



# wwPDB X-ray Structure Validation Summary Report ⓘ

Jan 3, 2024 – 01:06 am GMT

PDB ID : 5IBB  
Title : Structure of T. thermophilus 70S ribosome complex with mRNA, tRNA<sup>fMet</sup> and cognate tRNA<sup>Val</sup> in the A-site  
Authors : Rozov, A.; Demeshkina, N.; Yusupov, M.; Yusupova, G.  
Deposited on : 2016-02-22  
Resolution : 2.96 Å (reported)

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

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity : 4.02b-467  
Mogul : 1.8.4, CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.36  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.36

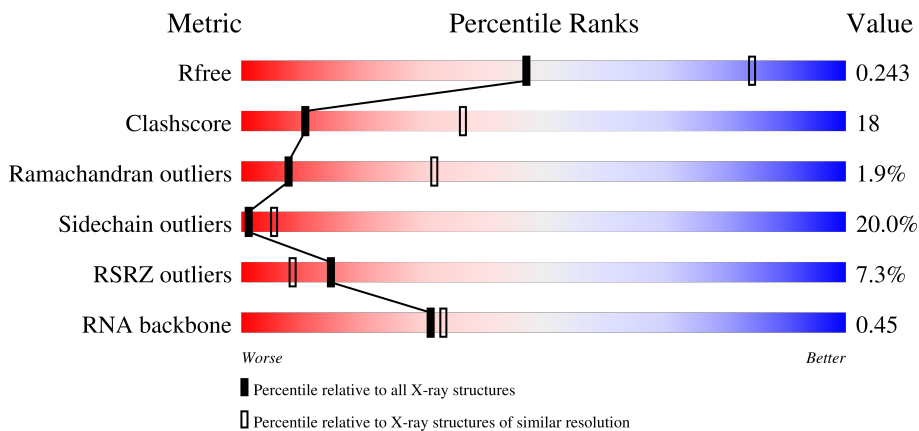
# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.96 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	130704	3104 (3.00-2.92)
Clashscore	141614	3462 (3.00-2.92)
Ramachandran outliers	138981	3340 (3.00-2.92)
Sidechain outliers	138945	3343 (3.00-2.92)
RSRZ outliers	127900	2986 (3.00-2.92)
RNA backbone	3102	1065 (3.22-2.70)

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

Mol	Chain	Length	Quality of chain
1	13	1522	
1	1G	1522	
2	12	256	
2	1E	256	

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

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Mol	Chain	Length	Quality of chain
15	6I	89	11% 54% 36% 8%
16	7A	88	% 50% 34% 9% 5%
16	7I	88	2% 42% 34% 17% 6%
17	8A	105	2% 53% 34% 7% 6%
17	8I	105	3% 40% 38% 13% 5%
18	9A	88	11% 42% 25% 8% 24%
18	9I	88	13% 40% 28% 9% 23%
19	AA	93	5% 23% 35% 5% 33%
19	AI	93	13% 39% 37% 11% 12%
20	BA	106	4% 44% 35% 13% 7%
20	BI	106	6% 26% 50% 13% 8%
21	1B	27	11% 44% 26% 11% 19%
21	1F	27	11% 48% 30% 7% 15%
22	1K	76	9% 26% 43% 18% 7% 5%
23	2K	77	% 47% 31% 19%
23	2L	77	44% 42% 10%
24	3K	76	14% 13% 37% 38% 8%
24	3L	76	12% 24% 39% 29% 7%
25	4K	30	7% 27% 17% 20% 7% 30%
25	4L	30	3% 23% 13% 20% 7% 37%
26	14	2917	% 39% 39% 15%
26	1H	2917	% 35% 42% 17%
27	16	122	% 45% 33% 20%
27	1J	122	34% 41% 21%
28	7I	229	26% 26% 24% 7% 42%

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Mol	Chain	Length	Quality of chain
28	79	229	
29	11	276	
29	19	276	
30	21	206	
30	29	206	
31	31	210	
31	39	210	
32	41	182	
32	49	182	
33	51	180	
33	59	180	
34	61	148	
34	69	148	
35	15	140	
35	58	140	
36	25	122	
36	68	122	
37	35	150	
37	78	150	
38	45	141	
38	88	141	
39	55	118	
39	98	118	
40	65	112	
40	A8	112	


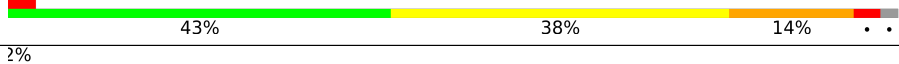

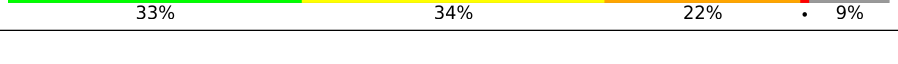
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Mol	Chain	Length	Quality of chain
41	75	146	
41	B8	146	
42	85	118	
42	C8	118	
43	95	101	
43	D8	101	
44	A5	113	
44	E8	113	
45	B5	96	
45	F8	96	
46	C5	110	
46	G8	110	
47	D5	206	
47	H8	206	
48	E5	85	
48	I8	85	
49	F5	98	
49	J8	98	
50	G5	72	
50	K8	72	
51	H5	60	
51	L8	60	
52	I5	71	
52	M8	71	
53	J5	60	

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Mol	Chain	Length	Quality of chain
53	N8	60	
54	L5	49	
54	P8	49	
55	M5	65	
55	Q8	65	
56	1L	76	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
57	MG	13	1643	-	-	-	X
57	MG	13	1650	-	-	-	X
57	MG	13	1671	-	-	-	X
57	MG	13	1678	-	-	-	X
57	MG	13	1687	-	-	-	X
57	MG	13	1690	-	-	-	X
57	MG	14	3007	-	-	-	X
57	MG	14	3031	-	-	-	X
57	MG	14	3083	-	-	-	X
57	MG	14	3087	-	-	-	X
57	MG	14	3092	-	-	-	X
57	MG	14	3094	-	-	-	X
57	MG	14	3097	-	-	-	X
57	MG	14	3110	-	-	-	X
57	MG	14	3111	-	-	-	X
57	MG	14	3112	-	-	-	X
57	MG	14	3134	-	-	-	X
57	MG	14	3137	-	-	-	X
57	MG	14	3152	-	-	-	X
57	MG	14	3157	-	-	-	X
57	MG	14	3162	-	-	-	X
57	MG	14	3163	-	-	-	X
57	MG	14	3172	-	-	-	X
57	MG	14	3174	-	-	-	X
57	MG	14	3189	-	-	-	X
57	MG	14	3205	-	-	-	X
57	MG	14	3214	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
57	MG	14	3226	-	-	-	X
57	MG	1G	1621	-	-	-	X
57	MG	1G	1630	-	-	-	X
57	MG	1H	3005	-	-	-	X
57	MG	1H	3009	-	-	-	X
57	MG	1H	3036	-	-	-	X
57	MG	1H	3058	-	-	-	X
57	MG	1H	3061	-	-	-	X
57	MG	1H	3072	-	-	-	X
57	MG	1H	3085	-	-	-	X
57	MG	1H	3086	-	-	-	X
57	MG	1H	3115	-	-	-	X
57	MG	1H	3120	-	-	-	X
57	MG	1H	3121	-	-	-	X
57	MG	1H	3123	-	-	-	X
57	MG	1H	3133	-	-	-	X
57	MG	1H	3179	-	-	-	X
57	MG	1H	3186	-	-	-	X
57	MG	1H	3187	-	-	-	X
57	MG	1H	3188	-	-	-	X
57	MG	1H	3189	-	-	-	X
57	MG	1H	3199	-	-	-	X
57	MG	1H	3204	-	-	-	X
57	MG	1H	3207	-	-	-	X
57	MG	1H	3211	-	-	-	X
57	MG	1H	3216	-	-	-	X
57	MG	1H	3217	-	-	-	X
57	MG	1H	3227	-	-	-	X
57	MG	1H	3232	-	-	-	X
57	MG	1H	3246	-	-	-	X
57	MG	1H	3260	-	-	-	X
57	MG	1H	3263	-	-	-	X
57	MG	1H	3274	-	-	-	X
57	MG	1H	3279	-	-	-	X
57	MG	1H	3282	-	-	-	X
57	MG	1H	3316	-	-	-	X
57	MG	1H	3317	-	-	-	X
57	MG	1H	3320	-	-	-	X
57	MG	2L	102	-	-	-	X
57	MG	2L	103	-	-	-	X
57	MG	4E	201	-	-	-	X
59	SF4	3E	301	-	-	X	-



## 2 Entry composition [i](#)

There are 61 unique types of molecules in this entry. The entry contains 296743 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
			Total	C	N	O	P			
1	13	1496	Total	C	N	O	P	0	0	0
			32157	14313	5960	10388	1496			
1	1G	1506	Total	C	N	O	P	0	0	0
			32371	14409	6001	10456	1505			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
13	1542	G	U	conflict	GB 55771382
1G	1542	G	U	conflict	GB 55771382

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	1E	235	Total	C	N	O	S	0	0	0
			1902	1215	340	342	5			
2	12	207	Total	C	N	O	S	0	0	0
			1696	1083	306	303	4			

- Molecule 3 is a protein called 30S ribosomal protein S3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	2E	205	Total	C	N	O	S	0	0	0
			1605	1011	313	280	1			
3	22	195	Total	C	N	O	S	0	0	0
			1537	973	297	266	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
4	3E	207	Total	C	N	O	S	0	0	0
			1698	1064	338	289	7			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
4	32	208	1702	1066	339	290	7	0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
5	4E	149	1142	722	216	200	4	0	0	0
5	42	149	1139	721	216	198	4	0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
6	5E	100	837	528	154	152	3	0	0	0
6	52	101	842	531	155	153	3	0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
7	6E	154	1242	770	250	216	6	0	0	0
7	62	140	1120	695	223	196	6	0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
8	7E	138	1115	705	215	192	3	0	0	0
8	72	137	1107	700	214	191	2	0	0	0

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
9	8E	126	1000	634	196	170	0	0	0
9	82	121	953	605	186	162	0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	1I	95	Total	C	N	O	S	0	0	0
			754	471	148	134	1			
10	1A	80	Total	C	N	O		0	0	0
			646	403	129	114				

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	2I	111	Total	C	N	O	S	0	0	0
			823	512	154	154	3			
11	2A	113	Total	C	N	O	S	0	0	0
			835	520	156	156	3			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	3I	122	Total	C	N	O	S	0	0	0
			956	603	193	159	1			
12	3A	122	Total	C	N	O	S	0	0	0
			956	603	193	159	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	4I	119	Total	C	N	O	S	0	0	0
			942	582	194	164	2			
13	4A	111	Total	C	N	O	S	0	0	0
			893	552	183	156	2			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
14	5I	60	Total	C	N	O	S	0	0	0
			491	312	104	71	4			
14	5A	59	Total	C	N	O	S	0	0	0
			486	309	103	70	4			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
15	6I	87	Total	C	N	O	S	0	0	0
			729	457	146	124	2			
15	6A	87	Total	C	N	O	S	0	0	0
			729	457	146	124	2			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
16	7I	83	Total	C	N	O	S	0	0	0
			700	443	139	117	1			
16	7A	84	Total	C	N	O	S	0	0	0
			705	446	140	118	1			

- Molecule 17 is a protein called 30S ribosomal protein S17.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
17	8I	100	Total	C	N	O	S	0	0	0
			834	534	155	143	2			
17	8A	99	Total	C	N	O	S	0	0	0
			823	528	151	142	2			

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
18	9I	68	Total	C	N	O	0	0	0
			549	352	105	92			
18	9A	67	Total	C	N	O	0	0	0
			544	349	104	91			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
19	AI	82	Total	C	N	O	S	0	0	0
			661	422	123	114	2			
19	AA	62	Total	C	N	O	S	0	0	0
			481	306	85	88	2			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
20	BI	97	Total	C	N	O	S	0	0	0
			746	461	157	126	2			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
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	22	Total	C	N	O	0	0	0
			188	116	44	28			

- Molecule 22 is a RNA chain called tRNAVal.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
22	1K	72	Total	C	N	O	P	0	0	0
			1540	688	274	506	72			

- Molecule 23 is a RNA chain called tRNAfMet.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
23	2K	77	Total	C	N	O	P	S	0	0	0
			1646	735	298	535	77	1			
23	2L	76	Total	C	N	O	P	S	0	0	0
			1626	726	296	527	76	1			

- Molecule 24 is a RNA chain called tRNAVal.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
24	3K	70	Total	C	N	O	P	0	0	0
			1491	665	268	488	70			
24	3L	71	Total	C	N	O	P	0	0	0
			1513	675	272	495	71			

- Molecule 25 is a RNA chain called mRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
25	4K	21	Total	C	N	O	P	0	0	0
			462	207	96	138	21			
25	4L	19	Total	C	N	O	P	0	0	0
			417	187	86	125	19			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
26	1H	2841	61195	27234	11446	19674	2841	0	0	0
26	14	2810	60535	26940	11330	19455	2810	0	0	0

There are 14 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
1H	161	U	UNK	conflict	GB 55771382
1H	654A	A	G	conflict	GB 55771382
1H	654E	C	G	conflict	GB 55771382
1H	654P	G	C	conflict	GB 55771382
1H	654T	A	C	conflict	GB 55771382
1H	1058	U	G	conflict	GB 55771382
1H	1080	A	C	conflict	GB 55771382
14	158	U	UNK	conflict	GB 55771382
14	654A	A	G	conflict	GB 55771382
14	654E	C	G	conflict	GB 55771382
14	654P	G	C	conflict	GB 55771382
14	654T	A	C	conflict	GB 55771382
14	1058	U	G	conflict	GB 55771382
14	1080	A	C	conflict	GB 55771382

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

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

- Molecule 28 is a protein called 50S ribosomal protein L1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
28	71	133	1033	651	194	187	1	0	0	0
28	79	57	456	283	91	82		0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
29	11	273	Total	C	N	O	S	0	0	0
			2120	1338	421	358	3			
29	19	274	Total	C	N	O	S	0	0	0
			2125	1341	422	359	3			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
30	21	202	Total	C	N	O	S	0	0	0
			1505	951	281	267	6			
30	29	204	Total	C	N	O	S	0	0	0
			1563	988	299	270	6			

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
32	41	179	Total	C	N	O	S	0	0	0
			1457	931	265	257	4			
32	49	181	Total	C	N	O	S	0	0	0
			1468	937	268	259	4			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
33	51	174	Total	C	N	O	S	0	0	0
			1328	842	249	236	1			
33	59	167	Total	C	N	O	S	0	0	0
			1283	815	239	228	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
34	61	146	Total	C	N	O	S	0	0	0
			1136	726	201	208	1			

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
35	58	137	1096	706	205	181	4	0	0	0
35	15	138	1104	712	206	182	4	0	0	0

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
38	88	141	1117	712	211	187	7	0	0	0
38	45	139	1104	705	209	184	6	0	0	0

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

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



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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
41	B8	136	1124	700	231	192	1	0	0	0
41	75	133	1109	691	228	189	1	0	0	0

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
43	D8	100	774	499	141	133	1	0	0	0
43	95	100	770	496	140	133	1	0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
44	E8	110	876	552	171	151	2	0	0	0
44	A5	111	886	558	174	152	2	0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
45	F8	95	Total	C	N	O	S	0	0	0
			743	482	134	126	1			
45	B5	94	Total	C	N	O	S	0	0	0
			735	477	133	125				

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
46	G8	103	Total	C	N	O	S	0	0	0
			777	501	145	126	5			
46	C5	104	Total	C	N	O	S	0	0	0
			794	510	152	127	5			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
47	H8	170	Total	C	N	O	S	0	0	0
			1365	870	246	246	3			
47	D5	133	Total	C	N	O	S	0	0	0
			1079	694	194	189	2			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
48	I8	77	Total	C	N	O	S	0	0	0
			611	378	129	103	1			
48	E5	76	Total	C	N	O	S	0	0	0
			603	372	128	102	1			

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
50	K8	68	Total	C	N	O	S	0	0	0
			575	358	116	100	1			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
50	G5	69	Total	C	N	O	S	0	0	0
			576	358	116	101	1			

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
52	M8	61	Total	C	N	O	S	0	0	0
			479	299	86	89	5			
52	I5	63	Total	C	N	O	S	0	0	0
			515	326	93	91	5			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
53	N8	56	Total	C	N	O	S	0	0	0
			437	275	87	70	5			
53	J5	56	Total	C	N	O	S	0	0	0
			434	272	87	70	5			

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

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

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

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

- Molecule 56 is a RNA chain called tRNAVal.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
56	1L	69	1469	656	262	482	69	0	0	0

- Molecule 57 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
57	13	148	Total 148	Mg 148	0	0
57	4E	1	Total 1	Mg 1	0	0
57	5E	1	Total 1	Mg 1	0	0
57	3I	1	Total 1	Mg 1	0	0
57	5I	1	Total 1	Mg 1	0	0
57	2K	4	Total 4	Mg 4	0	0
57	4K	2	Total 2	Mg 2	0	0
57	1H	548	Total 548	Mg 548	0	0
57	16	11	Total 11	Mg 11	0	0
57	11	2	Total 2	Mg 2	0	0
57	21	2	Total 2	Mg 2	0	0
57	31	2	Total 2	Mg 2	0	0
57	41	1	Total 1	Mg 1	0	0
57	68	2	Total 2	Mg 2	0	0
57	78	1	Total 1	Mg 1	0	0
57	88	3	Total 3	Mg 3	0	0
57	F8	1	Total 1	Mg 1	0	0
57	I8	1	Total 1	Mg 1	0	0

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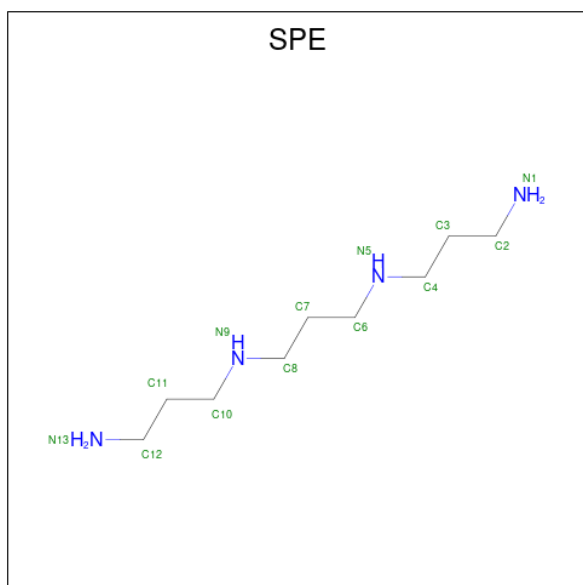
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
57	J8	1	Total Mg 1 1	0	0
57	L8	1	Total Mg 1 1	0	0
57	P8	1	Total Mg 1 1	0	0
57	Q8	1	Total Mg 1 1	0	0
57	1G	133	Total Mg 133 133	0	0
57	42	1	Total Mg 1 1	0	0
57	3A	1	Total Mg 1 1	0	0
57	4A	1	Total Mg 1 1	0	0
57	9A	1	Total Mg 1 1	0	0
57	2L	3	Total Mg 3 3	0	0
57	4L	2	Total Mg 2 2	0	0
57	14	445	Total Mg 445 445	0	0
57	1J	7	Total Mg 7 7	0	0
57	19	1	Total Mg 1 1	0	0
57	29	2	Total Mg 2 2	0	0
57	39	2	Total Mg 2 2	0	0
57	25	2	Total Mg 2 2	0	0
57	35	2	Total Mg 2 2	0	0
57	45	1	Total Mg 1 1	0	0
57	B5	1	Total Mg 1 1	0	0
57	C5	1	Total Mg 1 1	0	0

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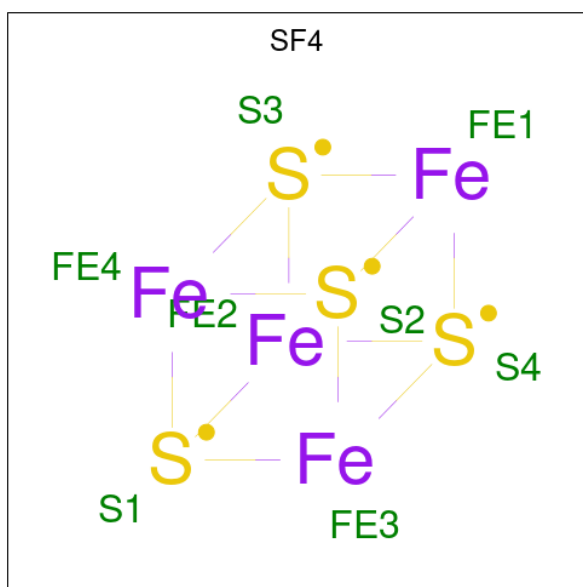
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
57	E5	1	Total Mg 1 1	0	0
57	M5	1	Total Mg 1 1	0	0

- Molecule 58 is THERMINE (three-letter code: SPE) (formula: C<sub>9</sub>H<sub>24</sub>N<sub>4</sub>).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
58	13	1	Total C N 13 9 4	0	0
58	1G	1	Total C N 13 9 4	0	0
58	14	1	Total C N 13 9 4	0	0
58	14	1	Total C N 13 9 4	0	0
58	1J	1	Total C N 13 9 4	0	0

- Molecule 59 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe<sub>4</sub>S<sub>4</sub>).



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

- Molecule 60 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

- Molecule 61 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
61	13	304	Total O 304 304	0	0
61	3E	1	Total O 1 1	0	0
61	4E	1	Total O 1 1	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
61	1I	2	Total O 2 2	0	0
61	2I	1	Total O 1 1	0	0
61	3I	2	Total O 2 2	0	0
61	5I	2	Total O 2 2	0	0
61	7I	2	Total O 2 2	0	0
61	1K	1	Total O 1 1	0	0
61	2K	6	Total O 6 6	0	0
61	3K	1	Total O 1 1	0	0
61	4K	11	Total O 11 11	0	0
61	1H	1133	Total O 1133 1133	0	0
61	16	15	Total O 15 15	0	0
61	11	16	Total O 16 16	0	0
61	21	8	Total O 8 8	0	0
61	31	4	Total O 4 4	0	0
61	58	1	Total O 1 1	0	0
61	78	11	Total O 11 11	0	0
61	98	2	Total O 2 2	0	0
61	A8	3	Total O 3 3	0	0
61	B8	1	Total O 1 1	0	0
61	E8	1	Total O 1 1	0	0
61	F8	1	Total O 1 1	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
61	I8	6	Total O 6 6	0	0
61	K8	1	Total O 1 1	0	0
61	L8	1	Total O 1 1	0	0
61	P8	1	Total O 1 1	0	0
61	Q8	5	Total O 5 5	0	0
61	1G	391	Total O 391 391	0	0
61	22	1	Total O 1 1	0	0
61	42	1	Total O 1 1	0	0
61	52	3	Total O 3 3	0	0
61	3A	1	Total O 1 1	0	0
61	7A	1	Total O 1 1	0	0
61	9A	3	Total O 3 3	0	0
61	BA	2	Total O 2 2	0	0
61	4L	14	Total O 14 14	0	0
61	14	1135	Total O 1135 1135	0	0
61	1J	18	Total O 18 18	0	0
61	19	8	Total O 8 8	0	0
61	29	6	Total O 6 6	0	0
61	39	6	Total O 6 6	0	0
61	25	11	Total O 11 11	0	0
61	35	9	Total O 9 9	0	0

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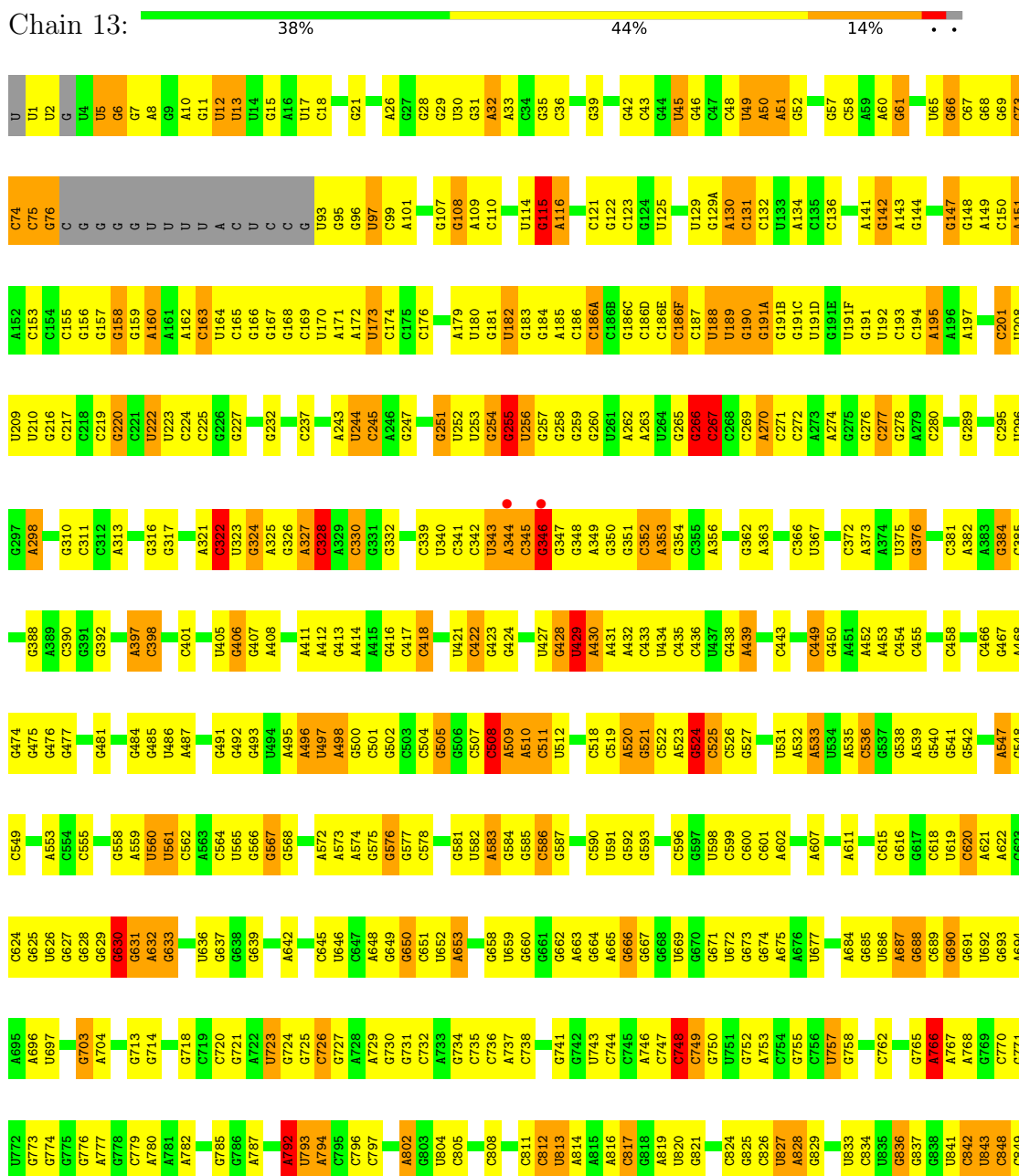
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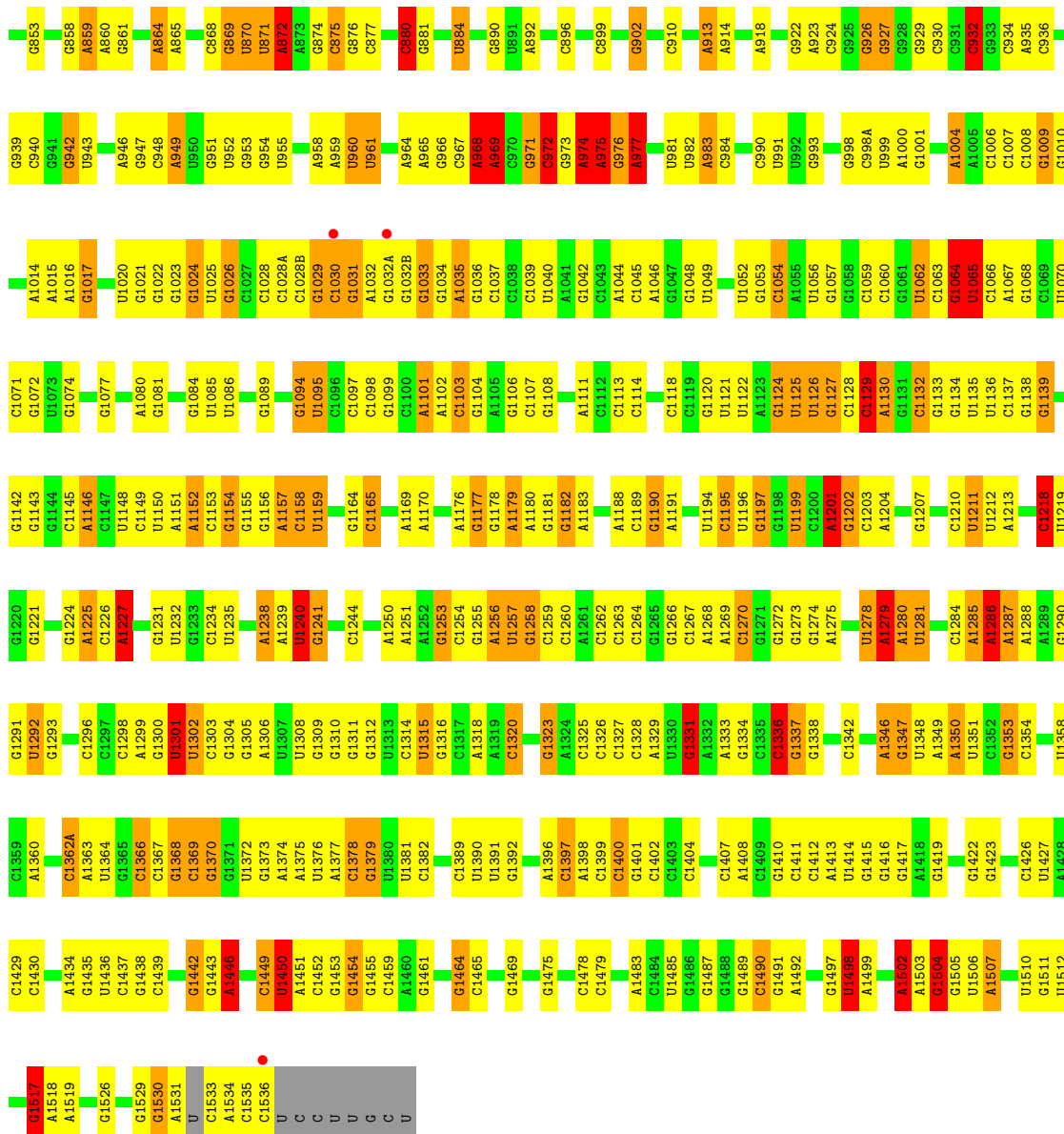
<b>Mol</b>	<b>Chain</b>	<b>Residues</b>	<b>Atoms</b>		<b>ZeroOcc</b>	<b>AltConf</b>
61	45	3	Total 3	O 3	0	0
61	55	1	Total 1	O 1	0	0
61	75	1	Total 1	O 1	0	0
61	85	1	Total 1	O 1	0	0
61	A5	1	Total 1	O 1	0	0
61	C5	3	Total 3	O 3	0	0
61	E5	5	Total 5	O 5	0	0
61	F5	3	Total 3	O 3	0	0
61	H5	1	Total 1	O 1	0	0
61	M5	7	Total 7	O 7	0	0

### 3 Residue-property plots

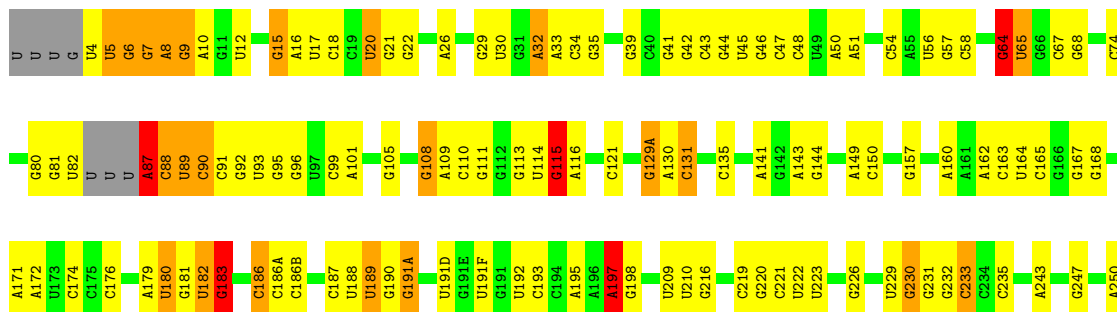
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

#### • Molecule 1: 16S ribosomal RNA

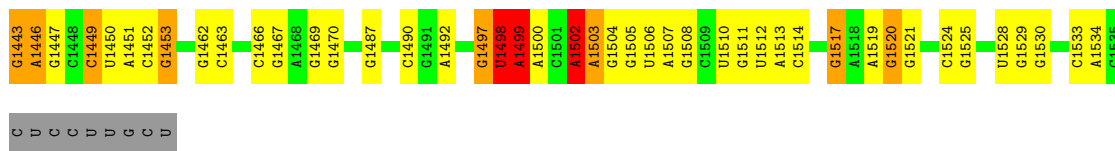




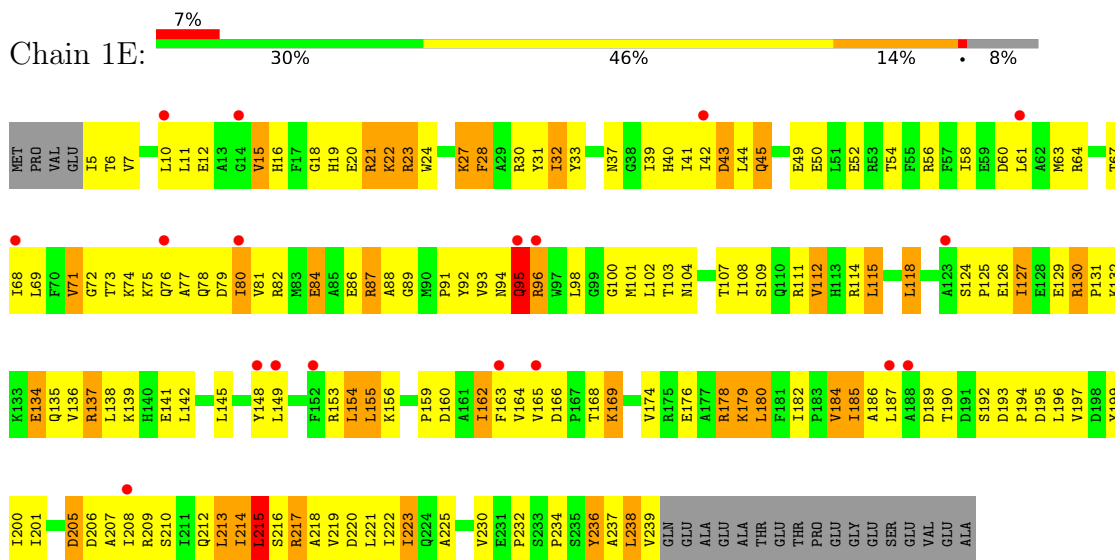
- Molecule 1: 16S ribosomal RNA



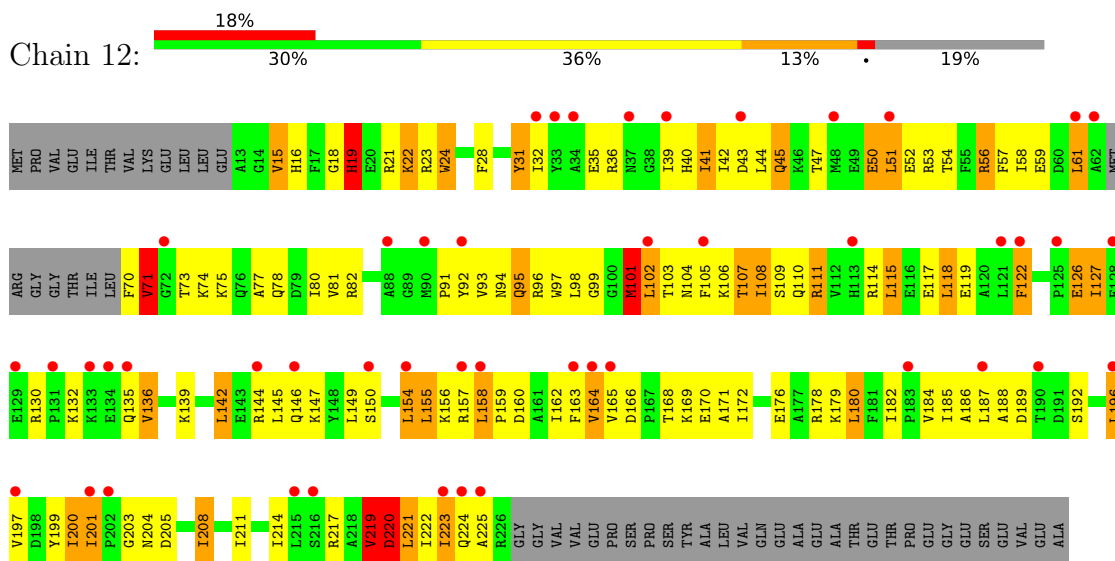
A1363	A1364	C1367	G1368	G1369	A1370	G1371	G1372	G1373	G1374	G1375	A1376	A1377	G1378	G1379	G1380	G1381	G1382	G1383	G1384	G1385	G1386	G1387	G1388	G1389	G1390	G1391	G1392	G1393	G1394	G1395	G1396	G1397	G1398	G1399	G1400	G1401	G1402	G1403	G1404	G1405	G1406	G1407	A1408	A1413	G1415	G1416	G1417	A1418	G1419	G1422	G1423	G1424	G1432	G1435	U1436	G1442																																																																																					
G1300	U1301	U1302	U1303	G1304	G1305	A1306	U1307	U1308	G1309	G1310	G1311	G1312	U1313	G1314	G1315	G1316	G1317	A1318	A1319	C1320	C1321	C1322	G1323	A1324	C1325	C1326	C1327	C1328	A1329	U1330	G1331	A1332	A1333	G1334	C1335	C1336	G1337	G1338	A1339	C1342	G1343	A1346	G1347	U1348	A1349	A1350	U1351	C1352	G1353	G1356	U1357	C1358	A1360	C1362A																																																																																							
G1222	C1223	G1224	A1225	C1226	A1227	C1228	U1232	U1233	U1234	U1235	A1238	A1239	U1240	G1241	A1245	C1246	C1249	A1250	A1251	G1255	A1256	U1257	U1258	C1259	C1260	A1268	A1269	G1272	G1273	G1274	A1275	G1276	U1277	A1278	A1279	A1280	U1281	C1282	G1283	G1284	A1285	A1286	A1287	A1288	A1289	G1290	G1291	U1292	C1296	C1297	C1298	A1299																																																																																									
C1158	U1159	G1160	C1161	C1162	A1167	A1169	A1170	G1171	C1172	G1173	G1174	G1175	A1176	G1177	G1178	A1179	A1180	G1181	G1182	A1183	G1184	G1185	G1186	C1187	A1188	C1189	G1190	A1191	C1192	G1193	U1194	C1195	U1196	G1197	G1198	U1199	C1200	A1201	G1202	C1203	A1204	U1205	G1206	G1207	C1208	C1209	C1210	C1211	U1212	A1213	C1214	G1215	G1216	C1217	C1218	U1219	G1220	G1221																																																																																			
U1020	G1021	G1022	G1023	G1024	U1025	G1026	C1027	A1028	C1028A	C1028B	G1029	G1030	G1031	A1032	G1032A	G1032B	G1033	C1037	C1038	C1039	U1040	A1041	G1042	C1043	A1046	G1047	U1048	G1049	C1051	U1052	G1053	A1054	A1055	U1056	G1057	G1058	C1059	C1060	G1061	C1062	U1063	G1064	G1068	C1069	U1070	G1071	C1072	U1073	G1074	G1077	A1080	G1081	G1084																																																																																								
A949	U950	G951	A859	U952	G953	C861	U957	A958	A959	A872	U960	A873	G962	G963	A964	A965	G966	C967	A968	A969	C893	G894	C895	A900	G903	A913	A914	A915	A918	A919	U920	U921	A922	A923	A924	G925	A926	G927	C931	G932	G933	A934	A935	C936	A937	A938	G939	C940	G941	G942	U943	G944	G945	A946	C947	C948																																																																																					
C856	C857	G858	A859	A860	C861	G869	U872	G773	A777	G778	G779	A780	C784	A787	A792	U793	A794	G800	U804	C805	C808	C809	C810	C811	C812	U813	A814	A815	A816	C817	C818	A819	U820	G821	C822	C826	U827	A828	C829	G836	G837	U841	U842	U843	G848	G851	G852	G853	G854	G855	G856	G857	G858	G859																																																																																							
G681	G682	G683	A684	G685	U686	A687	G688	C689	G690	G691	U692	G693	A694	A695	C701	A702	A706	C707	G617	U618	C620	A621	A622	A623	A624	C625	U626	G627	A628	G629	A630	G631	A632	C633	A640	U650	U651	U652	A653	A654	A655	A656	A657	A658	A659	U660	U661	U662	U663	U664	A665	U666	U667	U668	U669	U670	U671	U672	U673	U674	U675	U676	U677	U678	U679	U680	U681	U682	U683	U684	U685	U686	U687	U688	U689	U690	U691	U692	U693	U694	U695	U696	U697	U698	U699	U700	U701	U702	U703	U704	U705	U706	U707	U708	U709	U710	U711	U712	U713	U714	U715	U716	U717	U718	U719	U720	U721	U722	U723	U724	U725	U726	U727	U728	U729	U730	U731	U732	U733	U734	U735	U736	U737	U738	U739	U740	U741	U742	U743	U744	U745	U746	U747	U748	U749	U750	U751	U752	U753	U754	U755
C518	C519	A520	G521	C522	A523	U524	C525	C526	C527	C528	C529	G530	U531	A532	A533	U534	A535	C536	A537	A538	A539	G540	G541	G542	C543	G544	A545	A546	C547	A548	A549	A550	U551	U552	A553	C554	C555	C556	G557	G558	A559	U560	U561	C562	A563	C564	G567	A572	A573	G576	G577	A509	A510	C511	U512	U513	U514	U515	U516	U517	U518	U519	U520	U521	U522	U523	U524	U525	U526	U527	U528	U529	U530	U531	U532	U533	U534	U535	U536	U537	U538	U539	U540	U541	U542	U543	U544	U545	U546	U547	U548	U549	U550	U551	U552	U553	U554	U555	U556	U557	U558	U559	U560	U561	U562	U563	U564	U565	U566	U567	U568	U569	U570	U571	U572	U573	U574	U575	U576	U577	U578	U579	U580	U581	U582	U583															
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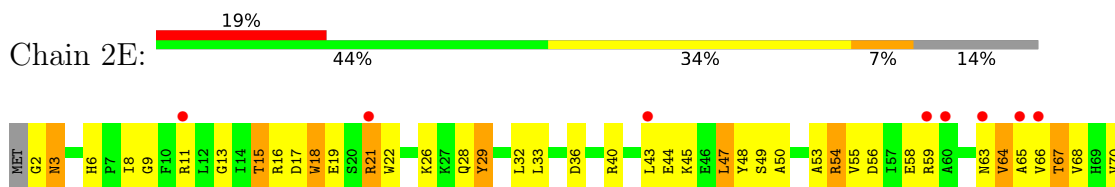
- Molecule 2: 30S ribosomal protein S2

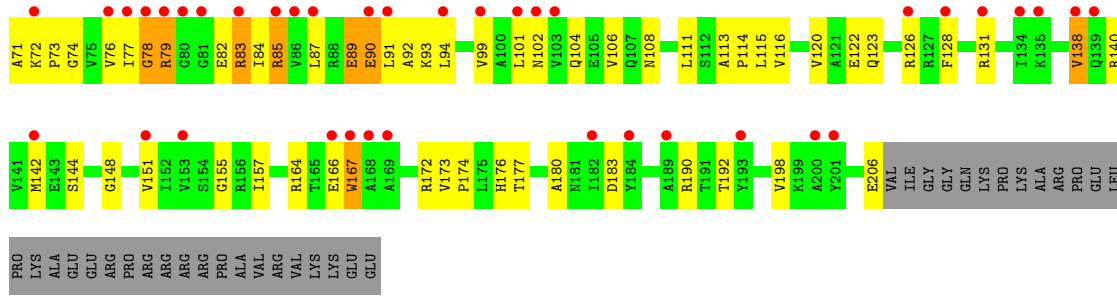


- Molecule 2: 30S ribosomal protein S2

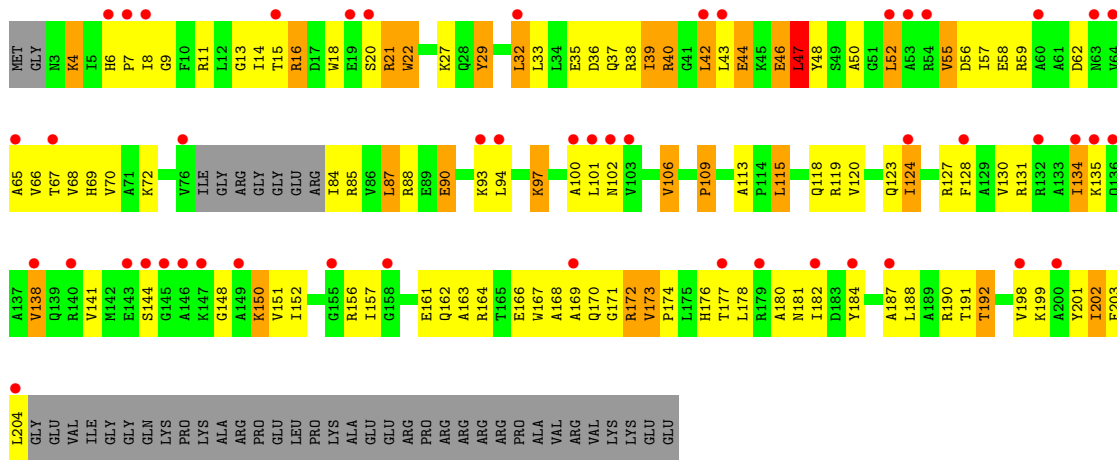


- Molecule 3: 30S ribosomal protein S3

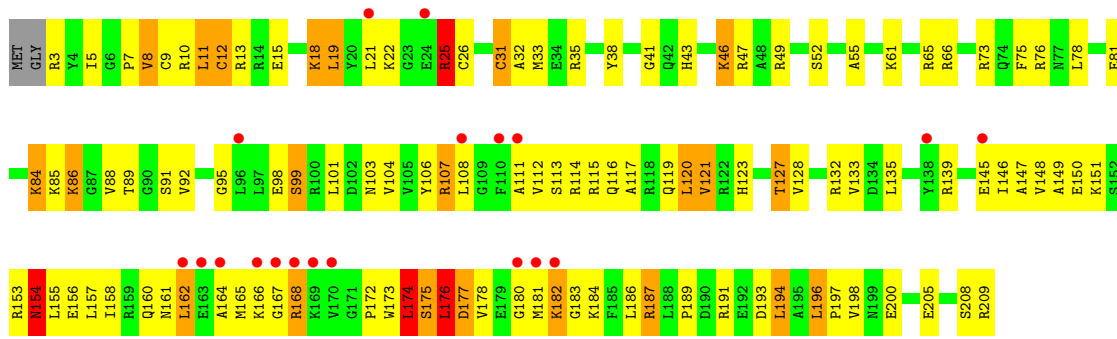




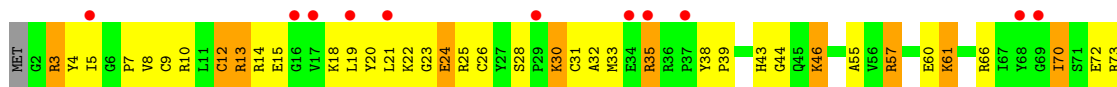
• Molecule 3: 30S ribosomal protein S3

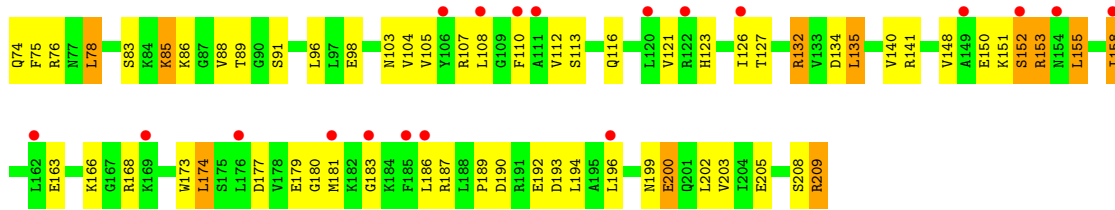


• Molecule 4: 30S ribosomal protein S4

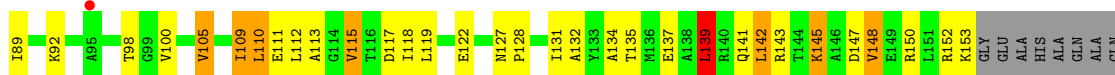
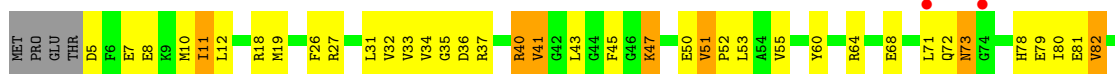


• Molecule 4: 30S ribosomal protein S4



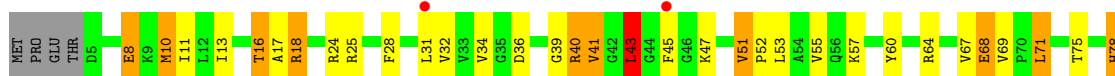


• Molecule 5: 30S ribosomal protein S5



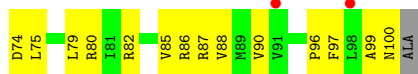
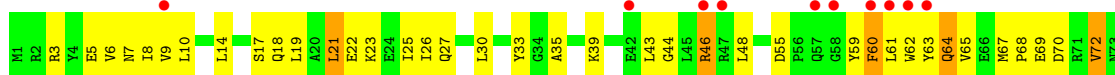
GLY

• Molecule 5: 30S ribosomal protein S5



ALA  
HIS  
ALA  
GLN  
ALA  
GLN  
GLY

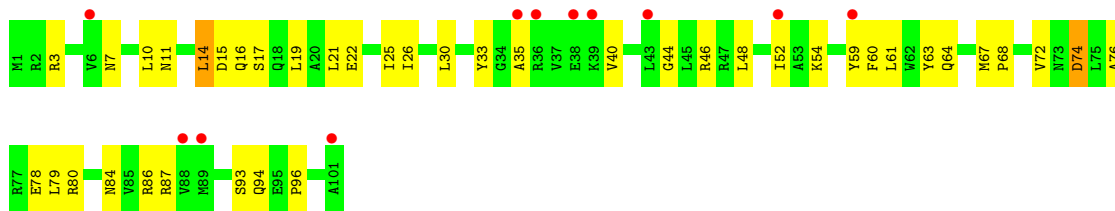
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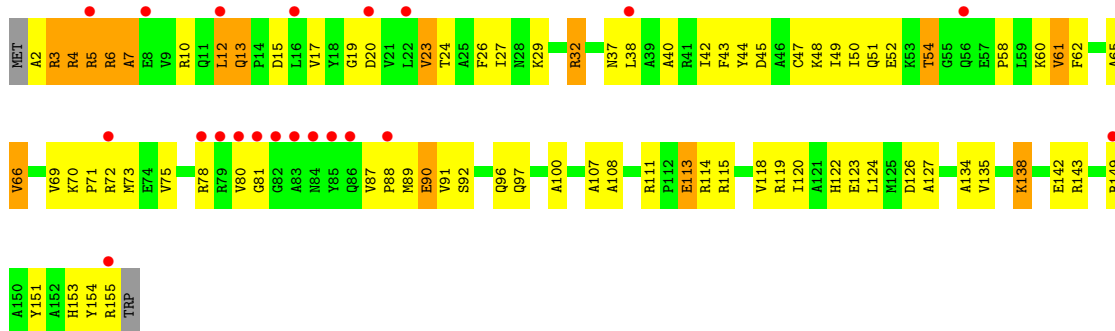
• Molecule 6: 30S ribosomal protein S6



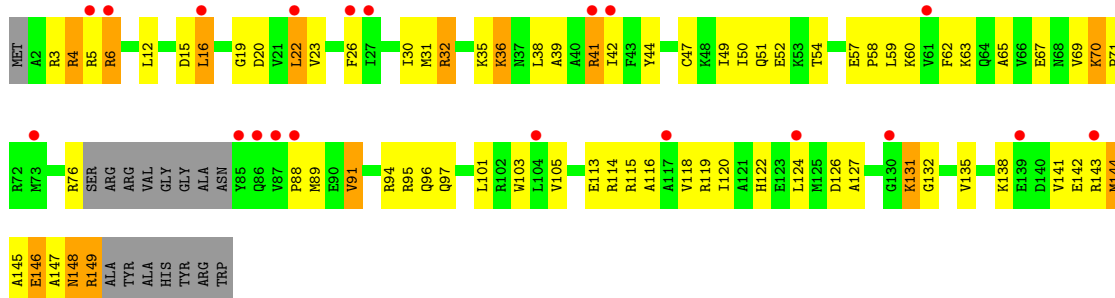




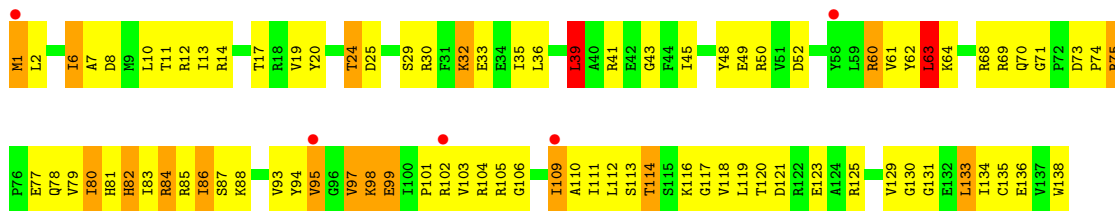
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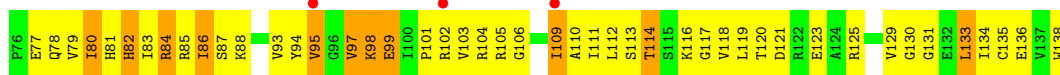
• Molecule 7: 30S ribosomal protein S7

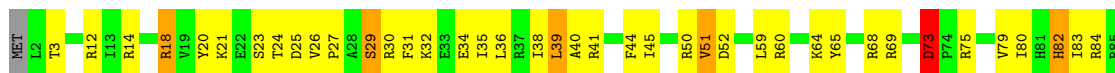


• Molecule 8: 30S ribosomal protein S8

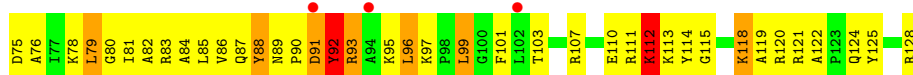


• Molecule 8: 30S ribosomal protein S8

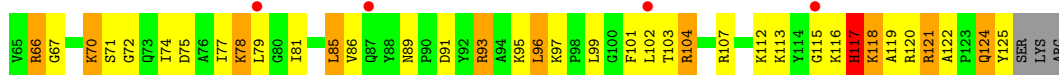
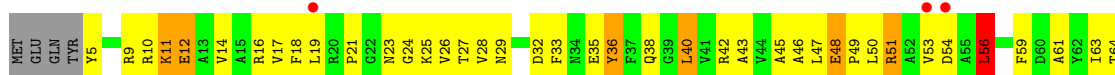




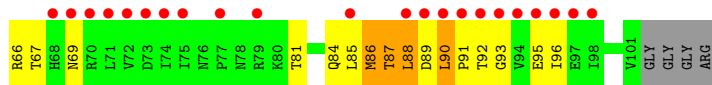
• Molecule 9: 30S ribosomal protein S9



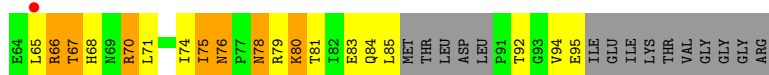
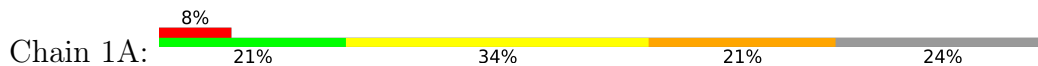
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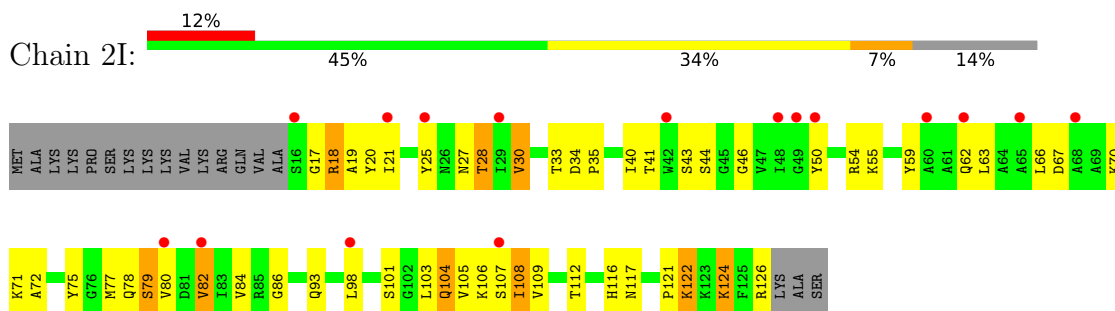
• Molecule 10: 30S ribosomal protein S10



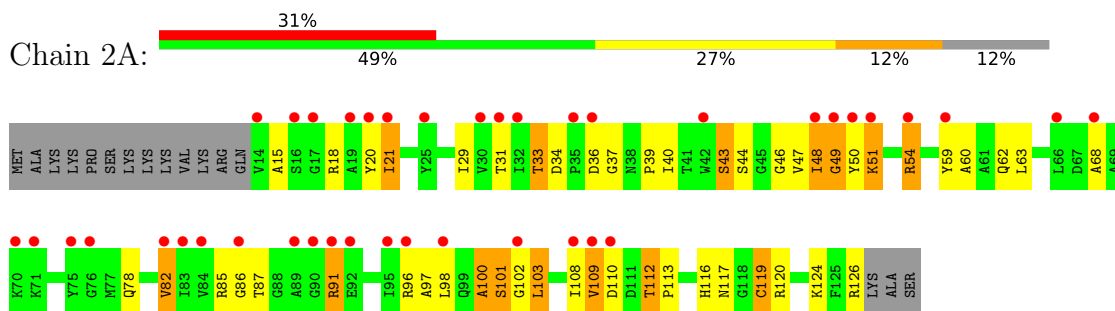
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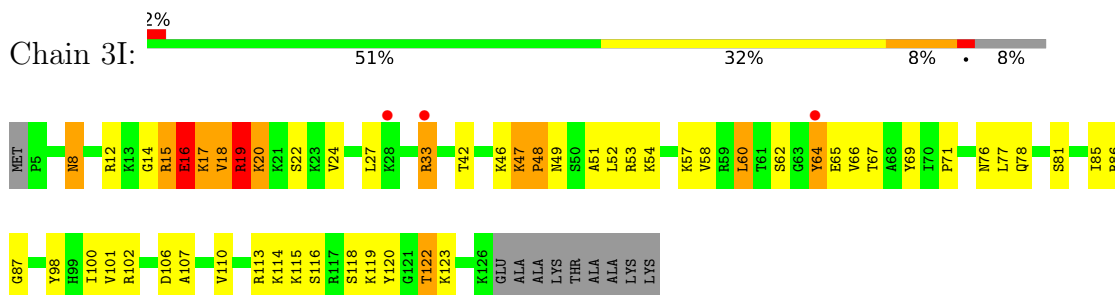
- Molecule 11: 30S ribosomal protein S11



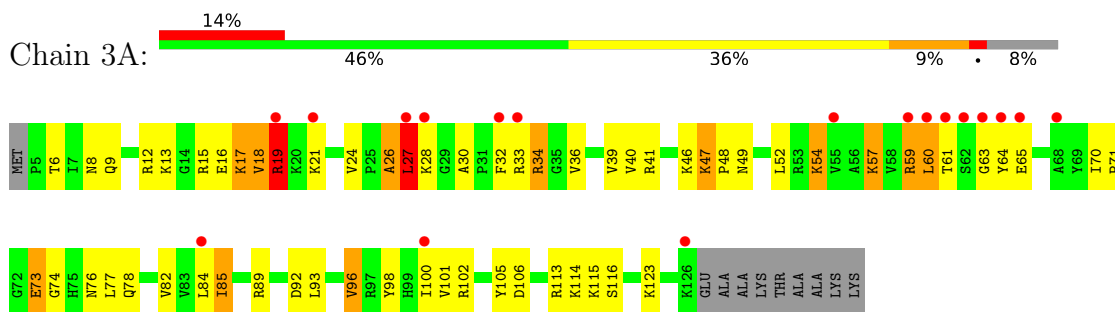
- Molecule 11: 30S ribosomal protein S11



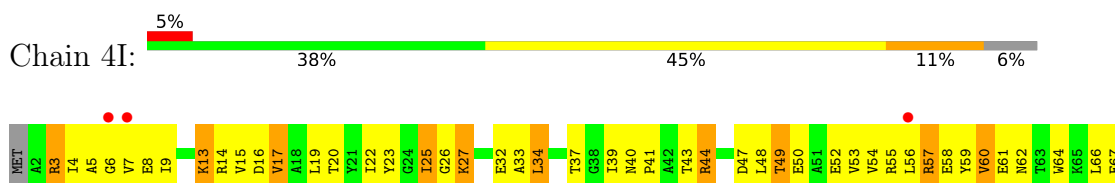
- Molecule 12: 30S ribosomal protein S12

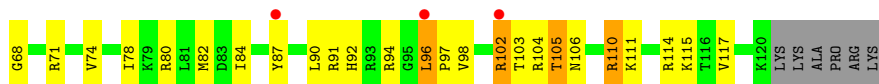


- Molecule 12: 30S ribosomal protein S12



- Molecule 13: 30S ribosomal protein S13

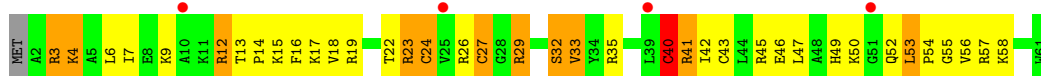




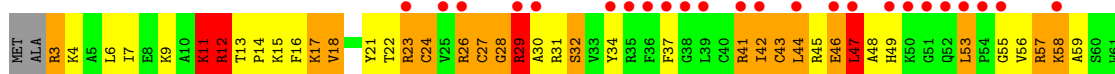
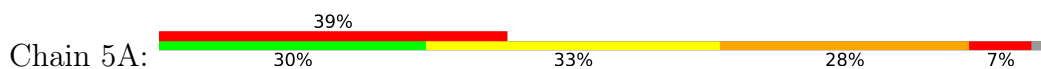
- Molecule 13: 30S ribosomal protein S13



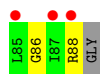
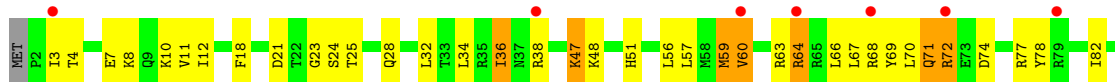
- Molecule 14: 30S ribosomal protein S14 type Z



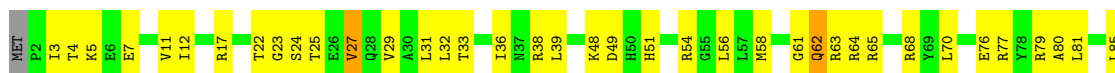
- Molecule 14: 30S ribosomal protein S14 type Z



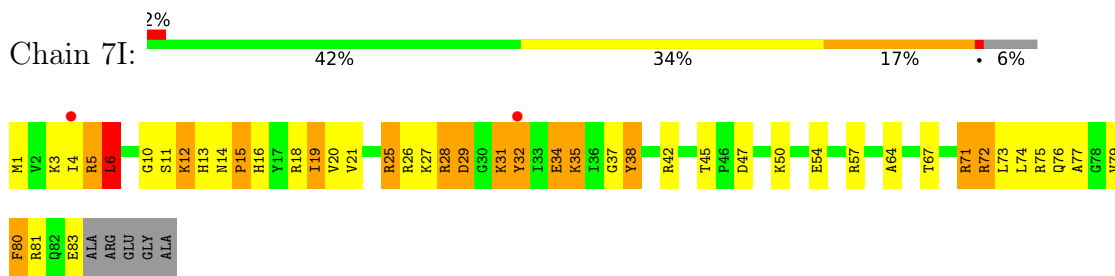
- Molecule 15: 30S ribosomal protein S15



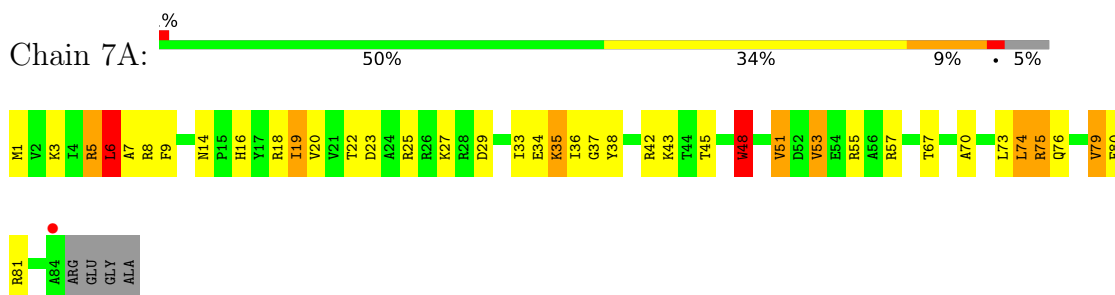
- Molecule 15: 30S ribosomal protein S15



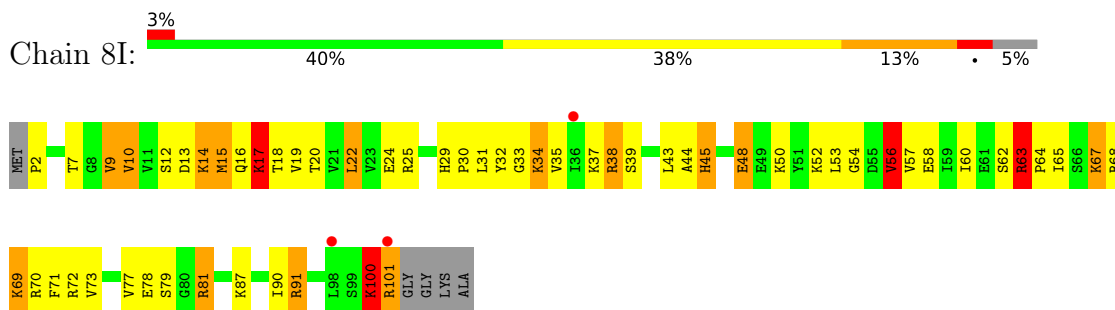
- Molecule 16: 30S ribosomal protein S16



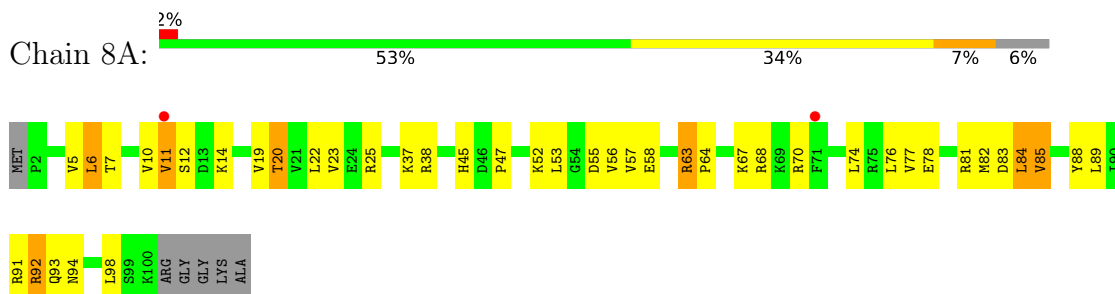
• Molecule 16: 30S ribosomal protein S16



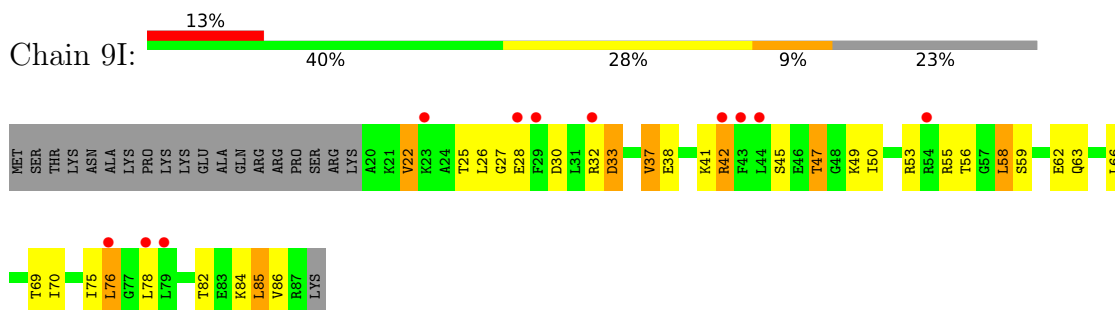
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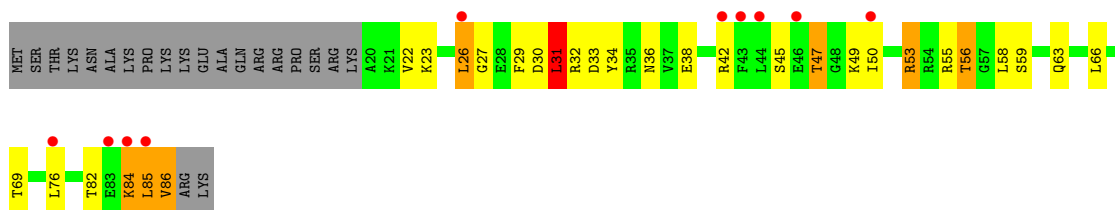
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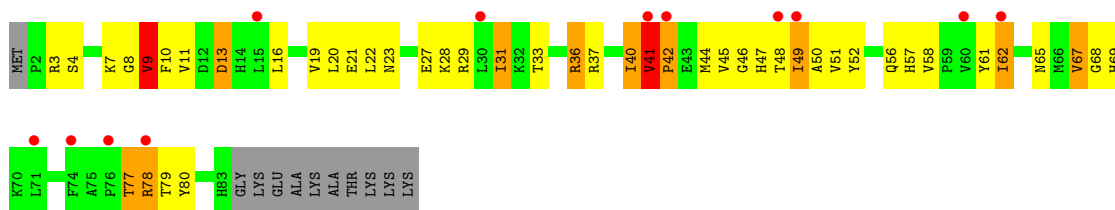
• Molecule 18: 30S ribosomal protein S18



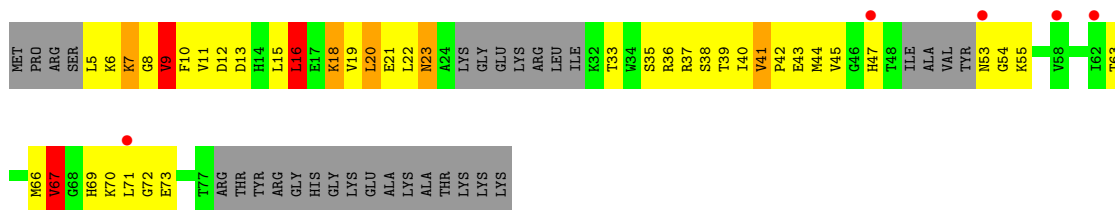
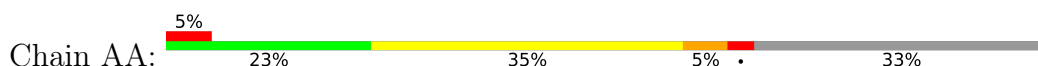
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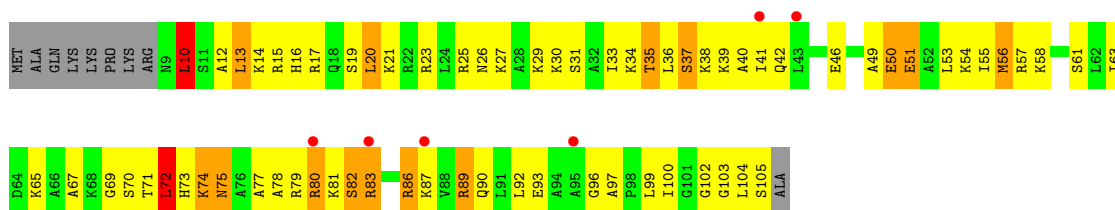
• Molecule 19: 30S ribosomal protein S19



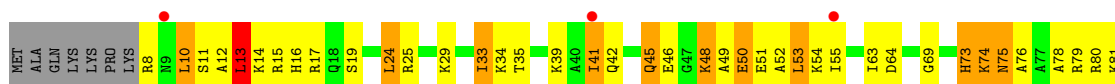
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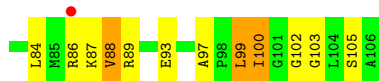


• Molecule 20: 30S ribosomal protein S20



• Molecule 20: 30S ribosomal protein S20

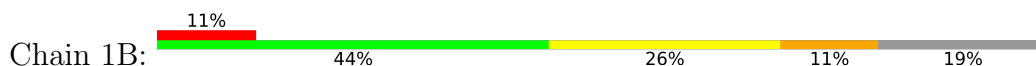




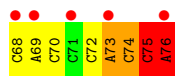
- Molecule 21: 30S ribosomal protein Thx



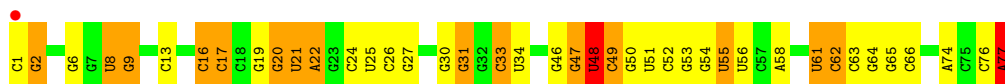
- Molecule 21: 30S ribosomal protein Thx



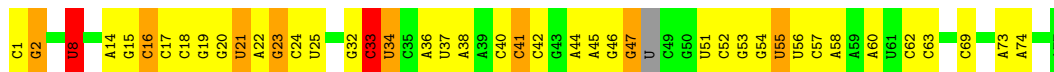
- Molecule 22: tRNAVal



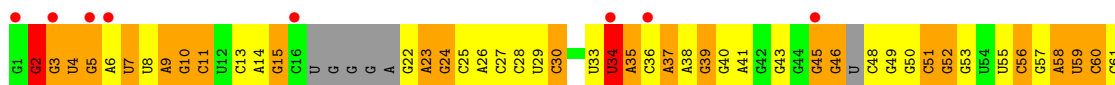
- Molecule 23: tRNAfMet

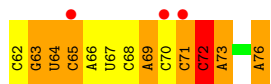


- Molecule 23: tRNAfMet

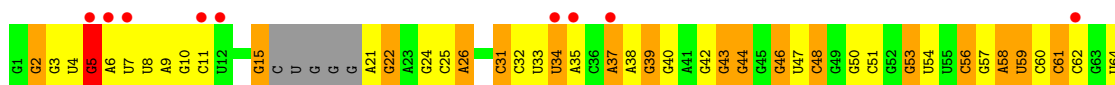
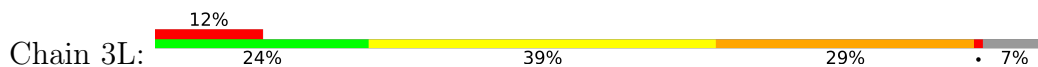


- Molecule 24: tRNAVal

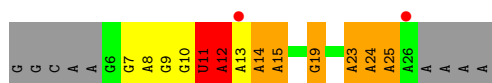
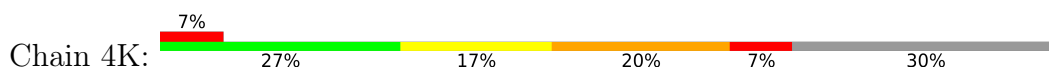




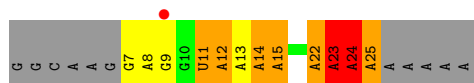
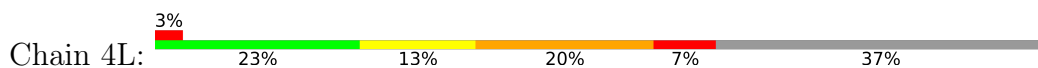
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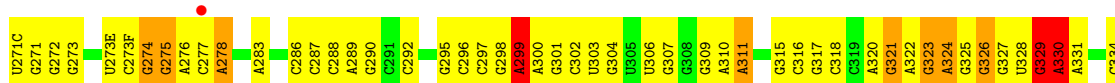
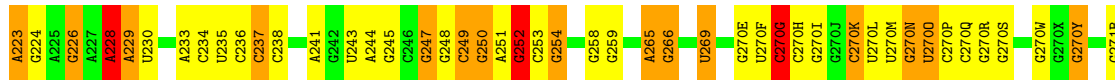
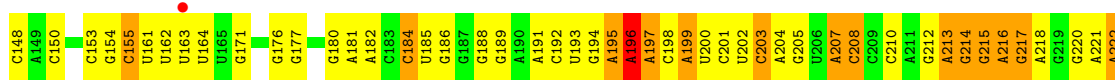
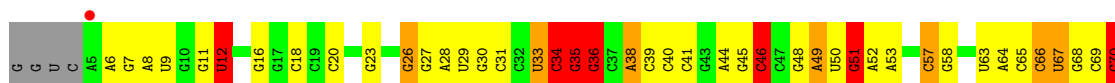
• Molecule 25: mRNA



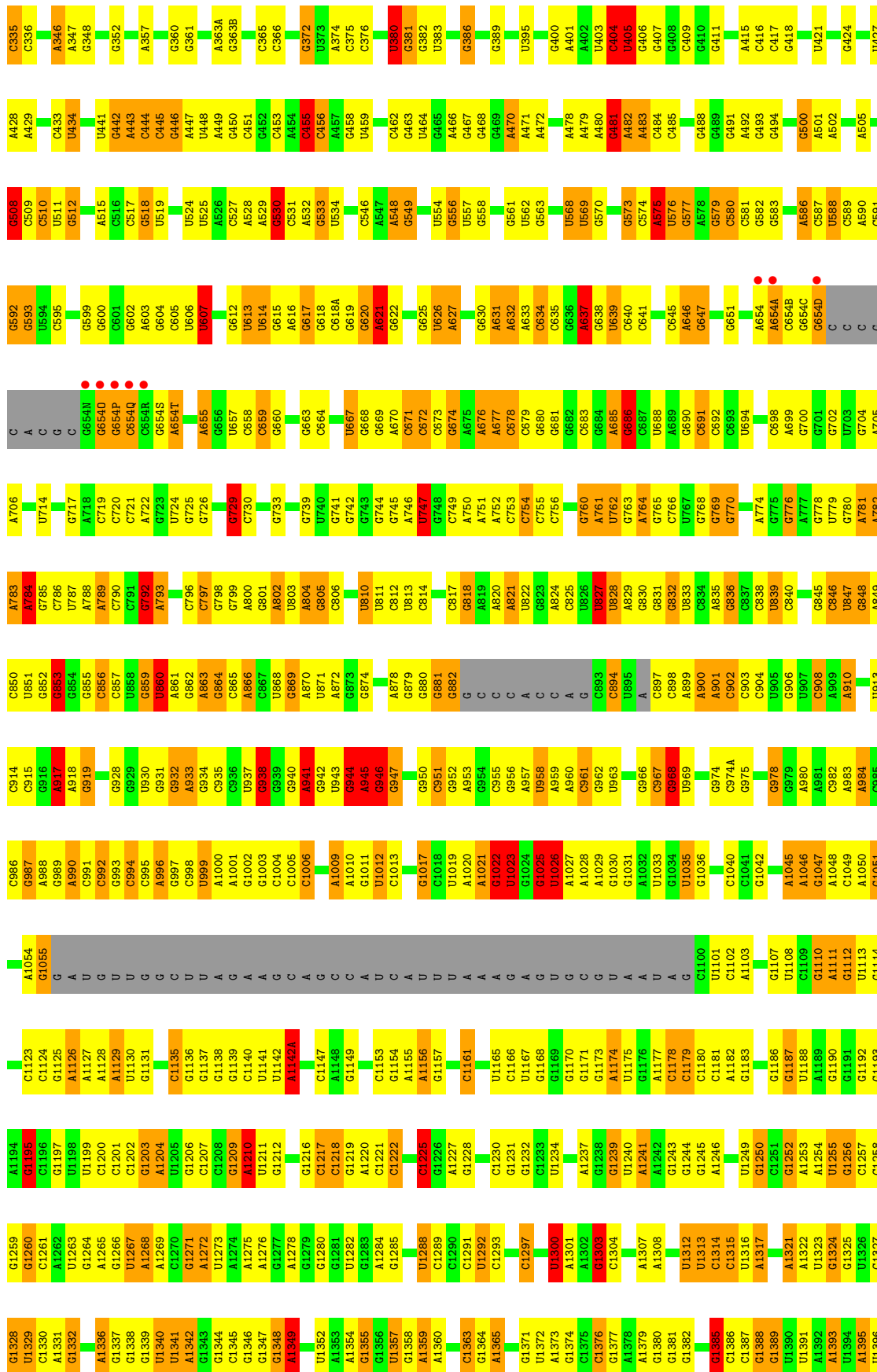
• Molecule 25: mRNA

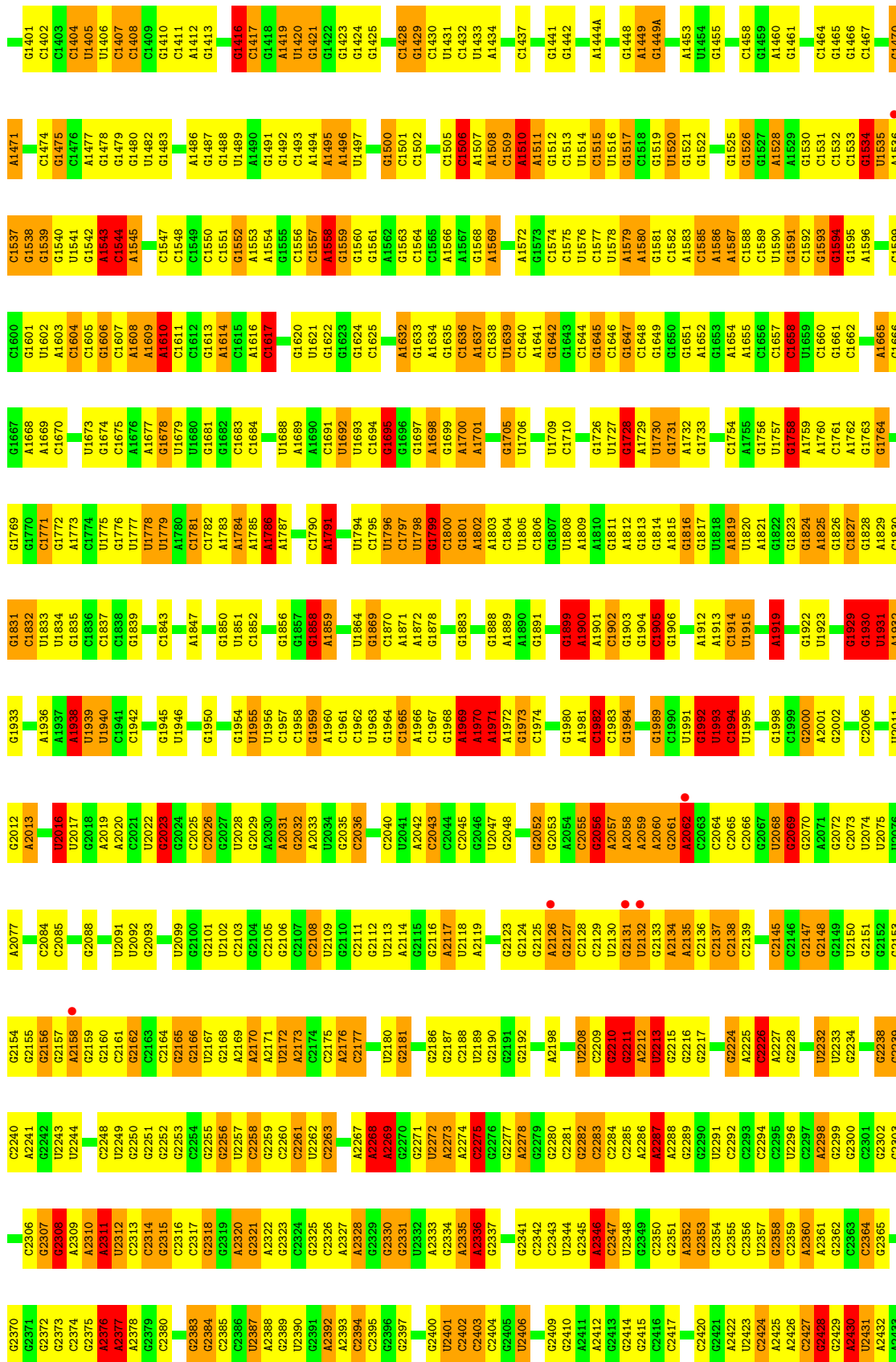


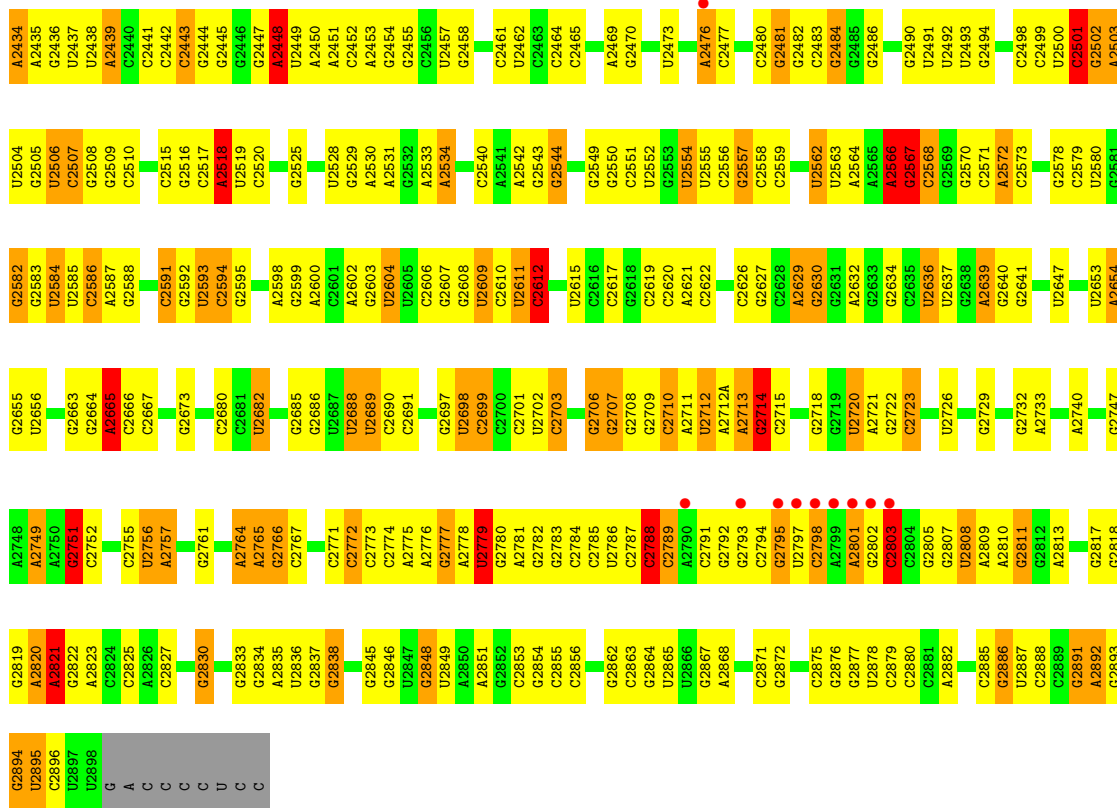
• Molecule 26: 23S ribosomal RNA



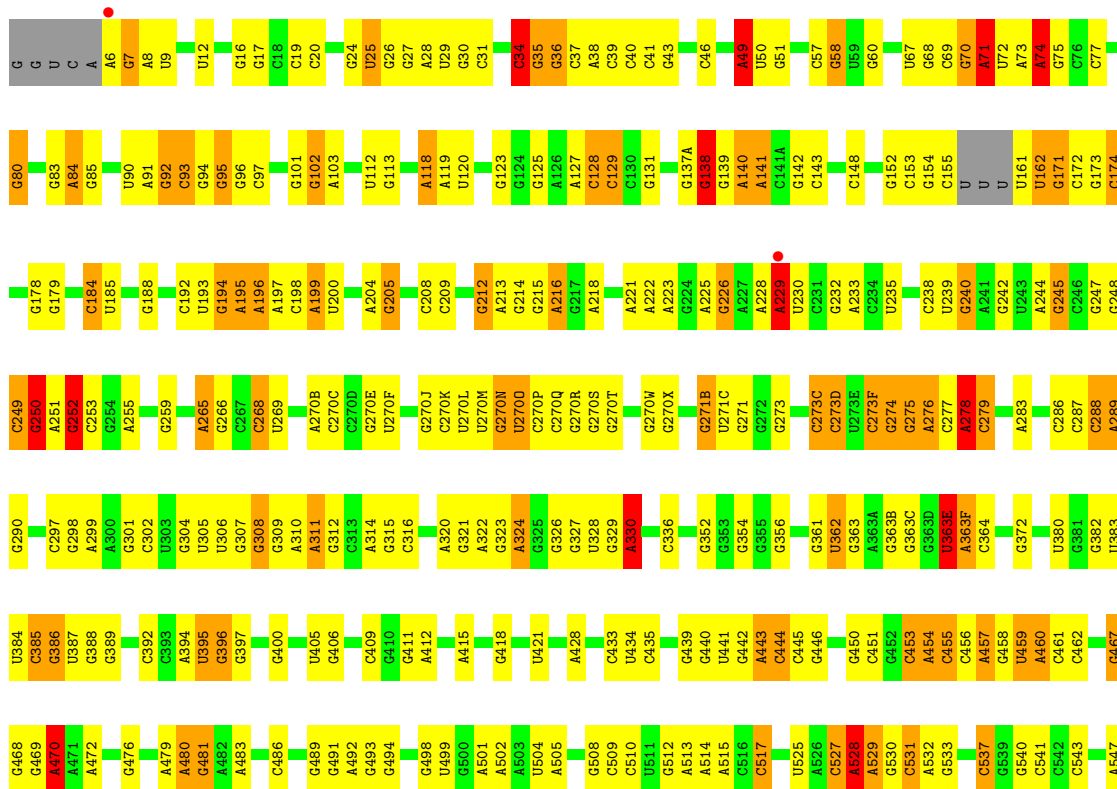






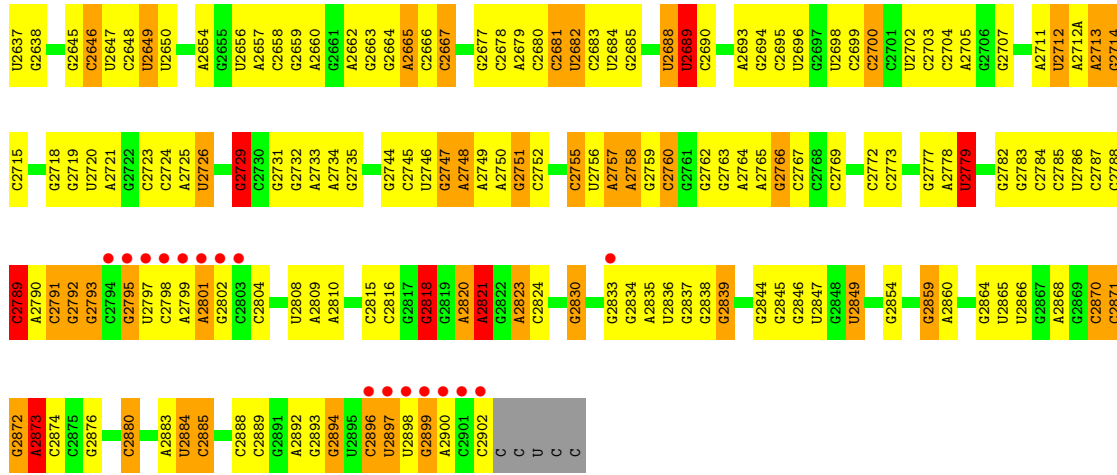


• Molecule 26: 23S ribosomal RNA

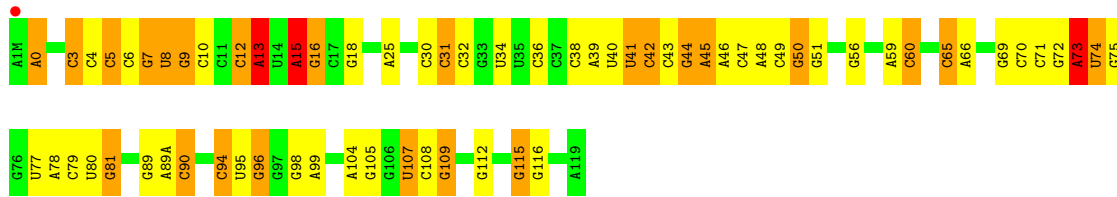


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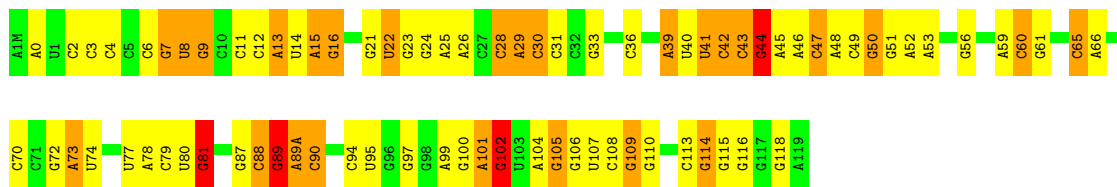
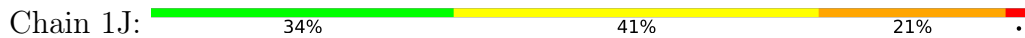
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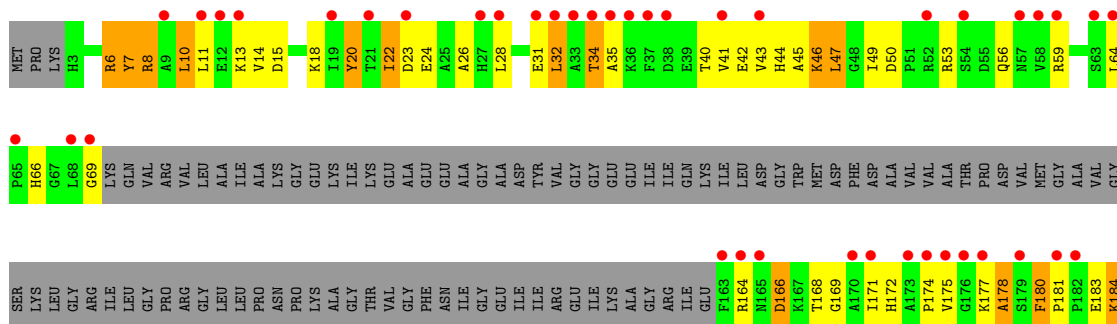
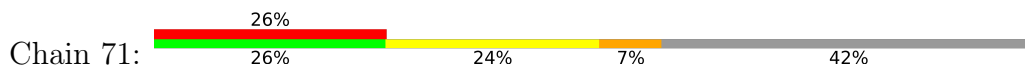
• Molecule 27: 5S ribosomal RNA

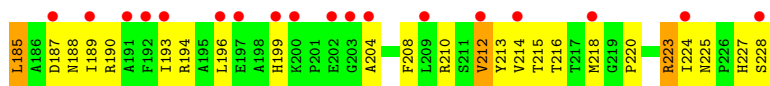


• Molecule 27: 5S ribosomal RNA

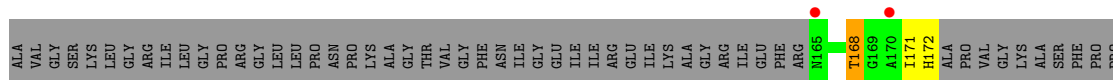
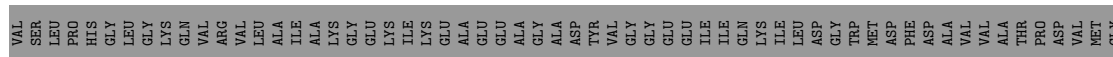
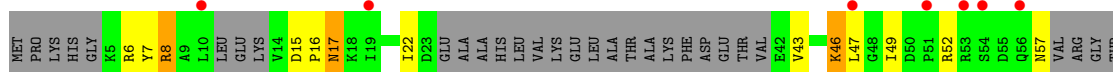


• Molecule 28: 50S ribosomal protein L1

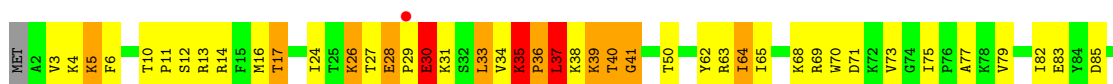




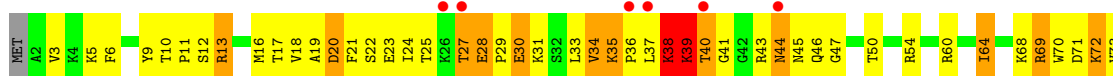
- Molecule 28: 50S ribosomal protein L1



- Molecule 29: 50S ribosomal protein L2

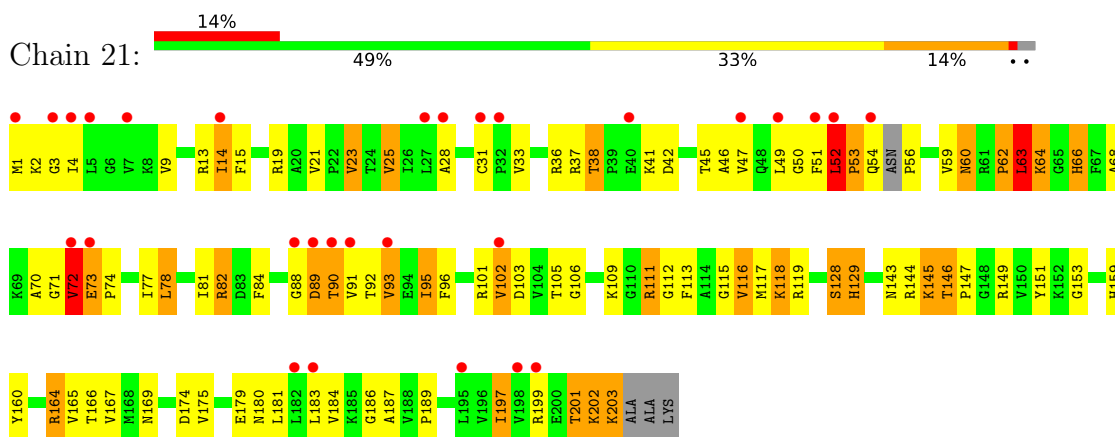


- Molecule 29: 50S ribosomal protein L2

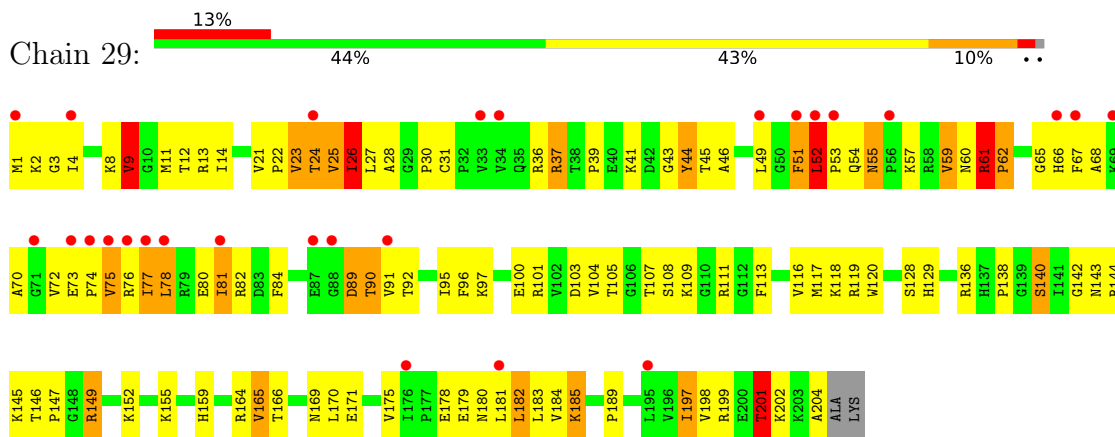


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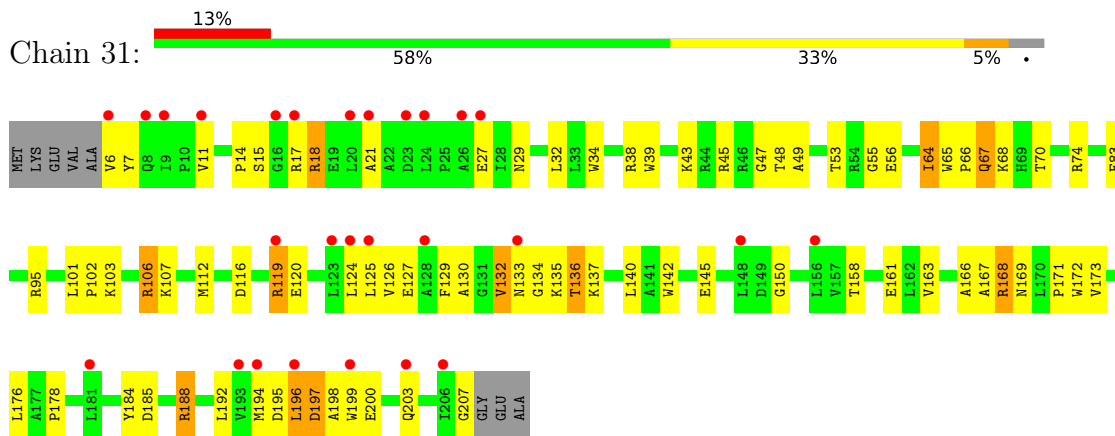
- Molecule 30: 50S ribosomal protein L3



- Molecule 30: 50S ribosomal protein L3



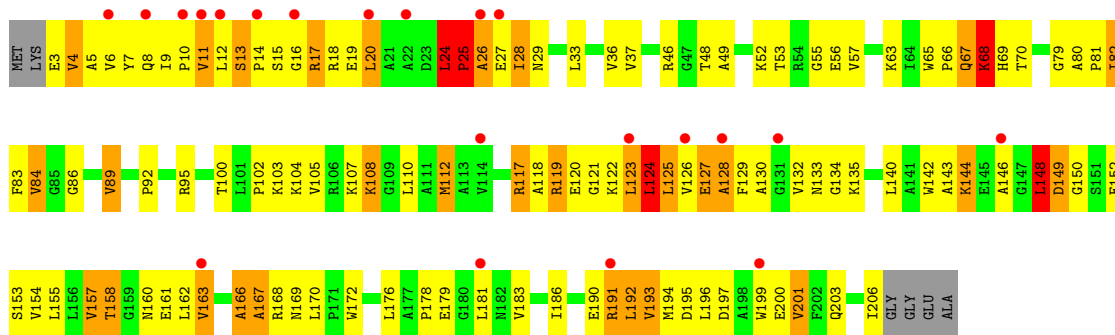
- Molecule 31: 50S ribosomal protein L4



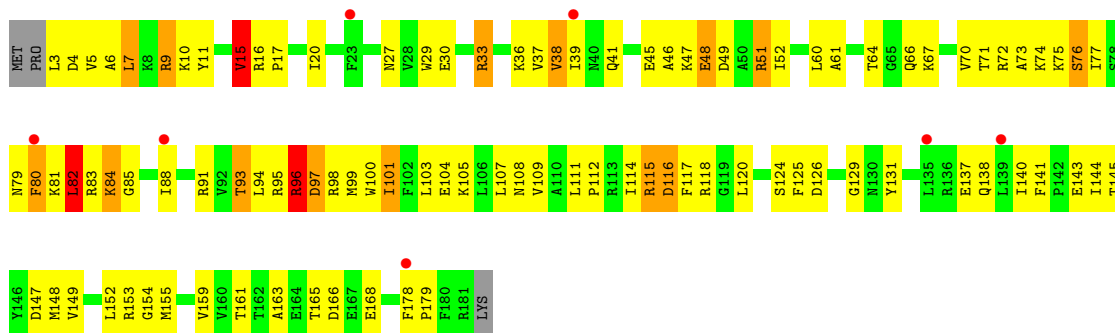
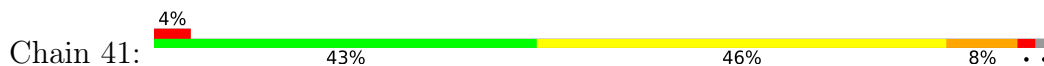
- Molecule 31: 50S ribosomal protein L4



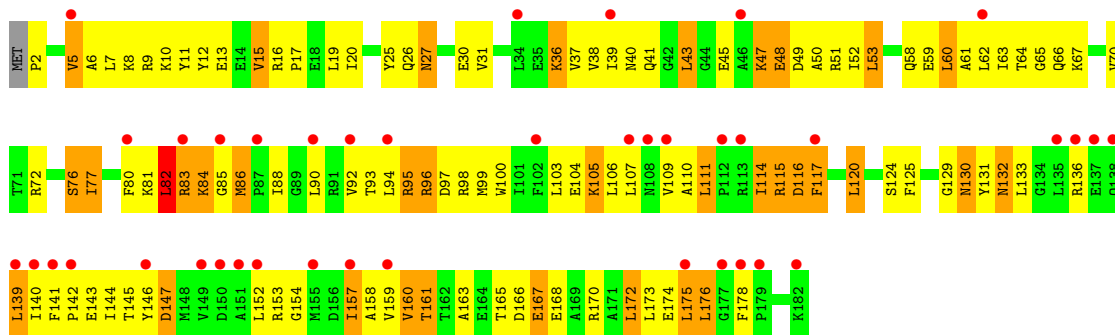




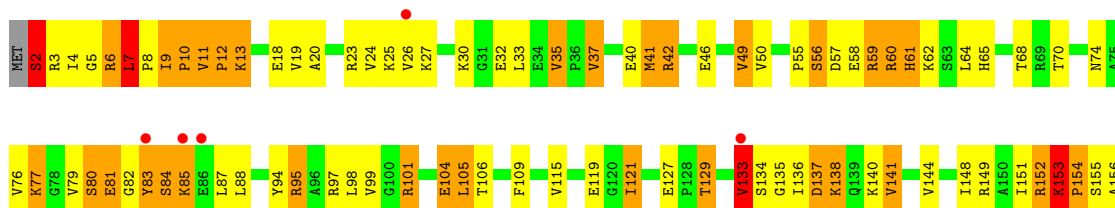
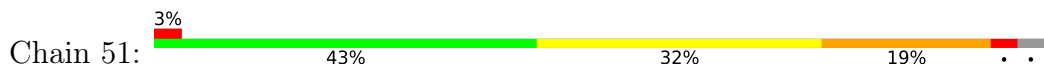
• Molecule 32: 50S ribosomal protein L5

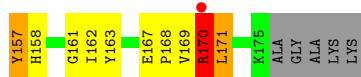


• Molecule 32: 50S ribosomal protein L5

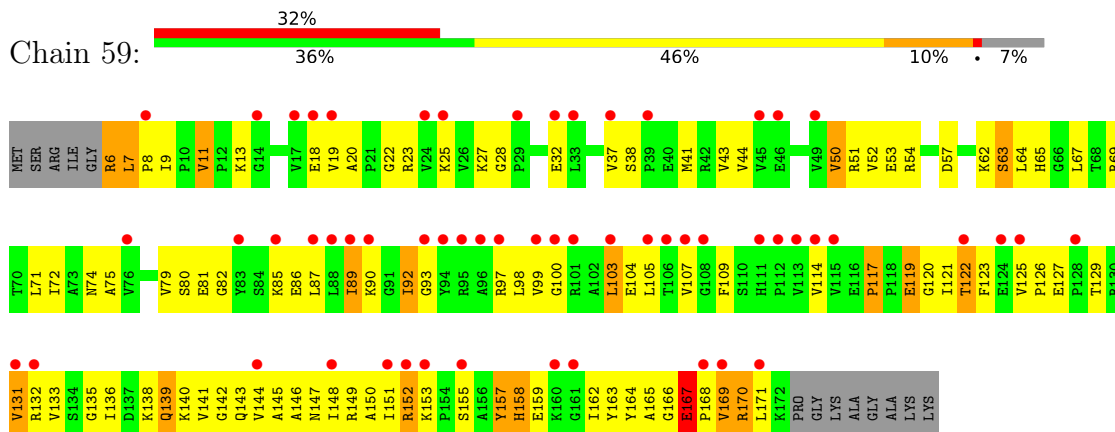


• Molecule 33: 50S ribosomal protein L6

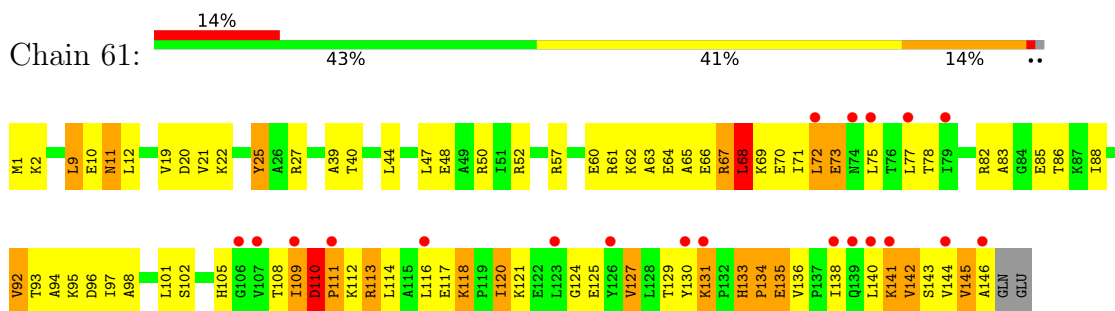




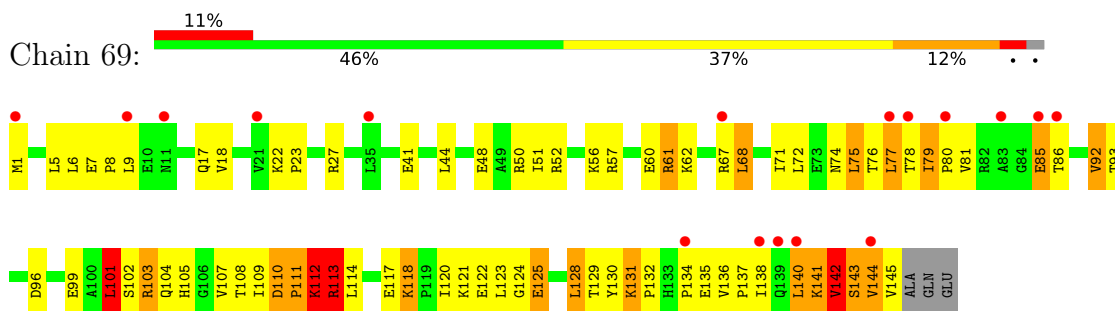
- Molecule 33: 50S ribosomal protein L6



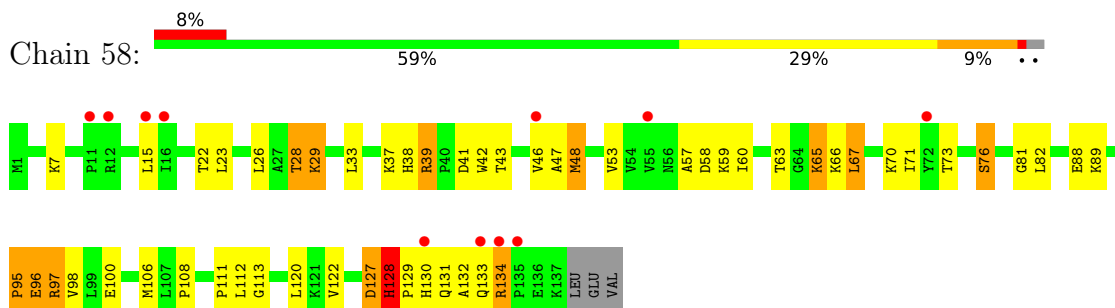
- Molecule 34: 50S ribosomal protein L9



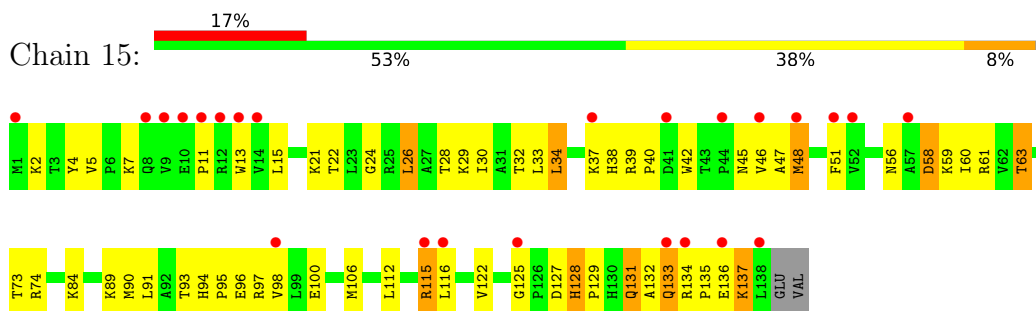
- Molecule 34: 50S ribosomal protein L9



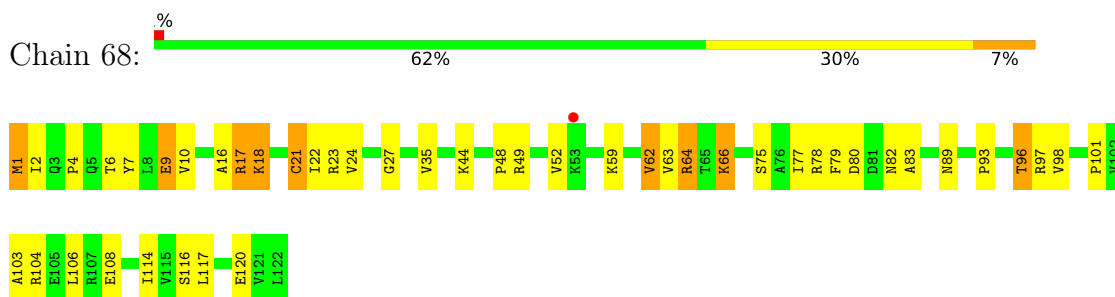
- Molecule 35: 50S ribosomal protein L13



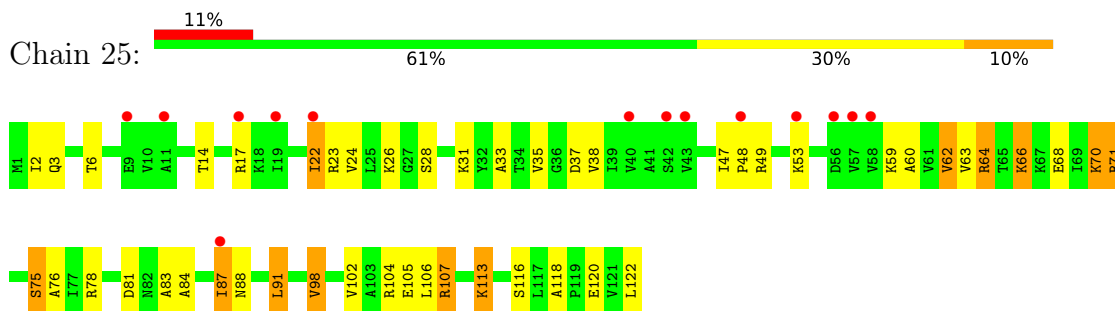
- Molecule 35: 50S ribosomal protein L13



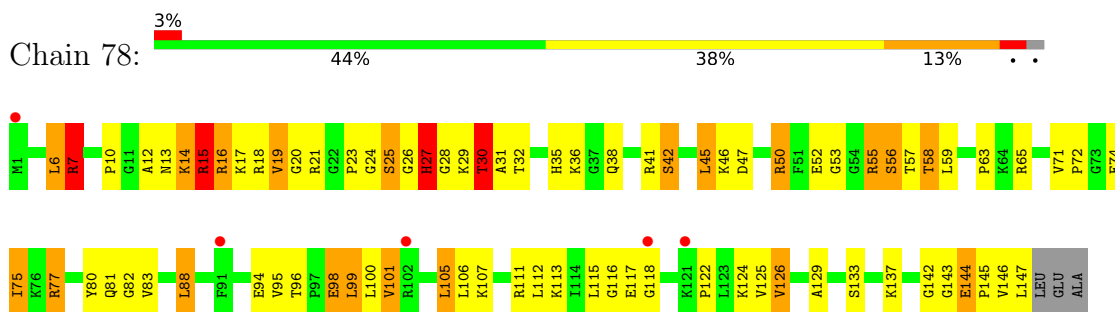
- Molecule 36: 50S ribosomal protein L14



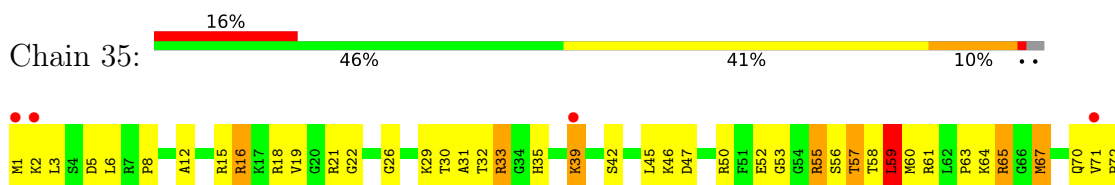
- Molecule 36: 50S ribosomal protein L14

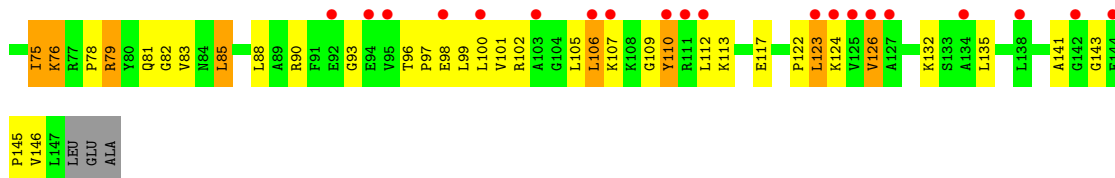


- Molecule 37: 50S ribosomal protein L15

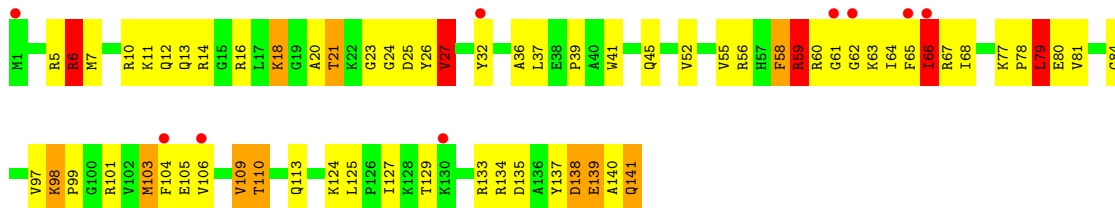


- Molecule 37: 50S ribosomal protein L15

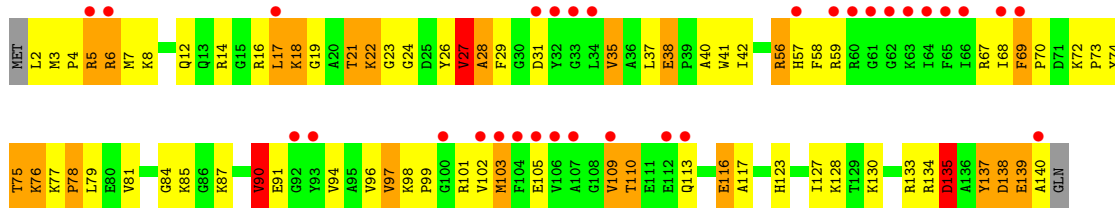




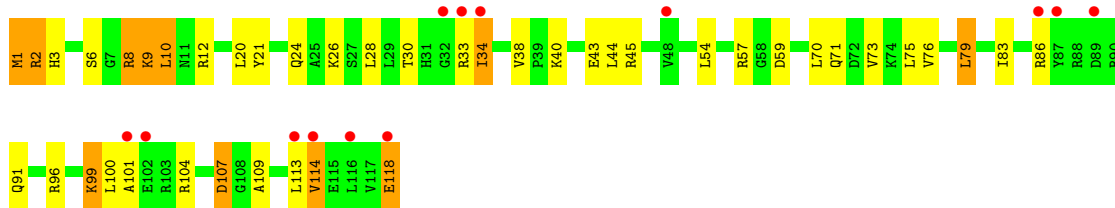
• Molecule 38: 50S ribosomal protein L16



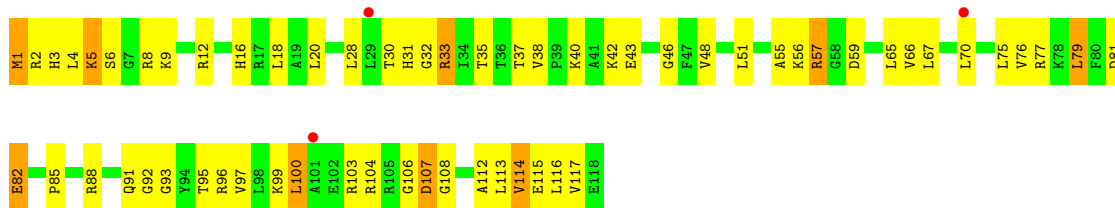
• Molecule 38: 50S ribosomal protein L16



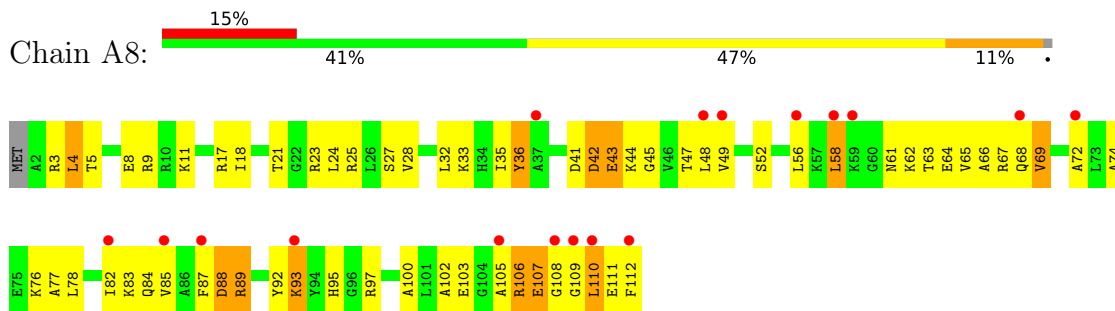
• Molecule 39: 50S ribosomal protein L17



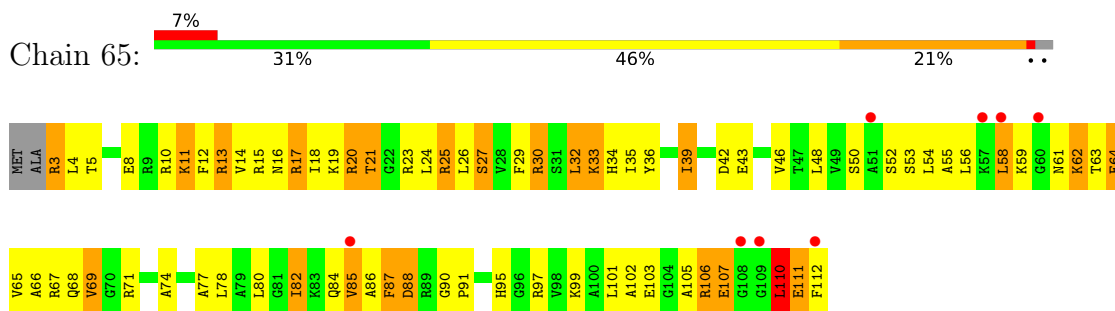
• Molecule 39: 50S ribosomal protein L17



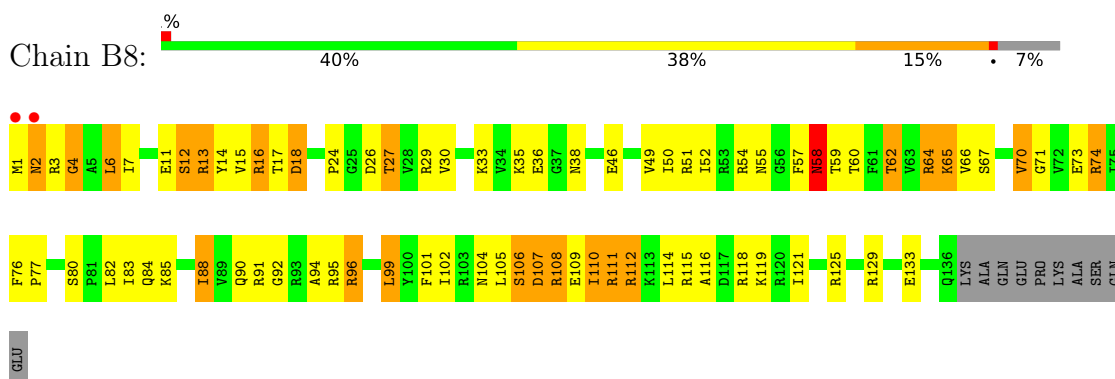
- Molecule 40: 50S ribosomal protein L18



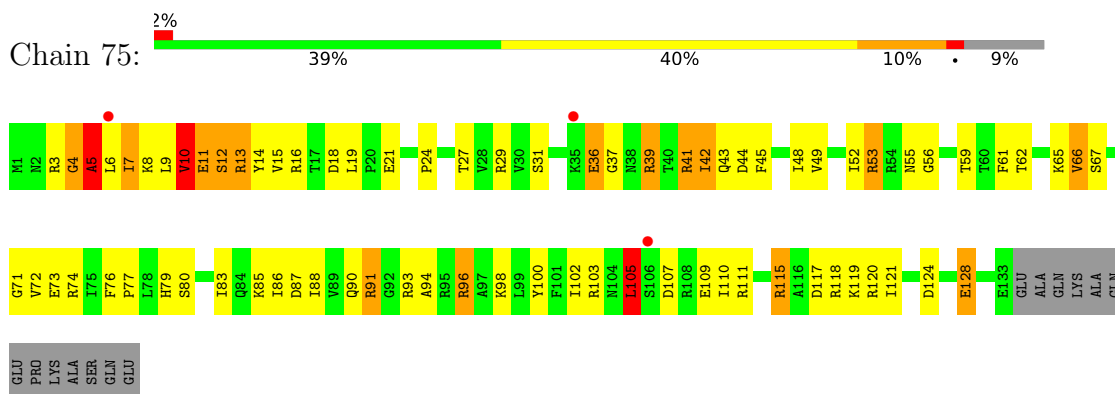
- Molecule 40: 50S ribosomal protein L18



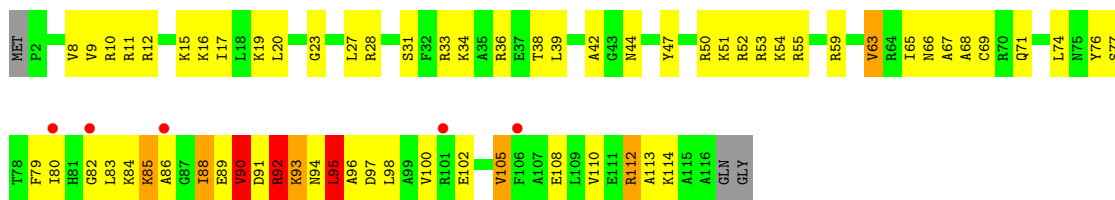
- Molecule 41: 50S ribosomal protein L19



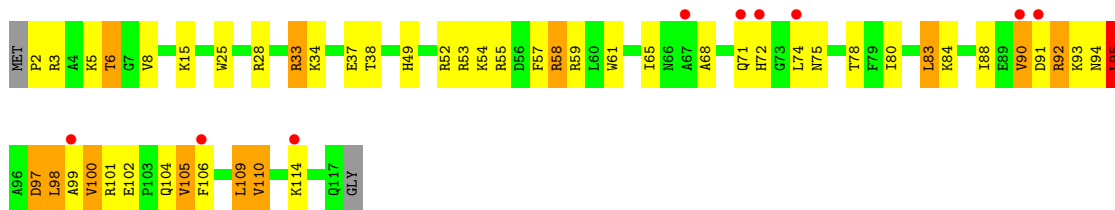
- Molecule 41: 50S ribosomal protein L19



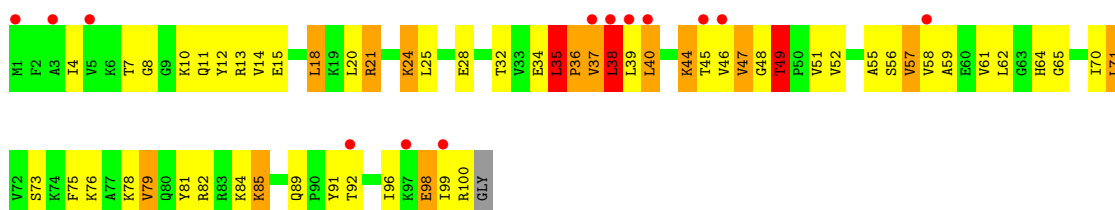
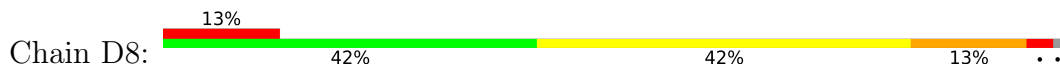
- Molecule 42: 50S ribosomal protein L20



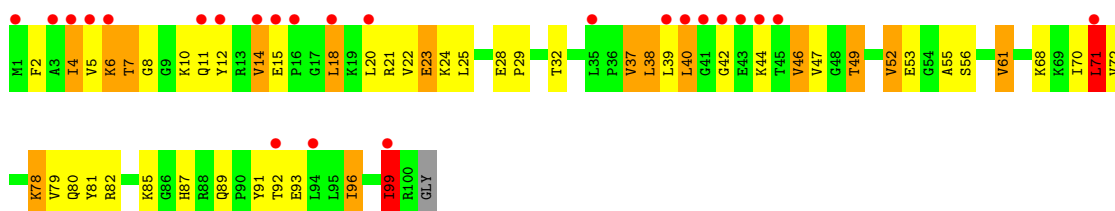
- Molecule 42: 50S ribosomal protein L20



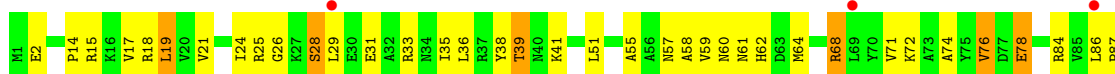
- Molecule 43: 50S ribosomal protein L21

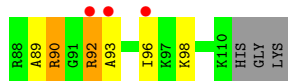


- Molecule 43: 50S ribosomal protein L21



- Molecule 44: 50S ribosomal protein L22

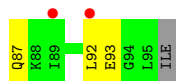
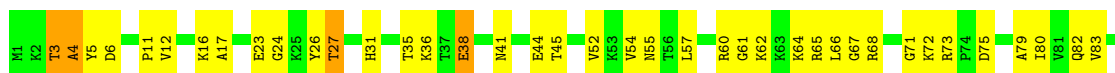




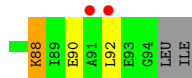
- Molecule 44: 50S ribosomal protein L22



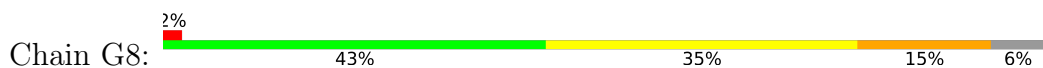
- Molecule 45: 50S ribosomal protein L23



- Molecule 45: 50S ribosomal protein L23

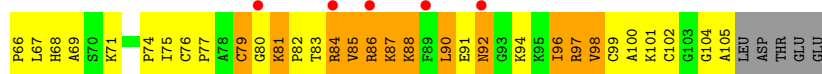


- Molecule 46: 50S ribosomal protein L24

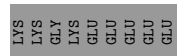
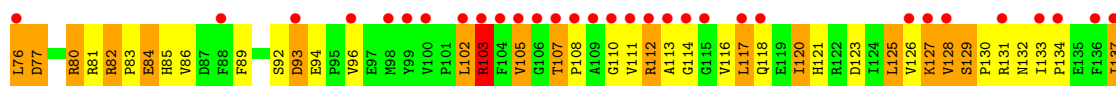
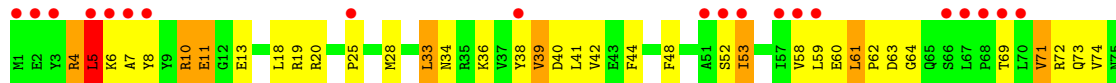


- Molecule 46: 50S ribosomal protein L24

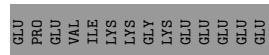
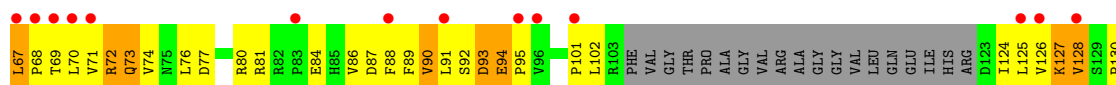
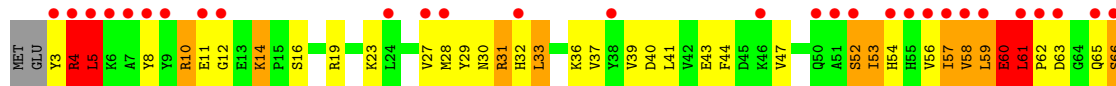
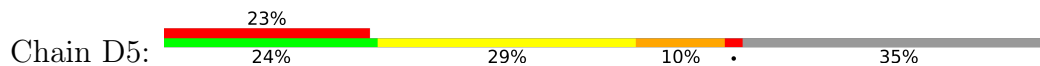




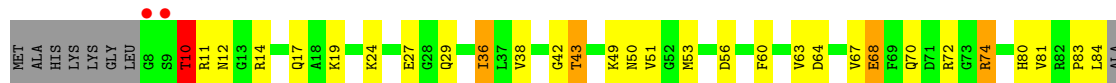
● Molecule 47: 50S ribosomal protein L25



● Molecule 47: 50S ribosomal protein L25

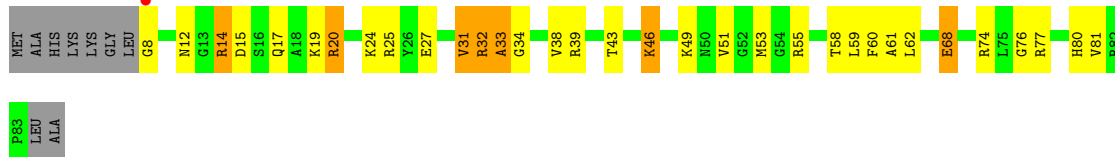


● Molecule 48: 50S ribosomal protein L27

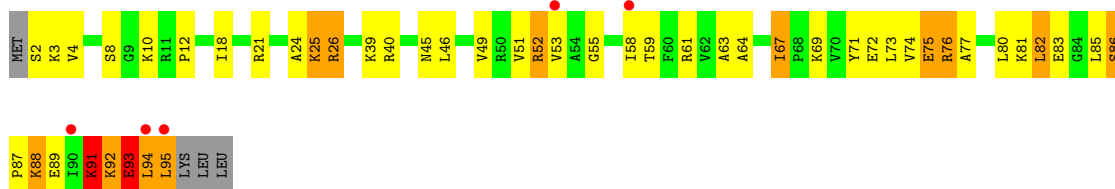


● Molecule 48: 50S ribosomal protein L27

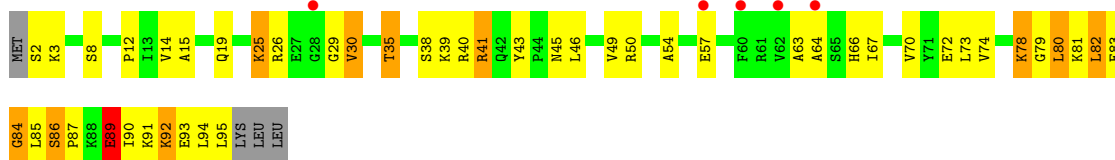




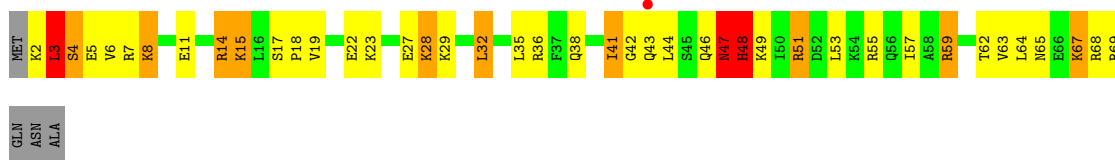
- Molecule 49: 50S ribosomal protein L28



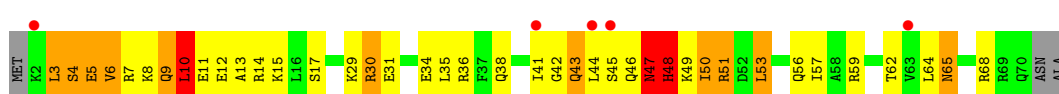
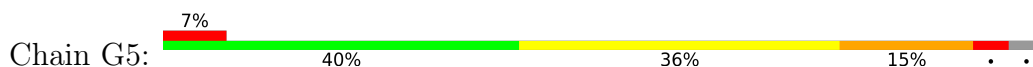
- Molecule 49: 50S ribosomal protein L28



- Molecule 50: 50S ribosomal protein L29



- Molecule 50: 50S ribosomal protein L29



- Molecule 51: 50S ribosomal protein L30

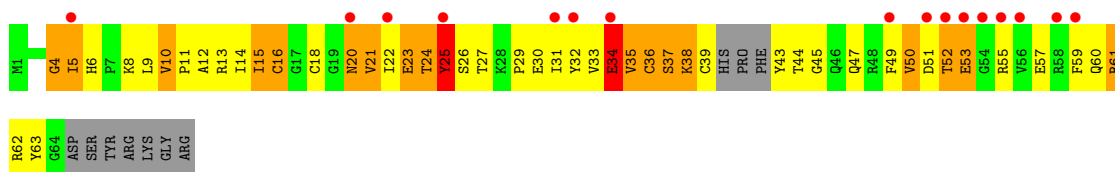
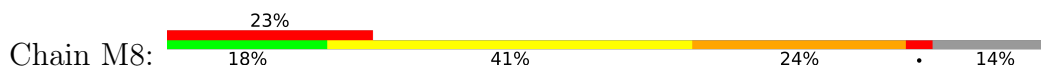




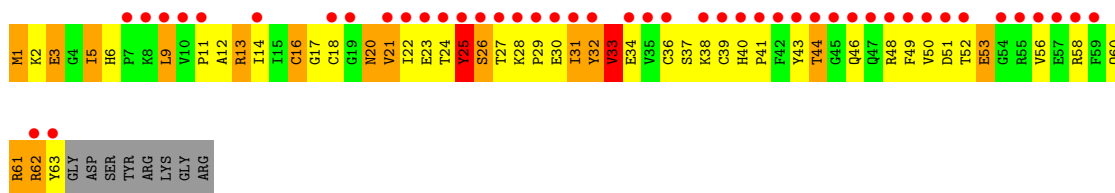
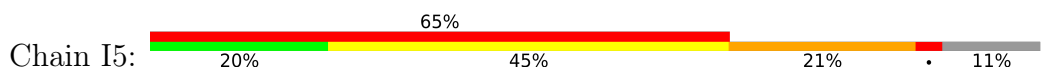
- Molecule 51: 50S ribosomal protein L30



- Molecule 52: 50S ribosomal protein L31



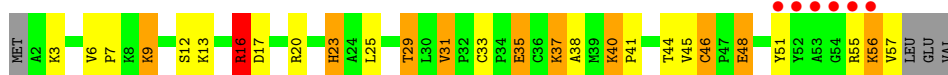
- Molecule 52: 50S ribosomal protein L31



- Molecule 53: 50S ribosomal protein L32



- Molecule 53: 50S ribosomal protein L32

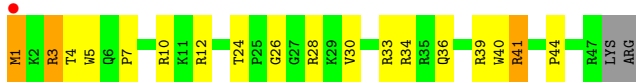


- Molecule 54: 50S ribosomal protein L34





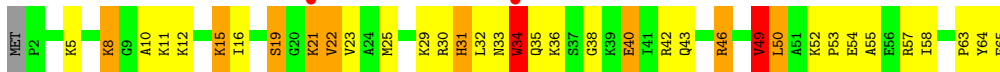
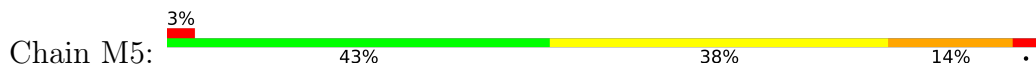
- Molecule 54: 50S ribosomal protein L34



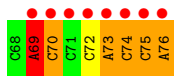
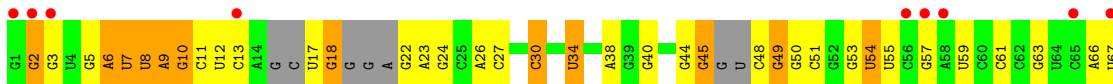
- Molecule 55: 50S ribosomal protein L35



- Molecule 55: 50S ribosomal protein L35



- Molecule 56: tRNAVal



## 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 448.90Å 620.80Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	146.68 – 2.96 146.68 – 2.96	Depositor EDS
% Data completeness (in resolution range)	99.8 (146.68-2.96) 89.3 (146.68-2.96)	Depositor EDS
$R_{merge}$	0.44	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	0.84 (at 2.96Å)	Xtrriage
Refinement program	PHENIX	Depositor
R, $R_{free}$	0.201 , 0.243 0.201 , 0.243	Depositor DCC
$R_{free}$ test set	2000 reflections (0.17%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	75.4	Xtrriage
Anisotropy	0.336	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.28 , 67.4	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	296743	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	97.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.49% of the height of the origin peak. No significant pseudotranslation is detected.*

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

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

## 5 Model quality i

### 5.1 Standard geometry i

Bond lengths and bond angles in the following residue types are not validated in this section: 5MU, H2U, PSU, OMC, CM0, ZN, 4SU, 7MG, MG, 6MZ, SPE, SF4

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	0.67	6/35994 (0.0%)	1.30	243/56171 (0.4%)
1	1G	0.61	1/36236 (0.0%)	1.22	170/56555 (0.3%)
2	12	0.39	0/1727	0.70	1/2326 (0.0%)
2	1E	0.40	0/1936	0.66	1/2611 (0.0%)
3	22	0.62	1/1560 (0.1%)	0.65	1/2104 (0.0%)
3	2E	0.49	1/1629 (0.1%)	0.67	0/2195
4	32	0.45	0/1732	0.65	0/2318
4	3E	0.48	0/1728	0.73	4/2313 (0.2%)
5	42	0.46	0/1155	0.67	1/1555 (0.1%)
5	4E	0.46	0/1158	0.70	1/1559 (0.1%)
6	52	0.47	0/855	0.63	0/1154
6	5E	0.48	0/850	0.64	0/1147
7	62	0.42	0/1132	0.66	1/1514 (0.1%)
7	6E	0.45	0/1259	0.57	0/1686
8	72	0.41	0/1127	0.63	0/1517
8	7E	0.43	0/1135	0.71	1/1527 (0.1%)
9	82	0.41	0/971	0.74	1/1304 (0.1%)
9	8E	0.50	1/1019 (0.1%)	0.76	1/1367 (0.1%)
10	1A	0.74	2/658 (0.3%)	0.68	0/885
10	1I	0.41	0/767	0.72	2/1034 (0.2%)
11	2A	0.46	0/850	0.66	0/1150
11	2I	0.46	0/838	0.67	0/1133
12	3A	0.56	0/972	0.73	1/1301 (0.1%)
12	3I	0.61	0/972	0.79	0/1301
13	4A	0.42	0/903	0.69	1/1211 (0.1%)
13	4I	0.48	0/952	0.73	1/1277 (0.1%)
14	5A	0.46	0/495	0.89	2/657 (0.3%)
14	5I	0.63	2/500 (0.4%)	0.90	3/664 (0.5%)
15	6A	0.47	0/740	0.63	0/987
15	6I	0.47	0/740	0.70	0/987
16	7A	0.45	0/721	0.74	1/970 (0.1%)
16	7I	0.47	0/716	0.76	1/963 (0.1%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
17	8A	0.46	0/836	0.61	0/1117
17	8I	0.55	1/847 (0.1%)	0.77	1/1131 (0.1%)
18	9A	0.51	0/549	0.75	1/732 (0.1%)
18	9I	0.46	0/554	0.69	0/739
19	AA	0.43	0/490	0.75	2/662 (0.3%)
19	AI	0.42	0/676	0.79	1/910 (0.1%)
20	BA	0.40	0/764	0.71	0/1007
20	BI	0.56	1/748 (0.1%)	0.81	2/986 (0.2%)
21	1B	0.44	0/192	0.65	0/252
21	1F	0.44	0/203	0.67	0/266
22	1K	0.64	0/1595	1.19	11/2475 (0.4%)
23	2K	0.77	0/1721	1.38	7/2682 (0.3%)
23	2L	0.67	0/1698	1.28	12/2644 (0.5%)
24	3K	0.54	0/1663	1.20	16/2585 (0.6%)
24	3L	0.56	0/1689	1.16	11/2628 (0.4%)
25	4K	0.72	0/520	1.23	3/808 (0.4%)
25	4L	0.64	0/470	1.23	4/732 (0.5%)
26	14	0.81	39/67798 (0.1%)	1.49	1064/105832 (1.0%)
26	1H	0.95	95/68537 (0.1%)	1.67	1647/106989 (1.5%)
27	16	0.79	0/2928	1.48	37/4568 (0.8%)
27	1J	0.73	0/2928	1.34	23/4568 (0.5%)
28	71	0.32	0/1055	0.62	0/1425
28	79	0.31	0/459	0.58	0/608
29	11	0.68	1/2170 (0.0%)	0.94	6/2926 (0.2%)
29	19	0.61	0/2175	0.86	2/2933 (0.1%)
30	21	0.58	0/1537	0.92	3/2081 (0.1%)
30	29	0.53	0/1596	0.85	1/2153 (0.0%)
31	31	0.58	0/1620	0.78	2/2194 (0.1%)
31	39	0.54	1/1637 (0.1%)	0.84	2/2218 (0.1%)
32	41	0.51	1/1481 (0.1%)	0.71	1/1994 (0.1%)
32	49	0.42	0/1492	0.72	3/2008 (0.1%)
33	51	0.54	0/1354	0.95	5/1833 (0.3%)
33	59	0.36	0/1308	0.67	2/1771 (0.1%)
34	61	0.46	0/1151	0.80	4/1558 (0.3%)
34	69	0.45	0/1146	0.75	2/1551 (0.1%)
35	15	0.47	1/1131 (0.1%)	0.72	0/1525
35	58	0.52	0/1123	0.74	1/1514 (0.1%)
36	25	0.51	0/942	0.70	0/1269
36	68	0.54	0/942	0.74	0/1269
37	35	0.55	0/1139	0.90	3/1514 (0.2%)
37	78	0.64	0/1139	1.03	6/1514 (0.4%)
38	45	0.65	2/1125 (0.2%)	0.83	1/1505 (0.1%)
38	88	0.71	0/1138	0.92	2/1523 (0.1%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
39	55	0.50	0/981	0.78	1/1312 (0.1%)
39	98	0.51	0/981	0.78	0/1312
40	65	0.52	0/886	0.83	0/1180
40	A8	0.56	0/891	0.78	0/1187
41	75	0.53	0/1123	0.83	4/1500 (0.3%)
41	B8	0.52	0/1138	0.82	1/1521 (0.1%)
42	85	0.52	0/977	0.73	0/1301
42	C8	0.57	0/968	0.85	4/1289 (0.3%)
43	95	0.49	0/781	0.81	1/1048 (0.1%)
43	D8	0.54	0/785	0.86	2/1052 (0.2%)
44	A5	0.54	0/897	0.76	1/1204 (0.1%)
44	E8	0.58	0/886	0.81	1/1189 (0.1%)
45	B5	0.53	0/749	0.72	1/1007 (0.1%)
45	F8	0.59	0/757	0.77	1/1017 (0.1%)
46	C5	0.54	0/807	0.89	0/1076
46	G8	0.64	0/790	0.93	3/1055 (0.3%)
47	D5	0.50	2/1103 (0.2%)	0.80	2/1494 (0.1%)
47	H8	0.48	0/1395	0.77	2/1890 (0.1%)
48	E5	0.62	0/611	0.83	0/814
48	I8	0.60	0/619	0.84	1/825 (0.1%)
49	F5	0.57	0/744	0.94	4/989 (0.4%)
49	J8	0.61	0/744	0.89	1/989 (0.1%)
50	G5	0.51	0/578	0.81	1/766 (0.1%)
50	K8	0.65	0/577	0.88	1/763 (0.1%)
51	H5	0.49	0/464	0.66	0/623
51	L8	0.49	0/464	0.73	0/623
52	I5	0.41	0/527	0.84	0/709
52	M8	0.54	0/486	0.87	2/652 (0.3%)
53	J5	0.51	0/448	0.83	1/606 (0.2%)
53	N8	0.58	0/451	0.75	0/610
54	L5	0.61	0/409	0.75	0/540
54	P8	0.78	0/409	0.96	3/540 (0.6%)
55	M5	0.61	1/524 (0.2%)	0.91	1/691 (0.1%)
55	Q8	0.67	0/524	0.96	2/691 (0.3%)
56	1L	0.53	0/1592	1.05	1/2472 (0.0%)
All	All	0.73	159/317359 (0.1%)	1.32	3368/475179 (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	5
2	1E	0	3
3	22	0	1
3	2E	0	1
4	32	0	2
4	3E	0	2
7	6E	0	1
8	72	0	2
8	7E	0	1
9	82	0	1
9	8E	0	2
10	1I	0	2
11	2A	0	2
12	3I	0	6
13	4A	0	4
13	4I	0	2
14	5A	0	5
14	5I	0	1
16	7I	0	1
17	8I	0	1
18	9I	0	1
19	AA	0	1
19	AI	0	1
20	BA	0	2
28	71	0	1
29	11	0	3
29	19	0	4
30	21	0	5
30	29	0	3
31	31	0	1
31	39	0	9
32	41	0	3
32	49	0	3
33	51	0	7
33	59	0	2
34	61	0	3
34	69	0	5
35	58	0	1
36	68	0	1
37	35	0	5
37	78	0	4
38	45	0	3
38	88	0	4

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Mol	Chain	#Chirality outliers	#Planarity outliers
39	55	0	1
39	98	0	2
40	65	0	1
40	A8	0	3
41	75	0	3
41	B8	0	4
42	85	0	4
42	C8	0	3
43	95	0	3
43	D8	0	3
44	A5	0	1
45	B5	0	1
45	F8	0	1
46	C5	0	2
46	G8	0	4
47	D5	0	3
47	H8	0	3
49	F5	0	2
49	J8	0	4
50	G5	0	2
50	K8	0	2
52	I5	0	3
52	M8	0	4
54	P8	0	1
55	M5	0	1
55	Q8	0	2
All	All	0	180

The worst 5 of 159 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	22	173	VAL	C-N	19.50	1.71	1.34
10	1A	38	ILE	C-N	14.98	1.62	1.34
26	1H	1698	A	N9-C4	-11.67	1.30	1.37
26	1H	783	A	N3-C4	-10.65	1.28	1.34
20	BI	97	ALA	C-N	10.36	1.53	1.34

The worst 5 of 3368 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	1H	1899	G	N3-C4-N9	-25.58	110.65	126.00
26	1H	945	A	N1-C6-N6	24.24	133.14	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	1H	945	A	C6-C5-N7	-23.79	115.65	132.30
26	1H	945	A	C5-N7-C8	-20.19	93.80	103.90
26	1H	1899	G	N3-C4-C5	19.48	138.34	128.60

There are no chirality outliers.

5 of 180 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	1E	15	VAL	Peptide
2	1E	236	TYR	Peptide
2	1E	95	GLN	Peptide
3	2E	78	GLY	Peptide
4	3E	154	ASN	Peptide

## 5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	13	32157	0	16234	739	0
1	1G	32371	0	16342	719	0
2	12	1696	0	1730	124	0
2	1E	1902	0	1949	157	0
3	22	1537	0	1603	116	0
3	2E	1605	0	1668	76	0
4	32	1702	0	1764	95	0
4	3E	1698	0	1760	125	0
5	42	1139	0	1202	85	0
5	4E	1142	0	1204	68	0
6	52	842	0	857	26	0
6	5E	837	0	852	39	0
7	62	1120	0	1167	82	0
7	6E	1242	0	1286	80	0
8	72	1107	0	1165	65	0
8	7E	1115	0	1177	92	0
9	82	953	0	983	106	0
9	8E	1000	0	1031	100	0
10	1A	646	0	662	81	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
10	1I	754	0	769	44	0
11	2A	835	0	847	42	0
11	2I	823	0	832	33	0
12	3A	956	0	1046	64	0
12	3I	956	0	1046	39	0
13	4A	893	0	946	72	0
13	4I	942	0	997	76	0
14	5A	486	0	525	65	0
14	5I	491	0	532	49	0
15	6A	729	0	768	33	0
15	6I	729	0	768	38	0
16	7A	705	0	725	58	0
16	7I	700	0	720	77	0
17	8A	823	0	891	32	0
17	8I	834	0	904	84	0
18	9A	544	0	605	26	0
18	9I	549	0	607	33	0
19	AA	481	0	468	39	0
19	AI	661	0	683	55	0
20	BA	762	0	861	44	0
20	BI	746	0	843	98	0
21	1B	188	0	195	12	0
21	1F	199	0	208	19	0
22	1K	1540	0	787	25	0
23	2K	1646	0	843	25	0
23	2L	1626	0	836	27	0
24	3K	1491	0	761	59	0
24	3L	1513	0	770	34	0
25	4K	462	0	230	11	0
25	4L	417	0	207	12	0
26	14	60535	0	30516	1082	0
26	1H	61195	0	30847	1152	0
27	16	2617	0	1328	54	0
27	1J	2617	0	1328	88	0
28	71	1033	0	1048	71	0
28	79	456	0	460	21	0
29	11	2120	0	2197	112	0
29	19	2125	0	2199	96	0
30	21	1505	0	1526	85	0
30	29	1563	0	1629	139	0
31	31	1585	0	1632	61	0
31	39	1602	0	1649	118	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
32	41	1457	0	1514	101	0
32	49	1468	0	1520	112	0
33	51	1328	0	1396	108	0
33	59	1283	0	1352	87	0
34	61	1136	0	1223	75	0
34	69	1131	0	1218	60	0
35	15	1104	0	1180	56	0
35	58	1096	0	1169	52	0
36	25	932	0	996	42	0
36	68	932	0	996	40	0
37	35	1122	0	1206	76	0
37	78	1122	0	1206	84	0
38	45	1104	0	1159	88	0
38	88	1117	0	1168	67	0
39	55	967	0	1033	45	0
39	98	967	0	1033	33	0
40	65	876	0	938	99	0
40	A8	881	0	943	58	0
41	75	1109	0	1170	74	0
41	B8	1124	0	1179	78	0
42	85	959	0	1019	59	0
42	C8	950	0	1011	85	0
43	95	770	0	838	48	0
43	D8	774	0	849	58	0
44	A5	886	0	948	38	0
44	E8	876	0	941	43	0
45	B5	735	0	785	37	0
45	F8	743	0	794	30	0
46	C5	794	0	886	81	0
46	G8	777	0	857	42	0
47	D5	1079	0	1088	86	0
47	H8	1365	0	1391	106	0
48	E5	603	0	620	36	0
48	I8	611	0	631	24	0
49	F5	737	0	813	44	0
49	J8	737	0	813	58	0
50	G5	576	0	625	33	0
50	K8	575	0	634	42	0
51	H5	459	0	512	41	0
51	L8	459	0	512	18	0
52	I5	515	0	514	46	0
52	M8	479	0	475	53	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
53	J5	434	0	454	25	0
53	N8	437	0	460	21	0
54	L5	401	0	436	15	0
54	P8	401	0	436	9	0
55	M5	516	0	582	32	0
55	Q8	516	0	582	32	0
56	1L	1469	0	752	37	0
57	11	2	0	0	0	0
57	13	148	0	0	0	0
57	14	445	0	0	0	0
57	16	11	0	0	0	0
57	19	1	0	0	0	0
57	1G	133	0	0	0	0
57	1H	548	0	0	0	0
57	1J	7	0	0	0	0
57	21	2	0	0	0	0
57	25	2	0	0	0	0
57	29	2	0	0	0	0
57	2K	4	0	0	0	0
57	2L	3	0	0	0	0
57	31	2	0	0	0	0
57	35	2	0	0	0	0
57	39	2	0	0	0	0
57	3A	1	0	0	0	0
57	3I	1	0	0	0	0
57	41	1	0	0	0	0
57	42	1	0	0	0	0
57	45	1	0	0	0	0
57	4A	1	0	0	0	0
57	4E	1	0	0	0	0
57	4K	2	0	0	0	0
57	4L	2	0	0	0	0
57	5E	1	0	0	0	0
57	5I	1	0	0	0	0
57	68	2	0	0	0	0
57	78	1	0	0	0	0
57	88	3	0	0	0	0
57	9A	1	0	0	0	0
57	B5	1	0	0	0	0
57	C5	1	0	0	0	0
57	E5	1	0	0	0	0
57	F8	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
57	I8	1	0	0	0	0
57	J8	1	0	0	0	0
57	L8	1	0	0	0	0
57	M5	1	0	0	0	0
57	P8	1	0	0	0	0
57	Q8	1	0	0	0	0
58	13	13	0	22	3	0
58	14	26	0	46	11	0
58	1G	13	0	24	0	0
58	1J	13	0	24	1	0
59	32	8	0	0	1	0
59	3E	8	0	0	3	0
60	5A	1	0	0	0	0
60	5I	1	0	0	0	0
60	C5	1	0	0	0	0
60	G8	1	0	0	0	0
61	11	16	0	0	6	0
61	13	304	0	0	17	0
61	14	1135	0	0	56	0
61	16	15	0	0	1	0
61	19	8	0	0	0	0
61	1G	391	0	0	17	0
61	1H	1133	0	0	86	0
61	1I	2	0	0	0	0
61	1J	18	0	0	1	0
61	1K	1	0	0	0	0
61	21	8	0	0	0	0
61	22	1	0	0	0	0
61	25	11	0	0	1	0
61	29	6	0	0	0	0
61	2I	1	0	0	0	0
61	2K	6	0	0	0	0
61	31	4	0	0	0	0
61	35	9	0	0	4	0
61	39	6	0	0	0	0
61	3A	1	0	0	0	0
61	3E	1	0	0	0	0
61	3I	2	0	0	0	0
61	3K	1	0	0	0	0
61	42	1	0	0	0	0
61	45	3	0	0	0	0
61	4E	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
61	4K	11	0	0	0	0
61	4L	14	0	0	1	0
61	52	3	0	0	0	0
61	55	1	0	0	0	0
61	58	1	0	0	0	0
61	5I	2	0	0	0	0
61	75	1	0	0	0	0
61	78	11	0	0	5	0
61	7A	1	0	0	0	0
61	7I	2	0	0	1	0
61	85	1	0	0	0	0
61	98	2	0	0	0	0
61	9A	3	0	0	3	0
61	A5	1	0	0	0	0
61	A8	3	0	0	1	0
61	B8	1	0	0	0	0
61	BA	2	0	0	0	0
61	C5	3	0	0	0	0
61	E5	5	0	0	0	0
61	E8	1	0	0	0	0
61	F5	3	0	0	0	0
61	F8	1	0	0	0	0
61	H5	1	0	0	0	0
61	I8	6	0	0	1	0
61	K8	1	0	0	0	0
61	L8	1	0	0	1	0
61	M5	7	0	0	1	0
61	P8	1	0	0	0	0
61	Q8	5	0	0	1	0
All	All	296743	0	197188	8820	0

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 18.

The worst 5 of 8820 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)
3:22:173:VAL:C	3:22:174:PRO:N	1.71	1.38
4:3E:25:ARG:NH1	59:3E:301:SF4:S3	2.12	1.23
19:AI:3:ARG:HE	19:AI:9:VAL:HG11	1.07	1.14
44:E8:89:ALA:O	44:E8:92:ARG:NH1	1.81	1.12

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
38:45:27:VAL:HB	38:45:28:ALA:HA	1.12	1.10

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

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

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	12	203/256 (79%)	172 (85%)	25 (12%)	6 (3%)	4	20
2	1E	231/256 (90%)	188 (81%)	41 (18%)	2 (1%)	17	51
3	22	191/239 (80%)	167 (87%)	24 (13%)	0	100	100
3	2E	203/239 (85%)	181 (89%)	22 (11%)	0	100	100
4	32	206/209 (99%)	183 (89%)	22 (11%)	1 (0%)	29	64
4	3E	205/209 (98%)	190 (93%)	15 (7%)	0	100	100
5	42	147/162 (91%)	140 (95%)	7 (5%)	0	100	100
5	4E	147/162 (91%)	140 (95%)	6 (4%)	1 (1%)	22	56
6	52	99/101 (98%)	97 (98%)	2 (2%)	0	100	100
6	5E	98/101 (97%)	93 (95%)	5 (5%)	0	100	100
7	62	136/156 (87%)	123 (90%)	13 (10%)	0	100	100
7	6E	152/156 (97%)	140 (92%)	12 (8%)	0	100	100
8	72	135/138 (98%)	125 (93%)	7 (5%)	3 (2%)	6	28
8	7E	136/138 (99%)	124 (91%)	11 (8%)	1 (1%)	22	56
9	82	119/128 (93%)	101 (85%)	17 (14%)	1 (1%)	19	53
9	8E	124/128 (97%)	101 (82%)	19 (15%)	4 (3%)	4	19
10	1A	76/105 (72%)	70 (92%)	6 (8%)	0	100	100
10	1I	93/105 (89%)	82 (88%)	10 (11%)	1 (1%)	14	46
11	2A	111/129 (86%)	102 (92%)	7 (6%)	2 (2%)	8	33

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
11	2I	109/129 (84%)	98 (90%)	10 (9%)	1 (1%)	17	51
12	3A	120/132 (91%)	101 (84%)	14 (12%)	5 (4%)	3	13
12	3I	120/132 (91%)	106 (88%)	11 (9%)	3 (2%)	5	25
13	4A	109/126 (86%)	98 (90%)	9 (8%)	2 (2%)	8	33
13	4I	117/126 (93%)	97 (83%)	20 (17%)	0	100	100
14	5A	57/61 (93%)	48 (84%)	8 (14%)	1 (2%)	8	33
14	5I	58/61 (95%)	48 (83%)	8 (14%)	2 (3%)	3	17
15	6A	85/89 (96%)	83 (98%)	2 (2%)	0	100	100
15	6I	85/89 (96%)	81 (95%)	4 (5%)	0	100	100
16	7A	82/88 (93%)	76 (93%)	5 (6%)	1 (1%)	13	43
16	7I	81/88 (92%)	79 (98%)	2 (2%)	0	100	100
17	8A	97/105 (92%)	91 (94%)	6 (6%)	0	100	100
17	8I	98/105 (93%)	89 (91%)	7 (7%)	2 (2%)	7	30
18	9A	65/88 (74%)	61 (94%)	4 (6%)	0	100	100
18	9I	66/88 (75%)	62 (94%)	3 (4%)	1 (2%)	10	38
19	AA	56/93 (60%)	49 (88%)	5 (9%)	2 (4%)	3	16
19	AI	80/93 (86%)	67 (84%)	8 (10%)	5 (6%)	1	6
20	BA	97/106 (92%)	85 (88%)	10 (10%)	2 (2%)	7	29
20	BI	95/106 (90%)	82 (86%)	13 (14%)	0	100	100
21	1B	20/27 (74%)	19 (95%)	1 (5%)	0	100	100
21	1F	21/27 (78%)	19 (90%)	2 (10%)	0	100	100
28	7I	129/229 (56%)	116 (90%)	12 (9%)	1 (1%)	19	53
28	79	45/229 (20%)	40 (89%)	4 (9%)	1 (2%)	6	28
29	11	271/276 (98%)	241 (89%)	21 (8%)	9 (3%)	4	18
29	19	272/276 (99%)	243 (89%)	25 (9%)	4 (2%)	10	38
30	21	200/206 (97%)	154 (77%)	37 (18%)	9 (4%)	2	12
30	29	202/206 (98%)	155 (77%)	35 (17%)	12 (6%)	1	7
31	31	200/210 (95%)	179 (90%)	18 (9%)	3 (2%)	10	38
31	39	202/210 (96%)	159 (79%)	35 (17%)	8 (4%)	3	14
32	41	177/182 (97%)	156 (88%)	18 (10%)	3 (2%)	9	34
32	49	179/182 (98%)	159 (89%)	19 (11%)	1 (1%)	25	60

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
33	51	172/180 (96%)	138 (80%)	23 (13%)	11 (6%)	1	5
33	59	165/180 (92%)	129 (78%)	30 (18%)	6 (4%)	3	16
34	61	144/148 (97%)	120 (83%)	21 (15%)	3 (2%)	7	29
34	69	143/148 (97%)	113 (79%)	27 (19%)	3 (2%)	7	29
35	15	136/140 (97%)	124 (91%)	11 (8%)	1 (1%)	22	56
35	58	135/140 (96%)	115 (85%)	17 (13%)	3 (2%)	6	28
36	25	120/122 (98%)	114 (95%)	6 (5%)	0	100	100
36	68	120/122 (98%)	116 (97%)	4 (3%)	0	100	100
37	35	145/150 (97%)	117 (81%)	27 (19%)	1 (1%)	22	56
37	78	145/150 (97%)	116 (80%)	21 (14%)	8 (6%)	2	8
38	45	137/141 (97%)	115 (84%)	19 (14%)	3 (2%)	6	28
38	88	139/141 (99%)	121 (87%)	12 (9%)	6 (4%)	2	12
39	55	116/118 (98%)	109 (94%)	6 (5%)	1 (1%)	17	51
39	98	116/118 (98%)	107 (92%)	7 (6%)	2 (2%)	9	34
40	65	108/112 (96%)	91 (84%)	16 (15%)	1 (1%)	17	51
40	A8	109/112 (97%)	92 (84%)	15 (14%)	2 (2%)	8	33
41	75	131/146 (90%)	120 (92%)	8 (6%)	3 (2%)	6	27
41	B8	134/146 (92%)	120 (90%)	12 (9%)	2 (2%)	10	38
42	85	114/118 (97%)	102 (90%)	12 (10%)	0	100	100
42	C8	113/118 (96%)	105 (93%)	3 (3%)	5 (4%)	2	12
43	95	98/101 (97%)	81 (83%)	14 (14%)	3 (3%)	4	19
43	D8	98/101 (97%)	88 (90%)	8 (8%)	2 (2%)	7	30
44	A5	109/113 (96%)	103 (94%)	5 (5%)	1 (1%)	17	51
44	E8	108/113 (96%)	100 (93%)	8 (7%)	0	100	100
45	B5	92/96 (96%)	81 (88%)	9 (10%)	2 (2%)	6	28
45	F8	93/96 (97%)	87 (94%)	5 (5%)	1 (1%)	14	46
46	C5	102/110 (93%)	71 (70%)	24 (24%)	7 (7%)	1	4
46	G8	101/110 (92%)	82 (81%)	15 (15%)	4 (4%)	3	14
47	D5	127/206 (62%)	102 (80%)	21 (16%)	4 (3%)	4	19
47	H8	168/206 (82%)	132 (79%)	32 (19%)	4 (2%)	6	26
48	E5	74/85 (87%)	66 (89%)	7 (10%)	1 (1%)	11	39

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
48	I8	75/85 (88%)	68 (91%)	6 (8%)	1 (1%)	12	41
49	F5	92/98 (94%)	80 (87%)	11 (12%)	1 (1%)	14	46
49	J8	92/98 (94%)	86 (94%)	4 (4%)	2 (2%)	6	28
50	G5	67/72 (93%)	62 (92%)	2 (3%)	3 (4%)	2	12
50	K8	66/72 (92%)	60 (91%)	3 (4%)	3 (4%)	2	12
51	H5	56/60 (93%)	55 (98%)	1 (2%)	0	100	100
51	L8	56/60 (93%)	51 (91%)	5 (9%)	0	100	100
52	I5	61/71 (86%)	28 (46%)	28 (46%)	5 (8%)	1	3
52	M8	57/71 (80%)	39 (68%)	13 (23%)	5 (9%)	1	3
53	J5	54/60 (90%)	50 (93%)	4 (7%)	0	100	100
53	N8	54/60 (90%)	49 (91%)	5 (9%)	0	100	100
54	L5	45/49 (92%)	42 (93%)	3 (7%)	0	100	100
54	P8	45/49 (92%)	43 (96%)	2 (4%)	0	100	100
55	M5	62/65 (95%)	54 (87%)	6 (10%)	2 (3%)	4	19
55	Q8	62/65 (95%)	52 (84%)	7 (11%)	3 (5%)	2	11
All	All	11163/12404 (90%)	9756 (87%)	1192 (11%)	215 (2%)	8	32

5 of 215 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
9	8E	111	ARG
18	9I	22	VAL
19	AI	41	VAL
30	21	77	ILE
37	78	25	SER

### 5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	12	179/220 (81%)	136 (76%)	43 (24%)	0	2

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	1E	202/220 (92%)	152 (75%)	50 (25%)	0	2
3	22	154/188 (82%)	119 (77%)	35 (23%)	1	3
3	2E	159/188 (85%)	127 (80%)	32 (20%)	1	5
4	32	180/181 (99%)	151 (84%)	29 (16%)	2	10
4	3E	180/181 (99%)	141 (78%)	39 (22%)	1	4
5	42	114/123 (93%)	88 (77%)	26 (23%)	1	3
5	4E	115/123 (94%)	93 (81%)	22 (19%)	1	6
6	52	90/90 (100%)	79 (88%)	11 (12%)	5	19
6	5E	90/90 (100%)	82 (91%)	8 (9%)	9	32
7	62	114/127 (90%)	91 (80%)	23 (20%)	1	5
7	6E	125/127 (98%)	101 (81%)	24 (19%)	1	6
8	72	118/119 (99%)	94 (80%)	24 (20%)	1	5
8	7E	119/119 (100%)	96 (81%)	23 (19%)	1	6
9	82	92/99 (93%)	67 (73%)	25 (27%)	0	1
9	8E	97/99 (98%)	77 (79%)	20 (21%)	1	4
10	1A	71/92 (77%)	46 (65%)	25 (35%)	0	1
10	1I	81/92 (88%)	66 (82%)	15 (18%)	1	7
11	2A	85/99 (86%)	69 (81%)	16 (19%)	1	7
11	2I	84/99 (85%)	69 (82%)	15 (18%)	2	7
12	3A	103/109 (94%)	84 (82%)	19 (18%)	1	7
12	3I	103/109 (94%)	86 (84%)	17 (16%)	2	9
13	4A	91/101 (90%)	62 (68%)	29 (32%)	0	1
13	4I	94/101 (93%)	72 (77%)	22 (23%)	1	3
14	5A	49/50 (98%)	26 (53%)	23 (47%)	0	0
14	5I	49/50 (98%)	35 (71%)	14 (29%)	0	1
15	6A	79/80 (99%)	74 (94%)	5 (6%)	18	48
15	6I	79/80 (99%)	70 (89%)	9 (11%)	5	21
16	7A	72/74 (97%)	60 (83%)	12 (17%)	2	9
16	7I	72/74 (97%)	55 (76%)	17 (24%)	1	3
17	8A	94/97 (97%)	78 (83%)	16 (17%)	2	9
17	8I	95/97 (98%)	72 (76%)	23 (24%)	0	2

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
18	9A	58/77 (75%)	45 (78%)	13 (22%)	1	3
18	9I	58/77 (75%)	43 (74%)	15 (26%)	0	2
19	AA	52/80 (65%)	41 (79%)	11 (21%)	1	4
19	AI	72/80 (90%)	60 (83%)	12 (17%)	2	9
20	BA	76/82 (93%)	56 (74%)	20 (26%)	0	2
20	BI	75/82 (92%)	57 (76%)	18 (24%)	0	2
21	1B	17/22 (77%)	13 (76%)	4 (24%)	1	3
21	1F	18/22 (82%)	15 (83%)	3 (17%)	2	9
28	71	109/181 (60%)	84 (77%)	25 (23%)	1	3
28	79	48/181 (26%)	37 (77%)	11 (23%)	1	3
29	11	214/218 (98%)	189 (88%)	25 (12%)	5	20
29	19	214/218 (98%)	179 (84%)	35 (16%)	2	9
30	21	155/166 (93%)	121 (78%)	34 (22%)	1	4
30	29	165/166 (99%)	145 (88%)	20 (12%)	5	19
31	31	161/166 (97%)	139 (86%)	22 (14%)	3	15
31	39	163/166 (98%)	129 (79%)	34 (21%)	1	4
32	41	153/156 (98%)	131 (86%)	22 (14%)	3	13
32	49	153/156 (98%)	112 (73%)	41 (27%)	0	2
33	51	143/148 (97%)	104 (73%)	39 (27%)	0	1
33	59	139/148 (94%)	113 (81%)	26 (19%)	1	7
34	61	122/124 (98%)	97 (80%)	25 (20%)	1	5
34	69	122/124 (98%)	93 (76%)	29 (24%)	0	2
35	15	117/119 (98%)	100 (86%)	17 (14%)	3	13
35	58	116/119 (98%)	100 (86%)	16 (14%)	3	14
36	25	100/100 (100%)	83 (83%)	17 (17%)	2	9
36	68	100/100 (100%)	88 (88%)	12 (12%)	5	19
37	35	114/116 (98%)	89 (78%)	25 (22%)	1	4
37	78	114/116 (98%)	91 (80%)	23 (20%)	1	5
38	45	109/111 (98%)	82 (75%)	27 (25%)	0	2
38	88	110/111 (99%)	92 (84%)	18 (16%)	2	9
39	55	101/101 (100%)	86 (85%)	15 (15%)	3	12

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
39	98	101/101 (100%)	85 (84%)	16 (16%)	2	10
40	65	87/88 (99%)	57 (66%)	30 (34%)	0	1
40	A8	87/88 (99%)	72 (83%)	15 (17%)	2	8
41	75	117/127 (92%)	98 (84%)	19 (16%)	2	10
41	B8	117/127 (92%)	90 (77%)	27 (23%)	1	3
42	85	93/94 (99%)	78 (84%)	15 (16%)	2	10
42	C8	92/94 (98%)	80 (87%)	12 (13%)	4	16
43	95	81/82 (99%)	60 (74%)	21 (26%)	0	2
43	D8	82/82 (100%)	60 (73%)	22 (27%)	0	2
44	A5	91/92 (99%)	74 (81%)	17 (19%)	1	7
44	E8	90/92 (98%)	80 (89%)	10 (11%)	6	22
45	B5	74/78 (95%)	64 (86%)	10 (14%)	4	15
45	F8	75/78 (96%)	69 (92%)	6 (8%)	12	37
46	C5	85/91 (93%)	62 (73%)	23 (27%)	0	1
46	G8	83/91 (91%)	65 (78%)	18 (22%)	1	4
47	D5	118/179 (66%)	90 (76%)	28 (24%)	1	2
47	H8	151/179 (84%)	112 (74%)	39 (26%)	0	2
48	E5	61/67 (91%)	53 (87%)	8 (13%)	4	16
48	I8	62/67 (92%)	53 (86%)	9 (14%)	3	13
49	F5	79/83 (95%)	65 (82%)	14 (18%)	2	8
49	J8	79/83 (95%)	65 (82%)	14 (18%)	2	8
50	G5	63/67 (94%)	42 (67%)	21 (33%)	0	1
50	K8	64/67 (96%)	48 (75%)	16 (25%)	0	2
51	H5	50/52 (96%)	39 (78%)	11 (22%)	1	4
51	L8	50/52 (96%)	40 (80%)	10 (20%)	1	5
52	I5	57/63 (90%)	39 (68%)	18 (32%)	0	1
52	M8	52/63 (82%)	33 (64%)	19 (36%)	0	0
53	J5	48/52 (92%)	34 (71%)	14 (29%)	0	1
53	N8	49/52 (94%)	39 (80%)	10 (20%)	1	5
54	L5	38/42 (90%)	33 (87%)	5 (13%)	4	16
54	P8	38/42 (90%)	32 (84%)	6 (16%)	2	10

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
55	M5	54/55 (98%)	42 (78%)	12 (22%)	1 3
55	Q8	54/55 (98%)	48 (89%)	6 (11%)	6 22
All	All	9419/10256 (92%)	7533 (80%)	1886 (20%)	1 5

5 of 1886 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	12	56	ARG
47	D5	73	GLN
10	1A	67	THR
46	C5	98	VAL
38	45	110	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 21 such sidechains are listed below:

Mol	Chain	Res	Type
30	29	54	GLN
32	49	130	ASN
50	G5	47	ASN
38	45	123	HIS
31	39	8	GLN

### 5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	13	1493/1522 (98%)	348 (23%)	34 (2%)
1	1G	1505/1522 (98%)	323 (21%)	33 (2%)
22	1K	67/76 (88%)	36 (53%)	4 (5%)
23	2K	76/77 (98%)	20 (26%)	1 (1%)
23	2L	75/77 (97%)	10 (13%)	2 (2%)
24	3K	67/76 (88%)	37 (55%)	3 (4%)
24	3L	69/76 (90%)	32 (46%)	1 (1%)
25	4K	19/30 (63%)	12 (63%)	2 (10%)
25	4L	18/30 (60%)	10 (55%)	2 (11%)
26	14	2803/2917 (96%)	638 (22%)	37 (1%)
26	1H	2836/2917 (97%)	590 (20%)	43 (1%)
27	16	121/122 (99%)	24 (19%)	0
27	1J	121/122 (99%)	34 (28%)	2 (1%)
56	1L	65/76 (85%)	24 (36%)	2 (3%)

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Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
All	All	9335/9640 (96%)	2138 (22%)	166 (1%)

5 of 2138 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	13	2	U
1	13	5	U
1	13	6	G
1	13	12	U
1	13	13	U

5 of 166 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	1G	1397	C
26	14	1497	U
1	1G	1533	C
26	14	101	G
26	14	2062	A

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
23	4SU	2L	8	23	18,21,22	1.94	3 (16%)	26,30,33	2.59	4 (15%)
23	OMC	2K	33	23	19,22,23	1.81	3 (15%)	26,31,34	1.09	3 (11%)
22	CM0	1K	34	22	22,26,27	3.97	7 (31%)	28,37,40	1.54	4 (14%)
56	PSU	1L	55	56	18,21,22	1.38	1 (5%)	22,30,33	1.51	4 (18%)
22	6MZ	1K	37	22	18,25,26	2.22	4 (22%)	16,36,39	2.30	3 (18%)
23	4SU	2K	8	23	18,21,22	1.91	3 (16%)	26,30,33	2.56	4 (15%)
23	5MU	2K	55	23,57	19,22,23	3.85	5 (26%)	28,32,35	3.22	8 (28%)



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
23	OMC	2L	33	23	19,22,23	1.80	4 (21%)	26,31,34	1.03	1 (3%)
23	5MU	2L	55	23	19,22,23	3.93	5 (26%)	28,32,35	3.04	9 (32%)
22	PSU	1K	55	22	18,21,22	1.36	1 (5%)	22,30,33	1.75	4 (18%)
22	H2U	1K	17	22	18,21,22	2.13	4 (22%)	21,30,33	2.38	5 (23%)
23	PSU	2L	56	23	18,21,22	1.14	1 (5%)	22,30,33	1.58	2 (9%)
23	7MG	2L	47	23	22,26,27	2.83	8 (36%)	29,39,42	3.00	10 (34%)
23	7MG	2K	47	23	22,26,27	3.09	6 (27%)	29,39,42	2.81	11 (37%)
23	PSU	2K	56	23	18,21,22	1.16	2 (11%)	22,30,33	2.02	4 (18%)
56	5MU	1L	54	56	19,22,23	3.87	5 (26%)	28,32,35	3.17	9 (32%)
22	5MU	1K	54	22	19,22,23	3.90	5 (26%)	28,32,35	2.99	7 (25%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
23	4SU	2L	8	23	-	0/7/25/26	0/2/2/2
23	OMC	2K	33	23	-	0/9/27/28	0/2/2/2
22	CM0	1K	34	22	-	6/12/30/31	0/2/2/2
56	PSU	1L	55	56	-	2/7/25/26	0/2/2/2
22	6MZ	1K	37	22	-	2/5/27/28	0/3/3/3
23	4SU	2K	8	23	-	0/7/25/26	0/2/2/2
23	5MU	2K	55	23,57	-	0/7/25/26	0/2/2/2
23	OMC	2L	33	23	-	0/9/27/28	0/2/2/2
23	5MU	2L	55	23	-	0/7/25/26	0/2/2/2
22	PSU	1K	55	22	-	2/7/25/26	0/2/2/2
22	H2U	1K	17	22	-	1/7/38/39	0/2/2/2
23	PSU	2L	56	23	-	0/7/25/26	0/2/2/2
23	7MG	2L	47	23	-	3/7/37/38	0/3/3/3
23	7MG	2K	47	23	-	0/7/37/38	0/3/3/3
23	PSU	2K	56	23	-	0/7/25/26	0/2/2/2
56	5MU	1L	54	56	-	0/7/25/26	0/2/2/2
22	5MU	1K	54	22	-	0/7/25/26	0/2/2/2

The worst 5 of 67 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	1K	34	CM0	C6-C5	14.10	1.50	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	1K	54	5MU	C2-N1	12.81	1.59	1.38
23	2L	55	5MU	C2-N1	12.78	1.59	1.38
56	1L	54	5MU	C2-N1	12.69	1.58	1.38
23	2K	55	5MU	C2-N1	12.54	1.58	1.38

The worst 5 of 92 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	2K	55	5MU	C5-C4-N3	10.74	124.48	115.31
56	1L	54	5MU	C5-C4-N3	10.28	124.09	115.31
22	1K	54	5MU	C5-C4-N3	10.26	124.07	115.31
23	2L	55	5MU	C5-C4-N3	9.92	123.78	115.31
23	2K	8	4SU	C4-N3-C2	-8.58	119.00	127.34

There are no chirality outliers.

5 of 16 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
22	1K	34	CM0	O4'-C4'-C5'-O5'
23	2L	47	7MG	C2'-C1'-N9-C8
22	1K	34	CM0	C3'-C4'-C5'-O5'
22	1K	34	CM0	O5-C7-C8-O8
22	1K	34	CM0	C6-C5-O5-C7

There are no ring outliers.

13 monomers are involved in 22 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
23	2L	8	4SU	2	0
23	2K	33	OMC	1	0
22	1K	34	CM0	1	0
23	2K	8	4SU	1	0
23	2K	55	5MU	3	0
23	2L	33	OMC	3	0
23	2L	55	5MU	3	0
22	1K	55	PSU	2	0
22	1K	17	H2U	2	0
23	2L	47	7MG	1	0
23	2K	47	7MG	2	0
56	1L	54	5MU	1	0
22	1K	54	5MU	1	0

## 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 1355 ligands modelled in this entry, 1348 are monoatomic - leaving 7 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
58	SPE	14	3445	26	12,12,12	0.58	0	11,11,11	0.89	0
59	SF4	32	301	4	0,12,12	-	-	-		
58	SPE	1J	208	-	12,12,12	0.40	0	11,11,11	0.88	0
58	SPE	13	1748	1	12,12,12	0.49	0	11,11,11	0.97	1 (9%)
58	SPE	14	3446	-	12,12,12	0.73	0	11,11,11	0.98	1 (9%)
59	SF4	3E	301	4	0,12,12	-	-	-		
58	SPE	1G	1733	-	12,12,12	0.40	0	11,11,11	0.91	0

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
58	SPE	14	3445	26	-	6/10/10/10	-
59	SF4	32	301	4	-	-	0/6/5/5
58	SPE	1J	208	-	-	5/10/10/10	-
58	SPE	13	1748	1	-	7/10/10/10	-
58	SPE	14	3446	-	-	5/10/10/10	-
59	SF4	3E	301	4	-	-	0/6/5/5
58	SPE	1G	1733	-	-	4/10/10/10	-

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
58	13	1748	SPE	C11-C10-N9	-2.43	105.58	112.14
58	14	3446	SPE	C11-C10-N9	-2.39	105.69	112.14

There are no chirality outliers.

5 of 27 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
58	14	3445	SPE	C2-C3-C4-N5
58	14	3446	SPE	N9-C10-C11-C12
58	13	1748	SPE	C2-C3-C4-N5
58	13	1748	SPE	N9-C10-C11-C12
58	13	1748	SPE	C7-C6-N5-C4

There are no ring outliers.

6 monomers are involved in 19 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
58	14	3445	SPE	5	0
59	32	301	SF4	1	0
58	1J	208	SPE	1	0
58	13	1748	SPE	3	0
58	14	3446	SPE	6	0
59	3E	301	SF4	3	0

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
2	1E	1
25	4K	1
3	22	1
10	1A	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	1E	78:GLN	C	79:ASP	N	4.14
1	4K	25:A	O3'	26:A	P	3.23
1	22	173:VAL	C	174:PRO	N	1.71
1	1A	38:ILE	C	39:PRO	N	1.62

## 6 Fit of model and data i

### 6.1 Protein, DNA and RNA chains i

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	1496/1522 (98%)	-0.40	5 (0%) 94 87	57, 98, 164, 235	0
1	1G	1506/1522 (98%)	-0.45	4 (0%) 94 87	68, 105, 166, 238	0
2	12	207/256 (80%)	1.12	47 (22%) 0 0	121, 148, 168, 185	0
2	1E	235/256 (91%)	0.46	18 (7%) 13 7	108, 135, 160, 171	0
3	22	195/239 (81%)	1.28	49 (25%) 0 0	113, 131, 152, 164	0
3	2E	205/239 (85%)	1.21	46 (22%) 0 0	85, 107, 142, 149	0
4	32	208/209 (99%)	0.84	30 (14%) 2 1	84, 101, 123, 132	0
4	3E	207/209 (99%)	0.55	19 (9%) 9 5	77, 103, 125, 132	0
5	42	149/162 (91%)	0.16	5 (3%) 45 29	91, 111, 128, 149	0
5	4E	149/162 (91%)	0.21	3 (2%) 65 48	79, 98, 118, 135	0
6	52	101/101 (100%)	0.84	11 (10%) 5 3	81, 97, 110, 131	0
6	5E	100/101 (99%)	0.91	12 (12%) 4 2	83, 99, 113, 123	0
7	62	140/156 (89%)	0.89	20 (14%) 2 1	103, 119, 131, 138	0
7	6E	154/156 (98%)	0.98	21 (13%) 3 1	98, 113, 138, 162	0
8	72	137/138 (99%)	-0.18	1 (0%) 87 76	90, 114, 125, 128	0
8	7E	138/138 (100%)	0.07	5 (3%) 42 28	87, 102, 113, 120	0
9	82	121/128 (94%)	0.41	7 (5%) 23 14	101, 144, 160, 164	0
9	8E	126/128 (98%)	0.66	12 (9%) 8 5	84, 133, 153, 157	0
10	1A	80/105 (76%)	0.31	8 (10%) 7 4	111, 138, 152, 156	0
10	1I	95/105 (90%)	2.01	48 (50%) 0 0	80, 127, 155, 159	0
11	2A	113/129 (87%)	1.68	40 (35%) 0 0	78, 103, 117, 120	0
11	2I	111/129 (86%)	0.91	16 (14%) 2 1	70, 99, 115, 125	0
12	3A	122/132 (92%)	0.84	18 (14%) 2 1	74, 91, 116, 132	0
12	3I	122/132 (92%)	0.30	3 (2%) 57 40	65, 76, 103, 112	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
13	4A	111/126 (88%)	0.33	4 (3%) 42 28	102, 129, 143, 152	0
13	4I	119/126 (94%)	0.30	6 (5%) 28 18	87, 111, 129, 139	0
14	5A	59/61 (96%)	1.73	24 (40%) 0 0	118, 129, 141, 142	0
14	5I	60/61 (98%)	0.43	4 (6%) 17 10	83, 97, 112, 119	0
15	6A	87/89 (97%)	-0.04	0 100 100	79, 100, 115, 117	0
15	6I	87/89 (97%)	0.80	10 (11%) 4 3	75, 94, 109, 116	0
16	7A	84/88 (95%)	0.03	1 (1%) 79 63	85, 98, 119, 145	0
16	7I	83/88 (94%)	0.13	2 (2%) 59 42	91, 107, 132, 147	0
17	8A	99/105 (94%)	0.14	2 (2%) 65 48	89, 100, 117, 120	0
17	8I	100/105 (95%)	0.32	3 (3%) 50 34	81, 98, 108, 115	0
18	9A	67/88 (76%)	0.87	10 (14%) 2 1	87, 101, 125, 129	0
18	9I	68/88 (77%)	0.94	11 (16%) 1 1	85, 100, 125, 128	0
19	AA	62/93 (66%)	0.27	5 (8%) 12 6	118, 142, 155, 158	0
19	AI	82/93 (88%)	0.77	12 (14%) 2 1	95, 110, 128, 136	0
20	BA	99/106 (93%)	0.43	4 (4%) 38 25	85, 104, 128, 140	0
20	BI	97/106 (91%)	0.25	6 (6%) 20 12	103, 117, 138, 145	0
21	1B	22/27 (81%)	0.92	3 (13%) 3 1	110, 116, 124, 134	0
21	1F	23/27 (85%)	0.76	3 (13%) 3 2	90, 98, 106, 108	0
22	1K	67/76 (88%)	0.62	7 (10%) 6 4	80, 167, 196, 203	0
23	2K	72/77 (93%)	-0.22	1 (1%) 75 59	68, 89, 116, 129	0
23	2L	71/77 (92%)	-0.04	0 100 100	78, 100, 132, 145	0
24	3K	70/76 (92%)	0.66	11 (15%) 2 1	71, 198, 222, 224	0
24	3L	71/76 (93%)	0.66	9 (12%) 3 2	78, 191, 215, 218	0
25	4K	21/30 (70%)	0.83	2 (9%) 8 5	69, 129, 212, 213	0
25	4L	19/30 (63%)	0.27	1 (5%) 26 16	85, 144, 210, 210	0
26	14	2810/2917 (96%)	-0.12	30 (1%) 80 65	54, 81, 180, 237	0
26	1H	2841/2917 (97%)	-0.12	27 (0%) 82 68	44, 70, 166, 244	0
27	16	122/122 (100%)	-0.66	1 (0%) 86 73	65, 87, 105, 180	0
27	1J	122/122 (100%)	-0.71	0 100 100	79, 106, 125, 185	0
28	71	133/229 (58%)	2.14	60 (45%) 0 0	136, 194, 219, 229	0
28	79	57/229 (24%)	0.84	11 (19%) 1 0	136, 178, 198, 205	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
29	11	273/276 (98%)	0.32	4 (1%) 73 57	44, 62, 78, 94	0
29	19	274/276 (99%)	0.84	24 (8%) 10 5	50, 72, 87, 102	0
30	21	202/206 (98%)	0.87	29 (14%) 2 1	49, 82, 115, 123	0
30	29	204/206 (99%)	0.78	27 (13%) 3 2	57, 88, 124, 135	0
31	31	202/210 (96%)	0.75	27 (13%) 3 1	46, 75, 108, 123	0
31	39	204/210 (97%)	0.66	21 (10%) 6 4	57, 95, 139, 164	0
32	41	179/182 (98%)	0.35	7 (3%) 39 25	75, 95, 124, 138	0
32	49	181/182 (99%)	1.04	40 (22%) 0 0	99, 118, 142, 156	0
33	51	174/180 (96%)	0.09	6 (3%) 45 29	76, 99, 116, 128	0
33	59	167/180 (92%)	1.60	57 (34%) 0 0	123, 190, 216, 225	0
34	61	146/148 (98%)	0.75	20 (13%) 3 1	75, 119, 134, 148	0
34	69	145/148 (97%)	0.57	17 (11%) 4 2	80, 115, 138, 144	0
35	15	138/140 (98%)	1.02	24 (17%) 1 1	76, 98, 124, 139	0
35	58	137/140 (97%)	0.55	11 (8%) 12 7	64, 84, 113, 134	0
36	25	122/122 (100%)	0.79	14 (11%) 4 3	68, 81, 97, 107	0
36	68	122/122 (100%)	0.49	1 (0%) 86 73	57, 72, 87, 93	0
37	35	147/150 (98%)	0.89	24 (16%) 1 1	58, 93, 121, 133	0
37	78	147/150 (98%)	0.32	5 (3%) 45 29	46, 77, 98, 106	0
38	45	139/141 (98%)	1.17	31 (22%) 0 0	70, 94, 112, 126	0
38	88	141/141 (100%)	0.45	9 (6%) 19 11	57, 74, 97, 117	0
39	55	118/118 (100%)	0.17	3 (2%) 57 40	61, 77, 92, 109	0
39	98	118/118 (100%)	0.80	13 (11%) 5 3	58, 76, 94, 104	0
40	65	110/112 (98%)	0.61	8 (7%) 15 8	82, 100, 119, 130	0
40	A8	111/112 (99%)	1.03	17 (15%) 2 1	73, 86, 104, 112	0
41	75	133/146 (91%)	0.17	3 (2%) 60 43	76, 88, 117, 142	0
41	B8	136/146 (93%)	0.04	2 (1%) 73 57	66, 83, 121, 152	0
42	85	116/118 (98%)	0.68	9 (7%) 13 7	65, 91, 116, 123	0
42	C8	115/118 (97%)	0.36	5 (4%) 35 22	57, 75, 96, 106	0
43	95	100/101 (99%)	1.23	24 (24%) 0 0	65, 108, 126, 132	0
43	D8	100/101 (99%)	0.92	13 (13%) 3 2	56, 92, 111, 125	0
44	A5	111/113 (98%)	0.61	7 (6%) 20 11	62, 73, 95, 128	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
44	E8	110/113 (97%)	0.47	6 (5%) 25 15	57, 69, 90, 101	0
45	B5	94/96 (97%)	0.41	7 (7%) 14 8	66, 80, 103, 111	0
45	F8	95/96 (98%)	0.13	2 (2%) 63 46	50, 66, 91, 99	0
46	C5	104/110 (94%)	1.58	26 (25%) 0 0	84, 110, 143, 150	0
46	G8	103/110 (93%)	0.21	2 (1%) 66 49	74, 91, 118, 125	0
47	D5	133/206 (64%)	1.70	48 (36%) 0 0	93, 123, 150, 159	0
47	H8	170/206 (82%)	2.15	78 (45%) 0 0	77, 112, 191, 198	0
48	E5	76/85 (89%)	0.06	1 (1%) 77 61	58, 82, 94, 108	0
48	I8	77/85 (90%)	-0.17	2 (2%) 56 39	54, 70, 87, 98	0
49	F5	94/98 (95%)	0.67	5 (5%) 26 16	61, 76, 117, 123	0
49	J8	94/98 (95%)	0.53	5 (5%) 26 16	49, 70, 115, 135	0
50	G5	69/72 (95%)	0.64	5 (7%) 15 8	77, 96, 113, 130	0
50	K8	68/72 (94%)	0.07	1 (1%) 73 57	60, 76, 94, 124	0
51	H5	58/60 (96%)	1.35	15 (25%) 0 0	73, 90, 118, 123	0
51	L8	58/60 (96%)	0.09	0 100 100	59, 75, 94, 101	0
52	I5	63/71 (88%)	3.48	46 (73%) 0 0	132, 174, 191, 195	0
52	M8	61/71 (85%)	1.37	16 (26%) 0 0	96, 137, 167, 174	0
53	J5	56/60 (93%)	0.62	6 (10%) 6 3	57, 81, 130, 140	0
53	N8	56/60 (93%)	1.22	10 (17%) 1 1	50, 83, 145, 155	0
54	L5	47/49 (95%)	0.18	1 (2%) 63 46	51, 61, 82, 96	0
54	P8	47/49 (95%)	0.05	0 100 100	44, 53, 68, 89	0
55	M5	64/65 (98%)	0.54	2 (3%) 49 32	64, 76, 89, 114	0
55	Q8	64/65 (98%)	0.06	1 (1%) 72 55	52, 64, 78, 91	0
56	1L	67/76 (88%)	1.41	17 (25%) 0 0	98, 180, 207, 210	0
All	All	20742/22044 (94%)	0.30	1522 (7%) 15 8	44, 93, 167, 244	0

The worst 5 of 1522 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
26	14	2902	C	15.3
46	C5	59	GLY	14.8
52	I5	52	THR	11.4
26	14	2901	C	11.2
43	D8	37	VAL	11.2

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

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
56	PSU	1L	55	20/21	0.73	0.29	118,133,146,147	0
22	H2U	1K	17	20/21	0.81	0.12	119,145,154,154	0
23	7MG	2L	47	24/25	0.84	0.16	92,112,117,118	0
22	PSU	1K	55	20/21	0.84	0.25	102,116,131,132	0
23	OMC	2L	33	21/22	0.90	0.18	83,94,97,100	0
56	5MU	1L	54	21/22	0.91	0.22	117,124,131,143	0
22	5MU	1K	54	21/22	0.92	0.19	100,106,117,129	0
23	PSU	2K	56	20/21	0.92	0.11	93,98,106,114	0
23	4SU	2L	8	20/21	0.93	0.15	104,106,109,112	0
23	PSU	2L	56	20/21	0.93	0.10	105,114,120,120	0
23	7MG	2K	47	24/25	0.94	0.12	90,98,109,111	0
23	4SU	2K	8	20/21	0.95	0.13	84,88,92,94	0
23	5MU	2K	55	21/22	0.95	0.12	99,102,106,113	0
22	CM0	1K	34	25/26	0.95	0.13	72,89,106,107	0
23	OMC	2K	33	21/22	0.96	0.17	72,79,82,89	0
23	5MU	2L	55	21/22	0.96	0.09	111,115,122,127	0
22	6MZ	1K	37	23/24	0.97	0.13	61,79,86,90	0

## 6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
57	MG	1G	1712	1/1	0.14	0.13	142,142,142,142	0
57	MG	13	1736	1/1	0.20	0.10	104,104,104,104	0
57	MG	1H	3246	1/1	0.24	0.48	72,72,72,72	0
57	MG	14	3386	1/1	0.28	0.15	93,93,93,93	0
57	MG	14	3438	1/1	0.31	0.12	101,101,101,101	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
57	MG	1H	3509	1/1	0.35	0.18	88,88,88,88	0
57	MG	14	3327	1/1	0.41	0.12	100,100,100,100	0
57	MG	14	3428	1/1	0.43	0.16	109,109,109,109	0
57	MG	1J	206	1/1	0.44	0.17	109,109,109,109	0
57	MG	14	3173	1/1	0.45	0.16	98,98,98,98	0
57	MG	1H	3216	1/1	0.45	0.54	89,89,89,89	0
57	MG	14	3436	1/1	0.46	0.22	96,96,96,96	0
57	MG	14	3174	1/1	0.46	0.45	83,83,83,83	0
57	MG	4L	101	1/1	0.46	0.09	110,110,110,110	0
57	MG	1G	1686	1/1	0.47	0.10	107,107,107,107	0
57	MG	1H	3118	1/1	0.47	0.33	83,83,83,83	0
57	MG	1G	1714	1/1	0.47	0.19	99,99,99,99	0
57	MG	1G	1630	1/1	0.47	0.49	106,106,106,106	0
57	MG	14	3214	1/1	0.48	0.76	93,93,93,93	0
57	MG	14	3349	1/1	0.49	0.07	105,105,105,105	0
57	MG	1G	1717	1/1	0.49	0.10	99,99,99,99	0
57	MG	13	1707	1/1	0.49	0.17	92,92,92,92	0
57	MG	1H	3205	1/1	0.51	0.32	90,90,90,90	0
57	MG	1H	3210	1/1	0.51	0.37	83,83,83,83	0
57	MG	13	1686	1/1	0.51	0.33	104,104,104,104	0
57	MG	13	1726	1/1	0.51	0.19	103,103,103,103	0
57	MG	14	3293	1/1	0.51	0.15	72,72,72,72	0
57	MG	1H	3198	1/1	0.51	0.22	108,108,108,108	0
57	MG	1H	3402	1/1	0.52	0.10	79,79,79,79	0
57	MG	14	3443	1/1	0.53	0.14	92,92,92,92	0
57	MG	1H	3515	1/1	0.53	0.16	98,98,98,98	0
57	MG	14	3423	1/1	0.54	0.37	92,92,92,92	0
57	MG	14	3216	1/1	0.54	0.14	106,106,106,106	0
57	MG	1G	1702	1/1	0.54	0.13	95,95,95,95	0
57	MG	1G	1675	1/1	0.54	0.12	107,107,107,107	0
57	MG	13	1671	1/1	0.54	0.79	91,91,91,91	0
57	MG	1G	1691	1/1	0.54	0.13	99,99,99,99	0
57	MG	13	1668	1/1	0.55	0.13	121,121,121,121	0
57	MG	1H	3274	1/1	0.55	0.46	83,83,83,83	0
57	MG	1H	3261	1/1	0.56	0.40	77,77,77,77	0
57	MG	1H	3266	1/1	0.56	0.29	89,89,89,89	0
57	MG	16	206	1/1	0.56	0.38	77,77,77,77	0
57	MG	13	1732	1/1	0.56	0.15	118,118,118,118	0
57	MG	1H	3010	1/1	0.56	0.25	78,78,78,78	0
57	MG	14	3422	1/1	0.56	0.17	100,100,100,100	0
57	MG	13	1645	1/1	0.57	0.30	78,78,78,78	0
57	MG	1G	1695	1/1	0.57	0.07	112,112,112,112	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
57	MG	1G	1715	1/1	0.57	0.12	119,119,119,119	0
57	MG	13	1654	1/1	0.57	0.09	113,113,113,113	0
57	MG	14	3405	1/1	0.58	0.09	91,91,91,91	0
57	MG	1H	3168	1/1	0.58	0.16	80,80,80,80	0
57	MG	14	3282	1/1	0.58	0.15	105,105,105,105	0
57	MG	1H	3188	1/1	0.58	0.68	95,95,95,95	0
57	MG	1H	3524	1/1	0.59	0.17	96,96,96,96	0
57	MG	1H	3295	1/1	0.59	0.15	70,70,70,70	0
57	MG	1H	3217	1/1	0.60	0.42	80,80,80,80	0
57	MG	1H	3061	1/1	0.60	0.45	76,76,76,76	0
57	MG	14	3409	1/1	0.60	0.25	95,95,95,95	0
57	MG	1G	1700	1/1	0.60	0.11	109,109,109,109	0
57	MG	14	3031	1/1	0.60	0.44	86,86,86,86	0
57	MG	39	302	1/1	0.60	0.30	67,67,67,67	0
57	MG	1H	3095	1/1	0.61	0.33	69,69,69,69	0
57	MG	1H	3238	1/1	0.61	0.36	87,87,87,87	0
57	MG	1G	1643	1/1	0.62	0.33	83,83,83,83	0
57	MG	1H	3520	1/1	0.62	0.11	97,97,97,97	0
57	MG	14	3157	1/1	0.62	0.69	89,89,89,89	0
57	MG	14	3291	1/1	0.62	0.14	90,90,90,90	0
57	MG	1G	1684	1/1	0.62	0.07	120,120,120,120	0
57	MG	1H	3182	1/1	0.62	0.26	90,90,90,90	0
57	MG	14	3284	1/1	0.63	0.11	72,72,72,72	0
57	MG	1G	1710	1/1	0.63	0.31	102,102,102,102	0
57	MG	1H	3289	1/1	0.63	0.31	78,78,78,78	0
57	MG	14	3208	1/1	0.63	0.20	78,78,78,78	0
57	MG	25	201	1/1	0.63	0.09	118,118,118,118	0
57	MG	1H	3525	1/1	0.64	0.08	134,134,134,134	0
57	MG	1H	3496	1/1	0.64	0.12	98,98,98,98	0
57	MG	1H	3212	1/1	0.64	0.19	65,65,65,65	0
57	MG	13	1677	1/1	0.64	0.29	92,92,92,92	0
57	MG	13	1743	1/1	0.64	0.13	153,153,153,153	0
57	MG	1H	3232	1/1	0.64	0.49	85,85,85,85	0
57	MG	14	3435	1/1	0.65	0.12	93,93,93,93	0
57	MG	14	3390	1/1	0.65	0.18	108,108,108,108	0
57	MG	14	3086	1/1	0.65	0.26	64,64,64,64	0
57	MG	13	1678	1/1	0.65	0.59	94,94,94,94	0
57	MG	1J	205	1/1	0.65	0.10	87,87,87,87	0
57	MG	14	3162	1/1	0.65	0.60	67,67,67,67	0
57	MG	1H	3077	1/1	0.65	0.25	56,56,56,56	0
57	MG	1H	3186	1/1	0.65	0.42	94,94,94,94	0
57	MG	1H	3104	1/1	0.66	0.29	88,88,88,88	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
57	MG	1H	3415	1/1	0.66	0.21	72,72,72,72	0
57	MG	13	1741	1/1	0.66	0.12	110,110,110,110	0
57	MG	1H	3500	1/1	0.66	0.09	93,93,93,93	0
57	MG	1G	1707	1/1	0.66	0.22	108,108,108,108	0
57	MG	1H	3508	1/1	0.66	0.08	84,84,84,84	0
57	MG	14	3092	1/1	0.66	0.49	81,81,81,81	0
57	MG	14	3147	1/1	0.66	0.10	69,69,69,69	0
57	MG	1H	3535	1/1	0.66	0.24	93,93,93,93	0
57	MG	13	1733	1/1	0.67	0.10	106,106,106,106	0
57	MG	14	3111	1/1	0.67	0.48	86,86,86,86	0
57	MG	14	3397	1/1	0.67	0.07	109,109,109,109	0
57	MG	14	3008	1/1	0.67	0.40	90,90,90,90	0
57	MG	1H	3180	1/1	0.67	0.38	88,88,88,88	0
57	MG	14	3295	1/1	0.67	0.29	90,90,90,90	0
57	MG	1G	1680	1/1	0.67	0.29	91,91,91,91	0
57	MG	14	3218	1/1	0.67	0.28	84,84,84,84	0
57	MG	1H	3263	1/1	0.68	0.47	91,91,91,91	0
57	MG	1H	3133	1/1	0.68	0.48	78,78,78,78	0
57	MG	1H	3439	1/1	0.68	0.05	95,95,95,95	0
57	MG	1H	3448	1/1	0.68	0.19	86,86,86,86	0
57	MG	1H	3479	1/1	0.68	0.17	75,75,75,75	0
57	MG	1H	3204	1/1	0.68	0.41	81,81,81,81	0
57	MG	1H	3211	1/1	0.68	0.49	79,79,79,79	0
57	MG	1H	3218	1/1	0.68	0.21	81,81,81,81	0
57	MG	1G	1701	1/1	0.68	0.08	101,101,101,101	0
57	MG	14	3416	1/1	0.69	0.05	89,89,89,89	0
57	MG	1H	3120	1/1	0.69	0.46	96,96,96,96	0
57	MG	14	3393	1/1	0.69	0.08	118,118,118,118	0
57	MG	1G	1719	1/1	0.69	0.06	119,119,119,119	0
57	MG	14	3136	1/1	0.69	0.12	127,127,127,127	0
57	MG	4K	101	1/1	0.69	0.27	86,86,86,86	0
57	MG	14	3053	1/1	0.70	0.08	72,72,72,72	0
57	MG	14	3189	1/1	0.70	0.66	85,85,85,85	0
57	MG	1H	3504	1/1	0.70	0.19	93,93,93,93	0
57	MG	14	3380	1/1	0.70	0.16	85,85,85,85	0
57	MG	1H	3103	1/1	0.70	0.30	82,82,82,82	0
57	MG	1H	3316	1/1	0.70	0.48	89,89,89,89	0
57	MG	1G	1728	1/1	0.70	0.05	114,114,114,114	0
57	MG	2L	102	1/1	0.70	0.63	90,90,90,90	0
57	MG	1H	3380	1/1	0.70	0.13	59,59,59,59	0
57	MG	1H	3154	1/1	0.70	0.14	66,66,66,66	0
57	MG	13	1650	1/1	0.70	0.40	85,85,85,85	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
57	MG	1H	3483	1/1	0.71	0.08	103,103,103,103	0
57	MG	1H	3321	1/1	0.71	0.37	90,90,90,90	0
57	MG	1H	3373	1/1	0.71	0.14	89,89,89,89	0
57	MG	13	1630	1/1	0.71	0.25	87,87,87,87	0
57	MG	1H	3250	1/1	0.71	0.38	93,93,93,93	0
57	MG	14	3298	1/1	0.71	0.24	56,56,56,56	0
57	MG	1H	3282	1/1	0.71	0.43	89,89,89,89	0
57	MG	1H	3260	1/1	0.71	0.43	98,98,98,98	0
57	MG	14	3376	1/1	0.71	0.12	78,78,78,78	0
57	MG	14	3083	1/1	0.71	0.68	87,87,87,87	0
57	MG	1H	3517	1/1	0.71	0.12	87,87,87,87	0
57	MG	1H	3199	1/1	0.71	0.42	78,78,78,78	0
57	MG	1H	3078	1/1	0.71	0.37	79,79,79,79	0
57	MG	14	3261	1/1	0.71	0.20	67,67,67,67	0
57	MG	1H	3227	1/1	0.72	0.41	79,79,79,79	0
57	MG	1H	3464	1/1	0.72	0.18	48,48,48,48	0
57	MG	14	3217	1/1	0.72	0.20	77,77,77,77	0
57	MG	14	3404	1/1	0.72	0.15	100,100,100,100	0
57	MG	14	3087	1/1	0.72	0.54	58,58,58,58	0
57	MG	1H	3155	1/1	0.72	0.21	91,91,91,91	0
57	MG	13	1683	1/1	0.72	0.20	72,72,72,72	0
57	MG	14	3134	1/1	0.72	0.42	71,71,71,71	0
57	MG	1H	3222	1/1	0.72	0.39	64,64,64,64	0
57	MG	14	3148	1/1	0.73	0.36	63,63,63,63	0
57	MG	1H	3009	1/1	0.73	0.43	77,77,77,77	0
57	MG	1H	3258	1/1	0.73	0.39	84,84,84,84	0
57	MG	13	1681	1/1	0.73	0.25	68,68,68,68	0
57	MG	1H	3036	1/1	0.73	0.75	70,70,70,70	0
57	MG	1G	1650	1/1	0.73	0.15	114,114,114,114	0
57	MG	14	3402	1/1	0.73	0.14	118,118,118,118	0
57	MG	1G	1651	1/1	0.73	0.15	105,105,105,105	0
57	MG	1H	3086	1/1	0.73	0.40	66,66,66,66	0
57	MG	1H	3422	1/1	0.73	0.14	101,101,101,101	0
57	MG	1H	3265	1/1	0.73	0.15	77,77,77,77	0
57	MG	1G	1685	1/1	0.74	0.12	91,91,91,91	0
57	MG	14	3396	1/1	0.74	0.14	109,109,109,109	0
57	MG	14	3097	1/1	0.74	0.43	90,90,90,90	0
57	MG	1H	3269	1/1	0.74	0.36	86,86,86,86	0
57	MG	14	3244	1/1	0.74	0.22	58,58,58,58	0
57	MG	1H	3072	1/1	0.74	0.66	72,72,72,72	0
57	MG	1H	3279	1/1	0.74	0.46	76,76,76,76	0
57	MG	14	3140	1/1	0.74	0.34	89,89,89,89	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
57	MG	1G	1731	1/1	0.74	0.08	114,114,114,114	0
57	MG	1G	1696	1/1	0.74	0.13	91,91,91,91	0
57	MG	14	3426	1/1	0.74	0.07	126,126,126,126	0
57	MG	1H	3434	1/1	0.74	0.19	68,68,68,68	0
57	MG	1H	3115	1/1	0.74	0.91	84,84,84,84	0
57	MG	1G	1652	1/1	0.74	0.33	94,94,94,94	0
57	MG	1G	1657	1/1	0.74	0.21	82,82,82,82	0
57	MG	1H	3443	1/1	0.74	0.14	53,53,53,53	0
57	MG	14	3207	1/1	0.74	0.28	85,85,85,85	0
57	MG	1H	3528	1/1	0.74	0.11	96,96,96,96	0
57	MG	1H	3121	1/1	0.74	0.94	80,80,80,80	0
57	MG	14	3391	1/1	0.74	0.24	103,103,103,103	0
57	MG	1H	3278	1/1	0.75	0.31	83,83,83,83	0
57	MG	1H	3322	1/1	0.75	0.32	100,100,100,100	0
57	MG	14	3094	1/1	0.75	0.94	70,70,70,70	0
57	MG	1H	3189	1/1	0.75	0.43	78,78,78,78	0
57	MG	13	1685	1/1	0.75	0.38	91,91,91,91	0
57	MG	14	3191	1/1	0.75	0.31	82,82,82,82	0
57	MG	14	3205	1/1	0.75	0.43	79,79,79,79	0
57	MG	13	1663	1/1	0.75	0.25	90,90,90,90	0
57	MG	1H	3187	1/1	0.75	1.20	81,81,81,81	0
57	MG	14	3077	1/1	0.75	0.20	84,84,84,84	0
57	MG	16	211	1/1	0.75	0.12	99,99,99,99	0
57	MG	13	1665	1/1	0.75	0.30	88,88,88,88	0
57	MG	1H	3294	1/1	0.76	0.15	90,90,90,90	0
57	MG	4E	201	1/1	0.76	0.46	85,85,85,85	0
57	MG	1H	3125	1/1	0.76	0.22	63,63,63,63	0
57	MG	1G	1644	1/1	0.76	0.37	107,107,107,107	0
57	MG	1G	1645	1/1	0.76	0.06	93,93,93,93	0
57	MG	14	3110	1/1	0.76	0.52	72,72,72,72	0
57	MG	14	3370	1/1	0.76	0.24	87,87,87,87	0
57	MG	2K	102	1/1	0.76	0.31	92,92,92,92	0
57	MG	13	1679	1/1	0.76	0.28	86,86,86,86	0
57	MG	14	3007	1/1	0.76	0.65	72,72,72,72	0
57	MG	14	3437	1/1	0.76	0.07	107,107,107,107	0
57	MG	1H	3005	1/1	0.76	0.72	74,74,74,74	0
57	MG	13	1643	1/1	0.76	0.42	86,86,86,86	0
57	MG	13	1625	1/1	0.76	0.31	93,93,93,93	0
57	MG	1H	3201	1/1	0.76	0.36	88,88,88,88	0
57	MG	1H	3221	1/1	0.76	0.28	64,64,64,64	0
57	MG	14	3172	1/1	0.76	0.49	82,82,82,82	0
57	MG	1H	3317	1/1	0.77	0.48	83,83,83,83	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
57	MG	13	1687	1/1	0.77	1.03	82,82,82,82	0
57	MG	14	3137	1/1	0.77	0.42	68,68,68,68	0
57	MG	14	3398	1/1	0.77	0.07	99,99,99,99	0
57	MG	14	3230	1/1	0.77	0.32	81,81,81,81	0
57	MG	1G	1647	1/1	0.77	0.26	102,102,102,102	0
57	MG	1H	3179	1/1	0.77	0.41	67,67,67,67	0
57	MG	14	3025	1/1	0.77	0.27	80,80,80,80	0
57	MG	14	3151	1/1	0.77	0.20	87,87,87,87	0
57	MG	1H	3117	1/1	0.77	0.37	54,54,54,54	0
57	MG	13	1702	1/1	0.77	0.08	107,107,107,107	0
57	MG	1G	1653	1/1	0.77	0.28	103,103,103,103	0
57	MG	1H	3185	1/1	0.77	0.35	90,90,90,90	0
57	MG	1H	3477	1/1	0.77	0.07	83,83,83,83	0
57	MG	1G	1619	1/1	0.77	0.29	86,86,86,86	0
57	MG	14	3351	1/1	0.77	0.18	104,104,104,104	0
57	MG	1G	1621	1/1	0.77	0.74	86,86,86,86	0
57	MG	1H	3157	1/1	0.77	0.13	73,73,73,73	0
57	MG	1G	1724	1/1	0.77	0.08	94,94,94,94	0
57	MG	1G	1638	1/1	0.77	0.11	93,93,93,93	0
57	MG	29	301	1/1	0.77	0.27	75,75,75,75	0
57	MG	1H	3519	1/1	0.77	0.10	83,83,83,83	0
57	MG	14	3215	1/1	0.77	0.18	72,72,72,72	0
57	MG	14	3226	1/1	0.78	0.46	83,83,83,83	0
57	MG	1H	3372	1/1	0.78	0.12	76,76,76,76	0
57	MG	1H	3273	1/1	0.78	0.14	69,69,69,69	0
57	MG	1H	3521	1/1	0.78	0.25	86,86,86,86	0
57	MG	13	1673	1/1	0.78	0.36	80,80,80,80	0
57	MG	14	3152	1/1	0.78	0.65	86,86,86,86	0
57	MG	1H	3397	1/1	0.78	0.17	58,58,58,58	0
57	MG	1H	3526	1/1	0.78	0.11	113,113,113,113	0
57	MG	1H	3308	1/1	0.78	0.35	56,56,56,56	0
57	MG	14	3082	1/1	0.78	0.33	90,90,90,90	0
57	MG	1H	3404	1/1	0.78	0.12	65,65,65,65	0
57	MG	1H	3313	1/1	0.78	0.17	74,74,74,74	0
57	MG	1H	3421	1/1	0.78	0.14	99,99,99,99	0
57	MG	1G	1616	1/1	0.78	0.32	88,88,88,88	0
57	MG	1G	1681	1/1	0.78	0.11	96,96,96,96	0
57	MG	1G	1723	1/1	0.78	0.16	94,94,94,94	0
57	MG	13	1651	1/1	0.78	0.29	97,97,97,97	0
57	MG	1H	3058	1/1	0.78	0.43	77,77,77,77	0
57	MG	13	1746	1/1	0.78	0.12	119,119,119,119	0
57	MG	13	1731	1/1	0.78	0.05	90,90,90,90	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
57	MG	2L	103	1/1	0.78	0.43	75,75,75,75	0
57	MG	1H	3542	1/1	0.79	0.33	90,90,90,90	0
57	MG	1H	3320	1/1	0.79	0.41	80,80,80,80	0
57	MG	14	3232	1/1	0.79	0.28	56,56,56,56	0
57	MG	1H	3101	1/1	0.79	0.14	65,65,65,65	0
57	MG	68	201	1/1	0.79	0.23	78,78,78,78	0
57	MG	13	1695	1/1	0.79	0.11	82,82,82,82	0
57	MG	1H	3206	1/1	0.79	0.24	91,91,91,91	0
57	MG	1H	3207	1/1	0.79	0.71	87,87,87,87	0
57	MG	1H	3171	1/1	0.79	0.30	90,90,90,90	0
57	MG	1H	3085	1/1	0.79	0.42	75,75,75,75	0
57	MG	13	1742	1/1	0.79	0.10	98,98,98,98	0
57	MG	1G	1692	1/1	0.79	0.09	105,105,105,105	0
57	MG	14	3348	1/1	0.79	0.10	101,101,101,101	0
57	MG	9A	101	1/1	0.79	0.25	115,115,115,115	0
57	MG	13	1614	1/1	0.79	0.28	88,88,88,88	0
57	MG	14	3355	1/1	0.79	0.14	107,107,107,107	0
57	MG	14	3112	1/1	0.79	0.43	99,99,99,99	0
57	MG	14	3374	1/1	0.79	0.11	83,83,83,83	0
57	MG	14	3131	1/1	0.79	0.35	70,70,70,70	0
57	MG	1H	3100	1/1	0.79	0.16	62,62,62,62	0
57	MG	1H	3416	1/1	0.79	0.06	89,89,89,89	0
57	MG	1H	3498	1/1	0.79	0.16	85,85,85,85	0
57	MG	1H	3420	1/1	0.79	0.07	102,102,102,102	0
57	MG	1G	1632	1/1	0.80	0.05	99,99,99,99	0
57	MG	14	3198	1/1	0.80	0.20	86,86,86,86	0
57	MG	1G	1711	1/1	0.80	0.12	108,108,108,108	0
57	MG	1H	3067	1/1	0.80	0.17	62,62,62,62	0
57	MG	1G	1683	1/1	0.80	0.04	113,113,113,113	0
57	MG	1H	3123	1/1	0.80	0.60	65,65,65,65	0
57	MG	1H	3348	1/1	0.80	0.14	49,49,49,49	0
57	MG	14	3081	1/1	0.80	0.35	81,81,81,81	0
57	MG	16	203	1/1	0.80	0.12	78,78,78,78	0
57	MG	13	1690	1/1	0.80	0.43	100,100,100,100	0
57	MG	1H	3184	1/1	0.80	0.24	93,93,93,93	0
57	MG	1H	3484	1/1	0.80	0.15	84,84,84,84	0
57	MG	1H	3374	1/1	0.80	0.11	86,86,86,86	0
57	MG	14	3243	1/1	0.80	0.08	82,82,82,82	0
57	MG	14	3163	1/1	0.80	0.84	84,84,84,84	0
57	MG	1H	3161	1/1	0.80	0.33	93,93,93,93	0
57	MG	1H	3003	1/1	0.80	0.47	65,65,65,65	0
57	MG	1H	3139	1/1	0.80	0.14	54,54,54,54	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
57	MG	1G	1676	1/1	0.80	0.07	100,100,100,100	0
58	SPE	1J	208	13/13	0.80	0.22	94,98,105,105	0
57	MG	1G	1664	1/1	0.81	0.19	73,73,73,73	0
57	MG	1G	1674	1/1	0.81	0.18	78,78,78,78	0
57	MG	1G	1620	1/1	0.81	0.27	79,79,79,79	0
57	MG	1H	3008	1/1	0.81	0.47	75,75,75,75	0
57	MG	14	3158	1/1	0.81	0.37	76,76,76,76	0
57	MG	13	1724	1/1	0.81	0.17	73,73,73,73	0
57	MG	13	1684	1/1	0.81	0.30	74,74,74,74	0
57	MG	1H	3330	1/1	0.81	0.17	47,47,47,47	0
57	MG	1H	3414	1/1	0.81	0.06	95,95,95,95	0
57	MG	1H	3165	1/1	0.81	0.20	59,59,59,59	0
57	MG	14	3177	1/1	0.81	0.31	82,82,82,82	0
57	MG	1H	3315	1/1	0.81	0.36	99,99,99,99	0
57	MG	1H	3518	1/1	0.81	0.12	101,101,101,101	0
57	MG	1G	1648	1/1	0.81	0.39	79,79,79,79	0
57	MG	14	3434	1/1	0.81	0.14	115,115,115,115	0
57	MG	1G	1694	1/1	0.81	0.10	94,94,94,94	0
57	MG	13	1657	1/1	0.81	0.41	80,80,80,80	0
57	MG	1H	3088	1/1	0.81	0.22	61,61,61,61	0
57	MG	1G	1697	1/1	0.81	0.07	110,110,110,110	0
57	MG	L8	101	1/1	0.81	0.35	86,86,86,86	0
57	MG	1J	201	1/1	0.81	0.29	86,86,86,86	0
57	MG	1H	3377	1/1	0.81	0.24	75,75,75,75	0
57	MG	14	3378	1/1	0.81	0.11	86,86,86,86	0
57	MG	14	3021	1/1	0.81	0.15	76,76,76,76	0
57	MG	1H	3523	1/1	0.81	0.23	84,84,84,84	0
57	MG	14	3387	1/1	0.81	0.12	89,89,89,89	0
57	MG	35	202	1/1	0.81	0.35	84,84,84,84	0
57	MG	14	3224	1/1	0.81	0.16	113,113,113,113	0
57	MG	1H	3340	1/1	0.82	0.31	70,70,70,70	0
57	MG	1H	3235	1/1	0.82	0.51	99,99,99,99	0
57	MG	14	3324	1/1	0.82	0.25	66,66,66,66	0
57	MG	1H	3364	1/1	0.82	0.12	72,72,72,72	0
57	MG	14	3343	1/1	0.82	0.08	87,87,87,87	0
57	MG	14	3411	1/1	0.82	0.27	93,93,93,93	0
57	MG	13	1740	1/1	0.82	0.05	132,132,132,132	0
57	MG	1H	3270	1/1	0.82	0.35	61,61,61,61	0
57	MG	1H	3527	1/1	0.82	0.11	107,107,107,107	0
57	MG	14	3220	1/1	0.82	0.29	73,73,73,73	0
57	MG	13	1723	1/1	0.82	0.12	83,83,83,83	0
57	MG	14	3168	1/1	0.82	0.27	87,87,87,87	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
57	MG	13	1691	1/1	0.82	0.20	65,65,65,65	0
57	MG	13	1688	1/1	0.82	0.52	72,72,72,72	0
57	MG	14	3379	1/1	0.82	0.09	99,99,99,99	0
57	MG	1H	3048	1/1	0.82	0.25	43,43,43,43	0
57	MG	14	3381	1/1	0.82	0.28	74,74,74,74	0
57	MG	1H	3462	1/1	0.82	0.20	53,53,53,53	0
57	MG	14	3256	1/1	0.82	0.16	54,54,54,54	0
57	MG	1H	3223	1/1	0.82	0.23	80,80,80,80	0
57	MG	1H	3084	1/1	0.82	0.60	68,68,68,68	0
57	MG	14	3062	1/1	0.82	0.86	71,71,71,71	0
57	MG	14	3395	1/1	0.82	0.10	91,91,91,91	0
57	MG	88	202	1/1	0.82	0.32	72,72,72,72	0
58	SPE	14	3446	13/13	0.82	0.28	68,79,87,89	0
57	MG	13	1728	1/1	0.82	0.14	112,112,112,112	0
57	MG	13	1662	1/1	0.83	0.19	76,76,76,76	0
57	MG	14	3104	1/1	0.83	0.19	84,84,84,84	0
57	MG	1G	1722	1/1	0.83	0.12	101,101,101,101	0
57	MG	1H	3122	1/1	0.83	0.27	67,67,67,67	0
57	MG	1G	1682	1/1	0.83	0.08	105,105,105,105	0
57	MG	1H	3296	1/1	0.83	0.30	81,81,81,81	0
57	MG	14	3133	1/1	0.83	0.29	58,58,58,58	0
57	MG	1H	3038	1/1	0.83	0.60	65,65,65,65	0
57	MG	1H	3311	1/1	0.83	0.20	93,93,93,93	0
57	MG	1H	3473	1/1	0.83	0.12	76,76,76,76	0
57	MG	14	3138	1/1	0.83	0.34	86,86,86,86	0
57	MG	14	3239	1/1	0.83	0.17	59,59,59,59	0
57	MG	13	1734	1/1	0.83	0.07	100,100,100,100	0
57	MG	13	1745	1/1	0.83	0.06	111,111,111,111	0
57	MG	1H	3111	1/1	0.83	0.50	73,73,73,73	0
57	MG	14	3149	1/1	0.83	0.67	71,71,71,71	0
57	MG	14	3274	1/1	0.83	0.14	81,81,81,81	0
57	MG	1H	3228	1/1	0.83	0.34	70,70,70,70	0
57	MG	1H	3486	1/1	0.83	0.10	89,89,89,89	0
57	MG	1H	3530	1/1	0.83	0.10	98,98,98,98	0
57	MG	14	3027	1/1	0.83	0.25	76,76,76,76	0
57	MG	1H	3183	1/1	0.83	0.25	73,73,73,73	0
57	MG	1H	3149	1/1	0.83	0.29	86,86,86,86	0
57	MG	14	3317	1/1	0.83	0.16	64,64,64,64	0
57	MG	14	3165	1/1	0.83	0.44	74,74,74,74	0
57	MG	13	1708	1/1	0.83	0.09	95,95,95,95	0
57	MG	14	3442	1/1	0.83	0.21	75,75,75,75	0
57	MG	1H	3327	1/1	0.83	0.11	65,65,65,65	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
57	MG	1G	1709	1/1	0.83	0.14	87,87,87,87	0
57	MG	1H	3087	1/1	0.83	0.38	79,79,79,79	0
57	MG	1G	1662	1/1	0.83	0.90	94,94,94,94	0
57	MG	14	3187	1/1	0.83	0.33	90,90,90,90	0
57	MG	14	3085	1/1	0.83	0.47	81,81,81,81	0
57	MG	13	1682	1/1	0.83	0.28	85,85,85,85	0
57	MG	35	201	1/1	0.83	0.16	86,86,86,86	0
57	MG	13	1672	1/1	0.83	0.83	86,86,86,86	0
57	MG	F8	101	1/1	0.83	0.42	86,86,86,86	0
57	MG	1H	3516	1/1	0.83	0.09	79,79,79,79	0
57	MG	13	1699	1/1	0.84	0.09	102,102,102,102	0
57	MG	14	3246	1/1	0.84	0.18	72,72,72,72	0
57	MG	1H	3522	1/1	0.84	0.20	91,91,91,91	0
57	MG	1H	3307	1/1	0.84	0.64	72,72,72,72	0
57	MG	14	3272	1/1	0.84	0.07	78,78,78,78	0
57	MG	1H	3418	1/1	0.84	0.09	86,86,86,86	0
57	MG	1G	1670	1/1	0.84	0.21	88,88,88,88	0
57	MG	14	3116	1/1	0.84	0.28	66,66,66,66	0
57	MG	1H	3220	1/1	0.84	0.15	89,89,89,89	0
57	MG	14	3406	1/1	0.84	0.10	90,90,90,90	0
57	MG	14	3190	1/1	0.84	0.33	79,79,79,79	0
57	MG	14	3410	1/1	0.84	0.07	116,116,116,116	0
57	MG	1G	1704	1/1	0.84	0.07	107,107,107,107	0
57	MG	1H	3248	1/1	0.84	0.39	96,96,96,96	0
57	MG	14	3421	1/1	0.84	0.20	98,98,98,98	0
57	MG	14	3301	1/1	0.84	0.07	117,117,117,117	0
57	MG	14	3314	1/1	0.84	0.13	83,83,83,83	0
57	MG	14	3199	1/1	0.84	0.56	68,68,68,68	0
57	MG	14	3427	1/1	0.84	0.18	92,92,92,92	0
57	MG	1H	3370	1/1	0.84	0.17	59,59,59,59	0
57	MG	1G	1678	1/1	0.84	0.15	73,73,73,73	0
57	MG	1H	3127	1/1	0.84	0.37	84,84,84,84	0
57	MG	14	3211	1/1	0.84	0.42	85,85,85,85	0
57	MG	14	3213	1/1	0.84	0.39	76,76,76,76	0
57	MG	1H	3158	1/1	0.84	0.48	71,71,71,71	0
57	MG	1H	3190	1/1	0.84	0.41	75,75,75,75	0
57	MG	14	3362	1/1	0.84	0.09	97,97,97,97	0
57	MG	1H	3281	1/1	0.84	0.21	67,67,67,67	0
57	MG	1H	3544	1/1	0.84	0.08	84,84,84,84	0
57	MG	13	1653	1/1	0.84	0.53	94,94,94,94	0
57	MG	1G	1720	1/1	0.84	0.05	106,106,106,106	0
57	MG	1H	3098	1/1	0.84	0.53	78,78,78,78	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
57	MG	13	1623	1/1	0.84	0.40	80,80,80,80	0
57	MG	14	3161	1/1	0.84	0.88	79,79,79,79	0
57	MG	1H	3325	1/1	0.84	0.38	88,88,88,88	0
57	MG	13	1697	1/1	0.84	0.11	78,78,78,78	0
57	MG	1G	1729	1/1	0.84	0.10	104,104,104,104	0
57	MG	14	3222	1/1	0.85	0.58	88,88,88,88	0
57	MG	14	3052	1/1	0.85	0.46	79,79,79,79	0
57	MG	41	201	1/1	0.85	0.11	62,62,62,62	0
57	MG	1H	3323	1/1	0.85	0.23	75,75,75,75	0
57	MG	14	3066	1/1	0.85	0.36	59,59,59,59	0
57	MG	14	3075	1/1	0.85	0.35	89,89,89,89	0
57	MG	1H	3449	1/1	0.85	0.41	80,80,80,80	0
57	MG	13	1727	1/1	0.85	0.17	90,90,90,90	0
57	MG	13	1669	1/1	0.85	0.30	92,92,92,92	0
57	MG	14	3394	1/1	0.85	0.14	63,63,63,63	0
57	MG	14	3252	1/1	0.85	0.25	62,62,62,62	0
57	MG	13	1642	1/1	0.85	0.17	72,72,72,72	0
57	MG	1H	3410	1/1	0.85	0.08	106,106,106,106	0
57	MG	14	3271	1/1	0.85	0.06	72,72,72,72	0
57	MG	1H	3332	1/1	0.85	0.15	50,50,50,50	0
57	MG	1H	3276	1/1	0.85	0.36	90,90,90,90	0
57	MG	14	3281	1/1	0.85	0.07	95,95,95,95	0
57	MG	2K	103	1/1	0.85	0.38	89,89,89,89	0
57	MG	14	3181	1/1	0.85	0.34	81,81,81,81	0
57	MG	14	3286	1/1	0.85	0.06	93,93,93,93	0
57	MG	14	3288	1/1	0.85	0.15	77,77,77,77	0
57	MG	1H	3350	1/1	0.85	0.20	57,57,57,57	0
57	MG	14	3420	1/1	0.85	0.08	96,96,96,96	0
57	MG	14	3292	1/1	0.85	0.11	85,85,85,85	0
57	MG	1H	3106	1/1	0.85	0.18	68,68,68,68	0
57	MG	1H	3108	1/1	0.85	0.32	69,69,69,69	0
57	MG	1H	3191	1/1	0.85	0.29	72,72,72,72	0
57	MG	42	201	1/1	0.85	0.11	116,116,116,116	0
57	MG	1H	3429	1/1	0.85	0.18	56,56,56,56	0
57	MG	14	3203	1/1	0.85	0.43	93,93,93,93	0
57	MG	1H	3537	1/1	0.85	0.21	61,61,61,61	0
57	MG	1H	3197	1/1	0.85	0.35	80,80,80,80	0
57	MG	14	3331	1/1	0.85	0.16	79,79,79,79	0
57	MG	14	3335	1/1	0.85	0.14	63,63,63,63	0
57	MG	1H	3436	1/1	0.85	0.12	65,65,65,65	0
57	MG	1H	3545	1/1	0.85	0.07	116,116,116,116	0
57	MG	1H	3511	1/1	0.85	0.05	92,92,92,92	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
57	MG	1H	3082	1/1	0.85	0.39	76,76,76,76	0
57	MG	14	3352	1/1	0.85	0.11	84,84,84,84	0
57	MG	1J	207	1/1	0.85	0.10	92,92,92,92	0
57	MG	16	208	1/1	0.85	0.37	79,79,79,79	0
57	MG	13	1700	1/1	0.85	0.07	86,86,86,86	0
57	MG	14	3367	1/1	0.85	0.08	99,99,99,99	0
57	MG	14	3368	1/1	0.85	0.12	74,74,74,74	0
57	MG	31	302	1/1	0.85	0.21	73,73,73,73	0
57	MG	M5	101	1/1	0.85	0.10	86,86,86,86	0
58	SPE	13	1748	13/13	0.85	0.24	60,77,82,87	0
58	SPE	1G	1733	13/13	0.85	0.10	98,101,104,105	0
57	MG	14	3032	1/1	0.85	0.45	80,80,80,80	0
57	MG	14	3041	1/1	0.85	0.63	76,76,76,76	0
57	MG	14	3276	1/1	0.86	0.07	95,95,95,95	0
57	MG	1H	3075	1/1	0.86	0.19	61,61,61,61	0
57	MG	1H	3145	1/1	0.86	0.61	62,62,62,62	0
57	MG	14	3283	1/1	0.86	0.09	71,71,71,71	0
57	MG	1H	3513	1/1	0.86	0.11	80,80,80,80	0
57	MG	1H	3424	1/1	0.86	0.05	100,100,100,100	0
57	MG	1G	1725	1/1	0.86	0.11	113,113,113,113	0
57	MG	1H	3303	1/1	0.86	0.47	76,76,76,76	0
57	MG	1H	3352	1/1	0.86	0.08	84,84,84,84	0
57	MG	14	3200	1/1	0.86	0.28	98,98,98,98	0
57	MG	1H	3099	1/1	0.86	0.37	84,84,84,84	0
57	MG	1H	3231	1/1	0.86	0.21	67,67,67,67	0
57	MG	3A	201	1/1	0.86	0.25	77,77,77,77	0
57	MG	4A	201	1/1	0.86	0.21	96,96,96,96	0
57	MG	14	3209	1/1	0.86	0.33	65,65,65,65	0
57	MG	14	3319	1/1	0.86	0.10	78,78,78,78	0
57	MG	13	1615	1/1	0.86	0.23	73,73,73,73	0
57	MG	1H	3444	1/1	0.86	0.10	73,73,73,73	0
57	MG	1G	1624	1/1	0.86	0.43	76,76,76,76	0
57	MG	1H	3233	1/1	0.86	0.19	110,110,110,110	0
57	MG	14	3004	1/1	0.86	0.23	73,73,73,73	0
57	MG	14	3429	1/1	0.86	0.09	99,99,99,99	0
57	MG	1H	3234	1/1	0.86	0.74	76,76,76,76	0
57	MG	1H	3458	1/1	0.86	0.14	82,82,82,82	0
57	MG	1H	3113	1/1	0.86	0.26	64,64,64,64	0
57	MG	1H	3378	1/1	0.86	0.09	65,65,65,65	0
57	MG	14	3353	1/1	0.86	0.12	90,90,90,90	0
57	MG	1H	3466	1/1	0.86	0.03	89,89,89,89	0
57	MG	14	3359	1/1	0.86	0.06	86,86,86,86	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
57	MG	1H	3124	1/1	0.86	0.52	73,73,73,73	0
57	MG	1H	3388	1/1	0.86	0.18	58,58,58,58	0
57	MG	1H	3277	1/1	0.86	0.53	82,82,82,82	0
57	MG	13	1632	1/1	0.86	0.39	90,90,90,90	0
57	MG	1H	3200	1/1	0.86	0.34	73,73,73,73	0
57	MG	13	1664	1/1	0.86	0.19	69,69,69,69	0
57	MG	1H	3164	1/1	0.86	0.14	64,64,64,64	0
57	MG	25	202	1/1	0.86	0.17	110,110,110,110	0
57	MG	1H	3284	1/1	0.86	0.34	71,71,71,71	0
57	MG	1H	3259	1/1	0.86	0.43	92,92,92,92	0
57	MG	14	3078	1/1	0.86	0.35	64,64,64,64	0
57	MG	1G	1666	1/1	0.86	0.08	103,103,103,103	0
57	MG	1H	3331	1/1	0.86	0.23	53,53,53,53	0
57	MG	14	3273	1/1	0.86	0.16	70,70,70,70	0
57	MG	13	1674	1/1	0.86	0.38	92,92,92,92	0
57	MG	1H	3488	1/1	0.87	0.07	88,88,88,88	0
57	MG	1G	1727	1/1	0.87	0.09	93,93,93,93	0
57	MG	14	3316	1/1	0.87	0.09	90,90,90,90	0
57	MG	1H	3493	1/1	0.87	0.05	102,102,102,102	0
57	MG	1G	1689	1/1	0.87	0.16	89,89,89,89	0
57	MG	14	3223	1/1	0.87	0.31	87,87,87,87	0
57	MG	1H	3224	1/1	0.87	0.44	90,90,90,90	0
57	MG	14	3225	1/1	0.87	0.11	95,95,95,95	0
57	MG	14	3334	1/1	0.87	0.07	94,94,94,94	0
57	MG	14	3415	1/1	0.87	0.10	101,101,101,101	0
57	MG	13	1660	1/1	0.87	0.50	96,96,96,96	0
57	MG	14	3419	1/1	0.87	0.20	110,110,110,110	0
57	MG	14	3341	1/1	0.87	0.08	91,91,91,91	0
57	MG	1H	3209	1/1	0.87	0.41	52,52,52,52	0
57	MG	1H	3042	1/1	0.87	0.41	67,67,67,67	0
57	MG	14	3093	1/1	0.87	0.24	79,79,79,79	0
57	MG	14	3424	1/1	0.87	0.13	94,94,94,94	0
57	MG	1H	3080	1/1	0.87	0.52	103,103,103,103	0
57	MG	14	3176	1/1	0.87	0.35	69,69,69,69	0
57	MG	1H	3292	1/1	0.87	0.23	84,84,84,84	0
57	MG	1H	3062	1/1	0.87	0.26	40,40,40,40	0
57	MG	14	3431	1/1	0.87	0.23	60,60,60,60	0
57	MG	14	3357	1/1	0.87	0.09	96,96,96,96	0
57	MG	13	1737	1/1	0.87	0.10	98,98,98,98	0
57	MG	1H	3394	1/1	0.87	0.07	74,74,74,74	0
57	MG	14	3268	1/1	0.87	0.13	86,86,86,86	0
57	MG	1H	3070	1/1	0.87	0.40	56,56,56,56	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
57	MG	14	3369	1/1	0.87	0.11	92,92,92,92	0
57	MG	1H	3450	1/1	0.87	0.20	59,59,59,59	0
57	MG	14	3129	1/1	0.87	0.47	75,75,75,75	0
57	MG	1H	3102	1/1	0.87	0.59	66,66,66,66	0
57	MG	1H	3202	1/1	0.87	0.98	82,82,82,82	0
57	MG	14	3201	1/1	0.87	0.73	95,95,95,95	0
57	MG	1H	3406	1/1	0.87	0.16	46,46,46,46	0
57	MG	1H	3338	1/1	0.87	0.17	63,63,63,63	0
57	MG	14	3383	1/1	0.87	0.14	92,92,92,92	0
57	MG	1G	1607	1/1	0.87	0.27	92,92,92,92	0
57	MG	1H	3275	1/1	0.87	0.60	67,67,67,67	0
57	MG	1H	3051	1/1	0.87	0.47	76,76,76,76	0
57	MG	1H	3312	1/1	0.87	0.23	94,94,94,94	0
57	MG	1H	3056	1/1	0.87	0.43	73,73,73,73	0
57	MG	1G	1623	1/1	0.87	0.49	75,75,75,75	0
58	SPE	14	3445	13/13	0.87	0.36	70,76,79,79	0
57	MG	1H	3360	1/1	0.87	0.15	76,76,76,76	0
57	MG	1H	3177	1/1	0.87	0.61	77,77,77,77	0
57	MG	1H	3019	1/1	0.88	0.30	61,61,61,61	0
57	MG	14	3155	1/1	0.88	0.30	80,80,80,80	0
57	MG	1H	3367	1/1	0.88	0.15	56,56,56,56	0
57	MG	1H	3309	1/1	0.88	0.72	74,74,74,74	0
57	MG	1G	1693	1/1	0.88	0.06	84,84,84,84	0
57	MG	14	3264	1/1	0.88	0.21	52,52,52,52	0
57	MG	1H	3105	1/1	0.88	0.43	79,79,79,79	0
57	MG	1H	3442	1/1	0.88	0.21	69,69,69,69	0
57	MG	1H	3089	1/1	0.88	0.28	66,66,66,66	0
57	MG	1H	3092	1/1	0.88	0.18	74,74,74,74	0
57	MG	1H	3445	1/1	0.88	0.16	44,44,44,44	0
57	MG	14	3056	1/1	0.88	0.32	80,80,80,80	0
57	MG	14	3280	1/1	0.88	0.11	97,97,97,97	0
57	MG	1H	3094	1/1	0.88	0.50	68,68,68,68	0
57	MG	1G	1633	1/1	0.88	0.17	89,89,89,89	0
57	MG	14	3072	1/1	0.88	0.16	57,57,57,57	0
57	MG	1G	1703	1/1	0.88	0.08	113,113,113,113	0
57	MG	1H	3242	1/1	0.88	0.12	74,74,74,74	0
57	MG	1H	3245	1/1	0.88	0.52	78,78,78,78	0
57	MG	1H	3452	1/1	0.88	0.09	75,75,75,75	0
57	MG	1H	3134	1/1	0.88	0.23	44,44,44,44	0
57	MG	14	3193	1/1	0.88	0.38	95,95,95,95	0
57	MG	1H	3391	1/1	0.88	0.19	50,50,50,50	0
57	MG	13	1647	1/1	0.88	0.27	91,91,91,91	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
57	MG	1H	3395	1/1	0.88	0.10	84,84,84,84	0
57	MG	1H	3249	1/1	0.88	0.30	68,68,68,68	0
57	MG	1H	3533	1/1	0.88	0.20	44,44,44,44	0
57	MG	14	3204	1/1	0.88	0.78	80,80,80,80	0
57	MG	1H	3474	1/1	0.88	0.09	82,82,82,82	0
57	MG	14	3323	1/1	0.88	0.12	83,83,83,83	0
57	MG	13	1620	1/1	0.88	0.29	57,57,57,57	0
57	MG	1G	1721	1/1	0.88	0.07	107,107,107,107	0
57	MG	1G	1661	1/1	0.88	0.18	99,99,99,99	0
57	MG	14	3332	1/1	0.88	0.10	80,80,80,80	0
57	MG	14	3210	1/1	0.88	0.17	80,80,80,80	0
57	MG	1H	3147	1/1	0.88	0.43	64,64,64,64	0
57	MG	1H	3286	1/1	0.88	0.29	87,87,87,87	0
57	MG	1H	3065	1/1	0.88	0.18	50,50,50,50	0
57	MG	1G	1669	1/1	0.88	0.11	99,99,99,99	0
57	MG	14	3126	1/1	0.88	0.22	75,75,75,75	0
57	MG	1H	3203	1/1	0.88	0.36	74,74,74,74	0
57	MG	13	1739	1/1	0.88	0.05	92,92,92,92	0
57	MG	1J	202	1/1	0.88	0.09	84,84,84,84	0
57	MG	13	1635	1/1	0.88	0.22	99,99,99,99	0
57	MG	13	1706	1/1	0.88	0.09	103,103,103,103	0
57	MG	1H	3297	1/1	0.88	0.17	78,78,78,78	0
57	MG	14	3358	1/1	0.88	0.09	88,88,88,88	0
57	MG	1H	3301	1/1	0.88	0.27	70,70,70,70	0
57	MG	1H	3502	1/1	0.88	0.10	90,90,90,90	0
57	MG	14	3366	1/1	0.88	0.12	98,98,98,98	0
57	MG	13	1637	1/1	0.88	0.11	79,79,79,79	0
57	MG	14	3227	1/1	0.88	0.27	76,76,76,76	0
57	MG	88	203	1/1	0.88	0.20	76,76,76,76	0
57	MG	1H	3267	1/1	0.88	0.53	68,68,68,68	0
57	MG	14	3238	1/1	0.88	0.15	66,66,66,66	0
57	MG	14	3375	1/1	0.88	0.06	84,84,84,84	0
57	MG	1H	3425	1/1	0.88	0.17	74,74,74,74	0
57	MG	1G	1605	1/1	0.88	0.31	82,82,82,82	0
57	MG	14	3039	1/1	0.89	0.41	65,65,65,65	0
57	MG	1H	3237	1/1	0.89	0.17	73,73,73,73	0
57	MG	13	1626	1/1	0.89	0.28	67,67,67,67	0
57	MG	14	3167	1/1	0.89	0.28	76,76,76,76	0
57	MG	1G	1698	1/1	0.89	0.12	105,105,105,105	0
57	MG	14	3385	1/1	0.89	0.13	80,80,80,80	0
57	MG	1H	3241	1/1	0.89	0.13	64,64,64,64	0
57	MG	1G	1637	1/1	0.89	0.12	113,113,113,113	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
57	MG	1H	3379	1/1	0.89	0.17	58,58,58,58	0
57	MG	14	3275	1/1	0.89	0.07	74,74,74,74	0
57	MG	1H	3495	1/1	0.89	0.06	94,94,94,94	0
57	MG	1H	3541	1/1	0.89	0.10	67,67,67,67	0
57	MG	14	3178	1/1	0.89	0.50	92,92,92,92	0
57	MG	14	3179	1/1	0.89	0.23	71,71,71,71	0
57	MG	1H	3172	1/1	0.89	0.25	84,84,84,84	0
57	MG	14	3183	1/1	0.89	0.61	65,65,65,65	0
57	MG	14	3400	1/1	0.89	0.09	76,76,76,76	0
57	MG	1G	1646	1/1	0.89	0.07	83,83,83,83	0
57	MG	14	3287	1/1	0.89	0.07	73,73,73,73	0
57	MG	13	1616	1/1	0.89	0.29	82,82,82,82	0
57	MG	1H	3128	1/1	0.89	0.14	79,79,79,79	0
57	MG	14	3408	1/1	0.89	0.07	111,111,111,111	0
57	MG	1H	3392	1/1	0.89	0.20	52,52,52,52	0
57	MG	16	204	1/1	0.89	0.26	70,70,70,70	0
57	MG	14	3294	1/1	0.89	0.11	114,114,114,114	0
57	MG	14	3413	1/1	0.89	0.27	81,81,81,81	0
57	MG	16	205	1/1	0.89	0.10	66,66,66,66	0
57	MG	1H	3130	1/1	0.89	0.72	87,87,87,87	0
57	MG	1H	3193	1/1	0.89	0.51	93,93,93,93	0
57	MG	14	3307	1/1	0.89	0.15	72,72,72,72	0
57	MG	1H	3447	1/1	0.89	0.12	66,66,66,66	0
57	MG	11	301	1/1	0.89	0.64	60,60,60,60	0
57	MG	1H	3304	1/1	0.89	0.42	85,85,85,85	0
57	MG	14	3099	1/1	0.89	0.34	77,77,77,77	0
57	MG	14	3425	1/1	0.89	0.10	91,91,91,91	0
57	MG	1H	3401	1/1	0.89	0.20	63,63,63,63	0
57	MG	1G	1667	1/1	0.89	0.12	90,90,90,90	0
57	MG	1G	1668	1/1	0.89	0.06	95,95,95,95	0
57	MG	1H	3195	1/1	0.89	0.16	59,59,59,59	0
57	MG	14	3113	1/1	0.89	0.31	57,57,57,57	0
57	MG	14	3432	1/1	0.89	0.15	103,103,103,103	0
57	MG	14	3433	1/1	0.89	0.11	69,69,69,69	0
57	MG	88	201	1/1	0.89	0.16	78,78,78,78	0
57	MG	5I	101	1/1	0.89	0.08	80,80,80,80	0
57	MG	1H	3006	1/1	0.89	0.43	71,71,71,71	0
57	MG	1H	3280	1/1	0.89	0.54	68,68,68,68	0
57	MG	J8	101	1/1	0.89	0.61	79,79,79,79	0
57	MG	13	1710	1/1	0.89	0.10	82,82,82,82	0
57	MG	P8	101	1/1	0.89	0.34	71,71,71,71	0
57	MG	1H	3214	1/1	0.89	0.26	86,86,86,86	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
57	MG	1H	3469	1/1	0.89	0.09	93,93,93,93	0
57	MG	1G	1611	1/1	0.89	0.68	77,77,77,77	0
57	MG	4L	102	1/1	0.89	0.11	108,108,108,108	0
57	MG	1H	3114	1/1	0.89	0.66	67,67,67,67	0
57	MG	1G	1618	1/1	0.89	0.24	89,89,89,89	0
57	MG	1H	3285	1/1	0.89	0.41	96,96,96,96	0
57	MG	14	3363	1/1	0.89	0.09	102,102,102,102	0
57	MG	14	3365	1/1	0.89	0.17	96,96,96,96	0
57	MG	1H	3371	1/1	0.89	0.14	56,56,56,56	0
57	MG	14	3236	1/1	0.89	0.15	70,70,70,70	0
57	MG	C5	201	1/1	0.89	0.08	103,103,103,103	0
57	MG	14	3154	1/1	0.89	0.14	87,87,87,87	0
57	MG	1H	3478	1/1	0.89	0.06	78,78,78,78	0
57	MG	13	1735	1/1	0.89	0.08	111,111,111,111	0
57	MG	1H	3287	1/1	0.89	0.39	78,78,78,78	0
57	MG	14	3160	1/1	0.89	0.32	92,92,92,92	0
57	MG	1G	1625	1/1	0.89	0.12	98,98,98,98	0
57	MG	14	3267	1/1	0.90	0.08	86,86,86,86	0
57	MG	1H	3456	1/1	0.90	0.15	41,41,41,41	0
57	MG	14	3035	1/1	0.90	0.85	79,79,79,79	0
57	MG	14	3384	1/1	0.90	0.07	88,88,88,88	0
57	MG	1H	3390	1/1	0.90	0.10	68,68,68,68	0
57	MG	14	3040	1/1	0.90	0.40	72,72,72,72	0
57	MG	14	3171	1/1	0.90	0.16	57,57,57,57	0
57	MG	14	3389	1/1	0.90	0.17	94,94,94,94	0
57	MG	1H	3162	1/1	0.90	0.32	68,68,68,68	0
57	MG	1H	3037	1/1	0.90	0.35	71,71,71,71	0
57	MG	14	3392	1/1	0.90	0.05	112,112,112,112	0
57	MG	2K	101	1/1	0.90	0.31	63,63,63,63	0
57	MG	1H	3531	1/1	0.90	0.21	76,76,76,76	0
57	MG	1G	1636	1/1	0.90	0.07	91,91,91,91	0
57	MG	14	3063	1/1	0.90	0.36	52,52,52,52	0
57	MG	1H	3167	1/1	0.90	0.14	60,60,60,60	0
57	MG	1H	3471	1/1	0.90	0.07	73,73,73,73	0
57	MG	14	3399	1/1	0.90	0.14	95,95,95,95	0
57	MG	13	1667	1/1	0.90	0.85	96,96,96,96	0
57	MG	14	3401	1/1	0.90	0.29	85,85,85,85	0
57	MG	1H	3044	1/1	0.90	0.67	81,81,81,81	0
57	MG	1H	3126	1/1	0.90	0.22	75,75,75,75	0
57	MG	1H	3176	1/1	0.90	0.34	62,62,62,62	0
57	MG	13	1738	1/1	0.90	0.10	70,70,70,70	0
57	MG	14	3407	1/1	0.90	0.04	83,83,83,83	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
57	MG	16	201	1/1	0.90	0.16	83,83,83,83	0
57	MG	14	3194	1/1	0.90	0.69	87,87,87,87	0
57	MG	14	3296	1/1	0.90	0.20	62,62,62,62	0
57	MG	13	1649	1/1	0.90	0.23	72,72,72,72	0
57	MG	14	3412	1/1	0.90	0.10	101,101,101,101	0
57	MG	1G	1713	1/1	0.90	0.13	113,113,113,113	0
57	MG	14	3305	1/1	0.90	0.10	78,78,78,78	0
57	MG	13	1609	1/1	0.90	0.25	71,71,71,71	0
57	MG	14	3418	1/1	0.90	0.09	101,101,101,101	0
57	MG	14	3308	1/1	0.90	0.23	58,58,58,58	0
57	MG	13	1730	1/1	0.90	0.08	81,81,81,81	0
57	MG	1G	1716	1/1	0.90	0.07	92,92,92,92	0
57	MG	1H	3255	1/1	0.90	0.23	73,73,73,73	0
57	MG	1G	1654	1/1	0.90	0.36	94,94,94,94	0
57	MG	13	1670	1/1	0.90	0.23	100,100,100,100	0
57	MG	14	3101	1/1	0.90	0.26	90,90,90,90	0
57	MG	1G	1660	1/1	0.90	0.28	75,75,75,75	0
57	MG	1H	3137	1/1	0.90	0.17	57,57,57,57	0
57	MG	1H	3356	1/1	0.90	0.12	75,75,75,75	0
57	MG	1H	3357	1/1	0.90	0.20	62,62,62,62	0
57	MG	1H	3423	1/1	0.90	0.08	66,66,66,66	0
57	MG	1G	1726	1/1	0.90	0.06	113,113,113,113	0
57	MG	1H	3358	1/1	0.90	0.15	40,40,40,40	0
57	MG	78	201	1/1	0.90	0.07	57,57,57,57	0
57	MG	13	1633	1/1	0.90	0.21	87,87,87,87	0
57	MG	1H	3299	1/1	0.90	0.13	78,78,78,78	0
57	MG	1G	1672	1/1	0.90	0.10	92,92,92,92	0
57	MG	1H	3140	1/1	0.90	0.20	40,40,40,40	0
57	MG	14	3440	1/1	0.90	0.10	98,98,98,98	0
57	MG	1H	3141	1/1	0.90	0.31	66,66,66,66	0
57	MG	13	1619	1/1	0.90	0.22	53,53,53,53	0
57	MG	13	1719	1/1	0.90	0.10	71,71,71,71	0
57	MG	1H	3116	1/1	0.90	0.18	82,82,82,82	0
57	MG	14	3229	1/1	0.90	0.17	90,90,90,90	0
57	MG	13	1624	1/1	0.90	0.12	93,93,93,93	0
57	MG	1H	3097	1/1	0.90	0.49	83,83,83,83	0
57	MG	1G	1610	1/1	0.90	0.24	69,69,69,69	0
57	MG	14	3005	1/1	0.90	0.30	50,50,50,50	0
57	MG	1H	3194	1/1	0.90	0.26	71,71,71,71	0
57	MG	1H	3119	1/1	0.90	0.21	62,62,62,62	0
57	MG	1H	3033	1/1	0.90	0.22	73,73,73,73	0
57	MG	14	3371	1/1	0.90	0.10	90,90,90,90	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
57	MG	14	3373	1/1	0.90	0.13	97,97,97,97	0
57	MG	E5	101	1/1	0.90	0.08	100,100,100,100	0
57	MG	14	3024	1/1	0.90	0.13	77,77,77,77	0
57	MG	14	3159	1/1	0.90	0.39	93,93,93,93	0
57	MG	1H	3386	1/1	0.90	0.16	48,48,48,48	0
57	MG	14	3377	1/1	0.90	0.09	64,64,64,64	0
57	MG	13	1656	1/1	0.90	0.25	87,87,87,87	0
57	MG	1H	3455	1/1	0.90	0.15	42,42,42,42	0
57	MG	14	3195	1/1	0.91	0.27	78,78,78,78	0
57	MG	14	3289	1/1	0.91	0.06	90,90,90,90	0
57	MG	14	3196	1/1	0.91	0.44	68,68,68,68	0
57	MG	1H	3181	1/1	0.91	0.16	94,94,94,94	0
57	MG	1H	3152	1/1	0.91	0.31	51,51,51,51	0
57	MG	1H	3027	1/1	0.91	0.35	84,84,84,84	0
57	MG	1G	1673	1/1	0.91	0.17	71,71,71,71	0
57	MG	14	3202	1/1	0.91	0.26	83,83,83,83	0
57	MG	Q8	101	1/1	0.91	0.26	81,81,81,81	0
57	MG	1H	3385	1/1	0.91	0.08	77,77,77,77	0
57	MG	1G	1606	1/1	0.91	0.13	84,84,84,84	0
57	MG	14	3123	1/1	0.91	0.38	60,60,60,60	0
57	MG	13	1718	1/1	0.91	0.07	88,88,88,88	0
57	MG	14	3313	1/1	0.91	0.15	87,87,87,87	0
57	MG	1H	3239	1/1	0.91	0.51	92,92,92,92	0
57	MG	1H	3208	1/1	0.91	0.44	78,78,78,78	0
57	MG	1G	1612	1/1	0.91	0.20	82,82,82,82	0
57	MG	1H	3109	1/1	0.91	0.34	79,79,79,79	0
57	MG	14	3002	1/1	0.91	0.70	68,68,68,68	0
57	MG	13	1602	1/1	0.91	0.26	78,78,78,78	0
57	MG	13	1613	1/1	0.91	0.18	81,81,81,81	0
57	MG	14	3330	1/1	0.91	0.13	64,64,64,64	0
57	MG	13	1603	1/1	0.91	0.12	116,116,116,116	0
57	MG	1H	3329	1/1	0.91	0.20	50,50,50,50	0
57	MG	14	3016	1/1	0.91	0.34	63,63,63,63	0
57	MG	1G	1622	1/1	0.91	0.35	85,85,85,85	0
57	MG	14	3338	1/1	0.91	0.08	81,81,81,81	0
57	MG	1H	3467	1/1	0.91	0.08	85,85,85,85	0
57	MG	1H	3163	1/1	0.91	0.20	74,74,74,74	0
57	MG	14	3346	1/1	0.91	0.07	92,92,92,92	0
57	MG	13	1646	1/1	0.91	0.32	97,97,97,97	0
57	MG	1G	1629	1/1	0.91	0.14	97,97,97,97	0
57	MG	14	3156	1/1	0.91	0.16	71,71,71,71	0
57	MG	1H	3251	1/1	0.91	0.22	77,77,77,77	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
57	MG	1H	3336	1/1	0.91	0.16	50,50,50,50	0
57	MG	1H	3536	1/1	0.91	0.17	60,60,60,60	0
57	MG	14	3356	1/1	0.91	0.10	67,67,67,67	0
57	MG	14	3235	1/1	0.91	0.21	65,65,65,65	0
57	MG	1H	3252	1/1	0.91	0.49	81,81,81,81	0
57	MG	1H	3254	1/1	0.91	0.90	75,75,75,75	0
57	MG	13	1636	1/1	0.91	0.28	103,103,103,103	0
57	MG	14	3241	1/1	0.91	0.09	100,100,100,100	0
57	MG	1H	3482	1/1	0.91	0.20	102,102,102,102	0
57	MG	1H	3349	1/1	0.91	0.19	67,67,67,67	0
57	MG	14	3439	1/1	0.91	0.14	99,99,99,99	0
57	MG	14	3166	1/1	0.91	0.76	82,82,82,82	0
57	MG	14	3441	1/1	0.91	0.26	102,102,102,102	0
57	MG	14	3247	1/1	0.91	0.19	60,60,60,60	0
57	MG	1H	3417	1/1	0.91	0.11	74,74,74,74	0
57	MG	14	3444	1/1	0.91	0.27	85,85,85,85	0
57	MG	1H	3192	1/1	0.91	0.27	76,76,76,76	0
57	MG	1H	3079	1/1	0.91	0.28	45,45,45,45	0
57	MG	13	1608	1/1	0.91	0.13	71,71,71,71	0
57	MG	1H	3494	1/1	0.91	0.09	98,98,98,98	0
57	MG	16	207	1/1	0.91	0.08	84,84,84,84	0
57	MG	1H	3169	1/1	0.91	0.93	82,82,82,82	0
57	MG	1H	3262	1/1	0.91	0.24	71,71,71,71	0
57	MG	13	1659	1/1	0.91	0.64	85,85,85,85	0
57	MG	1G	1655	1/1	0.91	0.14	70,70,70,70	0
57	MG	1H	3012	1/1	0.91	0.22	84,84,84,84	0
57	MG	1H	3306	1/1	0.91	0.29	70,70,70,70	0
57	MG	14	3185	1/1	0.91	0.12	76,76,76,76	0
57	MG	1H	3175	1/1	0.91	0.14	64,64,64,64	0
57	MG	13	1711	1/1	0.91	0.12	102,102,102,102	0
57	MG	1H	3023	1/1	0.91	0.12	72,72,72,72	0
57	MG	1H	3310	1/1	0.91	0.68	87,87,87,87	0
57	MG	14	3388	1/1	0.91	0.31	89,89,89,89	0
57	MG	1H	3148	1/1	0.91	0.22	80,80,80,80	0
57	MG	1H	3025	1/1	0.91	0.24	48,48,48,48	0
57	MG	1H	3272	1/1	0.92	0.31	80,80,80,80	0
57	MG	13	1606	1/1	0.92	0.33	77,77,77,77	0
57	MG	1H	3247	1/1	0.92	0.38	101,101,101,101	0
57	MG	1H	3066	1/1	0.92	0.18	65,65,65,65	0
57	MG	13	1747	1/1	0.92	0.11	110,110,110,110	0
57	MG	1H	3069	1/1	0.92	0.28	60,60,60,60	0
57	MG	1H	3166	1/1	0.92	0.26	56,56,56,56	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
57	MG	1G	1635	1/1	0.92	0.26	102,102,102,102	0
57	MG	14	3248	1/1	0.92	0.12	57,57,57,57	0
57	MG	1H	3512	1/1	0.92	0.17	97,97,97,97	0
57	MG	14	3417	1/1	0.92	0.11	89,89,89,89	0
57	MG	1H	3225	1/1	0.92	0.20	74,74,74,74	0
57	MG	1H	3253	1/1	0.92	0.66	71,71,71,71	0
57	MG	14	3103	1/1	0.92	0.81	75,75,75,75	0
57	MG	1H	3026	1/1	0.92	0.40	52,52,52,52	0
57	MG	14	3107	1/1	0.92	0.24	65,65,65,65	0
57	MG	1H	3408	1/1	0.92	0.08	69,69,69,69	0
57	MG	1H	3362	1/1	0.92	0.07	56,56,56,56	0
57	MG	13	1715	1/1	0.92	0.13	114,114,114,114	0
57	MG	1H	3365	1/1	0.92	0.15	62,62,62,62	0
57	MG	14	3115	1/1	0.92	0.41	48,48,48,48	0
57	MG	14	3006	1/1	0.92	0.25	79,79,79,79	0
57	MG	14	3117	1/1	0.92	0.14	58,58,58,58	0
57	MG	1H	3090	1/1	0.92	0.76	77,77,77,77	0
57	MG	1H	3369	1/1	0.92	0.26	54,54,54,54	0
57	MG	14	3127	1/1	0.92	0.35	62,62,62,62	0
57	MG	14	3015	1/1	0.92	0.24	73,73,73,73	0
57	MG	1H	3053	1/1	0.92	0.76	66,66,66,66	0
57	MG	1H	3419	1/1	0.92	0.07	78,78,78,78	0
57	MG	14	3022	1/1	0.92	0.35	44,44,44,44	0
57	MG	1H	3002	1/1	0.92	0.39	82,82,82,82	0
57	MG	1H	3153	1/1	0.92	0.23	82,82,82,82	0
57	MG	1G	1705	1/1	0.92	0.11	124,124,124,124	0
57	MG	13	1744	1/1	0.92	0.04	90,90,90,90	0
57	MG	14	3142	1/1	0.92	0.20	76,76,76,76	0
57	MG	14	3146	1/1	0.92	0.30	51,51,51,51	0
57	MG	1G	1602	1/1	0.92	0.11	81,81,81,81	0
57	MG	1G	1659	1/1	0.92	0.38	72,72,72,72	0
57	MG	1H	3059	1/1	0.92	0.42	72,72,72,72	0
57	MG	14	3302	1/1	0.92	0.13	86,86,86,86	0
57	MG	1H	3529	1/1	0.92	0.43	78,78,78,78	0
57	MG	1H	3213	1/1	0.92	0.26	77,77,77,77	0
57	MG	14	3049	1/1	0.92	0.32	57,57,57,57	0
57	MG	14	3310	1/1	0.92	0.14	64,64,64,64	0
57	MG	1H	3178	1/1	0.92	0.24	57,57,57,57	0
57	MG	1H	3428	1/1	0.92	0.16	68,68,68,68	0
57	MG	1H	3016	1/1	0.92	0.39	47,47,47,47	0
57	MG	1G	1615	1/1	0.92	0.39	91,91,91,91	0
57	MG	13	1622	1/1	0.92	0.35	74,74,74,74	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
57	MG	1G	1617	1/1	0.92	0.36	86,86,86,86	0
57	MG	1H	3435	1/1	0.92	0.10	60,60,60,60	0
57	MG	1H	3540	1/1	0.92	0.10	81,81,81,81	0
57	MG	1H	3298	1/1	0.92	0.14	83,83,83,83	0
57	MG	14	3231	1/1	0.92	0.67	80,80,80,80	0
57	MG	1H	3083	1/1	0.92	0.48	71,71,71,71	0
57	MG	1H	3271	1/1	0.92	0.31	77,77,77,77	0
57	MG	1H	3173	1/1	0.93	0.74	89,89,89,89	0
57	MG	13	1676	1/1	0.93	0.34	92,92,92,92	0
57	MG	14	3098	1/1	0.93	0.67	62,62,62,62	0
57	MG	1H	3020	1/1	0.93	0.26	47,47,47,47	0
57	MG	1H	3543	1/1	0.93	0.10	70,70,70,70	0
57	MG	1H	3257	1/1	0.93	0.36	51,51,51,51	0
57	MG	1H	3324	1/1	0.93	0.40	66,66,66,66	0
57	MG	1H	3431	1/1	0.93	0.09	60,60,60,60	0
57	MG	13	1704	1/1	0.93	0.10	77,77,77,77	0
57	MG	1H	3024	1/1	0.93	0.23	51,51,51,51	0
57	MG	14	3001	1/1	0.93	0.16	52,52,52,52	0
57	MG	14	3297	1/1	0.93	0.19	66,66,66,66	0
57	MG	1H	3229	1/1	0.93	0.38	64,64,64,64	0
57	MG	14	3299	1/1	0.93	0.21	58,58,58,58	0
57	MG	13	1720	1/1	0.93	0.04	100,100,100,100	0
57	MG	1H	3440	1/1	0.93	0.16	61,61,61,61	0
57	MG	13	1658	1/1	0.93	0.48	75,75,75,75	0
57	MG	13	1694	1/1	0.93	0.05	94,94,94,94	0
57	MG	1G	1641	1/1	0.93	0.11	88,88,88,88	0
57	MG	1H	3156	1/1	0.93	0.26	66,66,66,66	0
57	MG	31	301	1/1	0.93	0.26	63,63,63,63	0
57	MG	14	3130	1/1	0.93	0.39	70,70,70,70	0
57	MG	14	3018	1/1	0.93	0.34	78,78,78,78	0
57	MG	1G	1699	1/1	0.93	0.08	93,93,93,93	0
57	MG	14	3414	1/1	0.93	0.22	100,100,100,100	0
57	MG	1H	3028	1/1	0.93	0.42	62,62,62,62	0
57	MG	1H	3236	1/1	0.93	0.36	70,70,70,70	0
57	MG	1H	3268	1/1	0.93	0.66	92,92,92,92	0
57	MG	14	3026	1/1	0.93	0.12	69,69,69,69	0
57	MG	68	202	1/1	0.93	0.22	83,83,83,83	0
57	MG	14	3221	1/1	0.93	0.12	91,91,91,91	0
57	MG	14	3141	1/1	0.93	0.22	76,76,76,76	0
57	MG	14	3028	1/1	0.93	0.31	61,61,61,61	0
57	MG	1H	3399	1/1	0.93	0.19	54,54,54,54	0
57	MG	1H	3302	1/1	0.93	0.51	81,81,81,81	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
57	MG	13	1631	1/1	0.93	0.24	78,78,78,78	0
57	MG	1H	3107	1/1	0.93	0.43	72,72,72,72	0
57	MG	14	3344	1/1	0.93	0.08	88,88,88,88	0
57	MG	1H	3034	1/1	0.93	0.38	72,72,72,72	0
57	MG	1H	3407	1/1	0.93	0.04	77,77,77,77	0
57	MG	14	3043	1/1	0.93	0.39	83,83,83,83	0
57	MG	14	3046	1/1	0.93	0.42	76,76,76,76	0
57	MG	14	3234	1/1	0.93	0.11	56,56,56,56	0
57	MG	1H	3461	1/1	0.93	0.15	48,48,48,48	0
57	MG	1G	1658	1/1	0.93	0.26	84,84,84,84	0
57	MG	13	1709	1/1	0.93	0.04	69,69,69,69	0
57	MG	14	3054	1/1	0.93	0.27	49,49,49,49	0
57	MG	1H	3409	1/1	0.93	0.11	55,55,55,55	0
57	MG	1H	3131	1/1	0.93	0.34	75,75,75,75	0
57	MG	3I	201	1/1	0.93	0.26	64,64,64,64	0
57	MG	14	3064	1/1	0.93	0.30	62,62,62,62	0
57	MG	1G	1718	1/1	0.93	0.11	91,91,91,91	0
57	MG	14	3071	1/1	0.93	0.24	63,63,63,63	0
57	MG	14	3250	1/1	0.93	0.15	76,76,76,76	0
57	MG	1H	3112	1/1	0.93	0.32	79,79,79,79	0
57	MG	14	3074	1/1	0.93	0.27	81,81,81,81	0
57	MG	1J	203	1/1	0.93	0.23	91,91,91,91	0
57	MG	14	3257	1/1	0.93	0.14	69,69,69,69	0
57	MG	14	3260	1/1	0.93	0.12	55,55,55,55	0
57	MG	1H	3470	1/1	0.93	0.07	73,73,73,73	0
57	MG	19	301	1/1	0.93	0.39	57,57,57,57	0
57	MG	14	3076	1/1	0.93	0.17	89,89,89,89	0
57	MG	39	301	1/1	0.93	0.13	95,95,95,95	0
57	MG	1G	1609	1/1	0.93	0.44	96,96,96,96	0
57	MG	13	1618	1/1	0.93	0.58	60,60,60,60	0
57	MG	13	1644	1/1	0.93	0.06	82,82,82,82	0
57	MG	1H	3073	1/1	0.93	0.58	59,59,59,59	0
57	MG	1H	3314	1/1	0.93	0.19	88,88,88,88	0
57	MG	1H	3170	1/1	0.93	0.27	79,79,79,79	0
57	MG	1H	3074	1/1	0.93	0.41	73,73,73,73	0
57	MG	14	3182	1/1	0.93	0.12	82,82,82,82	0
57	MG	14	3279	1/1	0.93	0.26	83,83,83,83	0
57	MG	1H	3480	1/1	0.93	0.12	53,53,53,53	0
57	MG	13	1652	1/1	0.93	0.22	68,68,68,68	0
57	MG	14	3186	1/1	0.93	0.17	74,74,74,74	0
57	MG	1G	1730	1/1	0.93	0.06	94,94,94,94	0
57	MG	14	3108	1/1	0.94	0.84	77,77,77,77	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
57	MG	1H	3387	1/1	0.94	0.13	53,53,53,53	0
57	MG	13	1639	1/1	0.94	0.17	73,73,73,73	0
57	MG	1H	3032	1/1	0.94	0.19	56,56,56,56	0
57	MG	1G	1604	1/1	0.94	0.30	103,103,103,103	0
57	MG	1H	3481	1/1	0.94	0.07	80,80,80,80	0
57	MG	1H	3342	1/1	0.94	0.16	42,42,42,42	0
57	MG	1G	1708	1/1	0.94	0.04	140,140,140,140	0
57	MG	14	3118	1/1	0.94	0.09	73,73,73,73	0
57	MG	14	3122	1/1	0.94	0.29	84,84,84,84	0
57	MG	1H	3011	1/1	0.94	0.23	73,73,73,73	0
57	MG	13	1634	1/1	0.94	0.31	78,78,78,78	0
57	MG	14	3029	1/1	0.94	0.23	73,73,73,73	0
57	MG	14	3030	1/1	0.94	0.44	89,89,89,89	0
57	MG	1H	3013	1/1	0.94	0.32	37,37,37,37	0
57	MG	14	3212	1/1	0.94	0.33	94,94,94,94	0
57	MG	1H	3015	1/1	0.94	0.40	65,65,65,65	0
57	MG	14	3312	1/1	0.94	0.07	80,80,80,80	0
57	MG	14	3033	1/1	0.94	0.66	75,75,75,75	0
57	MG	14	3034	1/1	0.94	0.24	48,48,48,48	0
57	MG	1H	3489	1/1	0.94	0.09	69,69,69,69	0
57	MG	1H	3354	1/1	0.94	0.10	73,73,73,73	0
57	MG	1H	3230	1/1	0.94	0.22	87,87,87,87	0
57	MG	14	3320	1/1	0.94	0.18	46,46,46,46	0
57	MG	13	1661	1/1	0.94	0.20	92,92,92,92	0
57	MG	13	1693	1/1	0.94	0.12	84,84,84,84	0
57	MG	1H	3093	1/1	0.94	0.32	71,71,71,71	0
57	MG	14	3145	1/1	0.94	0.12	85,85,85,85	0
57	MG	13	1716	1/1	0.94	0.09	55,55,55,55	0
57	MG	1H	3045	1/1	0.94	0.22	42,42,42,42	0
57	MG	1H	3096	1/1	0.94	0.31	53,53,53,53	0
57	MG	1H	3453	1/1	0.94	0.19	58,58,58,58	0
57	MG	1H	3047	1/1	0.94	0.26	55,55,55,55	0
57	MG	14	3057	1/1	0.94	0.45	84,84,84,84	0
57	MG	14	3153	1/1	0.94	0.58	65,65,65,65	0
57	MG	1H	3510	1/1	0.94	0.07	70,70,70,70	0
57	MG	1G	1628	1/1	0.94	0.61	76,76,76,76	0
57	MG	1G	1677	1/1	0.94	0.07	97,97,97,97	0
57	MG	1H	3368	1/1	0.94	0.20	59,59,59,59	0
57	MG	14	3067	1/1	0.94	0.35	69,69,69,69	0
57	MG	1H	3457	1/1	0.94	0.09	45,45,45,45	0
57	MG	1G	1631	1/1	0.94	0.14	82,82,82,82	0
57	MG	14	3073	1/1	0.94	0.31	48,48,48,48	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
57	MG	1H	3022	1/1	0.94	0.33	41,41,41,41	0
57	MG	1H	3004	1/1	0.94	0.71	79,79,79,79	0
57	MG	1G	1634	1/1	0.94	0.18	93,93,93,93	0
57	MG	1H	3240	1/1	0.94	0.37	67,67,67,67	0
57	MG	1H	3463	1/1	0.94	0.17	48,48,48,48	0
57	MG	14	3080	1/1	0.94	0.34	51,51,51,51	0
57	MG	14	3169	1/1	0.94	0.14	53,53,53,53	0
57	MG	1G	1688	1/1	0.94	0.11	89,89,89,89	0
57	MG	13	1629	1/1	0.94	0.33	56,56,56,56	0
57	MG	14	3447	1/1	0.94	0.53	69,69,69,69	0
57	MG	1G	1690	1/1	0.94	0.08	114,114,114,114	0
57	MG	14	3262	1/1	0.94	0.16	66,66,66,66	0
57	MG	1H	3326	1/1	0.94	0.12	47,47,47,47	0
57	MG	1G	1639	1/1	0.94	0.12	103,103,103,103	0
57	MG	1G	1640	1/1	0.94	0.24	92,92,92,92	0
57	MG	14	3088	1/1	0.94	0.18	53,53,53,53	0
57	MG	14	3091	1/1	0.94	0.41	66,66,66,66	0
57	MG	13	1680	1/1	0.94	0.35	84,84,84,84	0
57	MG	14	3003	1/1	0.94	0.49	54,54,54,54	0
57	MG	1H	3244	1/1	0.94	0.32	77,77,77,77	0
57	MG	14	3184	1/1	0.94	0.25	72,72,72,72	0
57	MG	14	3277	1/1	0.94	0.17	59,59,59,59	0
57	MG	1H	3150	1/1	0.94	0.30	67,67,67,67	0
57	MG	14	3382	1/1	0.94	0.09	72,72,72,72	0
57	MG	1H	3151	1/1	0.94	0.12	59,59,59,59	0
57	MG	13	1638	1/1	0.94	0.08	78,78,78,78	0
57	MG	1H	3334	1/1	0.94	0.21	42,42,42,42	0
57	MG	14	3010	1/1	0.94	0.26	50,50,50,50	0
57	MG	14	3013	1/1	0.94	0.44	63,63,63,63	0
57	MG	14	3285	1/1	0.94	0.09	79,79,79,79	0
57	MG	14	3106	1/1	0.94	0.79	94,94,94,94	0
57	MG	13	1722	1/1	0.94	0.12	77,77,77,77	0
60	ZN	C5	202	1/1	0.94	0.12	151,151,151,151	0
57	MG	14	3188	1/1	0.95	0.51	76,76,76,76	0
57	MG	1G	1608	1/1	0.95	0.10	111,111,111,111	0
57	MG	1H	3319	1/1	0.95	0.17	56,56,56,56	0
57	MG	1H	3007	1/1	0.95	0.16	58,58,58,58	0
57	MG	1H	3001	1/1	0.95	0.29	61,61,61,61	0
57	MG	1H	3437	1/1	0.95	0.17	46,46,46,46	0
57	MG	1H	3393	1/1	0.95	0.10	69,69,69,69	0
57	MG	14	3121	1/1	0.95	0.28	55,55,55,55	0
57	MG	1H	3300	1/1	0.95	0.24	87,87,87,87	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
57	MG	1H	3539	1/1	0.95	0.11	45,45,45,45	0
57	MG	14	3124	1/1	0.95	0.35	82,82,82,82	0
57	MG	14	3125	1/1	0.95	0.47	70,70,70,70	0
57	MG	1H	3441	1/1	0.95	0.17	44,44,44,44	0
57	MG	1G	1671	1/1	0.95	0.09	86,86,86,86	0
57	MG	1H	3226	1/1	0.95	0.54	60,60,60,60	0
57	MG	14	3050	1/1	0.95	0.48	77,77,77,77	0
57	MG	14	3206	1/1	0.95	0.26	101,101,101,101	0
57	MG	1H	3196	1/1	0.95	0.18	56,56,56,56	0
57	MG	14	3403	1/1	0.95	0.06	83,83,83,83	0
57	MG	14	3132	1/1	0.95	0.30	78,78,78,78	0
57	MG	1H	3491	1/1	0.95	0.16	62,62,62,62	0
57	MG	14	3303	1/1	0.95	0.18	70,70,70,70	0
57	MG	1H	3492	1/1	0.95	0.07	83,83,83,83	0
57	MG	14	3055	1/1	0.95	0.29	50,50,50,50	0
57	MG	13	1617	1/1	0.95	0.69	78,78,78,78	0
57	MG	1H	3546	1/1	0.95	0.10	41,41,41,41	0
57	MG	14	3139	1/1	0.95	0.48	84,84,84,84	0
57	MG	14	3058	1/1	0.95	0.27	83,83,83,83	0
57	MG	13	1717	1/1	0.95	0.10	53,53,53,53	0
57	MG	1G	1626	1/1	0.95	0.24	68,68,68,68	0
57	MG	14	3143	1/1	0.95	0.42	54,54,54,54	0
57	MG	14	3219	1/1	0.95	0.43	54,54,54,54	0
57	MG	1H	3363	1/1	0.95	0.15	47,47,47,47	0
57	MG	1H	3146	1/1	0.95	0.64	58,58,58,58	0
57	MG	1H	3328	1/1	0.95	0.18	46,46,46,46	0
57	MG	14	3325	1/1	0.95	0.21	52,52,52,52	0
57	MG	14	3068	1/1	0.95	0.37	64,64,64,64	0
57	MG	14	3069	1/1	0.95	0.13	93,93,93,93	0
57	MG	14	3150	1/1	0.95	0.19	81,81,81,81	0
57	MG	1H	3366	1/1	0.95	0.16	63,63,63,63	0
57	MG	1H	3451	1/1	0.95	0.12	83,83,83,83	0
57	MG	1H	3129	1/1	0.95	0.51	69,69,69,69	0
57	MG	14	3336	1/1	0.95	0.07	65,65,65,65	0
57	MG	14	3337	1/1	0.95	0.11	57,57,57,57	0
57	MG	1G	1687	1/1	0.95	0.11	95,95,95,95	0
57	MG	14	3430	1/1	0.95	0.13	88,88,88,88	0
57	MG	16	210	1/1	0.95	0.06	78,78,78,78	0
57	MG	1H	3215	1/1	0.95	0.41	69,69,69,69	0
57	MG	14	3233	1/1	0.95	0.26	54,54,54,54	0
57	MG	1H	3174	1/1	0.95	0.20	37,37,37,37	0
57	MG	1H	3031	1/1	0.95	0.43	74,74,74,74	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
57	MG	1H	3288	1/1	0.95	0.29	77,77,77,77	0
57	MG	14	3350	1/1	0.95	0.10	61,61,61,61	0
57	MG	13	1705	1/1	0.95	0.18	83,83,83,83	0
57	MG	1H	3459	1/1	0.95	0.15	64,64,64,64	0
57	MG	1H	3337	1/1	0.95	0.19	44,44,44,44	0
57	MG	14	3084	1/1	0.95	0.30	87,87,87,87	0
57	MG	14	3164	1/1	0.95	0.32	80,80,80,80	0
57	MG	1G	1642	1/1	0.95	0.23	82,82,82,82	0
57	MG	13	1666	1/1	0.95	0.13	78,78,78,78	0
57	MG	14	3009	1/1	0.95	0.26	68,68,68,68	0
57	MG	1H	3376	1/1	0.95	0.09	45,45,45,45	0
57	MG	1H	3339	1/1	0.95	0.22	43,43,43,43	0
57	MG	14	3364	1/1	0.95	0.07	85,85,85,85	0
57	MG	14	3170	1/1	0.95	0.34	87,87,87,87	0
57	MG	14	3014	1/1	0.95	0.33	62,62,62,62	0
57	MG	4K	102	1/1	0.95	0.07	93,93,93,93	0
57	MG	1H	3076	1/1	0.95	0.16	39,39,39,39	0
57	MG	1H	3343	1/1	0.95	0.19	44,44,44,44	0
57	MG	14	3263	1/1	0.95	0.12	56,56,56,56	0
57	MG	14	3019	1/1	0.95	0.18	53,53,53,53	0
57	MG	14	3372	1/1	0.95	0.13	79,79,79,79	0
57	MG	1H	3344	1/1	0.95	0.13	46,46,46,46	0
57	MG	14	3100	1/1	0.95	0.31	61,61,61,61	0
57	MG	1H	3346	1/1	0.95	0.14	53,53,53,53	0
57	MG	B5	101	1/1	0.95	0.12	85,85,85,85	0
57	MG	14	3180	1/1	0.95	0.15	65,65,65,65	0
57	MG	1H	3472	1/1	0.95	0.16	62,62,62,62	0
57	MG	1G	1601	1/1	0.95	0.19	70,70,70,70	0
57	MG	1H	3426	1/1	0.95	0.05	76,76,76,76	0
57	MG	1H	3256	1/1	0.95	0.28	67,67,67,67	0
57	MG	1H	3476	1/1	0.95	0.12	68,68,68,68	0
57	MG	14	3278	1/1	0.95	0.12	80,80,80,80	0
57	MG	1H	3138	1/1	0.95	0.46	41,41,41,41	0
57	MG	1H	3389	1/1	0.95	0.12	68,68,68,68	0
57	MG	14	3175	1/1	0.96	0.08	107,107,107,107	0
57	MG	13	1689	1/1	0.96	0.40	85,85,85,85	0
57	MG	1H	3468	1/1	0.96	0.11	68,68,68,68	0
57	MG	1H	3029	1/1	0.96	0.21	63,63,63,63	0
57	MG	1H	3219	1/1	0.96	0.54	82,82,82,82	0
57	MG	14	3095	1/1	0.96	0.34	74,74,74,74	0
57	MG	1H	3063	1/1	0.96	0.17	53,53,53,53	0
57	MG	1H	3064	1/1	0.96	0.36	63,63,63,63	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
57	MG	14	3011	1/1	0.96	0.39	51,51,51,51	0
57	MG	14	3012	1/1	0.96	0.41	60,60,60,60	0
57	MG	13	1648	1/1	0.96	0.17	77,77,77,77	0
57	MG	14	3102	1/1	0.96	0.14	73,73,73,73	0
57	MG	1H	3534	1/1	0.96	0.12	92,92,92,92	0
57	MG	1H	3160	1/1	0.96	0.43	68,68,68,68	0
57	MG	14	3105	1/1	0.96	0.35	73,73,73,73	0
57	MG	1H	3475	1/1	0.96	0.06	83,83,83,83	0
57	MG	13	1610	1/1	0.96	0.35	73,73,73,73	0
57	MG	14	3192	1/1	0.96	0.39	82,82,82,82	0
57	MG	13	1692	1/1	0.96	0.16	61,61,61,61	0
57	MG	14	3020	1/1	0.96	0.42	61,61,61,61	0
57	MG	13	1621	1/1	0.96	0.21	56,56,56,56	0
57	MG	13	1612	1/1	0.96	0.21	76,76,76,76	0
57	MG	1H	3427	1/1	0.96	0.07	66,66,66,66	0
57	MG	2K	104	1/1	0.96	0.06	89,89,89,89	0
57	MG	13	1725	1/1	0.96	0.10	90,90,90,90	0
57	MG	1H	3040	1/1	0.96	0.32	36,36,36,36	0
57	MG	1H	3432	1/1	0.96	0.23	56,56,56,56	0
57	MG	14	3120	1/1	0.96	0.28	75,75,75,75	0
57	MG	1H	3485	1/1	0.96	0.06	83,83,83,83	0
57	MG	16	202	1/1	0.96	0.31	78,78,78,78	0
57	MG	1H	3433	1/1	0.96	0.13	61,61,61,61	0
57	MG	1H	3487	1/1	0.96	0.10	72,72,72,72	0
57	MG	1H	3381	1/1	0.96	0.10	48,48,48,48	0
57	MG	1H	3382	1/1	0.96	0.22	54,54,54,54	0
57	MG	1H	3490	1/1	0.96	0.11	65,65,65,65	0
57	MG	14	3036	1/1	0.96	0.26	47,47,47,47	0
57	MG	14	3037	1/1	0.96	0.34	57,57,57,57	0
57	MG	14	3315	1/1	0.96	0.10	86,86,86,86	0
57	MG	14	3038	1/1	0.96	0.36	69,69,69,69	0
57	MG	1H	3383	1/1	0.96	0.13	53,53,53,53	0
57	MG	1H	3264	1/1	0.96	0.25	59,59,59,59	0
57	MG	1H	3017	1/1	0.96	0.29	53,53,53,53	0
57	MG	1H	3043	1/1	0.96	0.41	66,66,66,66	0
57	MG	21	301	1/1	0.96	0.24	62,62,62,62	0
57	MG	1H	3341	1/1	0.96	0.18	48,48,48,48	0
57	MG	13	1627	1/1	0.96	0.24	85,85,85,85	0
57	MG	1H	3497	1/1	0.96	0.06	79,79,79,79	0
57	MG	1H	3305	1/1	0.96	0.23	71,71,71,71	0
57	MG	13	1696	1/1	0.96	0.15	83,83,83,83	0
57	MG	1H	3046	1/1	0.96	0.24	49,49,49,49	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
57	MG	14	3144	1/1	0.96	0.30	56,56,56,56	0
57	MG	1H	3446	1/1	0.96	0.07	60,60,60,60	0
57	MG	1H	3505	1/1	0.96	0.06	79,79,79,79	0
57	MG	14	3228	1/1	0.96	1.16	86,86,86,86	0
57	MG	14	3340	1/1	0.96	0.07	69,69,69,69	0
57	MG	1G	1656	1/1	0.96	0.23	66,66,66,66	0
57	MG	14	3060	1/1	0.96	0.55	56,56,56,56	0
57	MG	1H	3347	1/1	0.96	0.20	56,56,56,56	0
57	MG	1H	3021	1/1	0.96	0.34	63,63,63,63	0
57	MG	14	3347	1/1	0.96	0.07	101,101,101,101	0
57	MG	I8	101	1/1	0.96	0.05	69,69,69,69	0
57	MG	1H	3110	1/1	0.96	0.26	65,65,65,65	0
57	MG	1H	3396	1/1	0.96	0.14	64,64,64,64	0
57	MG	1H	3143	1/1	0.96	0.15	66,66,66,66	0
57	MG	1G	1663	1/1	0.96	0.20	76,76,76,76	0
57	MG	14	3070	1/1	0.96	0.33	82,82,82,82	0
57	MG	14	3240	1/1	0.96	0.12	62,62,62,62	0
57	MG	1H	3144	1/1	0.96	0.41	64,64,64,64	0
57	MG	1G	1665	1/1	0.96	0.20	78,78,78,78	0
57	MG	1H	3353	1/1	0.96	0.13	64,64,64,64	0
57	MG	13	1605	1/1	0.96	0.24	70,70,70,70	0
57	MG	14	3360	1/1	0.96	0.06	94,94,94,94	0
57	MG	1G	1603	1/1	0.96	0.26	79,79,79,79	0
57	MG	13	1714	1/1	0.96	0.08	100,100,100,100	0
57	MG	1H	3405	1/1	0.96	0.16	46,46,46,46	0
57	MG	1H	3052	1/1	0.96	0.35	50,50,50,50	0
57	MG	14	3253	1/1	0.96	0.22	53,53,53,53	0
57	MG	14	3254	1/1	0.96	0.17	52,52,52,52	0
57	MG	2L	101	1/1	0.96	0.53	77,77,77,77	0
57	MG	13	1641	1/1	0.96	0.25	68,68,68,68	0
57	MG	45	201	1/1	0.96	0.12	74,74,74,74	0
57	MG	13	1655	1/1	0.96	0.14	65,65,65,65	0
57	MG	1H	3057	1/1	0.96	0.26	72,72,72,72	0
57	MG	13	1701	1/1	0.96	0.04	69,69,69,69	0
57	MG	13	1749	1/1	0.96	0.14	78,78,78,78	0
57	MG	1H	3060	1/1	0.96	0.33	51,51,51,51	0
57	MG	14	3265	1/1	0.96	0.16	52,52,52,52	0
57	MG	14	3266	1/1	0.96	0.11	72,72,72,72	0
57	MG	1G	1614	1/1	0.96	0.29	82,82,82,82	0
57	MG	1G	1679	1/1	0.96	0.07	93,93,93,93	0
60	ZN	G8	201	1/1	0.96	0.10	131,131,131,131	0
57	MG	14	3089	1/1	0.96	0.43	79,79,79,79	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
57	MG	14	3339	1/1	0.97	0.14	49,49,49,49	0
57	MG	1H	3503	1/1	0.97	0.06	47,47,47,47	0
57	MG	1H	3333	1/1	0.97	0.21	67,67,67,67	0
57	MG	14	3342	1/1	0.97	0.11	82,82,82,82	0
57	MG	1H	3243	1/1	0.97	0.22	79,79,79,79	0
57	MG	1H	3335	1/1	0.97	0.12	53,53,53,53	0
57	MG	1H	3548	1/1	0.97	0.14	70,70,70,70	0
57	MG	14	3042	1/1	0.97	0.45	69,69,69,69	0
57	MG	13	1640	1/1	0.97	0.47	77,77,77,77	0
57	MG	14	3044	1/1	0.97	0.50	48,48,48,48	0
57	MG	14	3045	1/1	0.97	0.32	61,61,61,61	0
57	MG	1G	1613	1/1	0.97	0.34	83,83,83,83	0
57	MG	14	3047	1/1	0.97	0.26	81,81,81,81	0
57	MG	13	1628	1/1	0.97	0.39	79,79,79,79	0
57	MG	14	3354	1/1	0.97	0.09	73,73,73,73	0
57	MG	1H	3091	1/1	0.97	0.39	77,77,77,77	0
57	MG	14	3051	1/1	0.97	0.31	72,72,72,72	0
57	MG	1H	3438	1/1	0.97	0.12	50,50,50,50	0
57	MG	13	1607	1/1	0.97	0.26	80,80,80,80	0
57	MG	1H	3514	1/1	0.97	0.08	76,76,76,76	0
57	MG	13	1712	1/1	0.97	0.09	101,101,101,101	0
57	MG	14	3361	1/1	0.97	0.04	80,80,80,80	0
57	MG	1H	3290	1/1	0.97	0.13	87,87,87,87	0
57	MG	16	209	1/1	0.97	0.03	68,68,68,68	0
57	MG	1H	3291	1/1	0.97	0.20	78,78,78,78	0
57	MG	14	3059	1/1	0.97	0.26	70,70,70,70	0
57	MG	13	1675	1/1	0.97	0.18	104,104,104,104	0
57	MG	1H	3293	1/1	0.97	0.45	46,46,46,46	0
57	MG	1H	3413	1/1	0.97	0.12	59,59,59,59	0
57	MG	1H	3318	1/1	0.97	0.19	54,54,54,54	0
57	MG	14	3065	1/1	0.97	0.35	60,60,60,60	0
57	MG	1G	1627	1/1	0.97	0.20	77,77,77,77	0
57	MG	1H	3035	1/1	0.97	0.32	80,80,80,80	0
57	MG	13	1601	1/1	0.97	0.32	74,74,74,74	0
57	MG	1H	3049	1/1	0.97	0.43	69,69,69,69	0
57	MG	14	3237	1/1	0.97	0.15	56,56,56,56	0
57	MG	1H	3135	1/1	0.97	0.20	42,42,42,42	0
57	MG	14	3017	1/1	0.97	0.48	60,60,60,60	0
57	MG	14	3306	1/1	0.97	0.13	86,86,86,86	0
57	MG	1H	3050	1/1	0.97	0.30	54,54,54,54	0
57	MG	1H	3081	1/1	0.97	0.16	55,55,55,55	0
57	MG	14	3309	1/1	0.97	0.06	71,71,71,71	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
57	MG	5E	201	1/1	0.97	0.27	75,75,75,75	0
57	MG	1H	3454	1/1	0.97	0.13	48,48,48,48	0
57	MG	1H	3018	1/1	0.97	0.50	55,55,55,55	0
57	MG	14	3023	1/1	0.97	0.41	82,82,82,82	0
57	MG	13	1729	1/1	0.97	0.06	73,73,73,73	0
57	MG	1H	3532	1/1	0.97	0.12	103,103,103,103	0
57	MG	29	302	1/1	0.97	0.13	52,52,52,52	0
57	MG	1H	3068	1/1	0.97	0.57	71,71,71,71	0
57	MG	14	3318	1/1	0.97	0.07	75,75,75,75	0
57	MG	1H	3359	1/1	0.97	0.10	60,60,60,60	0
57	MG	1H	3054	1/1	0.97	0.29	37,37,37,37	0
57	MG	14	3322	1/1	0.97	0.12	64,64,64,64	0
57	MG	14	3255	1/1	0.97	0.17	52,52,52,52	0
57	MG	1H	3361	1/1	0.97	0.04	74,74,74,74	0
57	MG	1H	3055	1/1	0.97	0.26	60,60,60,60	0
57	MG	14	3258	1/1	0.97	0.09	71,71,71,71	0
57	MG	14	3329	1/1	0.97	0.11	60,60,60,60	0
57	MG	14	3259	1/1	0.97	0.06	63,63,63,63	0
57	MG	1H	3071	1/1	0.97	0.41	57,57,57,57	0
57	MG	1H	3430	1/1	0.97	0.14	61,61,61,61	0
57	MG	1H	3465	1/1	0.97	0.12	63,63,63,63	0
57	MG	1H	3283	1/1	0.97	0.35	146,146,146,146	0
57	MG	14	3090	1/1	0.97	0.49	65,65,65,65	0
57	MG	1G	1732	1/1	0.97	0.05	114,114,114,114	0
57	MG	1G	1734	1/1	0.97	0.16	84,84,84,84	0
57	MG	1H	3039	1/1	0.98	0.28	40,40,40,40	0
57	MG	14	3326	1/1	0.98	0.09	60,60,60,60	0
57	MG	13	1604	1/1	0.98	0.32	77,77,77,77	0
57	MG	14	3328	1/1	0.98	0.19	56,56,56,56	0
57	MG	1H	3142	1/1	0.98	0.12	64,64,64,64	0
57	MG	1H	3501	1/1	0.98	0.15	75,75,75,75	0
57	MG	1H	3041	1/1	0.98	0.25	51,51,51,51	0
57	MG	14	3128	1/1	0.98	0.33	88,88,88,88	0
57	MG	1H	3398	1/1	0.98	0.16	61,61,61,61	0
57	MG	14	3242	1/1	0.98	0.19	44,44,44,44	0
57	MG	14	3061	1/1	0.98	0.65	56,56,56,56	0
57	MG	1H	3460	1/1	0.98	0.14	48,48,48,48	0
57	MG	14	3245	1/1	0.98	0.17	56,56,56,56	0
57	MG	1H	3132	1/1	0.98	0.27	88,88,88,88	0
57	MG	14	3290	1/1	0.98	0.08	66,66,66,66	0
57	MG	14	3096	1/1	0.98	0.24	50,50,50,50	0
57	MG	1H	3506	1/1	0.98	0.09	61,61,61,61	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
57	MG	14	3249	1/1	0.98	0.18	60,60,60,60	0
57	MG	14	3135	1/1	0.98	0.21	69,69,69,69	0
57	MG	14	3345	1/1	0.98	0.08	83,83,83,83	0
57	MG	14	3251	1/1	0.98	0.18	63,63,63,63	0
57	MG	1H	3507	1/1	0.98	0.04	74,74,74,74	0
57	MG	1H	3400	1/1	0.98	0.13	59,59,59,59	0
57	MG	1H	3014	1/1	0.98	0.38	43,43,43,43	0
57	MG	1H	3384	1/1	0.98	0.07	61,61,61,61	0
57	MG	14	3300	1/1	0.98	0.20	73,73,73,73	0
57	MG	11	302	1/1	0.98	0.07	47,47,47,47	0
57	MG	1H	3403	1/1	0.98	0.17	50,50,50,50	0
57	MG	21	302	1/1	0.98	0.13	46,46,46,46	0
57	MG	14	3304	1/1	0.98	0.13	68,68,68,68	0
57	MG	1H	3355	1/1	0.98	0.13	67,67,67,67	0
57	MG	13	1703	1/1	0.98	0.14	66,66,66,66	0
57	MG	1H	3538	1/1	0.98	0.06	58,58,58,58	0
57	MG	1H	3159	1/1	0.98	0.29	74,74,74,74	0
57	MG	14	3109	1/1	0.98	0.52	74,74,74,74	0
57	MG	13	1611	1/1	0.98	0.11	85,85,85,85	0
57	MG	1H	3136	1/1	0.98	0.17	45,45,45,45	0
57	MG	13	1713	1/1	0.98	0.11	65,65,65,65	0
57	MG	14	3079	1/1	0.98	0.34	61,61,61,61	0
57	MG	14	3048	1/1	0.98	0.28	67,67,67,67	0
57	MG	14	3269	1/1	0.98	0.14	63,63,63,63	0
57	MG	1H	3375	1/1	0.98	0.18	48,48,48,48	0
57	MG	1H	3412	1/1	0.98	0.10	51,51,51,51	0
57	MG	1G	1649	1/1	0.98	0.37	89,89,89,89	0
57	MG	14	3119	1/1	0.98	0.37	79,79,79,79	0
57	MG	14	3321	1/1	0.98	0.07	64,64,64,64	0
57	MG	1G	1706	1/1	0.98	0.07	79,79,79,79	0
60	ZN	5I	102	1/1	0.98	0.11	98,98,98,98	0
57	MG	1H	3030	1/1	0.98	0.34	75,75,75,75	0
57	MG	13	1698	1/1	0.98	0.04	94,94,94,94	0
57	MG	1H	3351	1/1	0.99	0.11	59,59,59,59	0
57	MG	14	3270	1/1	0.99	0.09	65,65,65,65	0
57	MG	1H	3345	1/1	0.99	0.11	51,51,51,51	0
57	MG	14	3114	1/1	0.99	0.43	63,63,63,63	0
57	MG	1J	204	1/1	0.99	0.12	88,88,88,88	0
57	MG	13	1721	1/1	0.99	0.06	62,62,62,62	0
57	MG	14	3333	1/1	0.99	0.06	66,66,66,66	0
59	SF4	3E	301	8/8	0.99	0.17	86,90,100,103	0
59	SF4	32	301	8/8	0.99	0.15	90,99,108,116	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
57	MG	1H	3499	1/1	0.99	0.09	52,52,52,52	0
57	MG	1H	3411	1/1	0.99	0.09	80,80,80,80	0
60	ZN	5A	101	1/1	0.99	0.09	123,123,123,123	0
57	MG	14	3311	1/1	0.99	0.10	68,68,68,68	0
57	MG	1H	3547	1/1	1.00	0.28	61,61,61,61	0
57	MG	14	3197	1/1	1.00	0.20	78,78,78,78	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.