



wwPDB X-ray Structure Validation Summary Report ⓘ

Jun 2, 2020 – 09:14 am BST

PDB ID : 4WQR
Title : Complex of 70S ribosome with tRNA-Phe and mRNA with C-A mismatch in the first position in the A-site.
Authors : Rozov, A.; Demeshkina, N.; Yusupov, M.; Yusupova, G.
Deposited on : 2014-10-22
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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

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

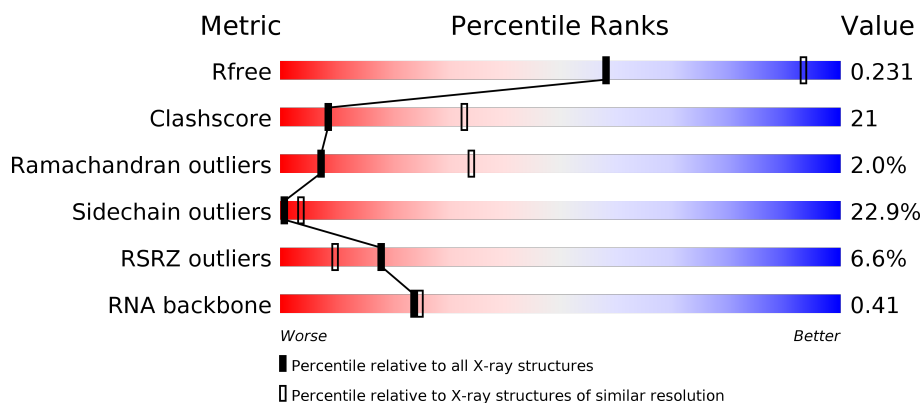
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.15 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}	130704	1665 (3.20-3.12)
Clashscore	141614	1804 (3.20-3.12)
Ramachandran outliers	138981	1770 (3.20-3.12)
Sidechain outliers	138945	1769 (3.20-3.12)
RSRZ outliers	127900	1616 (3.20-3.12)
RNA backbone	3102	1073 (3.50-2.82)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 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	
1	1G	1522	
2	12	256	
2	1E	256	

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


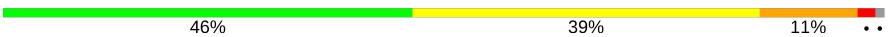
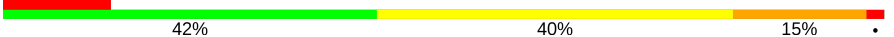


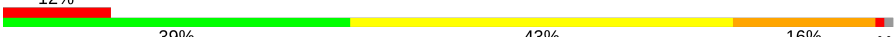

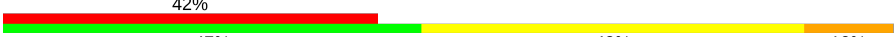
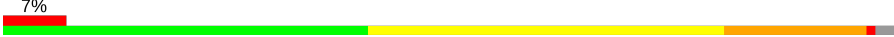

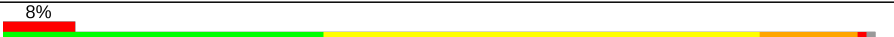


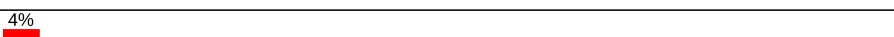








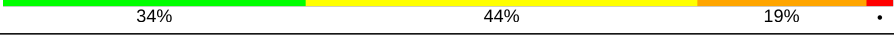


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Mol	Chain	Length	Quality of chain
15	6I	89	
16	7A	88	
16	7I	88	
17	8A	105	
17	8I	105	
18	9A	88	
18	9I	88	
19	AA	93	
19	AI	93	
20	BA	106	
20	BI	106	
21	1B	27	
21	1F	27	
22	1K	76	
22	1L	76	
23	2K	77	
23	2L	77	
24	3K	76	
24	3L	76	
25	4K	30	
25	4L	30	
26	14	2917	
26	1H	2917	
27	16	122	
27	1J	122	

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

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Mol	Chain	Length	Quality of chain
40	B8	146	
41	85	118	
41	C8	118	
42	95	101	
42	D8	101	
43	A5	113	
43	E8	113	
44	B5	96	
44	F8	96	
45	C5	110	
45	G8	110	
46	D5	206	
46	H8	206	
47	E5	85	
47	I8	85	
48	F5	98	
48	J8	98	
49	G5	72	
49	K8	72	
50	H5	60	
50	L8	60	
51	I5	71	
51	M8	71	
52	J5	60	
52	N8	60	

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Mol	Chain	Length	Quality of chain
53	K5	54	
53	O8	54	
54	L5	49	
54	P8	49	
55	M5	65	
55	Q8	65	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
56	MG	11	304	-	-	-	X
56	MG	13	1610	-	-	-	X
56	MG	13	1623	-	-	-	X
56	MG	13	1648	-	-	-	X
56	MG	13	1674	-	-	-	X
56	MG	13	1680	-	-	-	X
56	MG	13	1681	-	-	-	X
56	MG	13	1694	-	-	-	X
56	MG	13	1701	-	-	-	X
56	MG	13	1704	-	-	-	X
56	MG	14	3036	-	-	-	X
56	MG	14	3067	-	-	-	X
56	MG	14	3096	-	-	-	X
56	MG	14	3109	-	-	-	X
56	MG	14	3110	-	-	-	X
56	MG	14	3113	-	-	-	X
56	MG	14	3114	-	-	-	X
56	MG	14	3117	-	-	-	X
56	MG	14	3119	-	-	-	X
56	MG	14	3128	-	-	-	X
56	MG	14	3148	-	-	-	X
56	MG	14	3167	-	-	-	X
56	MG	14	3171	-	-	-	X
56	MG	14	3181	-	-	-	X
56	MG	14	3189	-	-	-	X
56	MG	14	3192	-	-	-	X
56	MG	14	3193	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
56	MG	14	3195	-	-	-	X
56	MG	14	3197	-	-	-	X
56	MG	14	3199	-	-	-	X
56	MG	14	3201	-	-	-	X
56	MG	14	3214	-	-	-	X
56	MG	14	3215	-	-	-	X
56	MG	14	3218	-	-	-	X
56	MG	14	3219	-	-	-	X
56	MG	14	3240	-	-	-	X
56	MG	14	3245	-	-	-	X
56	MG	14	3252	-	-	-	X
56	MG	14	3253	-	-	-	X
56	MG	14	3255	-	-	-	X
56	MG	14	3257	-	-	-	X
56	MG	16	205	-	-	-	X
56	MG	1G	1624	-	-	-	X
56	MG	1G	1628	-	-	-	X
56	MG	1G	1652	-	-	-	X
56	MG	1G	1654	-	-	-	X
56	MG	1G	1664	-	-	-	X
56	MG	1G	1669	-	-	-	X
56	MG	1G	1670	-	-	-	X
56	MG	1G	1677	-	-	-	X
56	MG	1G	1680	-	-	-	X
56	MG	1G	1682	-	-	-	X
56	MG	1H	3059	-	-	-	X
56	MG	1H	3067	-	-	-	X
56	MG	1H	3127	-	-	-	X
56	MG	1H	3176	-	-	-	X
56	MG	1H	3182	-	-	-	X
56	MG	1H	3184	-	-	-	X
56	MG	1H	3186	-	-	-	X
56	MG	1H	3199	-	-	-	X
56	MG	1H	3205	-	-	-	X
56	MG	1H	3216	-	-	-	X
56	MG	1H	3226	-	-	-	X
56	MG	1H	3227	-	-	-	X
56	MG	1H	3230	-	-	-	X
56	MG	1H	3236	-	-	-	X
56	MG	1H	3243	-	-	-	X
56	MG	1H	3259	-	-	-	X
56	MG	1H	3266	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
56	MG	1H	3268	-	-	-	X
56	MG	1H	3274	-	-	-	X
56	MG	1H	3279	-	-	-	X
56	MG	1H	3282	-	-	-	X
56	MG	1H	3285	-	-	-	X
56	MG	1H	3286	-	-	-	X
56	MG	1H	3290	-	-	-	X
56	MG	1H	3292	-	-	-	X
56	MG	1H	3293	-	-	-	X
56	MG	1H	3296	-	-	-	X
56	MG	1H	3301	-	-	-	X
56	MG	1H	3307	-	-	-	X
56	MG	1H	3327	-	-	-	X
56	MG	1H	3333	-	-	-	X
56	MG	1H	3335	-	-	-	X
56	MG	29	302	-	-	-	X
56	MG	2L	102	-	-	-	X
56	MG	4A	201	-	-	-	X
56	MG	P8	101	-	-	-	X
57	ZN	G8	201	-	-	-	X

2 Entry composition [i](#)

There are 58 unique types of molecules in this entry. The entry contains 300537 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	1498	Total	C	N	O	P	0	0	0
			32207	14334	5973	10402	1498			
1	1G	1497	Total	C	N	O	P	0	0	0
			32182	14324	5968	10394	1496			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	1E	237	Total	C	N	O	S	0	0	0
			1924	1228	344	347	5			
2	12	237	Total	C	N	O	S	0	0	0
			1924	1228	344	347	5			

- 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	206	Total	C	N	O	S	0	0	0
			1612	1016	314	281	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	3E	208	Total	C	N	O	S	0	0	0
			1703	1066	339	291	7			
4	32	208	Total	C	N	O	S	0	0	0
			1703	1066	339	291	7			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	4E	151	Total	C	N	O	S	0	0	0
			1155	729	218	204	4			
5	42	151	Total	C	N	O	S	0	0	0
			1155	729	218	204	4			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	5E	101	Total	C	N	O	S	0	0	0
			843	531	155	154	3			
6	52	101	Total	C	N	O	S	0	0	0
			843	531	155	154	3			

- Molecule 7 is a protein called 30S ribosomal protein S7.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	6E	155	Total	C	N	O	S	0	0	0
			1257	781	252	218	6			
7	62	155	Total	C	N	O	S	0	0	0
			1257	781	252	218	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
			1116	705	215	193	3			
8	72	138	Total	C	N	O	S	0	0	0
			1116	705	215	193	3			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	8E	127	Total	C	N	O		0	0	0
			1010	639	197	174				
9	82	127	Total	C	N	O		0	0	0
			1010	639	197	174				

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	2I	119	Total	C	N	O	S	0	0	0
			885	549	168	165	3			
11	2A	119	Total	C	N	O	S	0	0	0
			885	549	168	165	3			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	3I	125	Total	C	N	O	S	0	0	0
			975	614	196	164	1			
12	3A	125	Total	C	N	O	S	0	0	0
			975	614	196	164	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	4I	118	Total	C	N	O	S	0	0	0
			938	580	193	163	2			
13	4A	117	Total	C	N	O	S	0	0	0
			933	577	192	162	2			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
4I	119	ALA	GLY	conflict	UNP P80377
4A	119	ALA	GLY	conflict	UNP P80377

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
14	5I	60	Total	C	N	O	S	0	0	0
			492	312	104	72	4			
14	5A	58	Total	C	N	O	S	0	0	0
			476	303	99	70	4			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
15	6I	88	Total	C	N	O	S	0	0	0
			734	459	147	126	2			
15	6A	88	Total	C	N	O	S	0	0	0
			734	459	147	126	2			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
16	7I	84	Total	C	N	O	S	0	0	0
			705	446	140	118	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	100	Total	C	N	O	S	0	0	0
			834	534	155	143	2			

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
18	9I	72	Total	C	N	O	0	0	0
			591	376	117	98			
18	9A	72	Total	C	N	O	0	0	0
			591	376	117	98			

- 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
			647	413	119	113	2			
19	AA	78	Total	C	N	O	S	0	0	0
			624	398	115	109	2			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
20	BI	99	Total	C	N	O	S	0	0	0
			763	470	162	129	2			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
20	BA	99	Total	C	N	O	S	0	0	0
			763	470	162	129	2			

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
21	1F	25	Total	C	N	O	0	0	0
			217	134	52	31			
21	1B	25	Total	C	N	O	0	0	0
			217	134	52	31			

- Molecule 22 is a RNA chain called tRNA-Phe.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
22	1K	76	Total	C	N	O	P	S	0	0	0
			1626	729	290	531	75	1			
22	1L	76	Total	C	N	O	P	S	0	0	0
			1626	729	290	531	75	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			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
2K	18	C	U	conflict	GB 675817920
2L	18	C	U	conflict	GB 675817920

- Molecule 24 is a RNA chain called tRNA-Phe.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
24	3K	76	Total	C	N	O	P	0	0	0
			1619	723	290	531	75			
24	3L	76	Total	C	N	O	P	0	0	0
			1619	723	290	531	75			

- Molecule 25 is a RNA chain called mRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
25	4K	14	Total	C	N	O	P	0	0	0
			301	136	60	91	14			
25	4L	6	Total	C	N	O	P	0	0	0
			131	59	27	39	6			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
26	1H	2912	Total	C	N	O	P	0	0	0
			62707	27911	11722	20163	2911			
26	14	2909	Total	C	N	O	P	0	0	0
			62647	27884	11716	20139	2908			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
1H	161	U	-	insertion	GB 48268
1H	493	G	-	insertion	GB 48268
1H	1228	G	-	insertion	GB 48268
14	161	U	-	insertion	GB 48268
14	493	G	-	insertion	GB 48268
14	1228	G	-	insertion	GB 48268

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
29	21	205	Total	C	N	O	S	0	0	0
			1568	991	300	271	6			
29	29	205	Total	C	N	O	S	0	0	0
			1568	991	300	271	6			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
30	31	202	Total	C	N	O	S	0	0	0
			1585	1011	297	275	2			
30	39	208	Total	C	N	O	S	0	0	0
			1627	1037	304	283	3			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
31	41	181	Total	C	N	O	S	0	0	0
			1473	942	268	259	4			
31	49	181	Total	C	N	O	S	0	0	0
			1473	942	268	259	4			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
32	51	174	Total	C	N	O	S	0	0	0
			1336	848	251	236	1			
32	59	170	Total	C	N	O	S	0	0	0
			1307	829	245	232	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
33	61	146	Total	C	N	O	S	0	0	0
			1136	726	201	208	1			
33	69	146	Total	C	N	O	S	0	0	0
			1136	726	201	208	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
34	58	138	Total	C	N	O	S	0	0	0
			1104	712	206	182	4			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
34	15	138	Total	C	N	O	S	0	0	0
			1104	712	206	182	4			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
35	68	122	Total	C	N	O	S	0	0	0
			933	588	171	170	4			
35	25	122	Total	C	N	O	S	0	0	0
			933	588	171	170	4			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
36	78	150	Total	C	N	O	S	0	0	0
			1145	712	232	198	3			
36	35	150	Total	C	N	O	S	0	0	0
			1145	712	232	198	3			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
37	88	138	Total	C	N	O	S	0	0	0
			1087	693	208	180	6			
37	45	141	Total	C	N	O	S	0	0	0
			1122	715	212	188	7			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
38	98	118	Total	C	N	O	S	0	0	0
			968	604	203	160	1			
38	55	117	Total	C	N	O	S	0	0	0
			960	599	202	159				

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
39	A8	111	Total	C	N	O	0	0	0
			882	556	176	150			
39	65	111	Total	C	N	O	0	0	0
			882	556	176	150			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
40	B8	137	Total	C	N	O	S	0	0	0
			1141	710	234	196	1			
40	75	137	Total	C	N	O	S	0	0	0
			1141	710	234	196	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
41	C8	117	Total	C	N	O	S	0	0	0
			964	610	202	151	1			
41	85	117	Total	C	N	O	S	0	0	0
			964	610	202	151	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
42	D8	101	Total	C	N	O	S	0	0	0
			779	501	142	135	1			
42	95	101	Total	C	N	O	S	0	0	0
			779	501	142	135	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
43	E8	113	Total	C	N	O	S	0	0	0
			900	566	177	155	2			
43	A5	113	Total	C	N	O	S	0	0	0
			900	566	177	155	2			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
44	F8	94	Total	C	N	O	S	0	0	0
			742	482	134	125	1			
44	B5	93	Total	C	N	O		0	0	0
			730	474	132	124				

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
45	G8	104	Total	C	N	O	S	0	0	0
			791	510	149	127	5			
45	C5	104	Total	C	N	O	S	0	0	0
			794	510	152	127	5			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
46	H8	175	Total	C	N	O	S	0	0	0
			1397	892	251	251	3			
46	D5	179	Total	C	N	O	S	0	0	0
			1428	911	255	259	3			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
47	I8	80	Total	C	N	O	S	0	0	0
			627	388	132	106	1			
47	E5	77	Total	C	N	O	S	0	0	0
			613	379	129	104	1			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
I8	6	ALA	GLY	conflict	UNP P60493
I8	8	ALA	GLY	conflict	UNP P60493
E5	6	ALA	GLY	conflict	UNP P60493
E5	8	ALA	GLY	conflict	UNP P60493

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
48	J8	97	Total	C	N	O	S	0	0	0
			763	481	150	131	1			
48	F5	97	Total	C	N	O	S	0	0	0
			763	481	150	131	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
49	K8	67	Total	C	N	O	S	0	0	0
			563	349	114	99	1			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
49	G5	66	Total	C	N	O	S	0	0	0
			558	346	113	98	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
50	L8	57	Total	C	N	O		0	0	0
			452	288	88	76				
50	H5	59	Total	C	N	O		0	0	0
			469	298	90	81				

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
51	M8	66	Total	C	N	O	S	0	0	0
			533	335	96	97	5			
51	I5	63	Total	C	N	O	S	0	0	0
			515	326	93	91	5			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
52	N8	58	Total	C	N	O	S	0	0	0
			454	285	89	75	5			
52	J5	59	Total	C	N	O	S	0	0	0
			459	288	90	76	5			

- Molecule 53 is a protein called 50S ribosomal protein L33.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
53	O8	45	Total	C	N	O	S	0	0	0
			389	241	79	65	4			
53	K5	45	Total	C	N	O	S	0	0	0
			389	241	79	65	4			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
54	P8	48	Total	C	N	O	S	0	0	0
			418	257	104	55	2			
54	L5	46	Total	C	N	O	S	0	0	0
			398	245	98	53	2			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
55	Q8	60	Total	C	N	O	S	0	0	0
			480	306	98	74	2			
55	M5	60	Total	C	N	O	S	0	0	0
			477	303	98	74	2			

- Molecule 56 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
56	98	1	Total	Mg	0	0
			1	1		
56	P8	1	Total	Mg	0	0
			1	1		
56	85	1	Total	Mg	0	0
			1	1		
56	C5	1	Total	Mg	0	0
			1	1		
56	13	151	Total	Mg	0	0
			151	151		
56	1J	9	Total	Mg	0	0
			9	9		
56	35	1	Total	Mg	0	0
			1	1		
56	C8	1	Total	Mg	0	0
			1	1		
56	75	1	Total	Mg	0	0
			1	1		
56	16	13	Total	Mg	0	0
			13	13		
56	21	2	Total	Mg	0	0
			2	2		
56	31	1	Total	Mg	0	0
			1	1		
56	Q8	1	Total	Mg	0	0
			1	1		
56	L8	1	Total	Mg	0	0
			1	1		
56	3I	1	Total	Mg	0	0
			1	1		
56	I8	2	Total	Mg	0	0
			2	2		
56	5E	1	Total	Mg	0	0
			1	1		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
56	29	2	Total 2	Mg 2	0	0
56	2K	3	Total 3	Mg 3	0	0
56	J8	2	Total 2	Mg 2	0	0
56	4A	1	Total 1	Mg 1	0	0
56	AI	1	Total 1	Mg 1	0	0
56	1G	103	Total 103	Mg 103	0	0
56	11	4	Total 4	Mg 4	0	0
56	E8	1	Total 1	Mg 1	0	0
56	1H	529	Total 529	Mg 529	0	0
56	F5	1	Total 1	Mg 1	0	0
56	88	2	Total 2	Mg 2	0	0
56	49	1	Total 1	Mg 1	0	0
56	14	389	Total 389	Mg 389	0	0
56	78	2	Total 2	Mg 2	0	0
56	3E	2	Total 2	Mg 2	0	0
56	6A	1	Total 1	Mg 1	0	0
56	1K	2	Total 2	Mg 2	0	0
56	41	2	Total 2	Mg 2	0	0
56	2L	2	Total 2	Mg 2	0	0

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
57	32	1	Total 1	Zn 1	0	0
57	3E	1	Total 1	Zn 1	0	0
57	5I	1	Total 1	Zn 1	0	0
57	5A	1	Total 1	Zn 1	0	0
57	G8	1	Total 1	Zn 1	0	0
57	C5	1	Total 1	Zn 1	0	0

- Molecule 58 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
58	13	212	Total 212	O 212	0	0
58	3E	1	Total 1	O 1	0	0
58	4E	2	Total 2	O 2	0	0
58	8E	2	Total 2	O 2	0	0
58	1I	2	Total 2	O 2	0	0
58	3I	1	Total 1	O 1	0	0
58	5I	2	Total 2	O 2	0	0
58	1K	1	Total 1	O 1	0	0
58	3K	1	Total 1	O 1	0	0
58	4K	4	Total 4	O 4	0	0
58	1H	1097	Total 1097	O 1097	0	0
58	16	16	Total 16	O 16	0	0
58	11	9	Total 9	O 9	0	0
58	21	5	Total 5	O 5	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
58	31	10	Total 10	O 10	0	0
58	58	1	Total 1	O 1	0	0
58	78	4	Total 4	O 4	0	0
58	98	1	Total 1	O 1	0	0
58	C8	2	Total 2	O 2	0	0
58	D8	1	Total 1	O 1	0	0
58	E8	2	Total 2	O 2	0	0
58	G8	3	Total 3	O 3	0	0
58	I8	6	Total 6	O 6	0	0
58	L8	2	Total 2	O 2	0	0
58	P8	2	Total 2	O 2	0	0
58	Q8	2	Total 2	O 2	0	0
58	1G	99	Total 99	O 99	0	0
58	7A	2	Total 2	O 2	0	0
58	BA	1	Total 1	O 1	0	0
58	14	730	Total 730	O 730	0	0
58	1J	12	Total 12	O 12	0	0
58	19	11	Total 11	O 11	0	0
58	29	6	Total 6	O 6	0	0
58	39	7	Total 7	O 7	0	0
58	55	1	Total 1	O 1	0	0

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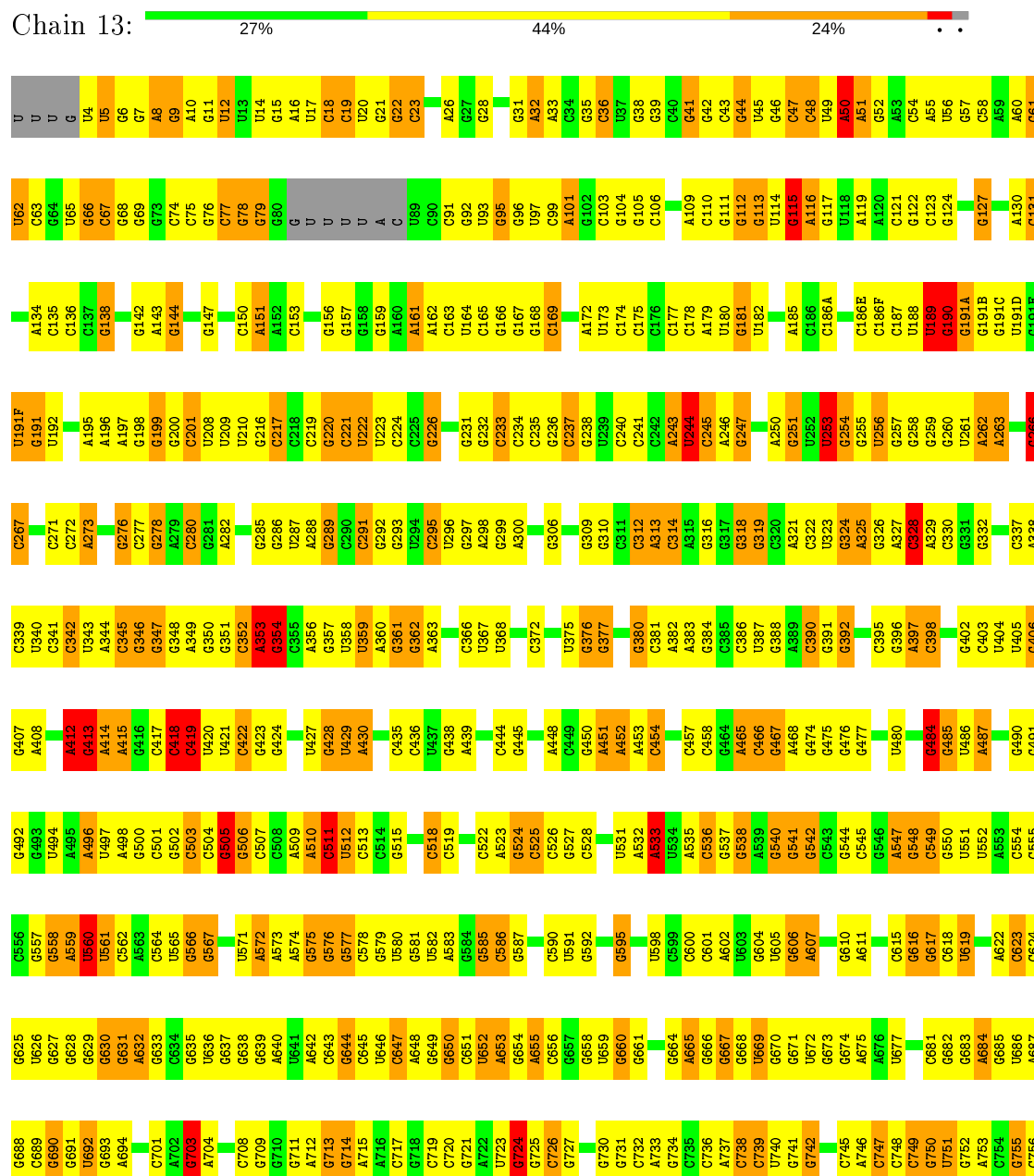
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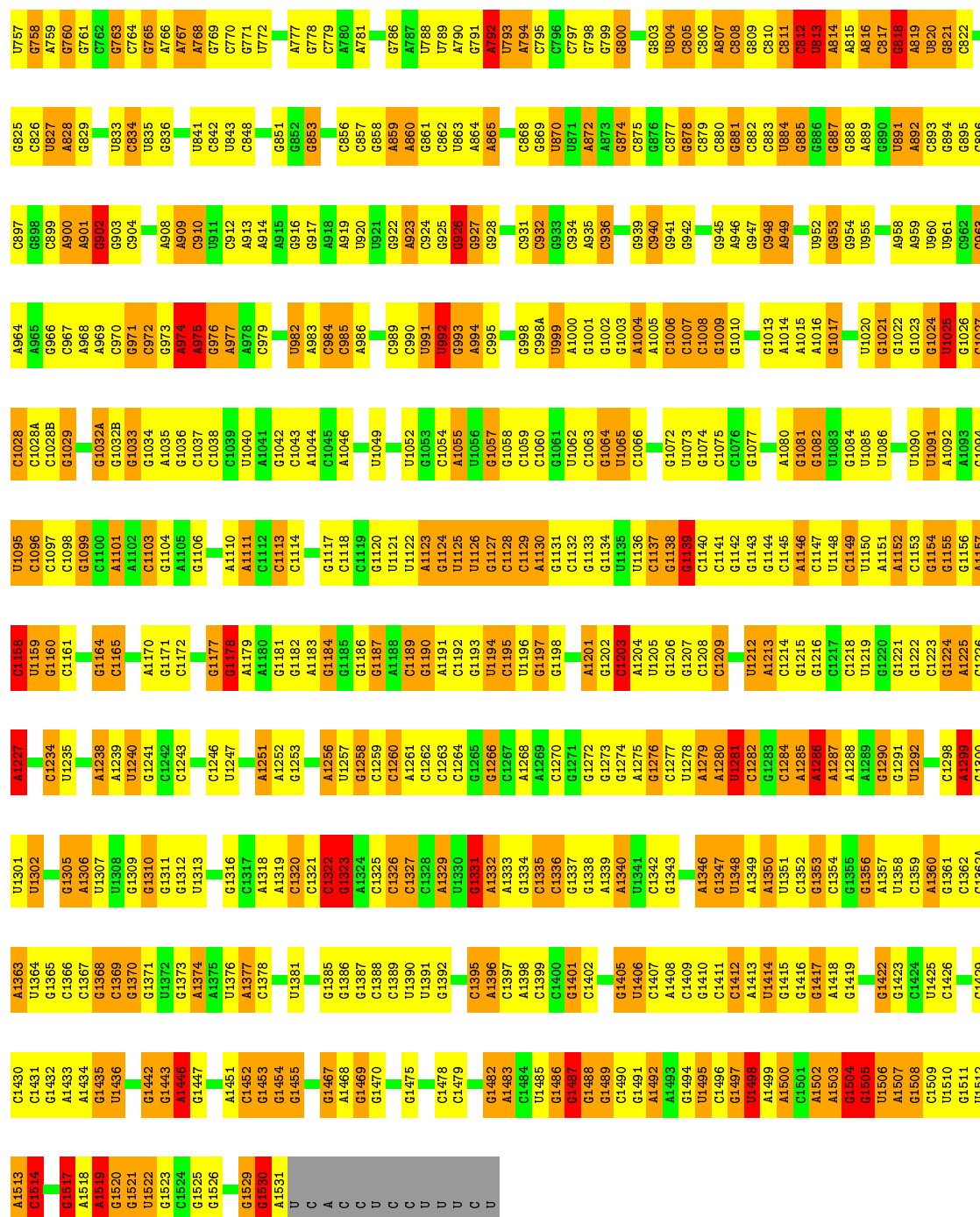
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
58	85	1	Total 1	O 1	0	0
58	A5	1	Total 1	O 1	0	0
58	H5	1	Total 1	O 1	0	0
58	L5	1	Total 1	O 1	0	0

3 Residue-property plots

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

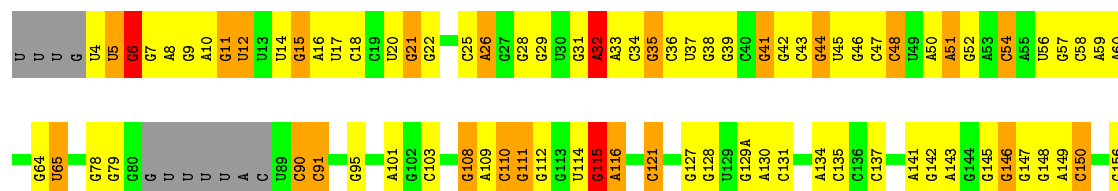
- Molecule 1: 16S ribosomal RNA



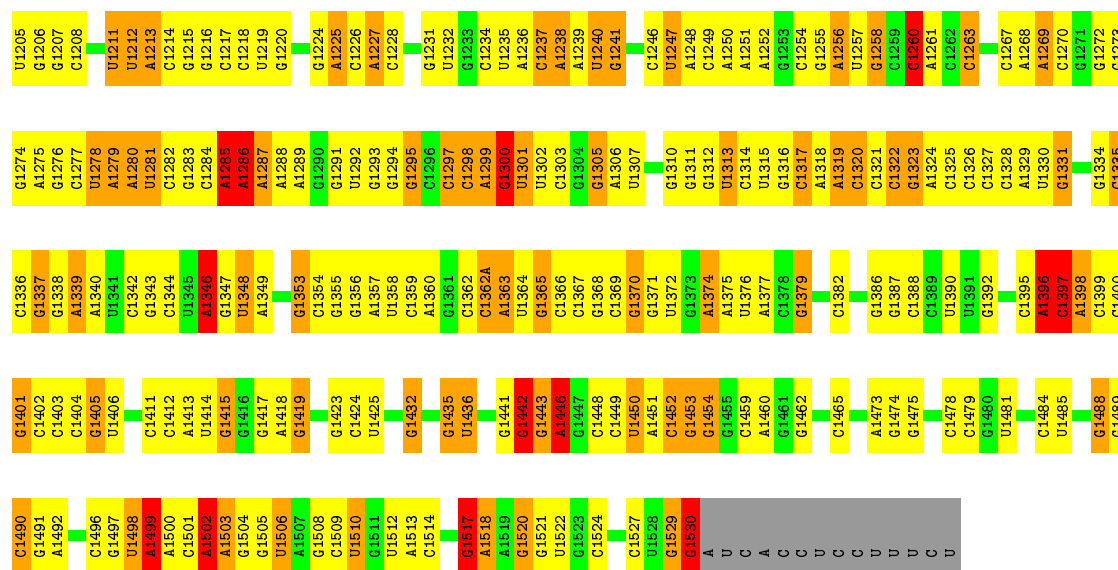


- Molecule 1: 16S ribosomal RNA

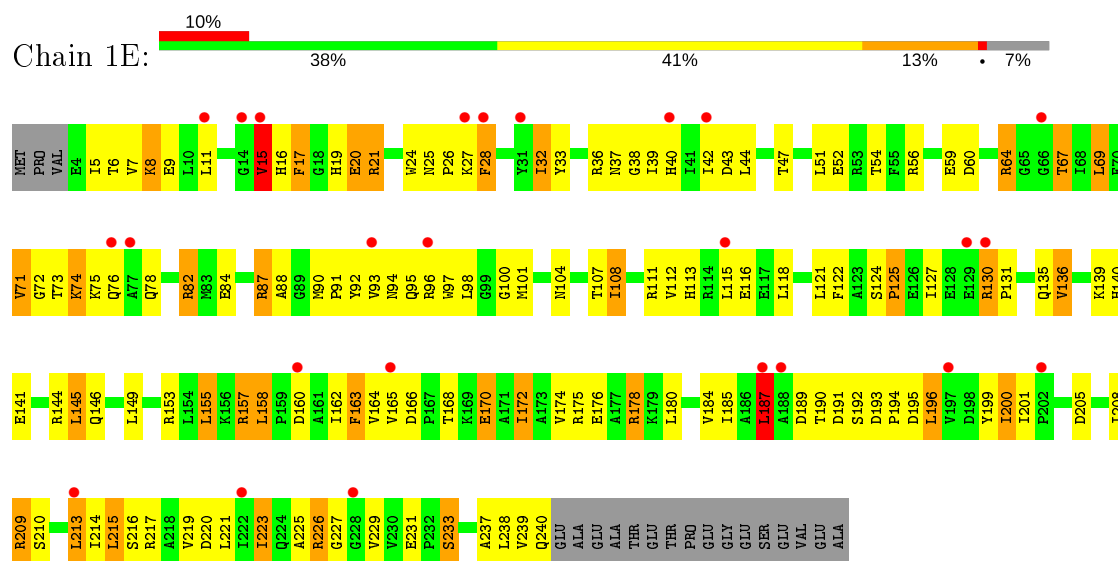
Chain 1G: 



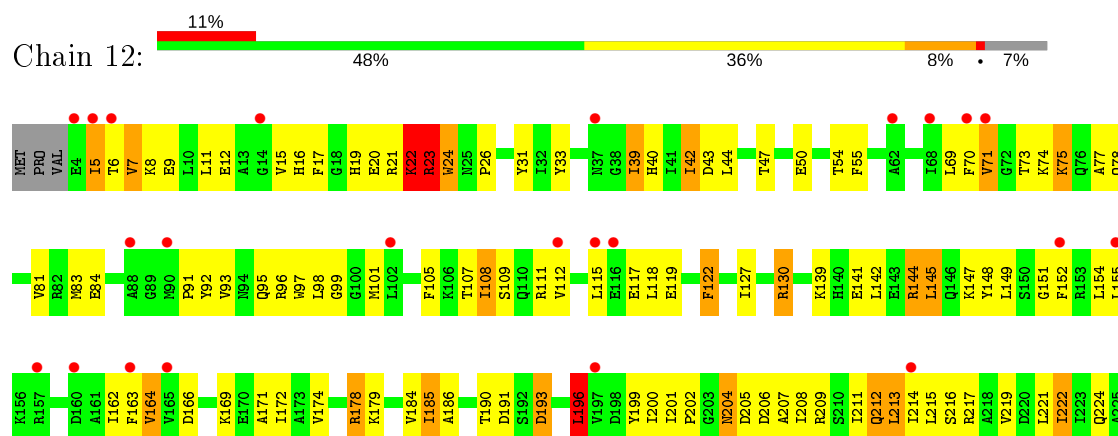
G1139	G1072	G1009	C947	C882	C508	C736	G662	C589	C525	C442	A373	G305	A238	G157
G1140	G1073	G1010	G948	C883	C509	A737	A663	C590	C526	C443	A374	G306	U229	A162
G1141	G1074	G1013	A949	U884	C511	C738	A664	G527	G527	C444	U375	G309	G230	C163
G1142	G1075	G1014	U950	G885	C512	G741	A665	C528	C528	G445	G376	G310	G231	U164
G1143	G1076	A1015	U952	G886	A814	G742	G666	G529	G530	G446	G377	G313	G232	C165
G1144	G1077	A1016	G953	G887	A815	U743	G667	U531	U531	G447	A382	A313	G233	G166
G1145	G1078	G1017	G954	G888	A816	U744	G668	U532	A532	A448	A383	A314	G234	G167
G1146	G1079	U1020	U955	A889	C517	C745	U669	U533	G533	C449	A384	A315	G235	G168
G1147	G1080	G1021	U956	G890	G818	C746	G670	U534	U534	G450	A385	G316	G236	U173
G1148	G1081	G1022	U957	U891	A819	C747	G671	U535	A535	A451	G388	G317	G237	C174
G1149	G1082	G1023	A958	G892	U820	C748	A674	U536	C536	A452	C390	G318	C240	C175
G1150	G1083	G1024	A959	G893	G821	C749	A675	G537	G537	A453	G391	G319	C241	C176
G1151	G1084	U1025	U960	G894	C822	G750	A676	U538	G538	C457	G392	C320	C242	C177
G1152	G1085	G1026	U961	G895	G823	C754	U677	U605	A539	C458	G393	A321	C243	C178
G1153	G1086	G1027	C962	C896	G824	C755	U678	U606	G540	C459	G394	A322	C244	C179
G1154	G1087	G1028	G963	G897	C825	C756	C680	A608	G541	C460	G395	A323	C245	C170
G1155	G1088	G1029	A964	G898	U826	C757	G681	A609	G542	A461	A397	U323	C246	U180
G1156	G1089	C1028A	A965	C899	A828	U757	G682	G543	G544	C462	A398	U324	C247	U181
G1157	G1090	C1028B	A966	A900	G829	G758	A684	G544	G545	C463	A399	U325	C248	U182
G1158	G1091	G1029	G967	A901	G830	U759	G685	G546	G547	C464	A400	G326	U249	U183
G1159	G1092	G1030	A968	G902	U831	G760	U686	A547	A547	C465	C401	A327	C250	G186A
G1160	G1093	G1031	A969	G903	U832	G761	A687	G548	G549	C466	C402	A328	C251	G186B
G1161	G1094	A1032	C904	G904	U833	G762	A688	G550	G551	C467	U404	C330	U252	G186C
G1162	G1095	G1032A	U905	U905	G836	G763	G689	U552	U552	C468	U405	G331	U253	C186D
G1163	G1096	G1032B	G906	G906	G837	C764	C680	U553	C554	C469	U406	G332	G254	
G1164	G1097	G1033	A907	A907	G838	G765	G690	C555	C556	U480	G407	G333	G255	
G1165	G1098	A1034	G973	C910	U841	A766	G691	C557	C558	G481	A408	C334	G256	C187
G1166	G1099	G1035	A974	G911	C942	C767	U692	A621	G559	G482	A409	G335	G257	U188
G1167	G1100	A1036	A975	U911	U843	U768	G693	G622	G560	C483	G410	G336	U261	U189
G1168	G1101	G1037	G976	C912	G848	G769	A694	G623	G561	C484	G411	G337	U262	G190
G1169	G1102	G1038	A977	C913	C849	U772	U695	G624	A559	C485	A412	G338	U263	G191A
G1170	G1103	G1039	A978	A914	U850	U773	U696	G625	U560	U486	A413	G339	U264	
G1171	G1104	U1040	A979	A915	G851	G774	C701	G626	U561	A487	G414	U340	U265	U191D
G1172	G1105	A1041	C980	G916	G852	G775	A702	G627	A562	C488	A415	C341	C267	G191E
G1173	G1106	G1042	U981	G917	G853	G776	A703	G628	C563	C489	G416	G342	C268	U191F
G1174	G1107	C1043	U982	A918	G854	A777	G704	G630	C564	G490	C417	G343	C269	G191
G1175	G1108	G1044	A983	A919	G855	C778	A705	G631	U565	C491	C418	G344	G270	U192
G1176	G1109	A1046	C984	A920	C856	C779	C707	A632	G566	A496	C419	G345	G271	C193
G1177	G1110	G1047	C985	G922	C857	A780	C708	G633	G567	U497	U420	G346	G272	C194
G1178	G1111	G1048	A986	A923	G858	A781	G709	U636	G568	A498	G421	G347	G273	
G1179	G1112	U1049	G987	C924	A859	A782	G710	G637	C569	C501	G422	G350	G280	A195
G1180	G1113	G1050	U991	G925	A860	C783	G711	G638	G570	G502	G423	G351	C281	A196
G1181	G1114	C1051	U992	G926	G861	C784	G712	G639	U571	G503	G424	C352	A282	A197
G1182	G1115	U1052	U993	G927	C862	G785	G713	A640	A572	C504	G425	C353	C283	G198
G1183	G1116	G1053	C994	C932	A865	A790	G714	U641	A573	C505	G426	C354	G284	G199
G1184	G1117	C1054	A994	G933	A866	G791	A715	A642	G574	G506	U427	C355	G285	G200
G1185	G1118	G1055	G995	C934	C867	A792	A716	U643	G575	A509	G428	A356	G286	C201
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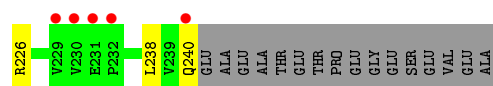


• Molecule 2: 30S ribosomal protein S2

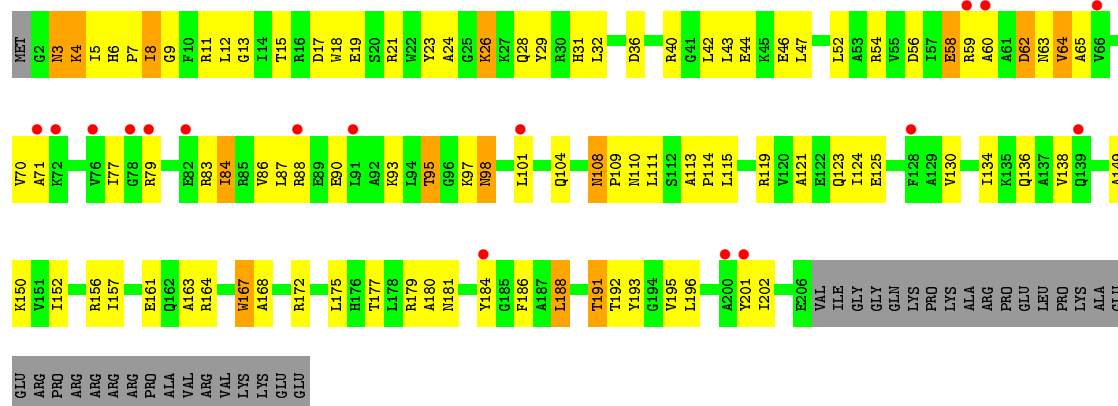


• Molecule 2: 30S ribosomal protein S2

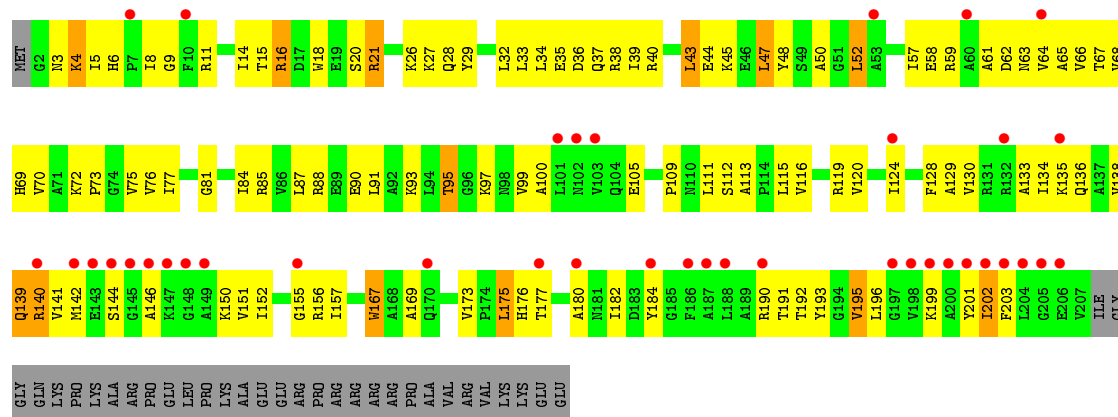




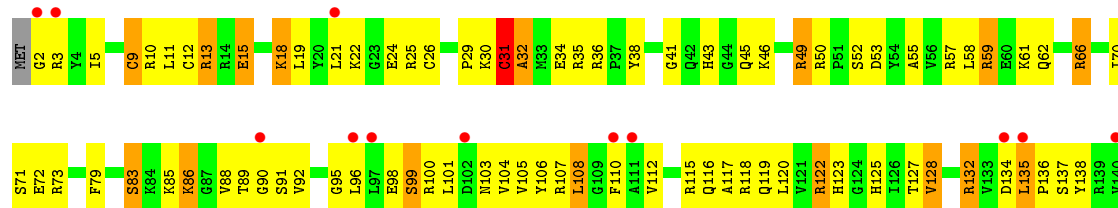
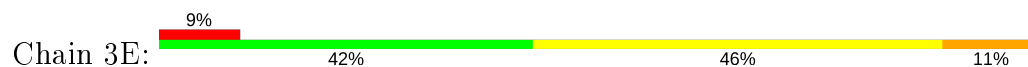
• Molecule 3: 30S ribosomal protein S3



• Molecule 3: 30S ribosomal protein S3

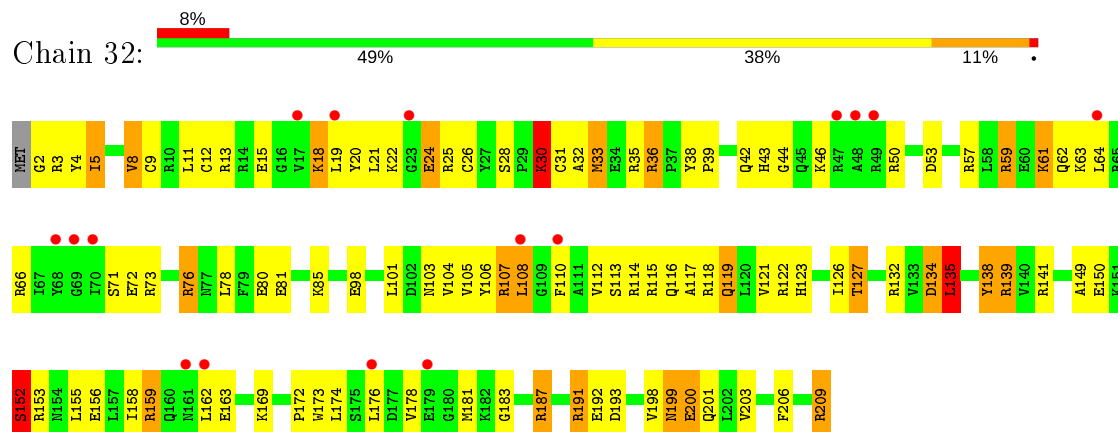


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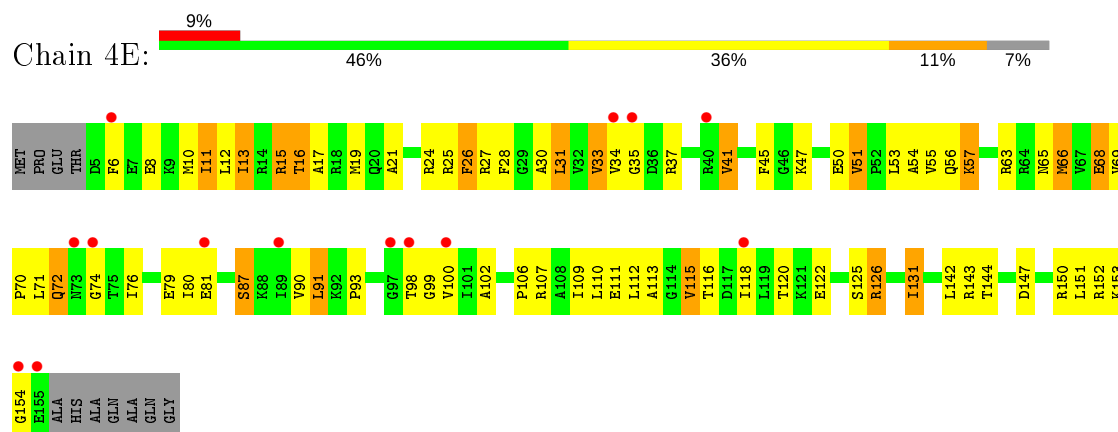




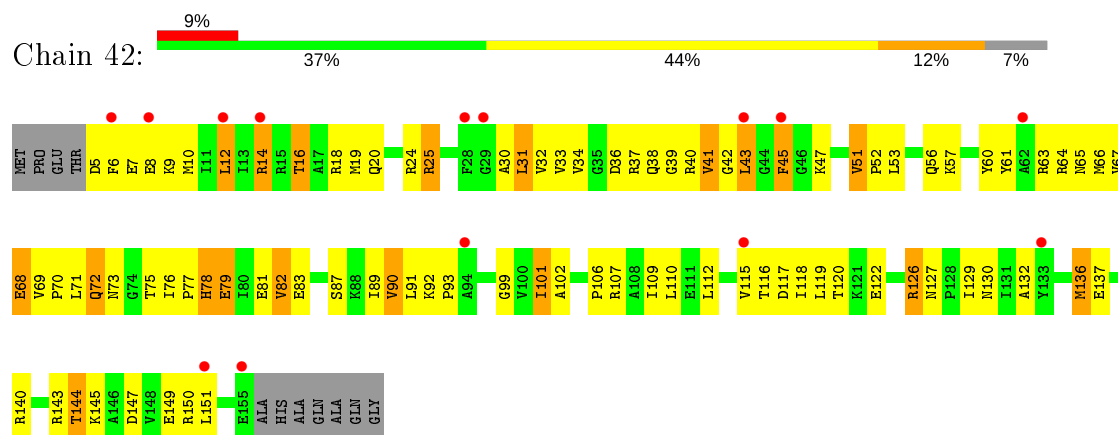
- Molecule 4: 30S ribosomal protein S4



- Molecule 5: 30S ribosomal protein S5



- Molecule 5: 30S ribosomal protein S5

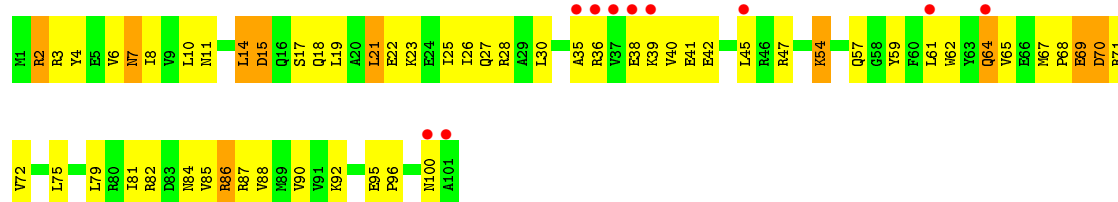


- Molecule 6: 30S ribosomal protein S6

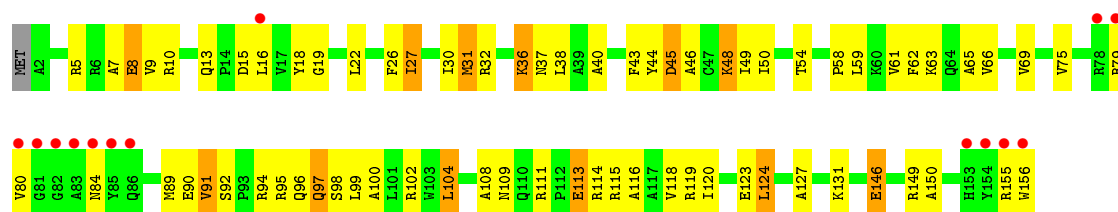




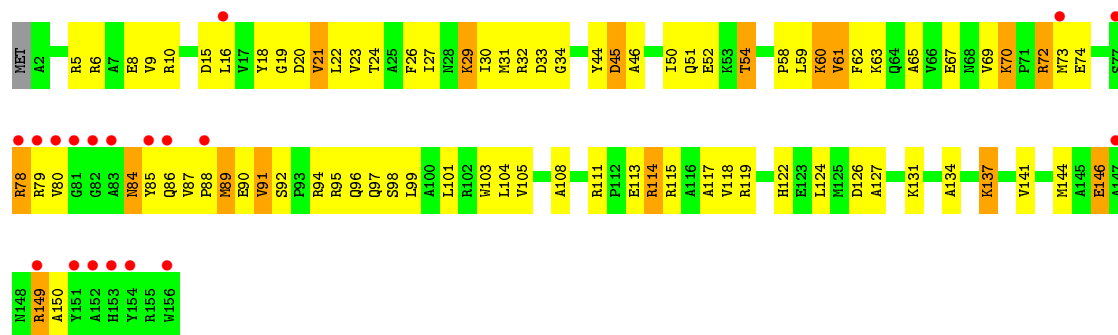
• Molecule 6: 30S ribosomal protein S6



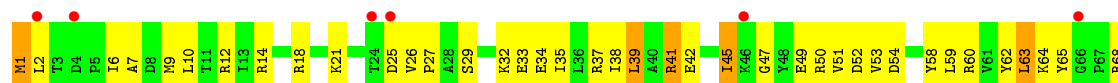
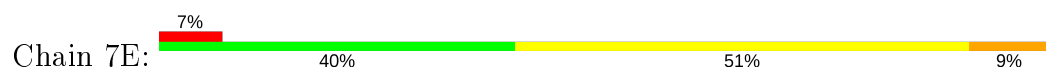
• Molecule 7: 30S ribosomal protein S7

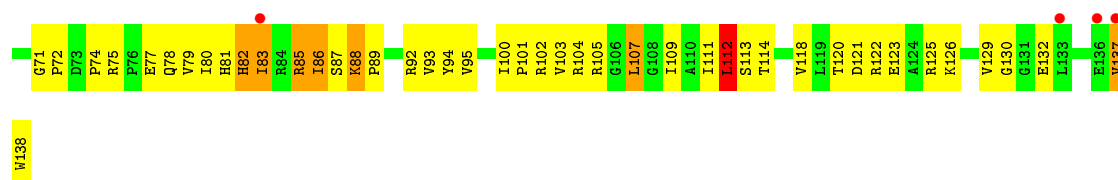


• Molecule 7: 30S ribosomal protein S7

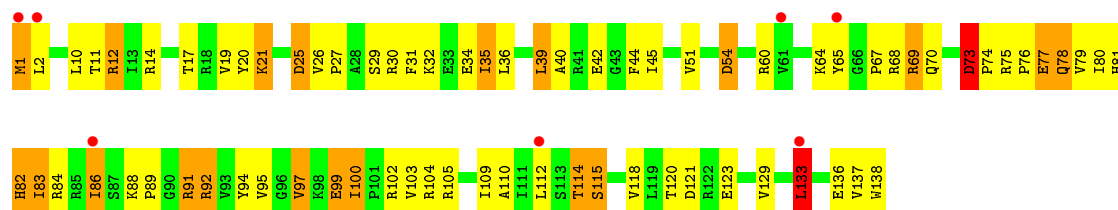


• Molecule 8: 30S ribosomal protein S8

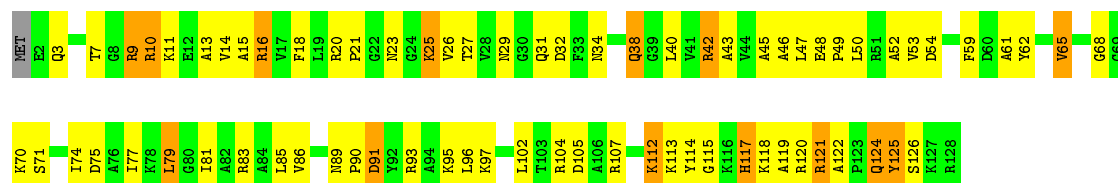




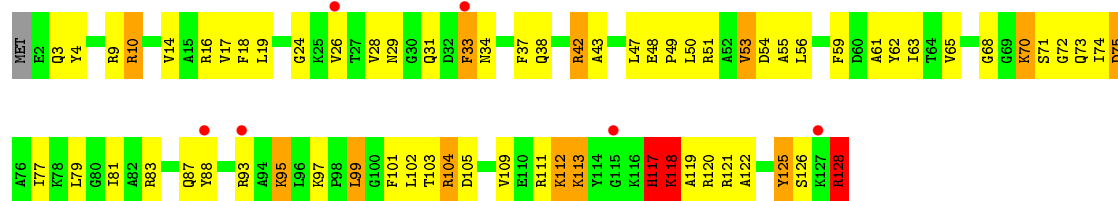
- Molecule 8: 30S ribosomal protein S8



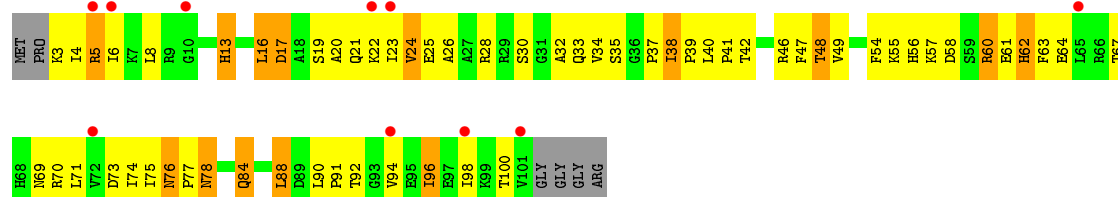
- Molecule 9: 30S ribosomal protein S9



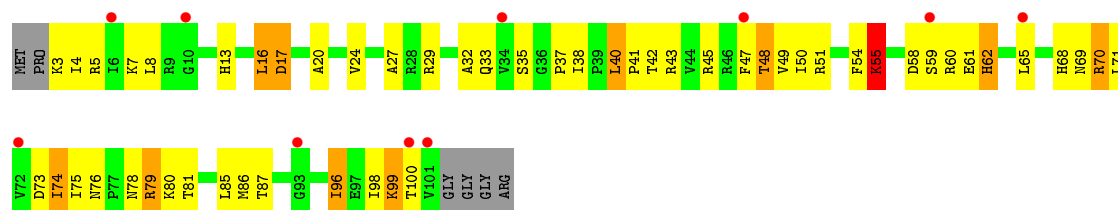
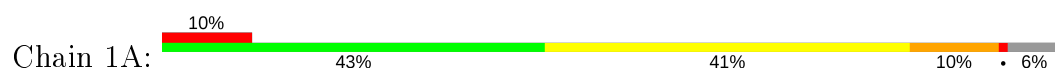
- Molecule 9: 30S ribosomal protein S9



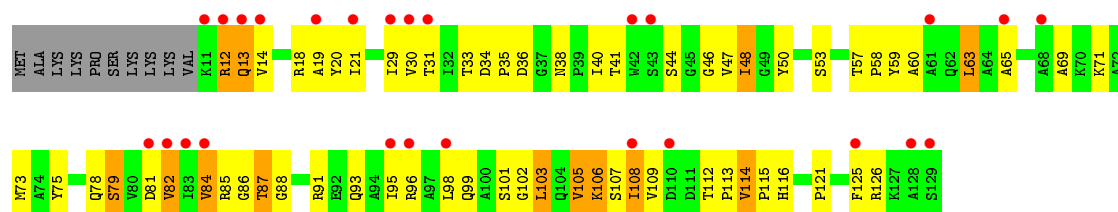
- Molecule 10: 30S ribosomal protein S10



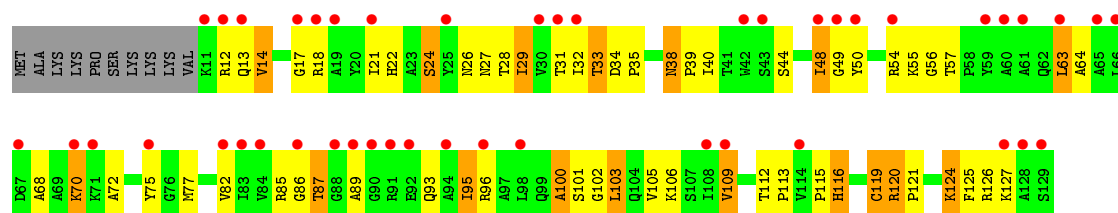
- Molecule 10: 30S ribosomal protein S10



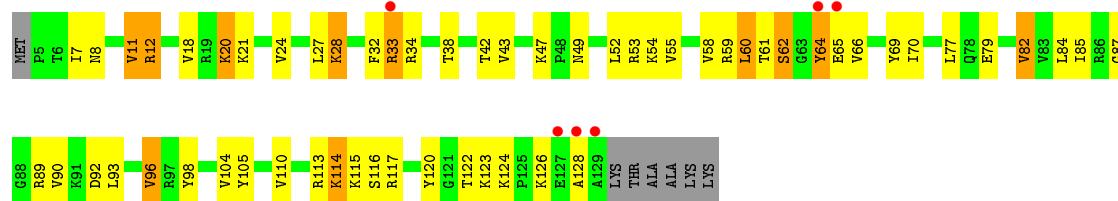
- Molecule 11: 30S ribosomal protein S11



- Molecule 11: 30S ribosomal protein S11



- Molecule 12: 30S ribosomal protein S12



- Molecule 12: 30S ribosomal protein S12

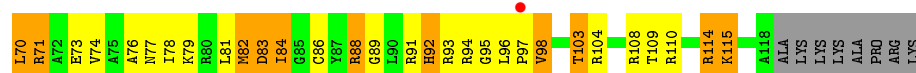




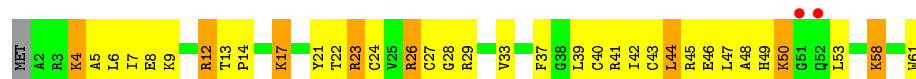
- Molecule 13: 30S ribosomal protein S13



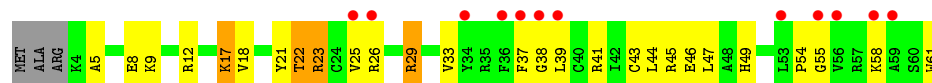
- Molecule 13: 30S ribosomal protein S13



- Molecule 14: 30S ribosomal protein S14 type Z



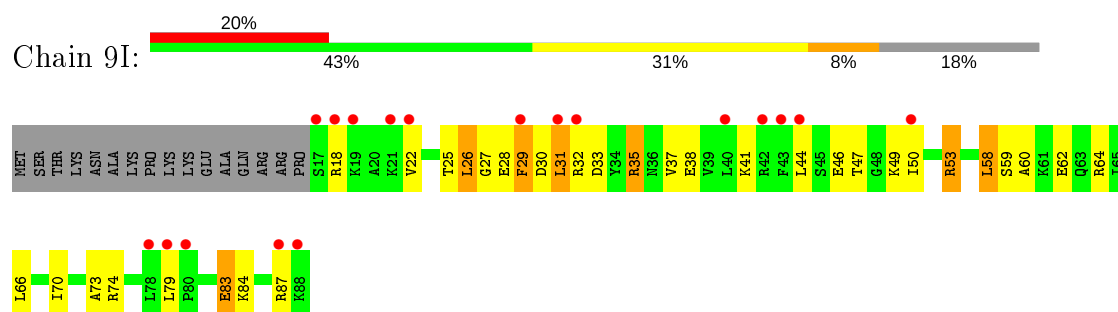
- Molecule 14: 30S ribosomal protein S14 type Z



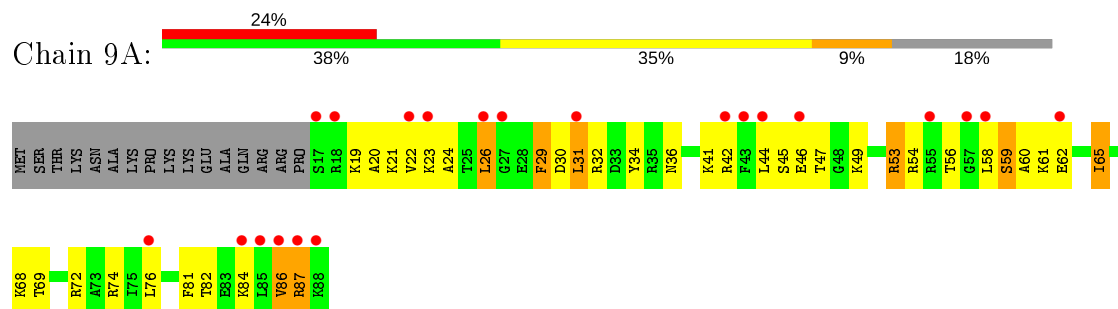
- Molecule 15: 30S ribosomal protein S15



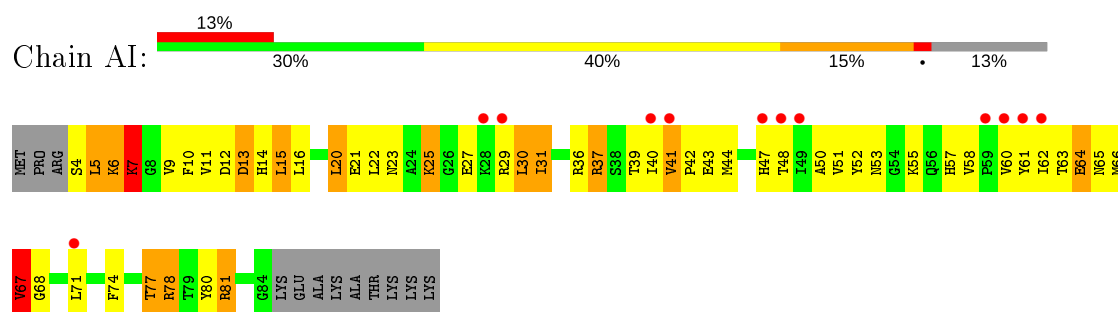
- Molecule 18: 30S ribosomal protein S18



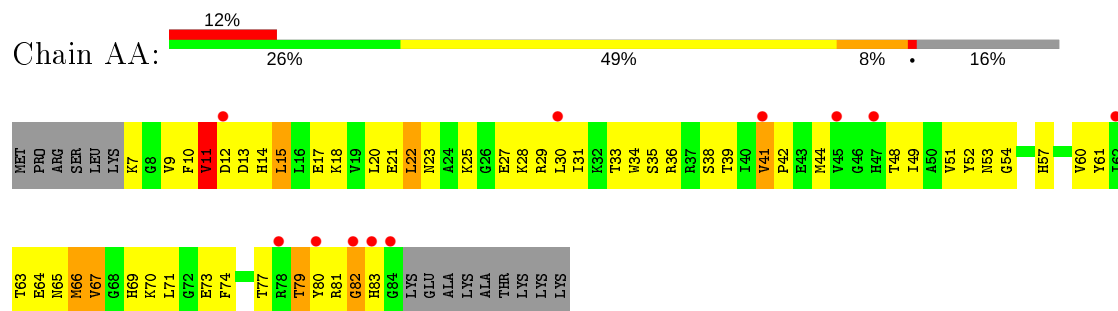
- Molecule 18: 30S ribosomal protein S18



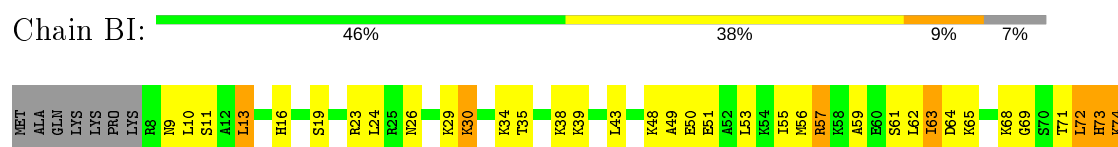
- Molecule 19: 30S ribosomal protein S19



- Molecule 19: 30S ribosomal protein S19

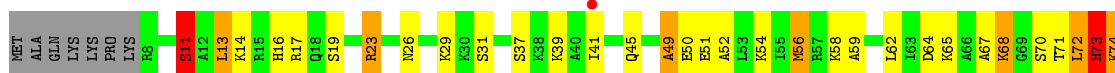


- Molecule 20: 30S ribosomal protein S20

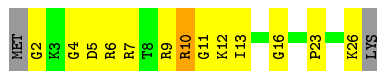




- Molecule 20: 30S ribosomal protein S20



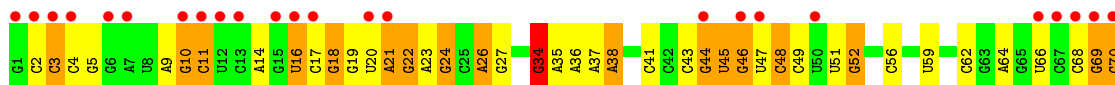
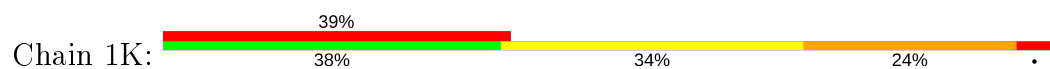
- Molecule 21: 30S ribosomal protein Thx



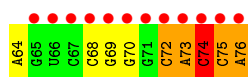
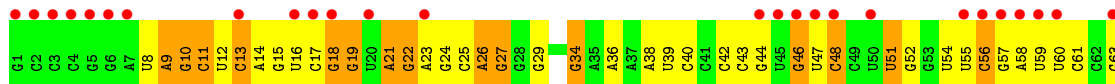
- Molecule 21: 30S ribosomal protein Thx



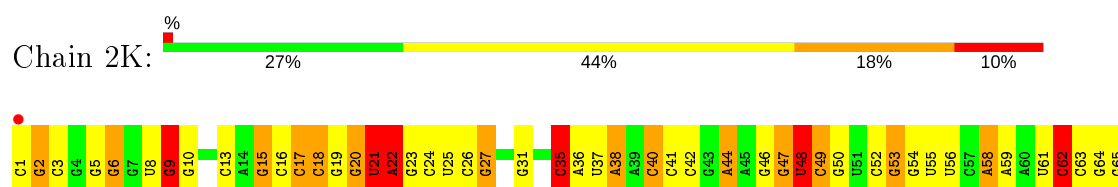
- Molecule 22: tRNA-Phe



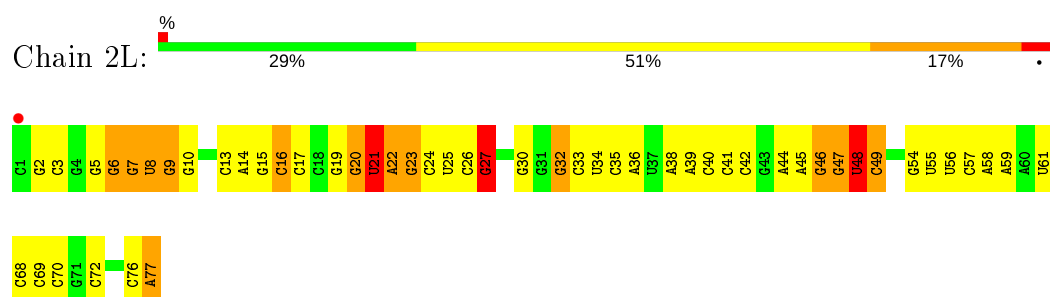
- Molecule 22: tRNA-Phe



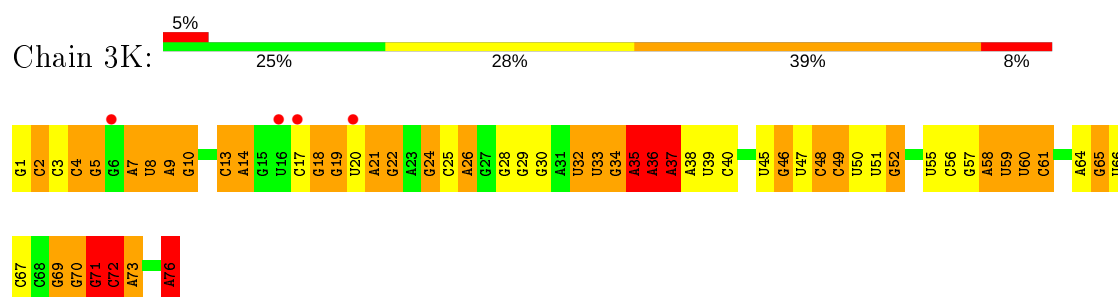
- Molecule 23: tRNA-fMet



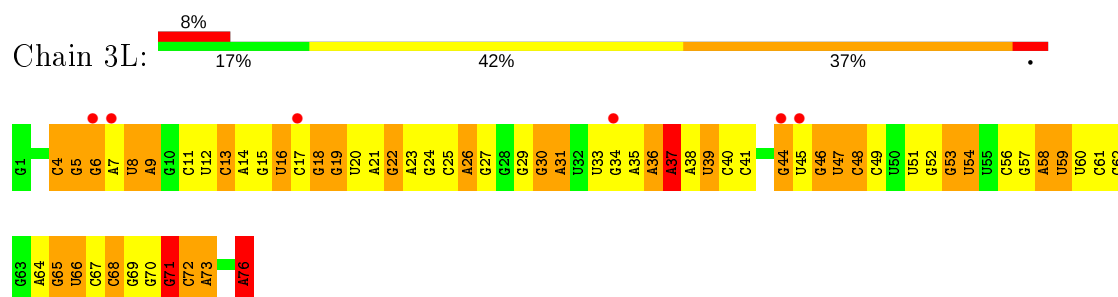
- Molecule 23: tRNA-fMet



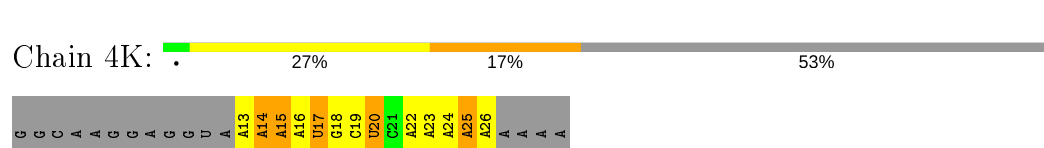
- Molecule 24: tRNA-Phe



- Molecule 24: tRNA-Phe



- Molecule 25: mRNA

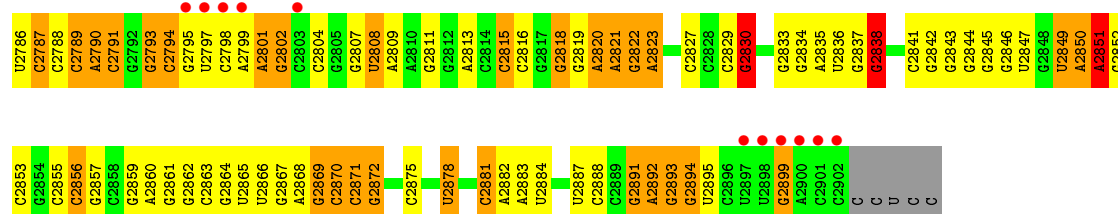


- Molecule 25: mRNA

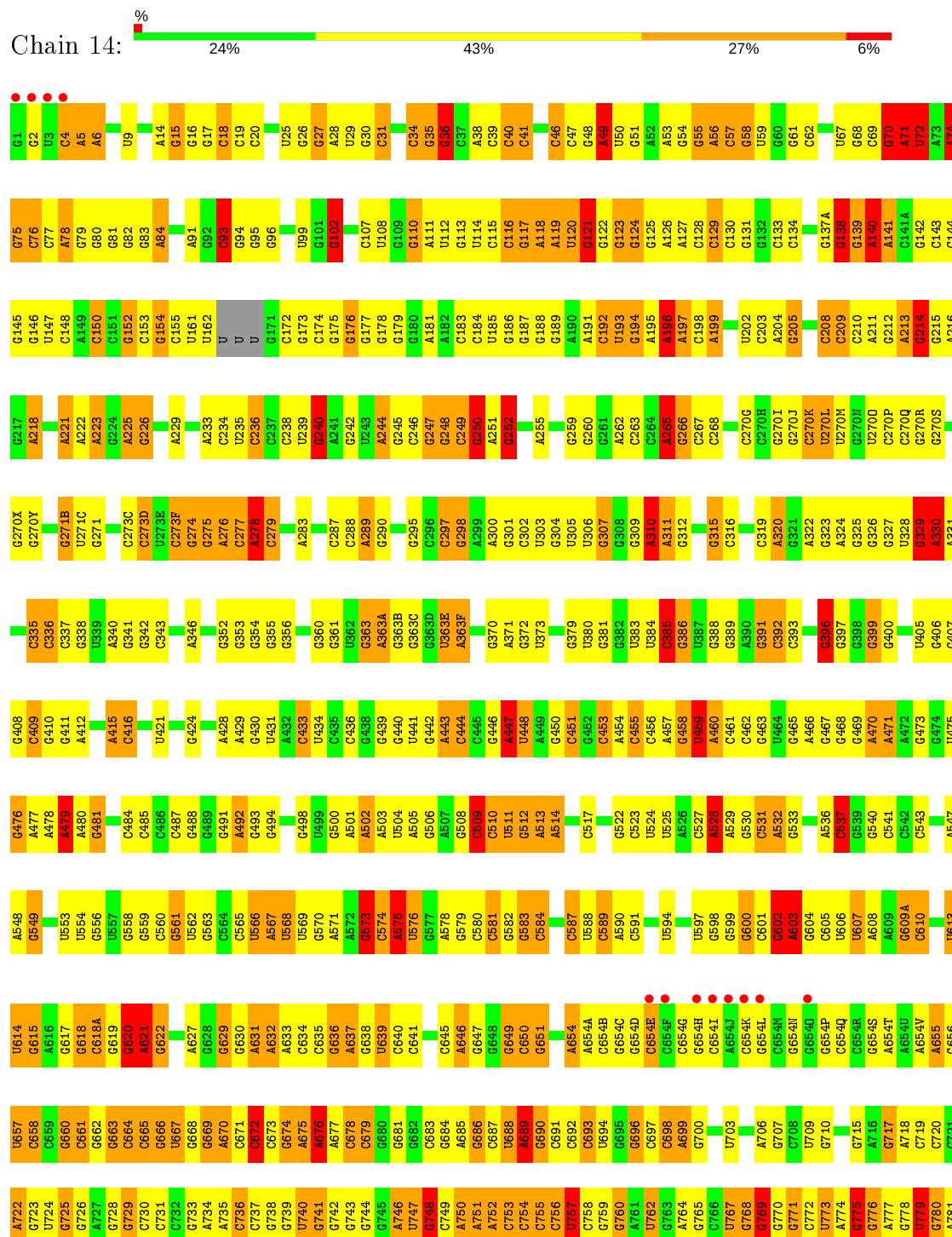


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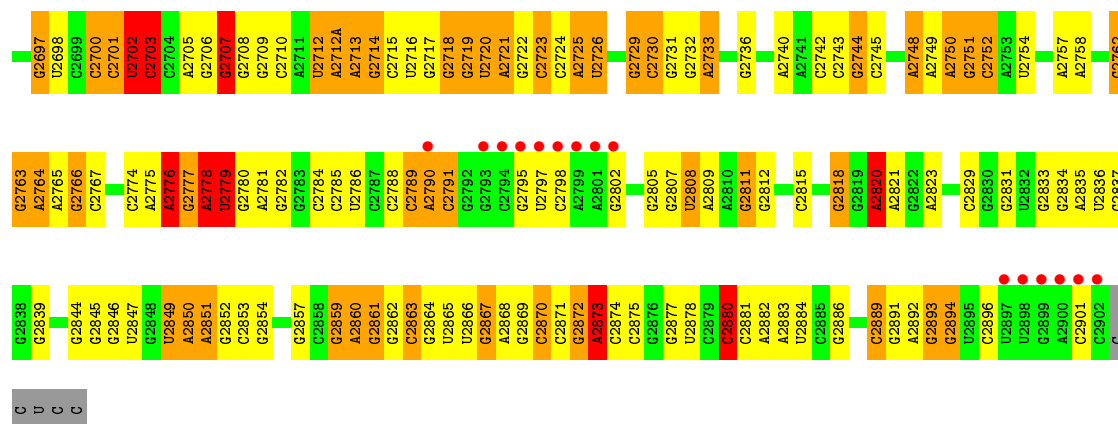


Molecule 26: 23S ribosomal RNA

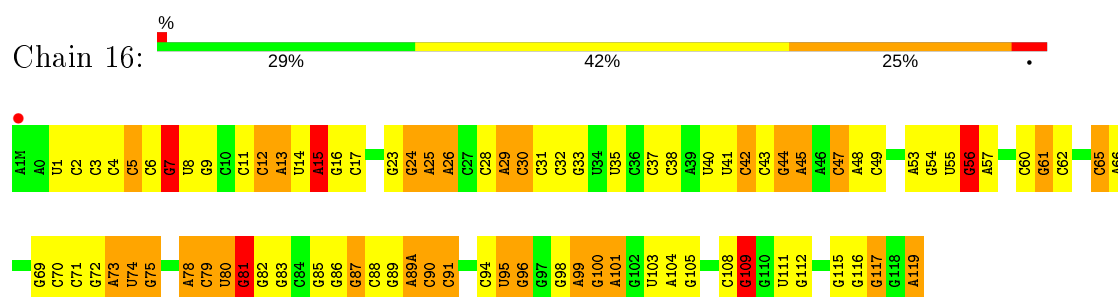


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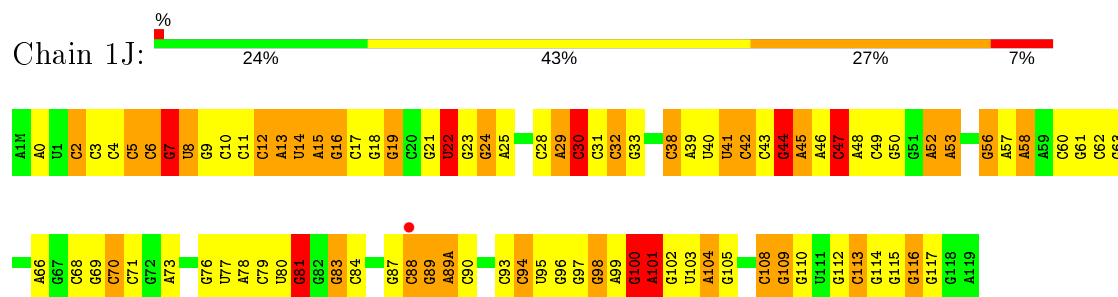
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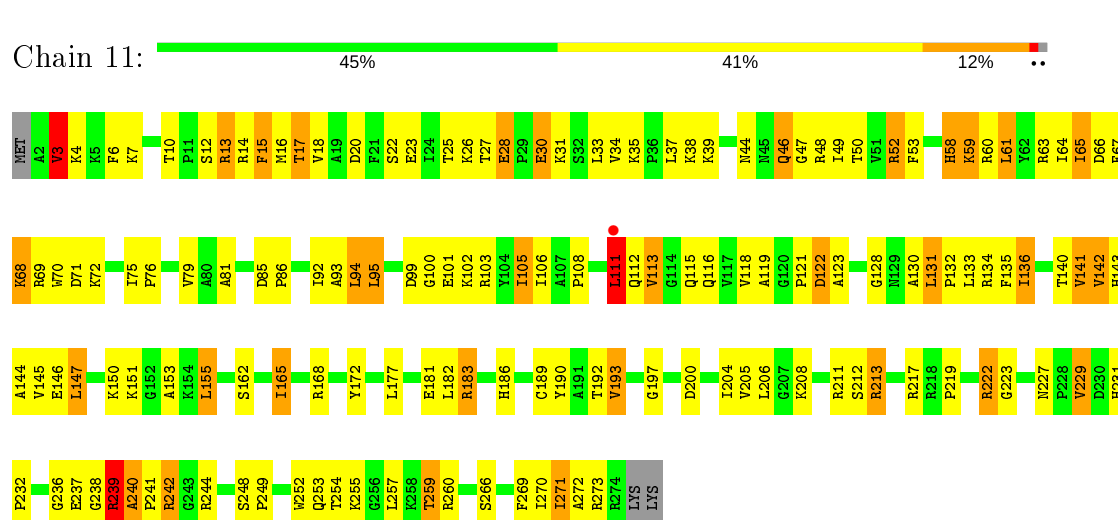
• Molecule 27: 5S ribosomal RNA



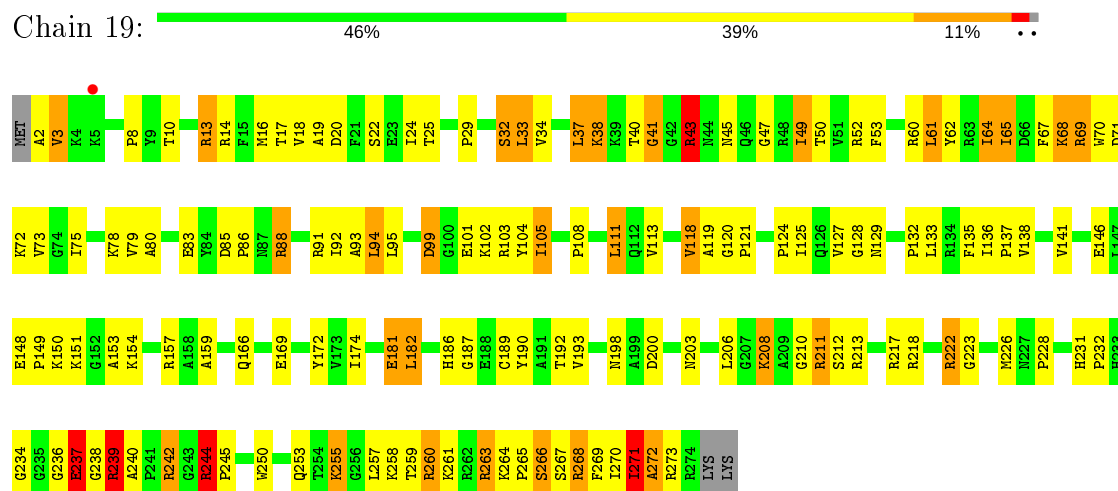
• Molecule 27: 5S ribosomal RNA



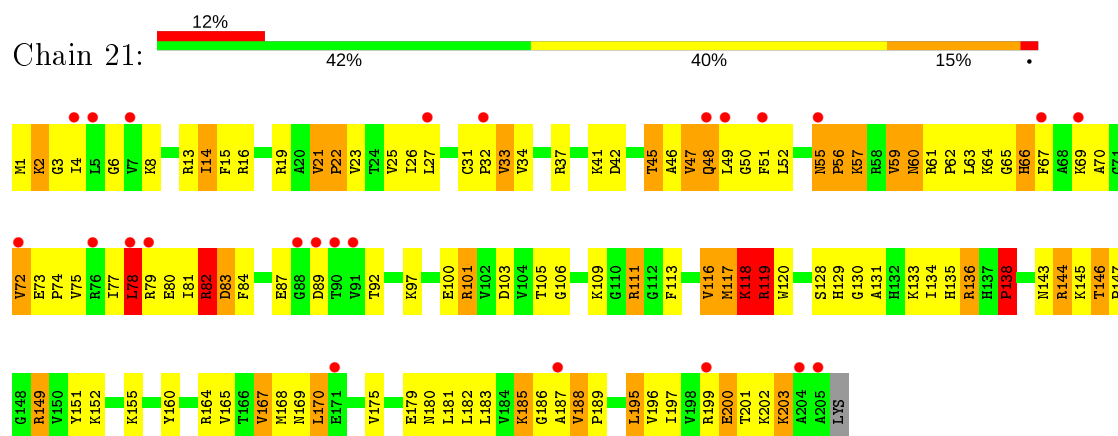
• Molecule 28: 50S ribosomal protein L2



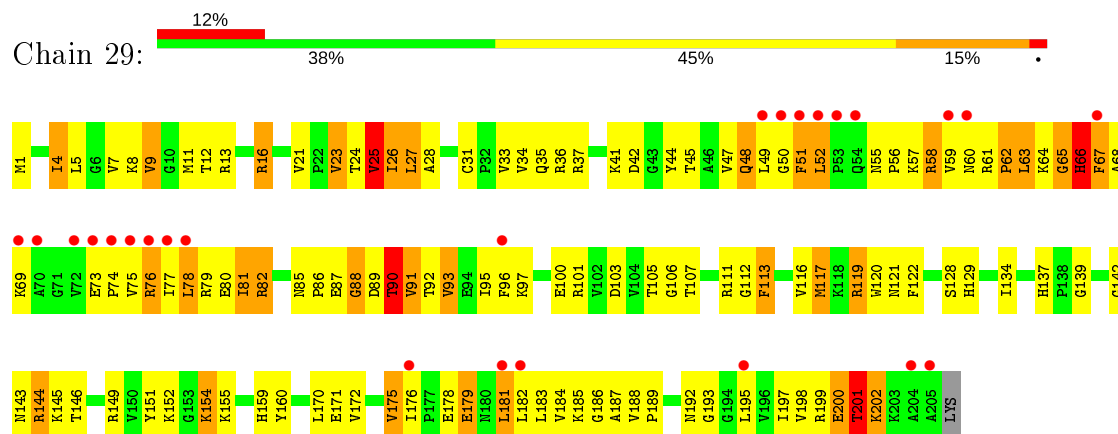
• Molecule 28: 50S ribosomal protein L2



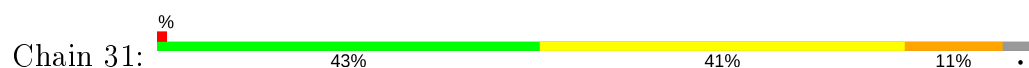
• Molecule 29: 50S ribosomal protein L3

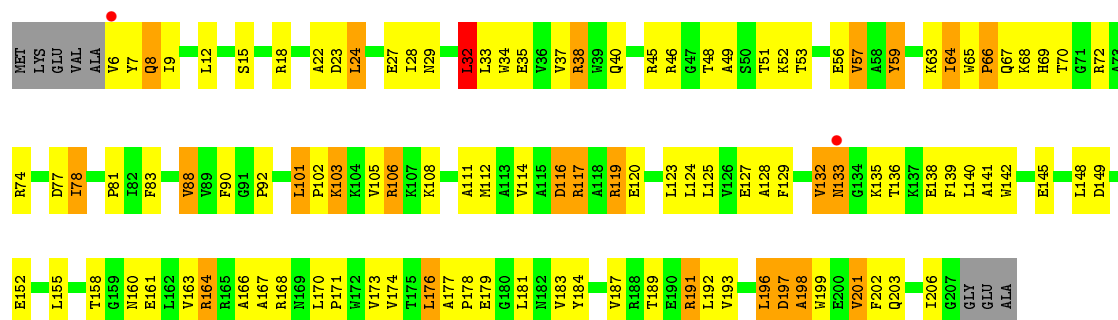


• Molecule 29: 50S ribosomal protein L3

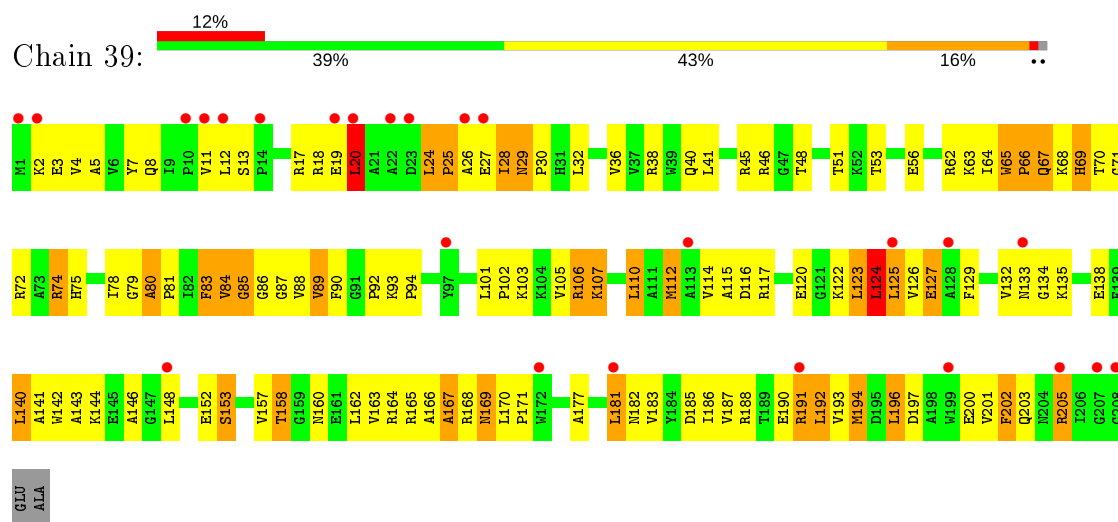


• Molecule 30: 50S ribosomal protein L4

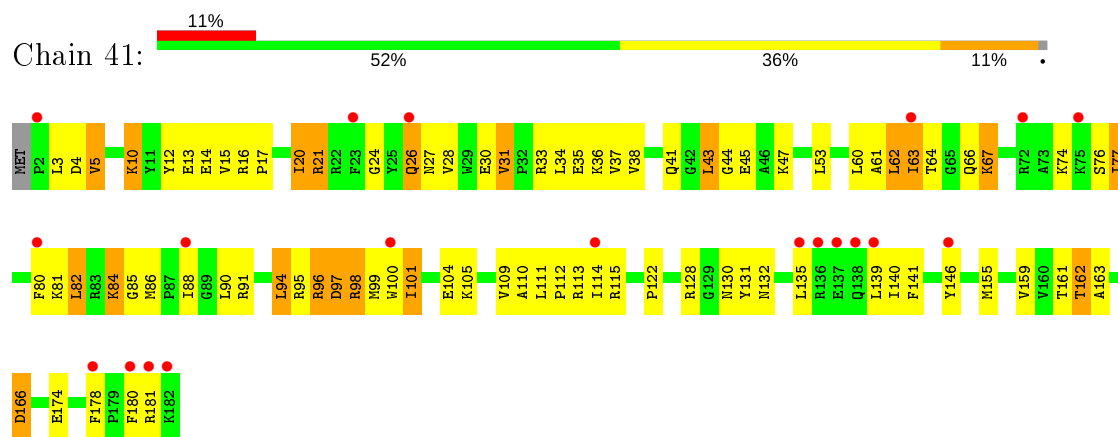




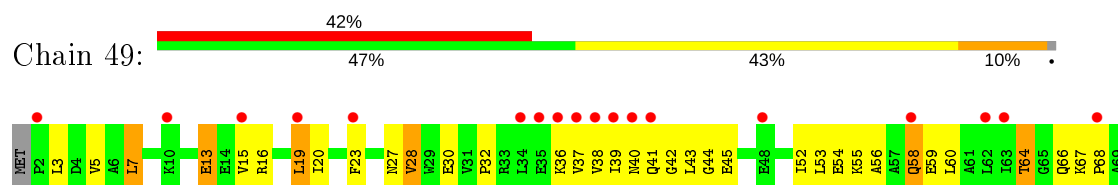
• Molecule 30: 50S ribosomal protein L4

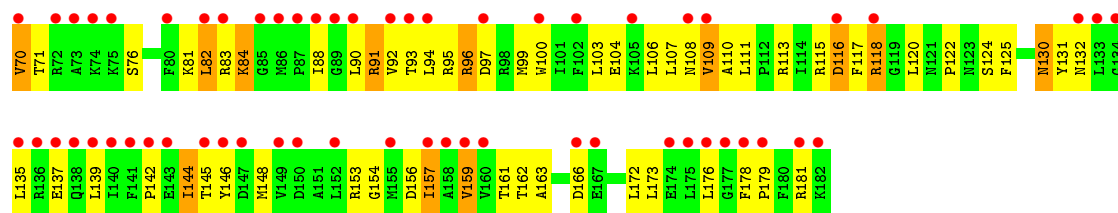


• Molecule 31: 50S ribosomal protein L5

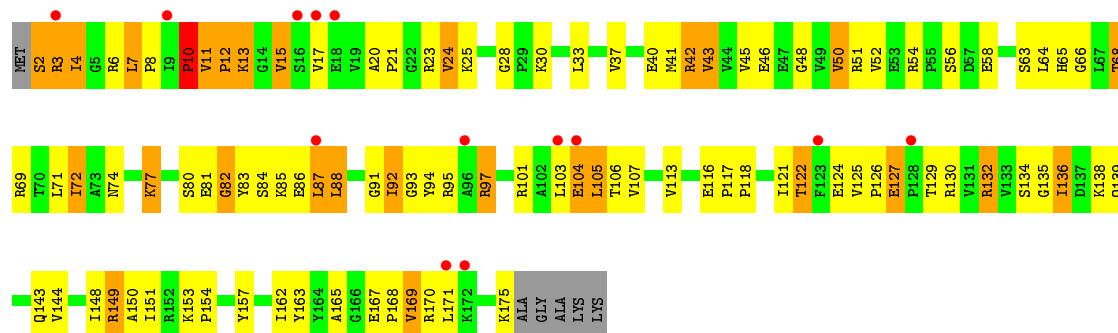
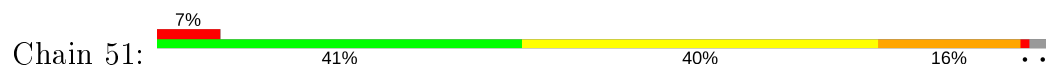


• Molecule 31: 50S ribosomal protein L5

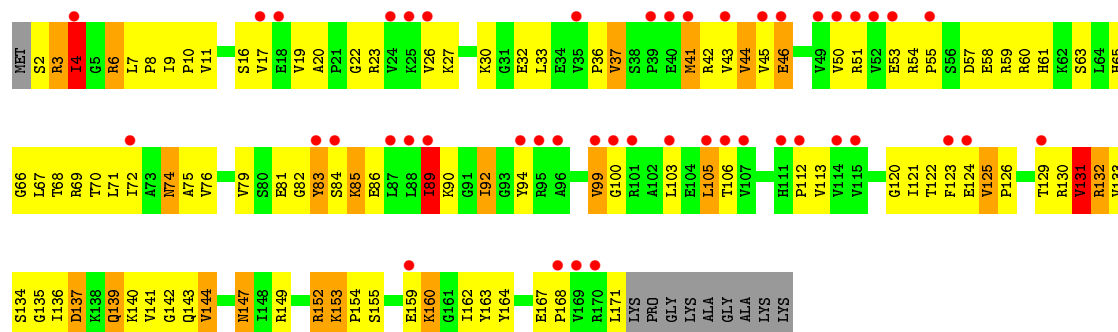




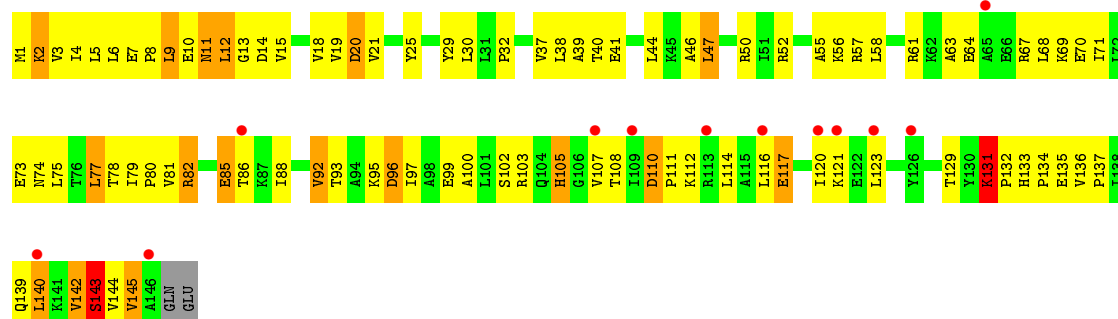
• Molecule 32: 50S ribosomal protein L6



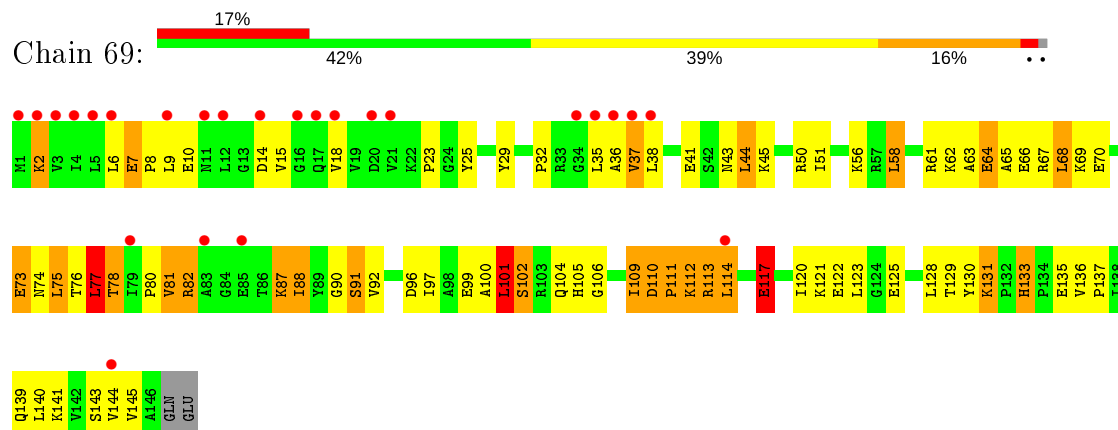
• Molecule 32: 50S ribosomal protein L6



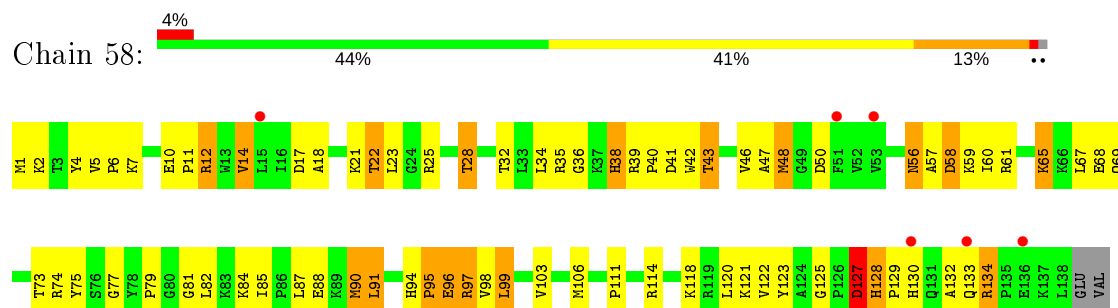
• Molecule 33: 50S ribosomal protein L9



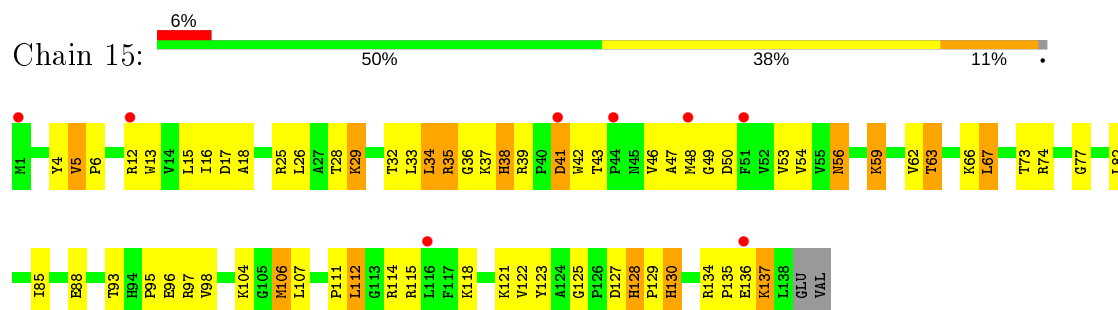
- Molecule 33: 50S ribosomal protein L9



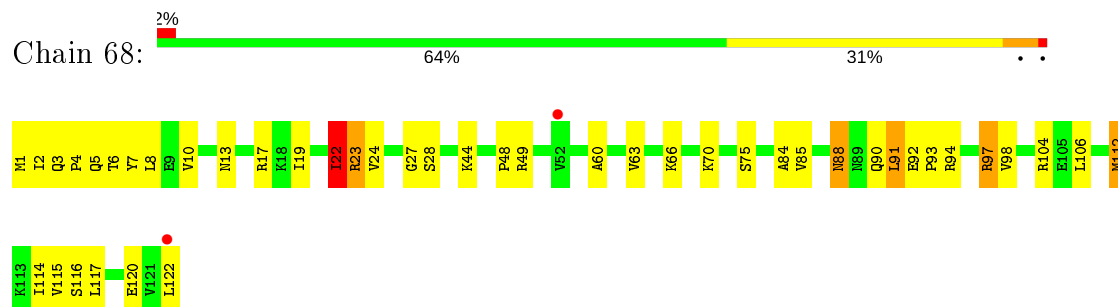
- Molecule 34: 50S ribosomal protein L13



- Molecule 34: 50S ribosomal protein L13

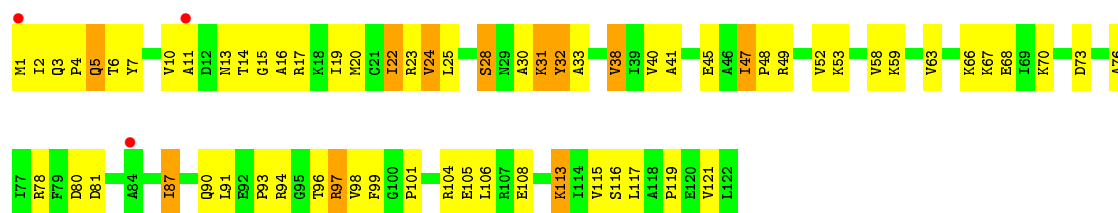


- Molecule 35: 50S ribosomal protein L14

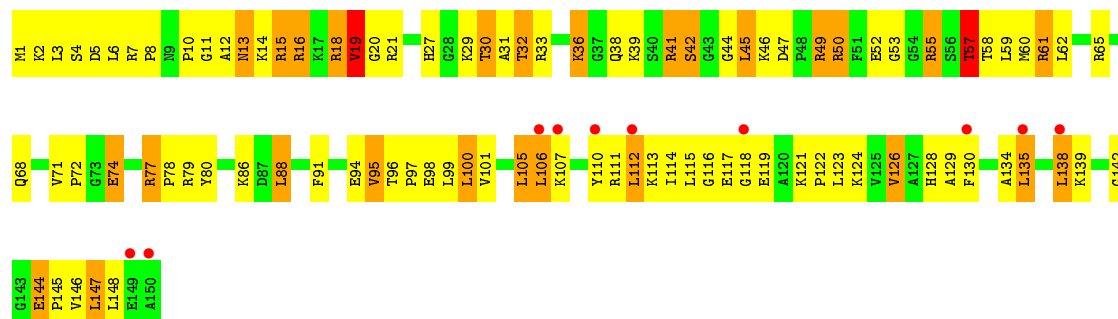


- Molecule 35: 50S ribosomal protein L14

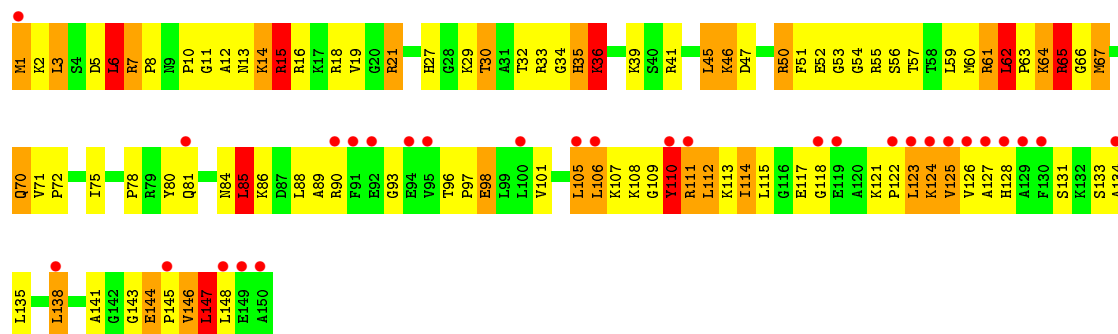




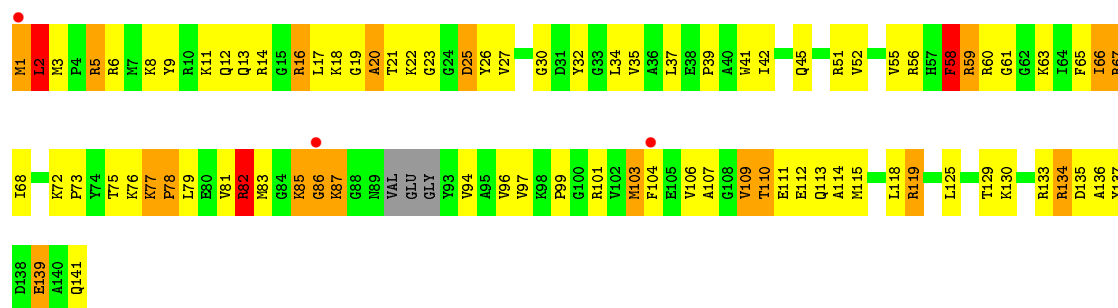
• Molecule 36: 50S ribosomal protein L15



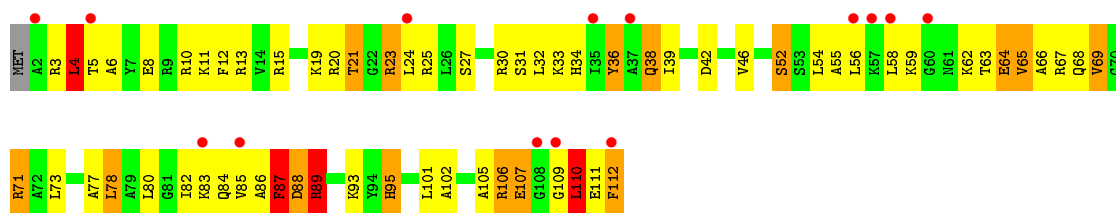
• Molecule 36: 50S ribosomal protein L15



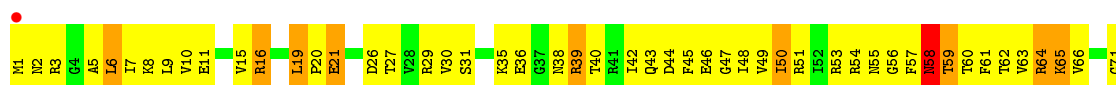
• Molecule 37: 50S ribosomal protein L16



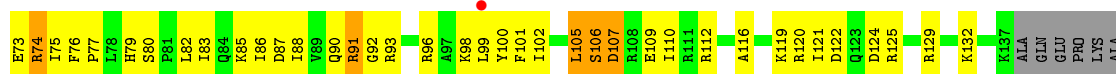
• Molecule 37: 50S ribosomal protein L16



• Molecule 40: 50S ribosomal protein L19

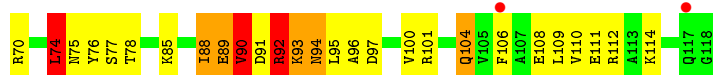


• Molecule 40: 50S ribosomal protein L19

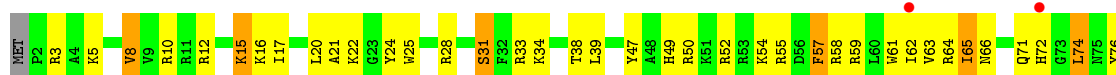


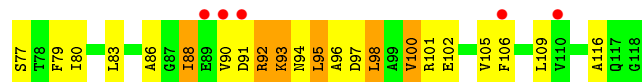
SER
GLN
GLU

• Molecule 41: 50S ribosomal protein L20

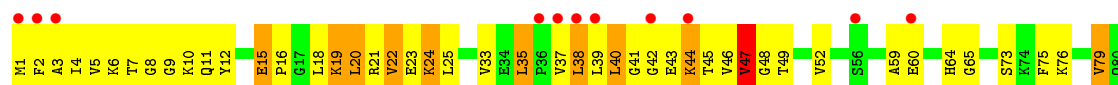
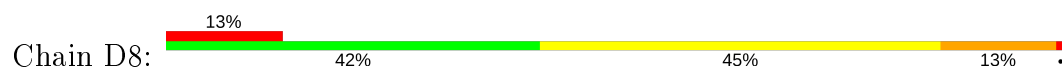


• Molecule 41: 50S ribosomal protein L20

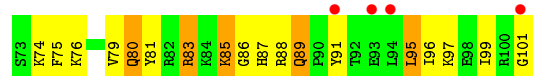
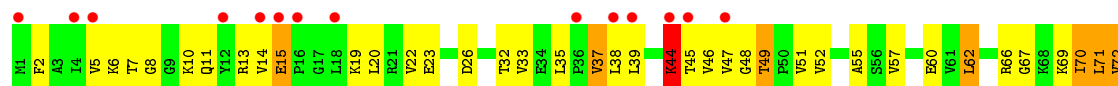
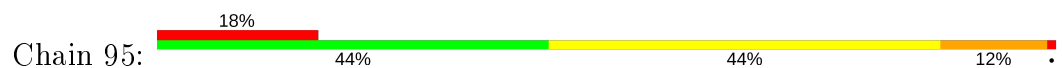




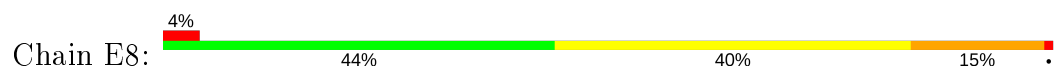
- Molecule 42: 50S ribosomal protein L21



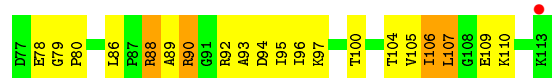
- Molecule 42: 50S ribosomal protein L21



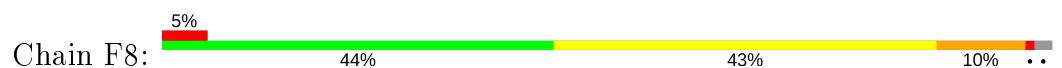
- Molecule 43: 50S ribosomal protein L22

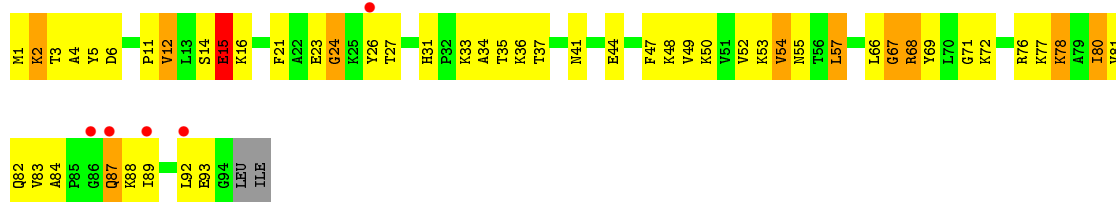


- Molecule 43: 50S ribosomal protein L22

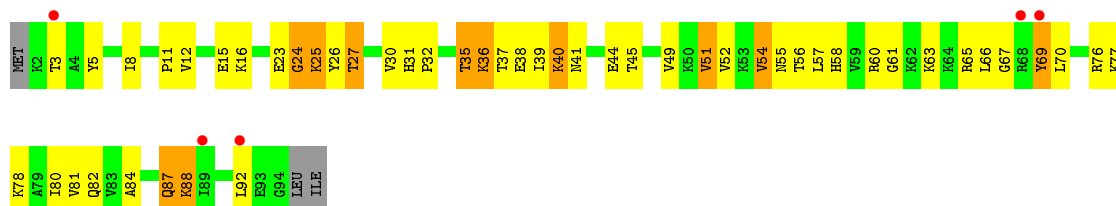


- Molecule 44: 50S ribosomal protein L23

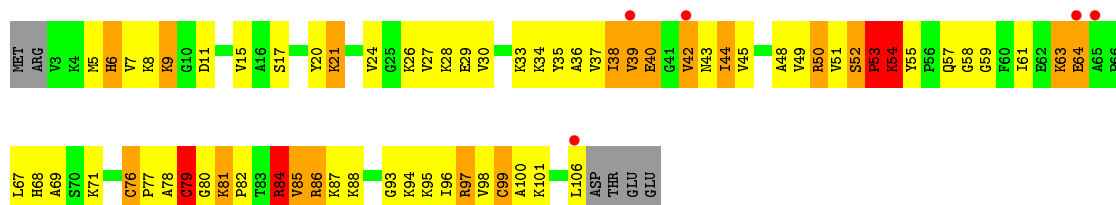




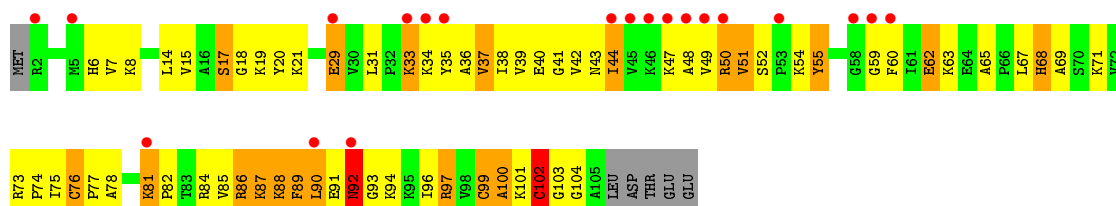
• Molecule 44: 50S ribosomal protein L23



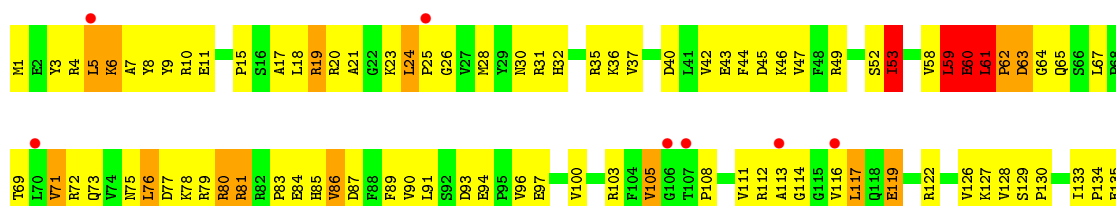
• Molecule 45: 50S ribosomal protein L24



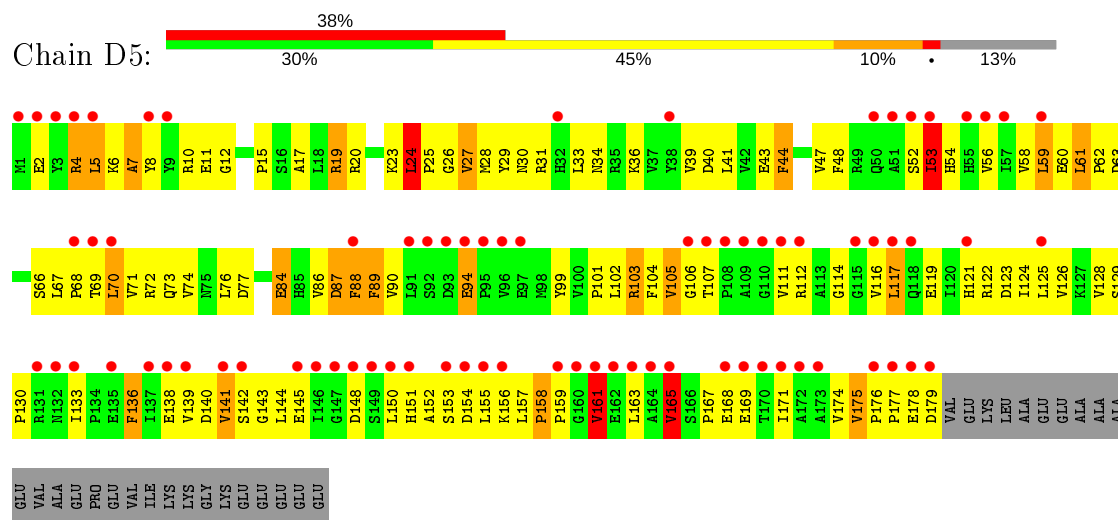
• Molecule 45: 50S ribosomal protein L24



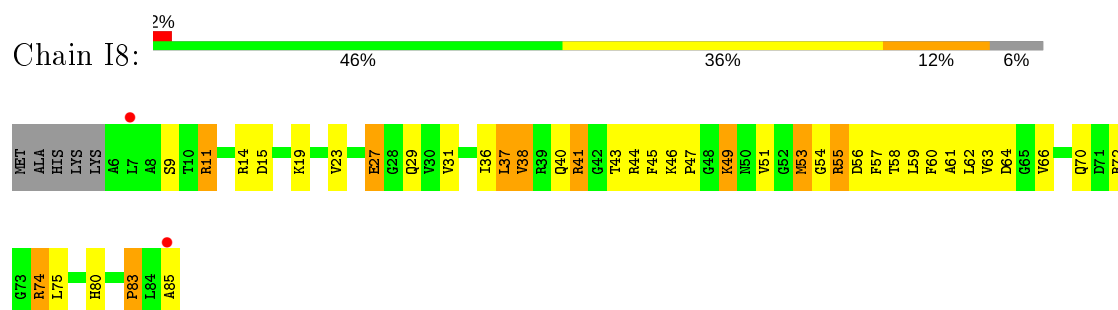
• Molecule 46: 50S ribosomal protein L25



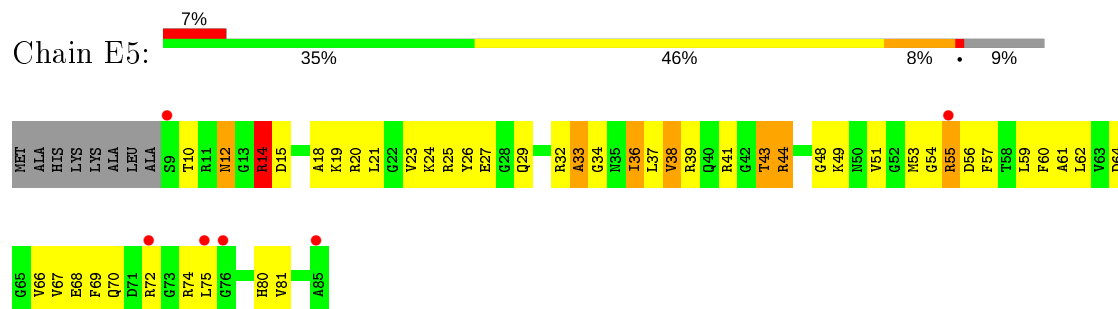
- Molecule 46: 50S ribosomal protein L25



- Molecule 47: 50S ribosomal protein L27



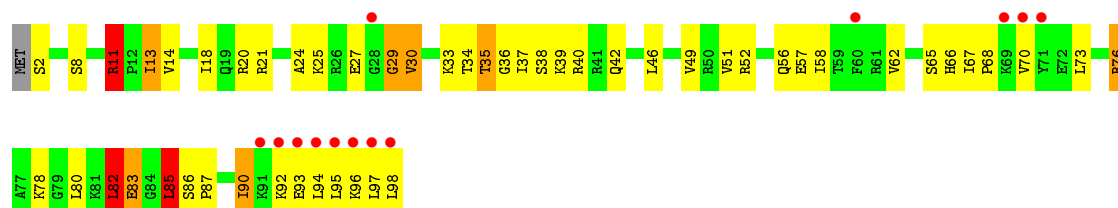
- Molecule 47: 50S ribosomal protein L27



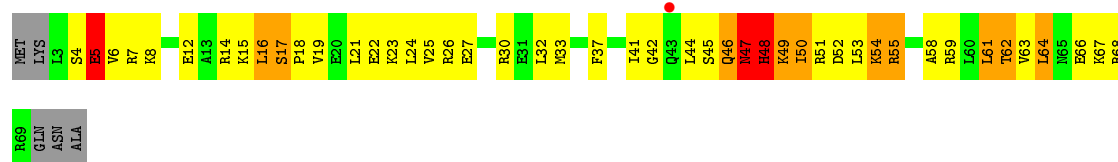
- Molecule 48: 50S ribosomal protein L28



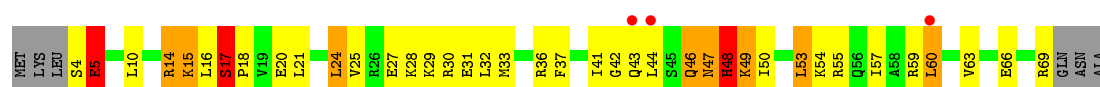
- Molecule 48: 50S ribosomal protein L28



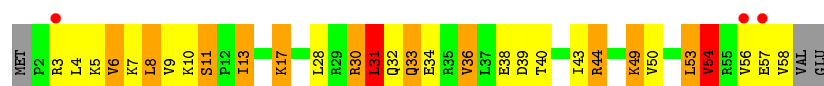
- Molecule 49: 50S ribosomal protein L29



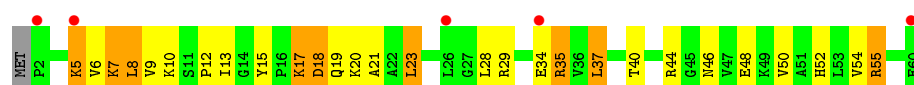
- Molecule 49: 50S ribosomal protein L29



- Molecule 50: 50S ribosomal protein L30

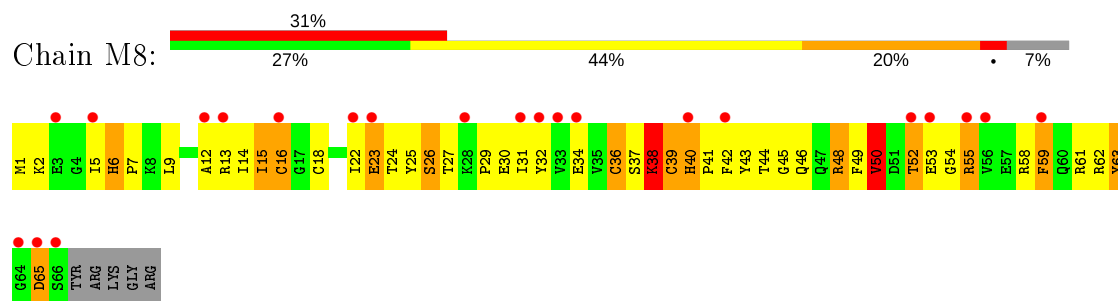


- Molecule 50: 50S ribosomal protein L30



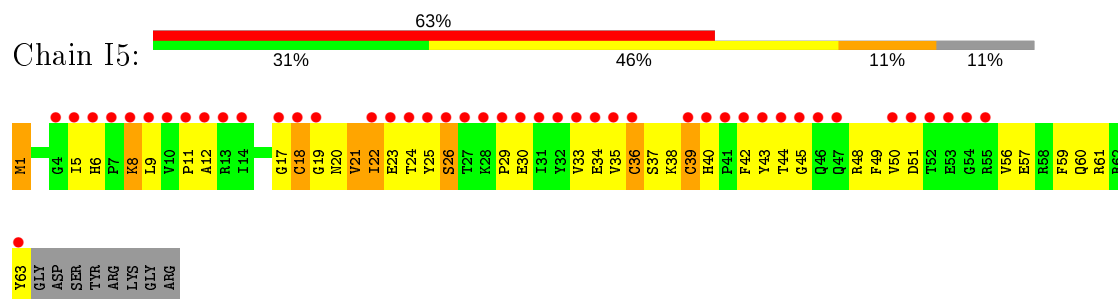
• Molecule 51: 50S ribosomal protein L31

Chain M8:



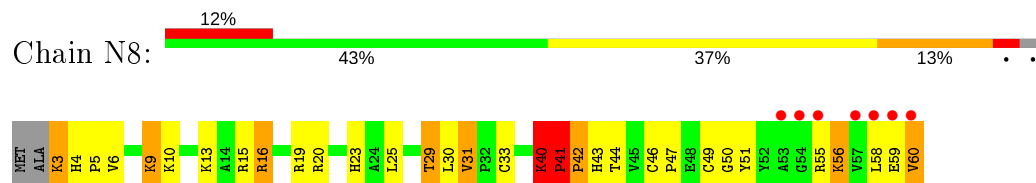
• Molecule 51: 50S ribosomal protein L31

Chain I5:



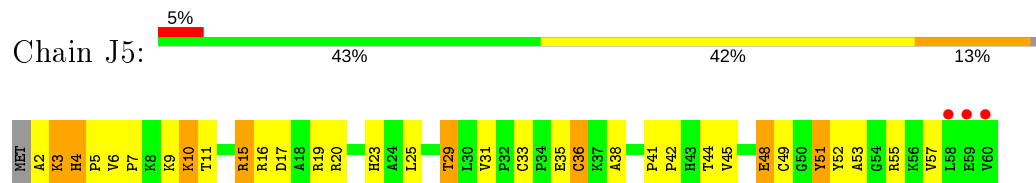
• Molecule 52: 50S ribosomal protein L32

Chain N8:



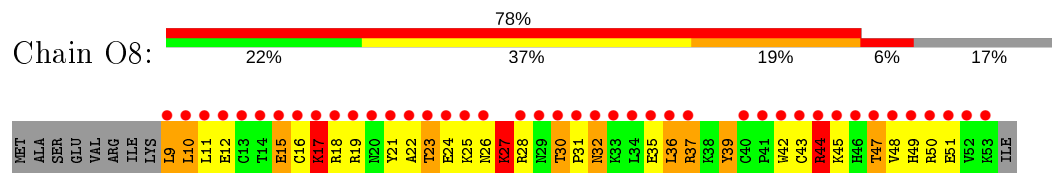
• Molecule 52: 50S ribosomal protein L32

Chain J5:



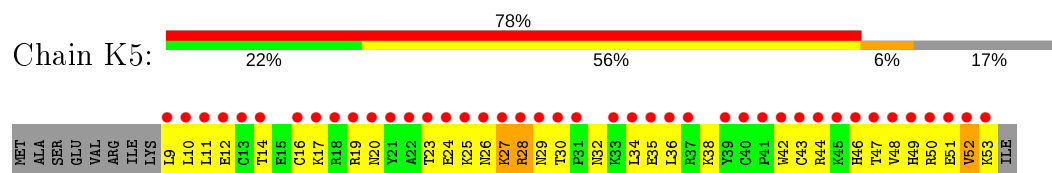
• Molecule 53: 50S ribosomal protein L33

Chain O8:



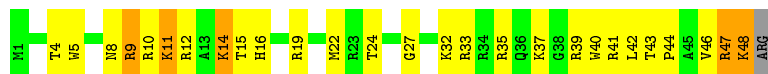
• Molecule 53: 50S ribosomal protein L33

Chain K5:



- Molecule 54: 50S ribosomal protein L34

Chain P8:  43% 45% 10%



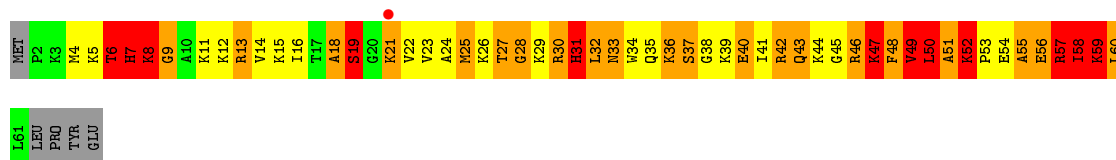
- Molecule 54: 50S ribosomal protein L34

Chain L5:  47% 39% 8% 6%



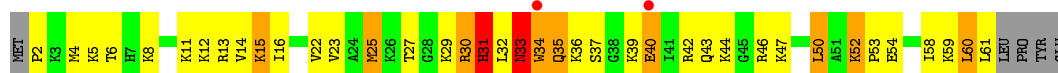
- Molecule 55: 50S ribosomal protein L35

Chain Q8:  2% 9% 32% 32% 18% 8%



- Molecule 55: 50S ribosomal protein L35

Chain M5:  3% 32% 43% 14% 8%



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	210.10Å 448.80Å 621.30Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	152.19 – 3.15 152.19 – 3.15	Depositor EDS
% Data completeness (in resolution range)	99.9 (152.19-3.15) 93.3 (152.19-3.15)	Depositor EDS
R_{merge}	0.37	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.89 (at 3.13Å)	Xtriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.189 , 0.231 0.189 , 0.231	Depositor DCC
R_{free} test set	2000 reflections (0.20%)	wwPDB-VP
Wilson B-factor (Å ²)	87.9	Xtriage
Anisotropy	0.303	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.27 , 87.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.27$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	300537	wwPDB-VP
Average B, all atoms (Å ²)	115.0	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: OMC, 5MU, ZN, MIA, MG, 4SU, 7MG, PSU

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	13	0.82	13/36052 (0.0%)	1.55	642/56266 (1.1%)
1	1G	0.71	2/36025 (0.0%)	1.38	354/56227 (0.6%)
2	12	0.37	0/1959	0.64	2/2642 (0.1%)
2	1E	0.45	0/1959	0.73	3/2642 (0.1%)
3	22	0.38	0/1636	0.62	0/2205
3	2E	0.51	0/1629	0.70	0/2195
4	32	0.50	0/1733	0.73	1/2318 (0.0%)
4	3E	0.65	2/1733 (0.1%)	0.78	2/2318 (0.1%)
5	42	0.48	0/1171	0.72	1/1576 (0.1%)
5	4E	0.55	0/1171	0.77	1/1576 (0.1%)
6	52	0.55	0/856	0.70	0/1154
6	5E	0.58	0/856	0.76	0/1154
7	62	0.44	0/1276	0.59	0/1709
7	6E	0.47	0/1276	0.61	0/1709
8	72	0.42	0/1136	0.67	1/1527 (0.1%)
8	7E	0.57	0/1136	0.78	2/1527 (0.1%)
9	82	0.40	0/1029	0.66	1/1379 (0.1%)
9	8E	0.47	0/1029	0.72	0/1379
10	1A	0.39	0/814	0.62	0/1095
10	1I	0.47	0/814	0.67	0/1095
11	2A	0.49	0/900	0.75	0/1213
11	2I	0.57	0/900	0.79	1/1213 (0.1%)
12	3A	0.61	0/991	0.81	1/1327 (0.1%)
12	3I	0.74	0/991	0.94	0/1327
13	4A	0.36	0/943	0.64	0/1265
13	4I	0.51	0/948	0.76	0/1272
14	5A	0.43	0/485	0.73	0/643
14	5I	0.66	1/501 (0.2%)	0.88	3/664 (0.5%)
15	6A	0.49	0/745	0.60	0/992
15	6I	0.60	0/745	0.82	0/992
16	7A	0.51	0/721	0.69	0/970
16	7I	0.52	0/721	0.73	0/970

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
17	8A	0.54	0/847	0.65	0/1131
17	8I	0.62	0/847	0.78	0/1131
18	9A	0.53	0/596	0.72	1/790 (0.1%)
18	9I	0.60	1/596 (0.2%)	0.79	0/790
19	AA	0.40	0/638	0.66	1/860 (0.1%)
19	AI	0.58	0/661	0.84	1/890 (0.1%)
20	BA	0.50	0/765	0.77	0/1007
20	BI	0.42	0/765	0.70	1/1007 (0.1%)
21	1B	0.55	0/221	0.64	0/288
21	1F	0.50	0/221	0.73	0/288
22	1K	0.53	0/1739	1.15	15/2708 (0.6%)
22	1L	0.44	0/1739	0.96	4/2708 (0.1%)
23	2K	1.13	6/1721 (0.3%)	1.67	45/2682 (1.7%)
23	2L	0.99	7/1721 (0.4%)	1.43	18/2682 (0.7%)
24	3K	0.52	0/1809	1.29	25/2819 (0.9%)
24	3L	0.48	2/1809 (0.1%)	1.14	15/2819 (0.5%)
25	4K	1.00	0/338	1.43	5/524 (1.0%)
25	4L	0.79	0/147	1.61	5/227 (2.2%)
26	14	0.99	121/70167 (0.2%)	1.77	2211/109541 (2.0%)
26	1H	1.20	257/70233 (0.4%)	2.06	3865/109643 (3.5%)
27	16	1.01	3/2928 (0.1%)	1.83	103/4568 (2.3%)
27	1J	0.83	1/2928 (0.0%)	1.53	48/4568 (1.1%)
28	11	0.96	3/2170 (0.1%)	1.14	13/2926 (0.4%)
28	19	0.80	0/2170	1.01	6/2926 (0.2%)
29	21	0.75	0/1601	0.99	3/2160 (0.1%)
29	29	0.76	0/1601	0.99	2/2160 (0.1%)
30	31	0.84	0/1620	1.02	5/2194 (0.2%)
30	39	0.67	0/1662	0.95	1/2249 (0.0%)
31	41	0.60	0/1498	0.86	2/2016 (0.1%)
31	49	0.44	0/1498	0.66	0/2016
32	51	0.64	0/1362	0.93	2/1841 (0.1%)
32	59	0.38	0/1332	0.69	1/1802 (0.1%)
33	61	0.55	0/1151	0.83	1/1558 (0.1%)
33	69	0.49	0/1151	0.79	4/1558 (0.3%)
34	15	0.53	0/1131	0.77	0/1525
34	58	0.65	0/1131	0.88	0/1525
35	25	0.66	0/943	0.83	0/1269
35	68	0.75	0/943	0.87	1/1269 (0.1%)
36	35	0.73	0/1162	1.15	6/1544 (0.4%)
36	78	0.81	0/1162	1.12	3/1544 (0.2%)
37	45	0.72	0/1143	0.96	1/1527 (0.1%)
37	88	0.96	3/1107 (0.3%)	1.15	7/1478 (0.5%)
38	55	0.71	0/974	0.93	1/1302 (0.1%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
38	98	0.67	0/982	1.00	4/1312 (0.3%)
39	65	0.57	0/892	0.96	3/1187 (0.3%)
39	A8	0.78	0/892	1.05	4/1187 (0.3%)
40	75	0.65	0/1155	0.79	0/1542
40	B8	0.70	0/1155	0.89	0/1542
41	85	0.64	0/982	0.81	0/1306
41	C8	0.80	0/982	0.97	5/1306 (0.4%)
42	95	0.67	0/790	0.91	2/1057 (0.2%)
42	D8	0.68	0/790	0.90	1/1057 (0.1%)
43	A5	0.74	0/911	0.88	1/1220 (0.1%)
43	E8	0.72	0/911	1.07	7/1220 (0.6%)
44	B5	0.83	0/744	0.89	0/1000
44	F8	0.96	2/756 (0.3%)	1.03	1/1014 (0.1%)
45	C5	0.78	0/807	0.97	1/1076 (0.1%)
45	G8	0.78	0/804	1.07	2/1073 (0.2%)
46	D5	0.45	0/1460	0.71	1/1982 (0.1%)
46	H8	0.56	0/1427	0.87	2/1935 (0.1%)
47	E5	0.65	0/621	0.94	1/827 (0.1%)
47	I8	0.87	0/635	1.03	0/847
48	F5	0.68	0/770	1.00	4/1022 (0.4%)
48	J8	0.81	0/770	1.00	2/1022 (0.2%)
49	G5	0.65	1/560 (0.2%)	0.84	1/741 (0.1%)
49	K8	0.88	0/565	1.08	1/748 (0.1%)
50	H5	0.54	0/474	0.78	0/635
50	L8	0.84	0/457	1.08	4/613 (0.7%)
51	I5	0.46	0/527	0.76	0/709
51	M8	0.64	0/545	0.84	0/733
52	J5	0.70	0/473	0.91	1/639 (0.2%)
52	N8	0.77	0/468	1.02	2/632 (0.3%)
53	K5	0.61	0/396	0.96	0/529
53	O8	0.83	1/396 (0.3%)	0.89	1/529 (0.2%)
54	L5	0.89	0/406	1.04	2/536 (0.4%)
54	P8	1.04	0/426	1.17	2/561 (0.4%)
55	M5	0.99	1/483 (0.2%)	1.14	1/634 (0.2%)
55	Q8	1.47	5/486 (1.0%)	1.86	11/638 (1.7%)
All	All	0.90	432/322727 (0.1%)	1.57	7504/483212 (1.6%)

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	1
2	1E	0	1
4	32	0	4
4	3E	0	1
9	82	0	2
10	1A	0	2
11	2A	0	2
12	3A	0	1
12	3I	0	1
15	6I	0	1
19	AI	0	2
20	BA	0	3
28	11	0	1
28	19	0	4
29	21	0	3
29	29	0	4
30	31	0	1
30	39	0	6
31	41	0	2
31	49	0	1
32	59	0	3
33	61	0	5
33	69	0	2
34	15	0	2
34	58	0	2
35	68	0	1
36	35	0	4
36	78	0	2
37	45	0	6
37	88	0	2
38	55	0	1
38	98	0	3
39	65	0	2
39	A8	0	2
40	75	0	1
40	B8	0	1
41	85	0	2
41	C8	0	2
42	95	0	1
43	A5	0	3
44	B5	0	2
44	F8	0	1
45	C5	0	3

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Mol	Chain	#Chirality outliers	#Planarity outliers
45	G8	0	3
46	D5	0	2
46	H8	0	2
47	I8	0	2
48	F5	0	1
48	J8	0	2
49	G5	0	3
49	K8	0	3
51	I5	0	2
51	M8	0	2
52	N8	0	2
53	K5	0	3
53	O8	0	3
55	M5	0	3
55	Q8	0	13
All	All	0	142

The worst 5 of 432 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	2L	21	U	C5-C6	18.43	1.50	1.34
23	2K	21	U	C5-C6	16.94	1.49	1.34
26	1H	774	A	N9-C4	-14.63	1.29	1.37
26	14	783	A	N9-C4	-13.79	1.29	1.37
26	1H	783	A	N9-C4	-12.87	1.30	1.37

The worst 5 of 7504 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	1H	1899	G	N3-C4-N9	-26.68	109.99	126.00
26	1H	676	A	C2-N3-C4	-22.63	99.29	110.60
26	1H	2430	A	C2-N3-C4	-22.43	99.39	110.60
26	1H	1899	G	N3-C4-C5	21.40	139.30	128.60
26	1H	783	A	C2-N3-C4	-21.20	100.00	110.60

There are no chirality outliers.

5 of 142 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	1E	15	VAL	Peptide
4	3E	31	CYS	Peptide

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Mol	Chain	Res	Type	Group
12	3I	87	GLY	Peptide
15	6I	87	ILE	Peptide
19	AI	6	LYS	Peptide

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	13	32207	0	16256	882	0
1	1G	32182	0	16244	875	0
2	12	1924	0	1975	85	0
2	1E	1924	0	1975	103	0
3	22	1612	0	1677	79	0
3	2E	1605	0	1668	65	0
4	32	1703	0	1763	94	0
4	3E	1703	0	1762	100	0
5	42	1155	0	1213	62	0
5	4E	1155	0	1213	54	0
6	52	843	0	857	44	0
6	5E	843	0	857	39	0
7	62	1257	0	1296	62	0
7	6E	1257	0	1296	49	0
8	72	1116	0	1177	57	0
8	7E	1116	0	1177	64	0
9	82	1010	0	1037	76	0
9	8E	1010	0	1037	61	0
10	1A	801	0	849	43	0
10	1I	801	0	849	62	0
11	2A	885	0	904	40	0
11	2I	885	0	904	44	0
12	3A	975	0	1062	47	0
12	3I	975	0	1062	43	0
13	4A	933	0	992	66	0
13	4I	938	0	997	50	0
14	5A	476	0	511	30	0
14	5I	492	0	529	29	0
15	6A	734	0	771	25	0
15	6I	734	0	771	29	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
16	7A	705	0	725	43	0
16	7I	705	0	725	54	0
17	8A	834	0	904	25	0
17	8I	834	0	904	51	0
18	9A	591	0	662	27	0
18	9I	591	0	662	29	0
19	AA	624	0	636	47	0
19	AI	647	0	665	57	0
20	BA	763	0	861	45	0
20	BI	763	0	861	44	0
21	1B	217	0	234	11	0
21	1F	217	0	234	13	0
22	1K	1626	0	834	28	0
22	1L	1626	0	834	41	0
23	2K	1646	0	845	38	0
23	2L	1646	0	845	39	0
24	3K	1619	0	822	52	0
24	3L	1619	0	822	60	0
25	4K	301	0	153	11	0
25	4L	131	0	66	5	0
26	14	62647	0	31580	1604	1
26	1H	62707	0	31607	1779	1
27	16	2617	0	1328	71	0
27	1J	2617	0	1328	99	0
28	11	2120	0	2197	122	0
28	19	2120	0	2197	117	0
29	21	1568	0	1634	107	0
29	29	1568	0	1634	117	0
30	31	1585	0	1632	104	0
30	39	1627	0	1680	101	0
31	41	1473	0	1535	77	0
31	49	1473	0	1535	70	0
32	51	1336	0	1418	94	0
32	59	1307	0	1382	73	0
33	61	1136	0	1223	63	0
33	69	1136	0	1223	56	0
34	15	1104	0	1180	55	0
34	58	1104	0	1180	70	0
35	25	933	0	996	48	0
35	68	933	0	996	41	0
36	35	1145	0	1228	113	0
36	78	1145	0	1228	119	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
37	45	1122	0	1179	84	0
37	88	1087	0	1129	83	0
38	55	960	0	1021	65	0
38	98	968	0	1033	72	0
39	65	882	0	943	62	0
39	A8	882	0	943	67	0
40	75	1141	0	1202	67	0
40	B8	1141	0	1202	76	0
41	85	964	0	1022	54	0
41	C8	964	0	1022	65	0
42	95	779	0	852	66	0
42	D8	779	0	852	40	0
43	A5	900	0	964	34	0
43	E8	900	0	964	50	0
44	B5	730	0	780	32	0
44	F8	742	0	803	56	0
45	C5	794	0	884	58	0
45	G8	791	0	882	57	0
46	D5	1428	0	1454	88	0
46	H8	1397	0	1430	85	0
47	E5	613	0	633	48	0
47	I8	627	0	642	34	0
48	F5	763	0	848	32	0
48	J8	763	0	848	38	0
49	G5	558	0	610	32	1
49	K8	563	0	612	41	1
50	H5	469	0	518	16	0
50	L8	452	0	503	33	0
51	I5	515	0	514	40	0
51	M8	533	0	526	48	0
52	J5	459	0	480	32	0
52	N8	454	0	475	33	0
53	K5	389	0	404	21	0
53	O8	389	0	404	31	0
54	L5	398	0	441	19	0
54	P8	418	0	467	22	0
55	M5	477	0	540	47	0
55	Q8	480	0	549	132	0
56	11	4	0	0	0	0
56	13	151	0	0	0	0
56	14	389	0	0	0	0
56	16	13	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
56	1G	103	0	0	0	0
56	1H	529	0	0	0	0
56	1J	9	0	0	0	0
56	1K	2	0	0	0	0
56	2I	2	0	0	0	0
56	29	2	0	0	0	0
56	2K	3	0	0	0	0
56	2L	2	0	0	0	0
56	3I	1	0	0	0	0
56	35	1	0	0	0	0
56	3E	2	0	0	0	0
56	3I	1	0	0	0	0
56	4I	2	0	0	0	0
56	49	1	0	0	0	0
56	4A	1	0	0	0	0
56	5E	1	0	0	0	0
56	6A	1	0	0	0	0
56	75	1	0	0	0	0
56	78	2	0	0	0	0
56	85	1	0	0	0	0
56	88	2	0	0	0	0
56	98	1	0	0	0	0
56	AI	1	0	0	0	0
56	C5	1	0	0	0	0
56	C8	1	0	0	0	0
56	E8	1	0	0	0	0
56	F5	1	0	0	0	0
56	I8	2	0	0	0	0
56	J8	2	0	0	0	0
56	L8	1	0	0	0	0
56	P8	1	0	0	0	0
56	Q8	1	0	0	0	0
57	32	1	0	0	0	0
57	3E	1	0	0	0	0
57	5A	1	0	0	0	0
57	5I	1	0	0	0	0
57	C5	1	0	0	0	0
57	G8	1	0	0	0	0
58	11	9	0	0	0	0
58	13	212	0	0	36	0
58	14	730	0	0	169	0
58	16	16	0	0	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
58	19	11	0	0	0	0
58	1G	99	0	0	22	0
58	1H	1097	0	0	264	0
58	1I	2	0	0	0	0
58	1J	12	0	0	3	0
58	1K	1	0	0	0	0
58	21	5	0	0	3	0
58	29	6	0	0	0	0
58	31	10	0	0	0	0
58	39	7	0	0	0	0
58	3E	1	0	0	0	0
58	3I	1	0	0	0	0
58	3K	1	0	0	0	0
58	4E	2	0	0	0	0
58	4K	4	0	0	0	0
58	55	1	0	0	0	0
58	58	1	0	0	0	0
58	5I	2	0	0	0	0
58	78	4	0	0	0	0
58	7A	2	0	0	0	0
58	85	1	0	0	0	0
58	8E	2	0	0	0	0
58	98	1	0	0	0	0
58	A5	1	0	0	0	0
58	BA	1	0	0	0	0
58	C8	2	0	0	1	0
58	D8	1	0	0	0	0
58	E8	2	0	0	0	0
58	G8	3	0	0	0	0
58	H5	1	0	0	0	0
58	I8	6	0	0	0	0
58	L5	1	0	0	0	0
58	L8	2	0	0	0	0
58	P8	2	0	0	0	0
58	Q8	2	0	0	0	0
All	All	300537	0	200491	9898	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 21.

The worst 5 of 9898 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)
4:32:9:CYS:SG	4:32:31:CYS:HB2	1.81	1.19
26:1H:2714:G:OP2	58:1H:3670:HOH:O	1.68	1.11
26:14:2593:U:O4	58:14:4084:HOH:O	1.72	1.07
36:78:19:VAL:HG12	36:78:21:ARG:H	1.15	1.07
26:1H:1614:A:OP1	58:1H:3921:HOH:O	1.73	1.06

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)
49:K8:17:SER:OG	26:14:307:G:OP1[2_564]	1.99	0.21
26:1H:277:C:O2'	49:G5:49:LYS:NZ[2_564]	2.13	0.07

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	12	235/256 (92%)	194 (83%)	38 (16%)	3 (1%)	12	44
2	1E	235/256 (92%)	198 (84%)	35 (15%)	2 (1%)	17	53
3	22	204/239 (85%)	180 (88%)	24 (12%)	0	100	100
3	2E	203/239 (85%)	179 (88%)	23 (11%)	1 (0%)	29	65
4	32	206/209 (99%)	181 (88%)	24 (12%)	1 (0%)	29	65
4	3E	206/209 (99%)	190 (92%)	14 (7%)	2 (1%)	15	51
5	42	149/162 (92%)	141 (95%)	8 (5%)	0	100	100
5	4E	149/162 (92%)	139 (93%)	9 (6%)	1 (1%)	22	59
6	52	99/101 (98%)	95 (96%)	4 (4%)	0	100	100
6	5E	99/101 (98%)	91 (92%)	8 (8%)	0	100	100
7	62	153/156 (98%)	146 (95%)	6 (4%)	1 (1%)	22	59
7	6E	153/156 (98%)	142 (93%)	11 (7%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
8	72	136/138 (99%)	126 (93%)	8 (6%)	2 (2%)	10	41
8	7E	136/138 (99%)	124 (91%)	11 (8%)	1 (1%)	22	59
9	82	125/128 (98%)	111 (89%)	13 (10%)	1 (1%)	19	55
9	8E	125/128 (98%)	107 (86%)	18 (14%)	0	100	100
10	1A	97/105 (92%)	91 (94%)	6 (6%)	0	100	100
10	1I	97/105 (92%)	90 (93%)	7 (7%)	0	100	100
11	2A	117/129 (91%)	102 (87%)	12 (10%)	3 (3%)	5	28
11	2I	117/129 (91%)	103 (88%)	13 (11%)	1 (1%)	17	53
12	3A	123/132 (93%)	100 (81%)	18 (15%)	5 (4%)	3	18
12	3I	123/132 (93%)	105 (85%)	18 (15%)	0	100	100
13	4A	115/126 (91%)	94 (82%)	19 (16%)	2 (2%)	9	38
13	4I	116/126 (92%)	94 (81%)	22 (19%)	0	100	100
14	5A	56/61 (92%)	47 (84%)	8 (14%)	1 (2%)	8	37
14	5I	58/61 (95%)	47 (81%)	9 (16%)	2 (3%)	3	21
15	6A	86/89 (97%)	82 (95%)	4 (5%)	0	100	100
15	6I	86/89 (97%)	77 (90%)	9 (10%)	0	100	100
16	7A	82/88 (93%)	77 (94%)	5 (6%)	0	100	100
16	7I	82/88 (93%)	75 (92%)	6 (7%)	1 (1%)	13	46
17	8A	98/105 (93%)	91 (93%)	7 (7%)	0	100	100
17	8I	98/105 (93%)	93 (95%)	5 (5%)	0	100	100
18	9A	70/88 (80%)	65 (93%)	5 (7%)	0	100	100
18	9I	70/88 (80%)	62 (89%)	7 (10%)	1 (1%)	11	43
19	AA	76/93 (82%)	61 (80%)	13 (17%)	2 (3%)	5	28
19	AI	79/93 (85%)	65 (82%)	10 (13%)	4 (5%)	2	13
20	BA	97/106 (92%)	84 (87%)	11 (11%)	2 (2%)	7	33
20	BI	97/106 (92%)	82 (84%)	14 (14%)	1 (1%)	15	51
21	1B	23/27 (85%)	21 (91%)	2 (9%)	0	100	100
21	1F	23/27 (85%)	21 (91%)	2 (9%)	0	100	100
28	11	271/276 (98%)	252 (93%)	14 (5%)	5 (2%)	8	37
28	19	271/276 (98%)	252 (93%)	14 (5%)	5 (2%)	8	37
29	21	203/206 (98%)	161 (79%)	30 (15%)	12 (6%)	1	11

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
29	29	203/206 (98%)	156 (77%)	35 (17%)	12 (6%)	1	11
30	31	200/210 (95%)	183 (92%)	15 (8%)	2 (1%)	15	51
30	39	206/210 (98%)	159 (77%)	41 (20%)	6 (3%)	4	25
31	41	179/182 (98%)	159 (89%)	17 (10%)	3 (2%)	9	38
31	49	179/182 (98%)	158 (88%)	20 (11%)	1 (1%)	25	62
32	51	172/180 (96%)	148 (86%)	17 (10%)	7 (4%)	3	18
32	59	168/180 (93%)	129 (77%)	34 (20%)	5 (3%)	4	24
33	61	144/148 (97%)	117 (81%)	23 (16%)	4 (3%)	5	26
33	69	144/148 (97%)	119 (83%)	21 (15%)	4 (3%)	5	26
34	15	136/140 (97%)	124 (91%)	11 (8%)	1 (1%)	22	59
34	58	136/140 (97%)	116 (85%)	16 (12%)	4 (3%)	4	25
35	25	120/122 (98%)	111 (92%)	9 (8%)	0	100	100
35	68	120/122 (98%)	111 (92%)	8 (7%)	1 (1%)	19	55
36	35	148/150 (99%)	114 (77%)	28 (19%)	6 (4%)	3	18
36	78	148/150 (99%)	121 (82%)	21 (14%)	6 (4%)	3	18
37	45	139/141 (99%)	114 (82%)	23 (16%)	2 (1%)	11	43
37	88	134/141 (95%)	110 (82%)	18 (13%)	6 (4%)	2	16
38	55	115/118 (98%)	104 (90%)	9 (8%)	2 (2%)	9	38
38	98	116/118 (98%)	97 (84%)	18 (16%)	1 (1%)	17	53
39	65	109/112 (97%)	87 (80%)	18 (16%)	4 (4%)	3	19
39	A8	109/112 (97%)	90 (83%)	18 (16%)	1 (1%)	17	53
40	75	135/146 (92%)	119 (88%)	15 (11%)	1 (1%)	22	59
40	B8	135/146 (92%)	122 (90%)	13 (10%)	0	100	100
41	85	115/118 (98%)	99 (86%)	15 (13%)	1 (1%)	17	53
41	C8	115/118 (98%)	101 (88%)	10 (9%)	4 (4%)	3	21
42	95	99/101 (98%)	78 (79%)	16 (16%)	5 (5%)	2	13
42	D8	99/101 (98%)	94 (95%)	3 (3%)	2 (2%)	7	34
43	A5	111/113 (98%)	100 (90%)	11 (10%)	0	100	100
43	E8	111/113 (98%)	101 (91%)	10 (9%)	0	100	100
44	B5	91/96 (95%)	82 (90%)	8 (9%)	1 (1%)	14	48
44	F8	92/96 (96%)	84 (91%)	7 (8%)	1 (1%)	14	48

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
45	C5	102/110 (93%)	75 (74%)	22 (22%)	5 (5%)	2	14
45	G8	102/110 (93%)	82 (80%)	14 (14%)	6 (6%)	1	11
46	D5	177/206 (86%)	130 (73%)	37 (21%)	10 (6%)	2	12
46	H8	173/206 (84%)	136 (79%)	28 (16%)	9 (5%)	2	13
47	E5	75/85 (88%)	66 (88%)	8 (11%)	1 (1%)	12	44
47	I8	78/85 (92%)	65 (83%)	12 (15%)	1 (1%)	12	44
48	F5	95/98 (97%)	88 (93%)	6 (6%)	1 (1%)	14	48
48	J8	95/98 (97%)	86 (90%)	7 (7%)	2 (2%)	7	33
49	G5	64/72 (89%)	59 (92%)	3 (5%)	2 (3%)	4	23
49	K8	65/72 (90%)	60 (92%)	3 (5%)	2 (3%)	4	23
50	H5	57/60 (95%)	53 (93%)	4 (7%)	0	100	100
50	L8	55/60 (92%)	50 (91%)	4 (7%)	1 (2%)	8	37
51	I5	61/71 (86%)	34 (56%)	24 (39%)	3 (5%)	2	14
51	M8	64/71 (90%)	40 (62%)	21 (33%)	3 (5%)	2	15
52	J5	57/60 (95%)	50 (88%)	6 (10%)	1 (2%)	8	37
52	N8	56/60 (93%)	48 (86%)	6 (11%)	2 (4%)	3	20
53	K5	43/54 (80%)	26 (60%)	14 (33%)	3 (7%)	1	7
53	O8	43/54 (80%)	28 (65%)	13 (30%)	2 (5%)	2	15
54	L5	44/49 (90%)	42 (96%)	2 (4%)	0	100	100
54	P8	46/49 (94%)	45 (98%)	1 (2%)	0	100	100
55	M5	58/65 (89%)	47 (81%)	9 (16%)	2 (3%)	3	21
55	Q8	58/65 (89%)	31 (53%)	16 (28%)	11 (19%)	0	0
All	All	11340/12054 (94%)	9786 (86%)	1332 (12%)	222 (2%)	7	34

5 of 222 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	1E	237	ALA
18	9I	22	VAL
29	21	83	ASP
32	51	169	VAL
36	78	57	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	205/220 (93%)	169 (82%)	36 (18%)	2	9
2	1E	205/220 (93%)	152 (74%)	53 (26%)	0	2
3	22	160/188 (85%)	134 (84%)	26 (16%)	2	10
3	2E	159/188 (85%)	128 (80%)	31 (20%)	1	7
4	32	180/181 (99%)	144 (80%)	36 (20%)	1	6
4	3E	180/181 (99%)	138 (77%)	42 (23%)	1	3
5	42	116/123 (94%)	84 (72%)	32 (28%)	0	1
5	4E	116/123 (94%)	88 (76%)	28 (24%)	0	2
6	52	90/90 (100%)	71 (79%)	19 (21%)	1	5
6	5E	90/90 (100%)	78 (87%)	12 (13%)	4	17
7	62	126/127 (99%)	97 (77%)	29 (23%)	1	3
7	6E	126/127 (99%)	99 (79%)	27 (21%)	1	5
8	72	119/119 (100%)	91 (76%)	28 (24%)	1	3
8	7E	119/119 (100%)	95 (80%)	24 (20%)	1	6
9	82	98/99 (99%)	77 (79%)	21 (21%)	1	5
9	8E	98/99 (99%)	77 (79%)	21 (21%)	1	5
10	1A	89/92 (97%)	71 (80%)	18 (20%)	1	6
10	1I	89/92 (97%)	71 (80%)	18 (20%)	1	6
11	2A	90/99 (91%)	64 (71%)	26 (29%)	0	1
11	2I	90/99 (91%)	71 (79%)	19 (21%)	1	5
12	3A	104/109 (95%)	85 (82%)	19 (18%)	1	8
12	3I	104/109 (95%)	84 (81%)	20 (19%)	1	7
13	4A	94/101 (93%)	70 (74%)	24 (26%)	0	2
13	4I	94/101 (93%)	72 (77%)	22 (23%)	1	3
14	5A	48/50 (96%)	40 (83%)	8 (17%)	2	9
14	5I	49/50 (98%)	37 (76%)	12 (24%)	0	2

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
15	6A	79/80 (99%)	65 (82%)	14 (18%)	2	8
15	6I	79/80 (99%)	70 (89%)	9 (11%)	5	23
16	7A	72/74 (97%)	57 (79%)	15 (21%)	1	5
16	7I	72/74 (97%)	52 (72%)	20 (28%)	0	1
17	8A	95/97 (98%)	77 (81%)	18 (19%)	1	7
17	8I	95/97 (98%)	73 (77%)	22 (23%)	1	3
18	9A	63/77 (82%)	46 (73%)	17 (27%)	0	1
18	9I	63/77 (82%)	51 (81%)	12 (19%)	1	7
19	AA	67/80 (84%)	50 (75%)	17 (25%)	0	2
19	AI	70/80 (88%)	49 (70%)	21 (30%)	0	1
20	BA	76/82 (93%)	64 (84%)	12 (16%)	2	11
20	BI	76/82 (93%)	61 (80%)	15 (20%)	1	6
21	1B	20/22 (91%)	18 (90%)	2 (10%)	7	28
21	1F	20/22 (91%)	19 (95%)	1 (5%)	24	57
28	11	214/218 (98%)	167 (78%)	47 (22%)	1	4
28	19	214/218 (98%)	173 (81%)	41 (19%)	1	7
29	21	165/166 (99%)	122 (74%)	43 (26%)	0	2
29	29	165/166 (99%)	125 (76%)	40 (24%)	0	2
30	31	161/166 (97%)	127 (79%)	34 (21%)	1	5
30	39	165/166 (99%)	124 (75%)	41 (25%)	0	2
31	41	155/156 (99%)	125 (81%)	30 (19%)	1	7
31	49	155/156 (99%)	127 (82%)	28 (18%)	1	8
32	51	145/148 (98%)	111 (77%)	34 (23%)	1	3
32	59	142/148 (96%)	105 (74%)	37 (26%)	0	2
33	61	122/124 (98%)	95 (78%)	27 (22%)	1	4
33	69	122/124 (98%)	89 (73%)	33 (27%)	0	1
34	15	117/119 (98%)	94 (80%)	23 (20%)	1	6
34	58	117/119 (98%)	90 (77%)	27 (23%)	1	3
35	25	100/100 (100%)	78 (78%)	22 (22%)	1	4
35	68	100/100 (100%)	89 (89%)	11 (11%)	6	24
36	35	116/116 (100%)	76 (66%)	40 (34%)	0	0

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles		
36	78	116/116 (100%)	85 (73%)	31 (27%)	0	1	
37	45	111/111 (100%)	85 (77%)	26 (23%)	1	3	
37	88	104/111 (94%)	78 (75%)	26 (25%)	0	2	
38	55	100/101 (99%)	80 (80%)	20 (20%)	1	6	
38	98	101/101 (100%)	73 (72%)	28 (28%)	0	1	
39	65	87/88 (99%)	60 (69%)	27 (31%)	0	1	
39	A8	87/88 (99%)	63 (72%)	24 (28%)	0	1	
40	75	120/127 (94%)	81 (68%)	39 (32%)	0	0	
40	B8	120/127 (94%)	89 (74%)	31 (26%)	0	2	
41	85	93/94 (99%)	74 (80%)	19 (20%)	1	5	
41	C8	93/94 (99%)	76 (82%)	17 (18%)	1	8	
42	95	82/82 (100%)	64 (78%)	18 (22%)	1	4	
42	D8	82/82 (100%)	57 (70%)	25 (30%)	0	1	
43	A5	92/92 (100%)	69 (75%)	23 (25%)	0	2	
43	E8	92/92 (100%)	66 (72%)	26 (28%)	0	1	
44	B5	74/78 (95%)	50 (68%)	24 (32%)	0	0	
44	F8	76/78 (97%)	60 (79%)	16 (21%)	1	5	
45	C5	85/91 (93%)	59 (69%)	26 (31%)	0	1	
45	G8	85/91 (93%)	59 (69%)	26 (31%)	0	1	
46	D5	158/179 (88%)	119 (75%)	39 (25%)	0	2	
46	H8	154/179 (86%)	128 (83%)	26 (17%)	2	9	
47	E5	62/67 (92%)	51 (82%)	11 (18%)	2	8	
47	I8	61/67 (91%)	45 (74%)	16 (26%)	0	2	
48	F5	82/83 (99%)	67 (82%)	15 (18%)	1	8	
48	J8	82/83 (99%)	61 (74%)	21 (26%)	0	2	
49	G5	62/67 (92%)	46 (74%)	16 (26%)	0	2	
49	K8	62/67 (92%)	42 (68%)	20 (32%)	0	0	
50	H5	51/52 (98%)	38 (74%)	13 (26%)	0	2	
50	L8	49/52 (94%)	33 (67%)	16 (33%)	0	0	
51	I5	57/63 (90%)	46 (81%)	11 (19%)	1	7	
51	M8	59/63 (94%)	42 (71%)	17 (29%)	0	1	

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
52	J5	51/52 (98%)	40 (78%)	11 (22%)	1	5
52	N8	51/52 (98%)	39 (76%)	12 (24%)	1	3
53	K5	44/52 (85%)	36 (82%)	8 (18%)	1	8
53	O8	44/52 (85%)	30 (68%)	14 (32%)	0	0
54	L5	39/42 (93%)	31 (80%)	8 (20%)	1	5
54	P8	41/42 (98%)	31 (76%)	10 (24%)	0	2
55	M5	49/55 (89%)	37 (76%)	12 (24%)	0	2
55	Q8	50/55 (91%)	30 (60%)	20 (40%)	0	0
All	All	9568/9998 (96%)	7376 (77%)	2192 (23%)	1	4

5 of 2192 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
48	J8	93	GLU
5	42	115	VAL
45	C5	33	LYS
50	L8	17	LYS
2	12	55	PHE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 28 such sidechains are listed below:

Mol	Chain	Res	Type
38	98	13	HIS
44	F8	82	GLN
45	C5	92	ASN
43	E8	62	HIS
44	F8	31	HIS

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	13	1495/1522 (98%)	358 (23%)	29 (1%)
1	1G	1495/1522 (98%)	366 (24%)	36 (2%)
22	1K	74/76 (97%)	36 (48%)	1 (1%)
22	1L	74/76 (97%)	32 (43%)	3 (4%)
23	2K	76/77 (98%)	21 (27%)	3 (3%)
23	2L	76/77 (98%)	19 (25%)	4 (5%)

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Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
24	3K	75/76 (98%)	39 (52%)	8 (10%)
24	3L	75/76 (98%)	41 (54%)	3 (4%)
25	4K	13/30 (43%)	6 (46%)	1 (7%)
25	4L	6/30 (20%)	2 (33%)	1 (16%)
26	14	2908/2917 (99%)	777 (26%)	51 (1%)
26	1H	2911/2917 (99%)	743 (25%)	61 (2%)
27	16	121/122 (99%)	21 (17%)	1 (0%)
27	1J	121/122 (99%)	35 (28%)	2 (1%)
All	All	9520/9640 (98%)	2496 (26%)	204 (2%)

5 of 2496 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	13	5	U
1	13	6	G
1	13	8	A
1	13	9	G
1	13	28	G

5 of 204 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
26	1H	2225	A
1	1G	429	U
26	14	2335	A
26	1H	2307	G
27	16	108	C

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

16 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
23	7MG	2L	47	23	22,26,27	3.53	7 (31%)	28,39,42	2.50	11 (39%)
23	7MG	2K	47	23	22,26,27	3.54	7 (31%)	28,39,42	2.70	13 (46%)
23	5MU	2L	55	23	15,22,23	2.21	3 (20%)	16,32,35	1.82	2 (12%)
23	OMC	2L	33	23	15,22,23	2.18	4 (26%)	17,31,34	1.68	3 (17%)
23	4SU	2K	8	23	14,21,22	3.36	2 (14%)	15,30,33	0.79	1 (6%)
22	PSU	1K	32	22	17,21,22	4.06	6 (35%)	20,30,33	3.38	5 (25%)
23	PSU	2K	56	23	17,21,22	4.07	5 (29%)	20,30,33	2.96	6 (30%)
22	PSU	1L	39	22	17,21,22	4.05	7 (41%)	20,30,33	3.62	5 (25%)
22	MIA	1K	37	22	24,31,32	2.35	5 (20%)	26,44,47	2.31	6 (23%)
22	PSU	1K	39	22	17,21,22	3.77	5 (29%)	20,30,33	3.28	4 (20%)
23	PSU	2L	56	23	17,21,22	4.03	6 (35%)	20,30,33	3.24	5 (25%)
22	PSU	1L	32	22	17,21,22	3.76	6 (35%)	20,30,33	3.42	7 (35%)
23	4SU	2L	8	23	14,21,22	3.30	2 (14%)	15,30,33	0.97	2 (13%)
23	OMC	2K	33	23	15,22,23	2.02	4 (26%)	17,31,34	1.50	2 (11%)
22	MIA	1L	37	22	24,31,32	2.45	4 (16%)	26,44,47	3.41	10 (38%)
23	5MU	2K	55	56,23	15,22,23	2.22	3 (20%)	16,32,35	1.98	2 (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
23	7MG	2L	47	23	-	3/7/37/38	0/3/3/3
23	7MG	2K	47	23	-	1/7/37/38	0/3/3/3
23	5MU	2L	55	23	-	0/5/25/26	0/2/2/2
23	OMC	2L	33	23	-	1/7/27/28	0/2/2/2
23	4SU	2K	8	23	-	0/5/25/26	0/2/2/2
22	PSU	1K	32	22	-	0/7/25/26	0/2/2/2
23	PSU	2K	56	23	-	0/7/25/26	0/2/2/2
22	PSU	1L	39	22	-	0/7/25/26	0/2/2/2
22	MIA	1K	37	22	-	5/11/33/34	0/3/3/3
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	PSU	1L	32	22	-	0/7/25/26	0/2/2/2
23	4SU	2L	8	23	-	0/5/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
23	OMC	2K	33	23	-	0/7/27/28	0/2/2/2
22	MIA	1L	37	22	-	7/11/33/34	0/3/3/3
23	5MU	2K	55	56,23	-	0/5/25/26	0/2/2/2

The worst 5 of 76 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	2K	56	PSU	C5-C1'	-14.36	1.40	1.52
22	1K	32	PSU	C5-C1'	-13.86	1.40	1.52
22	1L	39	PSU	C5-C1'	-13.23	1.41	1.52
23	2L	56	PSU	C5-C1'	-13.01	1.41	1.52
22	1K	39	PSU	C5-C1'	-12.71	1.41	1.52

The worst 5 of 84 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	1L	39	PSU	N1-C2-N3	-13.00	118.10	128.43
22	1K	32	PSU	N1-C2-N3	-11.65	119.17	128.43
22	1L	32	PSU	N1-C2-N3	-11.65	119.17	128.43
22	1L	37	MIA	C11-S10-C2	11.25	110.67	102.27
22	1K	39	PSU	N1-C2-N3	-11.20	119.53	128.43

There are no chirality outliers.

5 of 17 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
23	2L	47	7MG	C3'-C4'-C5'-O5'
23	2L	33	OMC	C2'-C1'-N1-C6
22	1K	37	MIA	C5-C6-N6-C12
22	1K	37	MIA	N1-C2-S10-C11
22	1K	37	MIA	N3-C2-S10-C11

There are no ring outliers.

11 monomers are involved in 23 short contacts:

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

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
23	2K	56	PSU	1	0
22	1L	39	PSU	1	0
22	1K	37	MIA	2	0
23	2L	56	PSU	1	0
23	2L	8	4SU	1	0
23	2K	55	5MU	2	0

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 1245 ligands modelled in this entry, 1245 are monoatomic - leaving 0 for Mogul analysis.

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.

No monomer is involved in short contacts.

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
1	13	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	13	1530:G	O3'	1531:A	P	3.03

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	1498/1522 (98%)	-0.66	0 100 100	61, 110, 194, 290	0
1	1G	1497/1522 (98%)	-0.67	2 (0%) 95 95	73, 129, 204, 306	0
2	12	237/256 (92%)	0.59	28 (11%) 4 2	151, 185, 205, 218	0
2	1E	237/256 (92%)	0.42	25 (10%) 6 3	119, 155, 183, 193	0
3	22	206/239 (86%)	1.05	39 (18%) 1 0	149, 166, 190, 202	0
3	2E	205/239 (85%)	0.48	17 (8%) 11 6	98, 122, 159, 171	0
4	32	208/209 (99%)	0.60	16 (7%) 13 6	107, 128, 153, 160	0
4	3E	208/209 (99%)	0.50	18 (8%) 10 5	92, 123, 146, 155	0
5	42	151/162 (93%)	0.67	14 (9%) 8 5	118, 139, 159, 195	0
5	4E	151/162 (93%)	0.54	14 (9%) 8 5	88, 109, 135, 174	0
6	52	101/101 (100%)	0.53	10 (9%) 7 4	92, 115, 133, 160	0
6	5E	101/101 (100%)	0.40	3 (2%) 50 33	87, 110, 132, 154	0
7	62	155/156 (99%)	0.44	19 (12%) 4 2	124, 143, 178, 199	0
7	6E	155/156 (99%)	0.08	14 (9%) 9 5	110, 129, 160, 179	0
8	72	138/138 (100%)	0.30	7 (5%) 28 15	115, 145, 160, 163	0
8	7E	138/138 (100%)	0.47	10 (7%) 15 8	93, 118, 128, 142	0
9	82	127/128 (99%)	0.55	6 (4%) 31 17	123, 171, 189, 197	0
9	8E	127/128 (99%)	-0.07	0 100 100	94, 149, 170, 180	0
10	1A	99/105 (94%)	0.60	10 (10%) 7 3	139, 174, 192, 197	0
10	1I	99/105 (94%)	0.69	10 (10%) 7 3	90, 148, 181, 187	0
11	2A	119/129 (92%)	1.74	45 (37%) 0 0	94, 125, 152, 183	0
11	2I	119/129 (92%)	1.36	26 (21%) 0 0	77, 113, 153, 182	0
12	3A	125/132 (94%)	1.17	30 (24%) 0 0	91, 114, 144, 175	0
12	3I	125/132 (94%)	0.41	6 (4%) 30 17	74, 84, 117, 179	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
13	4A	117/126 (92%)	0.41	12 (10%) 6 3	127, 171, 192, 200	0
13	4I	118/126 (93%)	0.05	3 (2%) 57 42	86, 127, 148, 156	0
14	5A	58/61 (95%)	0.90	12 (20%) 1 0	152, 166, 179, 184	0
14	5I	60/61 (98%)	-0.21	2 (3%) 46 29	92, 113, 128, 135	0
15	6A	88/89 (98%)	0.08	1 (1%) 80 70	96, 125, 143, 148	0
15	6I	88/89 (98%)	0.36	5 (5%) 23 12	82, 104, 122, 129	0
16	7A	84/88 (95%)	0.11	2 (2%) 59 43	100, 117, 142, 174	0
16	7I	84/88 (95%)	-0.41	0 100 100	110, 126, 158, 174	0
17	8A	100/105 (95%)	0.08	2 (2%) 65 50	105, 122, 138, 160	0
17	8I	100/105 (95%)	0.39	5 (5%) 28 15	97, 114, 125, 129	0
18	9A	72/88 (81%)	1.55	21 (29%) 0 0	106, 128, 167, 178	0
18	9I	72/88 (81%)	1.18	18 (25%) 0 0	90, 113, 143, 175	0
19	AA	78/93 (83%)	0.65	11 (14%) 2 1	160, 189, 203, 207	0
19	AI	81/93 (87%)	0.56	12 (14%) 2 1	103, 127, 156, 165	0
20	BA	99/106 (93%)	0.09	3 (3%) 50 33	97, 118, 150, 162	0
20	BI	99/106 (93%)	-0.45	0 100 100	115, 131, 165, 172	0
21	1B	25/27 (92%)	0.16	0 100 100	125, 153, 169, 189	0
21	1F	25/27 (92%)	-0.74	0 100 100	100, 112, 127, 154	0
22	1K	73/76 (96%)	2.25	30 (41%) 0 0	97, 221, 259, 264	0
22	1L	73/76 (96%)	3.30	38 (52%) 0 0	134, 254, 277, 285	0
23	2K	72/77 (93%)	-0.41	1 (1%) 75 63	73, 95, 128, 139	0
23	2L	72/77 (93%)	-0.26	1 (1%) 75 63	87, 121, 153, 165	0
24	3K	76/76 (100%)	-0.07	4 (5%) 26 13	77, 253, 279, 282	0
24	3L	76/76 (100%)	0.43	6 (7%) 12 6	89, 259, 278, 280	0
25	4K	14/30 (46%)	-0.25	0 100 100	76, 107, 151, 155	0
25	4L	6/30 (20%)	-0.25	0 100 100	100, 108, 158, 161	0
26	14	2909/2917 (99%)	-0.33	38 (1%) 77 66	53, 91, 249, 335	0
26	1H	2912/2917 (99%)	-0.34	30 (1%) 82 73	40, 77, 231, 309	0
27	16	122/122 (100%)	-0.71	1 (0%) 86 78	69, 98, 122, 202	0
27	1J	122/122 (100%)	-0.66	1 (0%) 86 78	89, 133, 162, 212	0
28	11	273/276 (98%)	0.13	1 (0%) 92 89	43, 66, 84, 98	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
28	19	273/276 (98%)	0.08	1 (0%) 92 89	54, 80, 97, 112	0
29	21	205/206 (99%)	0.57	24 (11%) 4 2	49, 94, 143, 161	0
29	29	205/206 (99%)	0.65	25 (12%) 4 2	64, 99, 146, 173	0
30	31	202/210 (96%)	-0.10	2 (0%) 82 73	47, 80, 119, 141	0
30	39	208/210 (99%)	0.66	25 (12%) 4 2	60, 109, 170, 198	0
31	41	181/182 (99%)	0.72	20 (11%) 5 3	83, 109, 145, 156	0
31	49	181/182 (99%)	1.91	76 (41%) 0 0	127, 154, 181, 199	0
32	51	174/180 (96%)	0.54	13 (7%) 14 7	85, 109, 129, 142	0
32	59	170/180 (94%)	1.31	46 (27%) 0 0	155, 205, 228, 248	0
33	61	146/148 (98%)	0.43	12 (8%) 11 6	80, 139, 157, 163	0
33	69	146/148 (98%)	0.81	25 (17%) 1 1	88, 135, 157, 168	0
34	15	138/140 (98%)	0.51	8 (5%) 23 12	85, 116, 149, 165	0
34	58	138/140 (98%)	0.18	6 (4%) 35 21	69, 95, 137, 156	0
35	25	122/122 (100%)	0.52	3 (2%) 57 42	73, 93, 108, 124	0
35	68	122/122 (100%)	0.33	2 (1%) 72 59	61, 80, 99, 112	0
36	35	150/150 (100%)	0.90	29 (19%) 1 0	62, 113, 145, 183	0
36	78	150/150 (100%)	0.28	10 (6%) 17 9	49, 85, 116, 166	0
37	45	141/141 (100%)	0.66	18 (12%) 3 2	81, 111, 145, 155	0
37	88	138/141 (97%)	0.11	3 (2%) 62 47	56, 83, 107, 138	0
38	55	117/118 (99%)	0.09	3 (2%) 56 40	64, 84, 99, 117	0
38	98	118/118 (100%)	0.28	2 (1%) 70 57	63, 87, 109, 120	0
39	65	111/112 (99%)	0.65	14 (12%) 3 2	98, 128, 148, 162	0
39	A8	111/112 (99%)	0.27	5 (4%) 33 19	75, 94, 123, 133	0
40	75	137/146 (93%)	0.13	4 (2%) 51 35	83, 101, 161, 195	0
40	B8	137/146 (93%)	-0.20	2 (1%) 73 61	76, 97, 154, 179	0
41	85	117/118 (99%)	0.45	7 (5%) 21 11	73, 104, 150, 174	0
41	C8	117/118 (99%)	0.04	2 (1%) 70 57	56, 82, 115, 134	0
42	95	101/101 (100%)	0.94	18 (17%) 1 1	71, 134, 155, 175	0
42	D8	101/101 (100%)	0.62	13 (12%) 3 2	61, 111, 141, 155	0
43	A5	113/113 (100%)	0.10	1 (0%) 84 75	66, 80, 117, 174	0
43	E8	113/113 (100%)	0.00	4 (3%) 44 27	58, 76, 112, 159	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
44	B5	93/96 (96%)	0.28	5 (5%) 25 13	71, 89, 113, 121	0
44	F8	94/96 (97%)	0.23	5 (5%) 26 13	56, 73, 97, 117	0
45	C5	104/110 (94%)	1.18	20 (19%) 1 0	89, 122, 160, 166	0
45	G8	104/110 (94%)	0.66	5 (4%) 30 17	75, 98, 142, 149	0
46	D5	179/206 (86%)	2.07	78 (43%) 0 0	124, 161, 240, 246	0
46	H8	175/206 (84%)	0.47	15 (8%) 10 5	86, 128, 212, 218	0
47	E5	77/85 (90%)	0.75	6 (7%) 13 6	77, 96, 116, 162	0
47	I8	80/85 (94%)	0.05	2 (2%) 57 42	58, 77, 114, 117	0
48	F5	97/98 (98%)	0.97	13 (13%) 3 2	63, 89, 143, 161	0
48	J8	97/98 (98%)	0.55	10 (10%) 6 3	54, 77, 128, 161	0
49	G5	66/72 (91%)	0.50	3 (4%) 33 19	89, 112, 130, 148	0
49	K8	67/72 (93%)	-0.00	1 (1%) 73 61	65, 81, 99, 132	0
50	H5	59/60 (98%)	0.82	5 (8%) 10 5	80, 109, 155, 173	0
50	L8	57/60 (95%)	0.59	3 (5%) 26 13	64, 83, 112, 120	0
51	I5	63/71 (88%)	3.80	45 (71%) 0 0	167, 206, 219, 221	0
51	M8	66/71 (92%)	1.61	22 (33%) 0 0	114, 161, 192, 200	0
52	J5	59/60 (98%)	0.17	3 (5%) 28 15	66, 91, 159, 212	0
52	N8	58/60 (96%)	0.70	7 (12%) 4 2	53, 100, 178, 183	0
53	K5	45/54 (83%)	6.24	42 (93%) 0 0	141, 181, 194, 201	0
53	O8	45/54 (83%)	4.71	42 (93%) 0 0	117, 148, 168, 171	0
54	L5	46/49 (93%)	-0.18	0 100 100	53, 63, 75, 87	0
54	P8	48/49 (97%)	-0.26	0 100 100	46, 51, 88, 113	0
55	M5	60/65 (92%)	0.30	2 (3%) 46 29	73, 86, 108, 133	0
55	Q8	60/65 (92%)	0.13	1 (1%) 70 57	61, 73, 104, 119	0
All	All	21056/21694 (97%)	0.13	1387 (6%) 18 10	40, 109, 201, 335	0

The worst 5 of 1387 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
26	14	2901	C	18.3
53	K5	13	CYS	17.4
53	K5	51	GLU	15.2
52	N8	60	VAL	14.4
22	1L	3	C	14.3

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

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
22	PSU	1L	39	20/21	0.86	0.20	113,140,153,154	0
23	4SU	2L	8	20/21	0.88	0.20	124,129,135,138	0
23	PSU	2L	56	20/21	0.90	0.11	121,128,134,135	0
22	PSU	1L	32	20/21	0.91	0.16	139,147,158,158	0
22	PSU	1K	32	20/21	0.92	0.12	112,119,129,131	0
22	PSU	1K	39	20/21	0.93	0.15	90,106,111,114	0
23	PSU	2K	56	20/21	0.93	0.10	97,104,114,116	0
22	MIA	1L	37	29/30	0.93	0.16	121,132,138,150	0
22	MIA	1K	37	29/30	0.94	0.18	88,98,114,119	0
23	4SU	2K	8	20/21	0.94	0.15	86,95,103,110	0
23	5MU	2L	55	21/22	0.95	0.11	126,131,137,141	0
23	OMC	2L	33	21/22	0.95	0.14	105,111,114,116	0
23	7MG	2K	47	24/25	0.95	0.11	97,107,122,130	0
23	5MU	2K	55	21/22	0.95	0.12	99,108,119,128	0
23	7MG	2L	47	24/25	0.97	0.11	130,140,145,148	0
23	OMC	2K	33	21/22	0.97	0.16	79,84,93,100	0

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 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	MG	6A	101	1/1	0.15	0.33	126,126,126,126	0
56	MG	14	3218	1/1	0.17	0.51	82,82,82,82	0
56	MG	13	1704	1/1	0.30	1.41	95,95,95,95	0
56	MG	13	1702	1/1	0.36	0.14	112,112,112,112	0
56	MG	13	1616	1/1	0.36	0.36	98,98,98,98	0
56	MG	75	201	1/1	0.37	0.34	108,108,108,108	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	1G	1669	1/1	0.40	0.65	103,103,103,103	0
56	MG	1H	3327	1/1	0.40	0.44	110,110,110,110	0
56	MG	1H	3279	1/1	0.41	0.48	100,100,100,100	0
56	MG	13	1732	1/1	0.43	0.11	132,132,132,132	0
56	MG	14	3197	1/1	0.43	0.42	94,94,94,94	0
56	MG	1G	1641	1/1	0.44	0.17	121,121,121,121	0
56	MG	1H	3182	1/1	0.44	0.67	82,82,82,82	0
56	MG	1H	3324	1/1	0.46	0.17	93,93,93,93	0
56	MG	13	1680	1/1	0.48	0.81	97,97,97,97	0
56	MG	1H	3059	1/1	0.49	0.71	63,63,63,63	0
56	MG	1G	1624	1/1	0.49	0.55	85,85,85,85	0
56	MG	1H	3294	1/1	0.51	0.24	122,122,122,122	0
56	MG	1H	3328	1/1	0.52	0.34	86,86,86,86	0
56	MG	1H	3127	1/1	0.52	0.43	84,84,84,84	0
56	MG	14	3219	1/1	0.52	1.15	89,89,89,89	0
56	MG	1H	3290	1/1	0.52	0.61	94,94,94,94	0
56	MG	29	302	1/1	0.53	0.51	85,85,85,85	0
56	MG	13	1708	1/1	0.53	0.14	116,116,116,116	0
56	MG	13	1710	1/1	0.54	0.13	125,125,125,125	0
56	MG	14	3255	1/1	0.54	0.67	94,94,94,94	0
56	MG	14	3240	1/1	0.54	1.67	103,103,103,103	0
56	MG	2L	102	1/1	0.54	0.74	103,103,103,103	0
56	MG	14	3114	1/1	0.55	0.48	72,72,72,72	0
56	MG	1H	3332	1/1	0.56	0.34	138,138,138,138	0
56	MG	14	3235	1/1	0.56	0.25	76,76,76,76	0
56	MG	13	1705	1/1	0.56	0.24	138,138,138,138	0
56	MG	1G	1620	1/1	0.56	0.36	111,111,111,111	0
56	MG	14	3258	1/1	0.57	0.28	90,90,90,90	0
56	MG	1H	3223	1/1	0.57	0.25	69,69,69,69	0
56	MG	13	1619	1/1	0.58	0.22	82,82,82,82	0
56	MG	13	1685	1/1	0.58	0.32	123,123,123,123	0
56	MG	14	3109	1/1	0.59	0.84	85,85,85,85	0
56	MG	1G	1685	1/1	0.59	0.17	139,139,139,139	0
56	MG	1H	3230	1/1	0.60	0.45	66,66,66,66	0
56	MG	13	1648	1/1	0.60	0.47	89,89,89,89	0
56	MG	14	3249	1/1	0.60	0.32	69,69,69,69	0
56	MG	1H	3297	1/1	0.60	0.21	80,80,80,80	0
56	MG	1H	3300	1/1	0.60	0.26	90,90,90,90	0
56	MG	1G	1612	1/1	0.60	0.18	94,94,94,94	0
56	MG	1G	1674	1/1	0.60	0.10	94,94,94,94	0
56	MG	14	3037	1/1	0.61	0.38	103,103,103,103	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	1G	1651	1/1	0.62	0.14	102,102,102,102	0
56	MG	1G	1678	1/1	0.62	0.22	114,114,114,114	0
56	MG	14	3096	1/1	0.62	0.66	78,78,78,78	0
56	MG	1H	3312	1/1	0.62	0.26	82,82,82,82	0
56	MG	16	209	1/1	0.62	0.26	90,90,90,90	0
56	MG	1H	3285	1/1	0.63	0.50	89,89,89,89	0
56	MG	1G	1619	1/1	0.64	0.21	130,130,130,130	0
56	MG	14	3119	1/1	0.65	0.54	88,88,88,88	0
56	MG	1H	3267	1/1	0.65	0.25	84,84,84,84	0
56	MG	1H	3333	1/1	0.65	0.60	99,99,99,99	0
56	MG	1G	1670	1/1	0.65	0.43	98,98,98,98	0
57	ZN	C5	202	1/1	0.65	0.12	181,181,181,181	0
56	MG	1H	3291	1/1	0.66	0.36	71,71,71,71	0
56	MG	14	3204	1/1	0.66	0.26	126,126,126,126	0
56	MG	13	1668	1/1	0.66	0.26	111,111,111,111	0
56	MG	13	1701	1/1	0.66	0.42	103,103,103,103	0
57	ZN	G8	201	1/1	0.66	0.46	188,188,188,188	0
56	MG	1G	1655	1/1	0.67	0.22	124,124,124,124	0
56	MG	1H	3296	1/1	0.67	0.68	81,81,81,81	0
56	MG	1H	3184	1/1	0.67	0.48	94,94,94,94	0
56	MG	1G	1677	1/1	0.67	0.45	106,106,106,106	0
56	MG	13	1695	1/1	0.67	0.12	88,88,88,88	0
56	MG	1H	3493	1/1	0.67	0.09	113,113,113,113	0
56	MG	1H	3120	1/1	0.67	0.18	68,68,68,68	0
56	MG	13	1696	1/1	0.67	0.23	137,137,137,137	0
56	MG	1H	3473	1/1	0.68	0.11	92,92,92,92	0
56	MG	1H	3148	1/1	0.68	0.38	47,47,47,47	0
56	MG	1G	1656	1/1	0.68	0.37	102,102,102,102	0
56	MG	14	3192	1/1	0.68	0.58	85,85,85,85	0
56	MG	1H	3304	1/1	0.68	0.28	79,79,79,79	0
56	MG	13	1743	1/1	0.68	0.05	156,156,156,156	0
56	MG	1H	3216	1/1	0.68	0.58	68,68,68,68	0
56	MG	1H	3225	1/1	0.69	0.34	79,79,79,79	0
56	MG	13	1671	1/1	0.69	0.27	110,110,110,110	0
56	MG	1H	3377	1/1	0.69	0.06	100,100,100,100	0
56	MG	3E	302	1/1	0.69	0.08	125,125,125,125	0
56	MG	14	3199	1/1	0.69	1.10	84,84,84,84	0
56	MG	13	1689	1/1	0.69	0.38	97,97,97,97	0
56	MG	1G	1654	1/1	0.69	0.56	86,86,86,86	0
56	MG	78	202	1/1	0.69	0.32	78,78,78,78	0
56	MG	C5	201	1/1	0.70	0.21	102,102,102,102	0
56	MG	1G	1684	1/1	0.70	0.15	113,113,113,113	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	1H	3106	1/1	0.70	0.20	78,78,78,78	0
56	MG	1H	3259	1/1	0.70	0.54	115,115,115,115	0
56	MG	1H	3292	1/1	0.70	0.72	79,79,79,79	0
56	MG	1H	3203	1/1	0.70	0.29	76,76,76,76	0
56	MG	1H	3282	1/1	0.70	0.46	68,68,68,68	0
56	MG	1H	3227	1/1	0.70	0.55	93,93,93,93	0
56	MG	14	3257	1/1	0.71	0.52	99,99,99,99	0
56	MG	14	3067	1/1	0.71	0.69	84,84,84,84	0
56	MG	AI	101	1/1	0.71	0.15	119,119,119,119	0
56	MG	13	1709	1/1	0.71	0.27	127,127,127,127	0
56	MG	1H	3318	1/1	0.71	0.18	86,86,86,86	0
56	MG	13	1636	1/1	0.71	0.14	93,93,93,93	0
56	MG	14	3082	1/1	0.71	0.37	97,97,97,97	0
56	MG	14	3036	1/1	0.71	0.59	68,68,68,68	0
56	MG	1G	1622	1/1	0.71	0.34	90,90,90,90	0
56	MG	13	1694	1/1	0.71	0.50	95,95,95,95	0
56	MG	13	1646	1/1	0.71	0.26	100,100,100,100	0
56	MG	1G	1636	1/1	0.71	0.31	94,94,94,94	0
56	MG	1H	3019	1/1	0.72	0.17	71,71,71,71	0
56	MG	13	1677	1/1	0.72	0.34	109,109,109,109	0
56	MG	1H	3244	1/1	0.72	0.22	89,89,89,89	0
56	MG	1H	3431	1/1	0.72	0.07	117,117,117,117	0
56	MG	1G	1682	1/1	0.72	0.66	102,102,102,102	0
56	MG	3E	301	1/1	0.72	0.19	128,128,128,128	0
56	MG	14	3245	1/1	0.72	0.40	84,84,84,84	0
56	MG	1G	1648	1/1	0.72	0.21	115,115,115,115	0
56	MG	13	1674	1/1	0.72	0.43	95,95,95,95	0
56	MG	13	1681	1/1	0.73	0.57	83,83,83,83	0
56	MG	14	3189	1/1	0.73	0.86	86,86,86,86	0
56	MG	4A	201	1/1	0.73	0.40	115,115,115,115	0
56	MG	1J	206	1/1	0.73	0.28	91,91,91,91	0
56	MG	1H	3183	1/1	0.73	0.21	76,76,76,76	0
56	MG	14	3201	1/1	0.73	0.52	86,86,86,86	0
56	MG	1H	3226	1/1	0.73	0.51	97,97,97,97	0
56	MG	11	304	1/1	0.73	0.70	68,68,68,68	0
56	MG	14	3361	1/1	0.73	0.07	115,115,115,115	0
56	MG	1H	3264	1/1	0.73	0.30	76,76,76,76	0
56	MG	14	3181	1/1	0.73	0.96	86,86,86,86	0
56	MG	13	1712	1/1	0.73	0.29	114,114,114,114	0
56	MG	14	3128	1/1	0.73	0.83	98,98,98,98	0
56	MG	14	3328	1/1	0.73	0.15	98,98,98,98	0
56	MG	14	3239	1/1	0.74	0.26	88,88,88,88	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	J8	102	1/1	0.74	0.31	66,66,66,66	0
56	MG	14	3193	1/1	0.74	0.44	74,74,74,74	0
56	MG	1H	3248	1/1	0.74	0.15	81,81,81,81	0
56	MG	14	3217	1/1	0.74	0.30	88,88,88,88	0
56	MG	1G	1639	1/1	0.74	0.39	99,99,99,99	0
56	MG	1H	3124	1/1	0.74	0.32	89,89,89,89	0
56	MG	1H	3489	1/1	0.74	0.14	86,86,86,86	0
56	MG	14	3371	1/1	0.74	0.08	108,108,108,108	0
56	MG	1H	3397	1/1	0.74	0.10	96,96,96,96	0
56	MG	14	3215	1/1	0.74	0.43	111,111,111,111	0
56	MG	1H	3286	1/1	0.74	0.70	91,91,91,91	0
56	MG	1G	1680	1/1	0.74	1.13	107,107,107,107	0
56	MG	14	3336	1/1	0.74	0.09	123,123,123,123	0
56	MG	14	3208	1/1	0.74	0.37	94,94,94,94	0
56	MG	1H	3176	1/1	0.74	0.65	90,90,90,90	0
56	MG	14	3253	1/1	0.74	0.47	86,86,86,86	0
56	MG	14	3252	1/1	0.74	0.53	117,117,117,117	0
56	MG	14	3196	1/1	0.75	0.27	91,91,91,91	0
56	MG	14	3228	1/1	0.75	0.06	192,192,192,192	0
56	MG	14	3148	1/1	0.75	0.46	75,75,75,75	0
56	MG	1H	3198	1/1	0.75	0.32	71,71,71,71	0
56	MG	1G	1628	1/1	0.75	0.47	76,76,76,76	0
56	MG	1H	3205	1/1	0.75	0.42	80,80,80,80	0
56	MG	1H	3095	1/1	0.75	0.32	78,78,78,78	0
56	MG	1H	3186	1/1	0.75	0.50	89,89,89,89	0
56	MG	1H	3255	1/1	0.75	0.33	68,68,68,68	0
56	MG	13	1610	1/1	0.75	0.40	72,72,72,72	0
56	MG	14	3117	1/1	0.76	0.44	84,84,84,84	0
56	MG	16	203	1/1	0.76	0.10	91,91,91,91	0
56	MG	1H	3268	1/1	0.76	1.00	80,80,80,80	0
56	MG	14	3028	1/1	0.76	0.36	81,81,81,81	0
56	MG	1G	1653	1/1	0.76	0.32	91,91,91,91	0
56	MG	1H	3335	1/1	0.76	0.41	97,97,97,97	0
56	MG	1G	1658	1/1	0.76	0.32	96,96,96,96	0
56	MG	14	3154	1/1	0.76	0.14	79,79,79,79	0
56	MG	14	3171	1/1	0.76	0.90	91,91,91,91	0
56	MG	1H	3067	1/1	0.76	0.41	74,74,74,74	0
56	MG	1H	3287	1/1	0.77	0.17	85,85,85,85	0
56	MG	14	3113	1/1	0.77	0.62	96,96,96,96	0
56	MG	13	1665	1/1	0.77	0.40	86,86,86,86	0
56	MG	16	206	1/1	0.77	0.29	76,76,76,76	0
56	MG	1H	3491	1/1	0.77	0.05	121,121,121,121	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	13	1699	1/1	0.77	0.24	98,98,98,98	0
56	MG	1H	3275	1/1	0.77	0.23	94,94,94,94	0
56	MG	1H	3047	1/1	0.77	0.25	71,71,71,71	0
56	MG	16	205	1/1	0.77	0.45	88,88,88,88	0
56	MG	14	3360	1/1	0.77	0.28	112,112,112,112	0
56	MG	14	3116	1/1	0.77	0.18	77,77,77,77	0
56	MG	1H	3179	1/1	0.77	0.27	59,59,59,59	0
56	MG	1G	1652	1/1	0.77	0.62	86,86,86,86	0
56	MG	1G	1668	1/1	0.77	0.23	116,116,116,116	0
56	MG	13	1737	1/1	0.77	0.05	122,122,122,122	0
56	MG	14	3110	1/1	0.77	0.51	88,88,88,88	0
56	MG	14	3214	1/1	0.78	0.73	81,81,81,81	0
56	MG	1H	3090	1/1	0.78	0.33	66,66,66,66	0
56	MG	1H	3243	1/1	0.78	0.62	88,88,88,88	0
56	MG	1H	3199	1/1	0.78	0.47	86,86,86,86	0
56	MG	1H	3269	1/1	0.78	0.40	99,99,99,99	0
56	MG	1G	1640	1/1	0.78	0.20	99,99,99,99	0
56	MG	1H	3281	1/1	0.78	0.30	60,60,60,60	0
56	MG	13	1623	1/1	0.78	0.42	85,85,85,85	0
56	MG	1H	3266	1/1	0.78	0.47	75,75,75,75	0
56	MG	1H	3232	1/1	0.78	0.15	90,90,90,90	0
56	MG	13	1683	1/1	0.78	0.31	78,78,78,78	0
56	MG	13	1688	1/1	0.78	0.15	102,102,102,102	0
56	MG	1H	3236	1/1	0.78	0.41	78,78,78,78	0
56	MG	1G	1607	1/1	0.78	0.29	92,92,92,92	0
56	MG	13	1678	1/1	0.78	0.19	110,110,110,110	0
56	MG	1H	3307	1/1	0.79	0.46	80,80,80,80	0
56	MG	P8	101	1/1	0.79	0.40	70,70,70,70	0
56	MG	1H	3247	1/1	0.79	0.38	65,65,65,65	0
56	MG	1H	3293	1/1	0.79	0.51	82,82,82,82	0
56	MG	13	1711	1/1	0.79	0.16	109,109,109,109	0
56	MG	1H	3252	1/1	0.79	0.38	83,83,83,83	0
56	MG	13	1741	1/1	0.79	0.04	138,138,138,138	0
56	MG	1H	3386	1/1	0.79	0.12	58,58,58,58	0
56	MG	14	3167	1/1	0.79	0.41	71,71,71,71	0
56	MG	1H	3301	1/1	0.79	0.54	84,84,84,84	0
56	MG	14	3195	1/1	0.79	0.99	96,96,96,96	0
56	MG	1G	1664	1/1	0.80	0.51	88,88,88,88	0
56	MG	16	207	1/1	0.80	0.36	87,87,87,87	0
56	MG	13	1670	1/1	0.80	0.40	92,92,92,92	0
56	MG	13	1640	1/1	0.80	0.10	95,95,95,95	0
56	MG	88	202	1/1	0.80	0.38	69,69,69,69	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	1H	3028	1/1	0.80	0.24	77,77,77,77	0
56	MG	14	3203	1/1	0.80	0.92	111,111,111,111	0
56	MG	1H	3289	1/1	0.80	0.45	77,77,77,77	0
56	MG	1H	3428	1/1	0.80	0.16	100,100,100,100	0
56	MG	13	1746	1/1	0.80	0.06	127,127,127,127	0
56	MG	1H	3121	1/1	0.80	0.61	88,88,88,88	0
56	MG	14	3334	1/1	0.80	0.09	116,116,116,116	0
56	MG	1G	1662	1/1	0.80	0.35	100,100,100,100	0
56	MG	1H	3274	1/1	0.80	0.47	87,87,87,87	0
56	MG	1H	3284	1/1	0.80	0.08	190,190,190,190	0
56	MG	14	3093	1/1	0.81	0.47	63,63,63,63	0
56	MG	1G	1661	1/1	0.81	1.07	87,87,87,87	0
56	MG	1H	3508	1/1	0.81	0.08	96,96,96,96	0
56	MG	1H	3174	1/1	0.81	0.19	78,78,78,78	0
56	MG	13	1707	1/1	0.81	0.11	104,104,104,104	0
56	MG	14	3243	1/1	0.81	0.87	81,81,81,81	0
56	MG	2K	101	1/1	0.81	0.34	86,86,86,86	0
56	MG	13	1687	1/1	0.81	0.90	79,79,79,79	0
56	MG	85	201	1/1	0.81	0.62	87,87,87,87	0
56	MG	14	3367	1/1	0.81	0.17	92,92,92,92	0
56	MG	14	3175	1/1	0.81	0.12	88,88,88,88	0
56	MG	14	3190	1/1	0.81	0.44	77,77,77,77	0
56	MG	Q8	101	1/1	0.81	0.21	53,53,53,53	0
56	MG	13	1682	1/1	0.81	0.50	92,92,92,92	0
56	MG	1H	3331	1/1	0.81	0.73	74,74,74,74	0
56	MG	14	3209	1/1	0.81	0.13	71,71,71,71	0
56	MG	14	3241	1/1	0.81	0.60	90,90,90,90	0
56	MG	1H	3330	1/1	0.81	0.40	94,94,94,94	0
56	MG	14	3188	1/1	0.81	0.24	83,83,83,83	0
56	MG	1H	3380	1/1	0.81	0.07	82,82,82,82	0
56	MG	13	1667	1/1	0.81	0.64	87,87,87,87	0
56	MG	14	3182	1/1	0.81	0.32	152,152,152,152	0
56	MG	13	1657	1/1	0.82	0.06	87,87,87,87	0
56	MG	1H	3295	1/1	0.82	0.24	94,94,94,94	0
56	MG	1H	3108	1/1	0.82	0.37	58,58,58,58	0
56	MG	13	1742	1/1	0.82	0.07	102,102,102,102	0
56	MG	14	3104	1/1	0.82	0.59	86,86,86,86	0
56	MG	14	3123	1/1	0.82	0.35	82,82,82,82	0
56	MG	1H	3214	1/1	0.82	0.26	79,79,79,79	0
56	MG	13	1649	1/1	0.82	0.37	79,79,79,79	0
56	MG	1H	3202	1/1	0.82	0.22	80,80,80,80	0
56	MG	1H	3138	1/1	0.82	0.46	69,69,69,69	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	1G	1613	1/1	0.82	1.03	87,87,87,87	0
56	MG	14	3132	1/1	0.82	0.26	75,75,75,75	0
56	MG	13	1679	1/1	0.82	0.18	95,95,95,95	0
56	MG	1G	1627	1/1	0.82	0.74	77,77,77,77	0
56	MG	1G	1665	1/1	0.82	0.59	104,104,104,104	0
56	MG	14	3068	1/1	0.82	0.31	73,73,73,73	0
56	MG	13	1639	1/1	0.82	0.33	98,98,98,98	0
56	MG	1H	3470	1/1	0.82	0.08	98,98,98,98	0
56	MG	1H	3135	1/1	0.82	0.48	68,68,68,68	0
56	MG	14	3142	1/1	0.83	0.65	73,73,73,73	0
56	MG	14	3330	1/1	0.83	0.05	104,104,104,104	0
56	MG	14	3187	1/1	0.83	0.71	62,62,62,62	0
56	MG	14	3118	1/1	0.83	0.46	92,92,92,92	0
56	MG	14	3282	1/1	0.83	0.08	92,92,92,92	0
56	MG	1H	3170	1/1	0.83	0.49	86,86,86,86	0
56	MG	1H	3466	1/1	0.83	0.07	106,106,106,106	0
56	MG	1H	3499	1/1	0.83	0.12	77,77,77,77	0
56	MG	1G	1673	1/1	0.83	0.38	138,138,138,138	0
56	MG	1H	3270	1/1	0.83	0.36	106,106,106,106	0
56	MG	1H	3404	1/1	0.83	0.09	86,86,86,86	0
56	MG	1H	3218	1/1	0.83	0.40	76,76,76,76	0
56	MG	14	3358	1/1	0.83	0.07	117,117,117,117	0
56	MG	1H	3165	1/1	0.83	0.30	68,68,68,68	0
56	MG	14	3232	1/1	0.83	0.98	109,109,109,109	0
56	MG	1H	3118	1/1	0.83	0.34	93,93,93,93	0
56	MG	14	3160	1/1	0.83	0.58	88,88,88,88	0
56	MG	14	3312	1/1	0.83	0.08	97,97,97,97	0
56	MG	1H	3105	1/1	0.83	0.75	68,68,68,68	0
56	MG	1H	3082	1/1	0.83	0.53	64,64,64,64	0
56	MG	1G	1630	1/1	0.83	0.62	76,76,76,76	0
56	MG	1G	1681	1/1	0.83	0.32	106,106,106,106	0
56	MG	1H	3143	1/1	0.83	0.27	68,68,68,68	0
56	MG	1H	3022	1/1	0.83	0.52	78,78,78,78	0
56	MG	14	3052	1/1	0.83	0.78	74,74,74,74	0
56	MG	14	3385	1/1	0.83	0.23	113,113,113,113	0
56	MG	1G	1701	1/1	0.83	0.09	128,128,128,128	0
56	MG	14	3231	1/1	0.83	0.41	77,77,77,77	0
56	MG	13	1615	1/1	0.84	0.31	103,103,103,103	0
56	MG	14	3130	1/1	0.84	0.39	75,75,75,75	0
56	MG	14	3226	1/1	0.84	0.36	83,83,83,83	0
56	MG	1G	1642	1/1	0.84	0.48	110,110,110,110	0
56	MG	1H	3068	1/1	0.84	0.29	67,67,67,67	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	13	1622	1/1	0.84	0.44	85,85,85,85	0
56	MG	11	302	1/1	0.84	0.26	82,82,82,82	0
56	MG	1H	3133	1/1	0.84	0.26	61,61,61,61	0
56	MG	1H	3026	1/1	0.84	0.51	85,85,85,85	0
56	MG	98	201	1/1	0.84	0.51	99,99,99,99	0
56	MG	14	3099	1/1	0.84	0.30	68,68,68,68	0
56	MG	1G	1699	1/1	0.84	0.11	122,122,122,122	0
56	MG	14	3216	1/1	0.84	0.55	70,70,70,70	0
56	MG	14	3254	1/1	0.84	0.57	81,81,81,81	0
56	MG	1J	204	1/1	0.84	0.70	100,100,100,100	0
56	MG	1H	3149	1/1	0.84	0.37	77,77,77,77	0
56	MG	14	3212	1/1	0.84	0.41	90,90,90,90	0
56	MG	1G	1697	1/1	0.84	0.10	108,108,108,108	0
56	MG	1G	1659	1/1	0.84	0.32	110,110,110,110	0
56	MG	1H	3242	1/1	0.84	0.41	86,86,86,86	0
56	MG	14	3122	1/1	0.84	0.30	81,81,81,81	0
56	MG	41	302	1/1	0.84	0.20	94,94,94,94	0
56	MG	1H	3122	1/1	0.84	0.50	78,78,78,78	0
56	MG	14	3365	1/1	0.85	0.15	87,87,87,87	0
56	MG	14	3329	1/1	0.85	0.08	89,89,89,89	0
56	MG	14	3378	1/1	0.85	0.11	92,92,92,92	0
56	MG	14	3324	1/1	0.85	0.10	107,107,107,107	0
56	MG	13	1700	1/1	0.85	0.16	100,100,100,100	0
56	MG	1H	3233	1/1	0.85	1.00	75,75,75,75	0
56	MG	1H	3083	1/1	0.85	0.31	55,55,55,55	0
56	MG	14	3071	1/1	0.85	0.21	88,88,88,88	0
56	MG	1H	3313	1/1	0.85	0.78	80,80,80,80	0
56	MG	14	3024	1/1	0.85	0.12	79,79,79,79	0
56	MG	1H	3461	1/1	0.85	0.09	105,105,105,105	0
56	MG	1H	3265	1/1	0.85	0.55	92,92,92,92	0
56	MG	13	1609	1/1	0.85	0.28	94,94,94,94	0
56	MG	1H	3123	1/1	0.85	0.67	73,73,73,73	0
56	MG	14	3103	1/1	0.85	0.14	52,52,52,52	0
56	MG	1H	3529	1/1	0.85	0.12	55,55,55,55	0
56	MG	2K	102	1/1	0.85	0.61	76,76,76,76	0
56	MG	1H	3204	1/1	0.85	0.53	76,76,76,76	0
56	MG	1H	3263	1/1	0.85	0.40	82,82,82,82	0
56	MG	14	3340	1/1	0.85	0.10	83,83,83,83	0
56	MG	14	3194	1/1	0.85	0.06	140,140,140,140	0
56	MG	1G	1605	1/1	0.85	0.19	101,101,101,101	0
56	MG	14	3206	1/1	0.85	0.33	90,90,90,90	0
56	MG	1H	3469	1/1	0.85	0.09	96,96,96,96	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	1G	1666	1/1	0.85	0.46	94,94,94,94	0
56	MG	L8	101	1/1	0.85	0.26	72,72,72,72	0
56	MG	13	1749	1/1	0.85	0.07	101,101,101,101	0
56	MG	1H	3094	1/1	0.86	0.33	76,76,76,76	0
56	MG	14	3363	1/1	0.86	0.17	96,96,96,96	0
56	MG	1H	3188	1/1	0.86	0.17	62,62,62,62	0
56	MG	1H	3260	1/1	0.86	0.46	82,82,82,82	0
56	MG	1H	3329	1/1	0.86	0.24	99,99,99,99	0
56	MG	1H	3079	1/1	0.86	0.23	52,52,52,52	0
56	MG	1H	3450	1/1	0.86	0.10	119,119,119,119	0
56	MG	1H	3151	1/1	0.86	0.23	71,71,71,71	0
56	MG	1H	3323	1/1	0.86	0.37	87,87,87,87	0
56	MG	14	3177	1/1	0.86	0.40	80,80,80,80	0
56	MG	14	3341	1/1	0.86	0.06	103,103,103,103	0
56	MG	1H	3234	1/1	0.86	0.23	74,74,74,74	0
56	MG	1H	3490	1/1	0.86	0.12	92,92,92,92	0
56	MG	14	3321	1/1	0.86	0.13	97,97,97,97	0
56	MG	14	3200	1/1	0.86	0.17	82,82,82,82	0
56	MG	1H	3273	1/1	0.86	0.42	97,97,97,97	0
56	MG	14	3100	1/1	0.86	0.31	70,70,70,70	0
56	MG	14	3041	1/1	0.86	0.69	76,76,76,76	0
56	MG	1H	3240	1/1	0.86	0.58	77,77,77,77	0
56	MG	1G	1671	1/1	0.86	0.37	96,96,96,96	0
56	MG	13	1684	1/1	0.86	1.20	95,95,95,95	0
56	MG	1H	3325	1/1	0.86	0.36	64,64,64,64	0
56	MG	1H	3070	1/1	0.86	0.54	74,74,74,74	0
56	MG	14	3038	1/1	0.86	0.26	74,74,74,74	0
56	MG	1J	207	1/1	0.86	0.20	109,109,109,109	0
56	MG	14	3124	1/1	0.86	0.36	81,81,81,81	0
56	MG	14	3359	1/1	0.86	0.09	97,97,97,97	0
56	MG	14	3178	1/1	0.86	0.18	95,95,95,95	0
56	MG	13	1676	1/1	0.86	0.10	104,104,104,104	0
56	MG	1H	3075	1/1	0.86	0.30	53,53,53,53	0
56	MG	1H	3087	1/1	0.86	0.22	72,72,72,72	0
56	MG	14	3173	1/1	0.86	0.53	82,82,82,82	0
56	MG	13	1656	1/1	0.87	0.23	83,83,83,83	0
56	MG	1K	102	1/1	0.87	0.51	93,93,93,93	0
56	MG	1H	3215	1/1	0.87	0.65	71,71,71,71	0
56	MG	14	3244	1/1	0.87	0.14	80,80,80,80	0
56	MG	11	301	1/1	0.87	0.40	48,48,48,48	0
56	MG	1H	3048	1/1	0.87	0.32	84,84,84,84	0
56	MG	1H	3132	1/1	0.87	0.70	74,74,74,74	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	1H	3235	1/1	0.87	0.57	82,82,82,82	0
56	MG	1H	3037	1/1	0.87	0.34	64,64,64,64	0
56	MG	14	3141	1/1	0.87	0.48	84,84,84,84	0
56	MG	41	301	1/1	0.87	0.09	77,77,77,77	0
56	MG	1G	1687	1/1	0.87	0.05	121,121,121,121	0
56	MG	1H	3308	1/1	0.87	0.56	81,81,81,81	0
56	MG	1H	3175	1/1	0.87	0.52	92,92,92,92	0
56	MG	14	3030	1/1	0.87	0.07	74,74,74,74	0
56	MG	1G	1644	1/1	0.87	0.50	74,74,74,74	0
56	MG	14	3234	1/1	0.87	0.64	80,80,80,80	0
56	MG	14	3224	1/1	0.87	0.38	90,90,90,90	0
56	MG	14	3086	1/1	0.87	0.25	53,53,53,53	0
56	MG	14	3207	1/1	0.87	0.40	93,93,93,93	0
56	MG	14	3191	1/1	0.87	0.23	94,94,94,94	0
56	MG	1H	3239	1/1	0.87	0.29	84,84,84,84	0
56	MG	1H	3299	1/1	0.87	0.47	93,93,93,93	0
56	MG	14	3126	1/1	0.87	0.37	71,71,71,71	0
56	MG	1G	1693	1/1	0.87	0.10	125,125,125,125	0
56	MG	11	303	1/1	0.87	0.66	75,75,75,75	0
56	MG	14	3156	1/1	0.87	0.23	80,80,80,80	0
56	MG	1H	3099	1/1	0.87	0.21	64,64,64,64	0
56	MG	1H	3116	1/1	0.87	0.13	61,61,61,61	0
56	MG	13	1654	1/1	0.87	0.16	105,105,105,105	0
56	MG	1H	3072	1/1	0.87	0.23	46,46,46,46	0
56	MG	1H	3527	1/1	0.87	0.10	69,69,69,69	0
56	MG	1H	3245	1/1	0.87	0.27	91,91,91,91	0
56	MG	16	204	1/1	0.87	0.42	86,86,86,86	0
56	MG	1G	1625	1/1	0.87	0.67	82,82,82,82	0
56	MG	14	3022	1/1	0.87	0.39	61,61,61,61	0
56	MG	1H	3378	1/1	0.87	0.09	83,83,83,83	0
56	MG	14	3229	1/1	0.87	0.31	82,82,82,82	0
56	MG	14	3384	1/1	0.87	0.07	110,110,110,110	0
56	MG	13	1713	1/1	0.87	0.12	77,77,77,77	0
56	MG	14	3220	1/1	0.87	0.16	77,77,77,77	0
56	MG	1H	3311	1/1	0.88	0.19	70,70,70,70	0
56	MG	1H	3098	1/1	0.88	0.38	74,74,74,74	0
56	MG	1G	1616	1/1	0.88	0.33	79,79,79,79	0
56	MG	1H	3298	1/1	0.88	0.51	73,73,73,73	0
56	MG	14	3276	1/1	0.88	0.15	64,64,64,64	0
56	MG	14	3108	1/1	0.88	0.43	64,64,64,64	0
56	MG	1J	203	1/1	0.88	0.20	79,79,79,79	0
56	MG	13	1675	1/1	0.88	0.22	92,92,92,92	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	1H	3159	1/1	0.88	0.20	65,65,65,65	0
56	MG	1H	3197	1/1	0.88	0.26	68,68,68,68	0
56	MG	14	3031	1/1	0.88	0.20	73,73,73,73	0
56	MG	14	3331	1/1	0.88	0.10	65,65,65,65	0
56	MG	1H	3212	1/1	0.88	0.68	92,92,92,92	0
56	MG	1H	3276	1/1	0.88	0.33	81,81,81,81	0
56	MG	14	3152	1/1	0.88	0.18	61,61,61,61	0
56	MG	1H	3189	1/1	0.88	0.29	77,77,77,77	0
56	MG	1H	3039	1/1	0.88	0.46	70,70,70,70	0
56	MG	1G	1643	1/1	0.88	0.38	79,79,79,79	0
56	MG	1H	3510	1/1	0.88	0.12	99,99,99,99	0
56	MG	1G	1608	1/1	0.88	0.18	90,90,90,90	0
56	MG	1H	3137	1/1	0.88	0.20	67,67,67,67	0
56	MG	14	3274	1/1	0.88	0.09	99,99,99,99	0
56	MG	14	3256	1/1	0.88	0.33	75,75,75,75	0
56	MG	13	1740	1/1	0.88	0.13	91,91,91,91	0
56	MG	13	1706	1/1	0.88	0.07	108,108,108,108	0
56	MG	14	3211	1/1	0.88	0.70	82,82,82,82	0
56	MG	1H	3334	1/1	0.88	0.20	77,77,77,77	0
56	MG	1H	3076	1/1	0.88	0.41	75,75,75,75	0
56	MG	14	3169	1/1	0.88	0.53	81,81,81,81	0
56	MG	1J	205	1/1	0.88	0.35	98,98,98,98	0
56	MG	14	3084	1/1	0.88	0.29	56,56,56,56	0
56	MG	1H	3496	1/1	0.88	0.12	59,59,59,59	0
56	MG	14	3372	1/1	0.88	0.15	88,88,88,88	0
56	MG	14	3168	1/1	0.88	0.38	74,74,74,74	0
56	MG	1G	1667	1/1	0.88	0.29	97,97,97,97	0
56	MG	14	3115	1/1	0.89	0.38	86,86,86,86	0
56	MG	1H	3231	1/1	0.89	0.20	63,63,63,63	0
56	MG	14	3279	1/1	0.89	0.04	95,95,95,95	0
56	MG	1H	3023	1/1	0.89	0.27	57,57,57,57	0
56	MG	14	3251	1/1	0.89	0.16	102,102,102,102	0
56	MG	1H	3344	1/1	0.89	0.11	48,48,48,48	0
56	MG	13	1686	1/1	0.89	0.22	106,106,106,106	0
56	MG	14	3097	1/1	0.89	0.56	80,80,80,80	0
56	MG	78	201	1/1	0.89	0.24	70,70,70,70	0
56	MG	1H	3129	1/1	0.89	0.24	77,77,77,77	0
56	MG	13	1650	1/1	0.89	0.37	98,98,98,98	0
56	MG	1H	3522	1/1	0.89	0.12	99,99,99,99	0
56	MG	1H	3156	1/1	0.89	0.40	78,78,78,78	0
56	MG	14	3032	1/1	0.89	0.35	60,60,60,60	0
56	MG	14	3210	1/1	0.89	0.49	88,88,88,88	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	16	210	1/1	0.89	0.28	97,97,97,97	0
56	MG	1H	3107	1/1	0.89	0.18	84,84,84,84	0
56	MG	14	3246	1/1	0.89	0.30	98,98,98,98	0
56	MG	14	3049	1/1	0.89	0.35	71,71,71,71	0
56	MG	1H	3427	1/1	0.89	0.13	78,78,78,78	0
56	MG	1G	1618	1/1	0.89	0.28	85,85,85,85	0
56	MG	1H	3464	1/1	0.89	0.07	111,111,111,111	0
56	MG	13	1750	1/1	0.89	0.09	97,97,97,97	0
56	MG	14	3094	1/1	0.89	0.19	82,82,82,82	0
56	MG	1H	3229	1/1	0.89	0.54	112,112,112,112	0
56	MG	1H	3144	1/1	0.89	0.25	78,78,78,78	0
56	MG	1H	3278	1/1	0.89	0.34	82,82,82,82	0
56	MG	13	1632	1/1	0.89	0.41	77,77,77,77	0
56	MG	1H	3406	1/1	0.89	0.15	86,86,86,86	0
56	MG	14	3236	1/1	0.89	0.40	89,89,89,89	0
56	MG	14	3335	1/1	0.89	0.05	91,91,91,91	0
56	MG	21	302	1/1	0.89	0.20	73,73,73,73	0
56	MG	1H	3096	1/1	0.89	0.33	70,70,70,70	0
56	MG	1H	3509	1/1	0.89	0.09	82,82,82,82	0
56	MG	13	1613	1/1	0.89	0.21	83,83,83,83	0
56	MG	1H	3207	1/1	0.89	0.35	79,79,79,79	0
56	MG	14	3112	1/1	0.89	0.87	90,90,90,90	0
56	MG	14	3149	1/1	0.89	0.51	89,89,89,89	0
56	MG	14	3133	1/1	0.89	0.50	82,82,82,82	0
56	MG	13	1641	1/1	0.89	0.25	90,90,90,90	0
56	MG	14	3092	1/1	0.89	0.39	68,68,68,68	0
56	MG	14	3120	1/1	0.89	0.48	78,78,78,78	0
56	MG	14	3164	1/1	0.89	0.20	74,74,74,74	0
56	MG	14	3131	1/1	0.89	0.58	93,93,93,93	0
56	MG	1H	3337	1/1	0.89	0.09	56,56,56,56	0
56	MG	1H	3315	1/1	0.89	0.24	77,77,77,77	0
56	MG	14	3098	1/1	0.89	0.38	53,53,53,53	0
56	MG	1H	3093	1/1	0.89	0.74	61,61,61,61	0
56	MG	14	3380	1/1	0.89	0.12	58,58,58,58	0
56	MG	1H	3110	1/1	0.90	0.40	64,64,64,64	0
56	MG	49	301	1/1	0.90	0.10	116,116,116,116	0
56	MG	1G	1690	1/1	0.90	0.08	90,90,90,90	0
56	MG	13	1727	1/1	0.90	0.13	117,117,117,117	0
56	MG	14	3069	1/1	0.90	0.44	63,63,63,63	0
56	MG	1H	3441	1/1	0.90	0.05	82,82,82,82	0
56	MG	1H	3467	1/1	0.90	0.04	86,86,86,86	0
56	MG	1H	3520	1/1	0.90	0.07	109,109,109,109	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	13	1664	1/1	0.90	0.38	71,71,71,71	0
56	MG	13	1658	1/1	0.90	0.39	92,92,92,92	0
56	MG	13	1724	1/1	0.90	0.14	102,102,102,102	0
56	MG	1H	3320	1/1	0.90	0.30	86,86,86,86	0
56	MG	13	1745	1/1	0.90	0.05	119,119,119,119	0
56	MG	1H	3190	1/1	0.90	0.43	88,88,88,88	0
56	MG	13	1645	1/1	0.90	0.46	83,83,83,83	0
56	MG	14	3180	1/1	0.90	0.59	93,93,93,93	0
56	MG	13	1617	1/1	0.90	0.42	70,70,70,70	0
56	MG	13	1693	1/1	0.90	0.40	109,109,109,109	0
56	MG	1H	3412	1/1	0.90	0.10	101,101,101,101	0
56	MG	1H	3200	1/1	0.90	0.17	98,98,98,98	0
56	MG	13	1635	1/1	0.90	0.57	73,73,73,73	0
56	MG	31	301	1/1	0.90	0.29	62,62,62,62	0
56	MG	I8	101	1/1	0.90	0.05	88,88,88,88	0
56	MG	13	1651	1/1	0.90	0.45	73,73,73,73	0
56	MG	14	3111	1/1	0.90	0.31	86,86,86,86	0
56	MG	14	3090	1/1	0.90	0.24	90,90,90,90	0
56	MG	13	1638	1/1	0.90	0.62	107,107,107,107	0
56	MG	1H	3213	1/1	0.90	0.69	86,86,86,86	0
56	MG	14	3305	1/1	0.90	0.14	112,112,112,112	0
56	MG	13	1662	1/1	0.90	0.40	113,113,113,113	0
56	MG	1H	3006	1/1	0.90	0.43	55,55,55,55	0
56	MG	1H	3516	1/1	0.90	0.06	100,100,100,100	0
56	MG	14	3316	1/1	0.90	0.10	82,82,82,82	0
56	MG	1G	1700	1/1	0.90	0.05	126,126,126,126	0
56	MG	1H	3102	1/1	0.90	0.42	75,75,75,75	0
56	MG	13	1725	1/1	0.90	0.14	90,90,90,90	0
56	MG	1H	3314	1/1	0.90	0.17	110,110,110,110	0
56	MG	13	1660	1/1	0.90	0.15	108,108,108,108	0
56	MG	1H	3321	1/1	0.90	0.17	72,72,72,72	0
56	MG	1J	202	1/1	0.90	0.27	81,81,81,81	0
56	MG	13	1634	1/1	0.90	0.28	80,80,80,80	0
56	MG	1H	3271	1/1	0.90	0.46	90,90,90,90	0
56	MG	1H	3253	1/1	0.90	0.49	64,64,64,64	0
56	MG	1H	3150	1/1	0.90	0.20	52,52,52,52	0
56	MG	1G	1696	1/1	0.90	0.05	98,98,98,98	0
56	MG	13	1738	1/1	0.90	0.08	113,113,113,113	0
56	MG	1H	3237	1/1	0.90	0.32	62,62,62,62	0
56	MG	14	3237	1/1	0.90	0.47	78,78,78,78	0
56	MG	1H	3097	1/1	0.91	0.38	41,41,41,41	0
56	MG	1H	3443	1/1	0.91	0.12	76,76,76,76	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	1H	3013	1/1	0.91	0.30	53,53,53,53	0
56	MG	1H	3310	1/1	0.91	0.30	82,82,82,82	0
56	MG	1H	3430	1/1	0.91	0.11	71,71,71,71	0
56	MG	14	3144	1/1	0.91	0.17	72,72,72,72	0
56	MG	1H	3419	1/1	0.91	0.11	53,53,53,53	0
56	MG	14	3260	1/1	0.91	0.15	62,62,62,62	0
56	MG	14	3176	1/1	0.91	0.24	71,71,71,71	0
56	MG	1H	3109	1/1	0.91	0.48	93,93,93,93	0
56	MG	14	3289	1/1	0.91	0.17	77,77,77,77	0
56	MG	13	1612	1/1	0.91	0.26	70,70,70,70	0
56	MG	13	1692	1/1	0.91	0.09	114,114,114,114	0
56	MG	1H	3283	1/1	0.91	0.26	67,67,67,67	0
56	MG	14	3165	1/1	0.91	0.38	81,81,81,81	0
56	MG	1J	208	1/1	0.91	0.05	109,109,109,109	0
56	MG	14	3170	1/1	0.91	0.46	88,88,88,88	0
56	MG	1H	3317	1/1	0.91	0.37	66,66,66,66	0
56	MG	14	3023	1/1	0.91	0.38	66,66,66,66	0
56	MG	13	1644	1/1	0.91	0.49	77,77,77,77	0
56	MG	1H	3058	1/1	0.91	0.73	69,69,69,69	0
56	MG	1H	3528	1/1	0.91	0.09	77,77,77,77	0
56	MG	14	3373	1/1	0.91	0.04	125,125,125,125	0
56	MG	1H	3038	1/1	0.91	0.26	76,76,76,76	0
56	MG	1H	3414	1/1	0.91	0.09	80,80,80,80	0
56	MG	14	3134	1/1	0.91	0.35	88,88,88,88	0
56	MG	14	3382	1/1	0.91	0.06	85,85,85,85	0
56	MG	14	3387	1/1	0.91	0.43	74,74,74,74	0
56	MG	1H	3027	1/1	0.91	0.56	64,64,64,64	0
56	MG	1H	3221	1/1	0.91	0.43	92,92,92,92	0
56	MG	1H	3507	1/1	0.91	0.04	94,94,94,94	0
56	MG	14	3313	1/1	0.91	0.07	81,81,81,81	0
56	MG	1H	3478	1/1	0.91	0.07	111,111,111,111	0
56	MG	13	1628	1/1	0.91	0.39	77,77,77,77	0
56	MG	1G	1609	1/1	0.91	0.23	101,101,101,101	0
56	MG	1H	3319	1/1	0.91	0.17	76,76,76,76	0
56	MG	1H	3158	1/1	0.91	0.37	55,55,55,55	0
56	MG	1H	3433	1/1	0.91	0.17	77,77,77,77	0
56	MG	14	3136	1/1	0.91	0.25	60,60,60,60	0
56	MG	16	202	1/1	0.91	0.41	66,66,66,66	0
56	MG	1G	1635	1/1	0.91	0.33	96,96,96,96	0
56	MG	1H	3224	1/1	0.91	0.55	89,89,89,89	0
56	MG	1H	3257	1/1	0.91	0.41	82,82,82,82	0
56	MG	1H	3360	1/1	0.91	0.04	105,105,105,105	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	14	3233	1/1	0.91	0.49	112,112,112,112	0
56	MG	1H	3178	1/1	0.91	0.31	68,68,68,68	0
56	MG	14	3186	1/1	0.91	0.27	86,86,86,86	0
56	MG	1H	3249	1/1	0.91	0.47	89,89,89,89	0
56	MG	13	1618	1/1	0.91	0.70	71,71,71,71	0
56	MG	1H	3136	1/1	0.91	0.29	66,66,66,66	0
56	MG	13	1715	1/1	0.91	0.09	116,116,116,116	0
56	MG	14	3102	1/1	0.91	0.76	76,76,76,76	0
56	MG	14	3076	1/1	0.91	0.30	79,79,79,79	0
56	MG	1G	1703	1/1	0.91	0.07	124,124,124,124	0
56	MG	16	208	1/1	0.91	0.13	70,70,70,70	0
56	MG	1G	1645	1/1	0.91	0.32	92,92,92,92	0
56	MG	13	1607	1/1	0.91	0.36	78,78,78,78	0
56	MG	1H	3130	1/1	0.91	0.49	82,82,82,82	0
56	MG	14	3266	1/1	0.91	0.06	69,69,69,69	0
56	MG	14	3007	1/1	0.91	0.34	54,54,54,54	0
56	MG	13	1697	1/1	0.91	0.51	75,75,75,75	0
56	MG	1H	3134	1/1	0.91	0.51	90,90,90,90	0
56	MG	1H	3164	1/1	0.91	0.26	70,70,70,70	0
56	MG	1H	3152	1/1	0.92	0.40	53,53,53,53	0
56	MG	1H	3455	1/1	0.92	0.08	111,111,111,111	0
56	MG	13	1744	1/1	0.92	0.05	144,144,144,144	0
56	MG	1G	1686	1/1	0.92	0.21	84,84,84,84	0
56	MG	14	3223	1/1	0.92	0.60	86,86,86,86	0
56	MG	14	3135	1/1	0.92	0.20	54,54,54,54	0
56	MG	1H	3457	1/1	0.92	0.08	91,91,91,91	0
56	MG	1G	1676	1/1	0.92	0.15	157,157,157,157	0
56	MG	35	201	1/1	0.92	0.39	76,76,76,76	0
56	MG	1H	3041	1/1	0.92	0.29	57,57,57,57	0
56	MG	14	3297	1/1	0.92	0.10	107,107,107,107	0
56	MG	14	3020	1/1	0.92	0.20	72,72,72,72	0
56	MG	1H	3025	1/1	0.92	0.18	86,86,86,86	0
56	MG	14	3259	1/1	0.92	0.18	67,67,67,67	0
56	MG	1H	3364	1/1	0.92	0.09	70,70,70,70	0
56	MG	14	3317	1/1	0.92	0.10	89,89,89,89	0
56	MG	1H	3161	1/1	0.92	0.33	66,66,66,66	0
56	MG	13	1633	1/1	0.92	0.53	73,73,73,73	0
56	MG	14	3151	1/1	0.92	0.53	52,52,52,52	0
56	MG	14	3287	1/1	0.92	0.08	99,99,99,99	0
56	MG	1H	3131	1/1	0.92	0.45	79,79,79,79	0
56	MG	14	3053	1/1	0.92	0.35	55,55,55,55	0
56	MG	1H	3103	1/1	0.92	0.33	76,76,76,76	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	1H	3115	1/1	0.92	0.24	59,59,59,59	0
56	MG	1H	3052	1/1	0.92	0.50	52,52,52,52	0
56	MG	1H	3241	1/1	0.92	0.42	70,70,70,70	0
56	MG	14	3294	1/1	0.92	0.10	69,69,69,69	0
56	MG	14	3184	1/1	0.92	0.35	53,53,53,53	0
56	MG	1H	3451	1/1	0.92	0.07	94,94,94,94	0
56	MG	1H	3483	1/1	0.92	0.06	117,117,117,117	0
56	MG	13	1726	1/1	0.92	0.10	91,91,91,91	0
56	MG	1H	3367	1/1	0.92	0.06	83,83,83,83	0
56	MG	14	3349	1/1	0.92	0.07	110,110,110,110	0
56	MG	1G	1629	1/1	0.92	0.39	89,89,89,89	0
56	MG	14	3326	1/1	0.92	0.05	110,110,110,110	0
56	MG	13	1748	1/1	0.92	0.06	156,156,156,156	0
56	MG	14	3375	1/1	0.92	0.10	61,61,61,61	0
56	MG	1H	3195	1/1	0.92	0.18	68,68,68,68	0
56	MG	13	1606	1/1	0.92	0.32	80,80,80,80	0
56	MG	1H	3101	1/1	0.92	0.27	80,80,80,80	0
56	MG	13	1690	1/1	0.92	0.15	96,96,96,96	0
56	MG	1H	3172	1/1	0.92	0.51	70,70,70,70	0
56	MG	14	3230	1/1	0.92	0.17	103,103,103,103	0
56	MG	14	3162	1/1	0.92	0.35	60,60,60,60	0
56	MG	13	1672	1/1	0.92	0.24	118,118,118,118	0
56	MG	14	3166	1/1	0.92	0.18	112,112,112,112	0
56	MG	1H	3503	1/1	0.92	0.07	115,115,115,115	0
56	MG	1G	1650	1/1	0.92	0.28	111,111,111,111	0
56	MG	13	1642	1/1	0.92	0.24	89,89,89,89	0
56	MG	1H	3445	1/1	0.92	0.10	91,91,91,91	0
56	MG	13	1655	1/1	0.92	0.37	80,80,80,80	0
56	MG	14	3227	1/1	0.92	0.28	103,103,103,103	0
56	MG	13	1747	1/1	0.92	0.09	140,140,140,140	0
56	MG	1H	3468	1/1	0.92	0.04	109,109,109,109	0
56	MG	1H	3114	1/1	0.92	0.12	59,59,59,59	0
56	MG	14	3261	1/1	0.92	0.14	54,54,54,54	0
56	MG	1H	3222	1/1	0.92	0.41	77,77,77,77	0
56	MG	1H	3462	1/1	0.92	0.09	81,81,81,81	0
56	MG	1H	3316	1/1	0.92	0.55	64,64,64,64	0
56	MG	1G	1626	1/1	0.92	0.48	78,78,78,78	0
56	MG	1H	3280	1/1	0.92	0.25	80,80,80,80	0
56	MG	1H	3492	1/1	0.92	0.11	108,108,108,108	0
56	MG	14	3157	1/1	0.92	0.24	107,107,107,107	0
56	MG	1H	3363	1/1	0.92	0.08	89,89,89,89	0
56	MG	14	3018	1/1	0.92	0.27	68,68,68,68	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	1H	3305	1/1	0.92	0.27	87,87,87,87	0
56	MG	14	3295	1/1	0.92	0.09	87,87,87,87	0
56	MG	1G	1675	1/1	0.92	0.57	96,96,96,96	0
56	MG	1H	3256	1/1	0.92	0.90	74,74,74,74	0
56	MG	1G	1637	1/1	0.92	0.26	124,124,124,124	0
56	MG	1H	3211	1/1	0.92	0.13	88,88,88,88	0
56	MG	14	3009	1/1	0.93	0.44	63,63,63,63	0
56	MG	13	1626	1/1	0.93	0.17	65,65,65,65	0
56	MG	13	1716	1/1	0.93	0.05	89,89,89,89	0
56	MG	1H	3350	1/1	0.93	0.13	43,43,43,43	0
56	MG	1H	3066	1/1	0.93	0.17	62,62,62,62	0
56	MG	1H	3494	1/1	0.93	0.06	95,95,95,95	0
56	MG	14	3377	1/1	0.93	0.10	52,52,52,52	0
56	MG	1H	3261	1/1	0.93	0.22	58,58,58,58	0
56	MG	1H	3435	1/1	0.93	0.08	95,95,95,95	0
56	MG	14	3143	1/1	0.93	0.75	70,70,70,70	0
56	MG	1H	3155	1/1	0.93	0.68	72,72,72,72	0
56	MG	14	3121	1/1	0.93	0.78	79,79,79,79	0
56	MG	14	3138	1/1	0.93	0.16	57,57,57,57	0
56	MG	14	3150	1/1	0.93	0.25	64,64,64,64	0
56	MG	14	3046	1/1	0.93	0.30	65,65,65,65	0
56	MG	14	3269	1/1	0.93	0.15	90,90,90,90	0
56	MG	1H	3154	1/1	0.93	0.15	66,66,66,66	0
56	MG	1H	3042	1/1	0.93	0.32	53,53,53,53	0
56	MG	1H	3089	1/1	0.93	0.16	44,44,44,44	0
56	MG	14	3348	1/1	0.93	0.05	97,97,97,97	0
56	MG	F5	101	1/1	0.93	0.47	74,74,74,74	0
56	MG	1H	3206	1/1	0.93	0.16	77,77,77,77	0
56	MG	14	3325	1/1	0.93	0.05	103,103,103,103	0
56	MG	1H	3442	1/1	0.93	0.08	100,100,100,100	0
56	MG	1H	3051	1/1	0.93	0.35	72,72,72,72	0
56	MG	14	3146	1/1	0.93	0.34	105,105,105,105	0
56	MG	1H	3193	1/1	0.93	0.41	67,67,67,67	0
56	MG	13	1608	1/1	0.93	0.18	75,75,75,75	0
56	MG	14	3356	1/1	0.93	0.09	85,85,85,85	0
56	MG	1H	3250	1/1	0.93	0.25	90,90,90,90	0
56	MG	1G	1692	1/1	0.93	0.07	111,111,111,111	0
56	MG	1H	3180	1/1	0.93	0.36	67,67,67,67	0
56	MG	1H	3086	1/1	0.93	0.47	67,67,67,67	0
56	MG	1H	3185	1/1	0.93	0.79	68,68,68,68	0
56	MG	14	3383	1/1	0.93	0.13	93,93,93,93	0
56	MG	13	1625	1/1	0.93	0.41	61,61,61,61	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	14	3339	1/1	0.93	0.09	85,85,85,85	0
56	MG	1G	1647	1/1	0.93	0.31	102,102,102,102	0
56	MG	C8	201	1/1	0.93	0.17	74,74,74,74	0
56	MG	1H	3254	1/1	0.93	0.23	84,84,84,84	0
56	MG	5E	201	1/1	0.93	0.23	93,93,93,93	0
56	MG	88	201	1/1	0.93	0.26	79,79,79,79	0
56	MG	1H	3142	1/1	0.93	0.23	101,101,101,101	0
56	MG	13	1721	1/1	0.93	0.07	94,94,94,94	0
56	MG	1H	3219	1/1	0.93	1.20	82,82,82,82	0
56	MG	1H	3390	1/1	0.93	0.12	55,55,55,55	0
56	MG	14	3155	1/1	0.93	0.19	82,82,82,82	0
56	MG	14	3075	1/1	0.93	0.43	61,61,61,61	0
56	MG	1H	3035	1/1	0.93	0.25	86,86,86,86	0
56	MG	14	3271	1/1	0.93	0.24	63,63,63,63	0
56	MG	13	1666	1/1	0.93	0.06	99,99,99,99	0
56	MG	1G	1633	1/1	0.93	0.33	92,92,92,92	0
56	MG	1H	3196	1/1	0.93	0.17	90,90,90,90	0
56	MG	1H	3054	1/1	0.93	0.22	53,53,53,53	0
56	MG	1H	3495	1/1	0.93	0.07	53,53,53,53	0
56	MG	14	3081	1/1	0.93	0.46	71,71,71,71	0
56	MG	1H	3475	1/1	0.93	0.08	77,77,77,77	0
56	MG	14	3021	1/1	0.93	0.31	80,80,80,80	0
56	MG	14	3161	1/1	0.93	0.57	70,70,70,70	0
56	MG	1H	3169	1/1	0.93	0.15	74,74,74,74	0
56	MG	14	3213	1/1	0.93	0.55	93,93,93,93	0
56	MG	14	3268	1/1	0.93	0.11	64,64,64,64	0
56	MG	13	1673	1/1	0.93	0.49	83,83,83,83	0
56	MG	1H	3157	1/1	0.93	0.39	65,65,65,65	0
56	MG	1H	3480	1/1	0.93	0.05	122,122,122,122	0
56	MG	14	3322	1/1	0.93	0.06	101,101,101,101	0
56	MG	1G	1695	1/1	0.93	0.04	103,103,103,103	0
56	MG	1H	3153	1/1	0.93	0.55	57,57,57,57	0
56	MG	13	1663	1/1	0.93	0.19	82,82,82,82	0
56	MG	14	3242	1/1	0.93	0.52	78,78,78,78	0
56	MG	14	3172	1/1	0.93	0.14	93,93,93,93	0
56	MG	14	3095	1/1	0.94	0.31	72,72,72,72	0
56	MG	14	3137	1/1	0.94	0.36	53,53,53,53	0
56	MG	14	3139	1/1	0.94	0.67	69,69,69,69	0
56	MG	14	3333	1/1	0.94	0.09	91,91,91,91	0
56	MG	1H	3359	1/1	0.94	0.06	102,102,102,102	0
56	MG	14	3202	1/1	0.94	0.10	115,115,115,115	0
56	MG	1H	3238	1/1	0.94	0.18	71,71,71,71	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	14	3055	1/1	0.94	0.32	60,60,60,60	0
56	MG	14	3280	1/1	0.94	0.09	88,88,88,88	0
56	MG	1H	3020	1/1	0.94	0.36	56,56,56,56	0
56	MG	13	1653	1/1	0.94	0.25	111,111,111,111	0
56	MG	14	3238	1/1	0.94	0.33	77,77,77,77	0
56	MG	14	3034	1/1	0.94	0.26	64,64,64,64	0
56	MG	1H	3085	1/1	0.94	0.43	74,74,74,74	0
57	ZN	5A	101	1/1	0.94	0.12	160,160,160,160	0
56	MG	14	3337	1/1	0.94	0.06	83,83,83,83	0
56	MG	14	3205	1/1	0.94	0.34	91,91,91,91	0
56	MG	1H	3309	1/1	0.94	0.19	87,87,87,87	0
56	MG	14	3063	1/1	0.94	0.27	62,62,62,62	0
56	MG	14	3353	1/1	0.94	0.05	99,99,99,99	0
56	MG	14	3362	1/1	0.94	0.06	78,78,78,78	0
56	MG	14	3299	1/1	0.94	0.08	82,82,82,82	0
56	MG	1H	3453	1/1	0.94	0.06	91,91,91,91	0
56	MG	1J	209	1/1	0.94	0.07	94,94,94,94	0
56	MG	1H	3021	1/1	0.94	0.21	58,58,58,58	0
56	MG	14	3327	1/1	0.94	0.10	120,120,120,120	0
56	MG	1H	3374	1/1	0.94	0.09	63,63,63,63	0
56	MG	14	3318	1/1	0.94	0.17	63,63,63,63	0
56	MG	13	1728	1/1	0.94	0.09	95,95,95,95	0
56	MG	1H	3117	1/1	0.94	0.56	63,63,63,63	0
56	MG	1H	3062	1/1	0.94	0.23	35,35,35,35	0
56	MG	13	1614	1/1	0.94	0.29	97,97,97,97	0
56	MG	1H	3456	1/1	0.94	0.05	111,111,111,111	0
56	MG	16	201	1/1	0.94	0.13	96,96,96,96	0
56	MG	14	3061	1/1	0.94	0.45	71,71,71,71	0
56	MG	1H	3084	1/1	0.94	0.19	66,66,66,66	0
56	MG	14	3198	1/1	0.94	0.06	82,82,82,82	0
56	MG	14	3283	1/1	0.94	0.13	57,57,57,57	0
56	MG	14	3379	1/1	0.94	0.09	60,60,60,60	0
56	MG	14	3145	1/1	0.94	0.24	90,90,90,90	0
56	MG	1G	1610	1/1	0.94	0.09	98,98,98,98	0
56	MG	1H	3063	1/1	0.94	0.46	47,47,47,47	0
56	MG	13	1691	1/1	0.94	0.26	101,101,101,101	0
56	MG	1H	3420	1/1	0.94	0.09	65,65,65,65	0
56	MG	1H	3078	1/1	0.94	0.18	60,60,60,60	0
56	MG	1H	3091	1/1	0.94	0.17	43,43,43,43	0
56	MG	1G	1631	1/1	0.94	0.34	89,89,89,89	0
56	MG	13	1611	1/1	0.94	0.26	70,70,70,70	0
56	MG	1H	3514	1/1	0.94	0.14	51,51,51,51	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	1H	3220	1/1	0.94	0.12	61,61,61,61	0
56	MG	1H	3351	1/1	0.94	0.15	50,50,50,50	0
56	MG	1H	3375	1/1	0.94	0.07	75,75,75,75	0
56	MG	14	3292	1/1	0.94	0.08	90,90,90,90	0
56	MG	1H	3444	1/1	0.94	0.04	97,97,97,97	0
56	MG	14	3221	1/1	0.94	0.46	88,88,88,88	0
56	MG	1H	3036	1/1	0.94	0.28	85,85,85,85	0
56	MG	14	3015	1/1	0.94	0.28	69,69,69,69	0
56	MG	1H	3417	1/1	0.94	0.13	65,65,65,65	0
56	MG	1H	3487	1/1	0.94	0.09	101,101,101,101	0
56	MG	1G	1638	1/1	0.94	0.11	154,154,154,154	0
56	MG	14	3074	1/1	0.94	0.49	63,63,63,63	0
56	MG	14	3366	1/1	0.94	0.15	83,83,83,83	0
56	MG	1H	3069	1/1	0.94	0.36	45,45,45,45	0
56	MG	14	3087	1/1	0.94	0.09	59,59,59,59	0
56	MG	16	211	1/1	0.94	0.07	84,84,84,84	0
56	MG	14	3153	1/1	0.94	0.15	60,60,60,60	0
56	MG	1H	3524	1/1	0.94	0.32	49,49,49,49	0
56	MG	1H	3379	1/1	0.94	0.05	79,79,79,79	0
56	MG	1H	3439	1/1	0.94	0.08	76,76,76,76	0
56	MG	1J	201	1/1	0.94	0.16	114,114,114,114	0
56	MG	1H	3145	1/1	0.94	0.28	49,49,49,49	0
56	MG	14	3051	1/1	0.94	0.72	71,71,71,71	0
56	MG	14	3129	1/1	0.94	0.44	76,76,76,76	0
56	MG	1H	3465	1/1	0.94	0.12	95,95,95,95	0
56	MG	1H	3031	1/1	0.94	0.25	63,63,63,63	0
56	MG	1H	3163	1/1	0.95	0.45	74,74,74,74	0
56	MG	14	3250	1/1	0.95	0.37	108,108,108,108	0
56	MG	1G	1663	1/1	0.95	0.28	89,89,89,89	0
56	MG	14	3225	1/1	0.95	0.09	96,96,96,96	0
56	MG	1H	3336	1/1	0.95	0.09	52,52,52,52	0
56	MG	14	3159	1/1	0.95	0.20	60,60,60,60	0
56	MG	1G	1646	1/1	0.95	0.19	84,84,84,84	0
56	MG	1H	3246	1/1	0.95	0.47	88,88,88,88	0
56	MG	1H	3014	1/1	0.95	0.42	57,57,57,57	0
56	MG	14	3278	1/1	0.95	0.10	84,84,84,84	0
56	MG	1H	3338	1/1	0.95	0.14	49,49,49,49	0
56	MG	1H	3388	1/1	0.95	0.15	63,63,63,63	0
56	MG	2K	103	1/1	0.95	0.32	59,59,59,59	0
56	MG	1H	3405	1/1	0.95	0.11	75,75,75,75	0
56	MG	1H	3349	1/1	0.95	0.10	70,70,70,70	0
56	MG	1H	3100	1/1	0.95	0.39	71,71,71,71	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	14	3174	1/1	0.95	0.27	96,96,96,96	0
56	MG	1H	3288	1/1	0.95	0.14	60,60,60,60	0
56	MG	1G	1691	1/1	0.95	0.05	119,119,119,119	0
56	MG	1H	3426	1/1	0.95	0.08	53,53,53,53	0
56	MG	1H	3504	1/1	0.95	0.05	75,75,75,75	0
56	MG	14	3070	1/1	0.95	0.52	59,59,59,59	0
56	MG	14	3364	1/1	0.95	0.14	77,77,77,77	0
56	MG	13	1718	1/1	0.95	0.12	88,88,88,88	0
56	MG	14	3105	1/1	0.95	0.51	75,75,75,75	0
56	MG	13	1652	1/1	0.95	0.07	79,79,79,79	0
56	MG	I8	102	1/1	0.95	0.07	67,67,67,67	0
56	MG	1H	3423	1/1	0.95	0.06	93,93,93,93	0
56	MG	14	3039	1/1	0.95	0.28	79,79,79,79	0
56	MG	14	3222	1/1	0.95	0.35	87,87,87,87	0
56	MG	1H	3092	1/1	0.95	0.23	52,52,52,52	0
56	MG	1H	3009	1/1	0.95	0.27	47,47,47,47	0
56	MG	1H	3277	1/1	0.95	0.47	84,84,84,84	0
56	MG	14	3315	1/1	0.95	0.13	71,71,71,71	0
56	MG	13	1659	1/1	0.95	0.12	107,107,107,107	0
56	MG	14	3311	1/1	0.95	0.07	82,82,82,82	0
56	MG	1H	3201	1/1	0.95	0.22	79,79,79,79	0
56	MG	14	3125	1/1	0.95	0.25	105,105,105,105	0
56	MG	1H	3119	1/1	0.95	1.25	86,86,86,86	0
56	MG	14	3044	1/1	0.95	0.93	82,82,82,82	0
56	MG	1H	3348	1/1	0.95	0.08	60,60,60,60	0
56	MG	14	3338	1/1	0.95	0.06	107,107,107,107	0
56	MG	1H	3030	1/1	0.95	0.28	70,70,70,70	0
56	MG	3I	201	1/1	0.95	0.24	70,70,70,70	0
56	MG	1H	3511	1/1	0.95	0.09	76,76,76,76	0
56	MG	1G	1679	1/1	0.95	0.44	105,105,105,105	0
56	MG	1H	3171	1/1	0.95	0.36	101,101,101,101	0
56	MG	13	1698	1/1	0.95	0.47	90,90,90,90	0
56	MG	14	3351	1/1	0.95	0.03	99,99,99,99	0
56	MG	14	3288	1/1	0.95	0.19	62,62,62,62	0
56	MG	1H	3518	1/1	0.95	0.13	74,74,74,74	0
56	MG	1H	3429	1/1	0.95	0.06	74,74,74,74	0
56	MG	1H	3512	1/1	0.95	0.15	44,44,44,44	0
56	MG	13	1723	1/1	0.95	0.12	105,105,105,105	0
56	MG	14	3307	1/1	0.95	0.09	70,70,70,70	0
56	MG	16	213	1/1	0.95	0.10	102,102,102,102	0
56	MG	1H	3479	1/1	0.95	0.11	67,67,67,67	0
56	MG	1H	3356	1/1	0.95	0.09	67,67,67,67	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	14	3029	1/1	0.95	0.31	84,84,84,84	0
56	MG	1H	3074	1/1	0.95	0.37	65,65,65,65	0
56	MG	14	3158	1/1	0.95	0.17	75,75,75,75	0
56	MG	1H	3046	1/1	0.95	0.34	80,80,80,80	0
56	MG	1H	3513	1/1	0.95	0.13	58,58,58,58	0
56	MG	14	3272	1/1	0.95	0.12	59,59,59,59	0
56	MG	1H	3146	1/1	0.95	0.20	42,42,42,42	0
56	MG	1H	3228	1/1	0.95	0.33	71,71,71,71	0
56	MG	13	1739	1/1	0.95	0.12	118,118,118,118	0
56	MG	1G	1611	1/1	0.95	0.60	91,91,91,91	0
56	MG	1H	3012	1/1	0.95	0.50	52,52,52,52	0
56	MG	1H	3210	1/1	0.95	0.17	95,95,95,95	0
56	MG	13	1703	1/1	0.95	0.92	91,91,91,91	0
56	MG	16	212	1/1	0.95	0.06	79,79,79,79	0
56	MG	14	3285	1/1	0.95	0.12	57,57,57,57	0
56	MG	1H	3486	1/1	0.95	0.09	61,61,61,61	0
56	MG	1G	1702	1/1	0.95	0.07	146,146,146,146	0
56	MG	1H	3402	1/1	0.95	0.16	49,49,49,49	0
56	MG	14	3016	1/1	0.95	0.30	68,68,68,68	0
56	MG	1H	3139	1/1	0.95	0.20	65,65,65,65	0
56	MG	14	3026	1/1	0.95	0.28	90,90,90,90	0
56	MG	1H	3505	1/1	0.95	0.07	78,78,78,78	0
56	MG	14	3381	1/1	0.95	0.10	79,79,79,79	0
56	MG	1H	3322	1/1	0.95	0.17	77,77,77,77	0
56	MG	1H	3272	1/1	0.95	0.50	71,71,71,71	0
56	MG	14	3057	1/1	0.95	0.38	80,80,80,80	0
56	MG	1H	3365	1/1	0.95	0.06	91,91,91,91	0
56	MG	1H	3191	1/1	0.95	0.22	59,59,59,59	0
56	MG	1H	3400	1/1	0.95	0.12	68,68,68,68	0
56	MG	1H	3126	1/1	0.95	0.46	88,88,88,88	0
56	MG	1H	3044	1/1	0.95	0.39	75,75,75,75	0
56	MG	1H	3181	1/1	0.95	0.23	99,99,99,99	0
56	MG	1H	3217	1/1	0.95	0.32	61,61,61,61	0
56	MG	1H	3500	1/1	0.95	0.07	80,80,80,80	0
56	MG	1H	3128	1/1	0.95	0.14	71,71,71,71	0
56	MG	14	3323	1/1	0.96	0.10	96,96,96,96	0
56	MG	14	3014	1/1	0.96	0.17	81,81,81,81	0
56	MG	1G	1698	1/1	0.96	0.08	91,91,91,91	0
56	MG	14	3163	1/1	0.96	0.56	71,71,71,71	0
56	MG	1H	3209	1/1	0.96	0.42	60,60,60,60	0
56	MG	14	3077	1/1	0.96	0.43	78,78,78,78	0
56	MG	1H	3521	1/1	0.96	0.13	49,49,49,49	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	1H	3438	1/1	0.96	0.11	52,52,52,52	0
56	MG	14	3079	1/1	0.96	0.55	69,69,69,69	0
56	MG	1H	3064	1/1	0.96	0.20	45,45,45,45	0
56	MG	1H	3053	1/1	0.96	0.27	48,48,48,48	0
56	MG	13	1714	1/1	0.96	0.10	62,62,62,62	0
56	MG	1H	3477	1/1	0.96	0.11	82,82,82,82	0
56	MG	1H	3447	1/1	0.96	0.12	81,81,81,81	0
56	MG	14	3089	1/1	0.96	0.49	87,87,87,87	0
56	MG	14	3293	1/1	0.96	0.12	68,68,68,68	0
56	MG	1G	1694	1/1	0.96	0.05	104,104,104,104	0
56	MG	13	1717	1/1	0.96	0.07	105,105,105,105	0
56	MG	1H	3471	1/1	0.96	0.08	94,94,94,94	0
56	MG	14	3376	1/1	0.96	0.11	65,65,65,65	0
56	MG	1H	3173	1/1	0.96	0.14	79,79,79,79	0
56	MG	1H	3208	1/1	0.96	0.22	71,71,71,71	0
56	MG	1G	1606	1/1	0.96	0.28	94,94,94,94	0
56	MG	1H	3354	1/1	0.96	0.09	61,61,61,61	0
56	MG	14	3319	1/1	0.96	0.05	88,88,88,88	0
56	MG	1H	3368	1/1	0.96	0.06	76,76,76,76	0
56	MG	1H	3326	1/1	0.96	0.35	94,94,94,94	0
56	MG	1H	3415	1/1	0.96	0.07	100,100,100,100	0
56	MG	1H	3192	1/1	0.96	0.36	81,81,81,81	0
56	MG	1G	1632	1/1	0.96	0.24	86,86,86,86	0
56	MG	13	1620	1/1	0.96	0.54	69,69,69,69	0
56	MG	14	3301	1/1	0.96	0.06	81,81,81,81	0
56	MG	1H	3125	1/1	0.96	0.62	77,77,77,77	0
56	MG	1G	1634	1/1	0.96	0.21	110,110,110,110	0
56	MG	1H	3401	1/1	0.96	0.07	50,50,50,50	0
56	MG	J8	101	1/1	0.96	0.30	72,72,72,72	0
56	MG	1H	3498	1/1	0.96	0.09	64,64,64,64	0
56	MG	1H	3057	1/1	0.96	0.32	40,40,40,40	0
56	MG	1H	3501	1/1	0.96	0.12	70,70,70,70	0
56	MG	13	1621	1/1	0.96	0.33	97,97,97,97	0
56	MG	14	3042	1/1	0.96	0.23	48,48,48,48	0
56	MG	1H	3488	1/1	0.96	0.09	102,102,102,102	0
56	MG	14	3080	1/1	0.96	0.35	54,54,54,54	0
56	MG	1H	3346	1/1	0.96	0.18	64,64,64,64	0
56	MG	1H	3409	1/1	0.96	0.05	83,83,83,83	0
56	MG	1G	1672	1/1	0.96	0.35	100,100,100,100	0
56	MG	1H	3262	1/1	0.96	0.17	57,57,57,57	0
56	MG	1H	3437	1/1	0.96	0.15	82,82,82,82	0
56	MG	1G	1683	1/1	0.96	0.26	123,123,123,123	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	1H	3045	1/1	0.96	0.35	75,75,75,75	0
56	MG	14	3066	1/1	0.96	0.52	65,65,65,65	0
56	MG	13	1751	1/1	0.96	0.21	70,70,70,70	0
56	MG	1H	3306	1/1	0.96	0.31	81,81,81,81	0
56	MG	14	3083	1/1	0.96	0.42	93,93,93,93	0
56	MG	1G	1604	1/1	0.96	0.20	95,95,95,95	0
56	MG	14	3033	1/1	0.96	0.27	69,69,69,69	0
56	MG	1H	3073	1/1	0.96	0.22	53,53,53,53	0
56	MG	1H	3303	1/1	0.96	0.21	88,88,88,88	0
56	MG	14	3011	1/1	0.96	0.56	57,57,57,57	0
56	MG	13	1647	1/1	0.96	0.54	75,75,75,75	0
56	MG	1H	3113	1/1	0.96	0.33	73,73,73,73	0
56	MG	1K	101	1/1	0.96	0.34	88,88,88,88	0
56	MG	1H	3526	1/1	0.96	0.15	46,46,46,46	0
56	MG	14	3045	1/1	0.96	0.56	60,60,60,60	0
56	MG	1H	3166	1/1	0.96	0.43	60,60,60,60	0
56	MG	1H	3162	1/1	0.96	0.17	55,55,55,55	0
56	MG	1H	3485	1/1	0.96	0.07	81,81,81,81	0
56	MG	14	3017	1/1	0.96	0.28	85,85,85,85	0
56	MG	1H	3410	1/1	0.96	0.12	62,62,62,62	0
56	MG	1G	1615	1/1	0.96	0.18	103,103,103,103	0
56	MG	14	3107	1/1	0.96	0.39	76,76,76,76	0
56	MG	1H	3369	1/1	0.96	0.14	70,70,70,70	0
56	MG	1H	3050	1/1	0.96	0.29	62,62,62,62	0
56	MG	14	3354	1/1	0.96	0.17	77,77,77,77	0
56	MG	E8	201	1/1	0.96	0.31	79,79,79,79	0
56	MG	1H	3422	1/1	0.96	0.09	83,83,83,83	0
56	MG	1H	3251	1/1	0.96	0.20	96,96,96,96	0
56	MG	14	3267	1/1	0.96	0.11	67,67,67,67	0
56	MG	1H	3399	1/1	0.96	0.09	67,67,67,67	0
56	MG	1H	3040	1/1	0.96	0.23	47,47,47,47	0
56	MG	1H	3372	1/1	0.96	0.14	65,65,65,65	0
56	MG	13	1637	1/1	0.96	0.62	59,59,59,59	0
56	MG	1H	3458	1/1	0.96	0.14	109,109,109,109	0
56	MG	1H	3403	1/1	0.96	0.20	48,48,48,48	0
56	MG	13	1733	1/1	0.96	0.11	101,101,101,101	0
56	MG	1H	3077	1/1	0.96	0.10	69,69,69,69	0
56	MG	1H	3177	1/1	0.96	0.23	62,62,62,62	0
56	MG	13	1719	1/1	0.96	0.14	64,64,64,64	0
56	MG	14	3183	1/1	0.96	0.45	83,83,83,83	0
56	MG	13	1605	1/1	0.96	0.33	81,81,81,81	0
56	MG	1H	3515	1/1	0.96	0.15	46,46,46,46	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	1H	3111	1/1	0.96	0.28	100,100,100,100	0
56	MG	1H	3413	1/1	0.96	0.08	71,71,71,71	0
56	MG	1H	3384	1/1	0.96	0.11	62,62,62,62	0
56	MG	14	3008	1/1	0.96	0.48	58,58,58,58	0
56	MG	14	3140	1/1	0.96	0.28	65,65,65,65	0
56	MG	1H	3484	1/1	0.96	0.10	89,89,89,89	0
56	MG	14	3343	1/1	0.96	0.04	100,100,100,100	0
56	MG	1H	3043	1/1	0.96	0.23	50,50,50,50	0
56	MG	14	3309	1/1	0.96	0.12	86,86,86,86	0
56	MG	1H	3446	1/1	0.96	0.05	84,84,84,84	0
56	MG	14	3054	1/1	0.96	0.43	59,59,59,59	0
56	MG	14	3352	1/1	0.96	0.08	106,106,106,106	0
56	MG	1G	1617	1/1	0.97	0.31	99,99,99,99	0
56	MG	1H	3371	1/1	0.97	0.15	53,53,53,53	0
56	MG	13	1604	1/1	0.97	0.31	89,89,89,89	0
56	MG	1H	3525	1/1	0.97	0.10	43,43,43,43	0
56	MG	13	1734	1/1	0.97	0.04	87,87,87,87	0
56	MG	14	3370	1/1	0.97	0.10	88,88,88,88	0
56	MG	14	3332	1/1	0.97	0.08	88,88,88,88	0
56	MG	14	3310	1/1	0.97	0.05	78,78,78,78	0
56	MG	1G	1603	1/1	0.97	0.40	83,83,83,83	0
56	MG	1G	1688	1/1	0.97	0.12	73,73,73,73	0
56	MG	14	3369	1/1	0.97	0.05	96,96,96,96	0
56	MG	14	3025	1/1	0.97	0.31	53,53,53,53	0
56	MG	1H	3436	1/1	0.97	0.07	79,79,79,79	0
56	MG	1H	3411	1/1	0.97	0.03	101,101,101,101	0
56	MG	14	3277	1/1	0.97	0.11	67,67,67,67	0
56	MG	1H	3361	1/1	0.97	0.04	105,105,105,105	0
56	MG	14	3347	1/1	0.97	0.10	75,75,75,75	0
56	MG	1H	3370	1/1	0.97	0.15	51,51,51,51	0
56	MG	1H	3391	1/1	0.97	0.10	53,53,53,53	0
56	MG	14	3262	1/1	0.97	0.10	88,88,88,88	0
56	MG	14	3320	1/1	0.97	0.09	72,72,72,72	0
56	MG	1H	3476	1/1	0.97	0.07	65,65,65,65	0
56	MG	1H	3049	1/1	0.97	0.21	74,74,74,74	0
56	MG	14	3389	1/1	0.97	0.21	62,62,62,62	0
56	MG	14	3047	1/1	0.97	0.30	59,59,59,59	0
56	MG	14	3040	1/1	0.97	0.43	49,49,49,49	0
56	MG	14	3306	1/1	0.97	0.17	49,49,49,49	0
56	MG	1H	3472	1/1	0.97	0.07	61,61,61,61	0
56	MG	1H	3497	1/1	0.97	0.10	51,51,51,51	0
56	MG	1H	3008	1/1	0.97	0.31	56,56,56,56	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	1G	1621	1/1	0.97	0.24	92,92,92,92	0
56	MG	1H	3024	1/1	0.97	0.30	53,53,53,53	0
56	MG	1H	3001	1/1	0.97	0.42	45,45,45,45	0
56	MG	1H	3056	1/1	0.97	0.33	54,54,54,54	0
56	MG	13	1643	1/1	0.97	0.36	96,96,96,96	0
56	MG	14	3019	1/1	0.97	0.50	56,56,56,56	0
56	MG	1H	3355	1/1	0.97	0.08	53,53,53,53	0
56	MG	14	3386	1/1	0.97	0.09	51,51,51,51	0
56	MG	14	3304	1/1	0.97	0.08	91,91,91,91	0
56	MG	1H	3459	1/1	0.97	0.10	64,64,64,64	0
56	MG	1H	3065	1/1	0.97	0.66	51,51,51,51	0
56	MG	1G	1657	1/1	0.97	0.48	87,87,87,87	0
56	MG	14	3073	1/1	0.97	0.38	58,58,58,58	0
56	MG	1H	3506	1/1	0.97	0.06	88,88,88,88	0
56	MG	14	3346	1/1	0.97	0.11	80,80,80,80	0
56	MG	14	3355	1/1	0.97	0.10	97,97,97,97	0
56	MG	1H	3347	1/1	0.97	0.16	59,59,59,59	0
56	MG	14	3012	1/1	0.97	0.46	49,49,49,49	0
56	MG	1H	3004	1/1	0.97	0.37	57,57,57,57	0
56	MG	14	3002	1/1	0.97	0.37	67,67,67,67	0
56	MG	1H	3061	1/1	0.97	0.42	61,61,61,61	0
56	MG	14	3065	1/1	0.97	0.48	49,49,49,49	0
56	MG	14	3273	1/1	0.97	0.08	53,53,53,53	0
56	MG	13	1729	1/1	0.97	0.08	111,111,111,111	0
56	MG	14	3314	1/1	0.97	0.08	64,64,64,64	0
56	MG	13	1669	1/1	0.97	0.23	142,142,142,142	0
56	MG	1H	3187	1/1	0.97	0.40	89,89,89,89	0
56	MG	14	3281	1/1	0.97	0.10	79,79,79,79	0
56	MG	14	3085	1/1	0.97	0.36	77,77,77,77	0
56	MG	1H	3339	1/1	0.97	0.11	50,50,50,50	0
56	MG	14	3059	1/1	0.97	0.27	59,59,59,59	0
56	MG	14	3048	1/1	0.97	0.40	65,65,65,65	0
56	MG	1H	3258	1/1	0.97	0.37	68,68,68,68	0
56	MG	1G	1614	1/1	0.97	0.64	78,78,78,78	0
56	MG	21	301	1/1	0.97	0.38	55,55,55,55	0
56	MG	13	1630	1/1	0.97	0.36	57,57,57,57	0
56	MG	14	3303	1/1	0.97	0.07	107,107,107,107	0
56	MG	1H	3394	1/1	0.97	0.16	54,54,54,54	0
56	MG	13	1631	1/1	0.97	0.27	82,82,82,82	0
56	MG	1H	3517	1/1	0.97	0.11	71,71,71,71	0
56	MG	14	3284	1/1	0.97	0.16	49,49,49,49	0
56	MG	14	3091	1/1	0.97	0.28	54,54,54,54	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	14	3147	1/1	0.97	0.25	95,95,95,95	0
56	MG	13	1629	1/1	0.97	0.25	87,87,87,87	0
56	MG	1G	1649	1/1	0.97	0.16	145,145,145,145	0
56	MG	14	3308	1/1	0.97	0.11	68,68,68,68	0
56	MG	1H	3382	1/1	0.97	0.13	60,60,60,60	0
56	MG	13	1627	1/1	0.97	0.24	57,57,57,57	0
56	MG	14	3027	1/1	0.97	0.25	91,91,91,91	0
56	MG	1H	3060	1/1	0.97	0.49	48,48,48,48	0
56	MG	14	3062	1/1	0.97	0.24	69,69,69,69	0
56	MG	1G	1623	1/1	0.97	0.37	114,114,114,114	0
56	MG	1H	3381	1/1	0.97	0.07	46,46,46,46	0
56	MG	1H	3343	1/1	0.97	0.14	48,48,48,48	0
56	MG	1H	3167	1/1	0.97	0.19	62,62,62,62	0
56	MG	1H	3418	1/1	0.97	0.14	56,56,56,56	0
56	MG	1H	3007	1/1	0.97	0.36	40,40,40,40	0
56	MG	14	3127	1/1	0.97	0.34	83,83,83,83	0
57	ZN	3E	303	1/1	0.97	0.39	110,110,110,110	0
56	MG	13	1602	1/1	0.97	0.37	68,68,68,68	0
56	MG	1H	3112	1/1	0.97	0.43	72,72,72,72	0
56	MG	13	1731	1/1	0.97	0.07	69,69,69,69	0
56	MG	14	3064	1/1	0.97	0.50	68,68,68,68	0
56	MG	14	3263	1/1	0.97	0.09	60,60,60,60	0
56	MG	1H	3032	1/1	0.97	0.36	46,46,46,46	0
56	MG	1H	3017	1/1	0.97	0.27	43,43,43,43	0
56	MG	14	3290	1/1	0.97	0.16	61,61,61,61	0
56	MG	14	3264	1/1	0.97	0.10	53,53,53,53	0
56	MG	1H	3362	1/1	0.97	0.11	72,72,72,72	0
56	MG	14	3357	1/1	0.97	0.14	82,82,82,82	0
56	MG	1H	3481	1/1	0.97	0.06	79,79,79,79	0
56	MG	13	1722	1/1	0.97	0.23	94,94,94,94	0
56	MG	14	3001	1/1	0.98	0.46	58,58,58,58	0
56	MG	1H	3302	1/1	0.98	0.14	81,81,81,81	0
56	MG	14	3302	1/1	0.98	0.11	73,73,73,73	0
56	MG	1G	1689	1/1	0.98	0.16	80,80,80,80	0
56	MG	1H	3482	1/1	0.98	0.16	66,66,66,66	0
56	MG	1H	3018	1/1	0.98	0.23	83,83,83,83	0
56	MG	14	3286	1/1	0.98	0.14	58,58,58,58	0
56	MG	1H	3345	1/1	0.98	0.10	47,47,47,47	0
56	MG	1H	3081	1/1	0.98	0.37	63,63,63,63	0
56	MG	1H	3357	1/1	0.98	0.10	52,52,52,52	0
56	MG	14	3350	1/1	0.98	0.06	84,84,84,84	0
56	MG	1H	3352	1/1	0.98	0.14	43,43,43,43	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	13	1624	1/1	0.98	0.70	71,71,71,71	0
56	MG	14	3101	1/1	0.98	0.16	55,55,55,55	0
56	MG	14	3300	1/1	0.98	0.13	47,47,47,47	0
56	MG	1H	3389	1/1	0.98	0.09	51,51,51,51	0
56	MG	1H	3452	1/1	0.98	0.09	69,69,69,69	0
56	MG	13	1603	1/1	0.98	0.36	74,74,74,74	0
56	MG	1H	3088	1/1	0.98	0.24	61,61,61,61	0
56	MG	14	3060	1/1	0.98	0.36	65,65,65,65	0
56	MG	1H	3387	1/1	0.98	0.12	57,57,57,57	0
56	MG	1H	3104	1/1	0.98	0.20	67,67,67,67	0
56	MG	1G	1660	1/1	0.98	0.07	92,92,92,92	0
56	MG	14	3003	1/1	0.98	0.39	45,45,45,45	0
56	MG	14	3058	1/1	0.98	0.50	49,49,49,49	0
56	MG	1H	3425	1/1	0.98	0.13	67,67,67,67	0
56	MG	1H	3016	1/1	0.98	0.40	61,61,61,61	0
56	MG	1H	3358	1/1	0.98	0.12	65,65,65,65	0
56	MG	1H	3002	1/1	0.98	0.27	30,30,30,30	0
56	MG	1H	3373	1/1	0.98	0.07	63,63,63,63	0
56	MG	14	3298	1/1	0.98	0.10	59,59,59,59	0
57	ZN	32	301	1/1	0.98	0.35	123,123,123,123	0
56	MG	13	1720	1/1	0.98	0.08	66,66,66,66	0
56	MG	14	3106	1/1	0.98	0.55	70,70,70,70	0
56	MG	1H	3140	1/1	0.98	0.34	59,59,59,59	0
56	MG	1H	3460	1/1	0.98	0.07	63,63,63,63	0
56	MG	1H	3341	1/1	0.98	0.13	49,49,49,49	0
56	MG	1H	3080	1/1	0.98	0.41	53,53,53,53	0
56	MG	14	3342	1/1	0.98	0.10	72,72,72,72	0
56	MG	14	3185	1/1	0.98	0.38	64,64,64,64	0
56	MG	1H	3392	1/1	0.98	0.19	42,42,42,42	0
56	MG	1H	3005	1/1	0.98	0.43	46,46,46,46	0
56	MG	1H	3160	1/1	0.98	0.26	92,92,92,92	0
56	MG	1H	3141	1/1	0.98	0.13	53,53,53,53	0
56	MG	1H	3448	1/1	0.98	0.04	68,68,68,68	0
56	MG	1H	3366	1/1	0.98	0.14	68,68,68,68	0
56	MG	13	1735	1/1	0.98	0.13	77,77,77,77	0
56	MG	14	3344	1/1	0.98	0.09	85,85,85,85	0
56	MG	14	3078	1/1	0.98	0.23	68,68,68,68	0
56	MG	1G	1602	1/1	0.98	0.46	72,72,72,72	0
56	MG	13	1736	1/1	0.98	0.15	86,86,86,86	0
56	MG	1H	3385	1/1	0.98	0.12	66,66,66,66	0
56	MG	1H	3474	1/1	0.98	0.06	91,91,91,91	0
56	MG	1H	3003	1/1	0.98	0.32	63,63,63,63	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	14	3056	1/1	0.98	0.35	64,64,64,64	0
56	MG	1H	3454	1/1	0.98	0.08	106,106,106,106	0
56	MG	14	3248	1/1	0.98	0.21	85,85,85,85	0
56	MG	13	1601	1/1	0.98	0.26	83,83,83,83	0
56	MG	1H	3011	1/1	0.98	0.39	54,54,54,54	0
56	MG	1H	3147	1/1	0.98	0.15	49,49,49,49	0
56	MG	1H	3407	1/1	0.98	0.08	84,84,84,84	0
56	MG	1H	3033	1/1	0.98	0.28	75,75,75,75	0
56	MG	14	3270	1/1	0.98	0.13	75,75,75,75	0
56	MG	1H	3523	1/1	0.98	0.50	37,37,37,37	0
56	MG	13	1730	1/1	0.98	0.10	75,75,75,75	0
56	MG	1H	3416	1/1	0.98	0.06	69,69,69,69	0
56	MG	1H	3502	1/1	0.98	0.10	49,49,49,49	0
56	MG	14	3345	1/1	0.98	0.07	72,72,72,72	0
56	MG	1H	3434	1/1	0.98	0.06	72,72,72,72	0
56	MG	1H	3463	1/1	0.98	0.07	82,82,82,82	0
56	MG	14	3374	1/1	0.98	0.06	57,57,57,57	0
56	MG	1H	3071	1/1	0.98	0.30	51,51,51,51	0
56	MG	1H	3449	1/1	0.98	0.07	66,66,66,66	0
56	MG	1H	3393	1/1	0.98	0.16	44,44,44,44	0
56	MG	1H	3034	1/1	0.98	0.37	91,91,91,91	0
56	MG	1H	3340	1/1	0.98	0.19	41,41,41,41	0
56	MG	1H	3408	1/1	0.98	0.13	58,58,58,58	0
56	MG	1H	3440	1/1	0.98	0.10	63,63,63,63	0
56	MG	14	3179	1/1	0.98	0.29	86,86,86,86	0
56	MG	1H	3396	1/1	0.98	0.04	79,79,79,79	0
56	MG	14	3004	1/1	0.98	0.31	53,53,53,53	0
56	MG	14	3265	1/1	0.98	0.11	61,61,61,61	0
56	MG	1H	3055	1/1	0.98	0.33	52,52,52,52	0
56	MG	14	3043	1/1	0.99	0.46	57,57,57,57	0
56	MG	14	3072	1/1	0.99	0.21	75,75,75,75	0
56	MG	14	3010	1/1	0.99	0.33	58,58,58,58	0
56	MG	2L	101	1/1	0.99	0.37	88,88,88,88	0
56	MG	1H	3383	1/1	0.99	0.05	48,48,48,48	0
56	MG	29	301	1/1	0.99	0.38	49,49,49,49	0
56	MG	1H	3168	1/1	0.99	0.49	84,84,84,84	0
56	MG	14	3013	1/1	0.99	0.28	66,66,66,66	0
56	MG	14	3035	1/1	0.99	0.47	71,71,71,71	0
56	MG	14	3275	1/1	0.99	0.12	71,71,71,71	0
56	MG	1G	1601	1/1	0.99	0.34	94,94,94,94	0
56	MG	1H	3015	1/1	0.99	0.16	57,57,57,57	0
57	ZN	5I	101	1/1	0.99	0.13	111,111,111,111	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	1H	3432	1/1	0.99	0.03	83,83,83,83	0
56	MG	14	3388	1/1	0.99	0.12	80,80,80,80	0
56	MG	1H	3376	1/1	0.99	0.06	70,70,70,70	0
56	MG	14	3291	1/1	0.99	0.14	54,54,54,54	0
56	MG	14	3006	1/1	0.99	0.56	60,60,60,60	0
56	MG	14	3005	1/1	0.99	0.46	48,48,48,48	0
56	MG	1H	3010	1/1	0.99	0.27	47,47,47,47	0
56	MG	1H	3395	1/1	0.99	0.14	48,48,48,48	0
56	MG	1H	3029	1/1	0.99	0.31	65,65,65,65	0
56	MG	14	3050	1/1	0.99	0.28	81,81,81,81	0
56	MG	1H	3194	1/1	0.99	0.32	48,48,48,48	0
56	MG	1H	3519	1/1	0.99	0.03	94,94,94,94	0
56	MG	1H	3424	1/1	0.99	0.14	49,49,49,49	0
56	MG	1H	3342	1/1	0.99	0.14	57,57,57,57	0
56	MG	14	3296	1/1	0.99	0.17	53,53,53,53	0
56	MG	1H	3421	1/1	0.99	0.18	64,64,64,64	0
56	MG	14	3368	1/1	0.99	0.12	53,53,53,53	0
56	MG	1H	3353	1/1	0.99	0.15	61,61,61,61	0
56	MG	14	3247	1/1	0.99	0.20	61,61,61,61	0
56	MG	1H	3398	1/1	0.99	0.13	63,63,63,63	0
56	MG	14	3088	1/1	0.99	0.32	44,44,44,44	0
56	MG	13	1661	1/1	0.99	0.15	95,95,95,95	0

6.5 Other polymers ⓘ

There are no such residues in this entry.