1/1	0.89	0.30	111,111,111,111	0
58	MG	14	3141	1/1	0.89	0.17	76,76,76,76	0
58	MG	1H	3125	1/1	0.89	0.16	75,75,75,75	0
58	MG	1H	3181	1/1	0.89	0.17	92,92,92,92	0
58	MG	1G	1668	1/1	0.89	0.09	138,138,138,138	0
58	MG	13	1669	1/1	0.89	0.13	120,120,120,120	0
58	MG	14	3034	1/1	0.89	0.18	96,96,96,96	0
58	MG	1H	3013	1/1	0.89	0.23	71,71,71,71	0
58	MG	1H	3186	1/1	0.89	0.18	96,96,96,96	0
58	MG	1G	1637	1/1	0.89	0.11	101,101,101,101	0
58	MG	13	1651	1/1	0.89	0.17	96,96,96,96	0
58	MG	14	3212	1/1	0.89	0.11	105,105,105,105	0
58	MG	14	3043	1/1	0.89	0.16	69,69,69,69	0
58	MG	13	1706	1/1	0.89	0.30	91,91,91,91	0
58	MG	1G	1609	1/1	0.89	0.10	113,113,113,113	0
58	MG	1H	3094	1/1	0.89	0.18	77,77,77,77	0
58	MG	1H	3190	1/1	0.89	0.14	108,108,108,108	0
58	MG	1H	3354	1/1	0.89	0.09	98,98,98,98	0
58	MG	14	3222	1/1	0.89	0.37	95,95,95,95	0
58	MG	1H	3193	1/1	0.89	0.26	104,104,104,104	0
58	MG	1H	3302	1/1	0.89	0.21	89,89,89,89	0
58	MG	1H	3095	1/1	0.89	0.40	95,95,95,95	0
58	MG	1H	3487	1/1	0.89	0.12	96,96,96,96	0
58	MG	14	3014	1/1	0.89	0.22	82,82,82,82	0
58	MG	13	1602	1/1	0.89	0.20	98,98,98,98	0
58	MG	1H	3278	1/1	0.89	0.30	90,90,90,90	0
58	MG	1H	3098	1/1	0.89	0.34	70,70,70,70	0
58	MG	16	204	1/1	0.89	0.09	106,106,106,106	0
58	MG	14	3175	1/1	0.89	0.20	93,93,93,93	0
58	MG	14	3237	1/1	0.89	0.14	181,181,181,181	0
58	MG	14	3406	1/1	0.89	0.06	121,121,121,121	0
58	MG	14	3176	1/1	0.89	0.19	96,96,96,96	0
58	MG	14	3020	1/1	0.89	0.23	93,93,93,93	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
58	MG	1H	3221	1/1	0.89	0.19	81,81,81,81	0
58	MG	1H	3251	1/1	0.89	0.15	75,75,75,75	0
58	MG	14	3069	1/1	0.89	0.15	106,106,106,106	0
58	MG	14	3074	1/1	0.89	0.27	70,70,70,70	0
58	MG	13	1701	1/1	0.89	0.17	103,103,103,103	0
58	MG	14	3248	1/1	0.89	0.23	89,89,89,89	0
58	MG	13	1642	1/1	0.89	0.14	104,104,104,104	0
58	MG	1H	3159	1/1	0.89	0.16	89,89,89,89	0
58	MG	1H	3287	1/1	0.89	0.28	96,96,96,96	0
58	MG	1H	3160	1/1	0.89	0.21	88,88,88,88	0
58	MG	13	1628	1/1	0.89	0.18	94,94,94,94	0
58	MG	14	3194	1/1	0.89	0.17	93,93,93,93	0
58	MG	14	3086	1/1	0.89	0.30	95,95,95,95	0
58	MG	13	1633	1/1	0.90	0.34	88,88,88,88	0
58	MG	1G	1655	1/1	0.90	0.07	176,176,176,176	0
58	MG	14	3017	1/1	0.90	0.25	68,68,68,68	0
58	MG	1H	3335	1/1	0.90	0.17	100,100,100,100	0
58	MG	1G	1657	1/1	0.90	0.07	163,163,163,163	0
58	MG	14	3221	1/1	0.90	0.10	80,80,80,80	0
58	MG	1H	3028	1/1	0.90	0.17	82,82,82,82	0
58	MG	14	3114	1/1	0.90	0.25	66,66,66,66	0
58	MG	14	3276	1/1	0.90	0.10	130,130,130,130	0
58	MG	1H	3144	1/1	0.90	0.27	89,89,89,89	0
58	MG	14	3169	1/1	0.90	0.19	69,69,69,69	0
58	MG	1H	3254	1/1	0.90	0.32	91,91,91,91	0
58	MG	13	1658	1/1	0.90	0.16	89,89,89,89	0
58	MG	14	3067	1/1	0.90	0.12	100,100,100,100	0
58	MG	1H	3092	1/1	0.90	0.19	76,76,76,76	0
58	MG	1H	3164	1/1	0.90	0.09	86,86,86,86	0
58	MG	1H	3108	1/1	0.90	0.33	92,92,92,92	0
58	MG	14	3178	1/1	0.90	0.21	94,94,94,94	0
58	MG	13	1638	1/1	0.90	0.27	82,82,82,82	0
58	MG	1H	3234	1/1	0.90	0.38	90,90,90,90	0
58	MG	14	3131	1/1	0.90	0.20	79,79,79,79	0
58	MG	13	1697	1/1	0.90	0.30	98,98,98,98	0
58	MG	1H	3151	1/1	0.90	0.07	90,90,90,90	0
58	MG	14	3081	1/1	0.90	0.17	89,89,89,89	0
58	MG	1H	3111	1/1	0.90	0.14	64,64,64,64	0
58	MG	1H	3153	1/1	0.90	0.12	86,86,86,86	0
58	MG	1H	3001	1/1	0.90	0.22	66,66,66,66	0
58	MG	14	3420	1/1	0.90	0.11	118,118,118,118	0
58	MG	14	3087	1/1	0.90	0.23	68,68,68,68	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
58	MG	2L	102	1/1	0.90	0.39	95,95,95,95	0
58	MG	1H	3270	1/1	0.90	0.20	87,87,87,87	0
58	MG	14	3040	1/1	0.90	0.20	72,72,72,72	0
58	MG	1H	3325	1/1	0.90	0.20	100,100,100,100	0
58	MG	1H	3299	1/1	0.90	0.25	94,94,94,94	0
58	MG	1H	3218	1/1	0.90	0.14	68,68,68,68	0
58	MG	29	302	1/1	0.90	0.17	94,94,94,94	0
58	MG	1H	3273	1/1	0.90	0.12	85,85,85,85	0
58	MG	1H	3096	1/1	0.90	0.23	76,76,76,76	0
58	MG	14	3048	1/1	0.90	0.17	90,90,90,90	0
58	MG	1H	3246	1/1	0.90	0.25	87,87,87,87	0
58	MG	13	1639	1/1	0.90	0.16	87,87,87,87	0
58	MG	16	202	1/1	0.90	0.11	102,102,102,102	0
58	MG	5E	202	1/1	0.90	0.06	111,111,111,111	0
58	MG	1H	3099	1/1	0.90	0.20	74,74,74,74	0
58	MG	1G	1651	1/1	0.91	0.07	128,128,128,128	0
58	MG	1H	3284	1/1	0.91	0.08	97,97,97,97	0
58	MG	14	3097	1/1	0.91	0.14	83,83,83,83	0
58	MG	14	3184	1/1	0.91	0.16	92,92,92,92	0
58	MG	1H	3044	1/1	0.91	0.15	68,68,68,68	0
58	MG	1H	3259	1/1	0.91	0.07	106,106,106,106	0
58	MG	14	3187	1/1	0.91	0.15	96,96,96,96	0
58	MG	1H	3026	1/1	0.91	0.18	80,80,80,80	0
58	MG	11	301	1/1	0.91	0.15	73,73,73,73	0
58	MG	1H	3170	1/1	0.91	0.07	92,92,92,92	0
58	MG	1H	3123	1/1	0.91	0.11	85,85,85,85	0
58	MG	1H	3140	1/1	0.91	0.20	89,89,89,89	0
58	MG	I8	101	1/1	0.91	0.21	70,70,70,70	0
58	MG	1H	3239	1/1	0.91	0.17	71,71,71,71	0
58	MG	13	1630	1/1	0.91	0.07	74,74,74,74	0
58	MG	1H	3293	1/1	0.91	0.25	94,94,94,94	0
58	MG	1G	1601	1/1	0.91	0.14	115,115,115,115	0
58	MG	14	3252	1/1	0.91	0.09	106,106,106,106	0
58	MG	1H	3142	1/1	0.91	0.23	89,89,89,89	0
58	MG	13	1741	1/1	0.91	0.15	88,88,88,88	0
58	MG	14	3159	1/1	0.91	0.17	81,81,81,81	0
58	MG	1H	3018	1/1	0.91	0.26	66,66,66,66	0
58	MG	1H	3052	1/1	0.91	0.19	69,69,69,69	0
58	MG	1G	1639	1/1	0.91	0.31	93,93,93,93	0
58	MG	14	3210	1/1	0.91	0.11	113,113,113,113	0
58	MG	1H	3042	1/1	0.91	0.20	59,59,59,59	0
58	MG	1H	3223	1/1	0.91	0.08	96,96,96,96	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
58	MG	1H	3147	1/1	0.91	0.32	93,93,93,93	0
58	MG	1H	3276	1/1	0.91	0.17	91,91,91,91	0
58	MG	14	3082	1/1	0.91	0.33	92,92,92,92	0
58	MG	1H	3014	1/1	0.91	0.11	65,65,65,65	0
58	MG	1H	3131	1/1	0.91	0.22	88,88,88,88	0
58	MG	1H	3279	1/1	0.91	0.13	106,106,106,106	0
58	MG	1H	3183	1/1	0.91	0.32	94,94,94,94	0
58	MG	1H	3104	1/1	0.91	0.18	66,66,66,66	0
58	MG	1H	3185	1/1	0.91	0.13	68,68,68,68	0
58	MG	14	3046	1/1	0.91	0.17	86,86,86,86	0
58	MG	1H	3078	1/1	0.91	0.15	80,80,80,80	0
58	MG	14	3229	1/1	0.91	0.14	93,93,93,93	0
58	MG	1H	3168	1/1	0.92	0.27	82,82,82,82	0
58	MG	1G	1675	1/1	0.92	0.09	150,150,150,150	0
58	MG	14	3236	1/1	0.92	0.07	121,121,121,121	0
58	MG	14	3072	1/1	0.92	0.24	84,84,84,84	0
58	MG	14	3164	1/1	0.92	0.16	93,93,93,93	0
58	MG	1G	1676	1/1	0.92	0.13	134,134,134,134	0
58	MG	1H	3050	1/1	0.92	0.14	74,74,74,74	0
58	MG	1H	3258	1/1	0.92	0.18	99,99,99,99	0
58	MG	1H	3059	1/1	0.92	0.09	110,110,110,110	0
58	MG	14	3203	1/1	0.92	0.18	84,84,84,84	0
58	MG	21	302	1/1	0.92	0.08	91,91,91,91	0
58	MG	14	3140	1/1	0.92	0.09	79,79,79,79	0
58	MG	1H	3171	1/1	0.92	0.46	83,83,83,83	0
58	MG	14	3173	1/1	0.92	0.10	96,96,96,96	0
58	MG	14	3209	1/1	0.92	0.16	90,90,90,90	0
58	MG	1H	3079	1/1	0.92	0.28	68,68,68,68	0
58	MG	14	3211	1/1	0.92	0.10	78,78,78,78	0
58	MG	1H	3133	1/1	0.92	0.07	83,83,83,83	0
58	MG	1H	3106	1/1	0.92	0.08	82,82,82,82	0
58	MG	14	3214	1/1	0.92	0.24	94,94,94,94	0
58	MG	1H	3012	1/1	0.92	0.35	93,93,93,93	0
58	MG	14	3358	1/1	0.92	0.08	107,107,107,107	0
58	MG	1H	3045	1/1	0.92	0.15	68,68,68,68	0
58	MG	14	3008	1/1	0.92	0.27	77,77,77,77	0
58	MG	1H	3192	1/1	0.92	0.25	85,85,85,85	0
58	MG	1H	3211	1/1	0.92	0.29	90,90,90,90	0
58	MG	1H	3041	1/1	0.92	0.14	73,73,73,73	0
58	MG	13	1654	1/1	0.92	0.15	111,111,111,111	0
58	MG	14	3305	1/1	0.92	0.10	127,127,127,127	0
58	MG	14	3154	1/1	0.92	0.09	84,84,84,84	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
58	MG	13	1607	1/1	0.92	0.08	101,101,101,101	0
58	MG	14	3268	1/1	0.92	0.23	84,84,84,84	0
58	MG	14	3225	1/1	0.92	0.21	95,95,95,95	0
58	MG	1H	3087	1/1	0.92	0.17	69,69,69,69	0
58	MG	14	3125	1/1	0.92	0.09	102,102,102,102	0
58	MG	14	3189	1/1	0.92	0.15	87,87,87,87	0
58	MG	14	3190	1/1	0.92	0.15	91,91,91,91	0
58	MG	1H	3068	1/1	0.92	0.24	70,70,70,70	0
58	MG	14	3099	1/1	0.92	0.12	91,91,91,91	0
58	MG	14	3160	1/1	0.92	0.14	98,98,98,98	0
58	MG	3I	201	1/1	0.93	0.10	87,87,87,87	0
58	MG	1H	3266	1/1	0.93	0.12	65,65,65,65	0
58	MG	13	1611	1/1	0.93	0.14	91,91,91,91	0
58	MG	14	3242	1/1	0.93	0.06	92,92,92,92	0
58	MG	14	3243	1/1	0.93	0.15	102,102,102,102	0
58	MG	13	1610	1/1	0.93	0.12	92,92,92,92	0
58	MG	1H	3007	1/1	0.93	0.13	65,65,65,65	0
58	MG	1H	3135	1/1	0.93	0.10	69,69,69,69	0
58	MG	14	3219	1/1	0.93	0.13	83,83,83,83	0
58	MG	14	3090	1/1	0.93	0.08	83,83,83,83	0
58	MG	14	3063	1/1	0.93	0.17	79,79,79,79	0
58	MG	1H	3352	1/1	0.93	0.19	75,75,75,75	0
58	MG	14	3401	1/1	0.93	0.05	127,127,127,127	0
58	MG	1H	3271	1/1	0.93	0.32	87,87,87,87	0
58	MG	14	3314	1/1	0.93	0.27	99,99,99,99	0
58	MG	1H	3103	1/1	0.93	0.35	72,72,72,72	0
58	MG	1G	1661	1/1	0.93	0.10	169,169,169,169	0
58	MG	14	3226	1/1	0.93	0.23	88,88,88,88	0
58	MG	13	1682	1/1	0.93	0.08	93,93,93,93	0
58	MG	13	1689	1/1	0.93	0.18	182,182,182,182	0
58	MG	14	3128	1/1	0.93	0.36	80,80,80,80	0
58	MG	14	3025	1/1	0.93	0.25	87,87,87,87	0
58	MG	14	3006	1/1	0.93	0.17	72,72,72,72	0
58	MG	13	1655	1/1	0.93	0.06	106,106,106,106	0
58	MG	14	3207	1/1	0.93	0.12	107,107,107,107	0
58	MG	1G	1613	1/1	0.93	0.12	114,114,114,114	0
58	MG	14	3079	1/1	0.93	0.11	87,87,87,87	0
58	MG	C8	201	1/1	0.93	0.24	74,74,74,74	0
58	MG	85	201	1/1	0.93	0.13	85,85,85,85	0
58	MG	13	1643	1/1	0.93	0.13	80,80,80,80	0
58	MG	14	3329	1/1	0.93	0.34	91,91,91,91	0
58	MG	1H	3130	1/1	0.93	0.12	79,79,79,79	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
58	MG	L5	101	1/1	0.93	0.32	96,96,96,96	0
60	ZN	G8	201	1/1	0.93	0.14	171,171,171,171	0
58	MG	1H	3228	1/1	0.94	0.31	74,74,74,74	0
58	MG	14	3340	1/1	0.94	0.15	91,91,91,91	0
58	MG	14	3077	1/1	0.94	0.10	83,83,83,83	0
58	MG	1H	3046	1/1	0.94	0.18	61,61,61,61	0
58	MG	1H	3442	1/1	0.94	0.13	63,63,63,63	0
58	MG	1H	3091	1/1	0.94	0.24	58,58,58,58	0
58	MG	14	3404	1/1	0.94	0.06	101,101,101,101	0
58	MG	13	1640	1/1	0.94	0.26	73,73,73,73	0
58	MG	13	1619	1/1	0.94	0.18	81,81,81,81	0
58	MG	14	3083	1/1	0.94	0.12	94,94,94,94	0
58	MG	14	3060	1/1	0.94	0.11	103,103,103,103	0
58	MG	1H	3197	1/1	0.94	0.35	68,68,68,68	0
58	MG	1H	3122	1/1	0.94	0.07	83,83,83,83	0
58	MG	1H	3114	1/1	0.94	0.08	77,77,77,77	0
58	MG	14	3064	1/1	0.94	0.11	86,86,86,86	0
58	MG	1H	3115	1/1	0.94	0.16	70,70,70,70	0
58	MG	1H	3238	1/1	0.94	0.07	83,83,83,83	0
58	MG	1H	3064	1/1	0.94	0.12	82,82,82,82	0
58	MG	14	3093	1/1	0.94	0.23	71,71,71,71	0
58	MG	14	3249	1/1	0.94	0.07	102,102,102,102	0
58	MG	13	1629	1/1	0.94	0.17	79,79,79,79	0
58	MG	1G	1653	1/1	0.94	0.07	118,118,118,118	0
58	MG	14	3070	1/1	0.94	0.10	94,94,94,94	0
58	MG	1H	3191	1/1	0.94	0.33	95,95,95,95	0
58	MG	14	3254	1/1	0.94	0.17	83,83,83,83	0
58	MG	1H	3353	1/1	0.94	0.14	96,96,96,96	0
58	MG	14	3127	1/1	0.94	0.20	67,67,67,67	0
58	MG	1G	1678	1/1	0.94	0.09	119,119,119,119	0
58	MG	1G	1607	1/1	0.95	0.07	109,109,109,109	0
58	MG	1H	3067	1/1	0.95	0.09	74,74,74,74	0
58	MG	14	3126	1/1	0.95	0.08	95,95,95,95	0
58	MG	14	3244	1/1	0.95	0.10	79,79,79,79	0
58	MG	14	3285	1/1	0.95	0.05	77,77,77,77	0
58	MG	13	1723	1/1	0.95	0.08	134,134,134,134	0
58	MG	1H	3058	1/1	0.95	0.07	76,76,76,76	0
58	MG	1H	3080	1/1	0.95	0.09	73,73,73,73	0
58	MG	1G	1677	1/1	0.95	0.06	185,185,185,185	0
58	MG	1H	3345	1/1	0.95	0.11	79,79,79,79	0
58	MG	13	1686	1/1	0.95	0.09	79,79,79,79	0
58	MG	1G	1615	1/1	0.95	0.18	142,142,142,142	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
58	MG	14	3172	1/1	0.95	0.12	75,75,75,75	0
58	MG	1H	3025	1/1	0.95	0.19	55,55,55,55	0
58	MG	16	206	1/1	0.95	0.07	89,89,89,89	0
58	MG	14	3100	1/1	0.95	0.07	107,107,107,107	0
58	MG	13	1622	1/1	0.95	0.11	99,99,99,99	0
58	MG	1H	3195	1/1	0.95	0.31	96,96,96,96	0
58	MG	1H	3245	1/1	0.95	0.05	100,100,100,100	0
58	MG	1H	3084	1/1	0.95	0.28	57,57,57,57	0
58	MG	14	3142	1/1	0.95	0.05	99,99,99,99	0
58	MG	14	3071	1/1	0.95	0.10	69,69,69,69	0
58	MG	13	1636	1/1	0.95	0.08	123,123,123,123	0
58	MG	14	3414	1/1	0.95	0.10	108,108,108,108	0
58	MG	14	3415	1/1	0.95	0.04	126,126,126,126	0
58	MG	14	3417	1/1	0.95	0.07	140,140,140,140	0
58	MG	14	3145	1/1	0.95	0.12	76,76,76,76	0
58	MG	1H	3265	1/1	0.95	0.30	100,100,100,100	0
58	MG	14	3306	1/1	0.95	0.09	129,129,129,129	0
58	MG	14	3307	1/1	0.95	0.05	80,80,80,80	0
58	MG	13	1615	1/1	0.95	0.12	90,90,90,90	0
58	MG	1H	3113	1/1	0.95	0.05	59,59,59,59	0
58	MG	1H	3411	1/1	0.95	0.07	94,94,94,94	0
58	MG	1H	3423	1/1	0.95	0.13	92,92,92,92	0
58	MG	1H	3438	1/1	0.95	0.13	110,110,110,110	0
58	MG	13	1601	1/1	0.95	0.12	86,86,86,86	0
58	MG	1H	3465	1/1	0.95	0.07	112,112,112,112	0
58	MG	1H	3479	1/1	0.95	0.07	91,91,91,91	0
58	MG	1H	3101	1/1	0.95	0.13	59,59,59,59	0
58	MG	1H	3483	1/1	0.95	0.05	119,119,119,119	0
58	MG	14	3118	1/1	0.95	0.12	73,73,73,73	0
58	MG	1H	3484	1/1	0.95	0.10	81,81,81,81	0
58	MG	14	3198	1/1	0.95	0.06	109,109,109,109	0
58	MG	14	3121	1/1	0.95	0.24	69,69,69,69	0
58	MG	1H	3485	1/1	0.95	0.08	83,83,83,83	0
58	MG	1H	3022	1/1	0.95	0.15	69,69,69,69	0
58	MG	14	3139	1/1	0.96	0.09	75,75,75,75	0
58	MG	1G	1617	1/1	0.96	0.06	159,159,159,159	0
58	MG	1H	3241	1/1	0.96	0.07	100,100,100,100	0
58	MG	14	3386	1/1	0.96	0.06	83,83,83,83	0
58	MG	14	3396	1/1	0.96	0.14	96,96,96,96	0
58	MG	13	1738	1/1	0.96	0.10	106,106,106,106	0
58	MG	1H	3015	1/1	0.96	0.53	77,77,77,77	0
58	MG	1H	3399	1/1	0.96	0.08	75,75,75,75	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
58	MG	1H	3061	1/1	0.96	0.35	79,79,79,79	0
58	MG	14	3012	1/1	0.96	0.22	67,67,67,67	0
58	MG	14	3038	1/1	0.96	0.16	67,67,67,67	0
58	MG	14	3092	1/1	0.96	0.10	91,91,91,91	0
58	MG	1H	3216	1/1	0.96	0.12	65,65,65,65	0
58	MG	1H	3040	1/1	0.96	0.21	71,71,71,71	0
58	MG	13	1736	1/1	0.96	0.07	126,126,126,126	0
58	MG	14	3180	1/1	0.96	0.20	81,81,81,81	0
58	MG	1H	3450	1/1	0.96	0.05	75,75,75,75	0
58	MG	1H	3451	1/1	0.96	0.10	85,85,85,85	0
58	MG	1H	3452	1/1	0.96	0.06	102,102,102,102	0
58	MG	1H	3459	1/1	0.96	0.15	102,102,102,102	0
58	MG	1G	1608	1/1	0.96	0.06	119,119,119,119	0
58	MG	14	3047	1/1	0.96	0.09	102,102,102,102	0
58	MG	1H	3463	1/1	0.96	0.13	103,103,103,103	0
58	MG	1H	3088	1/1	0.96	0.07	81,81,81,81	0
58	MG	45	203	1/1	0.96	0.47	104,104,104,104	0
58	MG	14	3050	1/1	0.96	0.05	87,87,87,87	0
58	MG	16	212	1/1	0.96	0.04	104,104,104,104	0
58	MG	1H	3470	1/1	0.96	0.05	85,85,85,85	0
58	MG	1H	3472	1/1	0.96	0.07	108,108,108,108	0
58	MG	1H	3249	1/1	0.96	0.05	83,83,83,83	0
58	MG	1H	3138	1/1	0.96	0.05	67,67,67,67	0
58	MG	1H	3004	1/1	0.96	0.12	60,60,60,60	0
60	ZN	C5	202	1/1	0.96	0.11	183,183,183,183	0
58	MG	13	1608	1/1	0.97	0.06	90,90,90,90	0
58	MG	14	3036	1/1	0.97	0.09	70,70,70,70	0
58	MG	13	1616	1/1	0.97	0.07	121,121,121,121	0
58	MG	14	3407	1/1	0.97	0.04	121,121,121,121	0
58	MG	1H	3306	1/1	0.97	0.09	77,77,77,77	0
58	MG	13	1665	1/1	0.97	0.05	105,105,105,105	0
58	MG	1H	3462	1/1	0.97	0.05	90,90,90,90	0
58	MG	1H	3401	1/1	0.97	0.04	71,71,71,71	0
58	MG	1H	3403	1/1	0.97	0.04	81,81,81,81	0
58	MG	1H	3055	1/1	0.97	0.05	74,74,74,74	0
58	MG	1H	3412	1/1	0.97	0.09	84,84,84,84	0
58	MG	1H	3201	1/1	0.97	0.46	97,97,97,97	0
58	MG	1H	3426	1/1	0.97	0.14	109,109,109,109	0
58	MG	1H	3433	1/1	0.97	0.15	113,113,113,113	0
58	MG	1H	3437	1/1	0.97	0.05	85,85,85,85	0
58	MG	13	1614	1/1	0.97	0.05	97,97,97,97	0
58	MG	1H	3233	1/1	0.97	0.04	93,93,93,93	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
58	MG	88	201	1/1	0.97	0.06	91,91,91,91	0
58	MG	1H	3448	1/1	0.97	0.07	88,88,88,88	0
58	MG	1H	3449	1/1	0.97	0.07	89,89,89,89	0
58	MG	14	3349	1/1	0.97	0.07	95,95,95,95	0
58	MG	14	3354	1/1	0.97	0.05	87,87,87,87	0
58	MG	1G	1670	1/1	0.97	0.05	112,112,112,112	0
58	MG	14	3366	1/1	0.97	0.04	114,114,114,114	0
58	MG	14	3368	1/1	0.97	0.05	87,87,87,87	0
58	MG	14	3372	1/1	0.97	0.07	134,134,134,134	0
58	MG	14	3381	1/1	0.97	0.09	116,116,116,116	0
58	MG	1G	1673	1/1	0.97	0.17	145,145,145,145	0
58	MG	1G	1674	1/1	0.97	0.04	124,124,124,124	0
58	MG	13	1726	1/1	0.98	0.05	91,91,91,91	0
58	MG	1H	3365	1/1	0.98	0.04	64,64,64,64	0
58	MG	1H	3443	1/1	0.98	0.11	80,80,80,80	0
58	MG	14	3364	1/1	0.98	0.10	105,105,105,105	0
58	MG	1H	3445	1/1	0.98	0.06	71,71,71,71	0
58	MG	14	3119	1/1	0.98	0.06	83,83,83,83	0
58	MG	14	3369	1/1	0.98	0.06	105,105,105,105	0
58	MG	1H	3447	1/1	0.98	0.04	115,115,115,115	0
58	MG	14	3374	1/1	0.98	0.10	107,107,107,107	0
58	MG	14	3375	1/1	0.98	0.10	117,117,117,117	0
58	MG	14	3376	1/1	0.98	0.04	124,124,124,124	0
58	MG	1H	3369	1/1	0.98	0.07	90,90,90,90	0
58	MG	14	3382	1/1	0.98	0.10	112,112,112,112	0
58	MG	1H	3375	1/1	0.98	0.04	81,81,81,81	0
58	MG	14	3388	1/1	0.98	0.06	88,88,88,88	0
58	MG	1H	3380	1/1	0.98	0.04	89,89,89,89	0
58	MG	14	3398	1/1	0.98	0.06	111,111,111,111	0
58	MG	1H	3384	1/1	0.98	0.12	87,87,87,87	0
58	MG	1H	3396	1/1	0.98	0.03	99,99,99,99	0
58	MG	14	3405	1/1	0.98	0.05	89,89,89,89	0
58	MG	1H	3454	1/1	0.98	0.11	96,96,96,96	0
58	MG	1H	3457	1/1	0.98	0.09	89,89,89,89	0
58	MG	14	3409	1/1	0.98	0.14	85,85,85,85	0
58	MG	14	3411	1/1	0.98	0.03	134,134,134,134	0
58	MG	13	1727	1/1	0.98	0.07	87,87,87,87	0
58	MG	1H	3461	1/1	0.98	0.09	97,97,97,97	0
58	MG	13	1731	1/1	0.98	0.03	108,108,108,108	0
58	MG	13	1734	1/1	0.98	0.05	131,131,131,131	0
58	MG	1H	3407	1/1	0.98	0.04	83,83,83,83	0
58	MG	1H	3467	1/1	0.98	0.03	115,115,115,115	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
58	MG	1H	3468	1/1	0.98	0.09	122,122,122,122	0
58	MG	P8	101	1/1	0.98	0.06	101,101,101,101	0
58	MG	13	1664	1/1	0.98	0.06	105,105,105,105	0
58	MG	1H	3471	1/1	0.98	0.05	128,128,128,128	0
58	MG	13	1737	1/1	0.98	0.08	116,116,116,116	0
58	MG	1H	3475	1/1	0.98	0.11	89,89,89,89	0
58	MG	1H	3417	1/1	0.98	0.04	77,77,77,77	0
58	MG	1H	3480	1/1	0.98	0.08	114,114,114,114	0
58	MG	1H	3418	1/1	0.98	0.06	86,86,86,86	0
58	MG	1H	3482	1/1	0.98	0.05	119,119,119,119	0
58	MG	1H	3420	1/1	0.98	0.03	81,81,81,81	0
58	MG	13	1656	1/1	0.98	0.05	105,105,105,105	0
58	MG	13	1717	1/1	0.98	0.07	123,123,123,123	0
58	MG	1H	3431	1/1	0.98	0.03	111,111,111,111	0
58	MG	14	3073	1/1	0.98	0.05	67,67,67,67	0
58	MG	14	3037	1/1	0.98	0.05	80,80,80,80	0
58	MG	13	1632	1/1	0.98	0.06	83,83,83,83	0
58	MG	1H	3434	1/1	0.98	0.07	82,82,82,82	0
60	ZN	5A	101	1/1	0.98	0.04	164,164,164,164	0
58	MG	13	1725	1/1	0.98	0.05	101,101,101,101	0
58	MG	1H	3430	1/1	0.99	0.05	81,81,81,81	0
58	MG	13	1718	1/1	0.99	0.06	110,110,110,110	0
58	MG	1H	3432	1/1	0.99	0.02	111,111,111,111	0
58	MG	13	1719	1/1	0.99	0.04	94,94,94,94	0
58	MG	13	1720	1/1	0.99	0.03	126,126,126,126	0
58	MG	1H	3435	1/1	0.99	0.07	85,85,85,85	0
58	MG	1H	3436	1/1	0.99	0.05	96,96,96,96	0
58	MG	1H	3358	1/1	0.99	0.02	70,70,70,70	0
58	MG	1H	3360	1/1	0.99	0.03	86,86,86,86	0
58	MG	1H	3439	1/1	0.99	0.03	72,72,72,72	0
58	MG	1H	3441	1/1	0.99	0.05	92,92,92,92	0
58	MG	1H	3362	1/1	0.99	0.04	71,71,71,71	0
58	MG	1H	3363	1/1	0.99	0.04	81,81,81,81	0
58	MG	1H	3364	1/1	0.99	0.08	74,74,74,74	0
58	MG	1H	3446	1/1	0.99	0.06	94,94,94,94	0
58	MG	13	1721	1/1	0.99	0.03	100,100,100,100	0
58	MG	1H	3366	1/1	0.99	0.03	73,73,73,73	0
58	MG	13	1722	1/1	0.99	0.03	99,99,99,99	0
58	MG	1H	3370	1/1	0.99	0.04	68,68,68,68	0
58	MG	1H	3371	1/1	0.99	0.03	77,77,77,77	0
58	MG	1H	3372	1/1	0.99	0.10	73,73,73,73	0
58	MG	1H	3453	1/1	0.99	0.05	93,93,93,93	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
58	MG	1H	3374	1/1	0.99	0.03	77,77,77,77	0
58	MG	1H	3455	1/1	0.99	0.05	87,87,87,87	0
58	MG	13	1711	1/1	0.99	0.08	85,85,85,85	0
58	MG	1H	3458	1/1	0.99	0.03	88,88,88,88	0
58	MG	1H	3376	1/1	0.99	0.02	106,106,106,106	0
58	MG	1H	3377	1/1	0.99	0.02	119,119,119,119	0
58	MG	1H	3378	1/1	0.99	0.04	90,90,90,90	0
58	MG	14	3344	1/1	0.99	0.09	91,91,91,91	0
58	MG	14	3345	1/1	0.99	0.04	80,80,80,80	0
58	MG	14	3346	1/1	0.99	0.04	81,81,81,81	0
58	MG	14	3347	1/1	0.99	0.04	87,87,87,87	0
58	MG	14	3348	1/1	0.99	0.03	86,86,86,86	0
58	MG	1H	3379	1/1	0.99	0.05	103,103,103,103	0
58	MG	14	3351	1/1	0.99	0.05	80,80,80,80	0
58	MG	14	3352	1/1	0.99	0.07	84,84,84,84	0
58	MG	14	3353	1/1	0.99	0.02	73,73,73,73	0
58	MG	1H	3464	1/1	0.99	0.07	95,95,95,95	0
58	MG	14	3355	1/1	0.99	0.03	92,92,92,92	0
58	MG	14	3356	1/1	0.99	0.03	85,85,85,85	0
58	MG	13	1724	1/1	0.99	0.04	99,99,99,99	0
58	MG	14	3359	1/1	0.99	0.02	94,94,94,94	0
58	MG	14	3360	1/1	0.99	0.04	78,78,78,78	0
58	MG	14	3361	1/1	0.99	0.02	79,79,79,79	0
58	MG	14	3362	1/1	0.99	0.03	86,86,86,86	0
58	MG	14	3363	1/1	0.99	0.10	80,80,80,80	0
58	MG	1H	3466	1/1	0.99	0.05	94,94,94,94	0
58	MG	14	3365	1/1	0.99	0.03	96,96,96,96	0
58	MG	1H	3381	1/1	0.99	0.06	80,80,80,80	0
58	MG	1H	3383	1/1	0.99	0.02	75,75,75,75	0
58	MG	1H	3469	1/1	0.99	0.13	124,124,124,124	0
58	MG	14	3370	1/1	0.99	0.03	94,94,94,94	0
58	MG	14	3371	1/1	0.99	0.04	95,95,95,95	0
58	MG	13	1712	1/1	0.99	0.03	98,98,98,98	0
58	MG	14	3373	1/1	0.99	0.02	86,86,86,86	0
58	MG	1H	3385	1/1	0.99	0.02	91,91,91,91	0
58	MG	1H	3386	1/1	0.99	0.03	109,109,109,109	0
58	MG	1H	3473	1/1	0.99	0.02	89,89,89,89	0
58	MG	14	3377	1/1	0.99	0.02	106,106,106,106	0
58	MG	14	3378	1/1	0.99	0.04	83,83,83,83	0
58	MG	14	3379	1/1	0.99	0.07	110,110,110,110	0
58	MG	14	3380	1/1	0.99	0.04	94,94,94,94	0
58	MG	1H	3474	1/1	0.99	0.03	110,110,110,110	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
58	MG	1H	3387	1/1	0.99	0.03	60,60,60,60	0
58	MG	14	3383	1/1	0.99	0.11	137,137,137,137	0
58	MG	14	3384	1/1	0.99	0.05	96,96,96,96	0
58	MG	14	3385	1/1	0.99	0.04	92,92,92,92	0
58	MG	1H	3476	1/1	0.99	0.04	122,122,122,122	0
58	MG	14	3387	1/1	0.99	0.03	88,88,88,88	0
58	MG	1H	3477	1/1	0.99	0.04	114,114,114,114	0
58	MG	14	3389	1/1	0.99	0.06	92,92,92,92	0
58	MG	14	3390	1/1	0.99	0.07	114,114,114,114	0
58	MG	14	3391	1/1	0.99	0.04	87,87,87,87	0
58	MG	14	3392	1/1	0.99	0.08	89,89,89,89	0
58	MG	14	3394	1/1	0.99	0.07	88,88,88,88	0
58	MG	14	3395	1/1	0.99	0.04	85,85,85,85	0
58	MG	1H	3478	1/1	0.99	0.02	95,95,95,95	0
58	MG	14	3397	1/1	0.99	0.06	103,103,103,103	0
58	MG	1H	3388	1/1	0.99	0.03	78,78,78,78	0
58	MG	14	3399	1/1	0.99	0.08	116,116,116,116	0
58	MG	14	3400	1/1	0.99	0.03	113,113,113,113	0
58	MG	1H	3390	1/1	0.99	0.03	74,74,74,74	0
58	MG	14	3402	1/1	0.99	0.03	83,83,83,83	0
58	MG	14	3403	1/1	0.99	0.08	114,114,114,114	0
58	MG	1H	3391	1/1	0.99	0.05	79,79,79,79	0
58	MG	1H	3392	1/1	0.99	0.04	81,81,81,81	0
58	MG	1H	3394	1/1	0.99	0.03	89,89,89,89	0
58	MG	1H	3395	1/1	0.99	0.07	103,103,103,103	0
58	MG	14	3408	1/1	0.99	0.02	130,130,130,130	0
58	MG	13	1713	1/1	0.99	0.08	117,117,117,117	0
58	MG	14	3410	1/1	0.99	0.03	91,91,91,91	0
58	MG	1H	3397	1/1	0.99	0.04	82,82,82,82	0
58	MG	14	3412	1/1	0.99	0.12	128,128,128,128	0
58	MG	14	3413	1/1	0.99	0.03	92,92,92,92	0
58	MG	1H	3398	1/1	0.99	0.08	76,76,76,76	0
58	MG	13	1714	1/1	0.99	0.03	98,98,98,98	0
58	MG	14	3416	1/1	0.99	0.04	124,124,124,124	0
58	MG	1H	3400	1/1	0.99	0.05	86,86,86,86	0
58	MG	14	3418	1/1	0.99	0.02	88,88,88,88	0
58	MG	14	3419	1/1	0.99	0.03	90,90,90,90	0
58	MG	13	1728	1/1	0.99	0.02	105,105,105,105	0
58	MG	1H	3402	1/1	0.99	0.03	76,76,76,76	0
58	MG	13	1729	1/1	0.99	0.03	96,96,96,96	0
58	MG	1H	3406	1/1	0.99	0.07	82,82,82,82	0
58	MG	13	1730	1/1	0.99	0.08	108,108,108,108	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
58	MG	1H	3410	1/1	0.99	0.03	97,97,97,97	0
58	MG	13	1715	1/1	0.99	0.05	113,113,113,113	0
58	MG	13	1732	1/1	0.99	0.11	127,127,127,127	0
58	MG	16	210	1/1	0.99	0.03	87,87,87,87	0
58	MG	16	211	1/1	0.99	0.02	92,92,92,92	0
58	MG	1H	3416	1/1	0.99	0.04	83,83,83,83	0
58	MG	1H	3308	1/1	0.99	0.07	81,81,81,81	0
58	MG	13	1733	1/1	0.99	0.06	102,102,102,102	0
58	MG	13	1716	1/1	0.99	0.05	108,108,108,108	0
58	MG	1H	3421	1/1	0.99	0.03	129,129,129,129	0
58	MG	1G	1671	1/1	0.99	0.07	121,121,121,121	0
58	MG	1H	3422	1/1	0.99	0.06	102,102,102,102	0
58	MG	13	1735	1/1	0.99	0.13	146,146,146,146	0
58	MG	1H	3424	1/1	0.99	0.02	81,81,81,81	0
58	MG	13	1613	1/1	0.99	0.02	109,109,109,109	0
59	SF4	3E	301	8/8	0.99	0.03	95,111,117,118	0
59	SF4	32	302	8/8	0.99	0.02	127,146,153,155	0
58	MG	1H	3427	1/1	0.99	0.02	106,106,106,106	0
58	MG	1H	3428	1/1	0.99	0.09	89,89,89,89	0
58	MG	1H	3429	1/1	0.99	0.03	82,82,82,82	0
58	MG	1H	3382	1/1	1.00	0.09	71,71,71,71	0
58	MG	14	3357	1/1	1.00	0.03	76,76,76,76	0
58	MG	1H	3460	1/1	1.00	0.06	86,86,86,86	0
58	MG	1H	3419	1/1	1.00	0.04	76,76,76,76	0
58	MG	1H	3368	1/1	1.00	0.04	76,76,76,76	0
58	MG	1H	3440	1/1	1.00	0.04	70,70,70,70	0
58	MG	1H	3393	1/1	1.00	0.01	95,95,95,95	0
58	MG	1H	3404	1/1	1.00	0.02	84,84,84,84	0
58	MG	14	3393	1/1	1.00	0.03	89,89,89,89	0
58	MG	1H	3405	1/1	1.00	0.03	75,75,75,75	0
58	MG	1H	3444	1/1	1.00	0.04	85,85,85,85	0
58	MG	1H	3359	1/1	1.00	0.02	71,71,71,71	0
58	MG	14	3367	1/1	1.00	0.02	86,86,86,86	0
58	MG	1G	1672	1/1	1.00	0.02	115,115,115,115	0
58	MG	1H	3425	1/1	1.00	0.02	77,77,77,77	0
58	MG	1H	3357	1/1	1.00	0.02	79,79,79,79	0
58	MG	1H	3408	1/1	1.00	0.05	72,72,72,72	0
58	MG	14	3343	1/1	1.00	0.06	87,87,87,87	0
58	MG	1H	3409	1/1	1.00	0.04	85,85,85,85	0
58	MG	1H	3361	1/1	1.00	0.01	72,72,72,72	0
58	MG	1H	3356	1/1	1.00	0.02	67,67,67,67	0
58	MG	1H	3373	1/1	1.00	0.02	86,86,86,86	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
58	MG	1H	3413	1/1	1.00	0.01	90,90,90,90	0
58	MG	1H	3414	1/1	1.00	0.06	79,79,79,79	0
58	MG	14	3350	1/1	1.00	0.01	116,116,116,116	0
58	MG	1H	3415	1/1	1.00	0.02	90,90,90,90	0
58	MG	1H	3456	1/1	1.00	0.02	68,68,68,68	0
60	ZN	5I	102	1/1	1.00	0.02	114,114,114,114	0
58	MG	1H	3389	1/1	1.00	0.02	71,71,71,71	0
58	MG	14	3002	1/1	1.00	0.01	65,65,65,65	0
58	MG	1H	3367	1/1	1.00	0.04	84,84,84,84	0

6.5 Other polymers [i](#)

There are no such residues in this entry.