



# wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 19, 2016 – 11:46 PM GMT

PDB ID : 4WSM  
Title : Complex of 70S ribosome with tRNA-Leu and mRNA with G-U mismatch in the first position in the A- and P-sites  
Authors : Rozov, A.; Demeshkina, N.; Yusupov, M.; Yusupova, G.  
Deposited on : 2014-10-28  
Resolution : 3.30 Å(reported)

This is a wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.  
We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)  
A user guide is available at  
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467  
Mogul : 1.7.1 (RC1), CSD as537be (2016)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026982  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : rb-20026982

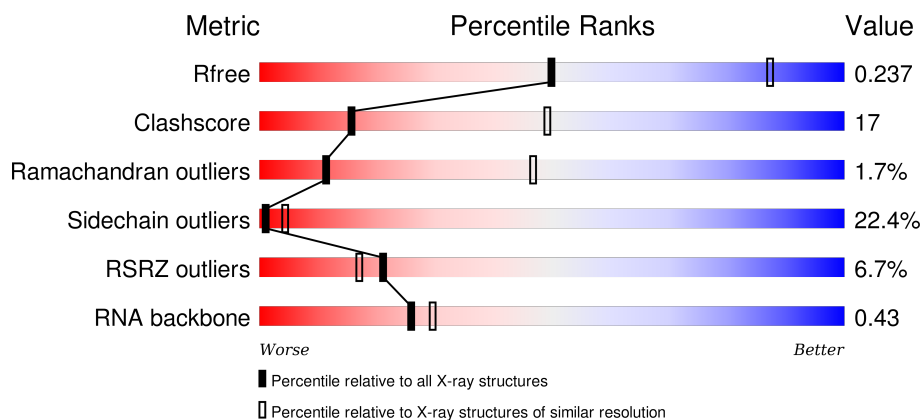
# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 3.30 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))
$R_{free}$	91344	2060 (3.40-3.20)
Clashscore	102246	1058 (3.38-3.22)
Ramachandran outliers	100387	1038 (3.38-3.22)
Sidechain outliers	100360	1037 (3.38-3.22)
RSRZ outliers	91569	2070 (3.40-3.20)
RNA backbone	2183	1005 (3.82-2.78)

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

Mol	Chain	Length	Quality of chain
1	13	1522	<div> <div>37%</div> <div>44%</div> <div>16%</div> <div>..</div> </div>
1	1G	1522	<div> <div>38%</div> <div>42%</div> <div>16%</div> <div>..</div> </div>
2	12	256	<div> <div>10%</div> <div>40%</div> <div>39%</div> <div>13%</div> <div>7%</div> </div>
2	1E	256	<div> <div>6%</div> <div>42%</div> <div>40%</div> <div>10%</div> <div>7%</div> </div>

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

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Mol	Chain	Length	Quality of chain
15	6I	89	
16	7A	88	
16	7I	88	
17	8A	105	
17	8I	105	
18	9A	88	
18	9I	88	
19	AA	93	
19	AI	93	
20	BA	106	
20	BI	106	
21	1B	27	
21	1F	27	
22	1K	87	
22	1L	87	
23	2K	87	
23	2L	87	
24	3K	87	
24	3L	87	
25	4K	60	
25	4L	60	
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	L5	49	
53	P8	49	
54	M5	65	
54	Q8	65	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
55	MG	13	1601	-	-	-	X
55	MG	13	1602	-	-	-	X
55	MG	13	1604	-	-	-	X
55	MG	13	1606	-	-	-	X
55	MG	13	1608	-	-	-	X
55	MG	13	1609	-	-	-	X
55	MG	13	1610	-	-	-	X
55	MG	13	1613	-	-	-	X
55	MG	13	1615	-	-	-	X
55	MG	13	1619	-	-	-	X
55	MG	13	1622	-	-	-	X
55	MG	13	1626	-	-	-	X
55	MG	13	1629	-	-	-	X
55	MG	13	1632	-	-	-	X
55	MG	13	1635	-	-	-	X
55	MG	13	1636	-	-	-	X
55	MG	13	1638	-	-	-	X
55	MG	13	1639	-	-	-	X
55	MG	13	1661	-	-	-	X
55	MG	13	1667	-	-	-	X
55	MG	13	1672	-	-	-	X
55	MG	13	1680	-	-	-	X
55	MG	13	1681	-	-	-	X
55	MG	13	1688	-	-	-	X
55	MG	13	1697	-	-	-	X
55	MG	13	1700	-	-	-	X
55	MG	13	1709	-	-	-	X
55	MG	13	1711	-	-	-	X
55	MG	13	1713	-	-	-	X
55	MG	13	1716	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
55	MG	13	1720	-	-	-	X
55	MG	13	1724	-	-	-	X
55	MG	13	1728	-	-	-	X
55	MG	13	1731	-	-	-	X
55	MG	14	3005	-	-	-	X
55	MG	14	3009	-	-	-	X
55	MG	14	3011	-	-	-	X
55	MG	14	3013	-	-	-	X
55	MG	14	3017	-	-	-	X
55	MG	14	3024	-	-	-	X
55	MG	14	3030	-	-	-	X
55	MG	14	3031	-	-	-	X
55	MG	14	3032	-	-	-	X
55	MG	14	3034	-	-	-	X
55	MG	14	3036	-	-	-	X
55	MG	14	3037	-	-	-	X
55	MG	14	3038	-	-	-	X
55	MG	14	3039	-	-	-	X
55	MG	14	3040	-	-	-	X
55	MG	14	3041	-	-	-	X
55	MG	14	3042	-	-	-	X
55	MG	14	3044	-	-	-	X
55	MG	14	3046	-	-	-	X
55	MG	14	3052	-	-	-	X
55	MG	14	3059	-	-	-	X
55	MG	14	3065	-	-	-	X
55	MG	14	3066	-	-	-	X
55	MG	14	3067	-	-	-	X
55	MG	14	3071	-	-	-	X
55	MG	14	3072	-	-	-	X
55	MG	14	3074	-	-	-	X
55	MG	14	3090	-	-	-	X
55	MG	14	3093	-	-	-	X
55	MG	14	3094	-	-	-	X
55	MG	14	3099	-	-	-	X
55	MG	14	3100	-	-	-	X
55	MG	14	3105	-	-	-	X
55	MG	14	3108	-	-	-	X
55	MG	14	3109	-	-	-	X
55	MG	14	3110	-	-	-	X
55	MG	14	3120	-	-	-	X
55	MG	14	3121	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
55	MG	14	3124	-	-	-	X
55	MG	14	3130	-	-	-	X
55	MG	14	3140	-	-	-	X
55	MG	14	3146	-	-	-	X
55	MG	14	3148	-	-	-	X
55	MG	14	3150	-	-	-	X
55	MG	14	3153	-	-	-	X
55	MG	14	3155	-	-	-	X
55	MG	14	3165	-	-	-	X
55	MG	14	3166	-	-	-	X
55	MG	14	3170	-	-	-	X
55	MG	14	3172	-	-	-	X
55	MG	14	3173	-	-	-	X
55	MG	14	3177	-	-	-	X
55	MG	14	3179	-	-	-	X
55	MG	14	3183	-	-	-	X
55	MG	14	3188	-	-	-	X
55	MG	14	3190	-	-	-	X
55	MG	14	3196	-	-	-	X
55	MG	14	3197	-	-	-	X
55	MG	14	3199	-	-	-	X
55	MG	14	3200	-	-	-	X
55	MG	14	3205	-	-	-	X
55	MG	14	3206	-	-	-	X
55	MG	14	3207	-	-	-	X
55	MG	14	3224	-	-	-	X
55	MG	14	3225	-	-	-	X
55	MG	14	3229	-	-	-	X
55	MG	14	3241	-	-	-	X
55	MG	14	3243	-	-	-	X
55	MG	14	3253	-	-	-	X
55	MG	14	3262	-	-	-	X
55	MG	14	3274	-	-	-	X
55	MG	14	3276	-	-	-	X
55	MG	14	3280	-	-	-	X
55	MG	14	3285	-	-	-	X
55	MG	14	3292	-	-	-	X
55	MG	14	3295	-	-	-	X
55	MG	14	3300	-	-	-	X
55	MG	14	3301	-	-	-	X
55	MG	14	3314	-	-	-	X
55	MG	14	3319	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
55	MG	14	3330	-	-	-	X
55	MG	14	3350	-	-	-	X
55	MG	14	3353	-	-	-	X
55	MG	14	3363	-	-	-	X
55	MG	14	3366	-	-	-	X
55	MG	14	3373	-	-	-	X
55	MG	14	3488	-	-	-	X
55	MG	14	3490	-	-	-	X
55	MG	16	201	-	-	-	X
55	MG	16	204	-	-	-	X
55	MG	1G	1602	-	-	-	X
55	MG	1G	1603	-	-	-	X
55	MG	1G	1604	-	-	-	X
55	MG	1G	1608	-	-	-	X
55	MG	1G	1613	-	-	-	X
55	MG	1G	1618	-	-	-	X
55	MG	1G	1619	-	-	-	X
55	MG	1G	1621	-	-	-	X
55	MG	1G	1622	-	-	-	X
55	MG	1G	1630	-	-	-	X
55	MG	1G	1641	-	-	-	X
55	MG	1G	1644	-	-	-	X
55	MG	1G	1649	-	-	-	X
55	MG	1G	1656	-	-	-	X
55	MG	1G	1672	-	-	-	X
55	MG	1G	1676	-	-	-	X
55	MG	1G	1685	-	-	-	X
55	MG	1G	1686	-	-	-	X
55	MG	1G	1687	-	-	-	X
55	MG	1G	1688	-	-	-	X
55	MG	1G	1695	-	-	-	X
55	MG	1G	1696	-	-	-	X
55	MG	1G	1701	-	-	-	X
55	MG	1G	1702	-	-	-	X
55	MG	1G	1704	-	-	-	X
55	MG	1G	1709	-	-	-	X
55	MG	1G	1710	-	-	-	X
55	MG	1G	1720	-	-	-	X
55	MG	1G	1722	-	-	-	X
55	MG	1G	1728	-	-	-	X
55	MG	1H	3001	-	-	-	X
55	MG	1H	3002	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
55	MG	1H	3003	-	-	-	X
55	MG	1H	3005	-	-	-	X
55	MG	1H	3009	-	-	-	X
55	MG	1H	3011	-	-	-	X
55	MG	1H	3016	-	-	-	X
55	MG	1H	3017	-	-	-	X
55	MG	1H	3018	-	-	-	X
55	MG	1H	3019	-	-	-	X
55	MG	1H	3021	-	-	-	X
55	MG	1H	3025	-	-	-	X
55	MG	1H	3029	-	-	-	X
55	MG	1H	3035	-	-	-	X
55	MG	1H	3038	-	-	-	X
55	MG	1H	3039	-	-	-	X
55	MG	1H	3040	-	-	-	X
55	MG	1H	3041	-	-	-	X
55	MG	1H	3043	-	-	-	X
55	MG	1H	3046	-	-	-	X
55	MG	1H	3052	-	-	-	X
55	MG	1H	3053	-	-	-	X
55	MG	1H	3055	-	-	-	X
55	MG	1H	3058	-	-	-	X
55	MG	1H	3060	-	-	-	X
55	MG	1H	3061	-	-	-	X
55	MG	1H	3066	-	-	-	X
55	MG	1H	3067	-	-	-	X
55	MG	1H	3071	-	-	-	X
55	MG	1H	3075	-	-	-	X
55	MG	1H	3076	-	-	-	X
55	MG	1H	3080	-	-	-	X
55	MG	1H	3083	-	-	-	X
55	MG	1H	3085	-	-	-	X
55	MG	1H	3087	-	-	-	X
55	MG	1H	3092	-	-	-	X
55	MG	1H	3096	-	-	-	X
55	MG	1H	3097	-	-	-	X
55	MG	1H	3098	-	-	-	X
55	MG	1H	3102	-	-	-	X
55	MG	1H	3103	-	-	-	X
55	MG	1H	3108	-	-	-	X
55	MG	1H	3110	-	-	-	X
55	MG	1H	3113	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
55	MG	1H	3115	-	-	-	X
55	MG	1H	3116	-	-	-	X
55	MG	1H	3118	-	-	-	X
55	MG	1H	3120	-	-	-	X
55	MG	1H	3121	-	-	-	X
55	MG	1H	3125	-	-	-	X
55	MG	1H	3130	-	-	-	X
55	MG	1H	3132	-	-	-	X
55	MG	1H	3135	-	-	-	X
55	MG	1H	3140	-	-	-	X
55	MG	1H	3142	-	-	-	X
55	MG	1H	3144	-	-	-	X
55	MG	1H	3148	-	-	-	X
55	MG	1H	3150	-	-	-	X
55	MG	1H	3152	-	-	-	X
55	MG	1H	3153	-	-	-	X
55	MG	1H	3161	-	-	-	X
55	MG	1H	3166	-	-	-	X
55	MG	1H	3168	-	-	-	X
55	MG	1H	3171	-	-	-	X
55	MG	1H	3173	-	-	-	X
55	MG	1H	3177	-	-	-	X
55	MG	1H	3180	-	-	-	X
55	MG	1H	3197	-	-	-	X
55	MG	1H	3209	-	-	-	X
55	MG	1H	3213	-	-	-	X
55	MG	1H	3216	-	-	-	X
55	MG	1H	3217	-	-	-	X
55	MG	1H	3226	-	-	-	X
55	MG	1H	3228	-	-	-	X
55	MG	1H	3244	-	-	-	X
55	MG	1H	3254	-	-	-	X
55	MG	1H	3263	-	-	-	X
55	MG	1H	3266	-	-	-	X
55	MG	1H	3268	-	-	-	X
55	MG	1H	3273	-	-	-	X
55	MG	1H	3279	-	-	-	X
55	MG	1H	3281	-	-	-	X
55	MG	1H	3283	-	-	-	X
55	MG	1H	3290	-	-	-	X
55	MG	1H	3299	-	-	-	X
55	MG	1H	3310	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
55	MG	1H	3314	-	-	-	X
55	MG	1H	3323	-	-	-	X
55	MG	1H	3326	-	-	-	X
55	MG	1H	3336	-	-	-	X
55	MG	1H	3344	-	-	-	X
55	MG	1H	3352	-	-	-	X
55	MG	1H	3355	-	-	-	X
55	MG	1H	3359	-	-	-	X
55	MG	1H	3363	-	-	-	X
55	MG	1H	3365	-	-	-	X
55	MG	1H	3369	-	-	-	X
55	MG	1H	3373	-	-	-	X
55	MG	1H	3377	-	-	-	X
55	MG	1H	3388	-	-	-	X
55	MG	1H	3395	-	-	-	X
55	MG	1H	3396	-	-	-	X
55	MG	1H	3405	-	-	-	X
55	MG	1H	3484	-	-	-	X
55	MG	1H	3509	-	-	-	X
55	MG	1H	3510	-	-	-	X
55	MG	1K	101	-	-	-	X
55	MG	29	301	-	-	-	X
55	MG	2L	101	-	-	-	X
56	ZN	3E	302	-	-	-	X
56	ZN	C5	201	-	-	-	X
56	ZN	G8	202	-	-	-	X

## 2 Entry composition [i](#)

There are 57 unique types of molecules in this entry. The entry contains 299429 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	1507	Total	C	N	O	P	0	0	0
			32389	14416	5999	10467	1507			
1	1G	1513	Total	C	N	O	P	0	0	0
			32511	14472	6018	10509	1512			

- 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
			1702	1066	339	290	7			
4	32	208	Total	C	N	O	S	0	0	0
			1702	1066	339	290	7			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	4E	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
			842	531	155	153	3			
6	52	101	Total	C	N	O	S	0	0	0
			842	531	155	153	3			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	6E	144	Total	C	N	O	S	0	0	0
			1157	718	230	203	6			
7	62	147	Total	C	N	O	S	0	0	0
			1200	750	237	207	6			

- Molecule 8 is a protein called 30S ribosomal protein S8.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	7E	138	Total	C	N	O	S	0	0	0
			1115	705	215	192	3			
8	72	138	Total	C	N	O	S	0	0	0
			1115	705	215	192	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
			1009	639	197	173			
9	82	124	Total	C	N	O	0	0	0
			983	624	190	169			

- 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	116	Total	C	N	O	S	0	0	0
			864	537	164	160	3			
11	2A	116	Total	C	N	O	S	0	0	0
			864	537	164	160	3			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	3I	122	Total	C	N	O	S	0	0	0
			956	603	193	159	1			
12	3A	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	116	Total	C	N	O	S	0	0	0
			928	574	191	161	2			
13	4A	116	Total	C	N	O	S	0	0	0
			928	574	191	161	2			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
14	5I	60	Total	C	N	O	S	0	0	0
			491	312	104	71	4			
14	5A	58	Total	C	N	O	S	0	0	0
			475	303	99	69	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
			733	459	147	125	2			
15	6A	88	Total	C	N	O	S	0	0	0
			733	459	147	125	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	99	Total	C	N	O	S	0	0	0
			823	528	151	142	2			

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
18	9I	67	Total	C	N	O	0	0	0
			550	352	107	91			
18	9A	69	Total	C	N	O	0	0	0
			564	361	110	93			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
19	AI	80	Total	C	N	O	S	0	0	0
			643	411	118	112	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
			762	470	162	128	2			
20	BA	99	Total	C	N	O	S	0	0	0
			762	470	162	128	2			

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
21	1F	23	Total	C	N	O	0	0	0
			199	122	48	29			
21	1B	25	Total	C	N	O	0	0	0
			217	134	52	31			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
22	1K	87	Total	C	N	O	P	0	0	0
			1863	831	333	612	87			
22	1L	87	Total	C	N	O	P	0	0	0
			1863	831	333	612	87			

- Molecule 23 is a RNA chain called tRNA-Leu.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
23	2K	79	Total	C	N	O	P	0	0	0
			1692	755	300	558	79			
23	2L	80	Total	C	N	O	P	0	0	0
			1712	764	303	565	80			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
24	3K	77	Total	C	N	O	P	0	0	0
			1646	733	292	544	77			
24	3L	75	Total	C	N	O	P	0	0	0
			1601	713	282	531	75			

- Molecule 25 is a RNA chain called mRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
25	4K	16	Total	C	N	O	P	0	0	0
			336	150	50	120	16			
25	4L	21	Total	C	N	O	P	0	0	0
			438	196	64	157	21			

- 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			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
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
			2126	1341	424	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			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
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			
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
			932	588	171	169	4			
35	25	122	Total	C	N	O	S	0	0	0
			932	588	171	169	4			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
36	78	147	Total	C	N	O	S	0	0	0
			1122	698	229	192	3			
36	35	150	Total	C	N	O	S	0	0	0
			1144	712	232	197	3			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
37	88	141	Total	C	N	O	S	0	0	0
			1121	715	212	187	7			
37	45	140	Total	C	N	O	S	0	0	0
			1113	710	211	186	6			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
38	98	118	Total	C	N	O	S	0	0	0
			967	604	203	159	1			
38	55	117	Total	C	N	O		0	0	0
			959	599	202	158				

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
39	A8	111	Total	C	N	O	0	0	0
			881	556	176	149			
39	65	111	Total	C	N	O	0	0	0
			881	556	176	149			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
40	B8	129	Total	C	N	O	S	0	0	0
			1081	674	223	183	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
			963	610	202	150	1			
41	85	117	Total	C	N	O	S	0	0	0
			963	610	202	150	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
			778	501	142	134	1			
42	95	101	Total	C	N	O	S	0	0	0
			778	501	142	134	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
43	E8	112	Total	C	N	O	S	0	0	0
			890	560	175	153	2			
43	A5	113	Total	C	N	O	S	0	0	0
			899	566	177	154	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	92	Total	C	N	O		0	0	0
			725	471	131	123				

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
45	G8	103	Total	C	N	O	S	0	0	0
			783	504	148	126	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	171	Total	C	N	O	S	0	0	0
			1373	876	247	247	3			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
46	D5	135	Total	C	N	O	S	0	0	0
			1120	720	202	195	3			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
47	I8	83	Total	C	N	O	S	0	0	0
			656	407	139	109	1			
47	E5	80	Total	C	N	O	S	0	0	0
			627	388	132	106	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	95	Total	C	N	O	S	0	0	0
			746	469	148	128	1			
48	F5	94	Total	C	N	O	S	0	0	0
			737	463	146	127	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
49	K8	68	Total	C	N	O	S	0	0	0
			575	358	116	100	1			
49	G5	67	Total	C	N	O	S	0	0	0
			567	351	115	100	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
			468	298	90	80			

- 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	55	Total	C	N	O	S	0	0	0
			429	269	86	69	5			
52	J5	56	Total	C	N	O	S	0	0	0
			434	272	87	70	5			

- Molecule 53 is a protein called 50S ribosomal protein L34.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
53	P8	47	Total	C	N	O	S	0	0	0
			409	251	102	54	2			
53	L5	47	Total	C	N	O	S	0	0	0
			409	251	102	54	2			

- Molecule 54 is a protein called 50S ribosomal protein L35.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
54	Q8	60	Total	C	N	O	S	0	0	0
			480	306	98	74	2			
54	M5	53	Total	C	N	O	S	0	0	0
			422	270	87	63	2			

- Molecule 55 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
55	98	1	Total	Mg	0	0
			1	1		
55	45	2	Total	Mg	0	0
			2	2		
55	P8	1	Total	Mg	0	0
			1	1		
55	85	2	Total	Mg	0	0
			2	2		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
55	32	1	Total 1	Mg 1	0	0
55	13	146	Total 146	Mg 146	0	0
55	1J	2	Total 2	Mg 2	0	0
55	16	5	Total 5	Mg 5	0	0
55	25	1	Total 1	Mg 1	0	0
55	21	2	Total 2	Mg 2	0	0
55	31	1	Total 1	Mg 1	0	0
55	3I	1	Total 1	Mg 1	0	0
55	I8	2	Total 2	Mg 2	0	0
55	5E	1	Total 1	Mg 1	0	0
55	29	3	Total 3	Mg 3	0	0
55	7A	1	Total 1	Mg 1	0	0
55	2K	3	Total 3	Mg 3	0	0
55	J8	1	Total 1	Mg 1	0	0
55	1G	143	Total 143	Mg 143	0	0
55	11	1	Total 1	Mg 1	0	0
55	1H	512	Total 512	Mg 512	0	0
55	E5	2	Total 2	Mg 2	0	0
55	88	4	Total 4	Mg 4	0	0
55	14	490	Total 490	Mg 490	0	0
55	78	1	Total 1	Mg 1	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
55	3E	1	Total 1	Mg 1	0	0
55	1K	1	Total 1	Mg 1	0	0
55	G8	1	Total 1	Mg 1	0	0
55	2L	2	Total 2	Mg 2	0	0

- Molecule 56 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
56	32	1	Total 1	Zn 1	0	0
56	3E	1	Total 1	Zn 1	0	0
56	5I	1	Total 1	Zn 1	0	0
56	5A	1	Total 1	Zn 1	0	0
56	G8	1	Total 1	Zn 1	0	0
56	C5	1	Total 1	Zn 1	0	0

- Molecule 57 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
57	13	74	Total 74	O 74	0	0
57	3E	1	Total 1	O 1	0	0
57	6I	1	Total 1	O 1	0	0
57	BI	1	Total 1	O 1	0	0
57	1H	552	Total 552	O 552	0	0
57	11	1	Total 1	O 1	0	0
57	21	1	Total 1	O 1	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
57	31	4	Total 4	O 4	0	0
57	78	2	Total 2	O 2	0	0
57	B8	1	Total 1	O 1	0	0
57	C8	2	Total 2	O 2	0	0
57	D8	1	Total 1	O 1	0	0
57	E8	1	Total 1	O 1	0	0
57	I8	3	Total 3	O 3	0	0
57	J8	1	Total 1	O 1	0	0
57	P8	1	Total 1	O 1	0	0
57	1G	73	Total 73	O 73	0	0
57	6A	2	Total 2	O 2	0	0
57	7A	1	Total 1	O 1	0	0
57	4L	2	Total 2	O 2	0	0
57	14	520	Total 520	O 520	0	0
57	19	8	Total 8	O 8	0	0
57	29	2	Total 2	O 2	0	0
57	39	4	Total 4	O 4	0	0
57	35	1	Total 1	O 1	0	0
57	55	2	Total 2	O 2	0	0
57	85	1	Total 1	O 1	0	0
57	A5	1	Total 1	O 1	0	0

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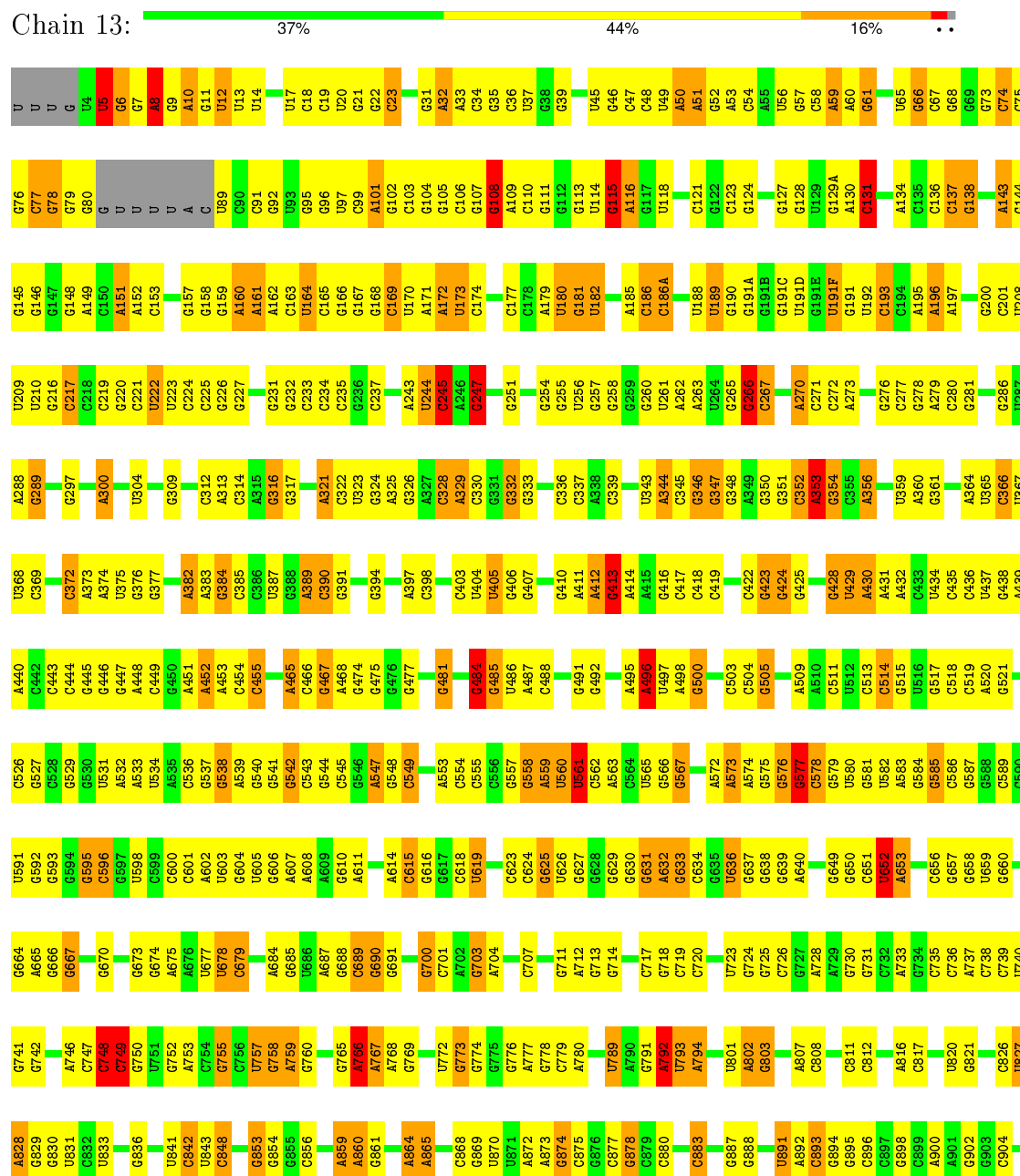
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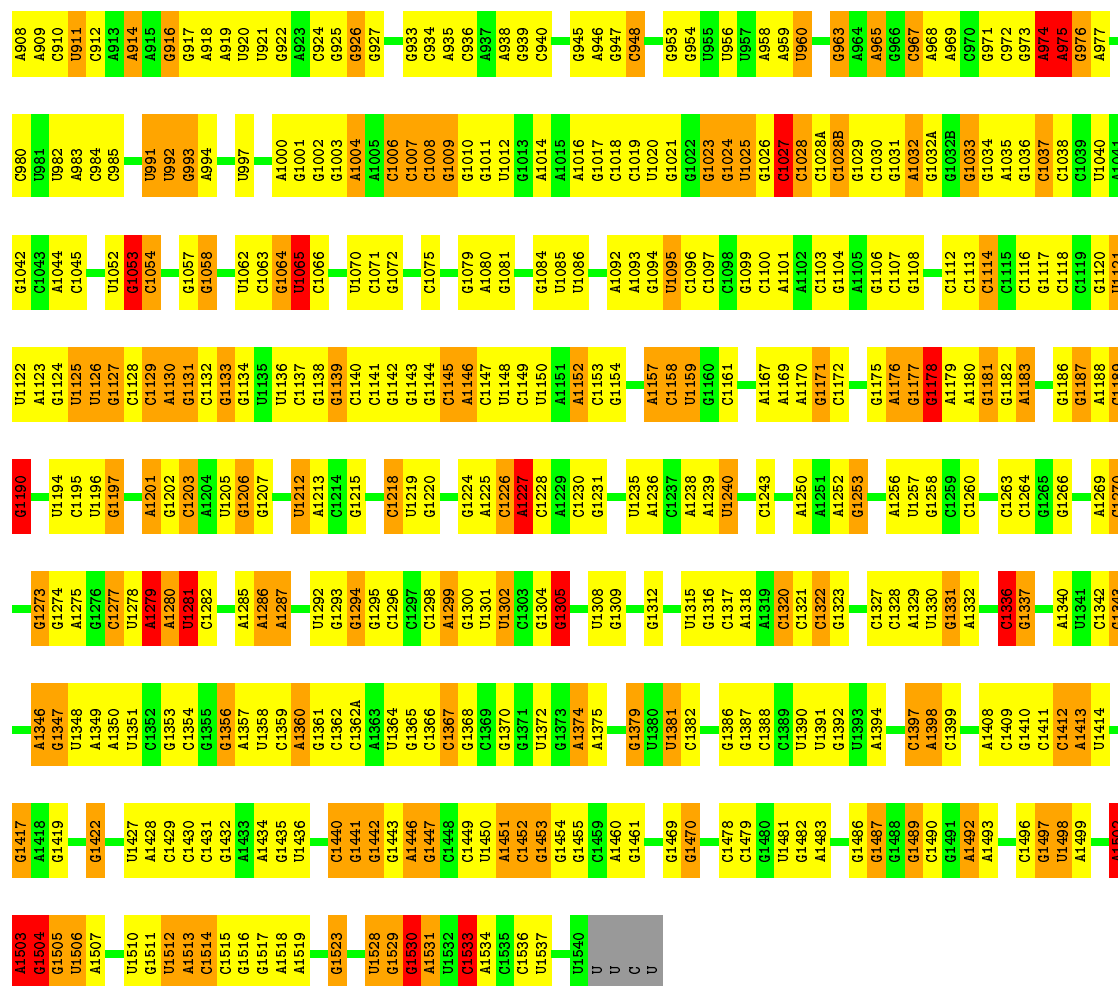
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57	M5	3	Total	O	0	0
			3	3		

### 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 errors 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 ( $\text{RSRZ} > 2$ ). 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.

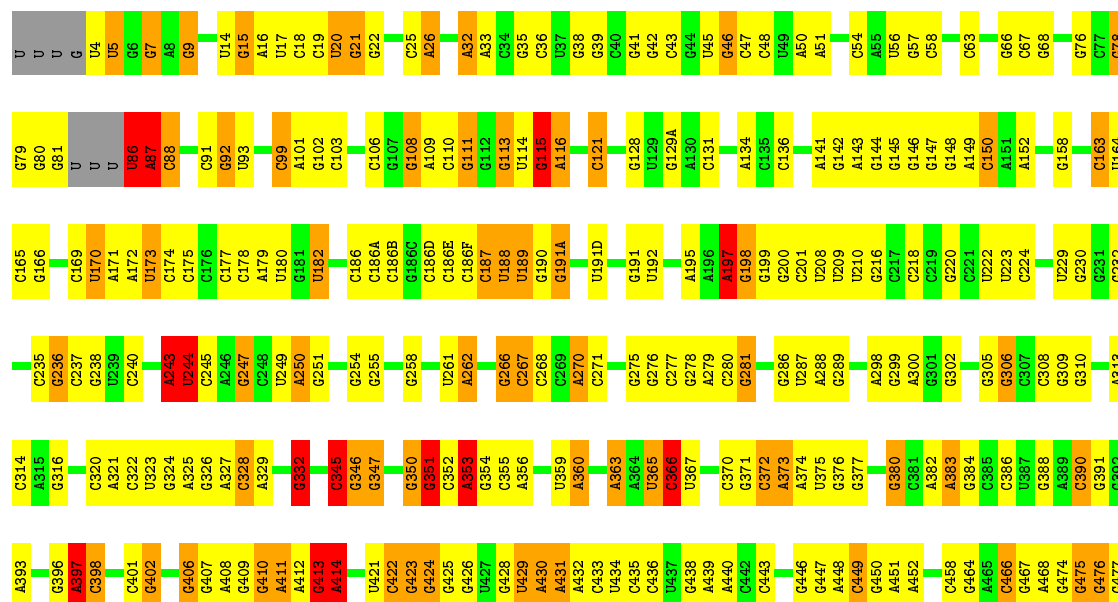
#### • Molecule 1: 16S ribosomal RNA

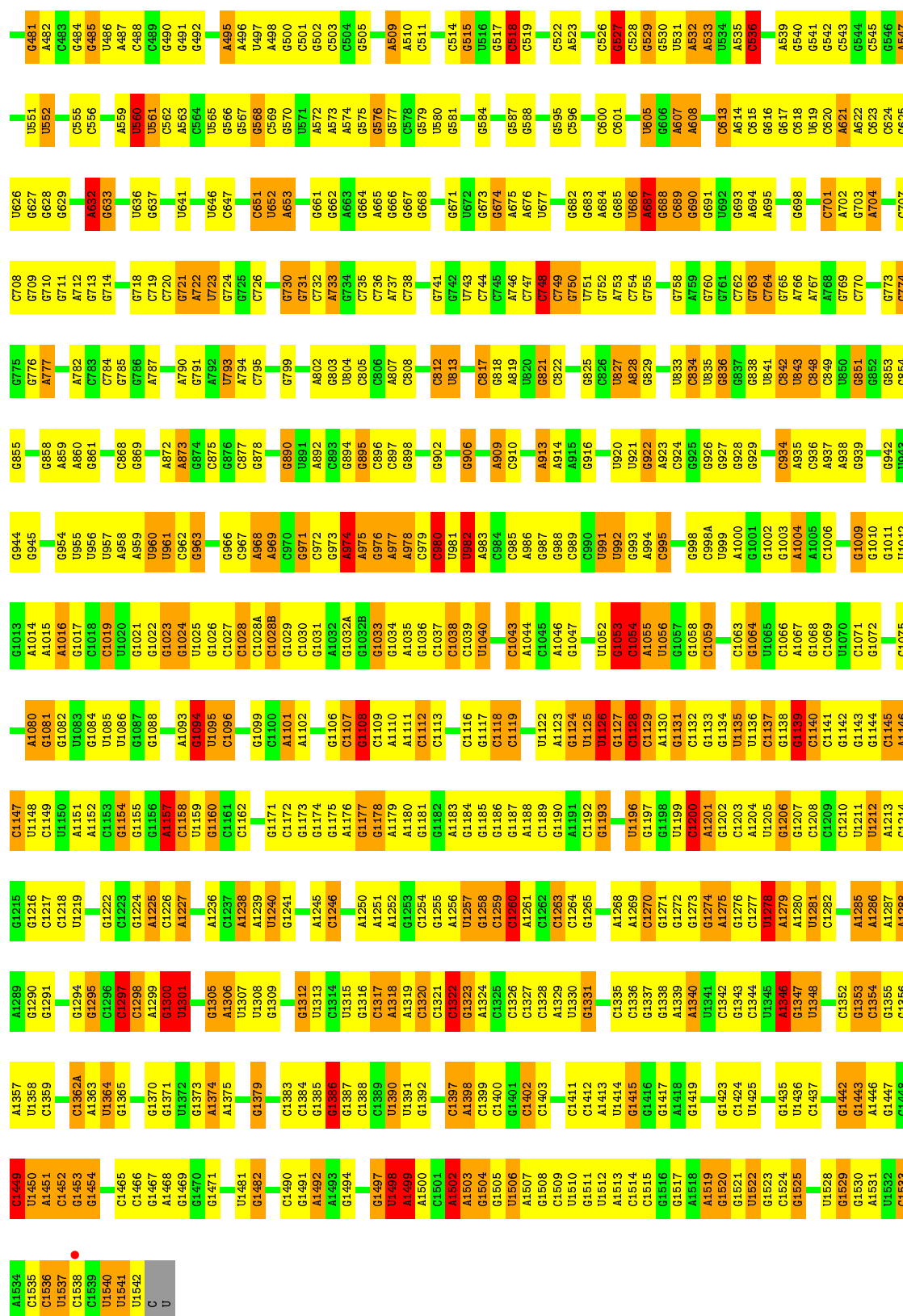




● Molecule 1: 16S ribosomal RNA

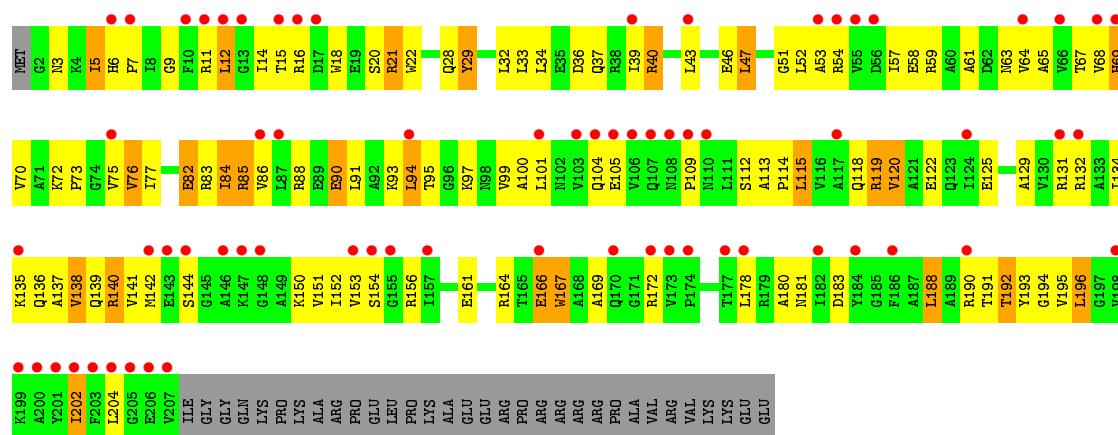
Chain 1G: 38% 42% 16%



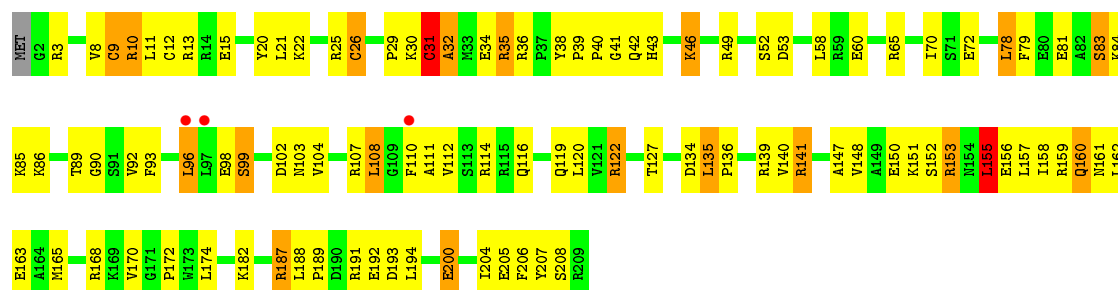




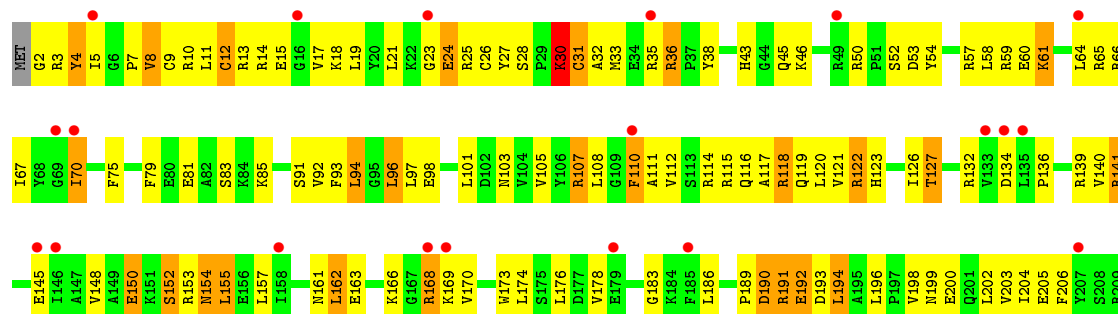
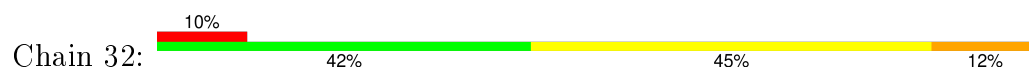




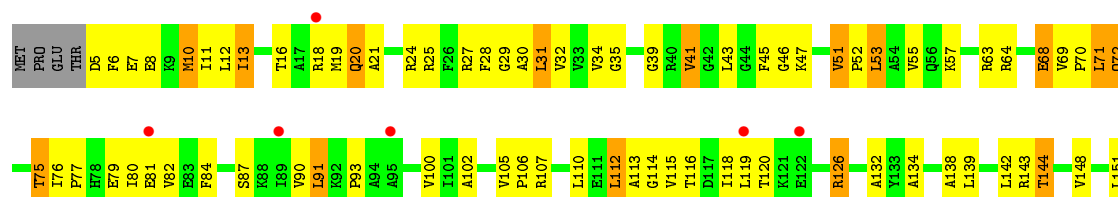
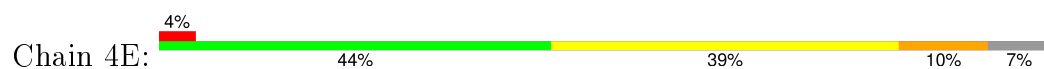
• Molecule 4: 30S ribosomal protein S4

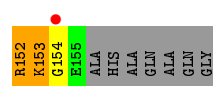


• Molecule 4: 30S ribosomal protein S4

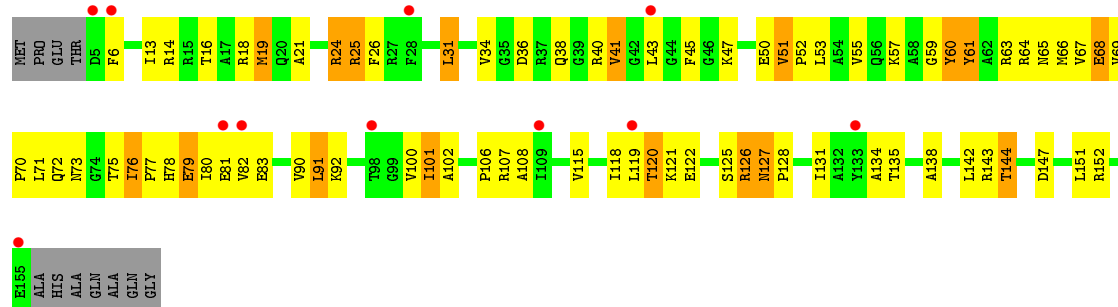


• Molecule 5: 30S ribosomal protein S5

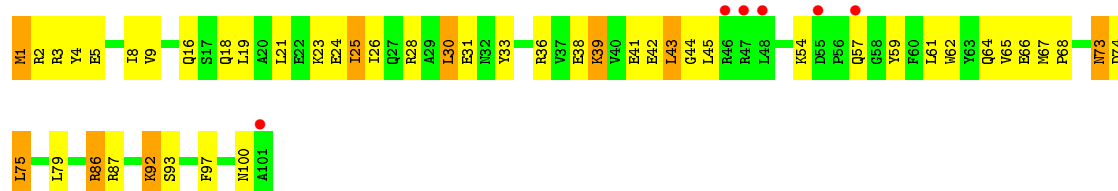




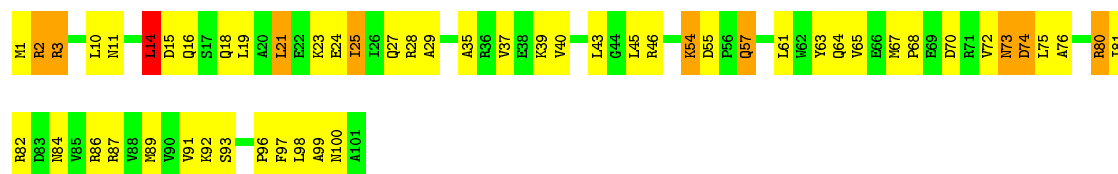
- Molecule 5: 30S ribosomal protein S5



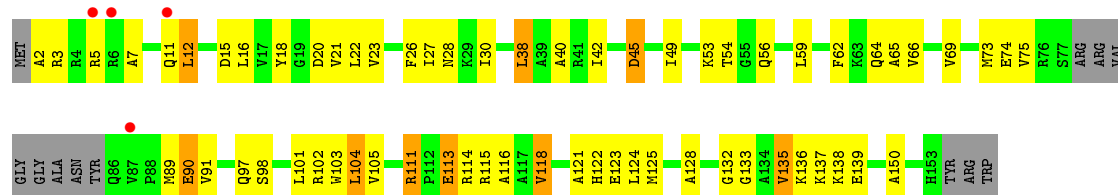
- Molecule 6: 30S ribosomal protein S6



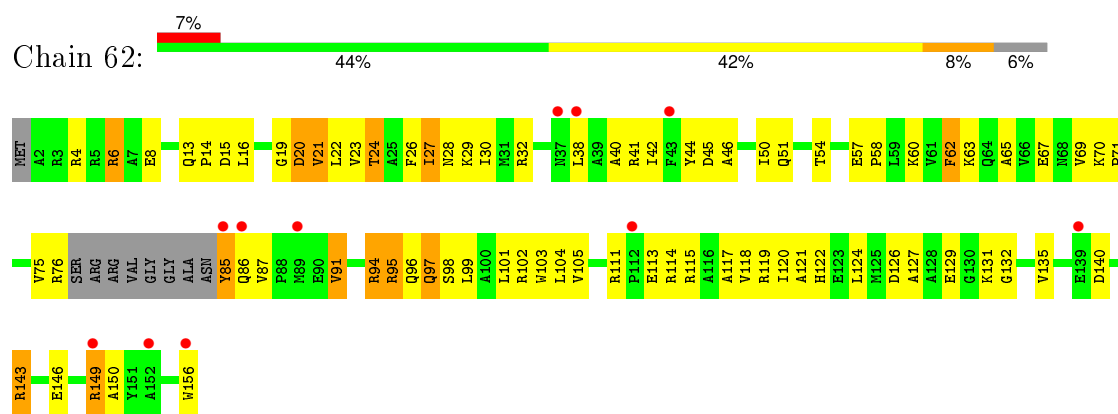
- Molecule 6: 30S ribosomal protein S6



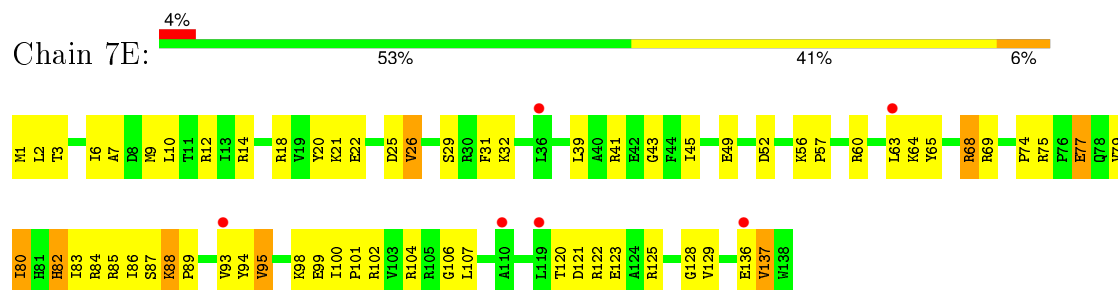
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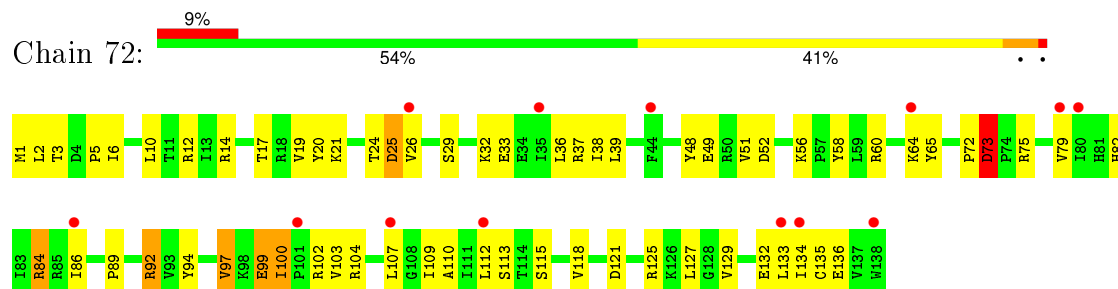
- Molecule 7: 30S ribosomal protein S7



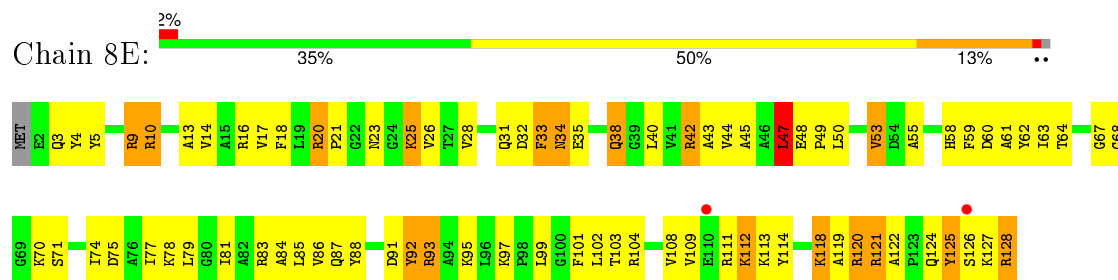
- Molecule 8: 30S ribosomal protein S8



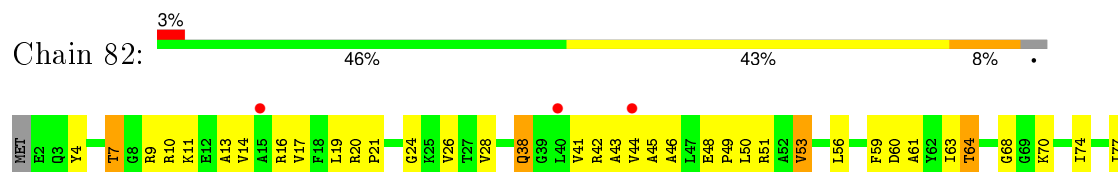
- Molecule 8: 30S ribosomal protein S8

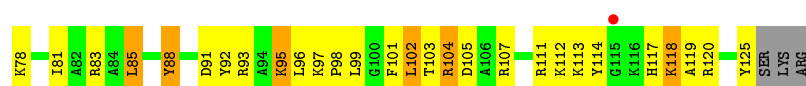


- Molecule 9: 30S ribosomal protein S9

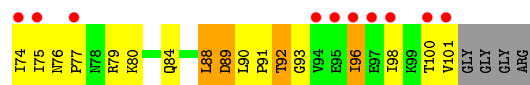
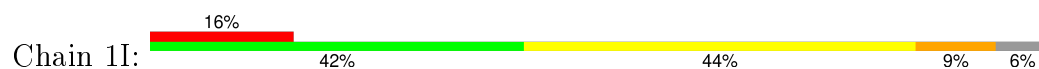


- Molecule 9: 30S ribosomal protein S9

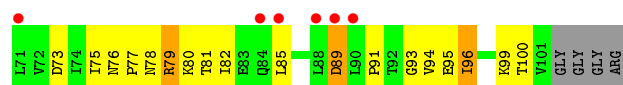




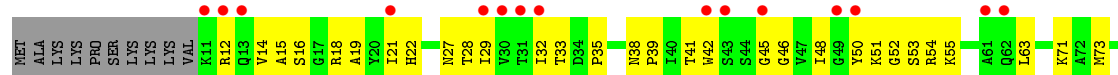
• Molecule 10: 30S ribosomal protein S10



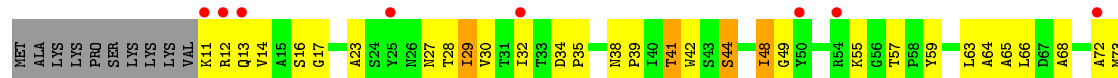
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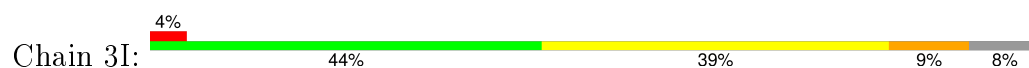
• Molecule 11: 30S ribosomal protein S11

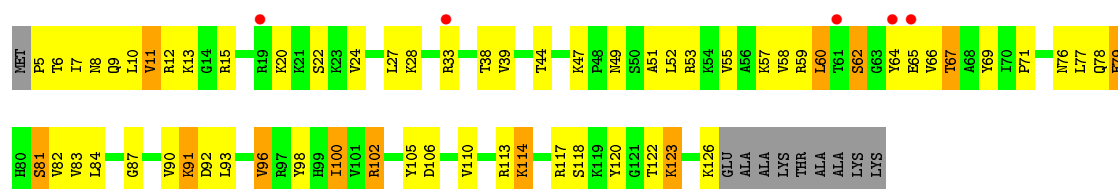


• Molecule 11: 30S ribosomal protein S11

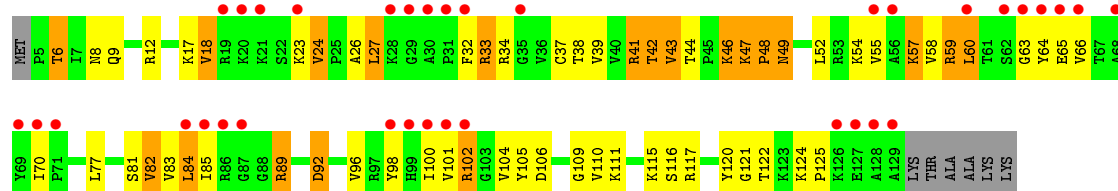


• Molecule 12: 30S ribosomal protein S12

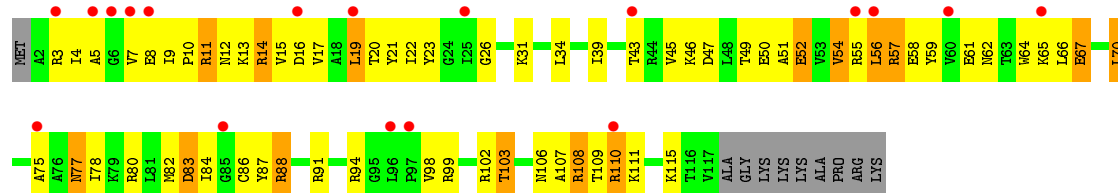




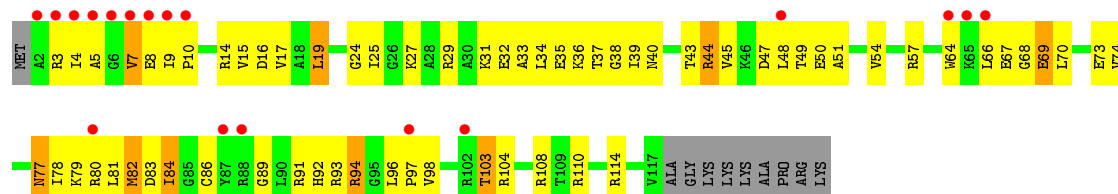
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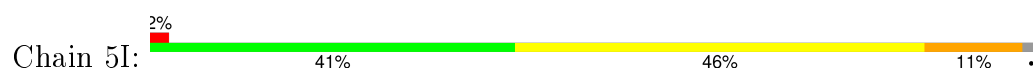
• Molecule 13: 30S ribosomal protein S13



• Molecule 13: 30S ribosomal protein S13

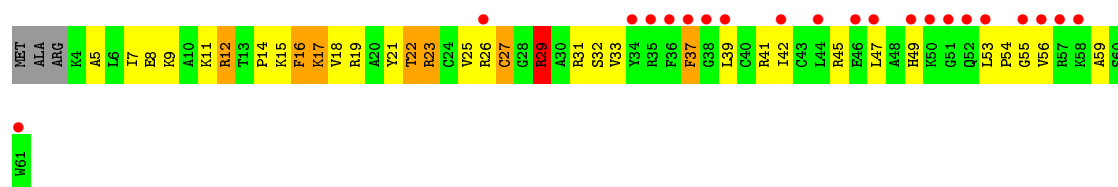


• Molecule 14: 30S ribosomal protein S14 type Z

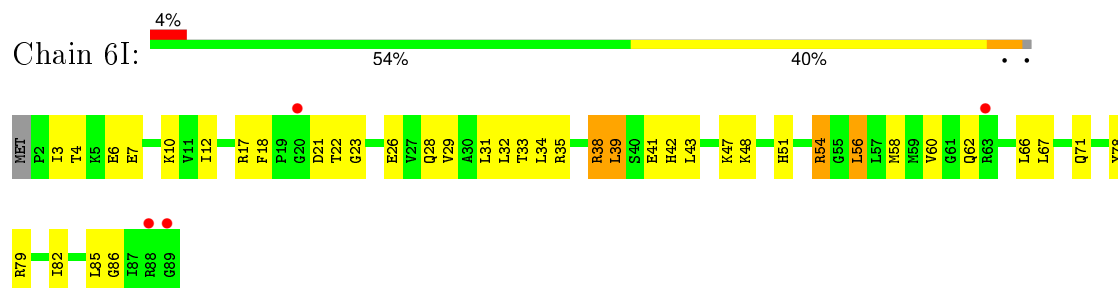


• Molecule 14: 30S ribosomal protein S14 type Z

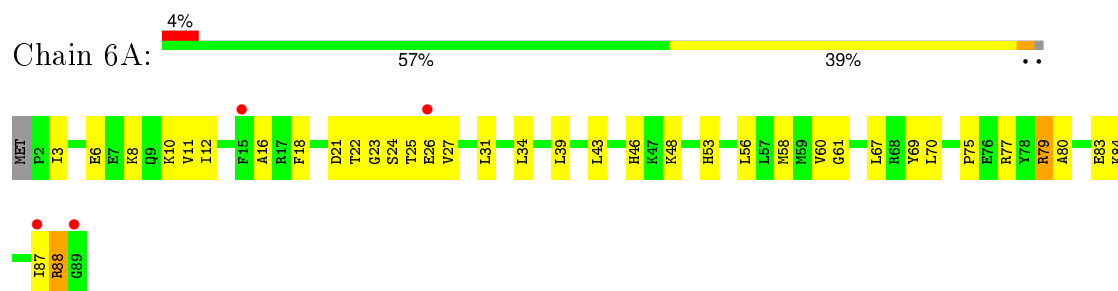




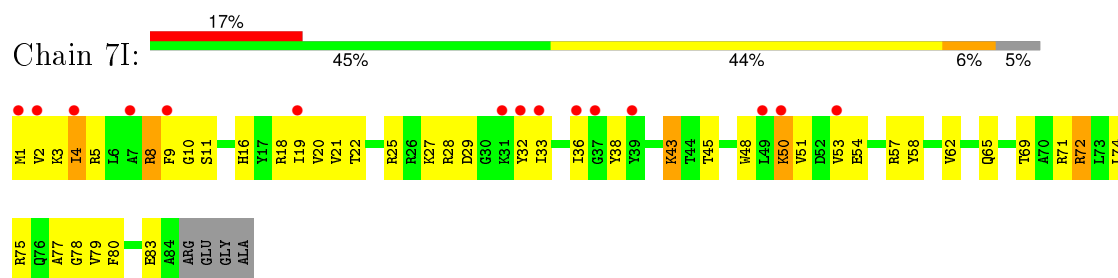
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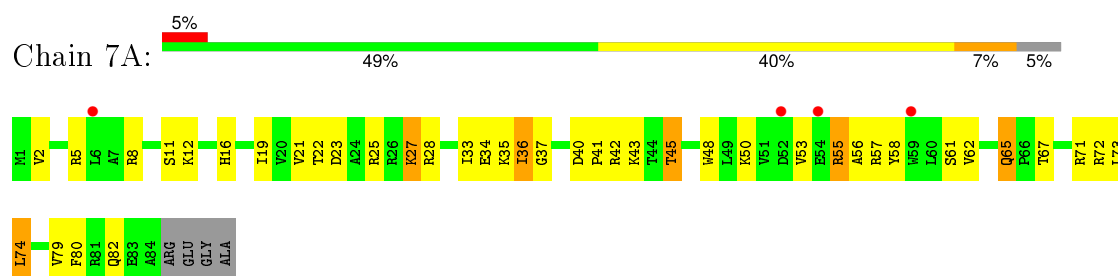
- Molecule 15: 30S ribosomal protein S15



- Molecule 16: 30S ribosomal protein S16

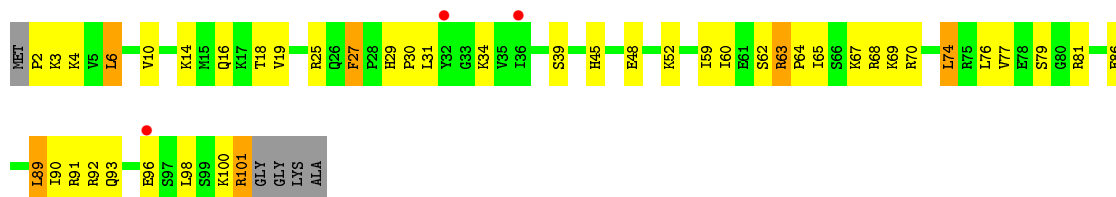


- Molecule 16: 30S ribosomal protein S16



- Molecule 17: 30S ribosomal protein S17

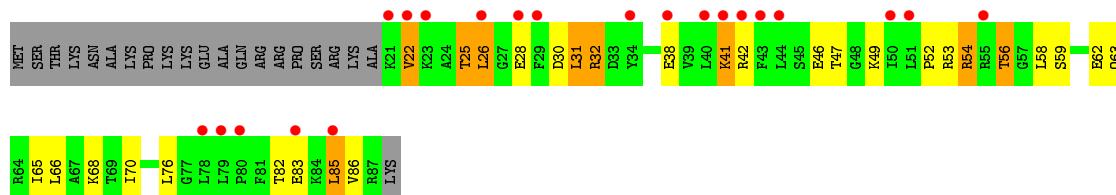




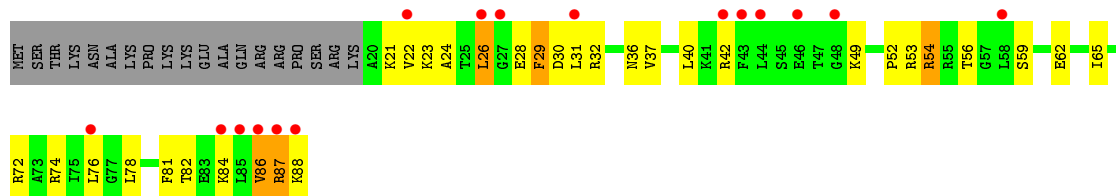
- Molecule 17: 30S ribosomal protein S17



- Molecule 18: 30S ribosomal protein S18



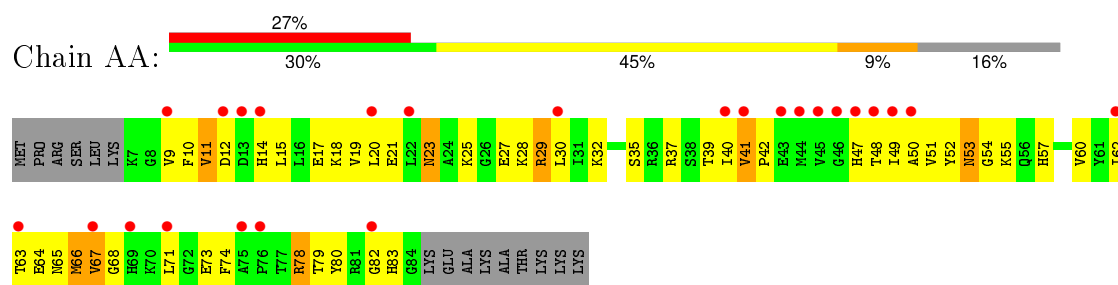
- Molecule 18: 30S ribosomal protein S18



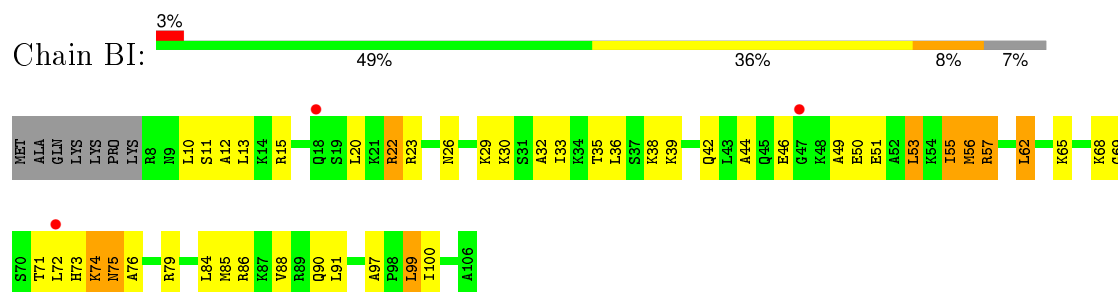
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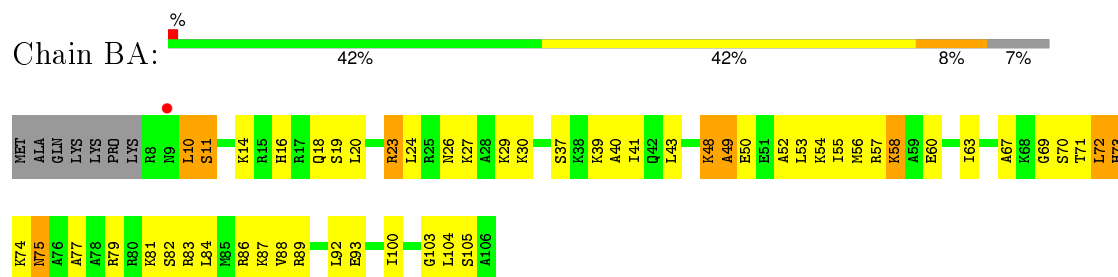
- Molecule 19: 30S ribosomal protein S19



- Molecule 20: 30S ribosomal protein S20



- Molecule 20: 30S ribosomal protein S20



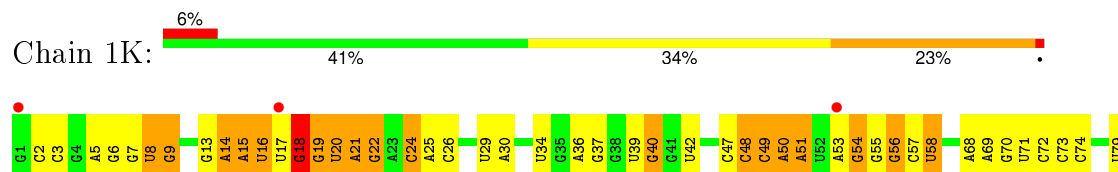
- Molecule 21: 30S ribosomal protein Thx



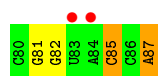
- Molecule 21: 30S ribosomal protein Thx



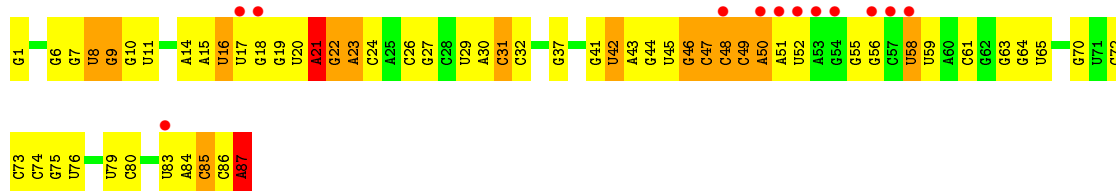
- Molecule 22: tRNA-Leu



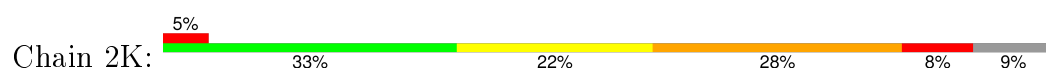




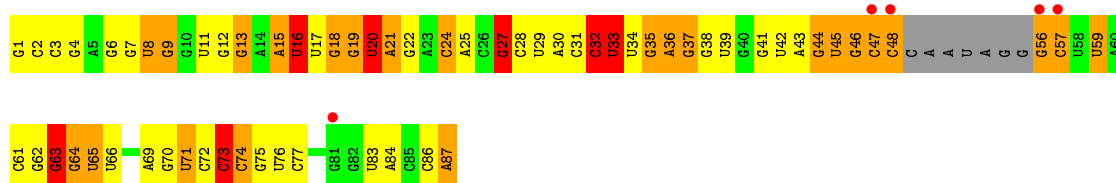
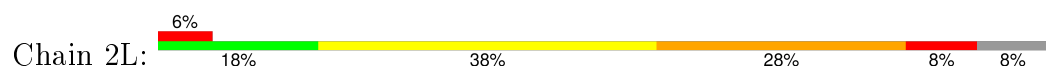
• Molecule 22: tRNA-Leu



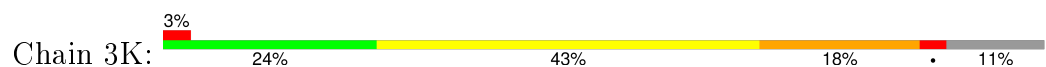
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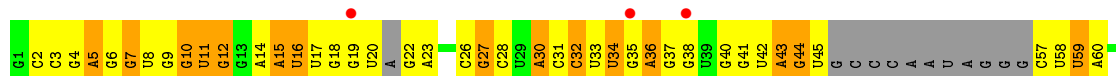
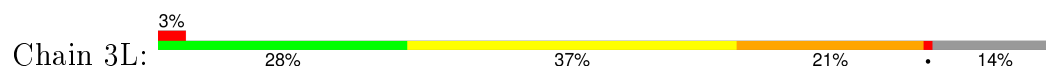
• Molecule 23: tRNA-Leu



• Molecule 24: tRNA-Leu



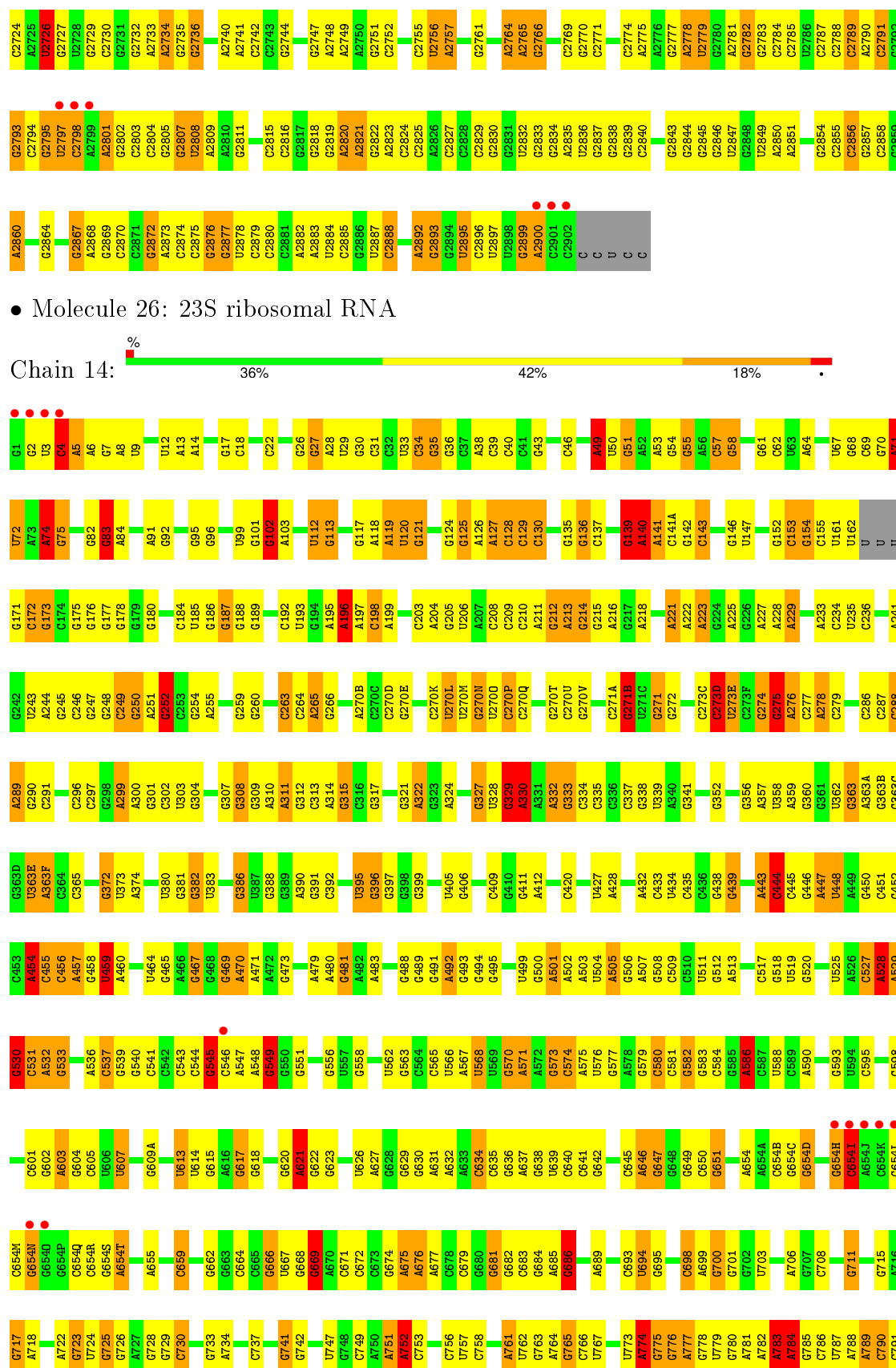
• Molecule 24: tRNA-Leu





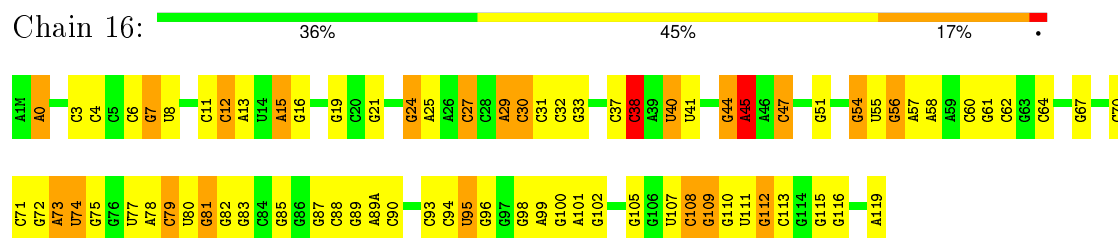




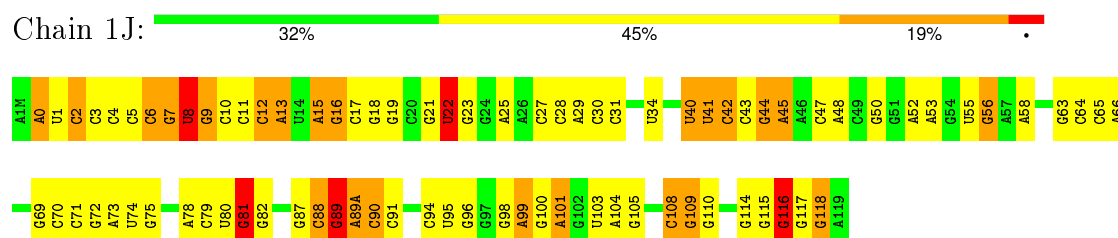


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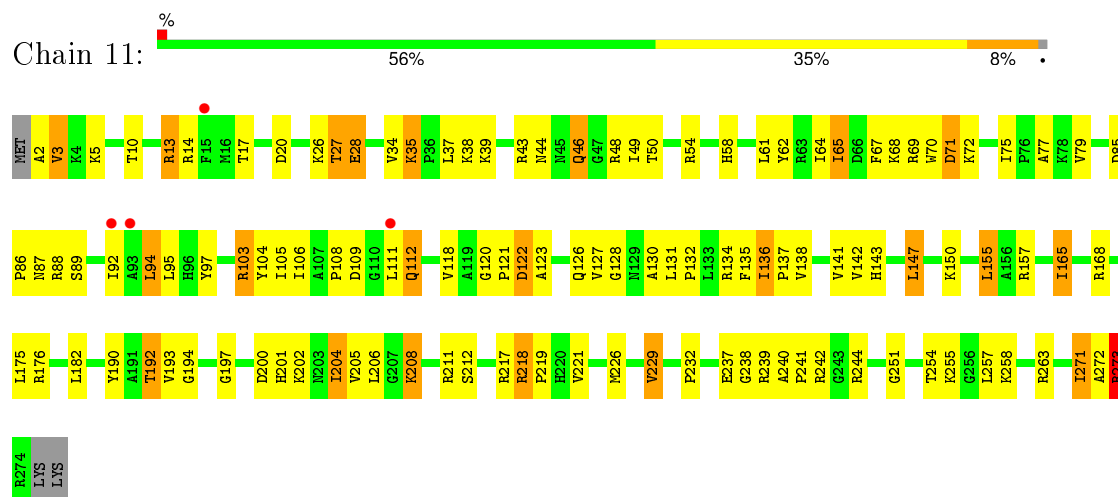
- Molecule 27: 5S ribosomal RNA



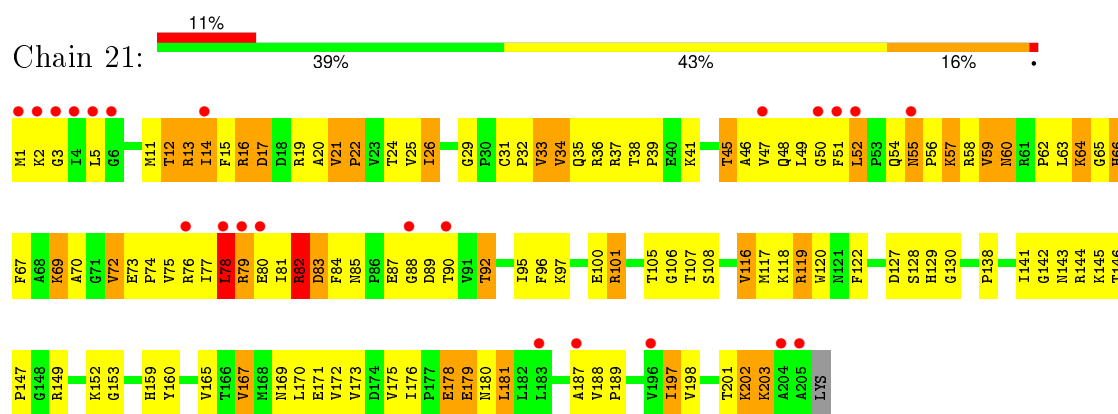
• Molecule 27: 5S ribosomal RNA



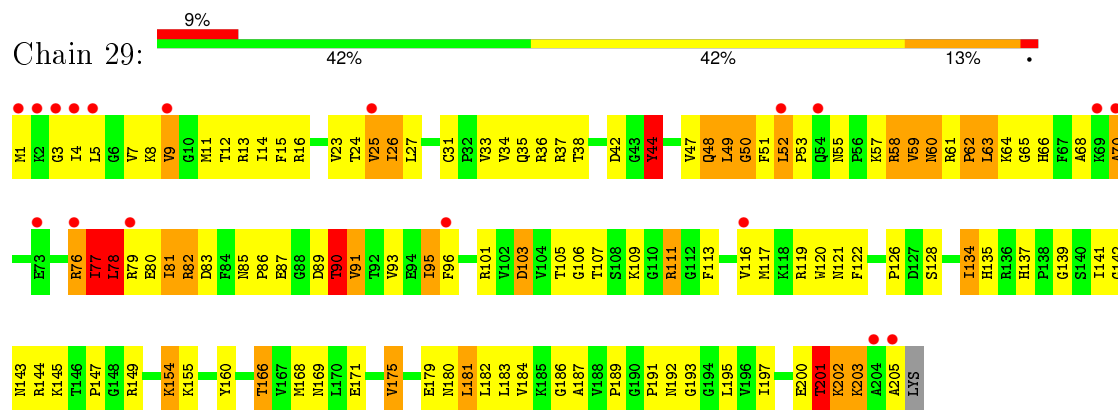
• Molecule 28: 50S ribosomal protein L2



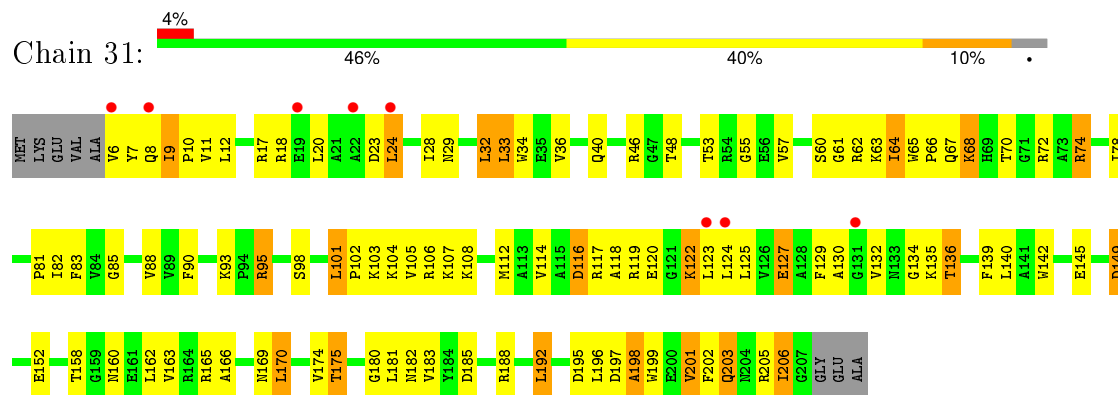




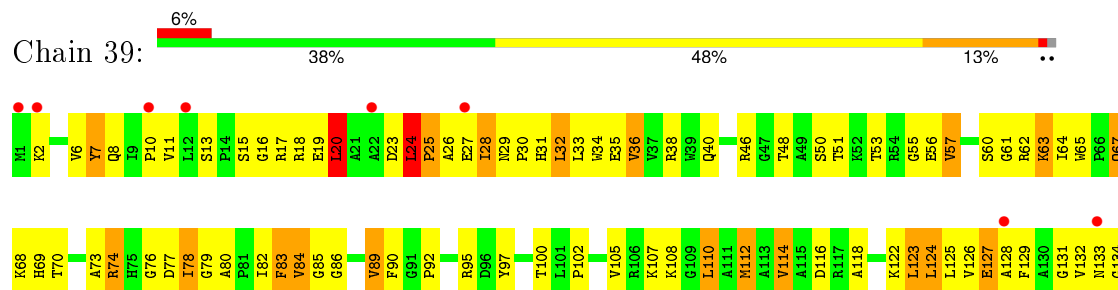
• Molecule 29: 50S ribosomal protein L3

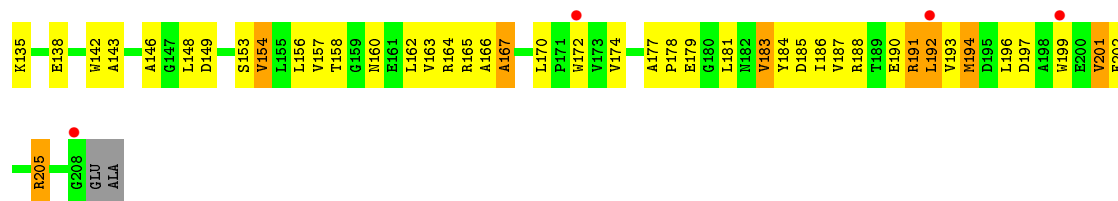


• Molecule 30: 50S ribosomal protein L4

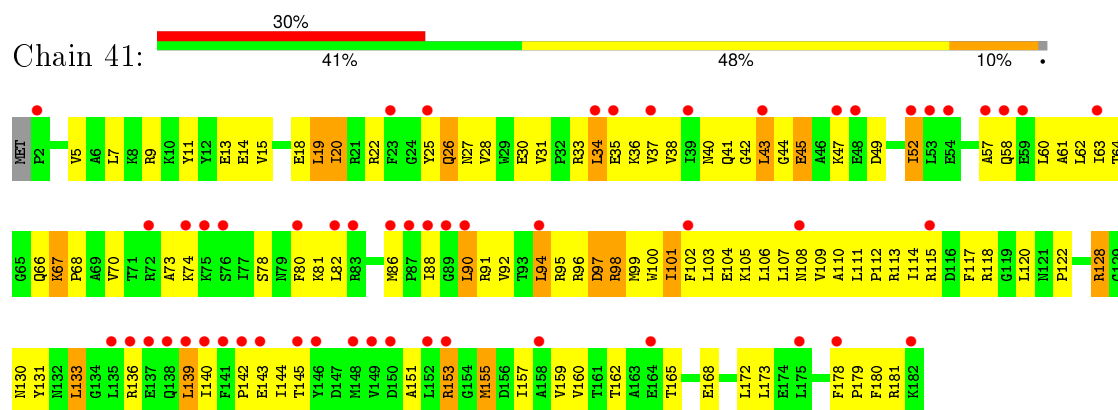


• Molecule 30: 50S ribosomal protein L4

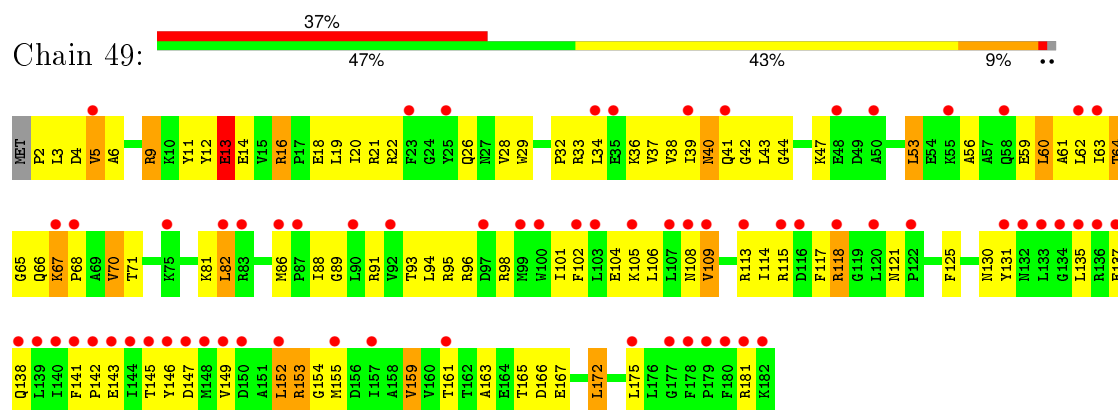




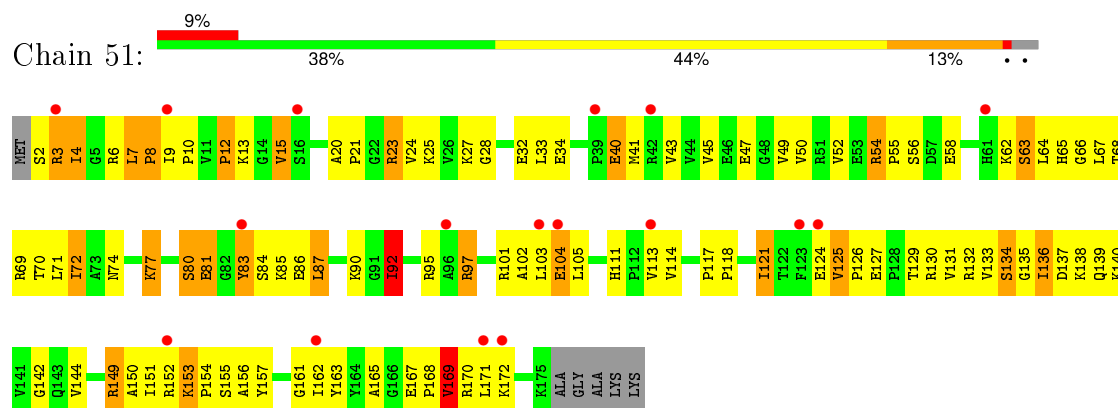
- Molecule 31: 50S ribosomal protein L5



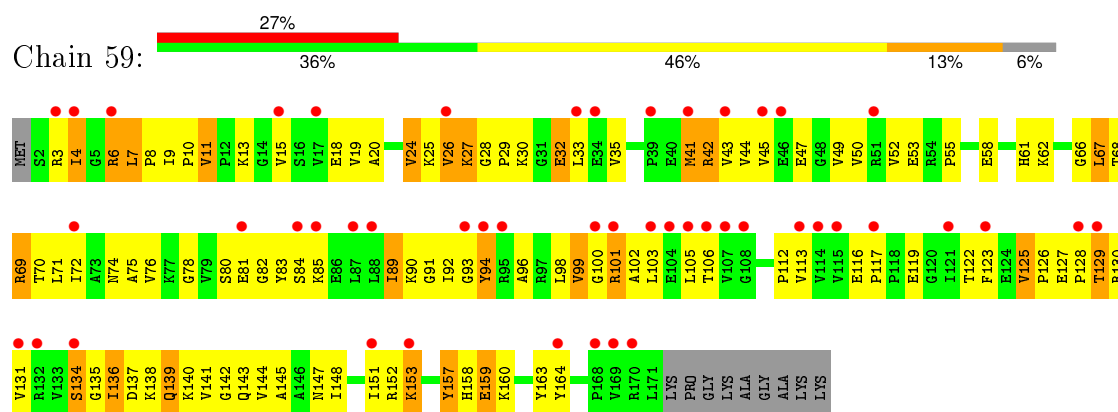
- Molecule 31: 50S ribosomal protein L5



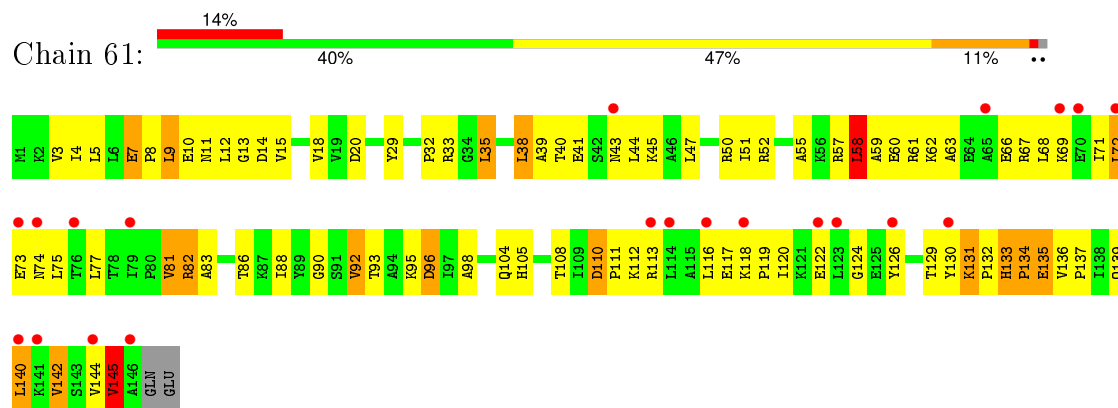
- Molecule 32: 50S ribosomal protein L6



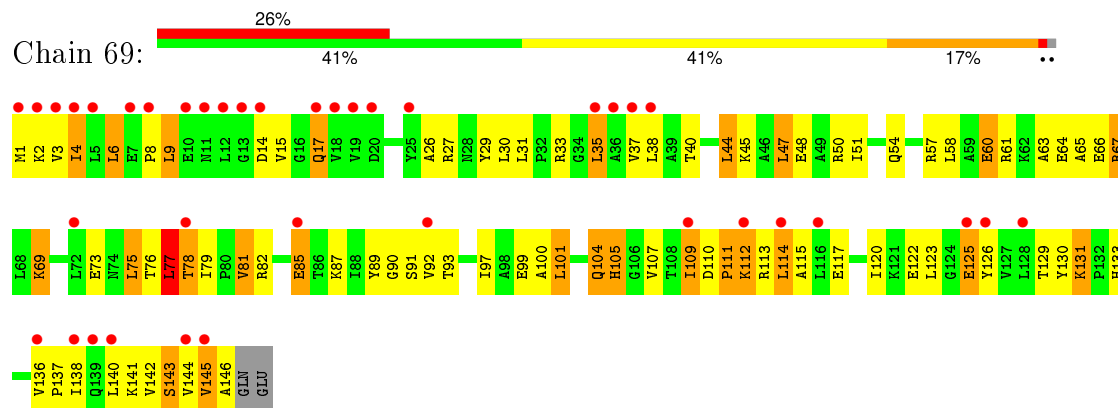
- Molecule 32: 50S ribosomal protein L6



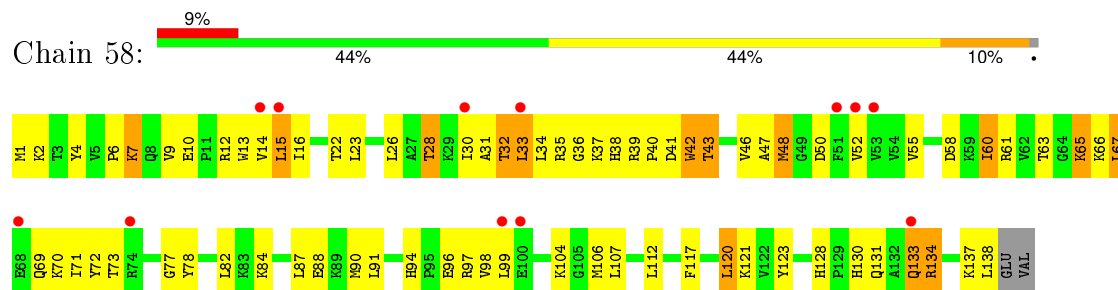
• Molecule 33: 50S ribosomal protein L9



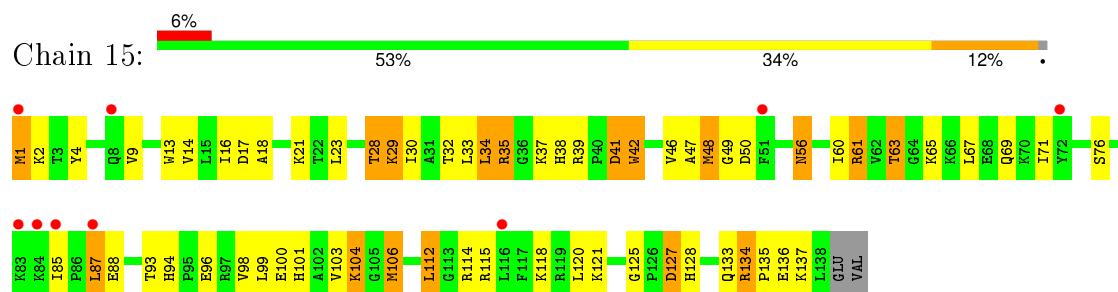
• Molecule 33: 50S ribosomal protein L9



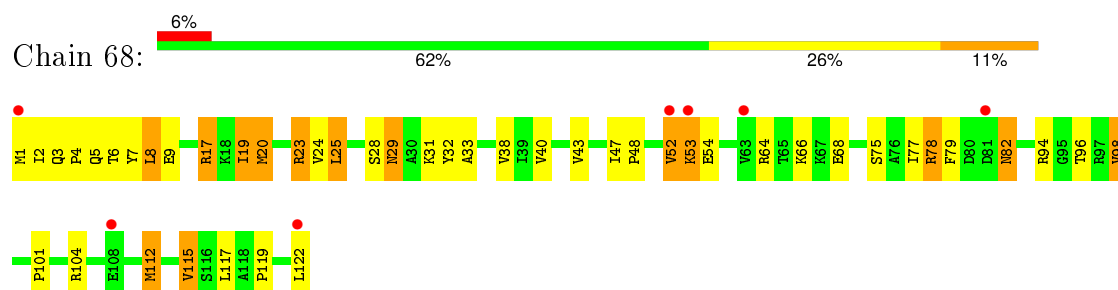
• Molecule 34: 50S ribosomal protein L13



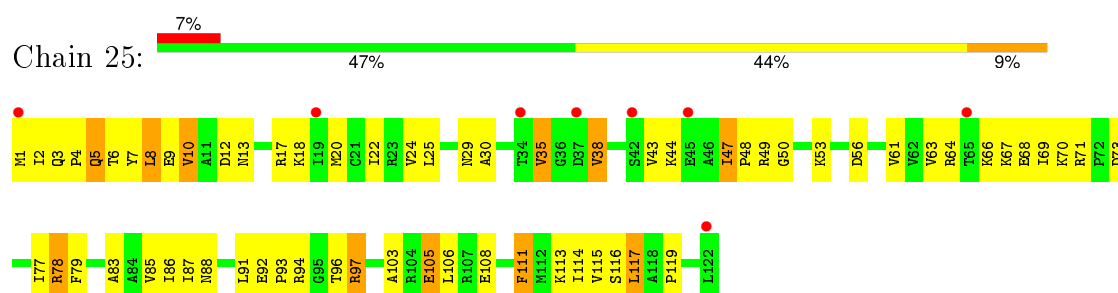
- Molecule 34: 50S ribosomal protein L13



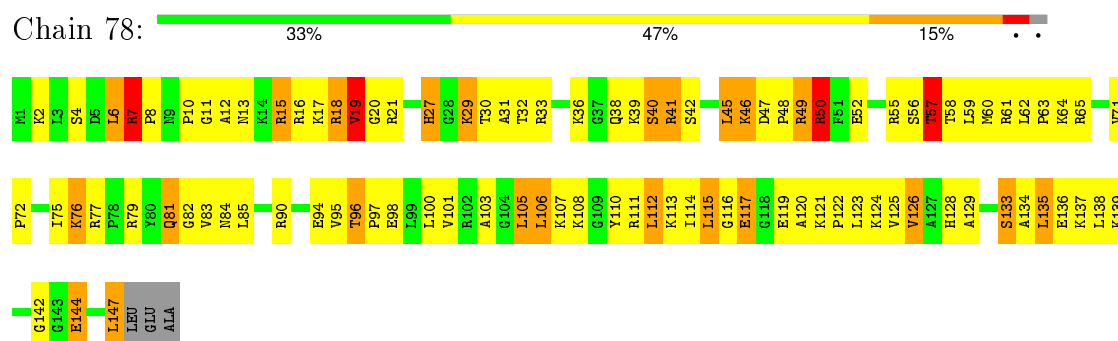
- Molecule 35: 50S ribosomal protein L14



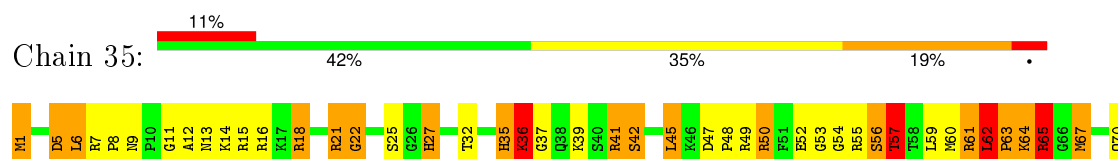
- Molecule 35: 50S ribosomal protein L14

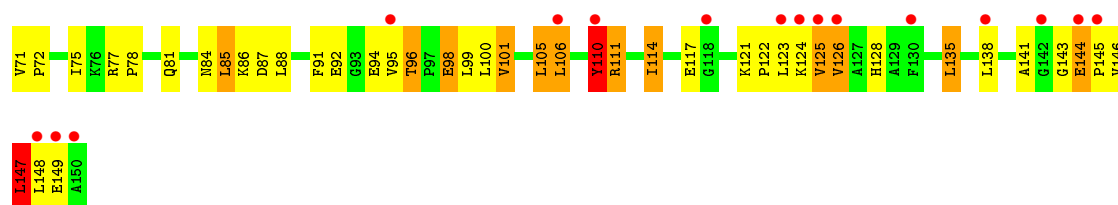


- Molecule 36: 50S ribosomal protein L15

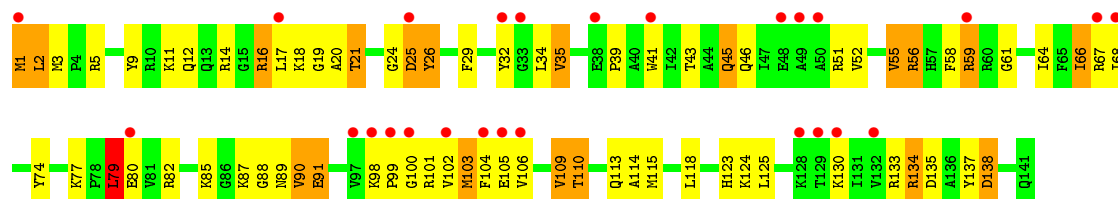


- Molecule 36: 50S ribosomal protein L15

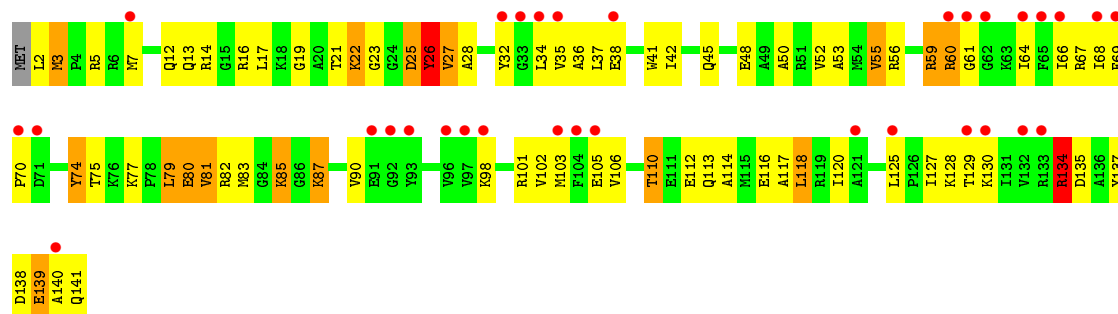
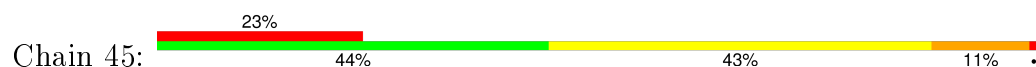




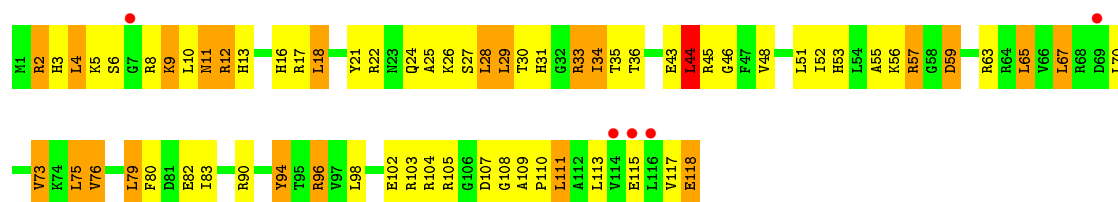
• Molecule 37: 50S ribosomal protein L16



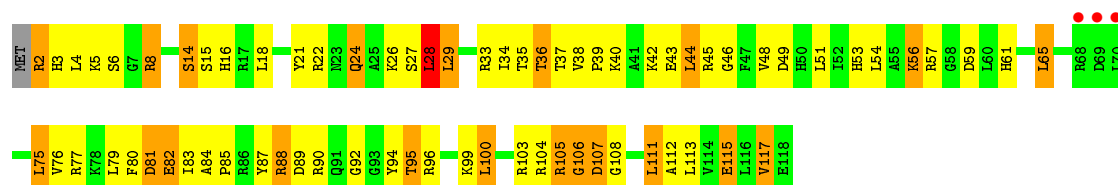
• Molecule 37: 50S ribosomal protein L16



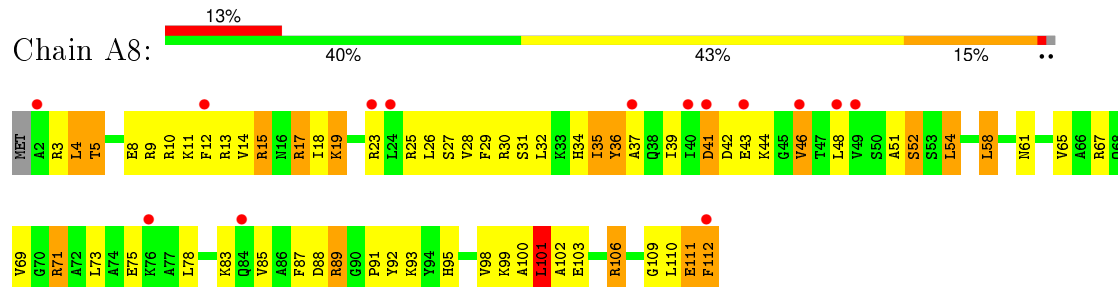
• Molecule 38: 50S ribosomal protein L17



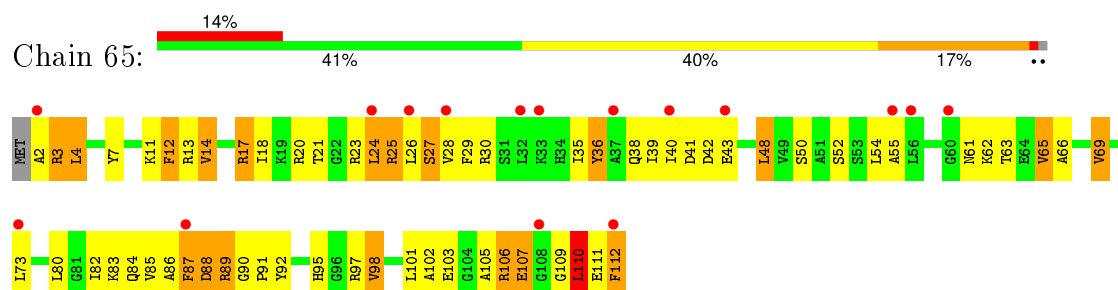
• Molecule 38: 50S ribosomal protein L17



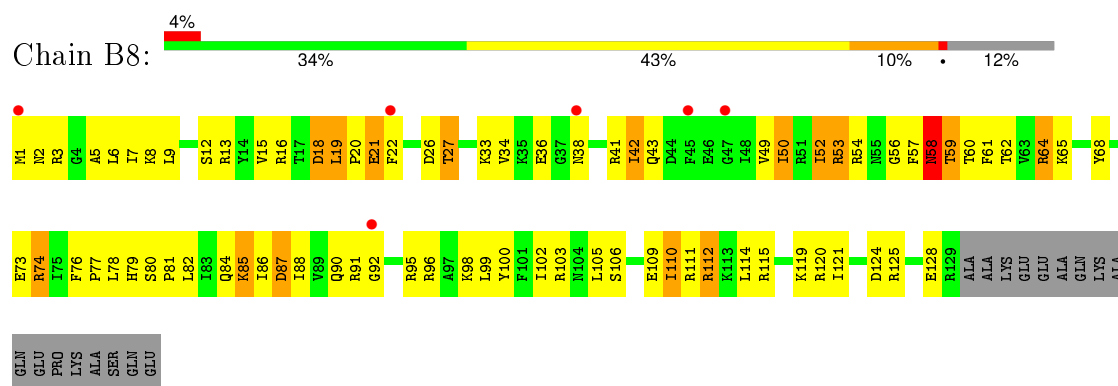
- Molecule 39: 50S ribosomal protein L18



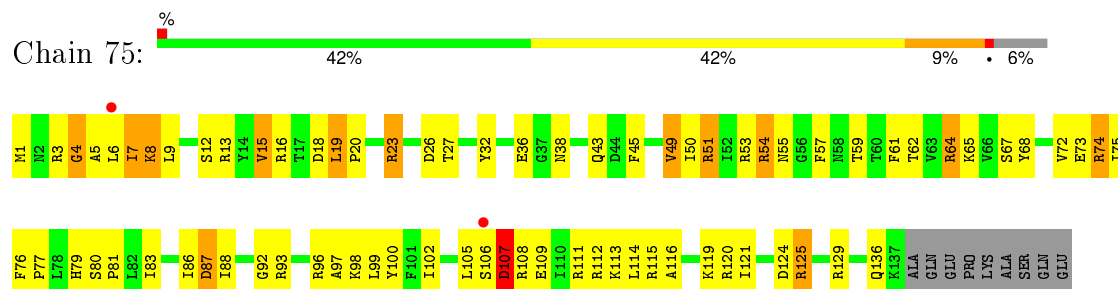
- Molecule 39: 50S ribosomal protein L18



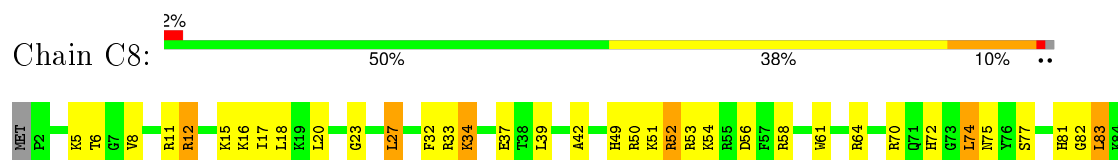
- Molecule 40: 50S ribosomal protein L19



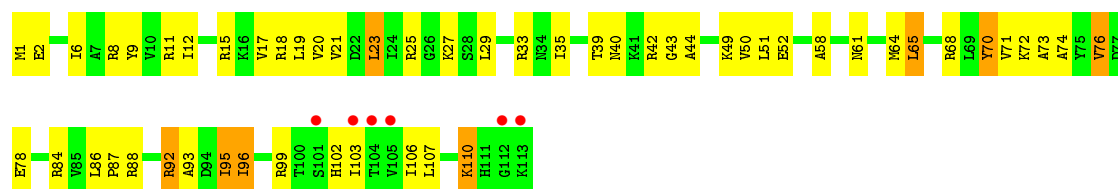
- Molecule 40: 50S ribosomal protein L19



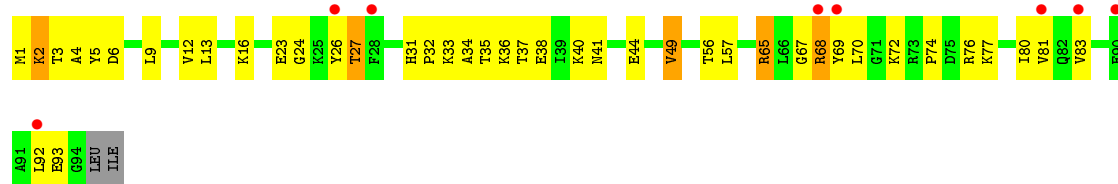
- Molecule 41: 50S ribosomal protein L20



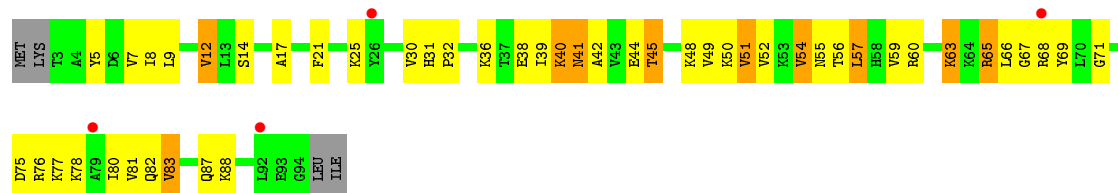




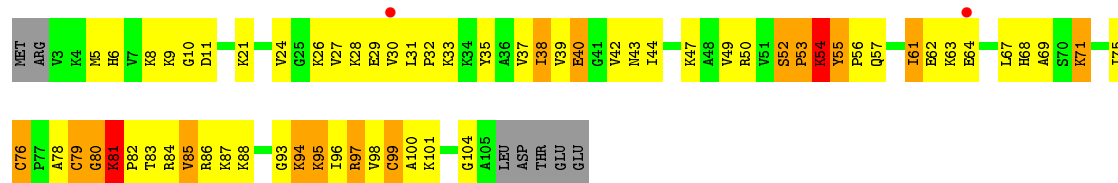
• Molecule 44: 50S ribosomal protein L23



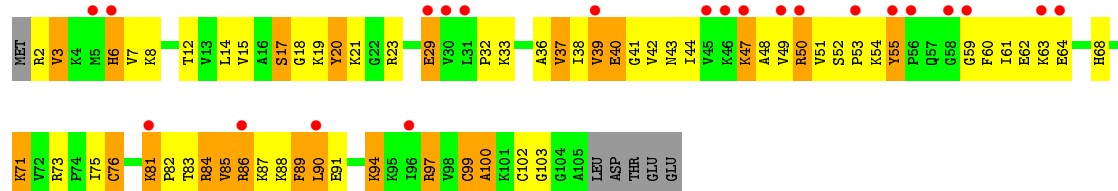
• Molecule 44: 50S ribosomal protein L23



• Molecule 45: 50S ribosomal protein L24



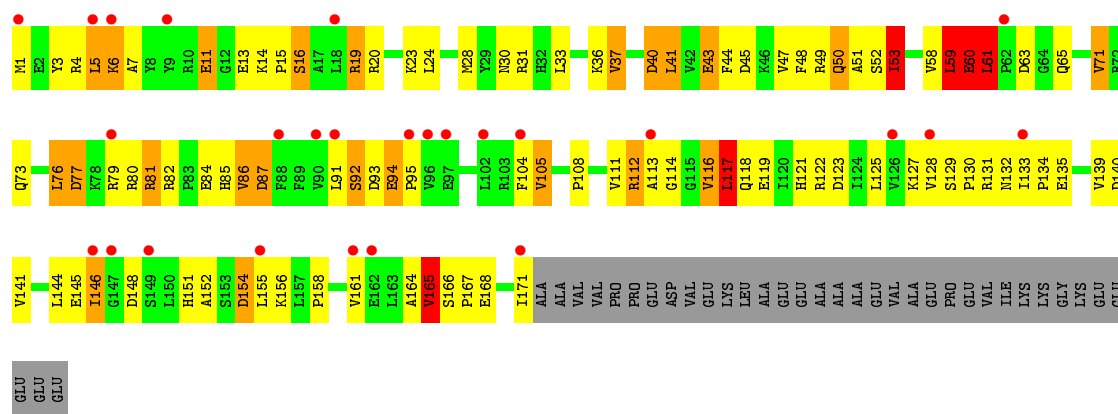
• Molecule 45: 50S ribosomal protein L24



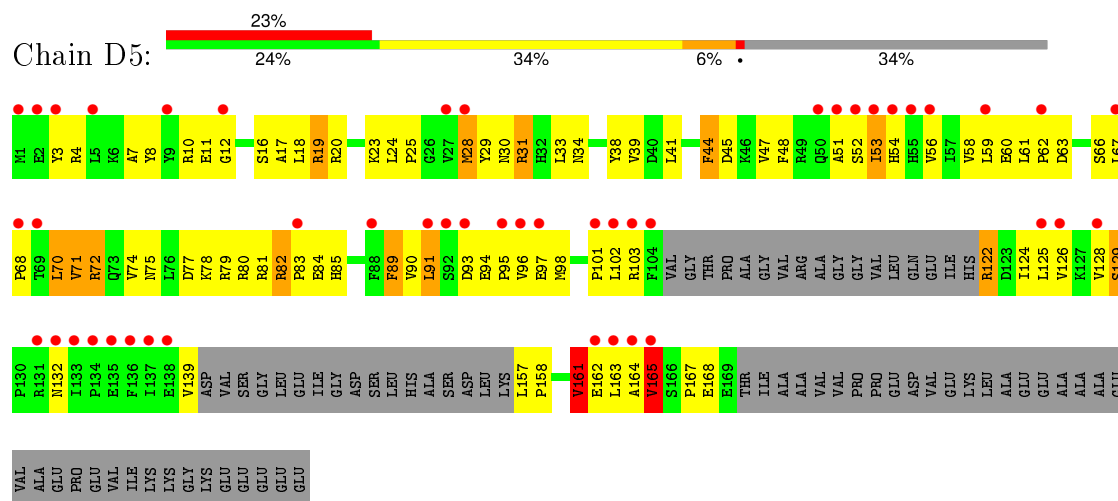
• Molecule 46: 50S ribosomal protein L25



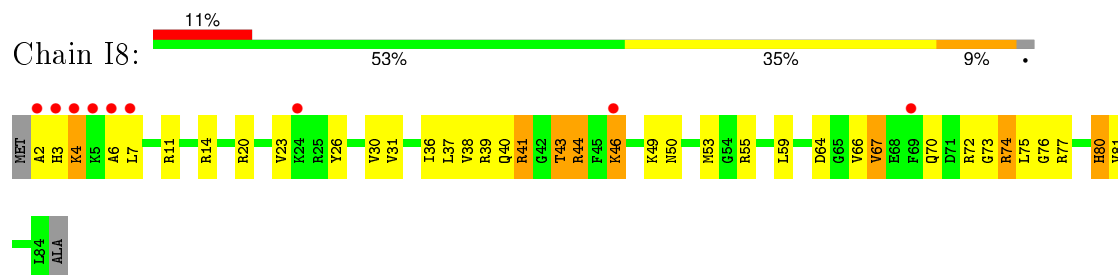




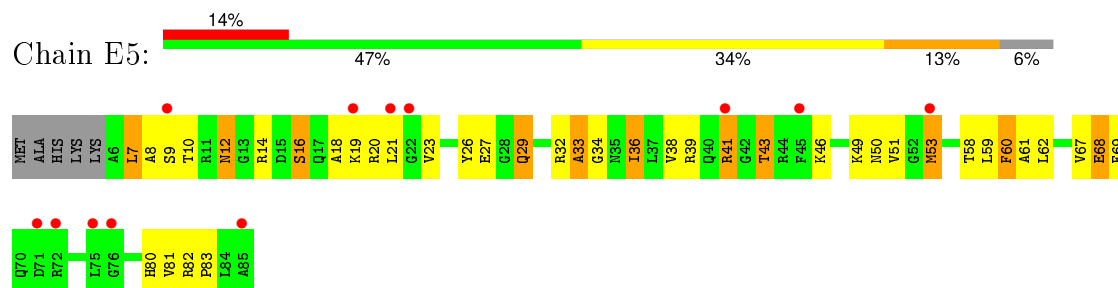
• Molecule 46: 50S ribosomal protein L25



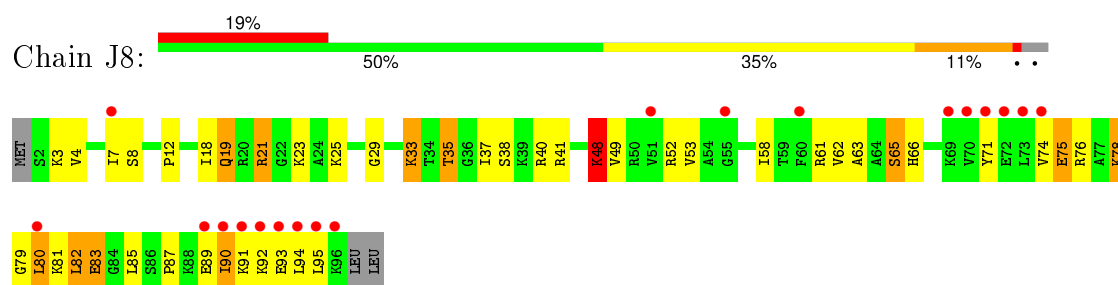
• Molecule 47: 50S ribosomal protein L27



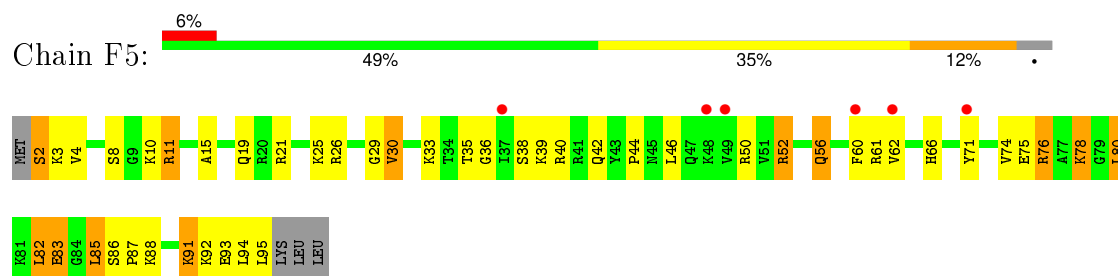
• Molecule 47: 50S ribosomal protein L27



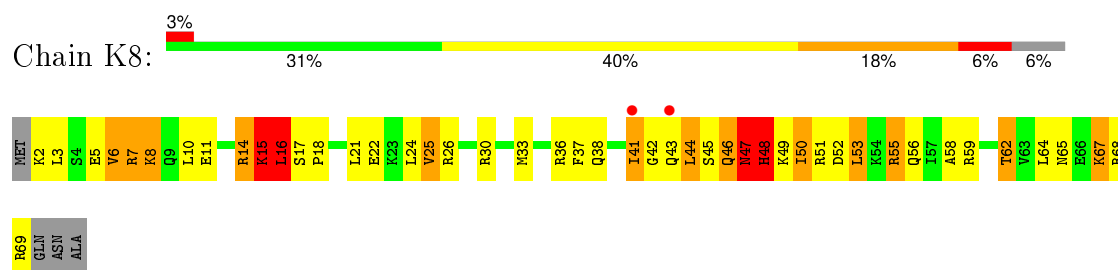
• Molecule 48: 50S ribosomal protein L28



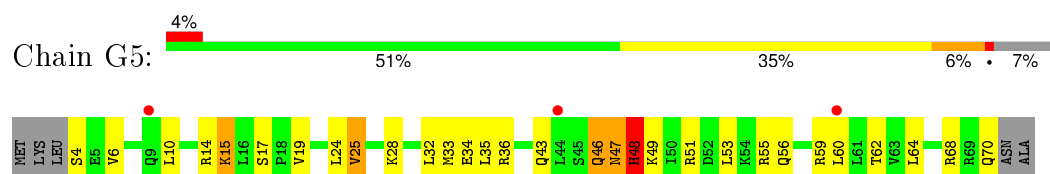
- Molecule 48: 50S ribosomal protein L28



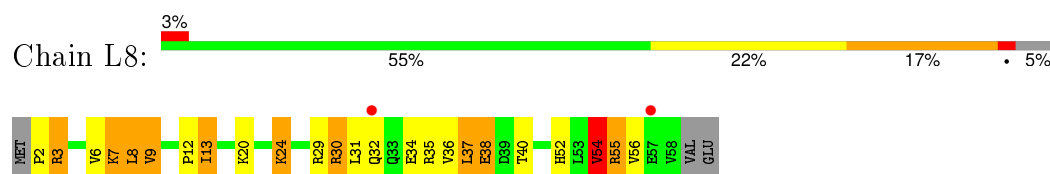
- Molecule 49: 50S ribosomal protein L29



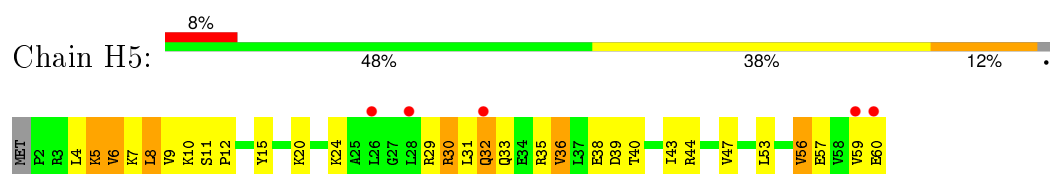
- Molecule 49: 50S ribosomal protein L29



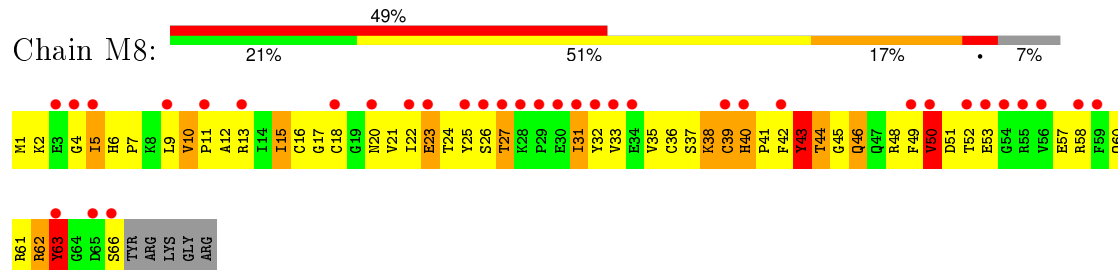
- Molecule 50: 50S ribosomal protein L30



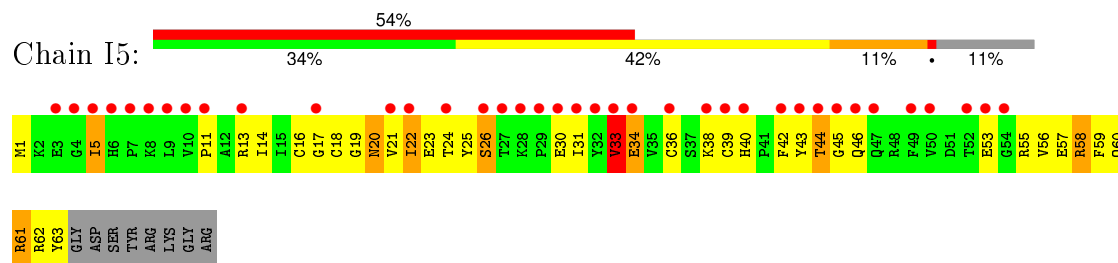
- Molecule 50: 50S ribosomal protein L30



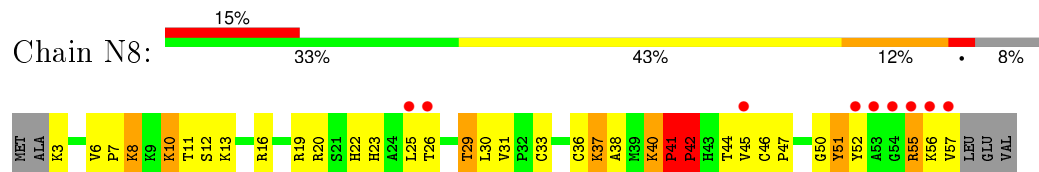
- Molecule 51: 50S ribosomal protein L31



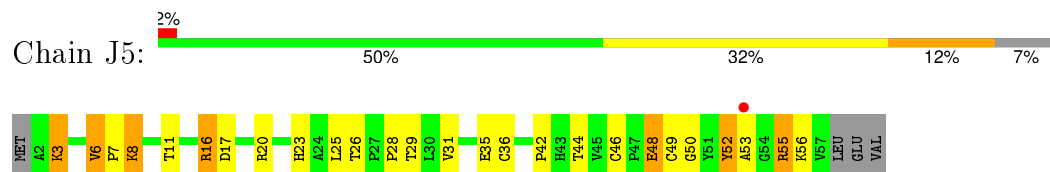
- Molecule 51: 50S ribosomal protein L31



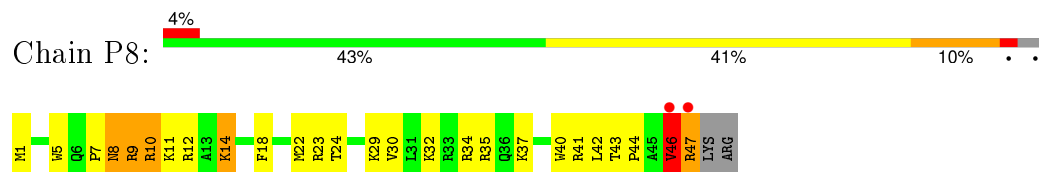
- Molecule 52: 50S ribosomal protein L32



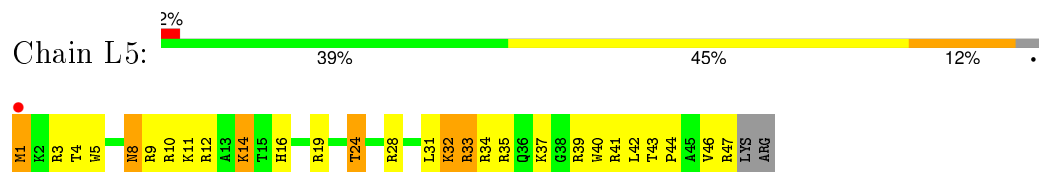
- Molecule 52: 50S ribosomal protein L32



- Molecule 53: 50S ribosomal protein L34



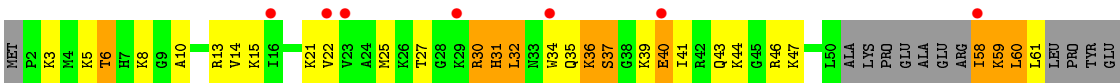
- Molecule 53: 50S ribosomal protein L34



- Molecule 54: 50S ribosomal protein L35



• Molecule 54: 50S ribosomal protein L35



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	209.50Å 449.90Å 618.70Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	153.31 – 3.30 153.31 – 3.30	Depositor EDS
% Data completeness (in resolution range)	100.0 (153.31-3.30) 93.1 (153.31-3.30)	Depositor EDS
$R_{merge}$	0.54	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.13 (at 3.33Å)	Xtriage
Refinement program	PHENIX	Depositor
R, $R_{free}$	0.185 , (Not available) 0.192 , 0.237	Depositor DCC
$R_{free}$ test set	2000 reflections (0.25%)	DCC
Wilson B-factor (Å <sup>2</sup> )	96.5	Xtriage
Anisotropy	0.275	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.26 , 81.4	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.43$ , $\langle L^2 \rangle = 0.25$	Xtriage
Outliers	0 of 867119 reflections	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	299429	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	116.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.56% of the height of the origin peak. No significant pseudotranslation is detected.*

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

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

## 5 Model quality ⓘ

### 5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: 5MU, MG, OMG, H2U, ZN, 1MG, 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	0.70	4/36254 (0.0%)	1.35	317/56581 (0.6%)
1	1G	0.66	0/36390	1.30	250/56793 (0.4%)
2	12	0.39	0/1959	0.67	2/2642 (0.1%)
2	1E	0.41	0/1959	0.67	2/2642 (0.1%)
3	22	0.44	0/1636	0.65	0/2205
3	2E	0.50	0/1629	0.66	1/2195 (0.0%)
4	32	0.54	1/1732 (0.1%)	0.76	1/2318 (0.0%)
4	3E	0.63	4/1732 (0.2%)	0.75	2/2318 (0.1%)
5	42	0.50	0/1171	0.73	0/1576
5	4E	0.54	0/1171	0.70	0/1576
6	52	0.52	0/855	0.72	2/1154 (0.2%)
6	5E	0.56	0/855	0.67	0/1154
7	62	0.43	0/1218	0.60	0/1632
7	6E	0.40	0/1171	0.57	0/1567
8	72	0.47	0/1135	0.65	0/1527
8	7E	0.51	0/1135	0.72	0/1527
9	82	0.41	0/1002	0.66	0/1346
9	8E	0.43	0/1028	0.65	0/1379
10	1A	0.40	0/814	0.63	0/1095
10	1I	0.47	0/814	0.70	0/1095
11	2A	0.48	0/879	0.70	0/1187
11	2I	0.47	0/879	0.72	1/1187 (0.1%)
12	3A	0.58	0/991	0.77	0/1327
12	3I	0.62	0/972	0.83	0/1301
13	4A	0.34	0/938	0.59	0/1258
13	4I	0.45	0/938	0.65	0/1258
14	5A	0.45	0/484	0.72	0/643
14	5I	0.64	1/500 (0.2%)	0.80	0/664
15	6A	0.51	0/744	0.64	0/992
15	6I	0.51	0/744	0.71	0/992
16	7A	0.52	0/721	0.70	0/970
16	7I	0.47	0/721	0.67	0/970

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
17	8A	0.56	0/836	0.66	0/1117
17	8I	0.52	0/847	0.73	0/1131
18	9A	0.53	0/569	0.78	0/757
18	9I	0.49	0/555	0.74	0/739
19	AA	0.39	0/638	0.66	0/860
19	AI	0.46	0/657	0.75	1/885 (0.1%)
20	BA	0.48	0/764	0.73	0/1007
20	BI	0.41	0/764	0.66	0/1007
21	1B	0.47	0/221	0.63	0/288
21	1F	0.41	0/203	0.65	0/266
22	1K	0.52	0/1988	1.13	11/3099 (0.4%)
22	1L	0.45	0/1988	1.06	9/3099 (0.3%)
23	2K	0.69	0/1746	1.39	17/2719 (0.6%)
23	2L	0.69	0/1768	1.47	21/2753 (0.8%)
24	3K	0.49	0/1838	1.12	6/2862 (0.2%)
24	3L	0.54	0/1786	1.13	4/2778 (0.1%)
25	4K	0.70	0/372	1.05	0/574
25	4L	0.60	0/485	1.03	1/749 (0.1%)
26	14	0.84	45/70167 (0.1%)	1.51	1106/109541 (1.0%)
26	1H	0.91	66/70233 (0.1%)	1.60	1430/109643 (1.3%)
27	16	0.75	0/2928	1.48	45/4568 (1.0%)
27	1J	0.71	0/2928	1.37	24/4568 (0.5%)
28	11	0.70	1/2176 (0.0%)	0.89	2/2933 (0.1%)
28	19	0.69	2/2170 (0.1%)	0.91	2/2926 (0.1%)
29	21	0.63	0/1601	0.91	2/2160 (0.1%)
29	29	0.67	0/1601	0.97	2/2160 (0.1%)
30	31	0.67	0/1620	0.82	0/2194
30	39	0.62	0/1662	0.90	0/2249
31	41	0.43	0/1498	0.66	1/2016 (0.0%)
31	49	0.37	0/1498	0.63	0/2016
32	51	0.57	0/1362	0.85	0/1841
32	59	0.38	0/1332	0.75	2/1802 (0.1%)
33	61	0.52	0/1151	0.78	2/1558 (0.1%)
33	69	0.48	0/1151	0.75	2/1558 (0.1%)
34	15	0.54	0/1131	0.71	0/1525
34	58	0.56	0/1131	0.79	1/1525 (0.1%)
35	25	0.64	0/942	0.81	2/1269 (0.2%)
35	68	0.61	0/942	0.76	0/1269
36	35	0.59	0/1161	0.99	1/1544 (0.1%)
36	78	0.64	0/1139	1.03	2/1514 (0.1%)
37	45	0.63	0/1134	0.82	0/1517
37	88	0.66	0/1142	0.92	3/1527 (0.2%)
38	55	0.62	0/973	0.87	1/1302 (0.1%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
38	98	0.53	0/981	0.85	2/1312 (0.2%)
39	65	0.55	0/891	0.91	1/1187 (0.1%)
39	A8	0.55	0/891	0.81	1/1187 (0.1%)
40	75	0.61	0/1155	0.77	0/1542
40	B8	0.64	0/1095	0.79	0/1463
41	85	0.59	0/981	0.79	0/1306
41	C8	0.67	0/981	0.88	2/1306 (0.2%)
42	95	0.66	0/789	0.85	2/1057 (0.2%)
42	D8	0.59	0/789	0.83	1/1057 (0.1%)
43	A5	0.68	0/910	0.87	0/1220
43	E8	0.64	0/901	0.83	0/1209
44	B5	0.69	0/739	0.81	0/993
44	F8	0.72	0/756	0.86	0/1014
45	C5	0.68	0/807	0.90	1/1076 (0.1%)
45	G8	0.71	0/796	0.98	5/1062 (0.5%)
46	D5	0.47	0/1145	0.67	0/1547
46	H8	0.47	0/1403	0.76	2/1901 (0.1%)
47	E5	0.63	0/635	0.89	0/848
47	I8	0.69	0/665	0.82	0/885
48	F5	0.65	0/744	0.87	1/989 (0.1%)
48	J8	0.67	0/753	0.93	3/1000 (0.3%)
49	G5	0.61	0/569	0.85	0/753
49	K8	0.68	0/577	0.92	1/763 (0.1%)
50	H5	0.48	0/473	0.63	0/635
50	L8	0.66	0/457	0.79	0/613
51	I5	0.44	0/527	0.79	0/709
51	M8	0.43	0/545	0.77	0/733
52	J5	0.60	0/448	0.82	0/606
52	N8	0.64	0/443	0.84	0/599
53	L5	0.65	0/417	0.83	0/550
53	P8	0.75	0/417	0.88	0/550
54	M5	0.71	0/426	0.97	1/556 (0.2%)
54	Q8	1.05	0/486	1.47	6/638 (0.9%)
All	All	0.74	124/322561 (0.0%)	1.33	3307/483352 (0.7%)

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

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	#Chirality outliers	#Planarity outliers
2	1E	0	3
4	32	0	3
4	3E	0	1
9	82	0	1
9	8E	0	1
10	1A	0	1
11	2A	0	1
12	3A	0	2
12	3I	0	1
13	4A	0	1
14	5A	0	1
19	AI	0	2
20	BA	0	2
28	11	0	1
28	19	0	3
29	21	0	4
29	29	0	8
30	31	0	1
30	39	0	6
31	49	0	1
33	61	0	3
33	69	0	3
34	15	0	1
36	35	0	7
36	78	0	2
37	45	0	5
37	88	0	3
38	55	0	2
38	98	0	1
40	75	0	2
40	B8	0	2
41	85	0	2
41	C8	0	1
42	95	0	1
43	A5	0	1
45	C5	0	4
45	G8	0	4
46	H8	0	3
47	E5	0	2
47	I8	0	2
48	F5	0	1
48	J8	0	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
49	G5	0	3
49	K8	0	5
51	I5	0	1
51	M8	0	3
52	J5	0	1
52	N8	0	2
53	P8	0	1
54	M5	0	2
54	Q8	0	12
All	All	0	128

The worst 5 of 124 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	1H	774	A	N9-C4	-14.53	1.29	1.37
26	14	783	A	N9-C4	-9.44	1.32	1.37
26	1H	71	A	N9-C4	-9.18	1.32	1.37
26	14	2518	A	N9-C4	-7.93	1.33	1.37
4	3E	12	CYS	CB-SG	7.85	1.95	1.82

The worst 5 of 3307 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	1H	1899	G	N3-C4-N9	-18.45	114.93	126.00
26	14	1332	G	N3-C4-N9	-15.36	116.78	126.00
26	1H	676	A	C2-N3-C4	-14.95	103.12	110.60
26	1H	783	A	C5-N7-C8	-14.89	96.45	103.90
26	14	1786	A	N7-C8-N9	14.75	121.17	113.80

There are no chirality outliers.

5 of 128 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	1E	15	VAL	Peptide
2	1E	169	LYS	Peptide
2	1E	237	ALA	Peptide
4	3E	31	CYS	Peptide
9	8E	47	LEU	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	32389	0	16350	718	0
1	1G	32511	0	16414	717	0
2	12	1924	0	1975	96	0
2	1E	1924	0	1975	88	0
3	22	1612	0	1677	83	0
3	2E	1605	0	1668	69	0
4	32	1702	0	1763	104	0
4	3E	1702	0	1763	77	0
5	42	1155	0	1213	52	0
5	4E	1155	0	1213	55	0
6	52	842	0	857	32	0
6	5E	842	0	857	33	0
7	62	1200	0	1238	51	0
7	6E	1157	0	1202	45	0
8	72	1115	0	1177	46	0
8	7E	1115	0	1177	42	0
9	82	983	0	1006	76	0
9	8E	1009	0	1037	68	0
10	1A	801	0	849	56	0
10	1I	801	0	849	53	0
11	2A	864	0	881	37	0
11	2I	864	0	881	39	0
12	3A	975	0	1062	41	0
12	3I	956	0	1046	47	0
13	4A	928	0	987	52	0
13	4I	928	0	987	55	0
14	5A	475	0	511	36	0
14	5I	491	0	529	31	0
15	6A	733	0	771	31	0
15	6I	733	0	771	25	0
16	7A	705	0	725	27	0
16	7I	705	0	725	40	0
17	8A	823	0	891	32	0
17	8I	834	0	904	39	0
18	9A	564	0	631	22	0
18	9I	550	0	613	23	0
19	AA	624	0	636	42	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
19	AI	643	0	662	43	0
20	BA	762	0	861	44	0
20	BI	762	0	861	40	0
21	1B	217	0	234	11	0
21	1F	199	0	208	9	0
22	1K	1863	0	942	41	0
22	1L	1863	0	942	40	0
23	2K	1692	0	859	47	0
23	2L	1712	0	870	62	0
24	3K	1646	0	830	36	0
24	3L	1601	0	809	30	0
25	4K	336	0	168	9	0
25	4L	438	0	220	11	0
26	14	62647	0	31582	1257	0
26	1H	62707	0	31614	1349	1
27	16	2617	0	1328	60	0
27	1J	2617	0	1328	70	0
28	11	2126	0	2208	88	0
28	19	2120	0	2197	86	0
29	21	1568	0	1634	96	0
29	29	1568	0	1634	104	0
30	31	1585	0	1632	84	0
30	39	1627	0	1680	94	0
31	41	1473	0	1535	92	0
31	49	1473	0	1535	67	0
32	51	1336	0	1418	80	0
32	59	1307	0	1382	73	0
33	61	1136	0	1223	59	0
33	69	1136	0	1223	57	0
34	15	1104	0	1180	49	0
34	58	1104	0	1180	56	0
35	25	932	0	996	43	0
35	68	932	0	996	35	0
36	35	1144	0	1228	82	0
36	78	1122	0	1206	97	0
37	45	1113	0	1167	64	0
37	88	1121	0	1179	66	0
38	55	959	0	1021	51	0
38	98	967	0	1033	58	0
39	65	881	0	943	59	0
39	A8	881	0	943	57	0
40	75	1141	0	1202	54	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
40	B8	1081	0	1141	63	0
41	85	963	0	1022	61	0
41	C8	963	0	1022	60	0
42	95	778	0	852	60	0
42	D8	778	0	852	37	0
43	A5	899	0	964	34	0
43	E8	890	0	951	31	0
44	B5	725	0	778	38	0
44	F8	742	0	803	30	0
45	C5	794	0	884	52	0
45	G8	783	0	870	46	0
46	D5	1120	0	1146	54	0
46	H8	1373	0	1402	75	0
47	E5	627	0	645	42	0
47	I8	656	0	679	32	0
48	F5	737	0	813	38	0
48	J8	746	0	826	34	0
49	G5	567	0	618	20	0
49	K8	575	0	634	38	0
50	H5	468	0	518	15	1
50	L8	452	0	503	19	0
51	I5	515	0	514	35	0
51	M8	533	0	526	52	0
52	J5	434	0	454	19	0
52	N8	429	0	449	31	0
53	L5	409	0	454	21	0
53	P8	409	0	454	18	0
54	M5	422	0	484	30	0
54	Q8	480	0	549	94	0
55	11	1	0	0	0	0
55	13	146	0	0	0	0
55	14	490	0	0	0	0
55	16	5	0	0	0	0
55	1G	143	0	0	0	0
55	1H	512	0	0	0	0
55	1J	2	0	0	0	0
55	1K	1	0	0	0	0
55	21	2	0	0	0	0
55	25	1	0	0	0	0
55	29	3	0	0	0	0
55	2K	3	0	0	0	0
55	2L	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
55	31	1	0	0	0	0
55	32	1	0	0	0	0
55	3E	1	0	0	0	0
55	3I	1	0	0	0	0
55	45	2	0	0	0	0
55	5E	1	0	0	0	0
55	78	1	0	0	0	0
55	7A	1	0	0	0	0
55	85	2	0	0	0	0
55	88	4	0	0	0	0
55	98	1	0	0	0	0
55	E5	2	0	0	0	0
55	G8	1	0	0	0	0
55	I8	2	0	0	0	0
55	J8	1	0	0	0	0
55	P8	1	0	0	0	0
56	32	1	0	0	0	0
56	3E	1	0	0	0	0
56	5A	1	0	0	0	0
56	5I	1	0	0	0	0
56	C5	1	0	0	0	0
56	G8	1	0	0	0	0
57	11	1	0	0	0	0
57	13	74	0	0	11	0
57	14	520	0	0	102	0
57	19	8	0	0	2	0
57	1G	73	0	0	6	0
57	1H	552	0	0	122	0
57	21	1	0	0	1	0
57	29	2	0	0	0	0
57	31	4	0	0	1	0
57	35	1	0	0	0	0
57	39	4	0	0	0	0
57	3E	1	0	0	0	0
57	4L	2	0	0	0	0
57	55	2	0	0	0	0
57	6A	2	0	0	0	0
57	6I	1	0	0	0	0
57	78	2	0	0	0	0
57	7A	1	0	0	0	0
57	85	1	0	0	0	0
57	A5	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
57	B8	1	0	0	0	0
57	BI	1	0	0	0	0
57	C8	2	0	0	1	0
57	D8	1	0	0	0	0
57	E8	1	0	0	0	0
57	I8	3	0	0	0	0
57	J8	1	0	0	0	0
57	M5	3	0	0	0	0
57	P8	1	0	0	0	0
All	All	299429	0	199511	8202	1

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 17.

The worst 5 of 8202 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:1H:2032:G:N7	57:1H:4116:HOH:O	1.81	1.11
2:12:185:ILE:HG22	2:12:199:TYR:HB2	1.39	1.04
26:1H:810:U:OP1	57:1H:4123:HOH:O	1.75	1.03
26:1H:2308:G:H1	26:1H:2311:A:H2	1.07	1.02
26:1H:763:G:OP1	57:1H:3623:HOH:O	1.80	1.00

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

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:1H:654(O):G:N2	50:H5:57:GLU:OE1[2_464]	2.18	0.02

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	12	235/256 (92%)	198 (84%)	35 (15%)	2 (1%)	21	60
2	1E	235/256 (92%)	200 (85%)	33 (14%)	2 (1%)	21	60
3	22	204/239 (85%)	181 (89%)	23 (11%)	0	100	100
3	2E	203/239 (85%)	185 (91%)	18 (9%)	0	100	100
4	32	206/209 (99%)	175 (85%)	30 (15%)	1 (0%)	34	71
4	3E	206/209 (99%)	194 (94%)	9 (4%)	3 (2%)	13	49
5	42	149/162 (92%)	139 (93%)	10 (7%)	0	100	100
5	4E	149/162 (92%)	142 (95%)	6 (4%)	1 (1%)	26	66
6	52	99/101 (98%)	97 (98%)	2 (2%)	0	100	100
6	5E	99/101 (98%)	94 (95%)	5 (5%)	0	100	100
7	62	143/156 (92%)	137 (96%)	6 (4%)	0	100	100
7	6E	140/156 (90%)	134 (96%)	6 (4%)	0	100	100
8	72	136/138 (99%)	125 (92%)	10 (7%)	1 (1%)	26	66
8	7E	136/138 (99%)	124 (91%)	11 (8%)	1 (1%)	26	66
9	82	122/128 (95%)	109 (89%)	12 (10%)	1 (1%)	24	62
9	8E	125/128 (98%)	106 (85%)	19 (15%)	0	100	100
10	1A	97/105 (92%)	90 (93%)	7 (7%)	0	100	100
10	1I	97/105 (92%)	90 (93%)	7 (7%)	0	100	100
11	2A	114/129 (88%)	103 (90%)	8 (7%)	3 (3%)	7	36
11	2I	114/129 (88%)	102 (90%)	10 (9%)	2 (2%)	11	46
12	3A	123/132 (93%)	99 (80%)	20 (16%)	4 (3%)	5	30
12	3I	120/132 (91%)	102 (85%)	18 (15%)	0	100	100
13	4A	114/126 (90%)	95 (83%)	18 (16%)	1 (1%)	21	60
13	4I	114/126 (90%)	95 (83%)	18 (16%)	1 (1%)	21	60
14	5A	56/61 (92%)	46 (82%)	9 (16%)	1 (2%)	11	46
14	5I	58/61 (95%)	49 (84%)	8 (14%)	1 (2%)	11	47
15	6A	86/89 (97%)	81 (94%)	5 (6%)	0	100	100
15	6I	86/89 (97%)	80 (93%)	6 (7%)	0	100	100
16	7A	82/88 (93%)	77 (94%)	5 (6%)	0	100	100
16	7I	82/88 (93%)	76 (93%)	6 (7%)	0	100	100
17	8A	97/105 (92%)	92 (95%)	5 (5%)	0	100	100
17	8I	98/105 (93%)	91 (93%)	7 (7%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
18	9A	67/88 (76%)	61 (91%)	6 (9%)	0	100	100
18	9I	65/88 (74%)	63 (97%)	1 (2%)	1 (2%)	13	49
19	AA	76/93 (82%)	62 (82%)	12 (16%)	2 (3%)	7	36
19	AI	78/93 (84%)	65 (83%)	11 (14%)	2 (3%)	7	36
20	BA	97/106 (92%)	87 (90%)	8 (8%)	2 (2%)	9	42
20	BI	97/106 (92%)	82 (84%)	15 (16%)	0	100	100
21	1B	23/27 (85%)	21 (91%)	2 (9%)	0	100	100
21	1F	21/27 (78%)	20 (95%)	1 (5%)	0	100	100
28	11	271/276 (98%)	257 (95%)	10 (4%)	4 (2%)	13	49
28	19	271/276 (98%)	247 (91%)	17 (6%)	7 (3%)	7	36
29	21	203/206 (98%)	162 (80%)	32 (16%)	9 (4%)	3	22
29	29	203/206 (98%)	154 (76%)	38 (19%)	11 (5%)	2	17
30	31	200/210 (95%)	183 (92%)	15 (8%)	2 (1%)	19	58
30	39	206/210 (98%)	165 (80%)	33 (16%)	8 (4%)	4	25
31	41	179/182 (98%)	156 (87%)	20 (11%)	3 (2%)	11	47
31	49	179/182 (98%)	153 (86%)	24 (13%)	2 (1%)	17	57
32	51	172/180 (96%)	148 (86%)	17 (10%)	7 (4%)	3	24
32	59	168/180 (93%)	131 (78%)	33 (20%)	4 (2%)	7	38
33	61	144/148 (97%)	117 (81%)	24 (17%)	3 (2%)	9	42
33	69	144/148 (97%)	116 (81%)	25 (17%)	3 (2%)	9	42
34	15	136/140 (97%)	119 (88%)	16 (12%)	1 (1%)	26	66
34	58	136/140 (97%)	118 (87%)	15 (11%)	3 (2%)	8	41
35	25	120/122 (98%)	115 (96%)	5 (4%)	0	100	100
35	68	120/122 (98%)	114 (95%)	6 (5%)	0	100	100
36	35	148/150 (99%)	115 (78%)	24 (16%)	9 (6%)	2	14
36	78	145/150 (97%)	117 (81%)	23 (16%)	5 (3%)	5	29
37	45	138/141 (98%)	109 (79%)	27 (20%)	2 (1%)	14	50
37	88	139/141 (99%)	115 (83%)	21 (15%)	3 (2%)	8	41
38	55	115/118 (98%)	101 (88%)	12 (10%)	2 (2%)	11	47
38	98	116/118 (98%)	101 (87%)	14 (12%)	1 (1%)	21	60
39	65	109/112 (97%)	87 (80%)	20 (18%)	2 (2%)	11	46

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
39	A8	109/112 (97%)	92 (84%)	16 (15%)	1 (1%)	21	60
40	75	135/146 (92%)	120 (89%)	14 (10%)	1 (1%)	26	66
40	B8	127/146 (87%)	113 (89%)	14 (11%)	0	100	100
41	85	115/118 (98%)	104 (90%)	10 (9%)	1 (1%)	21	60
41	C8	115/118 (98%)	104 (90%)	8 (7%)	3 (3%)	7	36
42	95	99/101 (98%)	77 (78%)	17 (17%)	5 (5%)	2	19
42	D8	99/101 (98%)	91 (92%)	6 (6%)	2 (2%)	9	43
43	A5	111/113 (98%)	104 (94%)	5 (4%)	2 (2%)	11	46
43	E8	110/113 (97%)	101 (92%)	9 (8%)	0	100	100
44	B5	90/96 (94%)	84 (93%)	4 (4%)	2 (2%)	8	41
44	F8	92/96 (96%)	83 (90%)	7 (8%)	2 (2%)	8	41
45	C5	102/110 (93%)	73 (72%)	24 (24%)	5 (5%)	3	19
45	G8	101/110 (92%)	78 (77%)	19 (19%)	4 (4%)	4	24
46	D5	129/206 (63%)	101 (78%)	24 (19%)	4 (3%)	5	32
46	H8	169/206 (82%)	137 (81%)	26 (15%)	6 (4%)	4	28
47	E5	78/85 (92%)	68 (87%)	9 (12%)	1 (1%)	15	52
47	I8	81/85 (95%)	74 (91%)	7 (9%)	0	100	100
48	F5	92/98 (94%)	82 (89%)	9 (10%)	1 (1%)	17	57
48	J8	93/98 (95%)	84 (90%)	7 (8%)	2 (2%)	8	41
49	G5	65/72 (90%)	61 (94%)	2 (3%)	2 (3%)	5	32
49	K8	66/72 (92%)	61 (92%)	2 (3%)	3 (4%)	3	21
50	H5	57/60 (95%)	55 (96%)	2 (4%)	0	100	100
50	L8	55/60 (92%)	53 (96%)	1 (2%)	1 (2%)	11	46
51	I5	61/71 (86%)	35 (57%)	23 (38%)	3 (5%)	3	19
51	M8	64/71 (90%)	41 (64%)	20 (31%)	3 (5%)	3	20
52	J5	54/60 (90%)	50 (93%)	4 (7%)	0	100	100
52	N8	53/60 (88%)	46 (87%)	5 (9%)	2 (4%)	4	26
53	L5	45/49 (92%)	44 (98%)	1 (2%)	0	100	100
53	P8	45/49 (92%)	41 (91%)	3 (7%)	1 (2%)	8	41
54	M5	49/65 (75%)	41 (84%)	7 (14%)	1 (2%)	9	43
54	Q8	58/65 (89%)	34 (59%)	18 (31%)	6 (10%)	1	4

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	11130/11946 (93%)	9701 (87%)	1242 (11%)	187 (2%)	11	47

5 of 187 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
29	21	83	ASP
32	51	169	VAL
36	78	57	THR
38	98	11	ASN
46	H8	165	VAL

### 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%)	158 (77%)	47 (23%)	1	4
2	1E	205/220 (93%)	164 (80%)	41 (20%)	1	6
3	22	160/188 (85%)	122 (76%)	38 (24%)	1	3
3	2E	159/188 (85%)	120 (76%)	39 (24%)	1	3
4	32	180/181 (99%)	144 (80%)	36 (20%)	1	6
4	3E	180/181 (99%)	151 (84%)	29 (16%)	3	14
5	42	116/123 (94%)	83 (72%)	33 (28%)	0	2
5	4E	116/123 (94%)	88 (76%)	28 (24%)	1	3
6	52	90/90 (100%)	66 (73%)	24 (27%)	0	2
6	5E	90/90 (100%)	75 (83%)	15 (17%)	3	13
7	62	121/127 (95%)	94 (78%)	27 (22%)	1	4
7	6E	118/127 (93%)	98 (83%)	20 (17%)	2	12
8	72	119/119 (100%)	101 (85%)	18 (15%)	3	16
8	7E	119/119 (100%)	96 (81%)	23 (19%)	2	7
9	82	95/99 (96%)	83 (87%)	12 (13%)	5	24
9	8E	98/99 (99%)	68 (69%)	30 (31%)	0	1

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
10	1A	89/92 (97%)	74 (83%)	15 (17%)	2	12
10	1I	89/92 (97%)	72 (81%)	17 (19%)	2	8
11	2A	88/99 (89%)	73 (83%)	15 (17%)	2	12
11	2I	88/99 (89%)	77 (88%)	11 (12%)	6	24
12	3A	104/109 (95%)	71 (68%)	33 (32%)	0	1
12	3I	103/109 (94%)	84 (82%)	19 (18%)	2	9
13	4A	94/101 (93%)	76 (81%)	18 (19%)	2	8
13	4I	94/101 (93%)	67 (71%)	27 (29%)	0	1
14	5A	48/50 (96%)	38 (79%)	10 (21%)	1	6
14	5I	49/50 (98%)	36 (74%)	13 (26%)	0	2
15	6A	79/80 (99%)	72 (91%)	7 (9%)	12	43
15	6I	79/80 (99%)	68 (86%)	11 (14%)	4	20
16	7A	72/74 (97%)	58 (81%)	14 (19%)	2	7
16	7I	72/74 (97%)	58 (81%)	14 (19%)	2	7
17	8A	94/97 (97%)	79 (84%)	15 (16%)	3	14
17	8I	95/97 (98%)	78 (82%)	17 (18%)	2	10
18	9A	60/77 (78%)	46 (77%)	14 (23%)	1	4
18	9I	59/77 (77%)	48 (81%)	11 (19%)	2	9
19	AA	67/80 (84%)	55 (82%)	12 (18%)	2	10
19	AI	70/80 (88%)	53 (76%)	17 (24%)	1	3
20	BA	76/82 (93%)	64 (84%)	12 (16%)	3	15
20	BI	76/82 (93%)	61 (80%)	15 (20%)	1	7
21	1B	20/22 (91%)	19 (95%)	1 (5%)	30	68
21	1F	18/22 (82%)	17 (94%)	1 (6%)	26	65
28	11	215/218 (99%)	175 (81%)	40 (19%)	2	9
28	19	214/218 (98%)	172 (80%)	42 (20%)	1	7
29	21	165/166 (99%)	124 (75%)	41 (25%)	1	3
29	29	165/166 (99%)	126 (76%)	39 (24%)	1	3
30	31	161/166 (97%)	126 (78%)	35 (22%)	1	5
30	39	165/166 (99%)	125 (76%)	40 (24%)	1	3
31	41	155/156 (99%)	122 (79%)	33 (21%)	1	5

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles		
31	49	155/156 (99%)	123 (79%)	32 (21%)	1	6	
32	51	145/148 (98%)	106 (73%)	39 (27%)	0	2	
32	59	142/148 (96%)	108 (76%)	34 (24%)	1	3	
33	61	122/124 (98%)	95 (78%)	27 (22%)	1	4	
33	69	122/124 (98%)	89 (73%)	33 (27%)	0	2	
34	15	117/119 (98%)	86 (74%)	31 (26%)	0	2	
34	58	117/119 (98%)	91 (78%)	26 (22%)	1	4	
35	25	100/100 (100%)	78 (78%)	22 (22%)	1	5	
35	68	100/100 (100%)	77 (77%)	23 (23%)	1	4	
36	35	116/116 (100%)	78 (67%)	38 (33%)	0	1	
36	78	114/116 (98%)	83 (73%)	31 (27%)	0	2	
37	45	110/111 (99%)	81 (74%)	29 (26%)	0	2	
37	88	111/111 (100%)	89 (80%)	22 (20%)	1	7	
38	55	100/101 (99%)	76 (76%)	24 (24%)	1	3	
38	98	101/101 (100%)	75 (74%)	26 (26%)	0	2	
39	65	87/88 (99%)	61 (70%)	26 (30%)	0	1	
39	A8	87/88 (99%)	64 (74%)	23 (26%)	0	2	
40	75	120/127 (94%)	87 (72%)	33 (28%)	0	2	
40	B8	115/127 (91%)	86 (75%)	29 (25%)	1	2	
41	85	93/94 (99%)	79 (85%)	14 (15%)	3	16	
41	C8	93/94 (99%)	77 (83%)	16 (17%)	2	12	
42	95	82/82 (100%)	61 (74%)	21 (26%)	0	2	
42	D8	82/82 (100%)	60 (73%)	22 (27%)	0	2	
43	A5	92/92 (100%)	74 (80%)	18 (20%)	1	7	
43	E8	91/92 (99%)	74 (81%)	17 (19%)	2	9	
44	B5	74/78 (95%)	56 (76%)	18 (24%)	1	3	
44	F8	76/78 (97%)	62 (82%)	14 (18%)	2	9	
45	C5	85/91 (93%)	61 (72%)	24 (28%)	0	2	
45	G8	84/91 (92%)	61 (73%)	23 (27%)	0	2	
46	D5	125/179 (70%)	94 (75%)	31 (25%)	1	3	
46	H8	152/179 (85%)	118 (78%)	34 (22%)	1	4	

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
47	E5	62/67 (92%)	48 (77%)	14 (23%)	1	4
47	I8	66/67 (98%)	50 (76%)	16 (24%)	1	3
48	F5	79/83 (95%)	60 (76%)	19 (24%)	1	3
48	J8	80/83 (96%)	62 (78%)	18 (22%)	1	4
49	G5	63/67 (94%)	49 (78%)	14 (22%)	1	4
49	K8	64/67 (96%)	46 (72%)	18 (28%)	0	2
50	H5	51/52 (98%)	39 (76%)	12 (24%)	1	4
50	L8	49/52 (94%)	36 (74%)	13 (26%)	0	2
51	I5	57/63 (90%)	44 (77%)	13 (23%)	1	4
51	M8	59/63 (94%)	42 (71%)	17 (29%)	0	1
52	J5	48/52 (92%)	37 (77%)	11 (23%)	1	4
52	N8	48/52 (92%)	35 (73%)	13 (27%)	0	2
53	L5	40/42 (95%)	28 (70%)	12 (30%)	0	1
53	P8	40/42 (95%)	29 (72%)	11 (28%)	0	2
54	M5	44/55 (80%)	31 (70%)	13 (30%)	0	1
54	Q8	50/55 (91%)	26 (52%)	24 (48%)	0	0
All	All	9404/9894 (95%)	7297 (78%)	2107 (22%)	1	4

5 of 2107 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
49	K8	6	VAL
5	42	41	VAL
45	C5	23	ARG
50	L8	40	THR
2	12	98	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 17 such sidechains are listed below:

Mol	Chain	Res	Type
44	F8	31	HIS
46	H8	73	GLN
29	29	55	ASN
37	88	12	GLN
32	59	61	HIS

### 5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	13	1505/1522 (98%)	327 (21%)	31 (2%)
1	1G	1512/1522 (99%)	370 (24%)	38 (2%)
22	1K	86/87 (98%)	23 (26%)	1 (1%)
22	1L	86/87 (98%)	31 (36%)	4 (4%)
23	2K	77/87 (88%)	31 (40%)	8 (10%)
23	2L	79/87 (90%)	32 (40%)	8 (10%)
24	3K	75/87 (86%)	35 (46%)	4 (5%)
24	3L	72/87 (82%)	34 (47%)	5 (6%)
25	4K	14/60 (23%)	6 (42%)	0
25	4L	19/60 (31%)	5 (26%)	0
26	14	2908/2917 (99%)	696 (23%)	40 (1%)
26	1H	2911/2917 (99%)	672 (23%)	52 (1%)
27	16	121/122 (99%)	21 (17%)	1 (0%)
27	1J	121/122 (99%)	36 (29%)	4 (3%)
All	All	9586/9764 (98%)	2319 (24%)	196 (2%)

5 of 2319 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	10	A

5 of 196 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
26	1H	2272	U
1	1G	509	A
26	14	2423	U
26	1H	2518	A
1	1G	197	A

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

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

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link

column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
22	1MG	1K	38	22	17,26,27	3.60	5 (29%)	19,39,42	2.38	2 (10%)
22	PSU	1K	39	22	15,21,22	0.94	1 (6%)	16,30,33	2.02	4 (25%)
22	5MU	1K	65	22	13,22,23	1.64	2 (15%)	16,32,35	1.44	1 (6%)
22	PSU	1K	66	22	15,21,22	1.09	1 (6%)	16,30,33	2.16	5 (31%)
22	1MG	1L	38	22	17,26,27	3.63	5 (29%)	19,39,42	2.29	1 (5%)
22	PSU	1L	39	22	15,21,22	1.09	2 (13%)	16,30,33	2.02	2 (12%)
22	5MU	1L	65	22	13,22,23	1.68	2 (15%)	16,32,35	1.33	1 (6%)
22	PSU	1L	66	22	15,21,22	0.92	1 (6%)	16,30,33	2.06	4 (25%)
23	H2U	2K	17	23	17,21,22	2.29	4 (23%)	23,30,33	3.03	4 (17%)
23	OMG	2K	18	23	18,26,27	5.80	6 (33%)	21,38,41	6.15	7 (33%)
23	1MG	2K	38	23	17,26,27	3.27	5 (29%)	19,39,42	2.02	3 (15%)
23	PSU	2K	39	23	15,21,22	0.93	1 (6%)	16,30,33	1.90	4 (25%)
23	5MU	2K	65	23	13,22,23	1.66	2 (15%)	16,32,35	1.41	1 (6%)
23	PSU	2K	66	23	15,21,22	1.17	2 (13%)	16,30,33	2.53	3 (18%)
23	H2U	2L	17	23	17,21,22	2.07	4 (23%)	23,30,33	2.79	5 (21%)
23	OMG	2L	18	23	18,26,27	5.76	6 (33%)	21,38,41	6.66	6 (28%)
23	1MG	2L	38	23	17,26,27	3.80	5 (29%)	19,39,42	2.51	3 (15%)
23	PSU	2L	39	23	15,21,22	0.97	1 (6%)	16,30,33	2.02	4 (25%)
23	5MU	2L	65	23	13,22,23	1.59	2 (15%)	16,32,35	1.45	1 (6%)
23	PSU	2L	66	23	15,21,22	1.08	1 (6%)	16,30,33	2.06	3 (18%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	1MG	1K	38	22	-	0/3/25/26	0/3/3/3
22	PSU	1K	39	22	-	0/7/25/26	0/2/2/2
22	5MU	1K	65	22	-	0/3/25/26	0/2/2/2
22	PSU	1K	66	22	-	0/7/25/26	0/2/2/2
22	1MG	1L	38	22	-	0/3/25/26	0/3/3/3
22	PSU	1L	39	22	-	0/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	5MU	1L	65	22	-	0/3/25/26	0/2/2/2
22	PSU	1L	66	22	-	0/7/25/26	0/2/2/2
23	H2U	2K	17	23	-	0/7/38/39	0/2/2/2
23	OMG	2K	18	23	-	0/5/27/28	0/3/3/3
23	1MG	2K	38	23	-	0/3/25/26	0/3/3/3
23	PSU	2K	39	23	-	0/7/25/26	0/2/2/2
23	5MU	2K	65	23	-	0/3/25/26	0/2/2/2
23	PSU	2K	66	23	-	0/7/25/26	0/2/2/2
23	H2U	2L	17	23	-	0/7/38/39	0/2/2/2
23	OMG	2L	18	23	-	0/5/27/28	0/3/3/3
23	1MG	2L	38	23	-	0/3/25/26	0/3/3/3
23	PSU	2L	39	23	-	0/7/25/26	0/2/2/2
23	5MU	2L	65	23	-	0/3/25/26	0/2/2/2
23	PSU	2L	66	23	-	0/7/25/26	0/2/2/2

The worst 5 of 58 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	2L	18	OMG	C8-N7	-13.70	1.08	1.34
23	2K	18	OMG	C8-N7	-13.11	1.09	1.34
23	2L	18	OMG	C6-N1	-4.43	1.25	1.33
23	2K	18	OMG	C6-N1	-4.22	1.25	1.33
23	2L	17	H2U	C6-N1	-3.98	1.42	1.47

The worst 5 of 64 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	2L	18	OMG	C6-C5-C4	-11.81	107.37	120.86
23	2K	18	OMG	C6-C5-C4	-11.40	107.84	120.86
23	2L	38	1MG	C1'-N9-C4	-10.07	115.57	126.81
22	1K	38	1MG	C1'-N9-C4	-9.55	116.15	126.81
22	1L	38	1MG	C1'-N9-C4	-9.27	116.46	126.81

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

10 monomers are involved in 13 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
22	1K	39	PSU	1	0
22	1L	65	5MU	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
23	2K	17	H2U	1	0
23	2K	18	OMG	2	0
23	2K	38	1MG	1	0
23	2L	18	OMG	2	0
23	2L	38	1MG	2	0
23	2L	39	PSU	2	0
23	2L	65	5MU	2	0
23	2L	66	PSU	2	0

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 1340 ligands modelled in this entry, 1340 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
25	4K	1
25	4L	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	4K	38:U	O3'	44:U	P	28.59
1	4L	40:U	O3'	44:U	P	16.09

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	13	1507/1522 (99%)	-0.64	0 100 100	70, 113, 194, 267	0
1	1G	1513/1522 (99%)	-0.67	1 (0%) 95 96	79, 120, 189, 288	0
2	12	237/256 (92%)	0.57	25 (10%) 8 7	133, 170, 199, 207	0
2	1E	237/256 (92%)	0.36	15 (6%) 23 19	116, 156, 187, 198	0
3	22	206/239 (86%)	1.52	68 (33%) 0 1	128, 150, 185, 189	0
3	2E	205/239 (85%)	0.66	20 (9%) 10 8	94, 120, 157, 169	0
4	32	208/209 (99%)	0.80	20 (9%) 10 9	100, 121, 146, 158	0
4	3E	208/209 (99%)	0.23	3 (1%) 78 73	91, 113, 135, 145	0
5	42	151/162 (93%)	0.52	11 (7%) 18 15	105, 124, 142, 169	0
5	4E	151/162 (93%)	0.36	7 (4%) 36 30	89, 108, 128, 159	0
6	52	101/101 (100%)	0.27	0 100 100	87, 107, 126, 138	0
6	5E	101/101 (100%)	0.55	6 (5%) 26 20	87, 109, 129, 140	0
7	62	147/156 (94%)	0.51	11 (7%) 17 14	123, 138, 159, 171	0
7	6E	144/156 (92%)	0.40	4 (2%) 56 50	118, 136, 154, 175	0
8	72	138/138 (100%)	0.70	13 (9%) 11 9	100, 125, 141, 147	0
8	7E	138/138 (100%)	0.45	6 (4%) 39 32	97, 116, 130, 141	0
9	82	124/128 (96%)	0.31	4 (3%) 51 44	112, 154, 172, 181	0
9	8E	127/128 (99%)	-0.02	2 (1%) 74 69	105, 145, 167, 173	0
10	1A	99/105 (94%)	0.94	16 (16%) 3 2	126, 158, 184, 196	0
10	1I	99/105 (94%)	1.07	17 (17%) 2 2	96, 144, 175, 179	0
11	2A	116/129 (89%)	1.14	20 (17%) 2 2	92, 114, 138, 155	0
11	2I	116/129 (89%)	0.96	22 (18%) 2 1	86, 117, 142, 184	0
12	3A	125/132 (94%)	1.18	35 (28%) 1 1	91, 108, 136, 189	0
12	3I	122/132 (92%)	0.49	5 (4%) 41 34	78, 86, 112, 144	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
13	4A	116/126 (92%)	0.98	18 (15%) 3 2	128, 165, 190, 202	0
13	4I	116/126 (92%)	0.96	18 (15%) 3 2	106, 146, 164, 175	0
14	5A	58/61 (95%)	1.29	21 (36%) 0 1	131, 143, 165, 167	0
14	5I	60/61 (98%)	0.02	1 (1%) 73 67	98, 110, 131, 142	0
15	6A	88/89 (98%)	0.26	4 (4%) 37 30	90, 113, 134, 136	0
15	6I	88/89 (98%)	0.34	4 (4%) 37 30	87, 108, 130, 139	0
16	7A	84/88 (95%)	0.42	4 (4%) 34 28	93, 108, 135, 169	0
16	7I	84/88 (95%)	0.82	15 (17%) 2 1	108, 120, 155, 187	0
17	8A	99/105 (94%)	0.52	9 (9%) 11 9	98, 112, 126, 131	0
17	8I	100/105 (95%)	0.12	3 (3%) 54 47	95, 113, 129, 133	0
18	9A	69/88 (78%)	1.37	16 (23%) 1 1	93, 115, 139, 172	0
18	9I	67/88 (76%)	1.47	21 (31%) 1 1	93, 111, 135, 144	0
19	AA	78/93 (83%)	1.43	25 (32%) 1 1	150, 182, 201, 206	0
19	AI	80/93 (86%)	1.02	18 (22%) 1 1	116, 149, 171, 175	0
20	BA	99/106 (93%)	0.08	1 (1%) 84 80	90, 115, 143, 158	0
20	BI	99/106 (93%)	0.36	3 (3%) 54 47	113, 132, 170, 175	0
21	1B	25/27 (92%)	0.98	6 (24%) 1 1	121, 142, 155, 172	0
21	1F	23/27 (85%)	0.24	0 100 100	115, 129, 133, 136	0
22	1K	83/87 (95%)	0.02	5 (6%) 25 20	95, 175, 257, 267	0
22	1L	83/87 (95%)	0.62	12 (14%) 3 3	111, 193, 298, 318	0
23	2K	73/87 (83%)	-0.06	4 (5%) 29 23	90, 130, 190, 235	0
23	2L	74/87 (85%)	0.21	5 (6%) 20 17	89, 140, 212, 243	0
24	3K	77/87 (88%)	0.04	3 (3%) 43 36	82, 248, 274, 282	0
24	3L	75/87 (86%)	-0.21	3 (4%) 42 34	82, 207, 221, 226	0
25	4K	16/60 (26%)	0.02	0 100 100	89, 147, 205, 218	0
25	4L	21/60 (35%)	0.16	2 (9%) 10 9	105, 147, 219, 221	0
26	14	2909/2917 (99%)	-0.35	35 (1%) 81 76	61, 91, 244, 328	0
26	1H	2912/2917 (99%)	-0.40	23 (0%) 87 84	55, 86, 243, 301	0
27	16	122/122 (100%)	-0.71	0 100 100	87, 113, 138, 224	0
27	1J	122/122 (100%)	-0.68	0 100 100	92, 126, 154, 207	0
28	11	273/276 (98%)	0.30	4 (1%) 76 71	55, 76, 93, 103	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
28	19	273/276 (98%)	0.53	11 (4%) 42 34	60, 81, 97, 113	0
29	21	205/206 (99%)	0.72	23 (11%) 7 5	63, 98, 141, 156	0
29	29	205/206 (99%)	0.68	18 (8%) 12 10	68, 96, 137, 158	0
30	31	202/210 (96%)	0.23	8 (3%) 42 34	59, 88, 127, 140	0
30	39	208/210 (99%)	0.59	12 (5%) 26 21	67, 106, 167, 200	0
31	41	181/182 (99%)	1.48	54 (29%) 1 1	113, 144, 175, 183	0
31	49	181/182 (99%)	1.84	68 (37%) 0 1	131, 162, 190, 207	0
32	51	174/180 (96%)	0.44	17 (9%) 10 8	93, 118, 133, 143	0
32	59	170/180 (94%)	1.33	48 (28%) 1 1	154, 211, 241, 256	0
33	61	146/148 (98%)	0.73	21 (14%) 3 3	86, 134, 157, 167	0
33	69	146/148 (98%)	1.09	38 (26%) 1 1	90, 135, 158, 166	0
34	15	138/140 (98%)	0.64	9 (6%) 22 18	79, 105, 142, 157	0
34	58	138/140 (98%)	0.48	12 (8%) 13 10	78, 100, 136, 154	0
35	25	122/122 (100%)	0.63	8 (6%) 22 17	77, 93, 110, 116	0
35	68	122/122 (100%)	0.72	7 (5%) 27 22	66, 89, 105, 114	0
36	35	150/150 (100%)	0.68	16 (10%) 8 6	68, 107, 146, 170	0
36	78	147/150 (98%)	-0.08	0 100 100	64, 92, 114, 126	0
37	45	140/141 (99%)	1.24	32 (22%) 1 1	77, 106, 132, 154	0
37	88	141/141 (100%)	1.02	26 (18%) 2 1	73, 95, 118, 143	0
38	55	117/118 (99%)	0.30	3 (2%) 59 53	68, 86, 107, 119	0
38	98	118/118 (100%)	0.56	5 (4%) 40 33	76, 94, 113, 126	0
39	65	111/112 (99%)	0.92	16 (14%) 3 3	91, 117, 141, 150	0
39	A8	111/112 (99%)	0.76	14 (12%) 5 4	90, 107, 127, 141	0
40	75	137/146 (93%)	0.12	2 (1%) 76 71	83, 101, 163, 193	0
40	B8	129/146 (88%)	0.44	6 (4%) 35 29	84, 103, 135, 159	0
41	85	117/118 (99%)	0.27	6 (5%) 32 25	69, 93, 134, 152	0
41	C8	117/118 (99%)	0.34	2 (1%) 73 67	65, 89, 124, 139	0
42	95	101/101 (100%)	0.58	7 (6%) 20 16	70, 121, 143, 174	0
42	D8	101/101 (100%)	1.00	15 (14%) 3 2	69, 110, 140, 150	0
43	A5	113/113 (100%)	0.61	6 (5%) 30 24	68, 80, 112, 185	0
43	E8	112/113 (99%)	0.65	6 (5%) 29 24	72, 84, 120, 154	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
44	B5	92/96 (95%)	0.43	4 (4%) 39 32	76, 92, 116, 127	0
44	F8	94/96 (97%)	0.65	8 (8%) 13 10	67, 81, 107, 132	0
45	C5	104/110 (94%)	1.26	22 (21%) 1 1	96, 121, 156, 170	0
45	G8	103/110 (93%)	0.32	2 (1%) 70 63	83, 103, 144, 153	0
46	D5	135/206 (65%)	1.58	47 (34%) 0 1	110, 142, 177, 191	0
46	H8	171/206 (83%)	1.04	26 (15%) 3 2	100, 140, 212, 221	0
47	E5	80/85 (94%)	0.89	12 (15%) 3 2	76, 92, 114, 143	0
47	I8	83/85 (97%)	0.75	9 (10%) 8 6	75, 88, 104, 115	0
48	F5	94/98 (95%)	0.56	6 (6%) 23 19	70, 88, 127, 146	0
48	J8	95/98 (96%)	1.02	19 (20%) 1 1	67, 85, 135, 140	0
49	G5	67/72 (93%)	0.51	3 (4%) 37 30	90, 112, 131, 146	0
49	K8	68/72 (94%)	0.23	2 (2%) 55 49	71, 90, 105, 126	0
50	H5	59/60 (98%)	0.57	5 (8%) 13 10	85, 101, 151, 166	0
50	L8	57/60 (95%)	0.29	2 (3%) 48 40	76, 94, 117, 137	0
51	I5	63/71 (88%)	2.59	38 (60%) 0 0	157, 205, 225, 231	0
51	M8	66/71 (92%)	2.18	35 (53%) 0 0	142, 184, 199, 204	0
52	J5	56/60 (93%)	0.06	1 (1%) 71 65	63, 85, 141, 149	0
52	N8	55/60 (91%)	0.80	9 (16%) 2 2	60, 100, 170, 184	0
53	L5	47/49 (95%)	0.05	1 (2%) 67 60	64, 69, 88, 95	0
53	P8	47/49 (95%)	-0.08	2 (4%) 39 32	57, 64, 82, 108	0
54	M5	53/65 (81%)	0.87	7 (13%) 4 3	68, 83, 101, 111	0
54	Q8	60/65 (92%)	0.29	2 (3%) 50 43	69, 84, 110, 124	0
All	All	20915/21710 (96%)	0.17	1392 (6%) 21 17	55, 108, 195, 328	0

The worst 5 of 1392 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
31	41	2	PRO	12.7
26	14	2902	C	11.9
26	14	2797	U	10.2
36	35	150	ALA	9.4
12	3A	128	ALA	9.3

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

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
22	5MU	1L	65	21/22	0.96	0.16	-	126,135,149,154	0
22	5MU	1K	65	21/22	0.92	0.15	-	109,126,139,143	0
22	PSU	1K	66	20/21	0.92	0.14	-	113,134,150,151	0
23	5MU	2L	65	21/22	0.94	0.13	-	116,128,142,149	0
23	OMG	2K	18	24/25	0.89	0.14	-	125,139,151,157	0
22	1MG	1K	38	24/25	0.95	0.15	-	93,100,106,107	0
23	PSU	2K	66	20/21	0.91	0.10	-	117,125,133,135	0
22	PSU	1K	39	20/21	0.93	0.15	-	97,105,110,111	0
22	PSU	1L	66	20/21	0.89	0.14	-	123,141,157,157	0
23	PSU	2L	39	20/21	0.95	0.13	-	95,108,114,117	0
23	H2U	2K	17	20/21	0.86	0.17	-	125,135,173,181	0
23	H2U	2L	17	20/21	0.90	0.16	-	129,137,180,190	0
23	PSU	2K	39	20/21	0.94	0.21	-	83,96,104,110	0
23	OMG	2L	18	24/25	0.93	0.16	-	136,144,154,157	0
22	PSU	1L	39	20/21	0.92	0.15	-	112,122,132,132	0
23	PSU	2L	66	20/21	0.93	0.11	-	120,131,136,140	0
22	1MG	1L	38	24/25	0.95	0.15	-	106,120,124,127	0
23	1MG	2L	38	24/25	0.96	0.13	-	103,110,121,121	0
23	1MG	2K	38	24/25	0.96	0.15	-	87,96,107,111	0
23	5MU	2K	65	21/22	0.97	0.08	-	119,125,131,134	0

## 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.



Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
55	MG	1H	3283	1/1	0.68	0.95	90.93	85,85,85,85	0
55	MG	14	3190	1/1	0.95	0.67	90.20	75,75,75,75	0
55	MG	14	3196	1/1	0.91	0.47	61.17	65,65,65,65	0
55	MG	14	3205	1/1	0.89	0.59	55.31	83,83,83,83	0
55	MG	13	1613	1/1	0.91	0.54	53.09	92,92,92,92	0
55	MG	14	3262	1/1	0.93	0.36	46.33	89,89,89,89	0
55	MG	1H	3314	1/1	0.68	0.69	42.75	92,92,92,92	0
55	MG	1H	3029	1/1	0.94	0.46	41.29	56,56,56,56	0
55	MG	14	3130	1/1	0.52	0.49	40.33	102,102,102,102	0
55	MG	1H	3279	1/1	0.65	0.66	39.28	86,86,86,86	0
55	MG	1H	3405	1/1	0.84	0.95	37.34	89,89,89,89	0
55	MG	13	1672	1/1	0.80	0.43	35.27	89,89,89,89	0
55	MG	14	3292	1/1	0.78	0.59	35.17	79,79,79,79	0
55	MG	1H	3363	1/1	0.95	0.67	35.05	54,54,54,54	0
55	MG	14	3373	1/1	0.92	1.13	34.77	74,74,74,74	0
55	MG	1H	3005	1/1	0.99	0.47	33.74	45,45,45,45	0
55	MG	13	1608	1/1	0.96	0.55	32.41	64,64,64,64	0
55	MG	14	3148	1/1	0.92	0.49	29.79	72,72,72,72	0
55	MG	14	3301	1/1	0.61	0.43	29.07	90,90,90,90	0
55	MG	1G	1685	1/1	0.94	0.44	28.34	92,92,92,92	0
55	MG	14	3350	1/1	0.92	0.41	27.60	84,84,84,84	0
55	MG	1H	3359	1/1	0.98	0.59	27.42	45,45,45,45	0
55	MG	14	3034	1/1	0.96	0.61	25.03	60,60,60,60	0
55	MG	14	3170	1/1	0.97	0.52	24.45	67,67,67,67	0
55	MG	1H	3108	1/1	0.98	0.68	24.20	58,58,58,58	0
55	MG	1H	3121	1/1	0.96	0.54	23.97	54,54,54,54	0
55	MG	14	3276	1/1	0.49	0.52	23.65	86,86,86,86	0
55	MG	1H	3130	1/1	0.96	0.53	23.53	70,70,70,70	0
55	MG	1G	1618	1/1	0.93	0.39	23.40	76,76,76,76	0
55	MG	14	3353	1/1	0.93	0.64	23.39	84,84,84,84	0
55	MG	14	3065	1/1	0.98	0.58	22.85	47,47,47,47	0
55	MG	14	3038	1/1	0.94	0.58	22.79	57,57,57,57	0
55	MG	14	3031	1/1	0.96	0.45	22.33	66,66,66,66	0
55	MG	1H	3125	1/1	0.77	0.60	21.86	73,73,73,73	0
55	MG	1H	3150	1/1	0.97	0.46	21.80	84,84,84,84	0
55	MG	1G	1687	1/1	0.93	0.40	21.31	101,101,101,101	0
55	MG	14	3146	1/1	0.98	0.40	21.07	73,73,73,73	0
55	MG	14	3044	1/1	0.95	0.75	21.04	79,79,79,79	0
55	MG	13	1724	1/1	0.95	0.46	20.36	63,63,63,63	0
55	MG	14	3071	1/1	0.94	0.57	19.80	48,48,48,48	0
55	MG	1H	3135	1/1	0.97	0.55	19.62	61,61,61,61	0
55	MG	13	1720	1/1	0.85	0.30	18.85	94,94,94,94	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
55	MG	1H	3018	1/1	0.93	0.54	18.85	46,46,46,46	0
55	MG	14	3319	1/1	0.71	0.44	18.49	89,89,89,89	0
55	MG	14	3109	1/1	0.93	0.48	18.47	66,66,66,66	0
55	MG	1H	3173	1/1	0.90	0.40	17.89	70,70,70,70	0
55	MG	14	3074	1/1	0.81	0.39	17.87	53,53,53,53	0
55	MG	13	1713	1/1	0.54	0.42	17.70	99,99,99,99	0
55	MG	14	3072	1/1	0.97	0.52	17.45	52,52,52,52	0
55	MG	14	3040	1/1	0.95	0.81	17.36	59,59,59,59	0
55	MG	1H	3103	1/1	0.98	0.43	17.15	48,48,48,48	0
55	MG	1H	3326	1/1	0.98	0.49	17.14	51,51,51,51	0
55	MG	1H	3017	1/1	0.95	0.47	17.11	56,56,56,56	0
55	MG	1H	3092	1/1	0.91	0.43	16.84	73,73,73,73	0
55	MG	14	3173	1/1	0.70	0.44	16.63	76,76,76,76	0
55	MG	14	3090	1/1	0.98	0.43	16.35	58,58,58,58	0
55	MG	1H	3083	1/1	0.95	0.36	16.22	55,55,55,55	0
55	MG	13	1601	1/1	0.98	0.36	16.10	63,63,63,63	0
55	MG	14	3120	1/1	0.65	0.29	15.55	69,69,69,69	0
55	MG	1H	3216	1/1	0.91	0.41	15.55	65,65,65,65	0
55	MG	1H	3152	1/1	0.94	0.41	15.52	54,54,54,54	0
55	MG	1H	3001	1/1	0.97	0.46	15.47	51,51,51,51	0
55	MG	1H	3336	1/1	0.81	0.27	15.33	70,70,70,70	0
55	MG	1H	3197	1/1	0.97	0.48	15.30	48,48,48,48	0
55	MG	1H	3365	1/1	0.96	0.28	15.30	46,46,46,46	0
55	MG	14	3243	1/1	0.71	0.39	15.24	75,75,75,75	0
55	MG	14	3066	1/1	0.99	0.42	15.23	62,62,62,62	0
55	MG	1H	3097	1/1	0.98	0.47	15.23	48,48,48,48	0
55	MG	1H	3011	1/1	0.98	0.33	15.16	49,49,49,49	0
55	MG	13	1626	1/1	0.95	0.56	15.07	68,68,68,68	0
55	MG	1H	3263	1/1	0.87	0.42	14.96	67,67,67,67	0
55	MG	14	3121	1/1	0.89	0.42	14.92	69,69,69,69	0
55	MG	1H	3344	1/1	0.92	0.34	14.76	85,85,85,85	0
55	MG	1H	3120	1/1	0.95	0.42	14.67	53,53,53,53	0
55	MG	1H	3003	1/1	0.99	0.45	14.65	58,58,58,58	0
55	MG	14	3229	1/1	0.42	0.56	14.62	77,77,77,77	0
55	MG	1H	3098	1/1	0.98	0.47	14.58	40,40,40,40	0
55	MG	13	1635	1/1	0.88	0.28	14.37	101,101,101,101	0
55	MG	14	3011	1/1	0.97	0.39	13.97	48,48,48,48	0
55	MG	14	3037	1/1	0.98	0.43	13.93	58,58,58,58	0
55	MG	13	1716	1/1	0.93	0.27	13.57	103,103,103,103	0
55	MG	14	3059	1/1	0.95	0.37	13.50	54,54,54,54	0
55	MG	14	3155	1/1	0.78	0.41	13.29	72,72,72,72	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
55	MG	1H	3161	1/1	0.85	0.39	13.08	80,80,80,80	0
55	MG	13	1638	1/1	0.97	0.39	12.95	74,74,74,74	0
55	MG	13	1681	1/1	0.95	0.27	12.94	91,91,91,91	0
55	MG	1H	3373	1/1	0.87	0.38	12.93	85,85,85,85	0
55	MG	1H	3039	1/1	0.94	0.40	12.73	66,66,66,66	0
55	MG	14	3140	1/1	0.87	0.26	12.60	108,108,108,108	0
55	MG	14	3009	1/1	0.98	0.44	12.56	62,62,62,62	0
55	MG	14	3274	1/1	0.87	0.25	12.50	83,83,83,83	0
55	MG	14	3067	1/1	0.97	0.38	12.32	54,54,54,54	0
55	MG	14	3207	1/1	0.97	0.49	12.18	92,92,92,92	0
55	MG	1G	1720	1/1	0.87	0.28	12.14	102,102,102,102	0
55	MG	14	3046	1/1	0.92	0.35	12.06	67,67,67,67	0
55	MG	1G	1603	1/1	0.98	0.49	12.03	65,65,65,65	0
55	MG	14	3024	1/1	0.97	0.38	11.99	79,79,79,79	0
55	MG	14	3224	1/1	0.94	0.48	11.91	73,73,73,73	0
55	MG	1H	3080	1/1	0.97	0.37	11.84	89,89,89,89	0
55	MG	13	1632	1/1	0.98	0.45	11.83	74,74,74,74	0
55	MG	13	1619	1/1	0.76	0.24	11.80	111,111,111,111	0
55	MG	1H	3281	1/1	0.95	0.36	11.64	65,65,65,65	0
55	MG	1H	3052	1/1	0.96	0.38	11.60	67,67,67,67	0
55	MG	14	3330	1/1	0.99	0.49	11.56	43,43,43,43	0
55	MG	1G	1686	1/1	0.96	0.26	11.52	108,108,108,108	0
55	MG	13	1697	1/1	0.95	0.52	11.50	67,67,67,67	0
55	MG	14	3093	1/1	0.97	0.32	11.41	60,60,60,60	0
55	MG	1H	3085	1/1	0.88	0.34	11.40	75,75,75,75	0
55	MG	13	1700	1/1	0.92	0.23	11.33	87,87,87,87	0
55	MG	1G	1728	1/1	0.81	0.26	11.25	92,92,92,92	0
55	MG	1G	1702	1/1	0.67	0.31	11.15	95,95,95,95	0
55	MG	14	3039	1/1	0.95	0.41	11.11	63,63,63,63	0
55	MG	14	3253	1/1	0.80	0.35	11.10	98,98,98,98	0
55	MG	14	3179	1/1	0.97	0.38	11.00	90,90,90,90	0
55	MG	1H	3009	1/1	0.96	0.32	10.99	56,56,56,56	0
55	MG	1H	3096	1/1	0.96	0.28	10.92	62,62,62,62	0
55	MG	1H	3310	1/1	0.97	0.35	10.91	52,52,52,52	0
55	MG	14	3150	1/1	0.86	0.25	10.87	92,92,92,92	0
55	MG	13	1629	1/1	0.93	0.30	10.81	65,65,65,65	0
55	MG	14	3032	1/1	0.84	0.48	10.80	71,71,71,71	0
55	MG	1G	1688	1/1	0.98	0.28	10.70	103,103,103,103	0
55	MG	1H	3118	1/1	0.95	0.39	10.61	74,74,74,74	0
55	MG	1G	1604	1/1	0.91	0.30	10.55	79,79,79,79	0
55	MG	14	3188	1/1	0.88	0.27	10.52	82,82,82,82	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
55	MG	13	1709	1/1	0.96	0.30	10.52	99,99,99,99	0
55	MG	1H	3035	1/1	0.97	0.32	10.44	82,82,82,82	0
55	MG	14	3013	1/1	0.99	0.30	10.43	66,66,66,66	0
55	MG	14	3100	1/1	0.97	0.28	10.32	77,77,77,77	0
55	MG	1H	3244	1/1	0.94	0.26	10.32	92,92,92,92	0
55	MG	14	3030	1/1	0.92	0.28	10.23	70,70,70,70	0
55	MG	1H	3002	1/1	0.98	0.39	10.13	53,53,53,53	0
55	MG	13	1667	1/1	0.87	0.32	10.07	88,88,88,88	0
55	MG	14	3036	1/1	0.93	0.28	9.97	71,71,71,71	0
55	MG	1H	3058	1/1	0.96	0.27	9.96	67,67,67,67	0
55	MG	13	1661	1/1	0.95	0.31	9.91	89,89,89,89	0
55	MG	1H	3153	1/1	0.87	0.23	9.58	79,79,79,79	0
55	MG	1G	1622	1/1	0.98	0.37	9.56	95,95,95,95	0
55	MG	1H	3171	1/1	0.77	0.24	9.53	80,80,80,80	0
55	MG	13	1604	1/1	0.96	0.30	9.44	71,71,71,71	0
55	MG	1H	3067	1/1	0.95	0.44	9.32	68,68,68,68	0
55	MG	13	1622	1/1	0.79	0.30	9.31	85,85,85,85	0
55	MG	14	3363	1/1	0.88	0.32	9.29	67,67,67,67	0
55	MG	1H	3019	1/1	0.98	0.56	8.86	51,51,51,51	0
55	MG	1H	3355	1/1	0.99	0.37	8.78	62,62,62,62	0
55	MG	1G	1710	1/1	0.93	0.40	8.72	87,87,87,87	0
55	MG	1H	3142	1/1	0.95	0.21	8.66	68,68,68,68	0
55	MG	1H	3510	1/1	0.89	0.48	8.63	65,65,65,65	0
55	MG	14	3124	1/1	0.85	0.24	8.52	77,77,77,77	0
55	MG	13	1728	1/1	0.95	0.29	8.49	80,80,80,80	0
55	MG	1H	3102	1/1	0.96	0.38	8.36	64,64,64,64	0
55	MG	1H	3140	1/1	0.91	0.32	8.31	82,82,82,82	0
55	MG	13	1606	1/1	0.98	0.29	8.21	89,89,89,89	0
55	MG	1G	1709	1/1	0.98	0.27	8.15	81,81,81,81	0
55	MG	14	3017	1/1	0.98	0.27	8.10	70,70,70,70	0
55	MG	1H	3395	1/1	0.76	0.28	8.04	100,100,100,100	0
55	MG	1H	3168	1/1	0.95	0.30	8.00	72,72,72,72	0
55	MG	1H	3132	1/1	0.77	0.29	7.94	63,63,63,63	0
55	MG	1H	3323	1/1	0.81	0.22	7.88	83,83,83,83	0
55	MG	14	3153	1/1	0.95	0.65	7.88	71,71,71,71	0
55	MG	13	1636	1/1	0.96	0.21	7.85	73,73,73,73	0
55	MG	14	3183	1/1	0.96	0.28	7.84	64,64,64,64	0
55	MG	13	1602	1/1	0.98	0.28	7.76	85,85,85,85	0
55	MG	1H	3041	1/1	0.94	0.21	7.74	72,72,72,72	0
55	MG	14	3488	1/1	0.97	0.57	7.73	64,64,64,64	0
55	MG	1G	1676	1/1	0.95	0.30	7.72	93,93,93,93	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
55	MG	1H	3290	1/1	0.91	0.28	7.55	71,71,71,71	0
55	MG	1G	1672	1/1	0.81	0.27	7.41	95,95,95,95	0
55	MG	1H	3071	1/1	0.91	0.37	7.39	74,74,74,74	0
55	MG	1G	1644	1/1	0.96	0.27	7.37	96,96,96,96	0
55	MG	1H	3299	1/1	0.78	0.20	7.31	79,79,79,79	0
55	MG	1H	3266	1/1	0.66	0.23	7.12	79,79,79,79	0
55	MG	14	3110	1/1	0.83	0.36	7.10	74,74,74,74	0
55	MG	1H	3055	1/1	0.99	0.25	6.93	66,66,66,66	0
55	MG	1G	1696	1/1	0.74	0.25	6.78	94,94,94,94	0
55	MG	1H	3268	1/1	0.85	0.27	6.69	66,66,66,66	0
55	MG	1H	3066	1/1	0.94	0.26	6.67	86,86,86,86	0
55	MG	14	3177	1/1	0.92	0.21	6.59	75,75,75,75	0
55	MG	14	3052	1/1	0.99	0.23	6.57	62,62,62,62	0
55	MG	1H	3021	1/1	0.99	0.38	6.53	43,43,43,43	0
55	MG	1H	3166	1/1	0.80	0.34	6.52	83,83,83,83	0
55	MG	14	3099	1/1	0.89	0.29	6.50	57,57,57,57	0
55	MG	1H	3254	1/1	0.96	0.29	6.49	56,56,56,56	0
55	MG	1H	3116	1/1	0.84	0.31	6.44	56,56,56,56	0
55	MG	1H	3213	1/1	0.78	0.25	6.34	55,55,55,55	0
55	MG	14	3197	1/1	0.98	0.29	6.32	82,82,82,82	0
55	MG	1H	3075	1/1	0.99	0.30	6.31	69,69,69,69	0
55	MG	1H	3226	1/1	0.68	0.23	6.24	93,93,93,93	0
55	MG	1H	3377	1/1	0.83	0.39	6.19	87,87,87,87	0
55	MG	1G	1602	1/1	0.98	0.38	6.18	80,80,80,80	0
55	MG	1G	1630	1/1	0.94	0.37	6.13	91,91,91,91	0
55	MG	1H	3484	1/1	0.92	0.25	6.00	104,104,104,104	0
55	MG	13	1615	1/1	0.94	0.24	5.92	88,88,88,88	0
55	MG	1H	3177	1/1	0.99	0.28	5.87	93,93,93,93	0
55	MG	1G	1722	1/1	0.90	0.32	5.86	84,84,84,84	0
55	MG	13	1731	1/1	0.88	0.19	5.84	82,82,82,82	0
55	MG	14	3172	1/1	0.98	0.38	5.65	69,69,69,69	0
55	MG	1H	3087	1/1	0.96	0.20	5.51	76,76,76,76	0
55	MG	1H	3352	1/1	0.76	0.23	5.45	87,87,87,87	0
55	MG	14	3005	1/1	0.98	0.29	5.44	62,62,62,62	0
55	MG	14	3366	1/1	0.92	0.24	5.43	89,89,89,89	0
55	MG	1H	3273	1/1	0.90	0.24	5.41	93,93,93,93	0
55	MG	14	3166	1/1	0.96	0.28	5.38	61,61,61,61	0
55	MG	14	3200	1/1	0.80	0.50	5.35	77,77,77,77	0
55	MG	1H	3509	1/1	0.95	0.46	5.32	47,47,47,47	0
55	MG	1G	1704	1/1	0.90	0.18	5.24	78,78,78,78	0
55	MG	1G	1621	1/1	0.98	0.28	5.16	80,80,80,80	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
55	MG	14	3108	1/1	0.98	0.30	5.09	61,61,61,61	0
55	MG	14	3241	1/1	0.92	0.23	5.02	83,83,83,83	0
55	MG	14	3285	1/1	0.82	0.33	4.94	72,72,72,72	0
55	MG	14	3490	1/1	0.96	0.53	4.75	81,81,81,81	0
55	MG	14	3280	1/1	0.72	0.17	4.67	87,87,87,87	0
55	MG	1H	3061	1/1	0.97	0.19	4.60	75,75,75,75	0
55	MG	1G	1701	1/1	0.68	0.19	4.58	119,119,119,119	0
55	MG	1G	1656	1/1	0.96	0.41	4.53	74,74,74,74	0
55	MG	29	301	1/1	0.85	0.42	4.52	88,88,88,88	0
55	MG	13	1688	1/1	0.83	0.18	4.43	92,92,92,92	0
55	MG	14	3041	1/1	0.98	0.33	4.39	53,53,53,53	0
55	MG	14	3206	1/1	0.97	0.23	4.37	92,92,92,92	0
55	MG	1H	3180	1/1	0.90	0.20	4.34	79,79,79,79	0
55	MG	2L	101	1/1	0.97	0.39	4.27	82,82,82,82	0
55	MG	14	3199	1/1	0.93	0.28	4.24	75,75,75,75	0
55	MG	16	201	1/1	0.83	0.20	4.12	97,97,97,97	0
55	MG	14	3300	1/1	0.98	0.28	4.07	64,64,64,64	0
55	MG	14	3042	1/1	0.97	0.38	4.06	47,47,47,47	0
55	MG	1H	3228	1/1	0.82	0.17	3.95	68,68,68,68	0
55	MG	13	1680	1/1	0.88	0.22	3.95	93,93,93,93	0
55	MG	1G	1649	1/1	0.90	0.20	3.91	109,109,109,109	0
55	MG	14	3094	1/1	0.97	0.30	3.90	60,60,60,60	0
55	MG	1H	3046	1/1	0.94	0.24	3.83	56,56,56,56	0
55	MG	1H	3060	1/1	0.98	0.35	3.75	59,59,59,59	0
55	MG	1H	3043	1/1	0.86	0.33	3.73	83,83,83,83	0
55	MG	1H	3148	1/1	0.97	0.31	3.73	75,75,75,75	0
55	MG	14	3314	1/1	0.92	0.21	3.72	90,90,90,90	0
55	MG	1H	3053	1/1	0.97	0.18	3.68	72,72,72,72	0
55	MG	1G	1613	1/1	0.72	0.21	3.46	92,92,92,92	0
55	MG	1H	3076	1/1	0.94	0.21	3.40	67,67,67,67	0
55	MG	13	1610	1/1	0.96	0.22	3.16	90,90,90,90	0
56	ZN	3E	302	1/1	0.98	0.36	3.15	86,86,86,86	0
55	MG	1G	1695	1/1	0.93	0.22	3.13	95,95,95,95	0
55	MG	1H	3025	1/1	0.90	0.24	3.08	55,55,55,55	0
55	MG	1H	3144	1/1	0.70	0.13	3.07	93,93,93,93	0
55	MG	14	3165	1/1	0.96	0.25	3.02	61,61,61,61	0
55	MG	1H	3369	1/1	0.92	0.20	2.97	86,86,86,86	0
55	MG	14	3225	1/1	0.93	0.18	2.96	87,87,87,87	0
55	MG	16	204	1/1	0.88	0.17	2.86	103,103,103,103	0
55	MG	1H	3217	1/1	0.93	0.22	2.77	56,56,56,56	0
56	ZN	C5	201	1/1	0.82	0.41	2.74	201,201,201,201	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
55	MG	14	3295	1/1	0.87	0.30	2.74	84,84,84,84	0
55	MG	1G	1641	1/1	0.95	0.19	2.73	91,91,91,91	0
55	MG	1H	3038	1/1	0.58	0.16	2.72	96,96,96,96	0
55	MG	1K	101	1/1	0.90	0.27	2.72	90,90,90,90	0
55	MG	1G	1608	1/1	0.98	0.20	2.68	99,99,99,99	0
55	MG	13	1609	1/1	0.95	0.29	2.67	80,80,80,80	0
56	ZN	G8	202	1/1	0.68	0.36	2.66	205,205,205,205	0
55	MG	1H	3016	1/1	0.98	0.26	2.56	70,70,70,70	0
55	MG	13	1639	1/1	0.90	0.17	2.46	85,85,85,85	0
55	MG	1H	3396	1/1	0.97	0.18	2.36	98,98,98,98	0
55	MG	1G	1619	1/1	0.98	0.21	2.32	105,105,105,105	0
55	MG	14	3105	1/1	0.87	0.18	2.28	90,90,90,90	0
55	MG	1H	3040	1/1	0.85	0.20	2.27	69,69,69,69	0
55	MG	1H	3113	1/1	0.93	0.17	2.26	78,78,78,78	0
55	MG	1H	3110	1/1	0.97	0.24	2.17	54,54,54,54	0
55	MG	1H	3115	1/1	0.94	0.26	2.07	73,73,73,73	0
55	MG	13	1711	1/1	0.86	0.15	2.05	107,107,107,107	0
55	MG	1H	3155	1/1	0.85	0.16	1.87	67,67,67,67	0
55	MG	14	3338	1/1	0.95	0.24	1.85	66,66,66,66	0
55	MG	1H	3388	1/1	0.82	0.45	1.75	90,90,90,90	0
55	MG	13	1696	1/1	0.78	0.23	1.75	73,73,73,73	0
55	MG	13	1674	1/1	0.77	0.20	1.66	112,112,112,112	0
55	MG	1H	3351	1/1	0.92	0.19	1.63	86,86,86,86	0
55	MG	1G	1713	1/1	0.86	0.26	1.63	100,100,100,100	0
55	MG	29	303	1/1	0.63	0.28	1.57	79,79,79,79	0
55	MG	13	1618	1/1	0.94	0.22	1.47	124,124,124,124	0
55	MG	1H	3209	1/1	0.99	0.51	1.46	63,63,63,63	0
55	MG	14	3118	1/1	0.89	0.19	1.44	69,69,69,69	0
55	MG	14	3026	1/1	0.81	0.10	1.38	83,83,83,83	0
55	MG	1G	1731	1/1	0.97	0.15	1.36	113,113,113,113	0
55	MG	11	301	1/1	0.82	0.34	1.29	53,53,53,53	0
55	MG	1H	3512	1/1	0.99	0.31	1.23	72,72,72,72	0
55	MG	14	3132	1/1	0.96	0.16	1.22	78,78,78,78	0
55	MG	14	3421	1/1	0.98	0.20	1.20	55,55,55,55	0
55	MG	14	3220	1/1	0.98	0.30	1.17	80,80,80,80	0
56	ZN	32	302	1/1	0.98	0.34	1.14	100,100,100,100	0
55	MG	85	201	1/1	0.90	0.22	1.11	83,83,83,83	0
55	MG	1G	1615	1/1	0.92	0.20	1.10	84,84,84,84	0
55	MG	1H	3186	1/1	0.82	0.15	1.02	76,76,76,76	0
55	MG	1G	1665	1/1	0.92	0.16	1.01	108,108,108,108	0
55	MG	14	3075	1/1	0.84	0.18	0.99	70,70,70,70	0
55	MG	1H	3093	1/1	0.99	0.18	0.98	60,60,60,60	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
55	MG	14	3103	1/1	0.88	0.18	0.97	73,73,73,73	0
55	MG	1H	3357	1/1	0.92	0.14	0.97	78,78,78,78	0
55	MG	1H	3044	1/1	0.91	0.23	0.84	63,63,63,63	0
55	MG	14	3117	1/1	0.96	0.19	0.72	73,73,73,73	0
55	MG	14	3249	1/1	0.91	0.13	0.59	100,100,100,100	0
55	MG	1J	201	1/1	0.98	0.18	0.57	115,115,115,115	0
55	MG	1G	1606	1/1	0.93	0.13	0.56	89,89,89,89	0
55	MG	1H	3045	1/1	0.91	0.18	0.52	64,64,64,64	0
55	MG	14	3106	1/1	0.94	0.22	0.47	80,80,80,80	0
55	MG	14	3302	1/1	0.99	0.16	0.46	85,85,85,85	0
55	MG	1G	1642	1/1	0.84	0.20	0.46	89,89,89,89	0
55	MG	14	3239	1/1	0.85	0.12	0.45	90,90,90,90	0
55	MG	2K	101	1/1	0.99	0.28	0.44	85,85,85,85	0
55	MG	1G	1646	1/1	0.97	0.19	0.39	109,109,109,109	0
55	MG	14	3193	1/1	0.79	0.36	0.39	83,83,83,83	0
55	MG	1H	3342	1/1	0.70	0.16	0.38	73,73,73,73	0
55	MG	2I	302	1/1	0.63	0.23	0.23	77,77,77,77	0
55	MG	1H	3498	1/1	0.91	0.21	0.19	100,100,100,100	0
55	MG	14	3340	1/1	0.82	0.27	0.17	66,66,66,66	0
55	MG	1H	3106	1/1	0.98	0.22	0.16	47,47,47,47	0
55	MG	13	1605	1/1	0.98	0.21	0.11	86,86,86,86	0
55	MG	1H	3418	1/1	0.98	0.17	0.03	71,71,71,71	0
55	MG	1G	1694	1/1	0.96	0.18	-0.16	80,80,80,80	0
55	MG	14	3475	1/1	0.97	0.16	-0.36	104,104,104,104	0
55	MG	1H	3095	1/1	0.95	0.17	-0.38	58,58,58,58	0
55	MG	13	1679	1/1	0.83	0.16	-0.43	135,135,135,135	0
55	MG	1G	1743	1/1	0.92	0.18	-0.49	98,98,98,98	0
55	MG	13	1729	1/1	0.79	0.10	-0.50	122,122,122,122	0
55	MG	13	1642	1/1	0.87	0.13	-0.63	85,85,85,85	0
55	MG	14	3126	1/1	0.78	0.14	-0.66	83,83,83,83	0
55	MG	88	302	1/1	0.88	0.18	-0.68	95,95,95,95	0
55	MG	1H	3375	1/1	0.91	0.18	-0.71	70,70,70,70	0
55	MG	1H	3415	1/1	0.97	0.16	-0.76	59,59,59,59	0
55	MG	14	3228	1/1	0.74	0.14	-0.77	78,78,78,78	0
55	MG	88	301	1/1	0.96	0.29	-0.78	82,82,82,82	0
55	MG	14	3448	1/1	0.93	0.11	-0.78	109,109,109,109	0
55	MG	1H	3417	1/1	0.98	0.15	-0.79	70,70,70,70	0
55	MG	1H	3191	1/1	0.89	0.13	-0.81	75,75,75,75	0
55	MG	1G	1692	1/1	0.94	0.10	-0.82	100,100,100,100	0
55	MG	14	3186	1/1	0.97	0.18	-0.85	69,69,69,69	0
55	MG	14	3477	1/1	0.97	0.13	-0.86	63,63,63,63	0
55	MG	1G	1691	1/1	0.99	0.08	-0.94	98,98,98,98	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
55	MG	1H	3349	1/1	0.89	0.15	-0.96	66,66,66,66	0
55	MG	1H	3442	1/1	0.97	0.14	-0.98	77,77,77,77	0
55	MG	45	202	1/1	0.93	0.15	-0.98	99,99,99,99	0
55	MG	1G	1611	1/1	0.98	0.10	-0.99	122,122,122,122	0
55	MG	14	3398	1/1	0.95	0.17	-0.99	66,66,66,66	0
56	ZN	5I	101	1/1	0.99	0.10	-1.00	109,109,109,109	0
55	MG	1G	1740	1/1	0.91	0.06	-1.08	112,112,112,112	0
55	MG	14	3240	1/1	0.97	0.13	-1.13	68,68,68,68	0
55	MG	14	3256	1/1	0.98	0.14	-1.17	95,95,95,95	0
56	ZN	5A	101	1/1	0.96	0.09	-1.19	125,125,125,125	0
55	MG	14	3462	1/1	0.97	0.16	-1.24	103,103,103,103	0
55	MG	1H	3437	1/1	0.99	0.13	-1.24	60,60,60,60	0
55	MG	1H	3511	1/1	0.89	0.09	-1.29	75,75,75,75	0
55	MG	1G	1738	1/1	0.62	0.07	-1.30	137,137,137,137	0
55	MG	13	1735	1/1	0.90	0.07	-1.33	111,111,111,111	0
55	MG	1H	3122	1/1	0.93	0.14	-1.35	68,68,68,68	0
55	MG	14	3409	1/1	0.94	0.16	-1.38	83,83,83,83	0
55	MG	13	1665	1/1	0.88	0.11	-1.40	103,103,103,103	0
55	MG	14	3456	1/1	0.82	0.13	-1.45	82,82,82,82	0
55	MG	14	3424	1/1	0.95	0.11	-1.47	72,72,72,72	0
55	MG	13	1714	1/1	0.91	0.08	-1.54	103,103,103,103	0
55	MG	14	3194	1/1	0.97	0.15	-1.58	66,66,66,66	0
55	MG	13	1732	1/1	0.89	0.06	-1.60	113,113,113,113	0
55	MG	14	3414	1/1	0.93	0.13	-1.61	85,85,85,85	0
55	MG	13	1745	1/1	0.98	0.13	-1.66	88,88,88,88	0
55	MG	14	3408	1/1	0.93	0.16	-1.70	63,63,63,63	0
55	MG	1H	3454	1/1	0.97	0.15	-1.73	94,94,94,94	0
55	MG	1H	3432	1/1	0.95	0.09	-1.73	58,58,58,58	0
55	MG	1H	3467	1/1	0.97	0.11	-1.79	67,67,67,67	0
55	MG	14	3397	1/1	0.99	0.15	-1.90	64,64,64,64	0
55	MG	1H	3505	1/1	0.98	0.09	-1.91	64,64,64,64	0
55	MG	14	3437	1/1	0.95	0.12	-2.02	88,88,88,88	0
55	MG	1H	3438	1/1	0.93	0.08	-2.02	75,75,75,75	0
55	MG	14	3022	1/1	0.92	0.09	-2.09	81,81,81,81	0
55	MG	1H	3424	1/1	0.95	0.13	-2.11	72,72,72,72	0
55	MG	14	3420	1/1	0.96	0.13	-2.12	91,91,91,91	0
55	MG	1H	3340	1/1	0.91	0.14	-2.22	75,75,75,75	0
55	MG	14	3287	1/1	0.93	0.08	-2.46	98,98,98,98	0
55	MG	13	1733	1/1	0.97	0.11	-2.49	95,95,95,95	0
55	MG	1H	3430	1/1	0.96	0.10	-2.49	87,87,87,87	0
55	MG	1H	3416	1/1	0.95	0.10	-2.53	60,60,60,60	0
55	MG	14	3461	1/1	0.85	0.06	-2.60	117,117,117,117	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
55	MG	14	3255	1/1	0.96	0.09	-2.60	90,90,90,90	0
55	MG	14	3489	1/1	0.85	0.07	-2.63	99,99,99,99	0
55	MG	14	3436	1/1	0.98	0.08	-2.65	69,69,69,69	0
55	MG	1H	3214	1/1	0.91	0.15	-2.66	56,56,56,56	0
55	MG	1H	3215	1/1	0.94	0.18	-2.75	45,45,45,45	0
55	MG	1G	1730	1/1	0.98	0.13	-2.80	77,77,77,77	0
55	MG	14	3426	1/1	0.98	0.11	-2.91	84,84,84,84	0
55	MG	13	1739	1/1	0.92	0.08	-2.91	111,111,111,111	0
55	MG	14	3445	1/1	0.90	0.10	-3.02	97,97,97,97	0
55	MG	1H	3473	1/1	0.94	0.12	-3.06	100,100,100,100	0
55	MG	1H	3485	1/1	0.94	0.07	-3.06	84,84,84,84	0
55	MG	14	3476	1/1	0.97	0.07	-3.10	65,65,65,65	0
55	MG	14	3481	1/1	0.93	0.11	-3.15	78,78,78,78	0
55	MG	14	3417	1/1	0.98	0.14	-3.21	72,72,72,72	0
55	MG	14	3401	1/1	0.90	0.15	-3.24	78,78,78,78	0
55	MG	14	3399	1/1	0.97	0.15	-3.24	75,75,75,75	0
55	MG	14	3346	1/1	0.98	0.14	-3.26	62,62,62,62	0
55	MG	1H	3421	1/1	0.94	0.11	-3.26	66,66,66,66	0
55	MG	1H	3137	1/1	0.97	0.11	-3.27	72,72,72,72	0
55	MG	14	3222	1/1	0.98	0.07	-3.49	73,73,73,73	0
55	MG	1H	3425	1/1	0.92	0.16	-3.61	62,62,62,62	0
55	MG	14	3400	1/1	0.64	0.10	-3.68	91,91,91,91	0
55	MG	1H	3466	1/1	0.95	0.08	-3.72	77,77,77,77	0
55	MG	1H	3475	1/1	0.90	0.09	-3.95	92,92,92,92	0
55	MG	14	3427	1/1	0.93	0.09	-4.01	97,97,97,97	0
55	MG	14	3403	1/1	0.92	0.06	-4.01	96,96,96,96	0
55	MG	14	3419	1/1	0.99	0.14	-4.11	56,56,56,56	0
55	MG	14	3406	1/1	0.97	0.13	-4.29	62,62,62,62	0
55	MG	14	3458	1/1	0.97	0.09	-4.42	91,91,91,91	0
55	MG	1H	3434	1/1	0.97	0.10	-4.53	72,72,72,72	0
55	MG	1H	3476	1/1	0.93	0.07	-4.56	119,119,119,119	0
55	MG	14	3405	1/1	0.93	0.09	-4.58	70,70,70,70	0
55	MG	14	3425	1/1	0.97	0.11	-4.86	66,66,66,66	0
55	MG	14	3402	1/1	0.96	0.13	-4.90	63,63,63,63	0
55	MG	1H	3444	1/1	0.95	0.04	-4.91	94,94,94,94	0
55	MG	1H	3502	1/1	0.98	0.10	-4.94	60,60,60,60	0
55	MG	14	3450	1/1	0.94	0.08	-5.34	65,65,65,65	0
55	MG	1H	3422	1/1	0.86	0.07	-5.39	85,85,85,85	0
55	MG	14	3416	1/1	0.93	0.11	-5.60	96,96,96,96	0
55	MG	1H	3440	1/1	0.99	0.10	-5.82	66,66,66,66	0
55	MG	14	3429	1/1	0.95	0.12	-5.90	72,72,72,72	0
55	MG	14	3433	1/1	0.85	0.10	-6.11	91,91,91,91	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
55	MG	14	3169	1/1	0.96	0.10	-6.14	55,55,55,55	0
55	MG	14	3412	1/1	0.95	0.11	-6.19	77,77,77,77	0
55	MG	1H	3458	1/1	0.98	0.06	-6.26	67,67,67,67	0
55	MG	1H	3489	1/1	0.95	0.09	-6.34	97,97,97,97	0
55	MG	1H	3433	1/1	0.97	0.08	-6.43	67,67,67,67	0
55	MG	1H	3464	1/1	0.90	0.07	-6.92	92,92,92,92	0
55	MG	1H	3483	1/1	0.98	0.08	-7.26	86,86,86,86	0
55	MG	14	3444	1/1	0.93	0.06	-7.51	106,106,106,106	0
55	MG	14	3482	1/1	0.96	0.11	-7.59	81,81,81,81	0
55	MG	1H	3446	1/1	0.86	0.11	-9.10	83,83,83,83	0
55	MG	1H	3439	1/1	0.98	0.11	-11.00	59,59,59,59	0
55	MG	13	1671	1/1	0.91	0.05	-11.67	106,106,106,106	0
55	MG	14	3422	1/1	0.84	0.13	-15.48	68,68,68,68	0
55	MG	1H	3179	1/1	0.89	0.28	-	71,71,71,71	0
55	MG	1H	3251	1/1	0.95	0.20	-	85,85,85,85	0
55	MG	1H	3462	1/1	0.94	0.09	-	91,91,91,91	0
55	MG	1H	3256	1/1	0.85	0.28	-	82,82,82,82	0
55	MG	1H	3257	1/1	0.82	0.34	-	82,82,82,82	0
55	MG	1G	1609	1/1	0.87	0.27	-	101,101,101,101	0
55	MG	1H	3348	1/1	0.91	0.35	-	88,88,88,88	0
55	MG	1G	1607	1/1	0.97	0.20	-	86,86,86,86	0
55	MG	14	3234	1/1	0.94	0.33	-	76,76,76,76	0
55	MG	14	3111	1/1	0.85	0.39	-	56,56,56,56	0
55	MG	1H	3431	1/1	0.97	0.06	-	74,74,74,74	0
55	MG	14	3236	1/1	0.69	0.32	-	119,119,119,119	0
55	MG	1H	3308	1/1	0.93	0.55	-	77,77,77,77	0
55	MG	14	3485	1/1	0.84	0.18	-	101,101,101,101	0
55	MG	13	1740	1/1	0.84	0.15	-	106,106,106,106	0
55	MG	1H	3366	1/1	0.96	0.16	-	76,76,76,76	0
55	MG	1H	3389	1/1	0.88	0.54	-	99,99,99,99	0
55	MG	1G	1659	1/1	0.72	0.61	-	83,83,83,83	0
55	MG	1G	1629	1/1	0.92	0.30	-	89,89,89,89	0
55	MG	13	1677	1/1	0.77	0.49	-	77,77,77,77	0
55	MG	13	1631	1/1	0.73	0.65	-	80,80,80,80	0
55	MG	1H	3451	1/1	0.80	0.07	-	105,105,105,105	0
55	MG	1H	3341	1/1	0.89	0.41	-	83,83,83,83	0
55	MG	14	3284	1/1	0.92	0.33	-	79,79,79,79	0
55	MG	1H	3291	1/1	0.96	0.35	-	117,117,117,117	0
55	MG	13	1675	1/1	0.77	0.32	-	87,87,87,87	0
55	MG	13	1645	1/1	0.86	0.48	-	84,84,84,84	0
55	MG	1H	3048	1/1	0.41	0.34	-	87,87,87,87	0
55	MG	1H	3506	1/1	0.98	0.08	-	81,81,81,81	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
55	MG	13	1668	1/1	0.98	0.38	-	78,78,78,78	0
55	MG	14	3168	1/1	0.93	0.39	-	66,66,66,66	0
55	MG	1H	3300	1/1	0.90	0.49	-	91,91,91,91	0
55	MG	14	3345	1/1	0.96	0.15	-	89,89,89,89	0
55	MG	14	3294	1/1	0.90	0.52	-	69,69,69,69	0
55	MG	14	3331	1/1	0.96	0.42	-	63,63,63,63	0
55	MG	1H	3492	1/1	0.89	0.20	-	101,101,101,101	0
55	MG	14	3382	1/1	0.67	0.35	-	91,91,91,91	0
55	MG	1G	1716	1/1	0.88	0.21	-	98,98,98,98	0
55	MG	14	3439	1/1	0.96	0.06	-	105,105,105,105	0
55	MG	1G	1707	1/1	0.69	0.57	-	92,92,92,92	0
55	MG	14	3077	1/1	0.97	0.46	-	63,63,63,63	0
55	MG	14	3440	1/1	0.94	0.04	-	105,105,105,105	0
55	MG	14	3079	1/1	0.95	0.56	-	46,46,46,46	0
55	MG	1H	3224	1/1	0.94	0.23	-	80,80,80,80	0
55	MG	1H	3264	1/1	0.85	0.24	-	86,86,86,86	0
55	MG	14	3305	1/1	0.86	0.52	-	89,89,89,89	0
55	MG	1H	3126	1/1	0.86	0.71	-	84,84,84,84	0
55	MG	14	3273	1/1	0.83	0.97	-	87,87,87,87	0
55	MG	14	3261	1/1	0.83	0.47	-	91,91,91,91	0
55	MG	13	1652	1/1	0.97	0.34	-	94,94,94,94	0
55	MG	1H	3267	1/1	0.82	0.46	-	85,85,85,85	0
55	MG	14	3246	1/1	0.83	0.34	-	97,97,97,97	0
55	MG	1H	3082	1/1	0.96	0.17	-	70,70,70,70	0
55	MG	14	3410	1/1	0.98	0.13	-	68,68,68,68	0
55	MG	1H	3086	1/1	0.79	0.50	-	84,84,84,84	0
55	MG	1G	1650	1/1	0.95	0.22	-	92,92,92,92	0
55	MG	1H	3154	1/1	0.78	0.42	-	81,81,81,81	0
55	MG	5E	201	1/1	0.98	0.20	-	92,92,92,92	0
55	MG	14	3145	1/1	0.82	0.38	-	79,79,79,79	0
55	MG	32	301	1/1	0.85	0.43	-	86,86,86,86	0
55	MG	1H	3297	1/1	0.97	0.29	-	87,87,87,87	0
55	MG	14	3393	1/1	0.71	0.69	-	79,79,79,79	0
55	MG	1G	1727	1/1	0.84	0.30	-	98,98,98,98	0
55	MG	14	3321	1/1	0.86	0.59	-	110,110,110,110	0
55	MG	1H	3471	1/1	0.98	0.15	-	90,90,90,90	0
55	MG	14	3443	1/1	0.96	0.11	-	74,74,74,74	0
55	MG	1H	3253	1/1	0.90	0.28	-	90,90,90,90	0
55	MG	13	1620	1/1	0.52	0.22	-	92,92,92,92	0
55	MG	14	3028	1/1	0.90	0.46	-	46,46,46,46	0
55	MG	1H	3246	1/1	0.97	0.29	-	90,90,90,90	0
55	MG	14	3349	1/1	0.94	0.32	-	95,95,95,95	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
55	MG	1H	3259	1/1	0.56	0.99	-	98,98,98,98	0
55	MG	1H	3143	1/1	0.93	0.31	-	96,96,96,96	0
55	MG	88	304	1/1	0.64	0.89	-	77,77,77,77	0
55	MG	1H	3211	1/1	0.80	0.49	-	104,104,104,104	0
55	MG	1H	3190	1/1	0.81	0.32	-	71,71,71,71	0
55	MG	1H	3465	1/1	0.85	0.11	-	108,108,108,108	0
55	MG	13	1727	1/1	0.72	0.46	-	90,90,90,90	0
55	MG	1H	3194	1/1	0.76	0.30	-	86,86,86,86	0
55	MG	1H	3495	1/1	0.61	0.07	-	112,112,112,112	0
55	MG	14	3068	1/1	0.94	0.52	-	57,57,57,57	0
55	MG	13	1666	1/1	0.85	0.47	-	78,78,78,78	0
55	MG	1H	3332	1/1	0.84	0.96	-	78,78,78,78	0
55	MG	14	3062	1/1	0.96	0.35	-	71,71,71,71	0
55	MG	14	3333	1/1	0.95	0.55	-	58,58,58,58	0
55	MG	1H	3474	1/1	0.91	0.09	-	102,102,102,102	0
55	MG	1H	3325	1/1	0.86	0.47	-	92,92,92,92	0
55	MG	1H	3022	1/1	0.97	0.37	-	57,57,57,57	0
55	MG	1H	3007	1/1	0.96	0.38	-	50,50,50,50	0
55	MG	13	1614	1/1	0.97	0.27	-	92,92,92,92	0
55	MG	1H	3441	1/1	0.75	0.09	-	103,103,103,103	0
55	MG	1H	3057	1/1	0.95	0.52	-	73,73,73,73	0
55	MG	13	1710	1/1	0.84	0.55	-	80,80,80,80	0
55	MG	1H	3353	1/1	0.93	0.45	-	75,75,75,75	0
55	MG	1H	3238	1/1	0.84	0.38	-	77,77,77,77	0
55	MG	14	3386	1/1	0.76	0.51	-	79,79,79,79	0
55	MG	14	3081	1/1	0.98	0.53	-	72,72,72,72	0
55	MG	14	3160	1/1	0.94	0.28	-	98,98,98,98	0
55	MG	1H	3167	1/1	0.87	0.24	-	75,75,75,75	0
55	MG	14	3339	1/1	0.92	0.42	-	71,71,71,71	0
55	MG	14	3404	1/1	0.95	0.21	-	105,105,105,105	0
55	MG	1H	3285	1/1	0.84	0.72	-	83,83,83,83	0
55	MG	1H	3015	1/1	0.99	0.52	-	53,53,53,53	0
55	MG	1H	3298	1/1	0.86	0.32	-	68,68,68,68	0
55	MG	1H	3337	1/1	0.74	0.32	-	82,82,82,82	0
55	MG	1H	3428	1/1	0.88	0.10	-	85,85,85,85	0
55	MG	1H	3088	1/1	0.98	0.48	-	44,44,44,44	0
55	MG	14	3003	1/1	0.95	0.27	-	63,63,63,63	0
55	MG	14	3252	1/1	0.41	0.73	-	97,97,97,97	0
55	MG	1H	3347	1/1	0.77	0.23	-	80,80,80,80	0
55	MG	1H	3293	1/1	0.83	0.44	-	78,78,78,78	0
55	MG	14	3086	1/1	0.84	0.30	-	77,77,77,77	0
55	MG	1H	3456	1/1	0.92	0.19	-	88,88,88,88	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
55	MG	1H	3436	1/1	0.97	0.10	-	77,77,77,77	0
55	MG	13	1643	1/1	0.88	0.12	-	104,104,104,104	0
55	MG	1H	3409	1/1	0.96	0.20	-	75,75,75,75	0
55	MG	1H	3084	1/1	0.98	0.38	-	65,65,65,65	0
55	MG	13	1647	1/1	0.88	0.31	-	93,93,93,93	0
55	MG	1H	3445	1/1	0.94	0.10	-	86,86,86,86	0
55	MG	1G	1635	1/1	0.91	0.50	-	82,82,82,82	0
55	MG	85	202	1/1	0.84	0.37	-	79,79,79,79	0
55	MG	1H	3141	1/1	0.97	0.23	-	50,50,50,50	0
55	MG	1G	1660	1/1	0.93	0.21	-	82,82,82,82	0
55	MG	1H	3212	1/1	0.94	0.36	-	71,71,71,71	0
55	MG	14	3184	1/1	0.97	0.50	-	59,59,59,59	0
55	MG	14	3396	1/1	0.99	0.11	-	79,79,79,79	0
55	MG	16	203	1/1	0.91	0.46	-	102,102,102,102	0
55	MG	13	1734	1/1	0.97	0.13	-	93,93,93,93	0
55	MG	1H	3289	1/1	0.90	0.18	-	80,80,80,80	0
55	MG	14	3329	1/1	0.97	0.58	-	58,58,58,58	0
55	MG	1H	3227	1/1	0.94	0.27	-	61,61,61,61	0
55	MG	14	3085	1/1	0.96	0.41	-	58,58,58,58	0
55	MG	1G	1682	1/1	0.95	0.15	-	80,80,80,80	0
55	MG	1G	1634	1/1	0.88	0.43	-	77,77,77,77	0
55	MG	14	3152	1/1	0.78	0.44	-	99,99,99,99	0
55	MG	1H	3408	1/1	0.88	0.26	-	82,82,82,82	0
55	MG	1H	3139	1/1	0.96	0.18	-	63,63,63,63	0
55	MG	14	3327	1/1	0.97	0.10	-	98,98,98,98	0
55	MG	1H	3401	1/1	0.84	0.37	-	80,80,80,80	0
55	MG	14	3167	1/1	0.83	0.24	-	50,50,50,50	0
55	MG	14	3226	1/1	0.81	0.41	-	92,92,92,92	0
55	MG	13	1658	1/1	0.75	0.39	-	82,82,82,82	0
55	MG	14	3230	1/1	0.67	0.46	-	85,85,85,85	0
55	MG	14	3438	1/1	0.86	0.26	-	117,117,117,117	0
55	MG	14	3267	1/1	0.95	0.25	-	74,74,74,74	0
55	MG	1H	3117	1/1	0.92	0.57	-	74,74,74,74	0
55	MG	1H	3090	1/1	0.83	0.50	-	77,77,77,77	0
55	MG	14	3309	1/1	0.82	0.29	-	95,95,95,95	0
55	MG	14	3455	1/1	0.93	0.13	-	121,121,121,121	0
55	MG	1H	3508	1/1	0.85	0.43	-	103,103,103,103	0
55	MG	1H	3176	1/1	0.92	0.47	-	59,59,59,59	0
55	MG	14	3266	1/1	0.94	0.20	-	69,69,69,69	0
55	MG	1H	3381	1/1	0.78	0.89	-	79,79,79,79	0
55	MG	1H	3006	1/1	0.98	0.40	-	53,53,53,53	0
55	MG	1H	3111	1/1	0.98	0.56	-	51,51,51,51	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
55	MG	1H	3237	1/1	0.91	0.25	-	74,74,74,74	0
55	MG	13	1723	1/1	0.82	0.47	-	88,88,88,88	0
55	MG	13	1644	1/1	0.89	0.88	-	91,91,91,91	0
55	MG	14	3020	1/1	0.85	0.48	-	80,80,80,80	0
55	MG	13	1715	1/1	0.89	0.59	-	88,88,88,88	0
55	MG	14	3388	1/1	0.70	0.72	-	94,94,94,94	0
55	MG	1G	1732	1/1	0.89	0.07	-	123,123,123,123	0
55	MG	14	3151	1/1	0.98	0.41	-	68,68,68,68	0
55	MG	1H	3318	1/1	0.91	0.18	-	50,50,50,50	0
55	MG	31	400	1/1	0.94	0.23	-	65,65,65,65	0
55	MG	1H	3320	1/1	0.94	0.24	-	82,82,82,82	0
55	MG	1H	3145	1/1	0.40	0.51	-	83,83,83,83	0
55	MG	1H	3174	1/1	0.85	0.41	-	74,74,74,74	0
55	MG	14	3158	1/1	0.94	0.41	-	68,68,68,68	0
55	MG	1G	1653	1/1	0.88	0.16	-	97,97,97,97	0
55	MG	1G	1711	1/1	0.91	0.42	-	88,88,88,88	0
55	MG	1H	3427	1/1	0.98	0.08	-	91,91,91,91	0
55	MG	1H	3099	1/1	0.88	0.46	-	59,59,59,59	0
55	MG	14	3010	1/1	0.97	0.35	-	54,54,54,54	0
55	MG	1H	3089	1/1	0.96	0.39	-	71,71,71,71	0
55	MG	14	3147	1/1	0.94	0.42	-	80,80,80,80	0
55	MG	13	1663	1/1	0.94	0.57	-	93,93,93,93	0
55	MG	1H	3287	1/1	0.87	0.28	-	75,75,75,75	0
55	MG	1H	3463	1/1	0.89	0.07	-	91,91,91,91	0
55	MG	14	3377	1/1	0.95	0.45	-	82,82,82,82	0
55	MG	14	3358	1/1	0.71	0.55	-	89,89,89,89	0
55	MG	1G	1742	1/1	0.69	0.09	-	131,131,131,131	0
55	MG	13	1692	1/1	0.96	0.56	-	52,52,52,52	0
55	MG	1G	1717	1/1	0.51	0.81	-	99,99,99,99	0
55	MG	1G	1674	1/1	0.67	0.25	-	113,113,113,113	0
55	MG	1G	1715	1/1	0.90	0.28	-	83,83,83,83	0
55	MG	P8	101	1/1	0.87	0.45	-	72,72,72,72	0
55	MG	1G	1733	1/1	0.97	0.06	-	93,93,93,93	0
55	MG	1H	3208	1/1	0.76	0.44	-	96,96,96,96	0
55	MG	14	3470	1/1	0.86	0.16	-	119,119,119,119	0
55	MG	1H	3157	1/1	0.94	0.68	-	60,60,60,60	0
55	MG	14	3171	1/1	0.56	0.45	-	103,103,103,103	0
55	MG	14	3007	1/1	0.99	0.50	-	68,68,68,68	0
55	MG	1G	1647	1/1	0.91	0.20	-	92,92,92,92	0
55	MG	13	1718	1/1	0.72	0.28	-	78,78,78,78	0
55	MG	14	3076	1/1	0.98	0.42	-	45,45,45,45	0
55	MG	14	3181	1/1	0.95	0.23	-	78,78,78,78	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
55	MG	1G	1670	1/1	0.80	0.33	-	117,117,117,117	0
55	MG	14	3131	1/1	0.77	0.49	-	93,93,93,93	0
55	MG	14	3286	1/1	0.89	0.54	-	91,91,91,91	0
55	MG	14	3019	1/1	0.95	0.26	-	80,80,80,80	0
55	MG	14	3175	1/1	0.68	0.89	-	95,95,95,95	0
55	MG	1H	3330	1/1	0.90	0.37	-	75,75,75,75	0
55	MG	1G	1658	1/1	0.83	0.77	-	78,78,78,78	0
55	MG	1H	3507	1/1	0.97	0.12	-	100,100,100,100	0
55	MG	13	1676	1/1	0.26	0.29	-	103,103,103,103	0
55	MG	13	1655	1/1	0.85	0.30	-	77,77,77,77	0
55	MG	1G	1729	1/1	0.56	0.51	-	89,89,89,89	0
55	MG	13	1705	1/1	0.74	0.61	-	102,102,102,102	0
55	MG	1G	1624	1/1	0.98	0.25	-	103,103,103,103	0
55	MG	14	3250	1/1	0.87	0.19	-	87,87,87,87	0
55	MG	14	3469	1/1	0.97	0.07	-	96,96,96,96	0
55	MG	1H	3151	1/1	0.90	0.27	-	81,81,81,81	0
55	MG	1H	3013	1/1	0.96	0.52	-	54,54,54,54	0
55	MG	1H	3360	1/1	0.97	0.37	-	70,70,70,70	0
55	MG	1G	1725	1/1	0.81	0.56	-	104,104,104,104	0
55	MG	14	3248	1/1	0.91	0.78	-	74,74,74,74	0
55	MG	13	1703	1/1	0.79	0.29	-	85,85,85,85	0
55	MG	14	3091	1/1	0.98	0.57	-	53,53,53,53	0
55	MG	14	3375	1/1	0.77	0.40	-	81,81,81,81	0
55	MG	14	3227	1/1	0.90	0.14	-	90,90,90,90	0
55	MG	14	3447	1/1	0.97	0.07	-	95,95,95,95	0
55	MG	1H	3091	1/1	0.98	0.46	-	58,58,58,58	0
55	MG	1H	3372	1/1	0.92	0.97	-	75,75,75,75	0
55	MG	14	3213	1/1	0.98	0.72	-	59,59,59,59	0
55	MG	14	3364	1/1	0.61	0.27	-	89,89,89,89	0
55	MG	1H	3315	1/1	0.88	0.40	-	92,92,92,92	0
55	MG	13	1708	1/1	0.93	0.41	-	81,81,81,81	0
55	MG	1G	1724	1/1	0.28	0.16	-	99,99,99,99	0
55	MG	1H	3261	1/1	0.73	0.30	-	85,85,85,85	0
55	MG	1H	3345	1/1	0.97	0.17	-	70,70,70,70	0
55	MG	1H	3339	1/1	0.90	0.23	-	88,88,88,88	0
55	MG	13	1662	1/1	0.83	0.11	-	98,98,98,98	0
55	MG	1H	3412	1/1	0.94	0.14	-	103,103,103,103	0
55	MG	14	3265	1/1	0.78	0.69	-	88,88,88,88	0
55	MG	1H	3455	1/1	0.96	0.12	-	62,62,62,62	0
55	MG	1H	3499	1/1	0.62	0.19	-	103,103,103,103	0
55	MG	1H	3027	1/1	0.99	0.43	-	51,51,51,51	0
55	MG	1H	3158	1/1	0.76	0.47	-	88,88,88,88	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
55	MG	13	1684	1/1	0.71	0.41	-	98,98,98,98	0
55	MG	1H	3453	1/1	0.94	0.08	-	89,89,89,89	0
55	MG	1G	1669	1/1	0.89	0.42	-	100,100,100,100	0
55	MG	14	3235	1/1	0.64	0.51	-	91,91,91,91	0
55	MG	14	3060	1/1	0.80	0.71	-	80,80,80,80	0
55	MG	13	1746	1/1	0.96	0.20	-	100,100,100,100	0
55	MG	E5	202	1/1	0.84	0.79	-	92,92,92,92	0
55	MG	1G	1637	1/1	0.85	0.46	-	84,84,84,84	0
55	MG	1H	3032	1/1	0.96	0.35	-	79,79,79,79	0
55	MG	14	3157	1/1	0.95	0.56	-	83,83,83,83	0
55	MG	1G	1620	1/1	0.94	0.26	-	88,88,88,88	0
55	MG	14	3318	1/1	0.83	0.25	-	77,77,77,77	0
55	MG	14	3348	1/1	0.88	0.35	-	86,86,86,86	0
55	MG	14	3291	1/1	0.93	0.52	-	91,91,91,91	0
55	MG	14	3096	1/1	0.64	0.57	-	62,62,62,62	0
55	MG	14	3057	1/1	0.97	0.49	-	45,45,45,45	0
55	MG	14	3371	1/1	0.84	0.57	-	91,91,91,91	0
55	MG	14	3078	1/1	0.86	0.61	-	68,68,68,68	0
55	MG	1H	3247	1/1	0.96	0.44	-	77,77,77,77	0
55	MG	14	3460	1/1	0.89	0.14	-	114,114,114,114	0
55	MG	14	3281	1/1	0.91	0.20	-	79,79,79,79	0
55	MG	1H	3493	1/1	0.79	0.20	-	122,122,122,122	0
55	MG	14	3283	1/1	0.93	0.56	-	101,101,101,101	0
55	MG	1H	3202	1/1	0.89	0.72	-	71,71,71,71	0
55	MG	1H	3203	1/1	0.36	0.27	-	110,110,110,110	0
55	MG	1G	1627	1/1	0.89	0.46	-	88,88,88,88	0
55	MG	14	3464	1/1	0.85	0.18	-	116,116,116,116	0
55	MG	1H	3327	1/1	0.86	0.55	-	83,83,83,83	0
55	MG	1H	3452	1/1	0.97	0.11	-	91,91,91,91	0
55	MG	1H	3399	1/1	0.88	0.48	-	94,94,94,94	0
55	MG	14	3233	1/1	0.67	0.69	-	91,91,91,91	0
55	MG	14	3045	1/1	0.95	0.52	-	55,55,55,55	0
55	MG	1G	1614	1/1	0.89	0.30	-	98,98,98,98	0
55	MG	1H	3049	1/1	0.97	0.35	-	89,89,89,89	0
55	MG	1H	3222	1/1	0.90	0.19	-	91,91,91,91	0
55	MG	1H	3074	1/1	0.94	0.31	-	59,59,59,59	0
55	MG	13	1623	1/1	0.94	0.46	-	94,94,94,94	0
55	MG	13	1741	1/1	0.85	0.05	-	128,128,128,128	0
55	MG	14	3328	1/1	0.94	0.40	-	38,38,38,38	0
55	MG	1H	3128	1/1	0.98	0.47	-	66,66,66,66	0
55	MG	14	3308	1/1	0.81	0.39	-	89,89,89,89	0
55	MG	1G	1671	1/1	0.94	0.51	-	84,84,84,84	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
55	MG	1H	3165	1/1	0.86	0.40	-	76,76,76,76	0
55	MG	1H	3258	1/1	0.96	0.11	-	92,92,92,92	0
55	MG	13	1737	1/1	0.88	0.11	-	114,114,114,114	0
55	MG	1H	3404	1/1	0.70	0.62	-	83,83,83,83	0
55	MG	14	3055	1/1	0.93	0.59	-	68,68,68,68	0
55	MG	1H	3262	1/1	0.66	0.25	-	93,93,93,93	0
55	MG	13	1640	1/1	0.94	0.30	-	73,73,73,73	0
55	MG	14	3390	1/1	0.78	0.29	-	70,70,70,70	0
55	MG	1H	3078	1/1	0.98	0.42	-	54,54,54,54	0
55	MG	1G	1705	1/1	0.78	0.38	-	105,105,105,105	0
55	MG	13	1712	1/1	0.87	0.61	-	86,86,86,86	0
55	MG	13	1673	1/1	0.14	0.50	-	145,145,145,145	0
55	MG	1H	3303	1/1	0.91	0.44	-	91,91,91,91	0
55	MG	14	3387	1/1	0.87	0.86	-	92,92,92,92	0
55	MG	13	1653	1/1	0.95	0.65	-	79,79,79,79	0
55	MG	I8	101	1/1	0.94	0.36	-	55,55,55,55	0
55	MG	1H	3047	1/1	0.96	0.10	-	96,96,96,96	0
55	MG	14	3343	1/1	0.92	0.32	-	75,75,75,75	0
55	MG	14	3459	1/1	0.87	0.10	-	122,122,122,122	0
55	MG	14	3187	1/1	0.76	0.31	-	81,81,81,81	0
55	MG	14	3351	1/1	0.90	0.42	-	104,104,104,104	0
55	MG	14	3354	1/1	0.92	0.77	-	76,76,76,76	0
55	MG	1G	1605	1/1	0.99	0.23	-	85,85,85,85	0
55	MG	1H	3133	1/1	0.87	0.40	-	79,79,79,79	0
55	MG	14	3352	1/1	0.71	0.50	-	99,99,99,99	0
55	MG	1H	3160	1/1	0.92	0.38	-	88,88,88,88	0
55	MG	14	3269	1/1	0.84	0.32	-	93,93,93,93	0
55	MG	13	1641	1/1	0.89	0.32	-	75,75,75,75	0
55	MG	14	3288	1/1	0.92	0.74	-	89,89,89,89	0
55	MG	1H	3392	1/1	0.77	0.30	-	86,86,86,86	0
55	MG	14	3159	1/1	0.59	0.41	-	102,102,102,102	0
55	MG	1H	3079	1/1	0.94	0.24	-	79,79,79,79	0
55	MG	98	201	1/1	0.90	0.62	-	71,71,71,71	0
55	MG	14	3143	1/1	0.90	0.72	-	64,64,64,64	0
55	MG	13	1698	1/1	0.74	0.40	-	89,89,89,89	0
55	MG	1H	3331	1/1	0.90	0.14	-	68,68,68,68	0
55	MG	13	1612	1/1	0.75	0.70	-	74,74,74,74	0
55	MG	1H	3472	1/1	0.95	0.06	-	86,86,86,86	0
55	MG	1H	3346	1/1	0.81	0.28	-	105,105,105,105	0
55	MG	13	1736	1/1	0.90	0.07	-	111,111,111,111	0
55	MG	14	3347	1/1	0.97	0.33	-	84,84,84,84	0
55	MG	1G	1632	1/1	0.78	0.28	-	81,81,81,81	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
55	MG	1G	1699	1/1	0.98	0.39	-	100,100,100,100	0
55	MG	14	3182	1/1	0.94	0.30	-	78,78,78,78	0
55	MG	14	3192	1/1	0.79	0.29	-	102,102,102,102	0
55	MG	13	1646	1/1	0.95	0.71	-	76,76,76,76	0
55	MG	1H	3182	1/1	0.97	0.58	-	59,59,59,59	0
55	MG	1H	3426	1/1	0.94	0.14	-	62,62,62,62	0
55	MG	14	3306	1/1	0.49	0.42	-	95,95,95,95	0
55	MG	14	3451	1/1	0.96	0.10	-	91,91,91,91	0
55	MG	14	3191	1/1	0.92	0.30	-	62,62,62,62	0
55	MG	16	205	1/1	0.85	0.40	-	87,87,87,87	0
55	MG	14	3370	1/1	0.85	0.56	-	88,88,88,88	0
55	MG	14	3463	1/1	0.75	0.09	-	119,119,119,119	0
55	MG	14	3209	1/1	0.93	0.23	-	91,91,91,91	0
55	MG	2L	102	1/1	0.95	0.35	-	71,71,71,71	0
55	MG	14	3125	1/1	0.91	0.47	-	75,75,75,75	0
55	MG	7A	101	1/1	0.82	0.17	-	85,85,85,85	0
55	MG	14	3218	1/1	0.97	0.35	-	57,57,57,57	0
55	MG	1H	3382	1/1	0.82	0.58	-	73,73,73,73	0
55	MG	1H	3479	1/1	0.75	0.07	-	103,103,103,103	0
55	MG	1G	1666	1/1	0.92	0.42	-	71,71,71,71	0
55	MG	1G	1667	1/1	0.93	0.20	-	84,84,84,84	0
55	MG	1H	3394	1/1	0.83	0.67	-	82,82,82,82	0
55	MG	1H	3028	1/1	0.96	0.32	-	52,52,52,52	0
55	MG	1H	3274	1/1	0.85	0.61	-	83,83,83,83	0
55	MG	1H	3504	1/1	0.87	0.14	-	95,95,95,95	0
55	MG	1H	3146	1/1	0.98	0.29	-	64,64,64,64	0
55	MG	14	3484	1/1	0.97	0.05	-	95,95,95,95	0
55	MG	1H	3386	1/1	0.95	0.59	-	87,87,87,87	0
55	MG	14	3407	1/1	0.97	0.16	-	66,66,66,66	0
55	MG	1H	3229	1/1	0.76	0.45	-	82,82,82,82	0
55	MG	1H	3147	1/1	0.94	0.33	-	81,81,81,81	0
55	MG	1H	3077	1/1	0.99	0.28	-	65,65,65,65	0
55	MG	14	3391	1/1	0.82	0.58	-	90,90,90,90	0
55	MG	1H	3107	1/1	0.93	0.85	-	76,76,76,76	0
55	MG	14	3457	1/1	0.92	0.05	-	103,103,103,103	0
55	MG	E5	201	1/1	0.95	0.24	-	62,62,62,62	0
55	MG	14	3113	1/1	0.95	0.26	-	76,76,76,76	0
55	MG	14	3001	1/1	0.76	0.71	-	81,81,81,81	0
55	MG	1H	3296	1/1	0.90	0.25	-	84,84,84,84	0
55	MG	14	3214	1/1	0.97	0.38	-	78,78,78,78	0
55	MG	1H	3178	1/1	0.94	0.50	-	69,69,69,69	0
55	MG	13	1654	1/1	0.93	0.29	-	78,78,78,78	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
55	MG	13	1730	1/1	0.72	0.15	-	95,95,95,95	0
55	MG	G8	201	1/1	0.97	0.30	-	65,65,65,65	0
55	MG	14	3237	1/1	0.91	0.16	-	65,65,65,65	0
55	MG	14	3307	1/1	0.75	0.31	-	91,91,91,91	0
55	MG	1H	3068	1/1	0.95	0.27	-	83,83,83,83	0
55	MG	13	1693	1/1	0.98	0.61	-	62,62,62,62	0
55	MG	14	3134	1/1	0.87	0.27	-	76,76,76,76	0
55	MG	14	3254	1/1	0.99	0.10	-	117,117,117,117	0
55	MG	14	3297	1/1	0.92	0.34	-	85,85,85,85	0
55	MG	14	3029	1/1	0.96	0.49	-	63,63,63,63	0
55	MG	1H	3362	1/1	0.96	0.38	-	56,56,56,56	0
55	MG	13	1625	1/1	0.96	0.50	-	78,78,78,78	0
55	MG	14	3357	1/1	0.87	0.38	-	93,93,93,93	0
55	MG	1G	1628	1/1	0.88	0.47	-	93,93,93,93	0
55	MG	1H	3461	1/1	0.97	0.10	-	67,67,67,67	0
55	MG	1H	3163	1/1	0.94	0.39	-	83,83,83,83	0
55	MG	1H	3491	1/1	0.86	0.04	-	122,122,122,122	0
55	MG	1G	1648	1/1	0.91	0.39	-	82,82,82,82	0
55	MG	14	3189	1/1	0.83	0.22	-	91,91,91,91	0
55	MG	1H	3193	1/1	0.41	0.32	-	116,116,116,116	0
55	MG	14	3341	1/1	0.93	0.41	-	77,77,77,77	0
55	MG	13	1704	1/1	0.84	0.41	-	93,93,93,93	0
55	MG	14	3176	1/1	0.89	0.71	-	63,63,63,63	0
55	MG	13	1611	1/1	0.92	0.31	-	115,115,115,115	0
55	MG	14	3311	1/1	0.81	0.45	-	103,103,103,103	0
55	MG	14	3238	1/1	0.74	0.16	-	98,98,98,98	0
55	MG	1H	3321	1/1	0.95	0.47	-	80,80,80,80	0
55	MG	21	301	1/1	0.93	0.36	-	64,64,64,64	0
55	MG	13	1656	1/1	0.96	0.41	-	63,63,63,63	0
55	MG	1H	3447	1/1	0.94	0.20	-	77,77,77,77	0
55	MG	14	3374	1/1	0.66	0.43	-	102,102,102,102	0
55	MG	14	3178	1/1	0.98	0.20	-	89,89,89,89	0
55	MG	14	3272	1/1	0.73	0.43	-	90,90,90,90	0
55	MG	14	3107	1/1	0.98	0.58	-	50,50,50,50	0
55	MG	14	3383	1/1	0.97	0.21	-	95,95,95,95	0
55	MG	14	3097	1/1	0.92	0.41	-	91,91,91,91	0
55	MG	1H	3503	1/1	0.94	0.22	-	76,76,76,76	0
55	MG	14	3356	1/1	0.97	0.27	-	77,77,77,77	0
55	MG	1H	3329	1/1	0.88	0.39	-	62,62,62,62	0
55	MG	1H	3338	1/1	0.59	0.61	-	82,82,82,82	0
55	MG	1H	3020	1/1	0.98	0.36	-	68,68,68,68	0
55	MG	14	3290	1/1	0.88	0.46	-	76,76,76,76	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
55	MG	14	3129	1/1	0.53	0.33	-	86,86,86,86	0
55	MG	14	3332	1/1	0.93	0.35	-	80,80,80,80	0
55	MG	1H	3162	1/1	0.89	0.47	-	89,89,89,89	0
55	MG	13	1725	1/1	0.96	0.57	-	71,71,71,71	0
55	MG	1H	3390	1/1	0.81	0.46	-	86,86,86,86	0
55	MG	1H	3334	1/1	0.92	0.23	-	75,75,75,75	0
55	MG	1H	3286	1/1	0.95	0.30	-	94,94,94,94	0
55	MG	14	3058	1/1	0.96	0.51	-	53,53,53,53	0
55	MG	1H	3316	1/1	0.92	0.44	-	87,87,87,87	0
55	MG	14	3095	1/1	0.98	0.36	-	54,54,54,54	0
55	MG	1H	3443	1/1	0.98	0.04	-	90,90,90,90	0
55	MG	1H	3250	1/1	0.79	1.87	-	97,97,97,97	0
55	MG	1H	3457	1/1	0.95	0.11	-	79,79,79,79	0
55	MG	1G	1693	1/1	0.68	0.34	-	109,109,109,109	0
55	MG	14	3369	1/1	0.58	0.68	-	105,105,105,105	0
55	MG	1H	3070	1/1	0.85	0.70	-	73,73,73,73	0
55	MG	1H	3282	1/1	0.94	0.34	-	89,89,89,89	0
55	MG	1H	3134	1/1	0.86	0.56	-	67,67,67,67	0
55	MG	1H	3205	1/1	0.97	0.43	-	75,75,75,75	0
55	MG	14	3310	1/1	0.82	0.24	-	84,84,84,84	0
55	MG	14	3467	1/1	0.91	0.09	-	97,97,97,97	0
55	MG	14	3049	1/1	0.96	0.25	-	80,80,80,80	0
55	MG	1G	1735	1/1	0.93	0.06	-	97,97,97,97	0
55	MG	1G	1737	1/1	0.94	0.06	-	93,93,93,93	0
55	MG	13	1603	1/1	0.97	0.26	-	73,73,73,73	0
55	MG	14	3278	1/1	0.87	0.51	-	69,69,69,69	0
55	MG	14	3195	1/1	0.96	0.47	-	69,69,69,69	0
55	MG	14	3271	1/1	0.92	0.80	-	75,75,75,75	0
55	MG	1H	3169	1/1	0.69	0.34	-	90,90,90,90	0
55	MG	1H	3313	1/1	0.55	0.45	-	98,98,98,98	0
55	MG	14	3312	1/1	0.79	0.40	-	96,96,96,96	0
55	MG	1H	3391	1/1	0.70	0.25	-	78,78,78,78	0
55	MG	1G	1625	1/1	0.68	0.37	-	99,99,99,99	0
55	MG	1G	1617	1/1	0.95	0.58	-	72,72,72,72	0
55	MG	1G	1708	1/1	0.74	0.58	-	66,66,66,66	0
55	MG	1H	3131	1/1	0.98	0.46	-	65,65,65,65	0
55	MG	1H	3260	1/1	0.92	0.47	-	85,85,85,85	0
55	MG	1H	3199	1/1	0.90	0.16	-	74,74,74,74	0
55	MG	14	3480	1/1	0.96	0.04	-	92,92,92,92	0
55	MG	14	3268	1/1	0.93	1.03	-	69,69,69,69	0
55	MG	14	3035	1/1	0.66	0.71	-	91,91,91,91	0
55	MG	1H	3008	1/1	0.94	0.26	-	64,64,64,64	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
55	MG	1H	3480	1/1	0.91	0.10	-	118,118,118,118	0
55	MG	14	3378	1/1	0.82	0.32	-	83,83,83,83	0
55	MG	14	3216	1/1	0.78	0.18	-	77,77,77,77	0
55	MG	1H	3101	1/1	0.96	0.49	-	60,60,60,60	0
55	MG	14	3468	1/1	0.93	0.32	-	107,107,107,107	0
55	MG	14	3008	1/1	0.97	0.37	-	61,61,61,61	0
55	MG	14	3244	1/1	0.85	0.78	-	75,75,75,75	0
55	MG	J8	101	1/1	0.98	0.47	-	65,65,65,65	0
55	MG	1H	3358	1/1	0.92	0.12	-	81,81,81,81	0
55	MG	14	3368	1/1	0.88	0.44	-	91,91,91,91	0
55	MG	1G	1700	1/1	0.82	0.45	-	99,99,99,99	0
55	MG	1H	3195	1/1	0.79	0.54	-	84,84,84,84	0
55	MG	13	1650	1/1	0.90	0.70	-	88,88,88,88	0
55	MG	1H	3482	1/1	0.94	0.06	-	83,83,83,83	0
55	MG	14	3466	1/1	0.95	0.12	-	103,103,103,103	0
55	MG	1H	3380	1/1	0.70	0.47	-	100,100,100,100	0
55	MG	14	3112	1/1	0.89	0.20	-	77,77,77,77	0
55	MG	1G	1633	1/1	0.89	0.70	-	73,73,73,73	0
55	MG	1H	3292	1/1	0.71	0.31	-	90,90,90,90	0
55	MG	14	3123	1/1	0.91	0.41	-	63,63,63,63	0
55	MG	14	3232	1/1	0.74	0.27	-	82,82,82,82	0
55	MG	1H	3403	1/1	0.94	0.56	-	79,79,79,79	0
55	MG	1H	3242	1/1	0.65	0.47	-	97,97,97,97	0
55	MG	1H	3023	1/1	0.97	0.45	-	48,48,48,48	0
55	MG	14	3380	1/1	0.90	0.78	-	93,93,93,93	0
55	MG	14	3142	1/1	0.92	0.49	-	77,77,77,77	0
55	MG	13	1670	1/1	0.60	0.29	-	99,99,99,99	0
55	MG	1H	3374	1/1	0.83	0.31	-	89,89,89,89	0
55	MG	13	1637	1/1	0.94	0.41	-	72,72,72,72	0
55	MG	78	201	1/1	0.91	0.21	-	74,74,74,74	0
55	MG	1H	3288	1/1	0.91	0.53	-	68,68,68,68	0
55	MG	14	3080	1/1	0.93	0.44	-	65,65,65,65	0
55	MG	13	1726	1/1	0.80	0.60	-	93,93,93,93	0
55	MG	14	3277	1/1	0.93	0.66	-	74,74,74,74	0
55	MG	14	3471	1/1	0.95	0.29	-	113,113,113,113	0
55	MG	14	3360	1/1	0.92	0.58	-	93,93,93,93	0
55	MG	14	3389	1/1	0.84	0.36	-	77,77,77,77	0
55	MG	1H	3054	1/1	0.98	0.52	-	51,51,51,51	0
55	MG	14	3204	1/1	0.70	0.56	-	89,89,89,89	0
55	MG	14	3012	1/1	0.93	0.41	-	48,48,48,48	0
55	MG	1H	3129	1/1	0.96	0.38	-	61,61,61,61	0
55	MG	2K	102	1/1	0.49	0.36	-	118,118,118,118	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
55	MG	1H	3423	1/1	0.79	0.13	-	110,110,110,110	0
55	MG	1H	3450	1/1	0.90	0.06	-	74,74,74,74	0
55	MG	1G	1726	1/1	0.88	0.54	-	90,90,90,90	0
55	MG	14	3064	1/1	0.99	0.58	-	54,54,54,54	0
55	MG	14	3139	1/1	0.94	0.31	-	98,98,98,98	0
55	MG	1H	3411	1/1	0.82	0.16	-	87,87,87,87	0
55	MG	1H	3387	1/1	0.94	0.46	-	73,73,73,73	0
55	MG	14	3315	1/1	0.85	0.36	-	92,92,92,92	0
55	MG	14	3016	1/1	0.93	0.43	-	74,74,74,74	0
55	MG	14	3334	1/1	0.94	0.35	-	76,76,76,76	0
55	MG	14	3418	1/1	0.92	0.13	-	72,72,72,72	0
55	MG	13	1743	1/1	0.77	0.09	-	142,142,142,142	0
55	MG	1G	1680	1/1	0.60	0.32	-	88,88,88,88	0
55	MG	14	3442	1/1	0.93	0.07	-	109,109,109,109	0
55	MG	14	3298	1/1	0.96	0.45	-	54,54,54,54	0
55	MG	1H	3188	1/1	0.55	0.47	-	92,92,92,92	0
55	MG	1G	1639	1/1	0.87	0.77	-	79,79,79,79	0
55	MG	1G	1651	1/1	0.88	0.09	-	93,93,93,93	0
55	MG	14	3116	1/1	0.78	0.43	-	65,65,65,65	0
55	MG	1G	1683	1/1	0.93	0.16	-	132,132,132,132	0
55	MG	1H	3235	1/1	0.86	0.61	-	88,88,88,88	0
55	MG	1H	3221	1/1	0.98	0.70	-	57,57,57,57	0
55	MG	1G	1612	1/1	0.92	0.10	-	88,88,88,88	0
55	MG	1H	3232	1/1	0.84	0.14	-	90,90,90,90	0
55	MG	1G	1741	1/1	0.96	0.07	-	105,105,105,105	0
55	MG	14	3324	1/1	0.78	0.43	-	80,80,80,80	0
55	MG	1H	3187	1/1	0.95	0.30	-	66,66,66,66	0
55	MG	14	3322	1/1	0.56	0.19	-	93,93,93,93	0
55	MG	14	3289	1/1	0.90	0.34	-	98,98,98,98	0
55	MG	1H	3231	1/1	0.95	0.15	-	90,90,90,90	0
55	MG	1H	3127	1/1	0.97	0.40	-	58,58,58,58	0
55	MG	1H	3063	1/1	0.89	0.45	-	90,90,90,90	0
55	MG	13	1722	1/1	0.65	0.26	-	106,106,106,106	0
55	MG	14	3379	1/1	0.89	0.45	-	107,107,107,107	0
55	MG	14	3104	1/1	0.91	0.32	-	87,87,87,87	0
55	MG	14	3299	1/1	0.99	0.43	-	64,64,64,64	0
55	MG	14	3053	1/1	0.89	0.33	-	69,69,69,69	0
55	MG	14	3337	1/1	0.93	0.36	-	64,64,64,64	0
55	MG	1H	3252	1/1	0.95	0.41	-	79,79,79,79	0
55	MG	1G	1626	1/1	0.97	0.34	-	80,80,80,80	0
55	MG	14	3070	1/1	0.91	0.23	-	57,57,57,57	0
55	MG	13	1621	1/1	0.95	0.39	-	75,75,75,75	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
55	MG	14	3395	1/1	0.70	0.21	-	98,98,98,98	0
55	MG	14	3115	1/1	0.76	0.39	-	77,77,77,77	0
55	MG	14	3474	1/1	0.91	0.06	-	107,107,107,107	0
55	MG	1H	3124	1/1	0.86	0.40	-	68,68,68,68	0
55	MG	1H	3136	1/1	0.97	0.47	-	72,72,72,72	0
55	MG	1H	3311	1/1	0.93	0.11	-	65,65,65,65	0
55	MG	13	1738	1/1	0.92	0.07	-	100,100,100,100	0
55	MG	14	3002	1/1	0.93	0.52	-	61,61,61,61	0
55	MG	1H	3384	1/1	0.72	0.36	-	79,79,79,79	0
55	MG	14	3102	1/1	0.98	0.17	-	62,62,62,62	0
55	MG	1H	3119	1/1	0.98	0.71	-	75,75,75,75	0
55	MG	13	1695	1/1	0.77	0.29	-	92,92,92,92	0
55	MG	1H	3081	1/1	0.89	0.53	-	85,85,85,85	0
55	MG	1H	3004	1/1	0.98	0.39	-	60,60,60,60	0
55	MG	14	3018	1/1	0.98	0.41	-	52,52,52,52	0
55	MG	1H	3350	1/1	0.91	0.26	-	79,79,79,79	0
55	MG	1H	3481	1/1	0.91	0.06	-	116,116,116,116	0
55	MG	13	1627	1/1	0.73	0.81	-	85,85,85,85	0
55	MG	1G	1690	1/1	0.79	0.41	-	97,97,97,97	0
55	MG	14	3138	1/1	0.96	0.59	-	83,83,83,83	0
55	MG	14	3004	1/1	0.96	0.28	-	59,59,59,59	0
55	MG	14	3304	1/1	0.86	0.45	-	109,109,109,109	0
55	MG	14	3185	1/1	0.92	0.24	-	74,74,74,74	0
55	MG	1H	3036	1/1	0.81	0.40	-	77,77,77,77	0
55	MG	2K	103	1/1	0.89	0.14	-	143,143,143,143	0
55	MG	14	3355	1/1	0.95	0.55	-	71,71,71,71	0
55	MG	1H	3249	1/1	0.95	0.38	-	80,80,80,80	0
55	MG	1H	3234	1/1	0.84	0.21	-	78,78,78,78	0
55	MG	1G	1661	1/1	0.94	0.46	-	65,65,65,65	0
55	MG	1H	3114	1/1	0.98	0.33	-	69,69,69,69	0
55	MG	14	3098	1/1	0.84	0.43	-	87,87,87,87	0
55	MG	14	3394	1/1	0.94	0.32	-	90,90,90,90	0
55	MG	1H	3319	1/1	0.68	0.53	-	102,102,102,102	0
55	MG	14	3465	1/1	0.84	0.19	-	115,115,115,115	0
55	MG	14	3454	1/1	0.81	0.04	-	111,111,111,111	0
55	MG	1H	3185	1/1	0.97	0.42	-	66,66,66,66	0
55	MG	14	3336	1/1	0.94	0.39	-	70,70,70,70	0
55	MG	14	3056	1/1	0.92	0.53	-	71,71,71,71	0
55	MG	13	1669	1/1	0.81	0.66	-	97,97,97,97	0
55	MG	1H	3034	1/1	0.89	0.22	-	54,54,54,54	0
55	MG	1H	3460	1/1	0.95	0.15	-	72,72,72,72	0
55	MG	1G	1698	1/1	0.85	0.24	-	112,112,112,112	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
55	MG	1H	3218	1/1	0.87	0.53	-	52,52,52,52	0
55	MG	14	3385	1/1	0.78	0.42	-	97,97,97,97	0
55	MG	1H	3494	1/1	0.57	0.15	-	125,125,125,125	0
55	MG	14	3025	1/1	0.98	0.27	-	82,82,82,82	0
55	MG	14	3015	1/1	0.99	0.37	-	69,69,69,69	0
55	MG	1H	3245	1/1	0.88	0.64	-	81,81,81,81	0
55	MG	14	3432	1/1	0.74	0.12	-	93,93,93,93	0
55	MG	1H	3241	1/1	0.66	0.42	-	92,92,92,92	0
55	MG	1H	3368	1/1	0.65	0.42	-	88,88,88,88	0
55	MG	1H	3429	1/1	0.91	0.08	-	91,91,91,91	0
55	MG	14	3264	1/1	0.69	0.37	-	78,78,78,78	0
55	MG	1H	3487	1/1	0.85	0.08	-	102,102,102,102	0
55	MG	14	3413	1/1	0.93	0.08	-	100,100,100,100	0
55	MG	13	1682	1/1	0.90	0.25	-	108,108,108,108	0
55	MG	13	1648	1/1	0.92	0.25	-	96,96,96,96	0
55	MG	1H	3031	1/1	0.97	0.31	-	57,57,57,57	0
55	MG	14	3323	1/1	0.75	0.41	-	79,79,79,79	0
55	MG	13	1691	1/1	0.97	0.37	-	89,89,89,89	0
55	MG	1H	3317	1/1	0.86	0.19	-	79,79,79,79	0
55	MG	13	1664	1/1	0.93	0.58	-	76,76,76,76	0
55	MG	14	3381	1/1	0.69	0.41	-	95,95,95,95	0
55	MG	14	3201	1/1	0.94	0.31	-	68,68,68,68	0
55	MG	1H	3322	1/1	0.93	0.27	-	109,109,109,109	0
55	MG	1H	3059	1/1	0.91	0.60	-	69,69,69,69	0
55	MG	1H	3328	1/1	0.93	0.33	-	70,70,70,70	0
55	MG	45	201	1/1	0.79	0.54	-	76,76,76,76	0
55	MG	1H	3354	1/1	0.69	0.21	-	107,107,107,107	0
55	MG	1H	3030	1/1	0.99	0.37	-	63,63,63,63	0
55	MG	1G	1675	1/1	0.84	0.16	-	102,102,102,102	0
55	MG	1H	3496	1/1	0.95	0.20	-	99,99,99,99	0
55	MG	13	1634	1/1	0.93	0.40	-	77,77,77,77	0
55	MG	1G	1643	1/1	0.97	0.27	-	78,78,78,78	0
55	MG	88	303	1/1	0.82	0.40	-	71,71,71,71	0
55	MG	14	3446	1/1	0.84	0.06	-	122,122,122,122	0
55	MG	14	3203	1/1	0.94	0.31	-	84,84,84,84	0
55	MG	14	3161	1/1	0.96	0.50	-	74,74,74,74	0
55	MG	1H	3033	1/1	0.62	0.24	-	92,92,92,92	0
55	MG	1H	3459	1/1	0.99	0.06	-	75,75,75,75	0
55	MG	1H	3105	1/1	0.96	0.49	-	50,50,50,50	0
55	MG	13	1742	1/1	0.91	0.11	-	111,111,111,111	0
55	MG	14	3441	1/1	0.94	0.03	-	102,102,102,102	0
55	MG	14	3275	1/1	0.77	0.47	-	96,96,96,96	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
55	MG	1H	3304	1/1	0.95	0.57	-	82,82,82,82	0
55	MG	1J	202	1/1	0.86	0.13	-	107,107,107,107	0
55	MG	1H	3470	1/1	0.92	0.14	-	79,79,79,79	0
55	MG	29	302	1/1	0.98	0.41	-	65,65,65,65	0
55	MG	1H	3104	1/1	0.78	0.64	-	77,77,77,77	0
55	MG	1H	3192	1/1	0.95	0.49	-	88,88,88,88	0
55	MG	14	3313	1/1	0.82	0.71	-	82,82,82,82	0
55	MG	1H	3243	1/1	0.85	0.56	-	69,69,69,69	0
55	MG	1G	1723	1/1	0.92	0.08	-	87,87,87,87	0
55	MG	16	202	1/1	0.94	0.23	-	90,90,90,90	0
55	MG	14	3061	1/1	0.98	0.45	-	62,62,62,62	0
55	MG	1H	3497	1/1	0.86	0.09	-	113,113,113,113	0
55	MG	1H	3206	1/1	0.71	0.59	-	69,69,69,69	0
55	MG	14	3006	1/1	0.98	0.42	-	54,54,54,54	0
55	MG	1H	3397	1/1	0.88	0.40	-	76,76,76,76	0
55	MG	14	3259	1/1	0.87	0.78	-	88,88,88,88	0
55	MG	1G	1623	1/1	0.90	0.47	-	89,89,89,89	0
55	MG	1H	3312	1/1	0.91	0.17	-	88,88,88,88	0
55	MG	1G	1631	1/1	0.83	0.53	-	88,88,88,88	0
55	MG	14	3212	1/1	0.96	0.37	-	88,88,88,88	0
55	MG	14	3296	1/1	0.86	0.63	-	94,94,94,94	0
55	MG	1G	1654	1/1	0.82	0.59	-	97,97,97,97	0
55	MG	1H	3062	1/1	0.82	0.38	-	70,70,70,70	0
55	MG	14	3198	1/1	0.88	0.14	-	95,95,95,95	0
55	MG	1H	3051	1/1	0.94	0.22	-	74,74,74,74	0
55	MG	14	3180	1/1	0.97	0.28	-	82,82,82,82	0
55	MG	1H	3200	1/1	0.90	0.32	-	68,68,68,68	0
55	MG	1H	3378	1/1	0.98	0.20	-	84,84,84,84	0
55	MG	1H	3305	1/1	0.88	0.36	-	96,96,96,96	0
55	MG	1H	3196	1/1	0.95	0.41	-	77,77,77,77	0
55	MG	1H	3407	1/1	0.91	0.82	-	102,102,102,102	0
55	MG	14	3361	1/1	0.95	0.21	-	88,88,88,88	0
55	MG	1H	3270	1/1	0.90	0.25	-	99,99,99,99	0
55	MG	1G	1601	1/1	0.54	0.35	-	91,91,91,91	0
55	MG	1H	3010	1/1	0.96	0.43	-	48,48,48,48	0
55	MG	14	3434	1/1	0.90	0.18	-	89,89,89,89	0
55	MG	13	1633	1/1	0.93	0.41	-	59,59,59,59	0
55	MG	1H	3294	1/1	0.83	0.31	-	96,96,96,96	0
55	MG	1G	1736	1/1	0.95	0.07	-	114,114,114,114	0
55	MG	14	3367	1/1	0.45	0.40	-	102,102,102,102	0
55	MG	14	3083	1/1	0.97	0.42	-	68,68,68,68	0
55	MG	1H	3175	1/1	0.36	0.68	-	112,112,112,112	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
55	MG	13	1701	1/1	0.95	0.41	-	83,83,83,83	0
55	MG	14	3316	1/1	0.93	0.31	-	78,78,78,78	0
55	MG	14	3043	1/1	0.85	0.92	-	83,83,83,83	0
55	MG	1G	1677	1/1	0.91	0.40	-	105,105,105,105	0
55	MG	14	3392	1/1	0.94	0.16	-	88,88,88,88	0
55	MG	1G	1610	1/1	0.86	0.29	-	86,86,86,86	0
55	MG	14	3376	1/1	0.95	0.21	-	59,59,59,59	0
55	MG	13	1657	1/1	0.73	0.23	-	90,90,90,90	0
55	MG	13	1687	1/1	0.95	0.74	-	90,90,90,90	0
55	MG	13	1628	1/1	0.98	0.47	-	64,64,64,64	0
55	MG	14	3431	1/1	0.90	0.06	-	86,86,86,86	0
55	MG	1H	3037	1/1	0.90	0.24	-	94,94,94,94	0
55	MG	1H	3284	1/1	0.95	0.21	-	69,69,69,69	0
55	MG	1H	3094	1/1	0.94	0.37	-	73,73,73,73	0
55	MG	1H	3220	1/1	0.96	0.39	-	55,55,55,55	0
55	MG	I8	102	1/1	0.89	0.12	-	108,108,108,108	0
55	MG	1H	3138	1/1	0.86	0.37	-	74,74,74,74	0
55	MG	14	3162	1/1	0.78	0.97	-	94,94,94,94	0
55	MG	1G	1712	1/1	0.74	0.12	-	87,87,87,87	0
55	MG	1H	3469	1/1	0.96	0.05	-	107,107,107,107	0
55	MG	1H	3383	1/1	0.86	0.26	-	90,90,90,90	0
55	MG	1G	1663	1/1	0.88	0.56	-	75,75,75,75	0
55	MG	14	3478	1/1	0.88	0.04	-	109,109,109,109	0
55	MG	14	3127	1/1	0.76	0.89	-	76,76,76,76	0
55	MG	1G	1718	1/1	0.95	0.40	-	76,76,76,76	0
55	MG	14	3069	1/1	0.98	0.36	-	65,65,65,65	0
55	MG	1H	3371	1/1	0.83	0.28	-	84,84,84,84	0
55	MG	1G	1616	1/1	0.92	0.53	-	62,62,62,62	0
55	MG	1G	1662	1/1	0.87	0.24	-	98,98,98,98	0
55	MG	13	1649	1/1	0.73	0.35	-	91,91,91,91	0
55	MG	14	3320	1/1	0.84	0.38	-	81,81,81,81	0
55	MG	14	3215	1/1	0.94	0.32	-	77,77,77,77	0
55	MG	14	3335	1/1	0.92	0.97	-	86,86,86,86	0
55	MG	1G	1681	1/1	0.95	0.17	-	86,86,86,86	0
55	MG	1H	3398	1/1	0.87	0.17	-	109,109,109,109	0
55	MG	1H	3343	1/1	0.76	0.77	-	90,90,90,90	0
55	MG	1H	3376	1/1	0.85	0.42	-	71,71,71,71	0
55	MG	14	3050	1/1	0.97	0.33	-	72,72,72,72	0
55	MG	14	3453	1/1	0.90	0.14	-	91,91,91,91	0
55	MG	13	1678	1/1	0.78	0.77	-	85,85,85,85	0
55	MG	13	1707	1/1	0.95	0.44	-	92,92,92,92	0
55	MG	14	3423	1/1	0.86	0.08	-	99,99,99,99	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
55	MG	14	3479	1/1	0.97	0.09	-	78,78,78,78	0
55	MG	1G	1721	1/1	0.94	0.17	-	102,102,102,102	0
55	MG	14	3114	1/1	0.97	0.50	-	81,81,81,81	0
55	MG	1H	3307	1/1	0.78	0.35	-	83,83,83,83	0
55	MG	1H	3414	1/1	0.89	0.58	-	97,97,97,97	0
55	MG	14	3073	1/1	0.95	0.34	-	70,70,70,70	0
55	MG	1H	3276	1/1	0.85	0.22	-	100,100,100,100	0
55	MG	13	1719	1/1	0.84	0.41	-	89,89,89,89	0
55	MG	1G	1636	1/1	0.93	0.20	-	93,93,93,93	0
55	MG	14	3027	1/1	0.92	0.25	-	85,85,85,85	0
55	MG	1G	1678	1/1	0.97	0.29	-	97,97,97,97	0
55	MG	14	3202	1/1	0.72	0.53	-	85,85,85,85	0
55	MG	14	3449	1/1	0.97	0.10	-	82,82,82,82	0
55	MG	1H	3012	1/1	0.99	0.29	-	52,52,52,52	0
55	MG	1H	3410	1/1	0.92	0.41	-	85,85,85,85	0
55	MG	1H	3219	1/1	0.91	0.28	-	64,64,64,64	0
55	MG	1H	3301	1/1	0.98	0.41	-	73,73,73,73	0
55	MG	1G	1638	1/1	0.96	0.38	-	95,95,95,95	0
55	MG	14	3303	1/1	0.92	0.41	-	71,71,71,71	0
55	MG	14	3122	1/1	0.93	0.61	-	84,84,84,84	0
55	MG	1H	3490	1/1	0.75	0.12	-	128,128,128,128	0
55	MG	1H	3056	1/1	0.91	0.34	-	75,75,75,75	0
55	MG	1H	3449	1/1	0.76	0.13	-	110,110,110,110	0
55	MG	1H	3230	1/1	0.89	0.50	-	84,84,84,84	0
55	MG	13	1699	1/1	0.90	0.61	-	72,72,72,72	0
55	MG	1G	1697	1/1	0.87	0.24	-	88,88,88,88	0
55	MG	3I	201	1/1	0.95	0.18	-	68,68,68,68	0
55	MG	13	1659	1/1	0.90	0.68	-	91,91,91,91	0
55	MG	14	3372	1/1	0.78	0.47	-	77,77,77,77	0
55	MG	1H	3278	1/1	0.90	0.42	-	84,84,84,84	0
55	MG	1H	3156	1/1	0.93	0.51	-	76,76,76,76	0
55	MG	14	3317	1/1	0.87	0.22	-	88,88,88,88	0
55	MG	14	3021	1/1	0.99	0.41	-	60,60,60,60	0
55	MG	13	1651	1/1	0.93	0.12	-	91,91,91,91	0
55	MG	1H	3477	1/1	0.94	0.05	-	92,92,92,92	0
55	MG	14	3279	1/1	0.94	0.38	-	80,80,80,80	0
55	MG	1H	3271	1/1	0.95	0.36	-	77,77,77,77	0
55	MG	14	3326	1/1	0.85	0.42	-	88,88,88,88	0
55	MG	1H	3149	1/1	0.96	0.65	-	74,74,74,74	0
55	MG	1H	3367	1/1	0.91	0.14	-	77,77,77,77	0
55	MG	1H	3478	1/1	0.86	0.05	-	118,118,118,118	0
55	MG	1H	3239	1/1	0.98	0.35	-	93,93,93,93	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
55	MG	14	3119	1/1	0.64	0.41	-	90,90,90,90	0
55	MG	14	3258	1/1	0.96	0.23	-	101,101,101,101	0
55	MG	25	201	1/1	0.72	0.32	-	107,107,107,107	0
55	MG	14	3023	1/1	0.93	0.26	-	56,56,56,56	0
55	MG	1G	1689	1/1	0.43	0.23	-	103,103,103,103	0
55	MG	14	3087	1/1	0.92	0.34	-	84,84,84,84	0
55	MG	1H	3393	1/1	0.94	0.22	-	58,58,58,58	0
55	MG	14	3342	1/1	0.82	0.59	-	99,99,99,99	0
55	MG	1H	3419	1/1	0.98	0.10	-	88,88,88,88	0
55	MG	14	3054	1/1	0.78	0.34	-	72,72,72,72	0
55	MG	14	3221	1/1	0.76	0.64	-	92,92,92,92	0
55	MG	1H	3164	1/1	0.77	0.50	-	66,66,66,66	0
55	MG	14	3047	1/1	0.98	0.25	-	67,67,67,67	0
55	MG	13	1607	1/1	0.94	0.18	-	77,77,77,77	0
55	MG	14	3282	1/1	0.84	0.47	-	89,89,89,89	0
55	MG	14	3435	1/1	0.96	0.09	-	117,117,117,117	0
55	MG	1H	3275	1/1	0.90	0.24	-	89,89,89,89	0
55	MG	14	3144	1/1	0.92	0.43	-	61,61,61,61	0
55	MG	14	3164	1/1	0.84	0.46	-	101,101,101,101	0
55	MG	14	3260	1/1	0.96	0.10	-	95,95,95,95	0
55	MG	14	3344	1/1	0.98	0.15	-	73,73,73,73	0
55	MG	13	1683	1/1	0.79	0.75	-	83,83,83,83	0
55	MG	14	3208	1/1	0.85	0.39	-	74,74,74,74	0
55	MG	14	3247	1/1	0.60	0.50	-	78,78,78,78	0
55	MG	1H	3204	1/1	0.81	0.34	-	83,83,83,83	0
55	MG	13	1690	1/1	0.86	0.61	-	90,90,90,90	0
55	MG	1H	3486	1/1	0.94	0.07	-	129,129,129,129	0
55	MG	1H	3400	1/1	0.50	0.45	-	94,94,94,94	0
55	MG	1G	1703	1/1	0.90	0.35	-	106,106,106,106	0
55	MG	1G	1664	1/1	0.92	0.32	-	95,95,95,95	0
55	MG	1H	3050	1/1	0.95	0.53	-	65,65,65,65	0
55	MG	1H	3413	1/1	0.89	0.24	-	89,89,89,89	0
55	MG	14	3452	1/1	0.94	0.17	-	94,94,94,94	0
55	MG	13	1717	1/1	0.85	0.37	-	100,100,100,100	0
55	MG	14	3359	1/1	0.81	0.43	-	90,90,90,90	0
55	MG	1H	3123	1/1	0.96	0.30	-	64,64,64,64	0
55	MG	13	1721	1/1	0.71	0.40	-	84,84,84,84	0
55	MG	13	1689	1/1	0.84	0.18	-	92,92,92,92	0
55	MG	14	3365	1/1	0.94	0.41	-	89,89,89,89	0
55	MG	1G	1668	1/1	0.86	0.49	-	96,96,96,96	0
55	MG	1H	3072	1/1	0.98	0.31	-	33,33,33,33	0
55	MG	14	3325	1/1	0.93	0.14	-	72,72,72,72	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
55	MG	1H	3100	1/1	0.95	0.30	-	65,65,65,65	0
55	MG	14	3486	1/1	0.79	0.07	-	138,138,138,138	0
55	MG	14	3257	1/1	0.98	0.34	-	78,78,78,78	0
55	MG	1H	3295	1/1	0.79	0.34	-	87,87,87,87	0
55	MG	13	1616	1/1	0.90	0.21	-	102,102,102,102	0
55	MG	1G	1714	1/1	0.89	0.38	-	94,94,94,94	0
55	MG	1G	1719	1/1	0.47	0.31	-	118,118,118,118	0
55	MG	1H	3468	1/1	0.92	0.13	-	106,106,106,106	0
55	MG	1H	3069	1/1	0.94	0.32	-	69,69,69,69	0
55	MG	14	3242	1/1	0.91	0.24	-	98,98,98,98	0
55	MG	1H	3335	1/1	0.32	0.31	-	101,101,101,101	0
55	MG	14	3219	1/1	0.90	0.37	-	86,86,86,86	0
55	MG	1G	1640	1/1	0.91	0.52	-	90,90,90,90	0
55	MG	14	3088	1/1	0.97	0.32	-	73,73,73,73	0
55	MG	1H	3042	1/1	0.95	0.32	-	84,84,84,84	0
55	MG	1H	3435	1/1	0.96	0.08	-	80,80,80,80	0
55	MG	1G	1657	1/1	0.63	0.22	-	92,92,92,92	0
55	MG	14	3473	1/1	0.96	0.17	-	61,61,61,61	0
55	MG	1H	3356	1/1	0.88	0.32	-	100,100,100,100	0
55	MG	14	3483	1/1	0.92	0.12	-	104,104,104,104	0
55	MG	1H	3448	1/1	0.94	0.06	-	86,86,86,86	0
55	MG	14	3210	1/1	0.90	0.26	-	86,86,86,86	0
55	MG	14	3136	1/1	0.95	0.36	-	71,71,71,71	0
55	MG	1H	3201	1/1	0.96	0.24	-	62,62,62,62	0
55	MG	1H	3184	1/1	0.91	0.41	-	75,75,75,75	0
55	MG	1H	3277	1/1	0.97	0.30	-	74,74,74,74	0
55	MG	13	1686	1/1	0.55	0.56	-	93,93,93,93	0
55	MG	14	3174	1/1	0.95	0.52	-	61,61,61,61	0
55	MG	14	3362	1/1	0.88	0.22	-	77,77,77,77	0
55	MG	14	3487	1/1	0.93	0.12	-	103,103,103,103	0
55	MG	1H	3406	1/1	0.75	0.56	-	87,87,87,87	0
55	MG	1H	3236	1/1	0.98	0.18	-	72,72,72,72	0
55	MG	1H	3207	1/1	0.89	0.32	-	86,86,86,86	0
55	MG	14	3293	1/1	0.84	0.36	-	72,72,72,72	0
55	MG	1G	1655	1/1	0.63	0.33	-	108,108,108,108	0
55	MG	14	3051	1/1	0.97	0.45	-	55,55,55,55	0
55	MG	1G	1673	1/1	0.87	0.14	-	97,97,97,97	0
55	MG	14	3211	1/1	0.90	0.55	-	74,74,74,74	0
55	MG	14	3430	1/1	0.97	0.08	-	69,69,69,69	0
55	MG	14	3411	1/1	0.96	0.10	-	88,88,88,88	0
55	MG	1H	3255	1/1	0.98	0.21	-	72,72,72,72	0
55	MG	1H	3333	1/1	0.85	0.64	-	85,85,85,85	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
55	MG	14	3128	1/1	0.86	0.53	-	89,89,89,89	0
55	MG	1G	1706	1/1	0.93	0.38	-	91,91,91,91	0
55	MG	1H	3370	1/1	0.97	0.29	-	75,75,75,75	0
55	MG	14	3063	1/1	0.97	0.34	-	69,69,69,69	0
55	MG	1H	3225	1/1	0.81	0.39	-	80,80,80,80	0
55	MG	14	3082	1/1	0.86	0.45	-	76,76,76,76	0
55	MG	1H	3361	1/1	0.77	0.72	-	78,78,78,78	0
55	MG	14	3163	1/1	0.91	0.33	-	81,81,81,81	0
55	MG	1H	3280	1/1	0.94	0.18	-	92,92,92,92	0
55	MG	14	3149	1/1	0.85	0.37	-	77,77,77,77	0
55	MG	1H	3240	1/1	0.86	0.49	-	74,74,74,74	0
55	MG	14	3033	1/1	0.94	0.32	-	77,77,77,77	0
55	MG	1H	3223	1/1	0.77	0.31	-	68,68,68,68	0
55	MG	1H	3109	1/1	0.95	0.69	-	39,39,39,39	0
55	MG	1H	3306	1/1	0.92	0.33	-	84,84,84,84	0
55	MG	13	1685	1/1	0.92	0.45	-	103,103,103,103	0
55	MG	1G	1679	1/1	0.85	0.27	-	88,88,88,88	0
55	MG	1H	3170	1/1	0.87	0.40	-	75,75,75,75	0
55	MG	3E	301	1/1	0.87	0.47	-	109,109,109,109	0
55	MG	14	3156	1/1	0.88	0.42	-	82,82,82,82	0
55	MG	14	3384	1/1	0.87	0.24	-	92,92,92,92	0
55	MG	1G	1734	1/1	0.96	0.07	-	108,108,108,108	0
55	MG	14	3101	1/1	0.84	0.15	-	89,89,89,89	0
55	MG	1H	3159	1/1	0.97	0.26	-	76,76,76,76	0
55	MG	13	1694	1/1	0.89	0.76	-	88,88,88,88	0
55	MG	1H	3272	1/1	0.72	0.54	-	85,85,85,85	0
55	MG	14	3014	1/1	0.93	0.21	-	77,77,77,77	0
55	MG	1H	3026	1/1	0.99	0.27	-	53,53,53,53	0
55	MG	14	3428	1/1	0.92	0.06	-	95,95,95,95	0
55	MG	13	1744	1/1	0.87	0.08	-	117,117,117,117	0
55	MG	1H	3065	1/1	0.81	0.35	-	80,80,80,80	0
55	MG	1H	3198	1/1	0.68	0.34	-	113,113,113,113	0
55	MG	13	1617	1/1	0.94	0.32	-	83,83,83,83	0
55	MG	1H	3488	1/1	0.98	0.10	-	66,66,66,66	0
55	MG	13	1624	1/1	0.95	0.37	-	92,92,92,92	0
55	MG	14	3084	1/1	0.85	0.42	-	86,86,86,86	0
55	MG	14	3472	1/1	0.97	0.05	-	103,103,103,103	0
55	MG	1H	3064	1/1	0.98	0.32	-	95,95,95,95	0
55	MG	13	1630	1/1	0.97	0.27	-	65,65,65,65	0
55	MG	1H	3302	1/1	0.89	0.46	-	86,86,86,86	0
55	MG	1H	3024	1/1	0.94	0.44	-	58,58,58,58	0
55	MG	1H	3500	1/1	0.91	0.07	-	105,105,105,105	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
55	MG	14	3415	1/1	0.99	0.09	-	71,71,71,71	0
55	MG	14	3141	1/1	0.91	0.45	-	78,78,78,78	0
55	MG	1H	3265	1/1	0.90	0.33	-	65,65,65,65	0
55	MG	1H	3248	1/1	0.56	0.42	-	106,106,106,106	0
55	MG	1H	3181	1/1	0.85	0.79	-	92,92,92,92	0
55	MG	1H	3364	1/1	0.96	0.56	-	75,75,75,75	0
55	MG	14	3133	1/1	0.81	0.85	-	76,76,76,76	0
55	MG	1H	3172	1/1	0.86	0.34	-	103,103,103,103	0
55	MG	14	3092	1/1	0.96	0.83	-	64,64,64,64	0
55	MG	13	1702	1/1	0.54	0.22	-	96,96,96,96	0
55	MG	1G	1645	1/1	0.73	0.22	-	80,80,80,80	0
55	MG	1H	3379	1/1	0.95	0.71	-	69,69,69,69	0
55	MG	1H	3112	1/1	0.93	0.69	-	69,69,69,69	0
55	MG	1H	3402	1/1	0.79	0.51	-	86,86,86,86	0
55	MG	13	1706	1/1	0.46	0.38	-	95,95,95,95	0
55	MG	1H	3269	1/1	0.86	0.32	-	99,99,99,99	0
55	MG	1H	3183	1/1	0.56	0.47	-	90,90,90,90	0
55	MG	1G	1684	1/1	0.96	0.10	-	109,109,109,109	0
55	MG	14	3263	1/1	0.87	0.44	-	92,92,92,92	0
55	MG	14	3217	1/1	0.80	0.32	-	98,98,98,98	0
55	MG	1H	3233	1/1	0.87	0.48	-	100,100,100,100	0
55	MG	14	3089	1/1	0.92	0.48	-	89,89,89,89	0
55	MG	1H	3073	1/1	0.64	0.66	-	68,68,68,68	0
55	MG	1H	3501	1/1	0.94	0.07	-	105,105,105,105	0
55	MG	14	3135	1/1	0.94	0.39	-	75,75,75,75	0
55	MG	1H	3014	1/1	0.97	0.50	-	40,40,40,40	0
55	MG	1G	1652	1/1	0.93	0.28	-	99,99,99,99	0
55	MG	1H	3309	1/1	0.95	0.34	-	78,78,78,78	0
55	MG	1H	3210	1/1	0.88	0.46	-	82,82,82,82	0
55	MG	14	3048	1/1	0.98	0.44	-	66,66,66,66	0
55	MG	14	3137	1/1	0.93	0.51	-	77,77,77,77	0
55	MG	1H	3420	1/1	0.97	0.06	-	99,99,99,99	0
55	MG	1H	3189	1/1	0.94	0.41	-	85,85,85,85	0
55	MG	14	3245	1/1	0.93	0.44	-	81,81,81,81	0
55	MG	1G	1739	1/1	0.90	0.24	-	107,107,107,107	0
55	MG	1H	3324	1/1	0.59	0.44	-	89,89,89,89	0
55	MG	1H	3385	1/1	0.93	0.22	-	106,106,106,106	0
55	MG	14	3251	1/1	0.94	0.54	-	74,74,74,74	0
55	MG	14	3270	1/1	0.70	0.36	-	87,87,87,87	0
55	MG	14	3154	1/1	0.91	0.47	-	81,81,81,81	0
55	MG	14	3231	1/1	0.87	0.49	-	79,79,79,79	0
55	MG	14	3223	1/1	0.57	0.40	-	118,118,118,118	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
55	MG	13	1660	1/1	0.86	0.17	-	99,99,99,99	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.