wwPDB X-ray Structure Validation Summary Report (i)

Aug 1, 2016 – 11:06 PM EDT

PDB ID	:	5IB7
Title	:	Structure of T. thermophilus 70S ribosome complex with mRNA, tRNAfMet, near-cognate tRNALys with U-G mismatch in the A-site and antibiotic paromomycin
Authors	:	Rozov, A.; Demeshkina, N.; Yusupov, M.; Yusupova, G.
Deposited on	:	2016-02-22
Resolution	:	2.99 Å(reported)

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

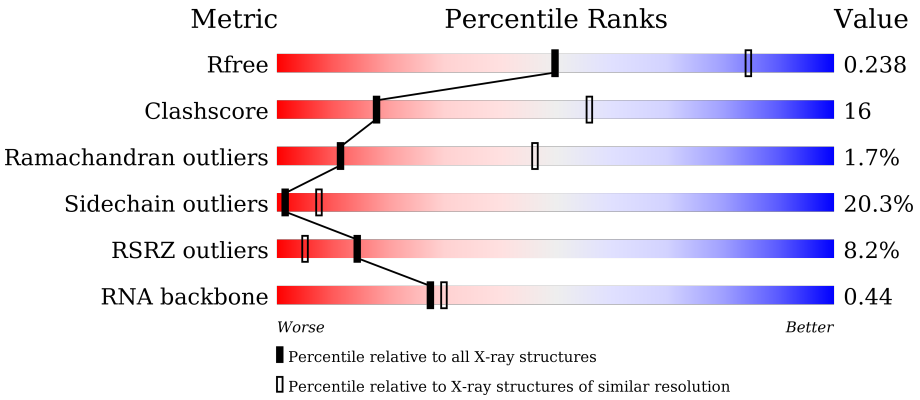
MolProbity	:	4.02b-467
Mogul	:	1.7.1 (RC1), CSD as537be (2016)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20027939
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	rb-20027939

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 2.99 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	1578 (3.00-3.00)
Clashscore	102246	1912 (3.00-3.00)
Ramachandran outliers	100387	1853 (3.00-3.00)
Sidechain outliers	100360	1856 (3.00-3.00)
RSRZ outliers	91569	1592 (3.00-3.00)
RNA backbone	2183	1036 (3.40-2.60)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria. 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 <=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	37% 45% 15%
1	1G	1522	% 39% 44% 14%
2	12	256	10% 34% 36% 9% 19%
2	1E	256	5% 39% 38% 12% 10%

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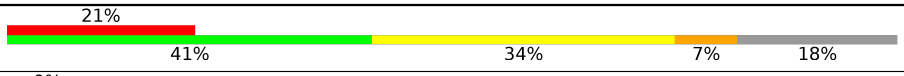
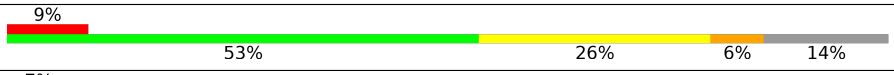
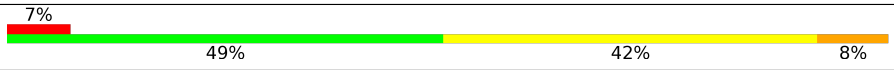
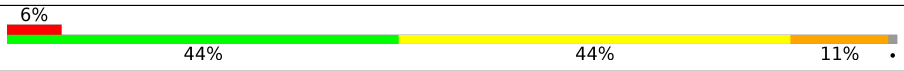
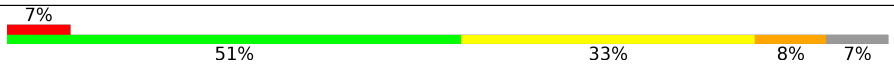
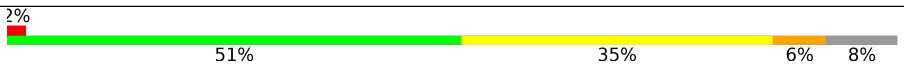
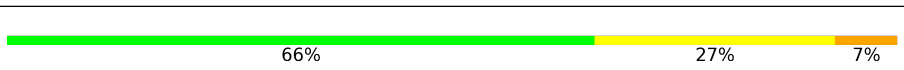
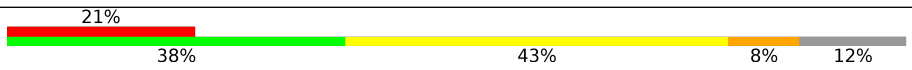
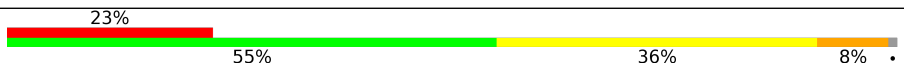
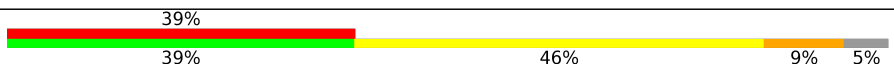
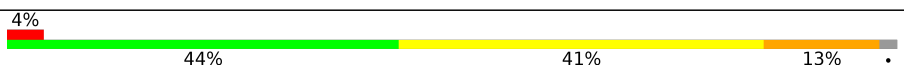
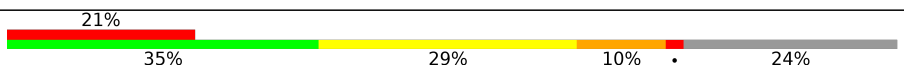
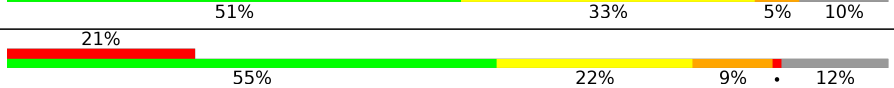
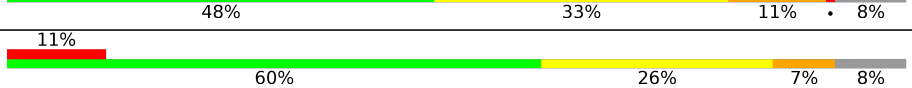
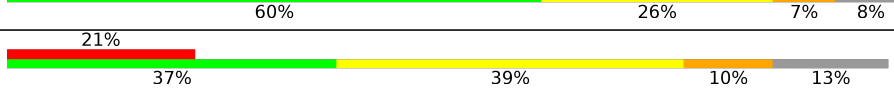
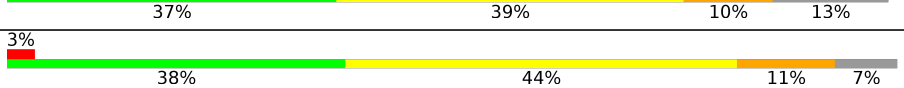
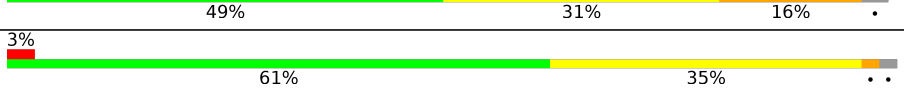
Mol	Chain	Length	Quality of chain
3	22	239	
3	2E	239	
4	32	209	
4	3E	209	
5	42	162	
5	4E	162	
6	52	101	
6	5E	101	
7	62	156	
7	6E	156	
8	72	138	
8	7E	138	
9	82	128	
9	8E	128	
10	1A	105	
10	1I	105	
11	2A	129	
11	2I	129	
12	3A	132	
12	3I	132	
13	4A	126	
13	4I	126	
14	5A	61	
14	5I	61	
15	6A	89	

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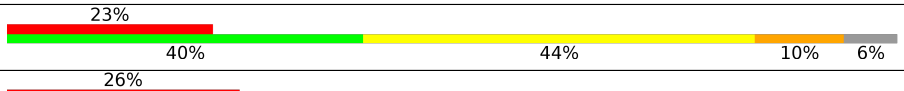
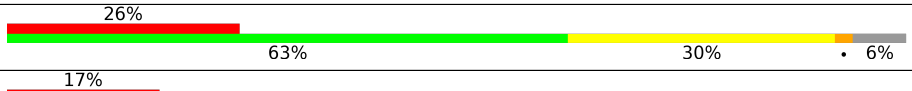
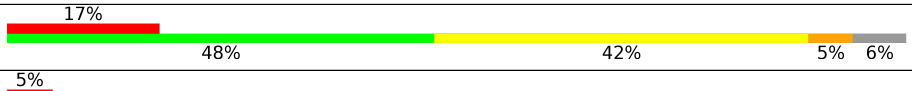
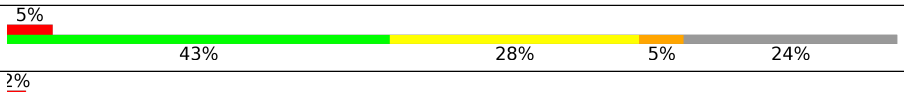
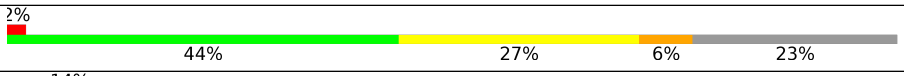
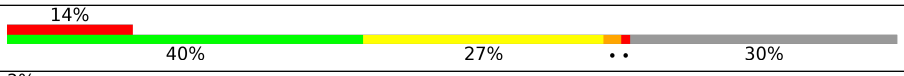
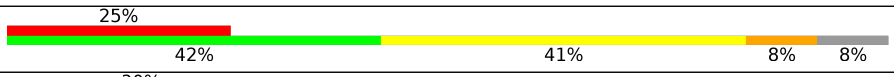
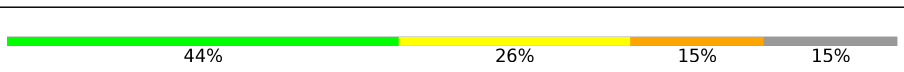
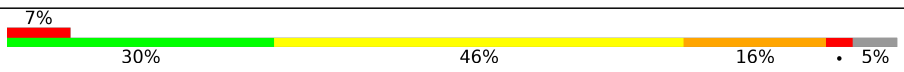
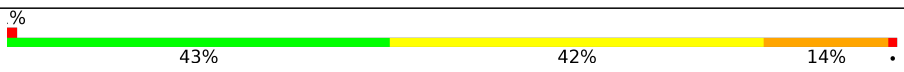
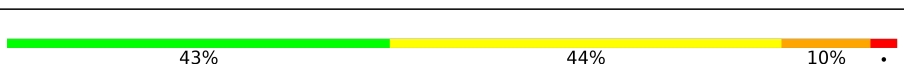
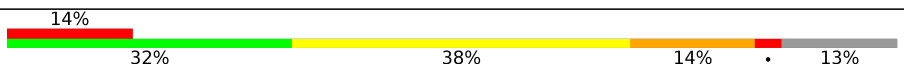
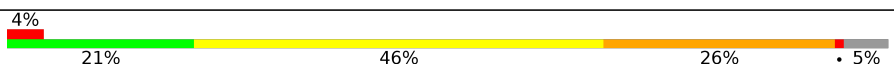
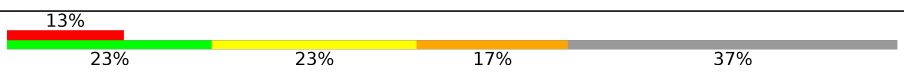
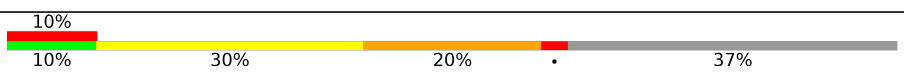
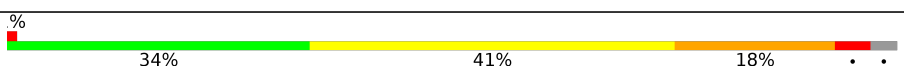
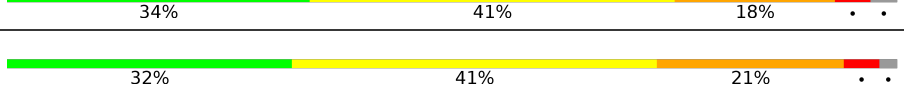
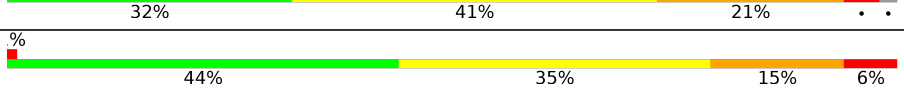
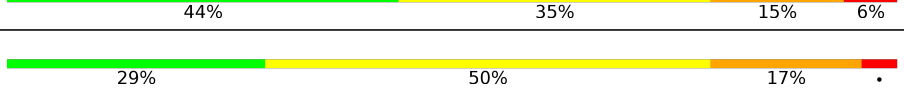
Mol	Chain	Length	Quality of chain
15	6I	89	
16	7A	88	
16	7I	88	
17	8A	105	
17	8I	105	
18	9A	88	
18	9I	88	
19	AA	93	
19	AI	93	
20	BA	106	
20	BI	106	
21	1B	27	
21	1F	27	
22	1K	76	
23	2K	77	
23	2L	77	
24	1L	76	
24	3K	76	
24	3L	76	
25	4K	30	
25	4L	30	
26	14	2917	
26	1H	2917	
27	16	122	
27	1J	122	

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Mol	Chain	Length	Quality of chain
28	71	229	9% 28% 23% 6% 42%
29	11	276	2% 53% 36% 9%
29	19	276	3% 55% 33% 10%
30	21	206	5% 44% 35% 17%
30	29	206	19% 46% 40% 12%
31	31	210	4% 51% 36% 9%
31	39	210	7% 40% 43% 13%
32	41	182	12% 51% 40% 7%
32	49	182	26% 46% 43% 10%
33	51	180	3% 52% 26% 17%
33	59	180	51% 47% 31% 14% 6%
34	61	148	11% 52% 34% 11%
34	69	148	8% 49% 38% 10%
35	15	140	18% 52% 35% 11%
35	58	140	13% 54% 32% 11%
36	25	122	11% 48% 41% 11%
36	68	122	2% 61% 34%
37	35	150	14% 43% 41% 12%
37	78	150	7% 37% 41% 15% 5%
38	45	141	19% 43% 42% 13%
38	88	141	7% 51% 35% 13%
39	55	118	5% 51% 41% 8%
39	98	118	10% 47% 40% 13%
40	65	112	20% 40% 43% 13%
40	A8	112	16% 38% 47% 13%

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Mol	Chain	Length	Quality of chain
41	75	146	5% 41% 38% 11% • 9%
41	B8	146	3% 36% 39% 16% • 8%
42	85	118	3% 56% 31% 11% •
42	C8	118	3% 58% 29% 9% • •
43	95	101	22% 56% 36% 6% ••
43	D8	101	15% 49% 39% 10% • •
44	A5	113	4% 64% 27% 7% •
44	E8	113	7% 58% 31% 8% •
45	B5	96	16% 54% 35% 8% •
45	F8	96	% 68% 23% 8% •
46	C5	110	33% 42% 36% 14% • 5%
46	G8	110	5% 46% 34% 13% • 6%
47	D5	206	34% 34% 40% 11% • 14%
47	H8	206	32% 43% 29% 8% • 17%
48	E5	85	15% 47% 34% 7% • 11%
48	I8	85	6% 49% 31% 11% 9%
49	F5	98	18% 52% 35% 9% •
49	J8	98	9% 49% 37% 9% • •
50	G5	72	7% 43% 43% 7% • •
50	K8	72	% 35% 40% 15% • 6%
51	H5	60	48% 57% 37% • •
51	L8	60	3% 52% 40% 5% •
52	M8	71	23% 35% 32% 14% • 15%
53	J5	60	12% 53% 37% • 7%
53	N8	60	43% 28% 7% • 20%

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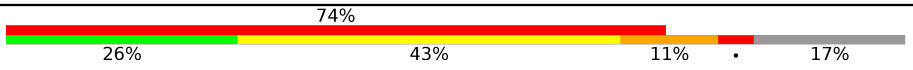
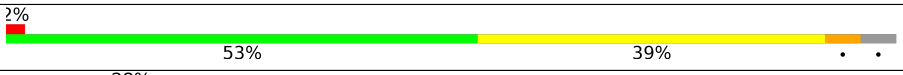
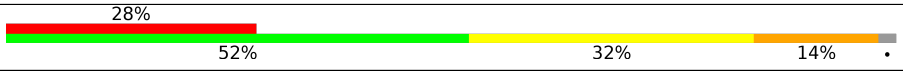
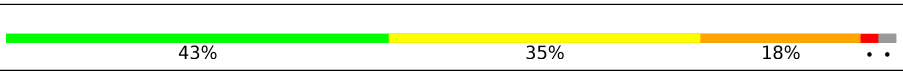
Mol	Chain	Length	Quality of chain
54	O8	54	
55	L5	49	
55	P8	49	
56	M5	65	
56	Q8	65	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
57	MG	13	1601	-	-	-	X
57	MG	13	1614	-	-	-	X
57	MG	13	1623	-	-	-	X
57	MG	13	1624	-	-	-	X
57	MG	13	1627	-	-	-	X
57	MG	13	1628	-	-	-	X
57	MG	13	1629	-	-	-	X
57	MG	13	1633	-	-	-	X
57	MG	13	1635	-	-	-	X
57	MG	13	1636	-	-	-	X
57	MG	13	1645	-	-	-	X
57	MG	13	1654	-	-	-	X
57	MG	13	1659	-	-	-	X
57	MG	13	1661	-	-	-	X
57	MG	13	1668	-	-	-	X
57	MG	13	1669	-	-	-	X
57	MG	13	1670	-	-	-	X
57	MG	14	3007	-	-	-	X
57	MG	14	3008	-	-	-	X
57	MG	14	3014	-	-	-	X
57	MG	14	3015	-	-	-	X
57	MG	14	3016	-	-	-	X
57	MG	14	3023	-	-	-	X
57	MG	14	3028	-	-	-	X
57	MG	14	3030	-	-	-	X
57	MG	14	3031	-	-	-	X
57	MG	14	3034	-	-	-	X
57	MG	14	3035	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
57	MG	14	3042	-	-	-	X
57	MG	14	3046	-	-	-	X
57	MG	14	3048	-	-	-	X
57	MG	14	3054	-	-	-	X
57	MG	14	3059	-	-	-	X
57	MG	14	3061	-	-	-	X
57	MG	14	3062	-	-	-	X
57	MG	14	3064	-	-	-	X
57	MG	14	3070	-	-	-	X
57	MG	14	3072	-	-	-	X
57	MG	14	3074	-	-	-	X
57	MG	14	3076	-	-	-	X
57	MG	14	3077	-	-	-	X
57	MG	14	3080	-	-	-	X
57	MG	14	3088	-	-	-	X
57	MG	14	3089	-	-	-	X
57	MG	14	3090	-	-	-	X
57	MG	14	3092	-	-	-	X
57	MG	14	3097	-	-	-	X
57	MG	14	3099	-	-	-	X
57	MG	14	3100	-	-	-	X
57	MG	14	3107	-	-	-	X
57	MG	14	3108	-	-	-	X
57	MG	14	3114	-	-	-	X
57	MG	14	3117	-	-	-	X
57	MG	14	3118	-	-	-	X
57	MG	14	3119	-	-	-	X
57	MG	14	3122	-	-	-	X
57	MG	14	3124	-	-	-	X
57	MG	14	3125	-	-	-	X
57	MG	14	3126	-	-	-	X
57	MG	14	3134	-	-	-	X
57	MG	14	3136	-	-	-	X
57	MG	14	3139	-	-	-	X
57	MG	14	3142	-	-	-	X
57	MG	14	3145	-	-	-	X
57	MG	14	3151	-	-	-	X
57	MG	14	3171	-	-	-	X
57	MG	14	3179	-	-	-	X
57	MG	14	3181	-	-	-	X
57	MG	14	3191	-	-	-	X
57	MG	14	3194	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
57	MG	14	3198	-	-	-	X
57	MG	14	3203	-	-	-	X
57	MG	14	3205	-	-	-	X
57	MG	14	3208	-	-	-	X
57	MG	14	3224	-	-	-	X
57	MG	14	3233	-	-	-	X
57	MG	14	3236	-	-	-	X
57	MG	14	3237	-	-	-	X
57	MG	14	3248	-	-	-	X
57	MG	16	202	-	-	-	X
57	MG	16	203	-	-	-	X
57	MG	19	301	-	-	-	X
57	MG	1G	1614	-	-	-	X
57	MG	1G	1636	-	-	-	X
57	MG	1H	3002	-	-	-	X
57	MG	1H	3009	-	-	-	X
57	MG	1H	3011	-	-	-	X
57	MG	1H	3013	-	-	-	X
57	MG	1H	3015	-	-	-	X
57	MG	1H	3029	-	-	-	X
57	MG	1H	3034	-	-	-	X
57	MG	1H	3040	-	-	-	X
57	MG	1H	3041	-	-	-	X
57	MG	1H	3042	-	-	-	X
57	MG	1H	3045	-	-	-	X
57	MG	1H	3056	-	-	-	X
57	MG	1H	3059	-	-	-	X
57	MG	1H	3061	-	-	-	X
57	MG	1H	3066	-	-	-	X
57	MG	1H	3067	-	-	-	X
57	MG	1H	3074	-	-	-	X
57	MG	1H	3076	-	-	-	X
57	MG	1H	3078	-	-	-	X
57	MG	1H	3079	-	-	-	X
57	MG	1H	3082	-	-	-	X
57	MG	1H	3085	-	-	-	X
57	MG	1H	3098	-	-	-	X
57	MG	1H	3102	-	-	-	X
57	MG	1H	3105	-	-	-	X
57	MG	1H	3108	-	-	-	X
57	MG	1H	3121	-	-	-	X
57	MG	1H	3130	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
57	MG	1H	3133	-	-	-	X
57	MG	1H	3140	-	-	-	X
57	MG	1H	3143	-	-	-	X
57	MG	1H	3151	-	-	-	X
57	MG	1H	3165	-	-	-	X
57	MG	1H	3167	-	-	-	X
57	MG	1H	3172	-	-	-	X
57	MG	1H	3175	-	-	-	X
57	MG	1H	3178	-	-	-	X
57	MG	1H	3181	-	-	-	X
57	MG	1H	3186	-	-	-	X
57	MG	1H	3187	-	-	-	X
57	MG	1H	3188	-	-	-	X
57	MG	1H	3200	-	-	-	X
57	MG	1H	3203	-	-	-	X
57	MG	1H	3205	-	-	-	X
57	MG	1H	3212	-	-	-	X
57	MG	1H	3221	-	-	-	X
57	MG	1H	3235	-	-	-	X
57	MG	1H	3264	-	-	-	X
57	MG	1H	3321	-	-	-	X
57	MG	2L	101	-	-	-	X
59	SF4	32	302	-	-	X	-
61	SPE	14	3436	-	-	-	X
61	SPE	14	3437	-	-	-	X

2 Entry composition

There are 62 unique types of molecules in this entry. The entry contains 297444 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a RNA chain called 16S ribosomal RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	13	1499	Total	C	N	O	P	0	0	0
			32223	14342	5973	10409	1499			
1	1G	1508	Total	C	N	O	P	0	0	0
			32414	14427	6005	10474	1508			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
13	1542	G	-	expression tag	GB 55771382
13	1543	C	-	expression tag	GB 55771382
13	1544	U	-	expression tag	GB 55771382
1G	1542	G	-	expression tag	GB 55771382
1G	1543	C	-	expression tag	GB 55771382
1G	1544	U	-	expression tag	GB 55771382

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	1E	231	Total	C	N	O	S	0	0	0
			1874	1199	334	336	5			
2	12	207	Total	C	N	O	S	0	0	0
			1696	1083	306	303	4			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	2E	205	Total	C	N	O	S	0	0	0
			1605	1011	313	280	1			
3	22	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
4	3E	207	Total	C	N	O	S	0	0	0
			1698	1064	338	289	7			
4	32	208	Total	C	N	O	S	0	0	0
			1702	1066	339	290	7			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	4E	149	Total	C	N	O	S	0	0	0
			1142	722	216	200	4			
5	42	150	Total	C	N	O	S	0	0	0
			1141	719	217	201	4			

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	6E	154	Total	C	N	O	S	0	0	0
			1242	770	250	216	6			
7	62	138	Total	C	N	O	S	0	0	0
			1110	689	221	194	6			

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

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

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
9	8E	126	Total	C	N	O	0	0	0
			1000	634	196	170			

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
9	82	121	Total	C	N	O	0	0	0
			953	605	186	162			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	1I	94	Total	C	N	O	S	0	0	0
			749	468	147	133	1			
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	121	Total	C	N	O	S	0	0	0
			947	597	191	158	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	4I	117	Total	C	N	O	S	0	0	0
			933	577	192	162	2			
13	4A	109	Total	C	N	O	S	0	0	0
			879	544	181	152	2			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
14	5I	59	Total	C	N	O	S	0	0	0
			486	309	103	70	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	99	Total	C	N	O	S	0	0	0
			823	528	151	142	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	65	Total	C	N	O	S	0	0	0
			510	324	92	92	2			

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

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

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
22	1K	72	Total	C	N	O	P	S	0	0	0
			1542	691	269	509	72	1			

- 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	77	Total	C	N	O	P	S	0	0	0
			1646	735	298	535	77	1			

- Molecule 24 is a RNA chain called tRNALys.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
24	3K	70	Total	C	N	O	P	0	0	0
			1483	664	260	490	69			
24	1L	66	Total	C	N	O	P	0	0	0
			1401	626	244	465	66			
24	3L	72	Total	C	N	O	P	0	0	0
			1528	684	270	503	71			

- Molecule 25 is a RNA chain called mRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
25	4K	19	Total	C	N	O	P	0	0	0
			420	188	89	124	19			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
25	4L	19	Total	C	N	O	P	0	0	0
			419	188	89	123	19			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
26	1H	2860	Total	C	N	O	P	0	0	0
			61609	27418	11525	19806	2860			
26	14	2826	Total	C	N	O	P	0	0	0
			60877	27092	11393	19566	2826			

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	1059B	U	G	conflict	GB 55771382
1H	1080	A	C	conflict	GB 55771382
14	158	U	UNK	conflict	GB 55771382
14	654A	A	G	conflict	GB 55771382
14	654E	C	G	conflict	GB 55771382
14	654P	G	C	conflict	GB 55771382
14	654T	A	C	conflict	GB 55771382
14	1058	U	G	conflict	GB 55771382
14	1080	A	C	conflict	GB 55771382

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
28	71	132	Total	C	N	O	S	0	0	0
			1027	648	193	185	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
29	11	273	Total	C	N	O	S	0	0	0
			2120	1338	421	358	3			
29	19	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	203	Total	C	N	O	S	0	0	0
			1546	978	295	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	180	Total	C	N	O	S	0	0	0
			1459	931	266	258	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	169	Total	C	N	O	S	0	0	0
			1295	823	241	230	1			

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
35	58	137	Total	C	N	O	S	0	0	0
			1096	706	205	181	4			
35	15	137	Total	C	N	O	S	0	0	0
			1096	707	205	181	3			

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
38	88	141	Total	C	N	O	S	0	0	0
			1117	712	211	187	7			
38	45	138	Total	C	N	O	S	0	0	0
			1099	702	208	183	6			

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
41	B8	135	Total	C	N	O	S	0	0	0
			1119	697	230	191	1			
41	75	133	Total	C	N	O	S	0	0	0
			1109	691	228	189	1			

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
45	F8	95	Total	C	N	O	S	0	0	0
			750	488	135	126	1			
45	B5	94	Total	C	N	O		0	0	0
			735	477	133	125				

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
46	G8	103	Total	C	N	O	S	0	0	0
			783	504	148	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	177	Total	C	N	O	S	0	0	0
			1411	901	253	255	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	96	Total	C	N	O	S	0	0	0
			747	469	148	129	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			
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	60	Total	C	N	O	S	0	0	0
			475	300	84	86	5			

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

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

- Molecule 54 is a protein called 50S ribosomal protein L33.

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

- Molecule 55 is a protein called 50S ribosomal protein L34.

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

- Molecule 56 is a protein called 50S ribosomal protein L35.

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

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
57	45	2	Total 2	Mg 2	0	0
57	P8	1	Total 1	Mg 1	0	0
57	32	1	Total 1	Mg 1	0	0
57	C5	1	Total 1	Mg 1	0	0
57	13	140	Total 140	Mg 140	0	0
57	1J	8	Total 8	Mg 8	0	0
57	5I	1	Total 1	Mg 1	0	0
57	35	1	Total 1	Mg 1	0	0
57	4L	1	Total 1	Mg 1	0	0
57	16	11	Total 11	Mg 11	0	0
57	42	1	Total 1	Mg 1	0	0
57	25	1	Total 1	Mg 1	0	0
57	M5	1	Total 1	Mg 1	0	0
57	21	3	Total 3	Mg 3	0	0
57	31	2	Total 2	Mg 2	0	0
57	Q8	1	Total 1	Mg 1	0	0
57	4I	1	Total 1	Mg 1	0	0
57	3I	1	Total 1	Mg 1	0	0

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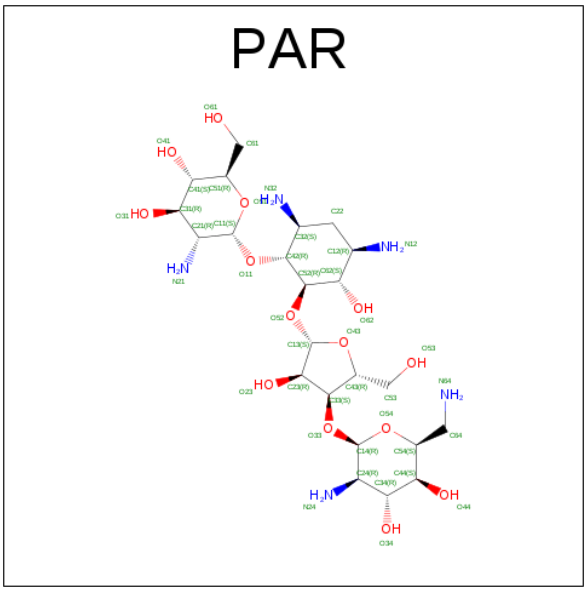
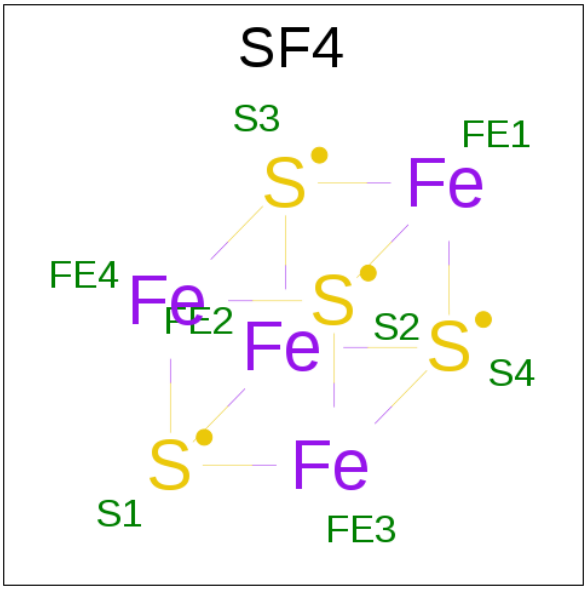
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
57	I8	2	Total Mg 2 2	0	0
57	52	1	Total Mg 1 1	0	0
57	29	1	Total Mg 1 1	0	0
57	7A	1	Total Mg 1 1	0	0
57	2K	2	Total Mg 2 2	0	0
57	39	2	Total Mg 2 2	0	0
57	1G	102	Total Mg 102 102	0	0
57	1H	525	Total Mg 525 525	0	0
57	E5	1	Total Mg 1 1	0	0
57	88	3	Total Mg 3 3	0	0
57	14	435	Total Mg 435 435	0	0
57	78	1	Total Mg 1 1	0	0
57	19	1	Total Mg 1 1	0	0
57	41	1	Total Mg 1 1	0	0
57	2L	2	Total Mg 2 2	0	0

- Molecule 58 is PAROMOMYCIN (three-letter code: PAR) (formula: $C_{23}H_{45}N_5O_{14}$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
58	13	1	Total	C	N	O	0	0
			42	23	5	14		
58	1G	1	Total	C	N	O	0	0
			42	23	5	14		

- Molecule 59 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe_4S_4).

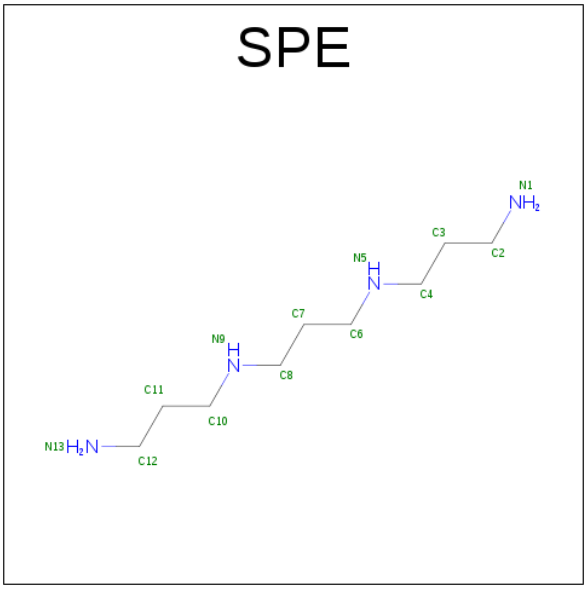


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
59	3E	1	Total	Fe	S		0	0
			8	4	4			
59	32	1	Total	Fe	S		0	0
			8	4	4			

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

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

- Molecule 61 is THERMINE (three-letter code: SPE) (formula: $C_9H_{24}N_4$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
61	1G	1	Total C N 13 9 4	0	0
61	14	1	Total C N 13 9 4	0	0
61	14	1	Total C N 13 9 4	0	0

- Molecule 62 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
62	13	320	Total O 320 320	0	0
62	4E	3	Total O 3 3	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
62	8E	2	Total O 2 2	0	0
62	1I	2	Total O 2 2	0	0
62	3I	2	Total O 2 2	0	0
62	5I	2	Total O 2 2	0	0
62	6I	3	Total O 3 3	0	0
62	7I	1	Total O 1 1	0	0
62	BI	2	Total O 2 2	0	0
62	1F	1	Total O 1 1	0	0
62	1K	2	Total O 2 2	0	0
62	2K	8	Total O 8 8	0	0
62	4K	5	Total O 5 5	0	0
62	1H	1470	Total O 1470 1470	0	0
62	16	12	Total O 12 12	0	0
62	11	17	Total O 17 17	0	0
62	21	7	Total O 7 7	0	0
62	31	5	Total O 5 5	0	0
62	41	1	Total O 1 1	0	0
62	58	2	Total O 2 2	0	0
62	78	10	Total O 10 10	0	0
62	B8	1	Total O 1 1	0	0
62	C8	3	Total O 3 3	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
62	F8	2	Total O 2 2	0	0
62	G8	2	Total O 2 2	0	0
62	I8	6	Total O 6 6	0	0
62	J8	4	Total O 4 4	0	0
62	L8	3	Total O 3 3	0	0
62	P8	1	Total O 1 1	0	0
62	Q8	5	Total O 5 5	0	0
62	1G	317	Total O 317 317	0	0
62	32	1	Total O 1 1	0	0
62	52	4	Total O 4 4	0	0
62	1A	1	Total O 1 1	0	0
62	6A	2	Total O 2 2	0	0
62	7A	5	Total O 5 5	0	0
62	9A	2	Total O 2 2	0	0
62	BA	2	Total O 2 2	0	0
62	2L	6	Total O 6 6	0	0
62	4L	6	Total O 6 6	0	0
62	14	1144	Total O 1144 1144	0	0
62	1J	12	Total O 12 12	0	0
62	19	15	Total O 15 15	0	0
62	29	4	Total O 4 4	0	0

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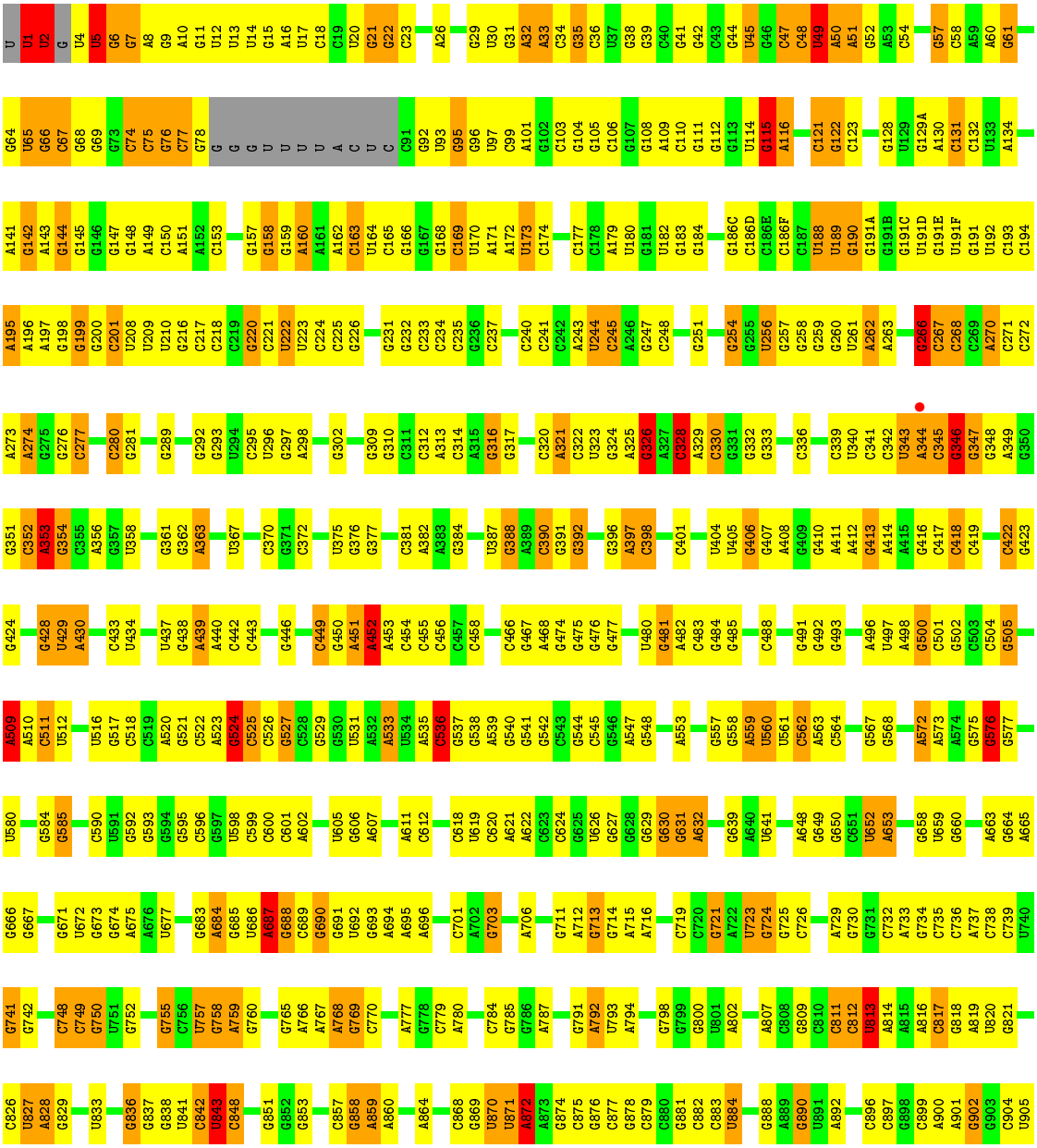
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
62	39	5	Total O 5 5	0	0
62	15	1	Total O 1 1	0	0
62	25	6	Total O 6 6	0	0
62	35	8	Total O 8 8	0	0
62	55	3	Total O 3 3	0	0
62	85	2	Total O 2 2	0	0
62	A5	1	Total O 1 1	0	0
62	B5	1	Total O 1 1	0	0
62	C5	3	Total O 3 3	0	0
62	F5	1	Total O 1 1	0	0
62	H5	2	Total O 2 2	0	0
62	M5	9	Total O 9 9	0	0

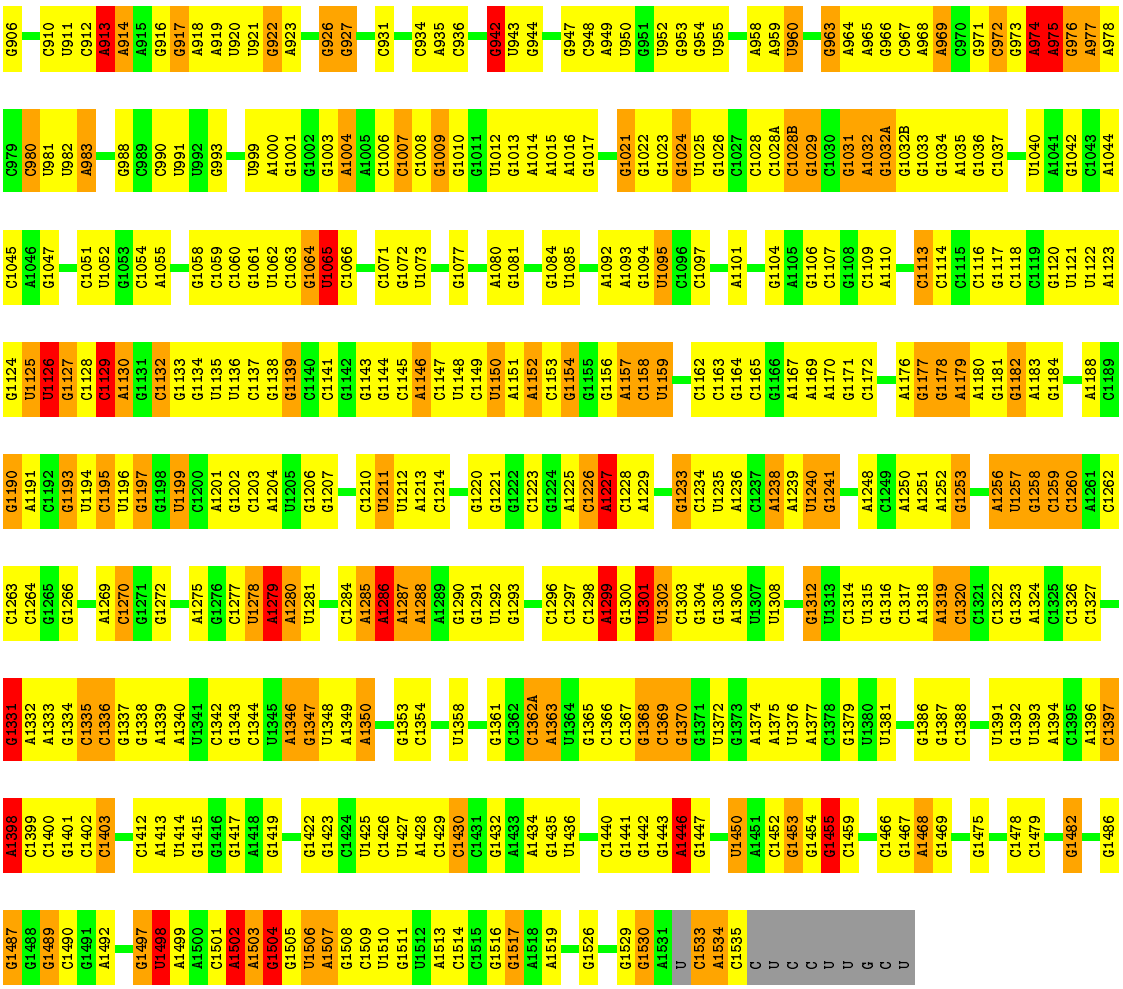
3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (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

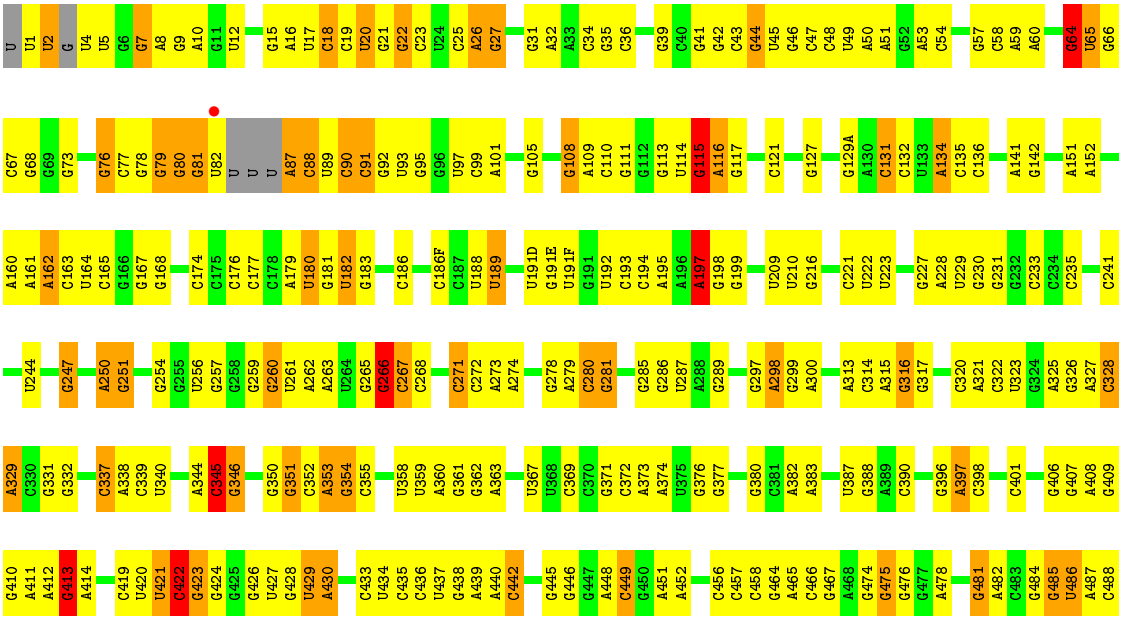
Chain 13: 37% 45% 15%

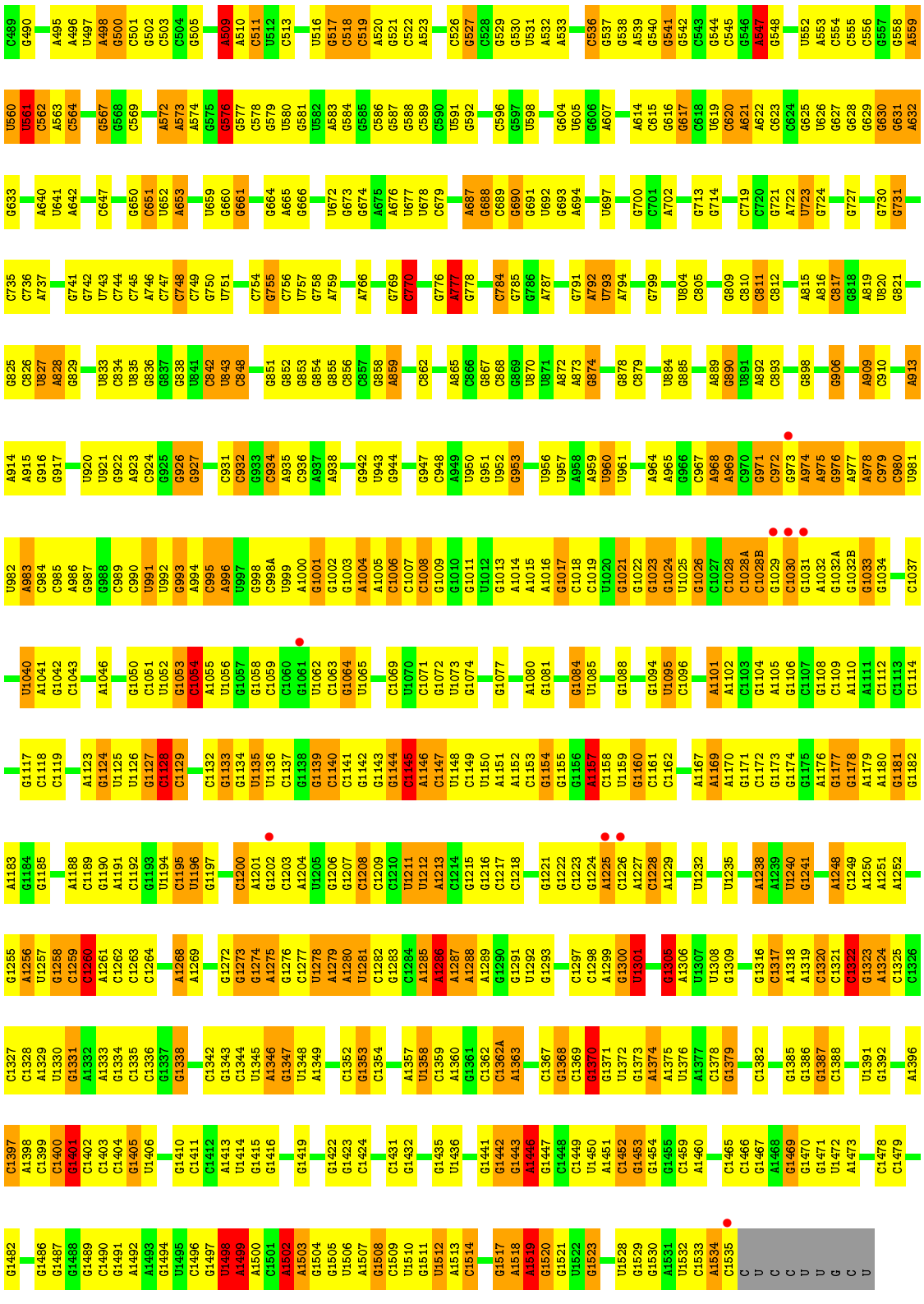




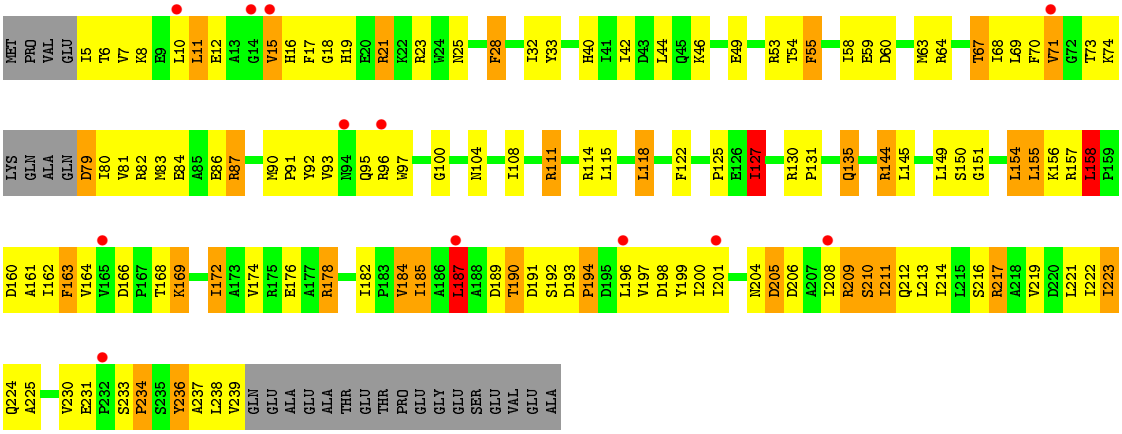
• Molecule 1: 16S ribosomal RNA

Chain 1G:



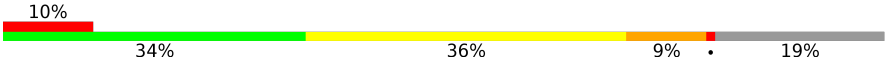


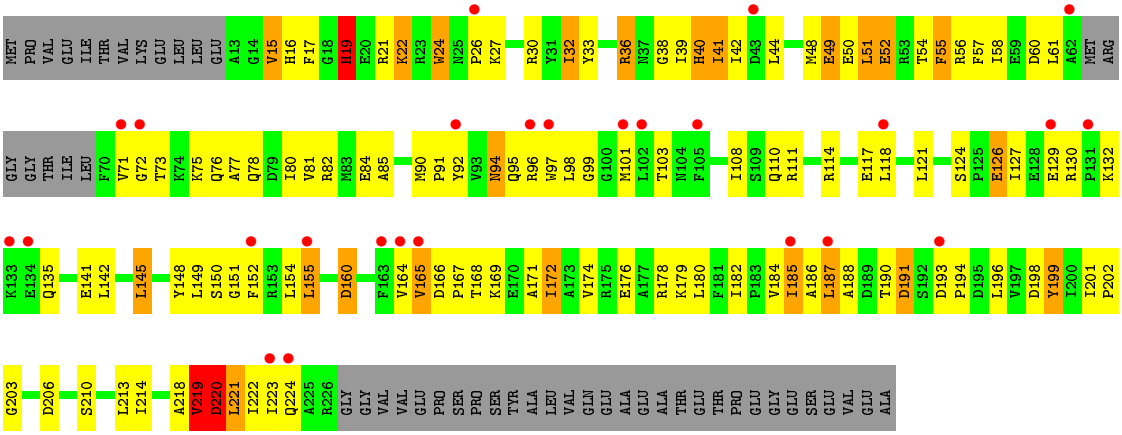
• Molecule 2: 30S ribosomal protein S2



• Molecule 2: 30S ribosomal protein S2

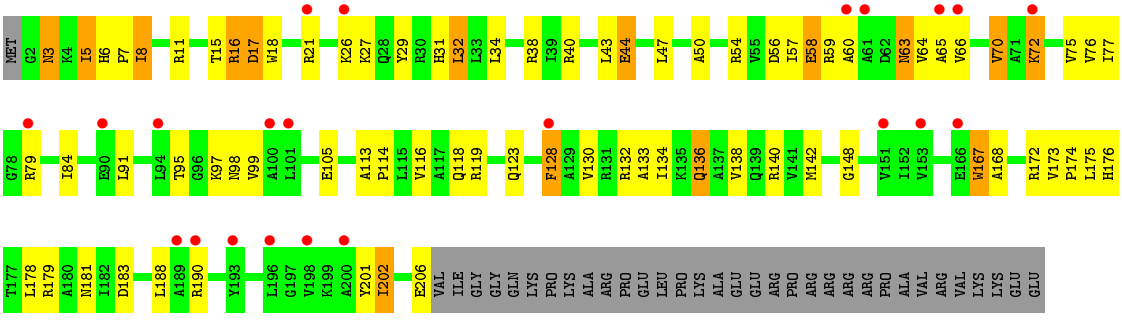
Chain 12:





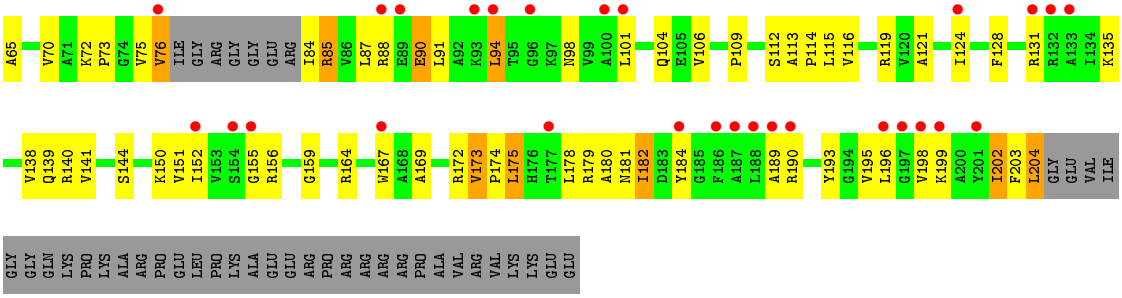
• Molecule 3: 30S ribosomal protein S3

Chain 2E:



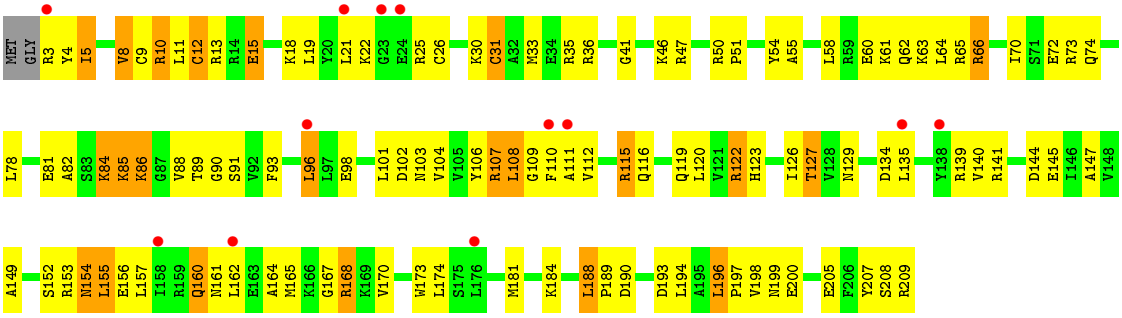
• Molecule 3: 30S ribosomal protein S3

Chain 22:



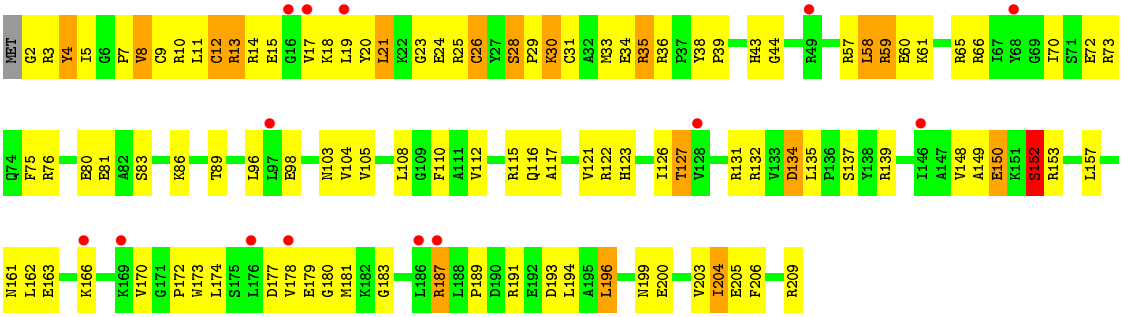
• Molecule 4: 30S ribosomal protein S4

Chain 3E:



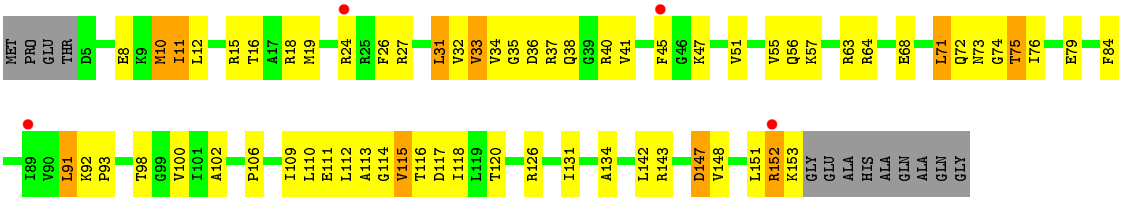
• Molecule 4: 30S ribosomal protein S4

Chain 32:



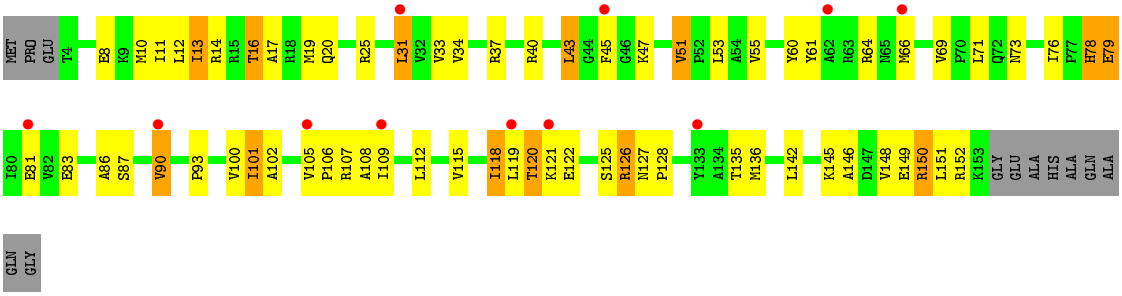
• Molecule 5: 30S ribosomal protein S5

Chain 4E:

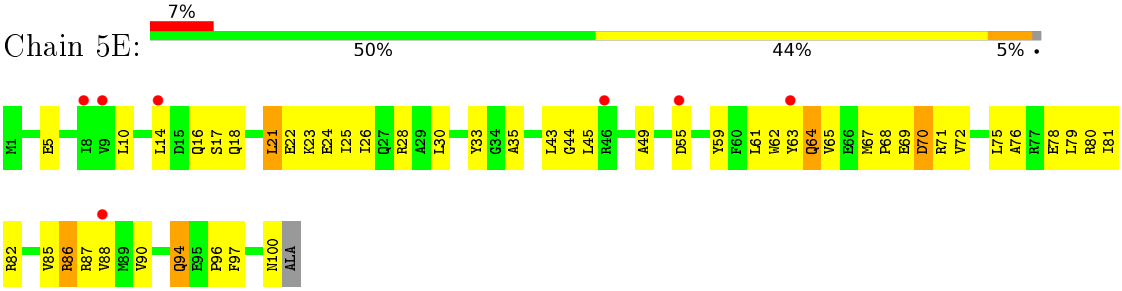


• Molecule 5: 30S ribosomal protein S5

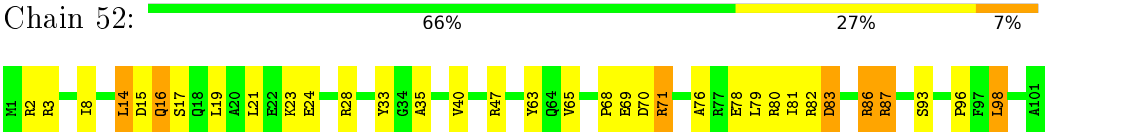
Chain 42:



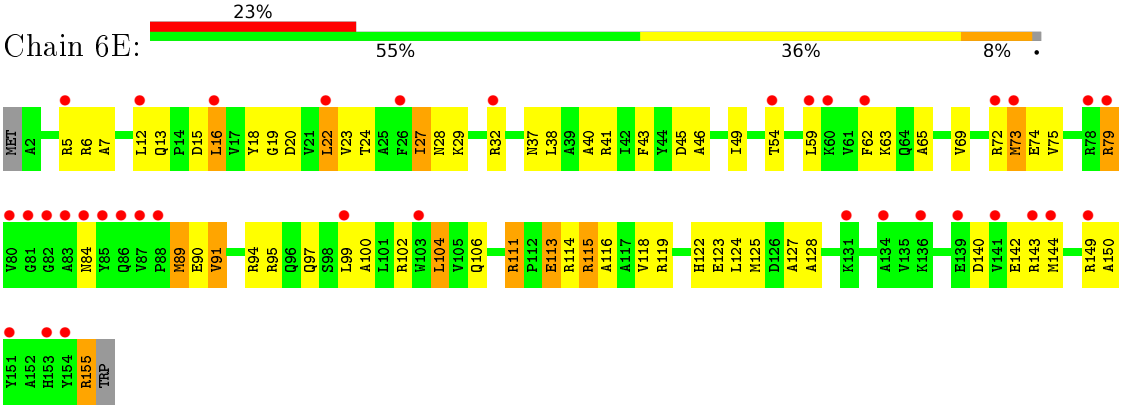
- Molecule 6: 30S ribosomal protein S6



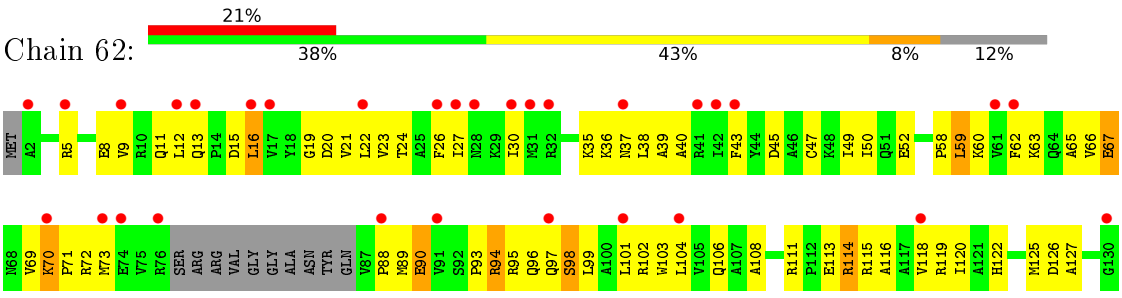
- Molecule 6: 30S ribosomal protein S6

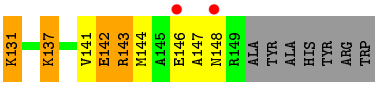


- Molecule 7: 30S ribosomal protein S7



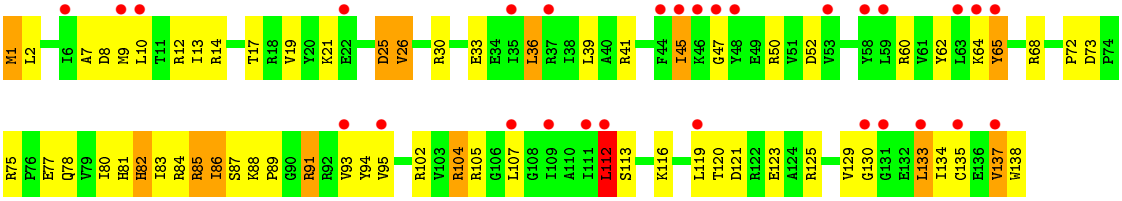
- Molecule 7: 30S ribosomal protein S7





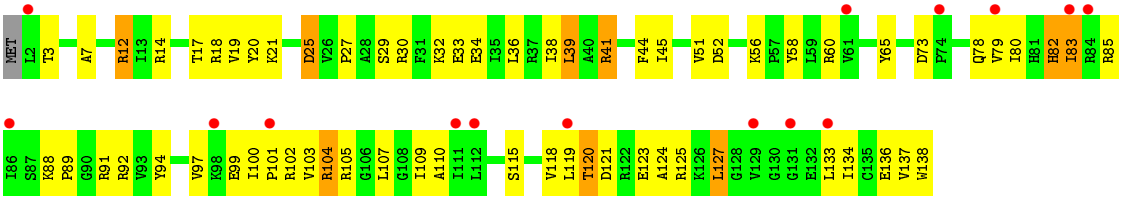
• Molecule 8: 30S ribosomal protein S8

Chain 7E:



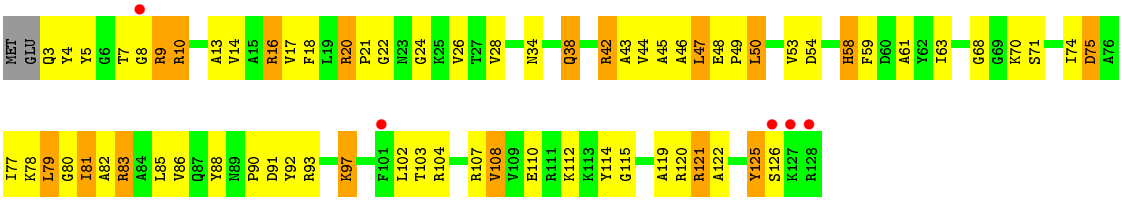
• Molecule 8: 30S ribosomal protein S8

Chain 72:



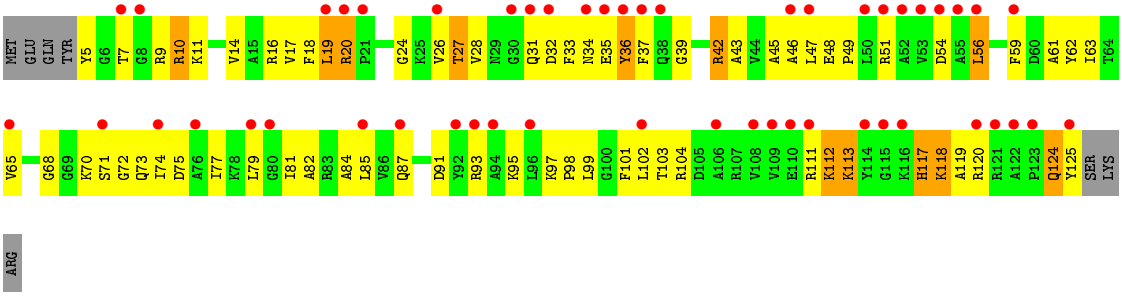
• Molecule 9: 30S ribosomal protein S9

Chain 8E:



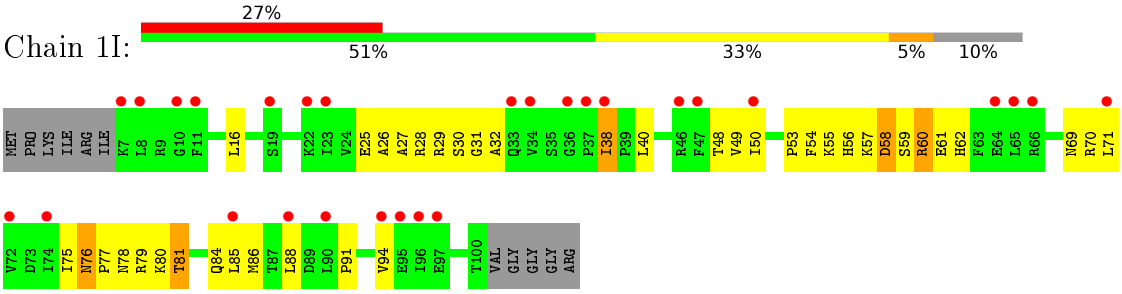
• Molecule 9: 30S ribosomal protein S9

Chain 82:



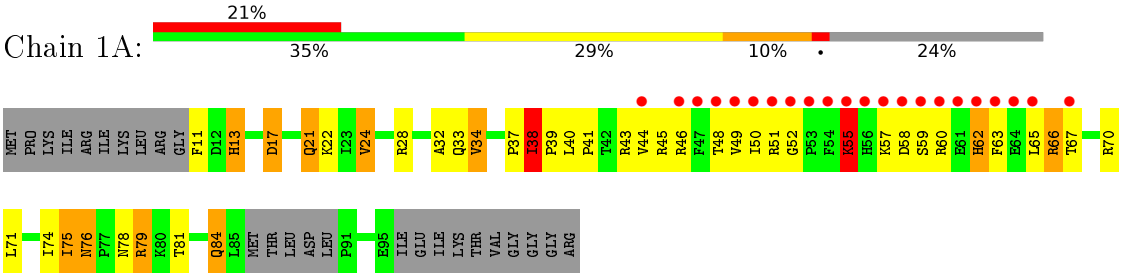
• Molecule 10: 30S ribosomal protein S10

Chain 1I:



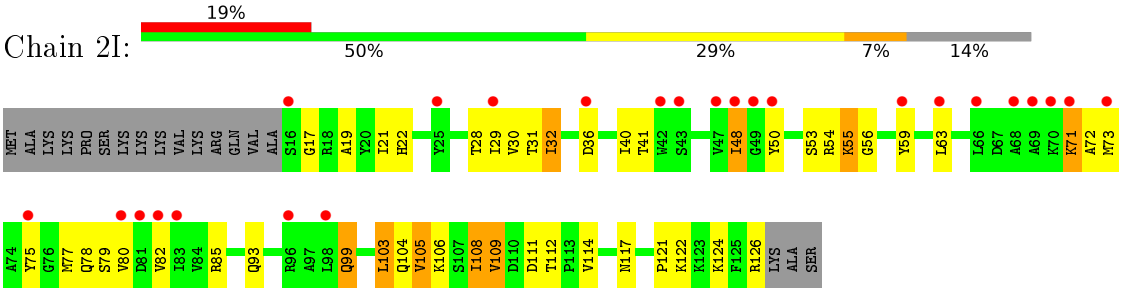
• Molecule 10: 30S ribosomal protein S10

Chain 1A:



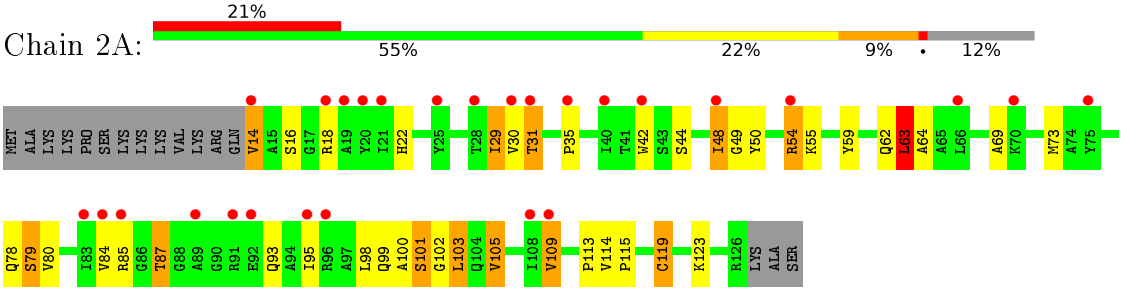
• Molecule 11: 30S ribosomal protein S11

Chain 2I:



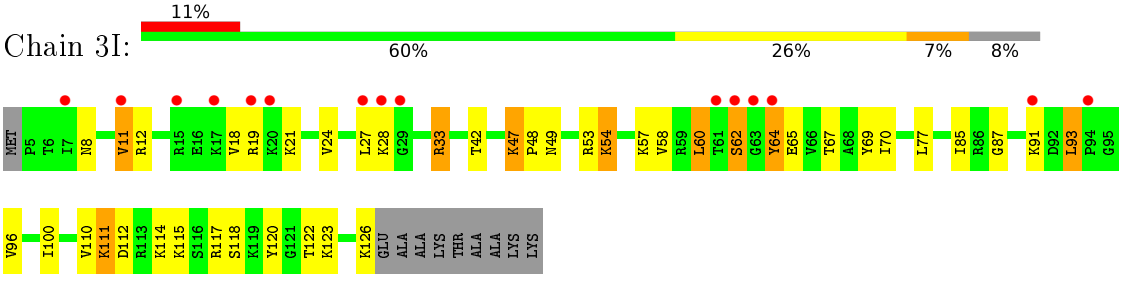
• Molecule 11: 30S ribosomal protein S11

Chain 2A:



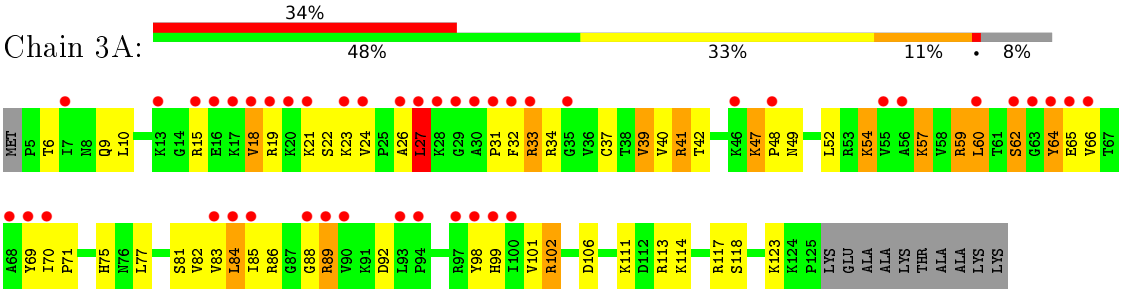
• Molecule 12: 30S ribosomal protein S12

Chain 3I:



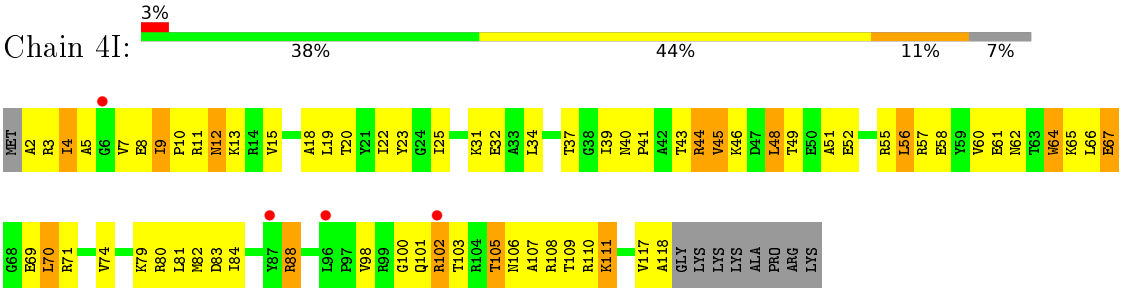
• Molecule 12: 30S ribosomal protein S12

Chain 3A:



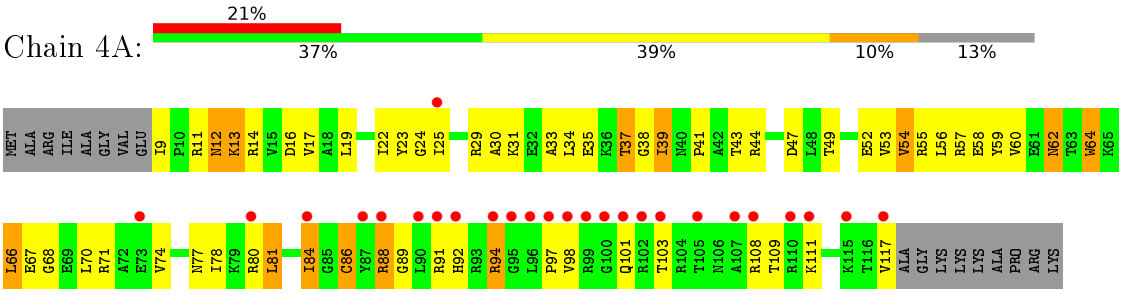
• Molecule 13: 30S ribosomal protein S13

Chain 4I:



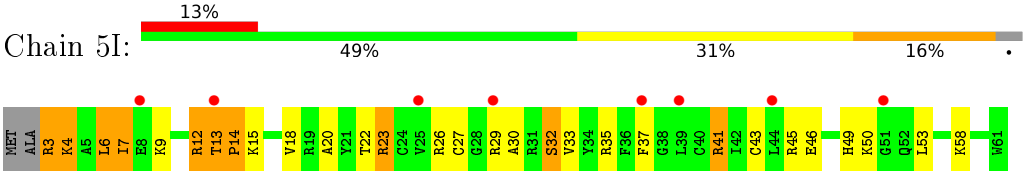
• Molecule 13: 30S ribosomal protein S13

Chain 4A:



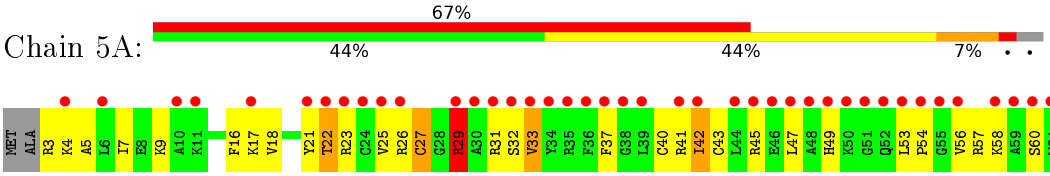
• Molecule 14: 30S ribosomal protein S14 type Z

Chain 5I:



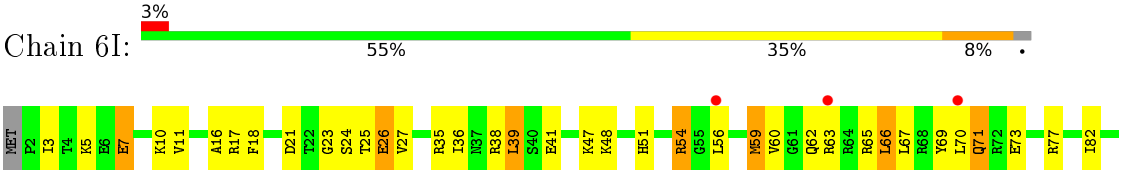
• Molecule 14: 30S ribosomal protein S14 type Z

Chain 5A:



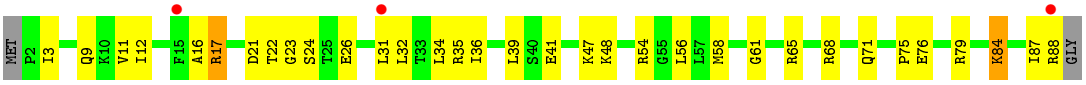
• Molecule 15: 30S ribosomal protein S15

Chain 6I:



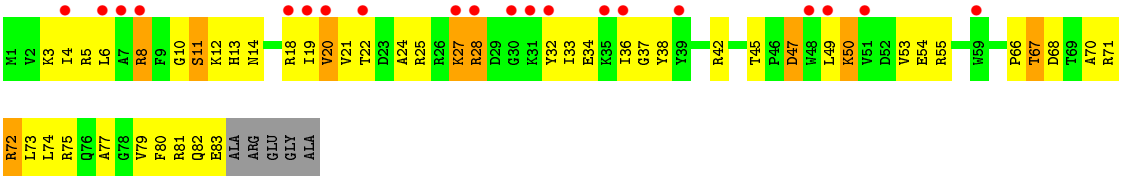
- Molecule 15: 30S ribosomal protein S15

Chain 6A:



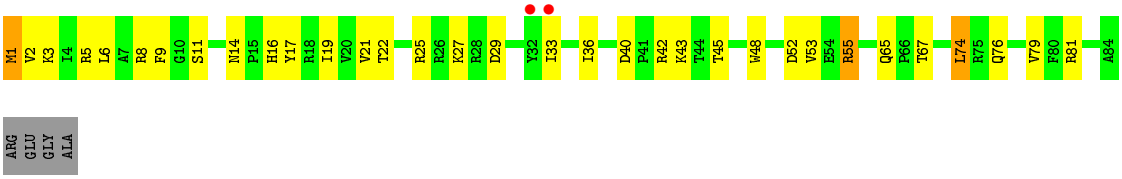
- Molecule 16: 30S ribosomal protein S16

Chain 7I:



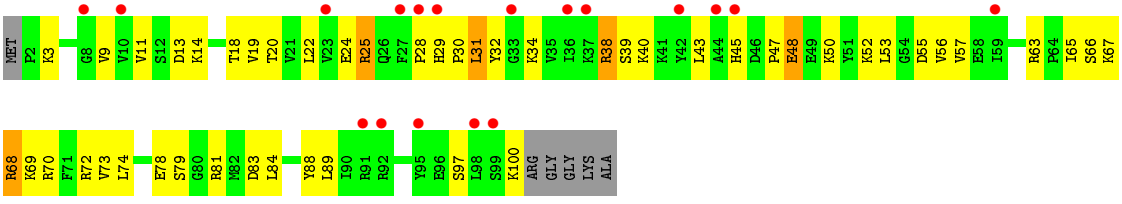
- Molecule 16: 30S ribosomal protein S16

Chain 7A:



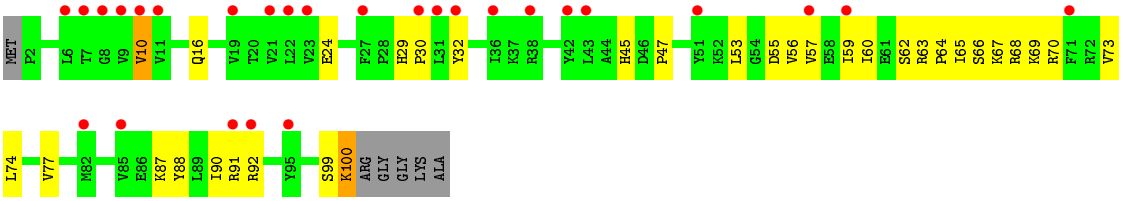
- Molecule 17: 30S ribosomal protein S17

Chain 8I:



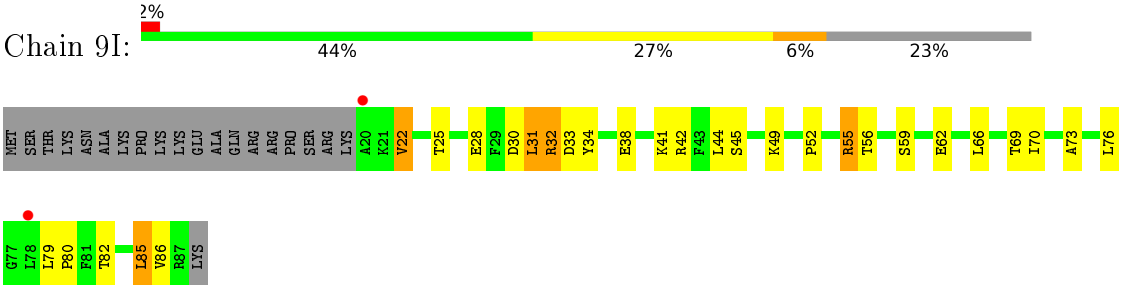
- Molecule 17: 30S ribosomal protein S17

Chain 8A:



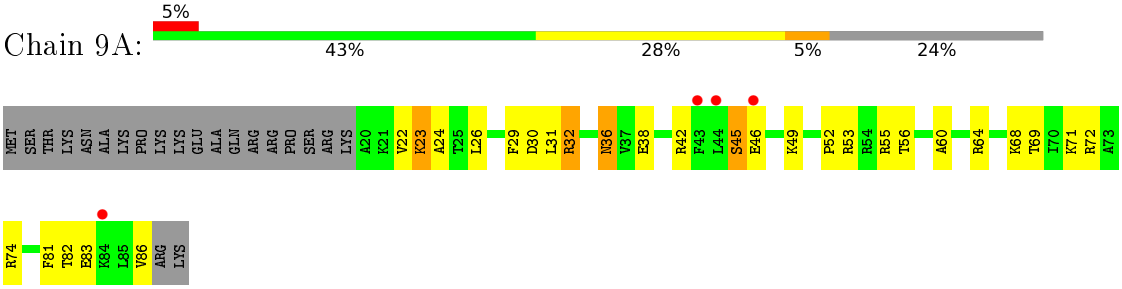
• Molecule 18: 30S ribosomal protein S18

Chain 9I:



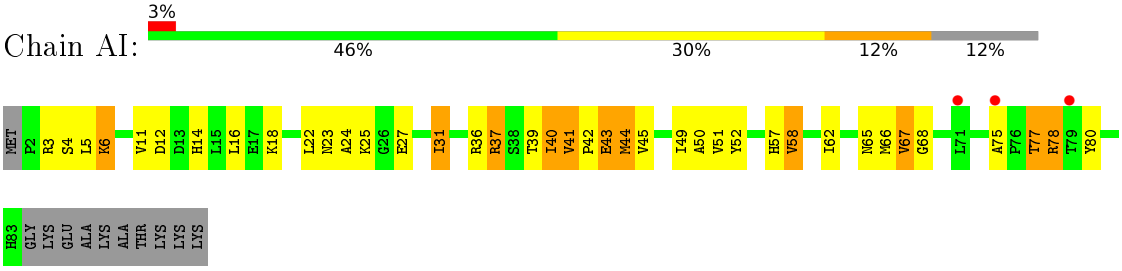
• Molecule 18: 30S ribosomal protein S18

Chain 9A:



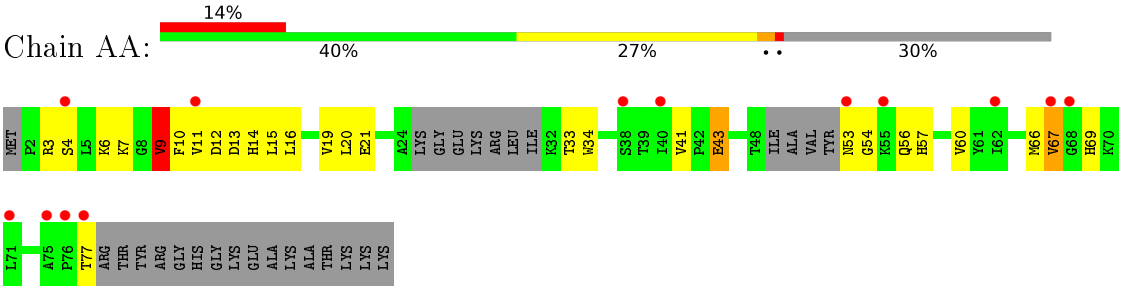
• Molecule 19: 30S ribosomal protein S19

Chain AI:



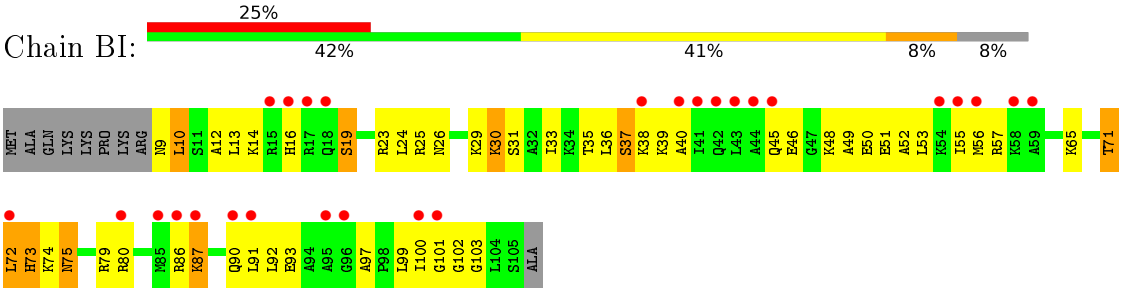
• Molecule 19: 30S ribosomal protein S19

Chain AA:



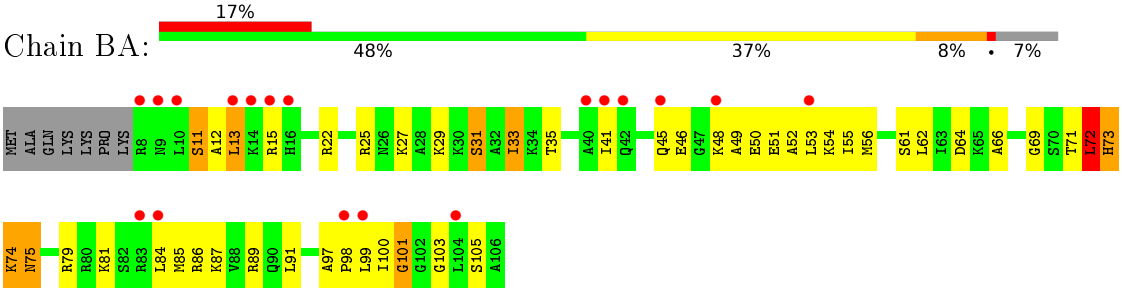
• Molecule 20: 30S ribosomal protein S20

Chain BI:



• Molecule 20: 30S ribosomal protein S20

Chain BA:

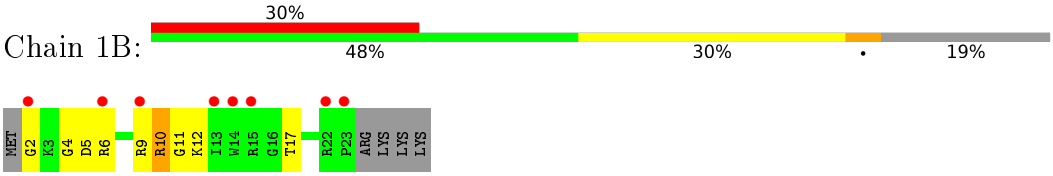


• Molecule 21: 30S ribosomal protein Thx

Chain 1F:

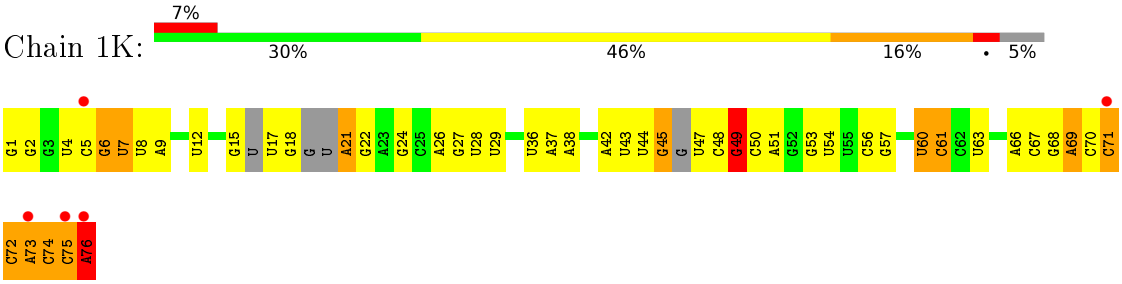
• Molecule 21: 30S ribosomal protein Thx

Chain 1B:



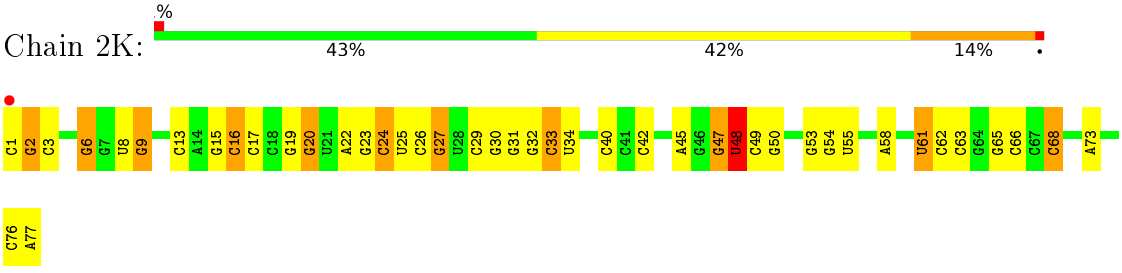
• Molecule 22: tRNALys

Chain 1K:



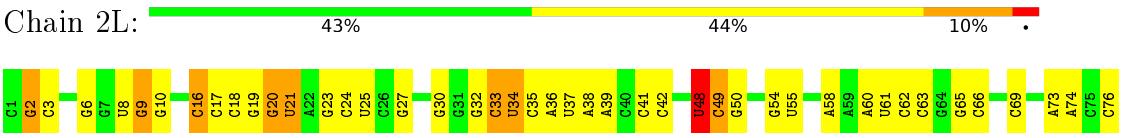
• Molecule 23: tRNAfMet

Chain 2K:



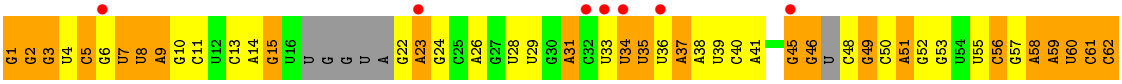
• Molecule 23: tRNAfMet

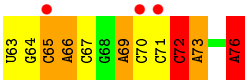
Chain 2L:



- Molecule 24: tRNALys

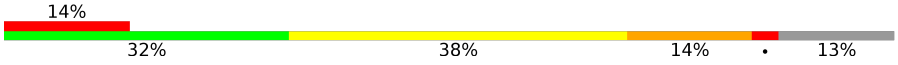
Chain 3K:

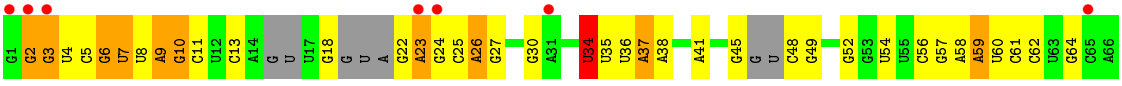


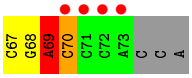


- Molecule 24: tRNALys

Chain 1L:

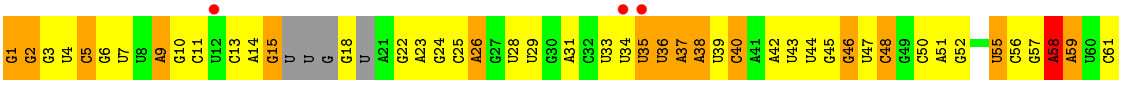


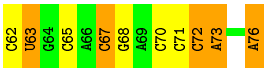




- Molecule 24: tRNALys

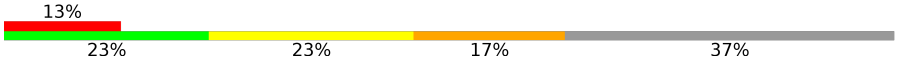
Chain 3L:

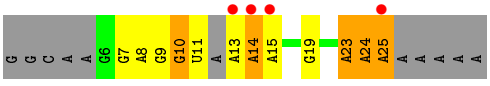




- Molecule 25: mRNA

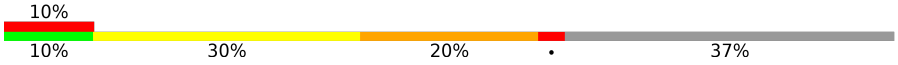
Chain 4K:

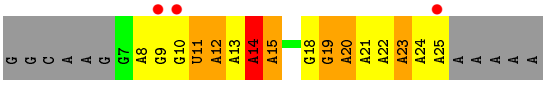




- Molecule 25: mRNA

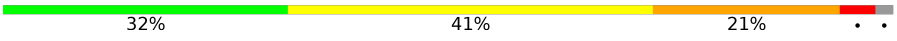
Chain 4L:

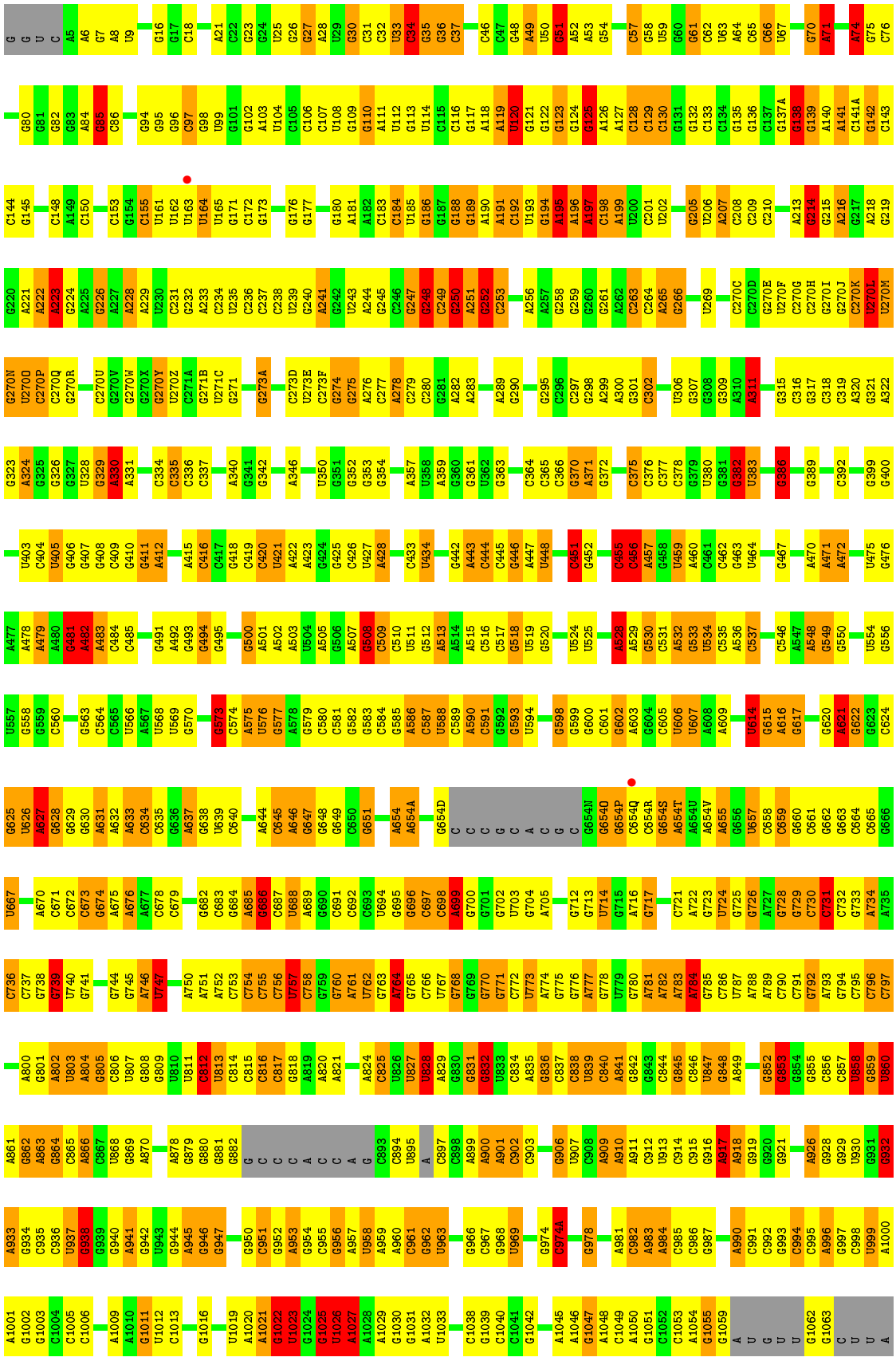


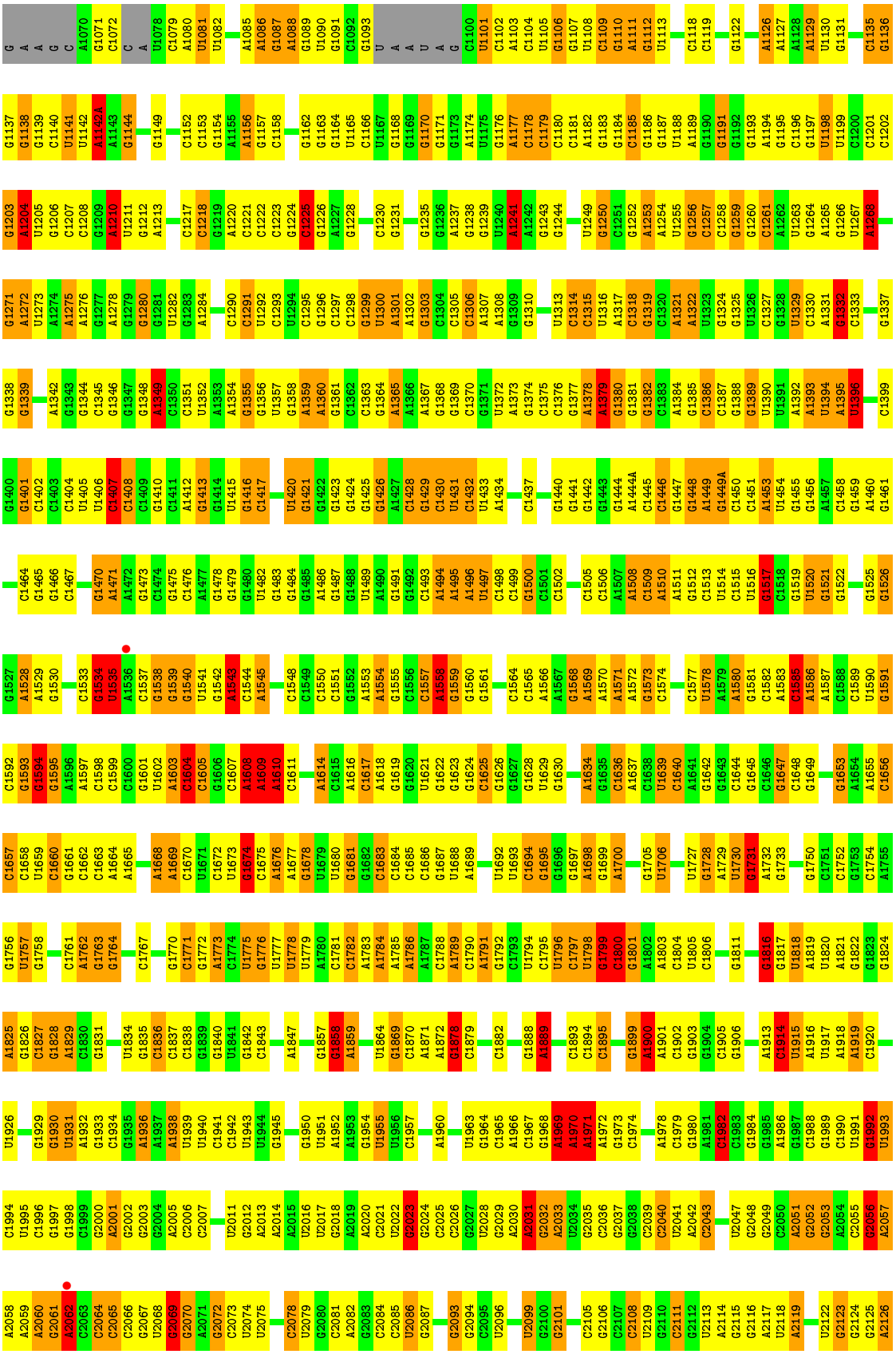


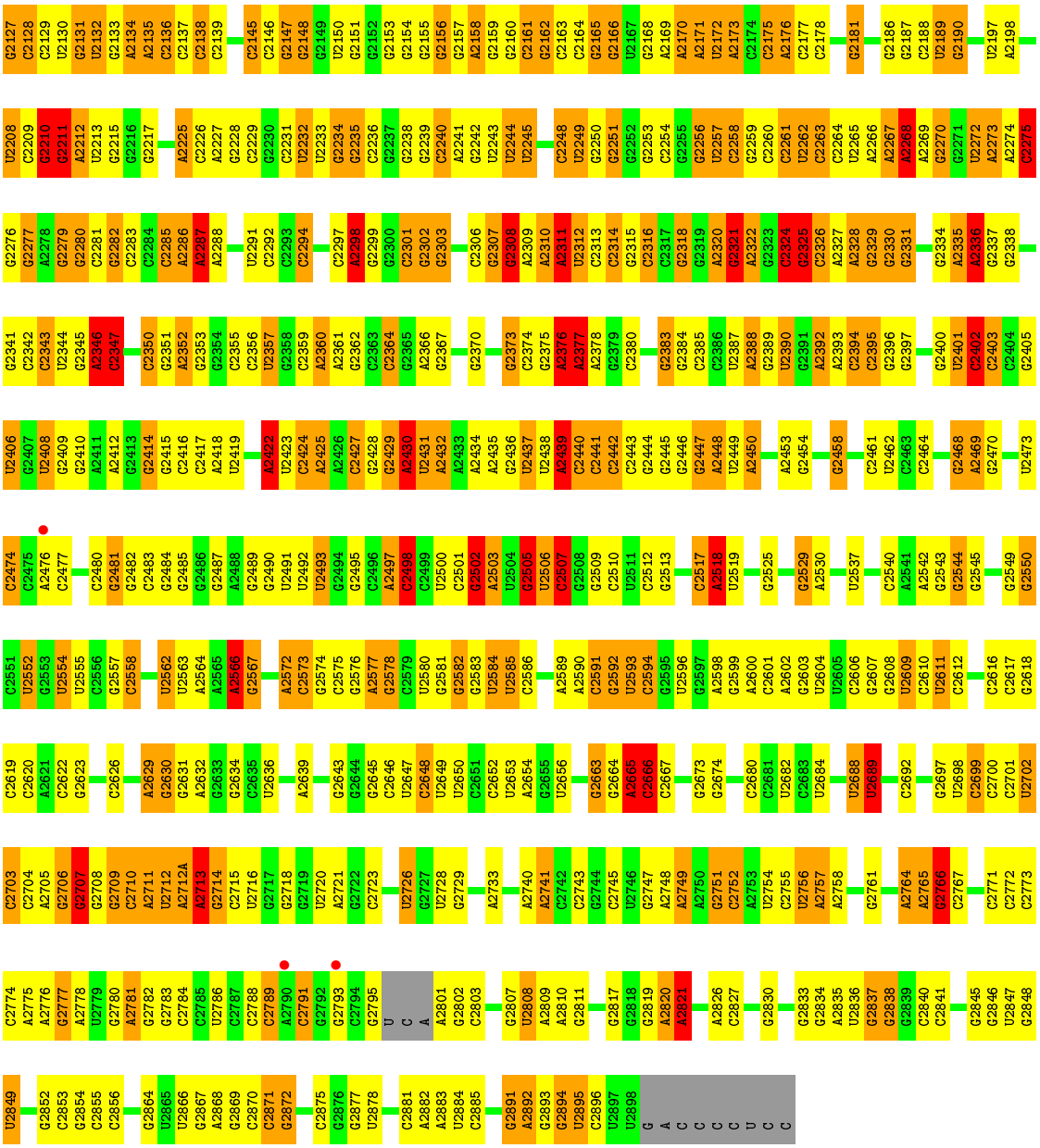
- Molecule 26: 23S ribosomal RNA

Chain 1H:



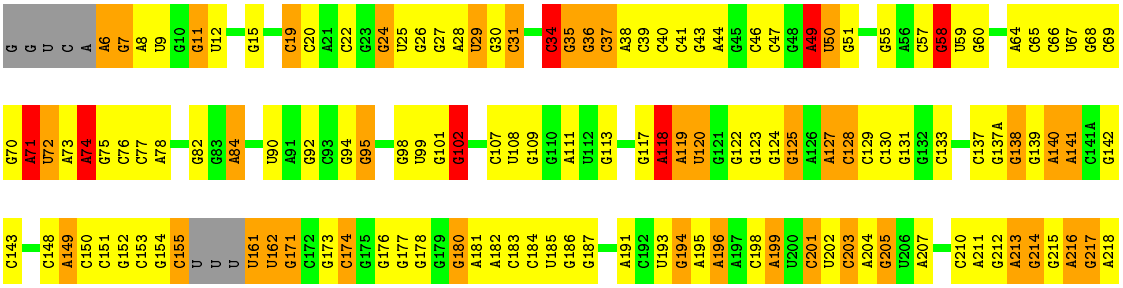


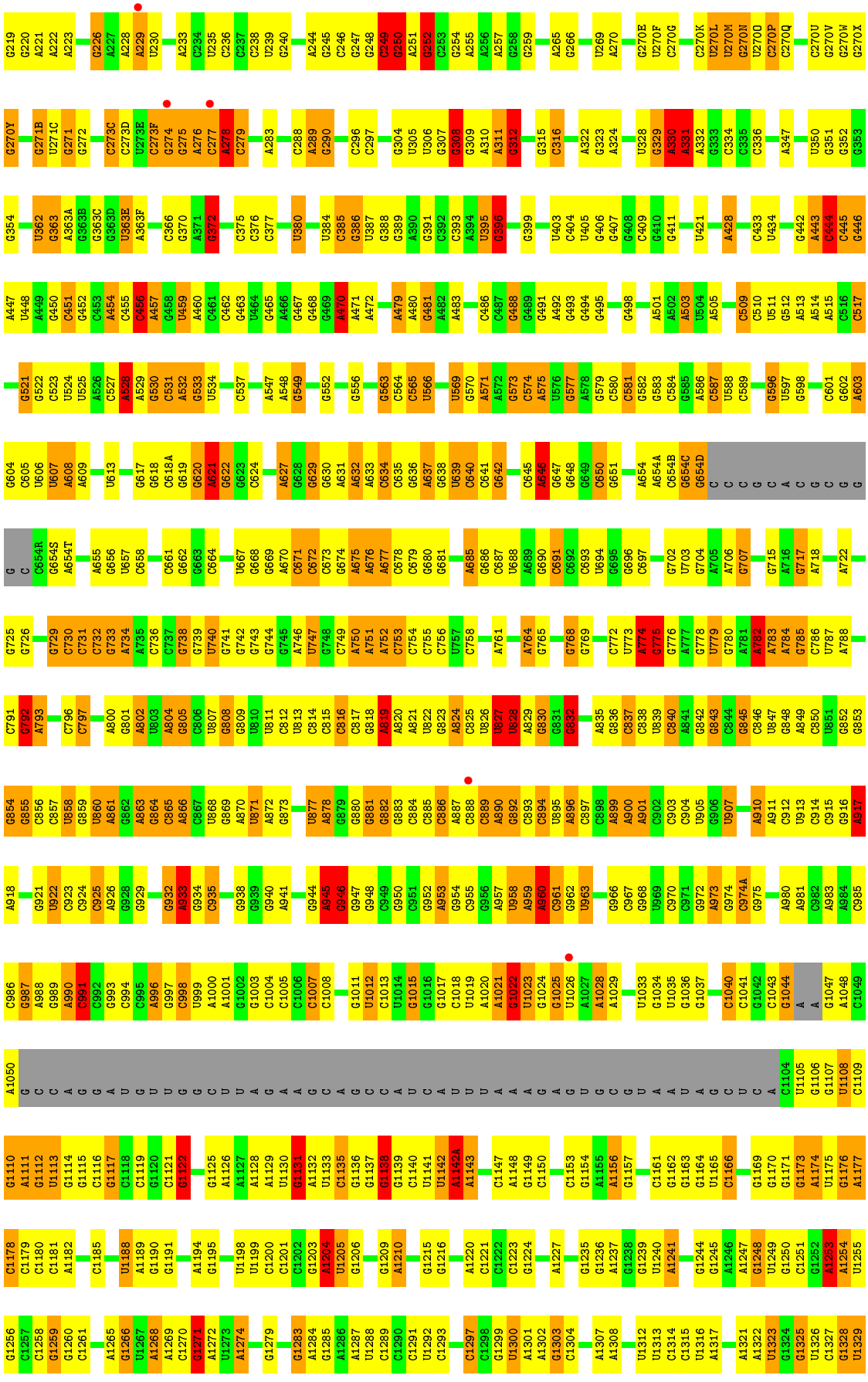


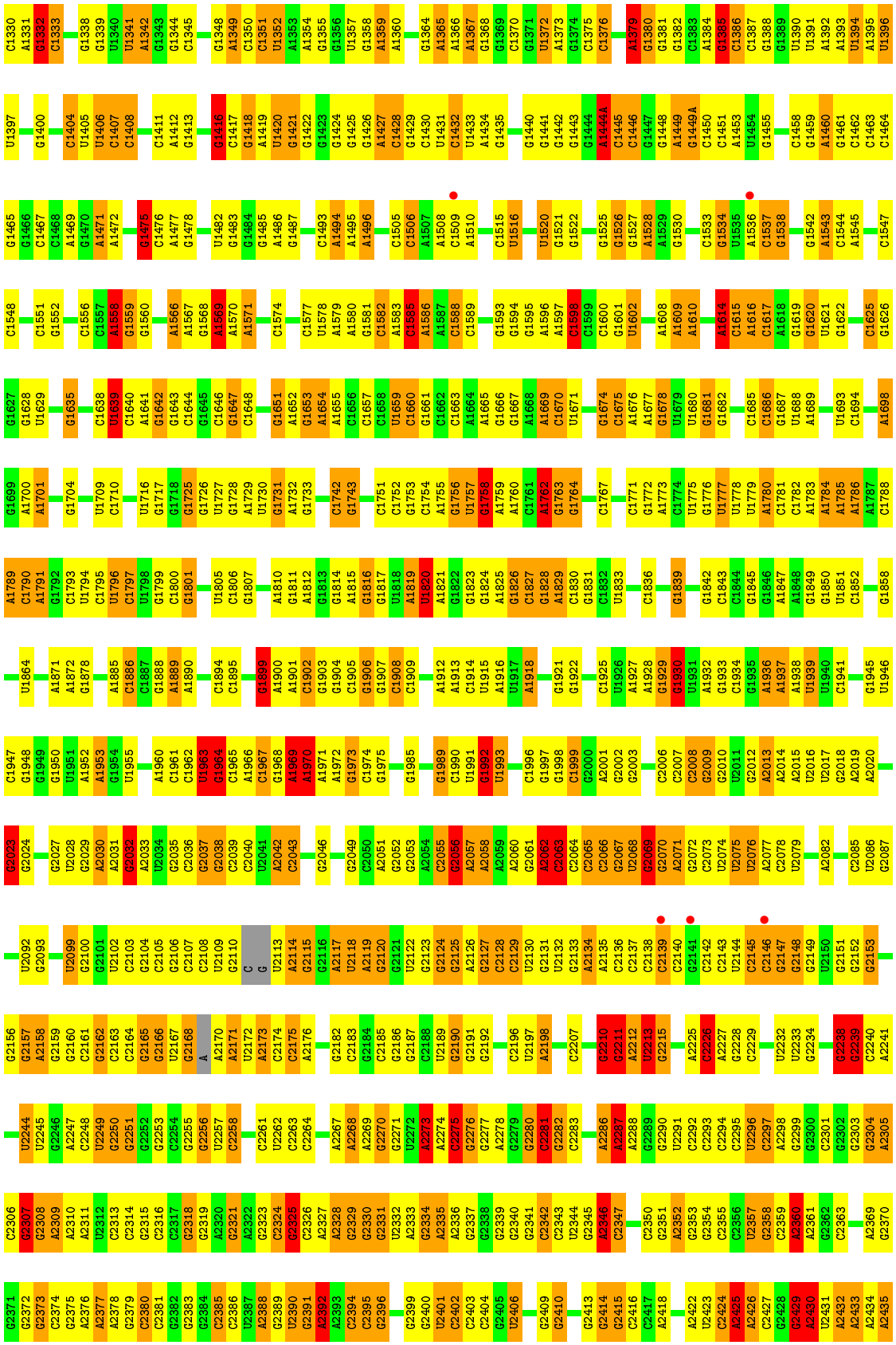


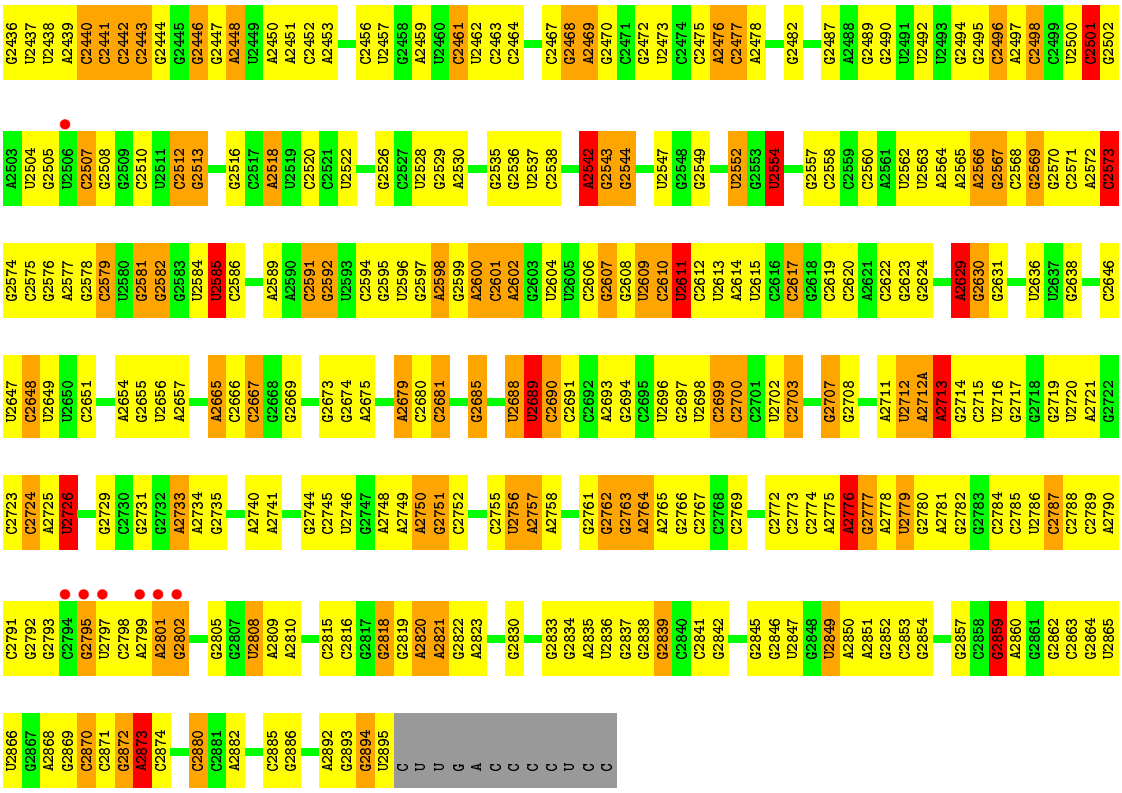
• Molecule 26: 23S ribosomal RNA

Chain 14:



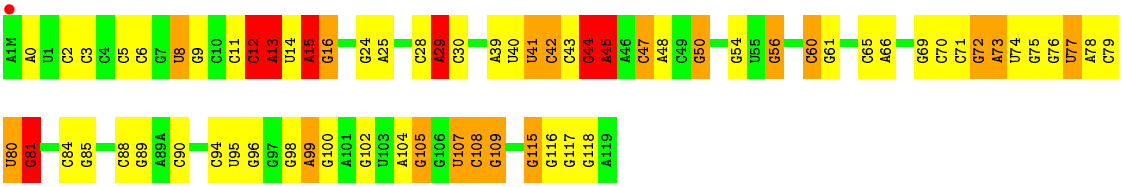






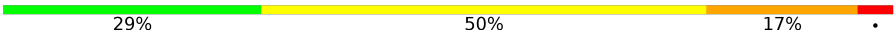
• Molecule 27: 5S ribosomal RNA

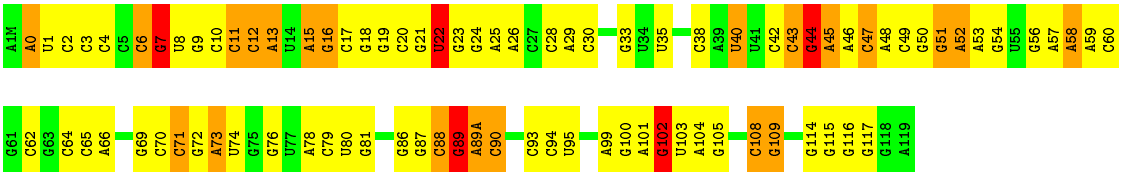
Chain 16:



• Molecule 27: 5S ribosomal RNA

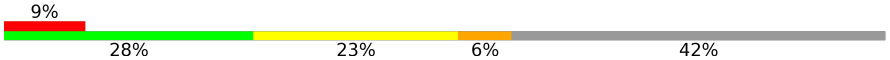
Chain 1J:

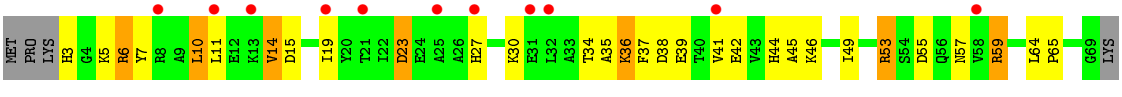


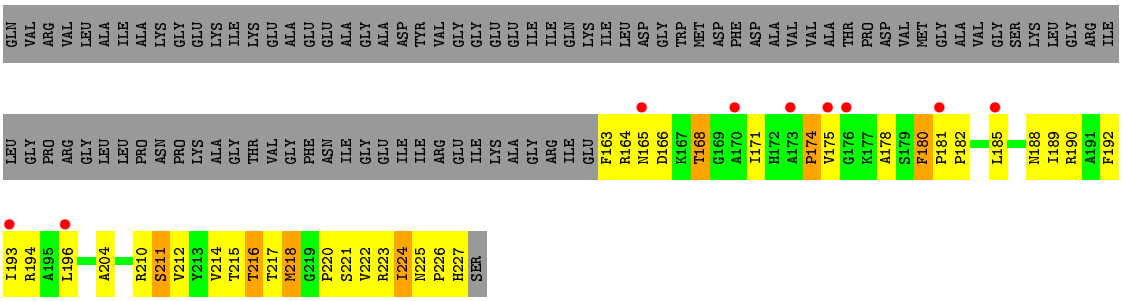


• Molecule 28: 50S ribosomal protein L1

Chain 71:

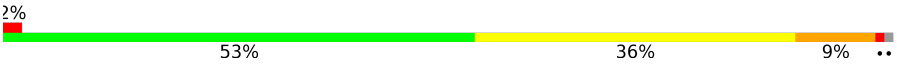


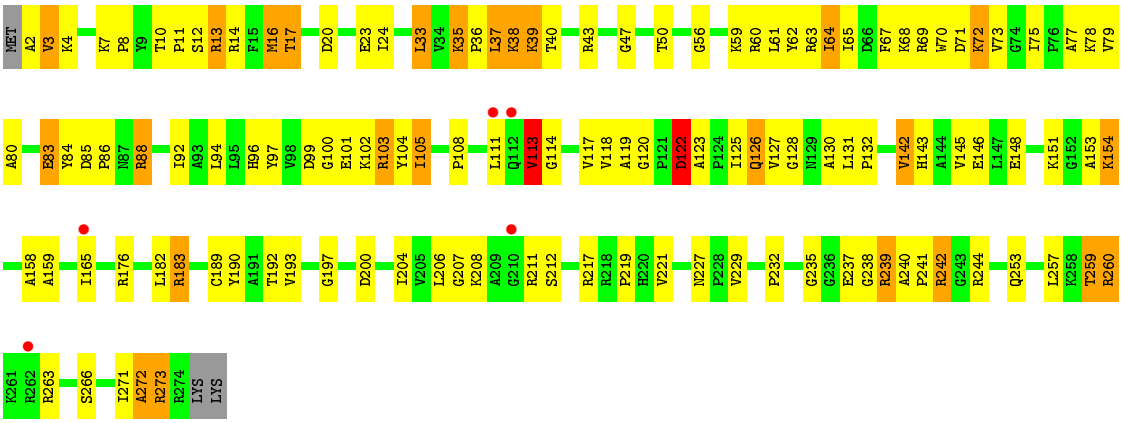




• Molecule 29: 50S ribosomal protein L2

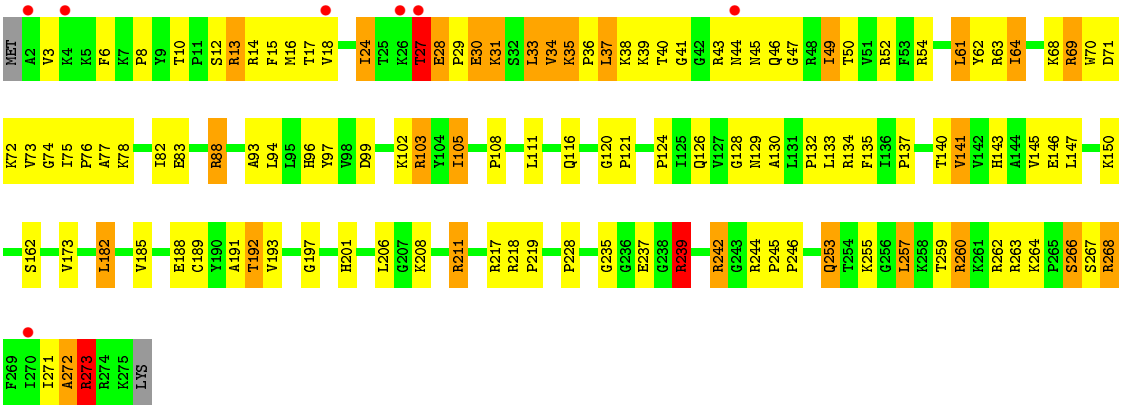
Chain 11:





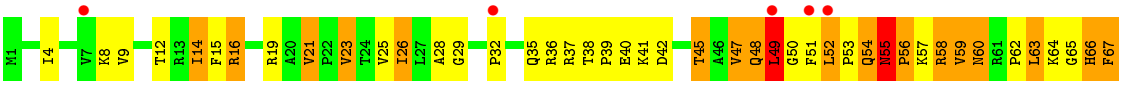
• Molecule 29: 50S ribosomal protein L2

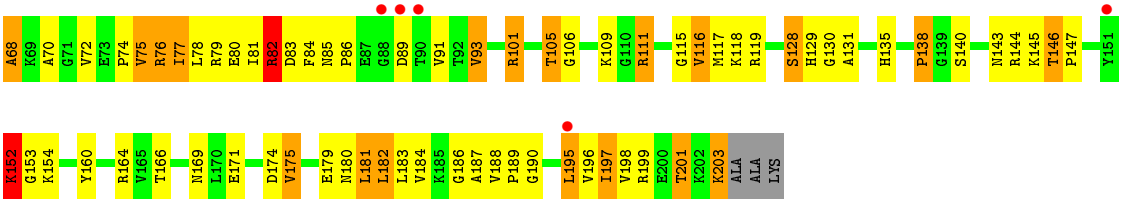
Chain 19:



• Molecule 30: 50S ribosomal protein L3

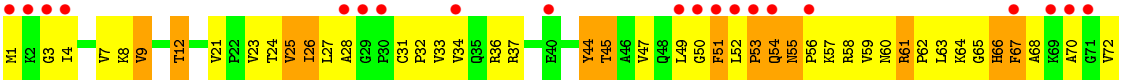
Chain 21:

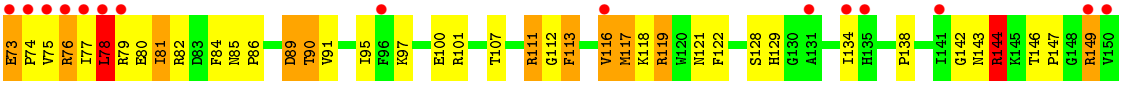


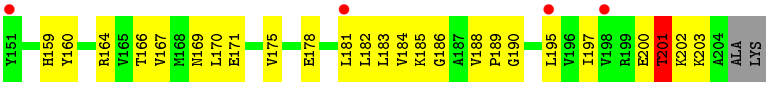


• Molecule 30: 50S ribosomal protein L3

Chain 29:

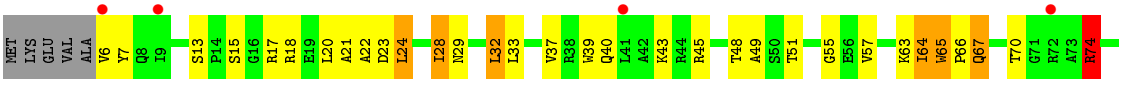


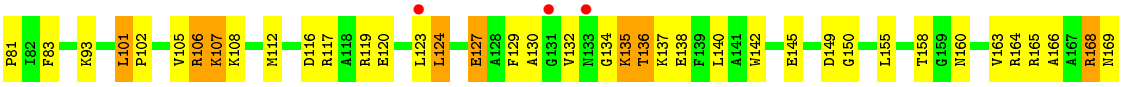




• Molecule 31: 50S ribosomal protein L4

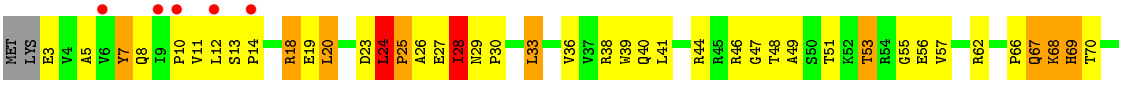
Chain 31:

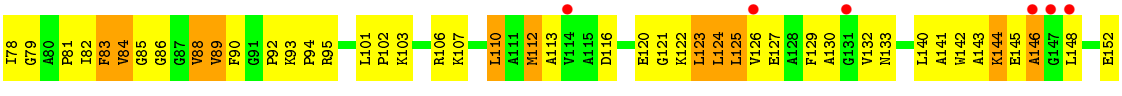


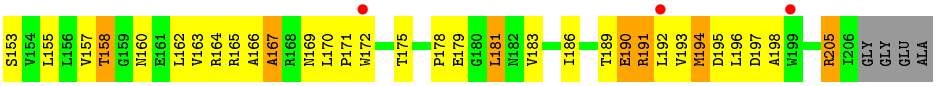


• Molecule 31: 50S ribosomal protein L4

Chain 39:

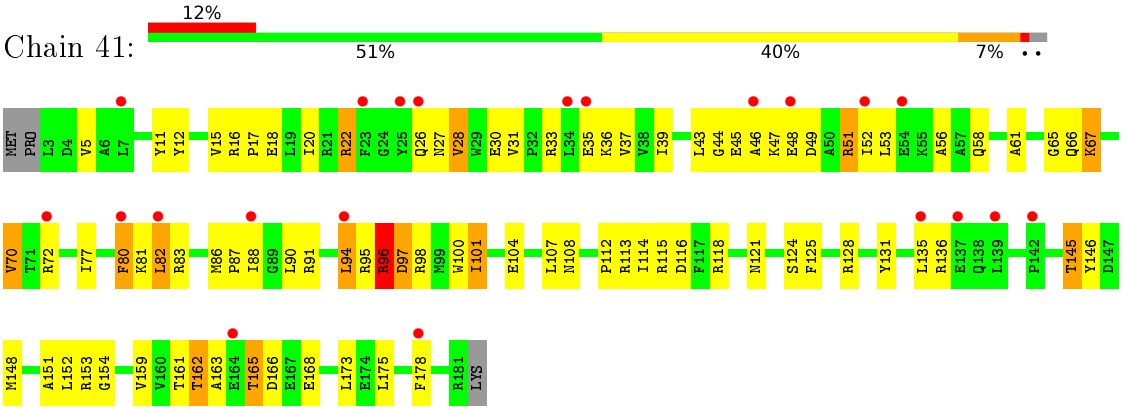






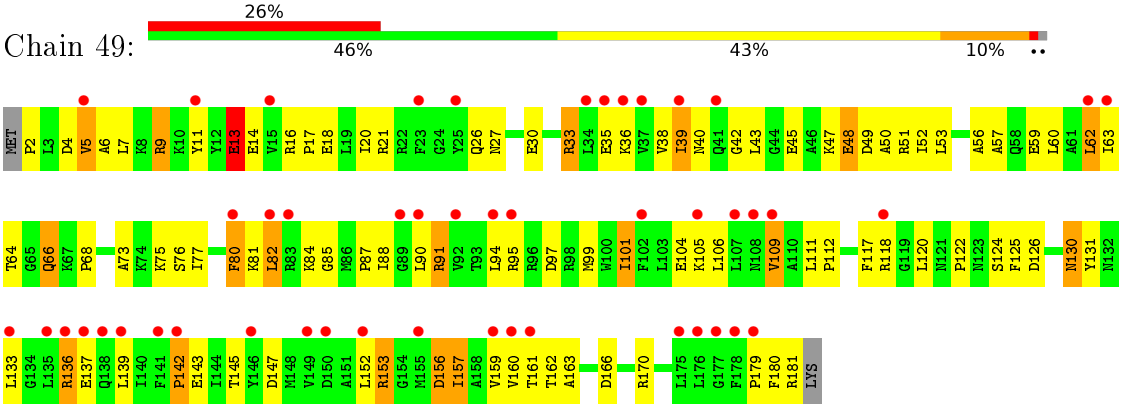
• Molecule 32: 50S ribosomal protein L5

Chain 41:



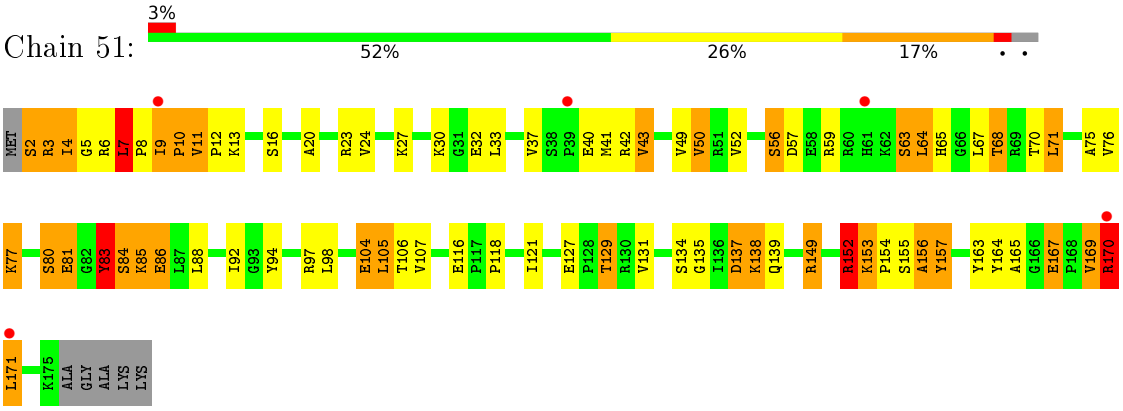
• Molecule 32: 50S ribosomal protein L5

Chain 49:



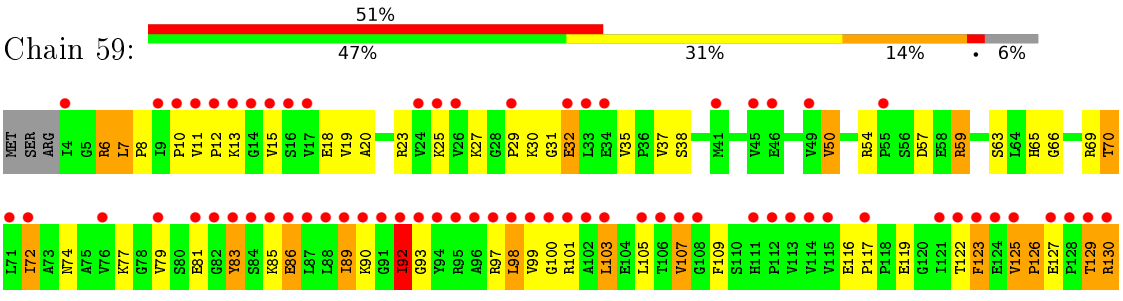
• Molecule 33: 50S ribosomal protein L6

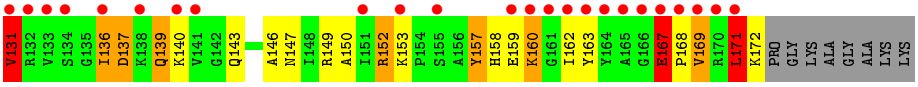
Chain 51:



• Molecule 33: 50S ribosomal protein L6

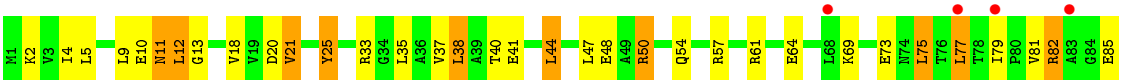
Chain 59:

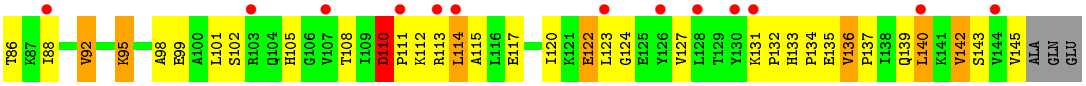




• Molecule 34: 50S ribosomal protein L9

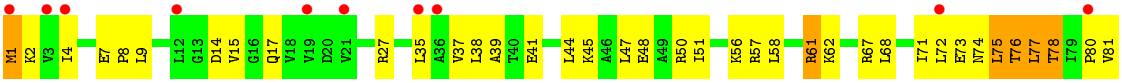
Chain 61:

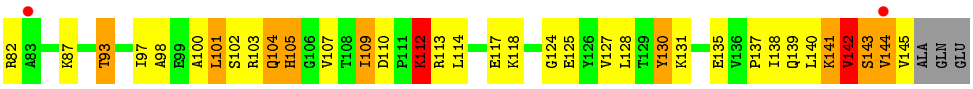




• Molecule 34: 50S ribosomal protein L9

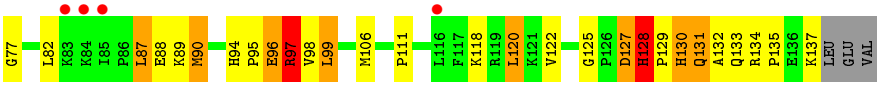
Chain 69:





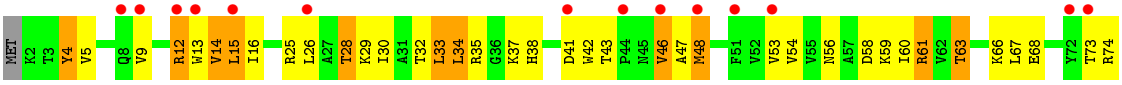
• Molecule 35: 50S ribosomal protein L13

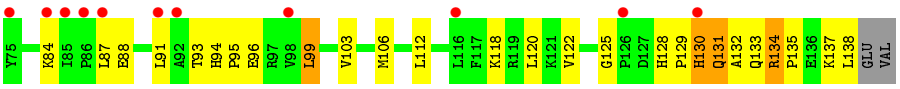
Chain 58:



• Molecule 35: 50S ribosomal protein L13

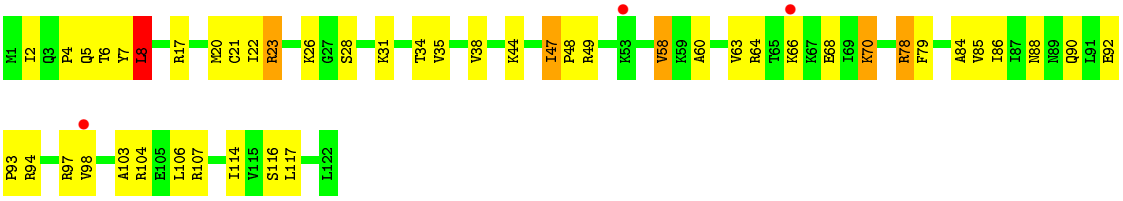
Chain 15:





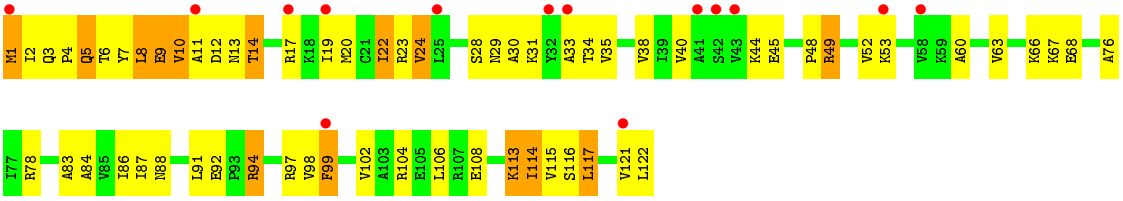
• Molecule 36: 50S ribosomal protein L14

Chain 68:



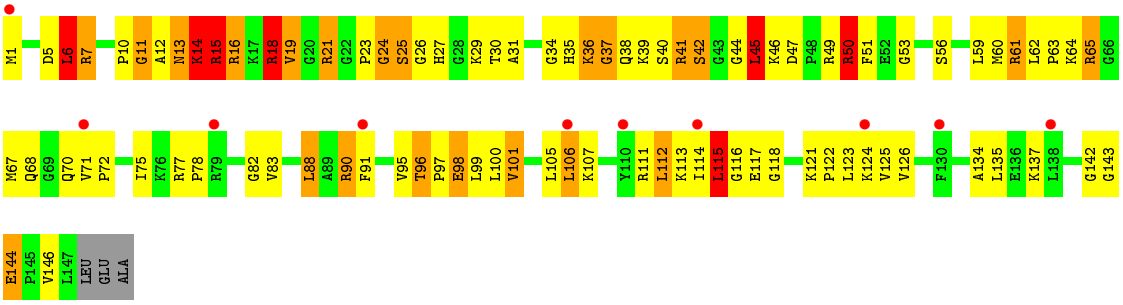
• Molecule 36: 50S ribosomal protein L14

Chain 25:



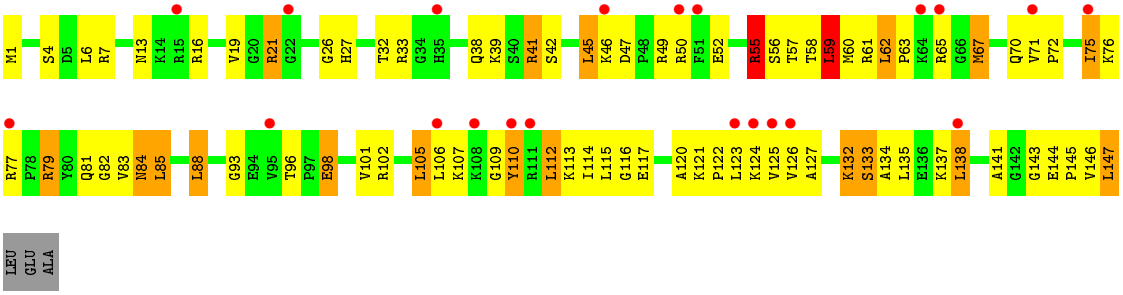
• Molecule 37: 50S ribosomal protein L15

Chain 78:



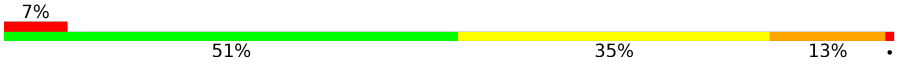
• Molecule 37: 50S ribosomal protein L15

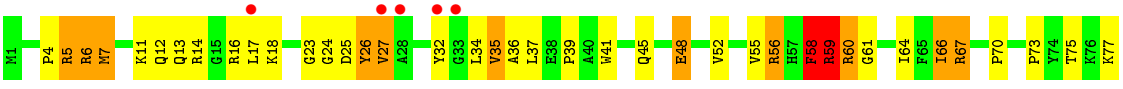
Chain 35:

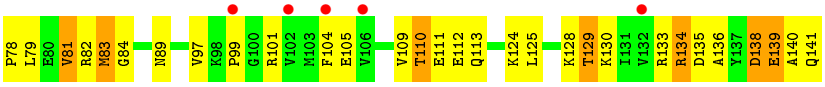


• Molecule 38: 50S ribosomal protein L16

Chain 88:

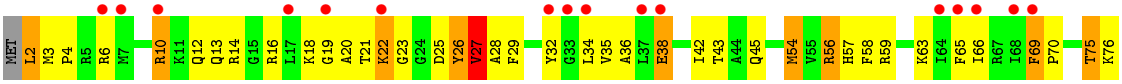






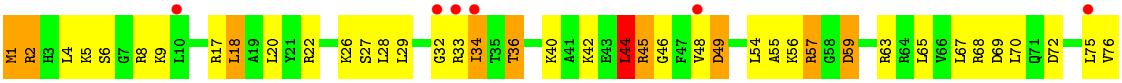
• Molecule 38: 50S ribosomal protein L16

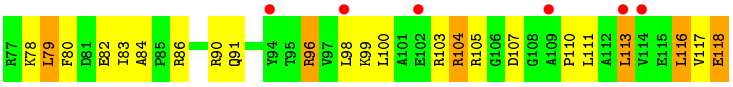
Chain 45:



• Molecule 39: 50S ribosomal protein L17

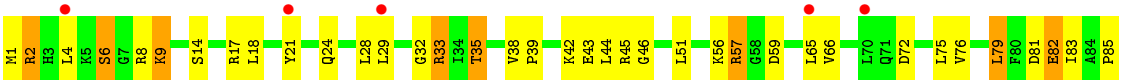
Chain 98:

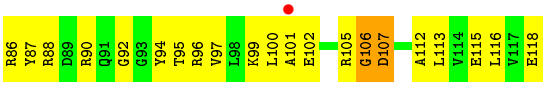




• Molecule 39: 50S ribosomal protein L17

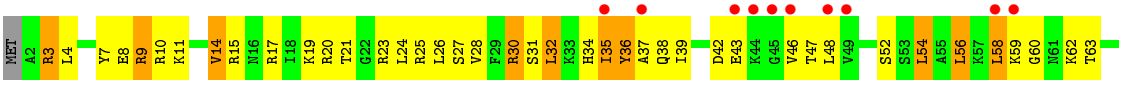
Chain 55:





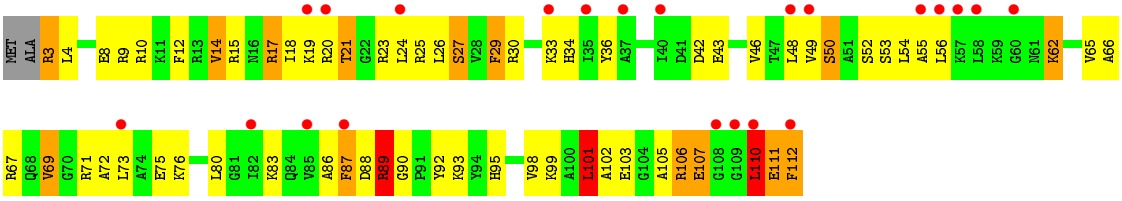
• Molecule 40: 50S ribosomal protein L18

Chain A8:



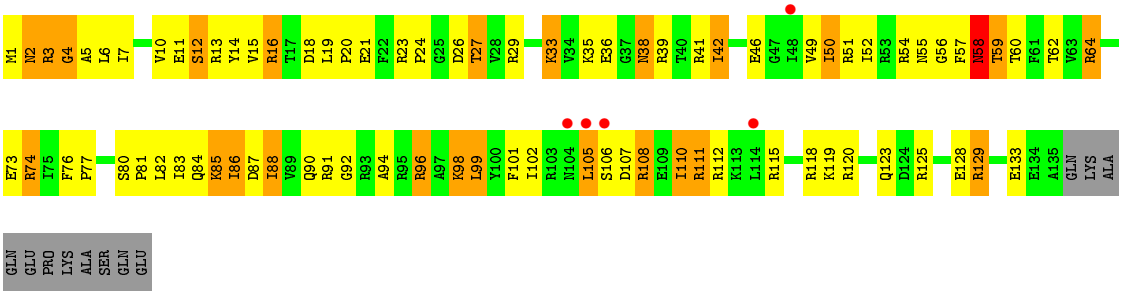
• Molecule 40: 50S ribosomal protein L18

Chain 65:



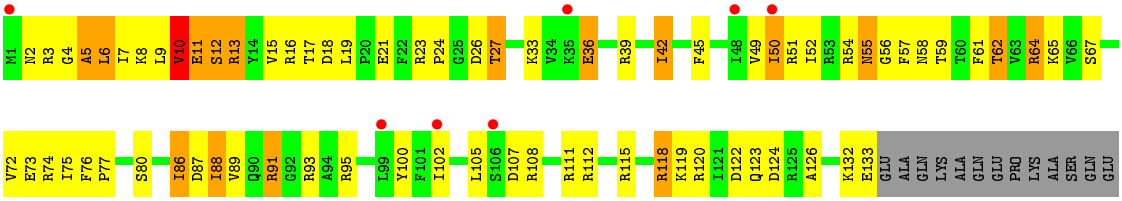
• Molecule 41: 50S ribosomal protein L19

Chain B8:



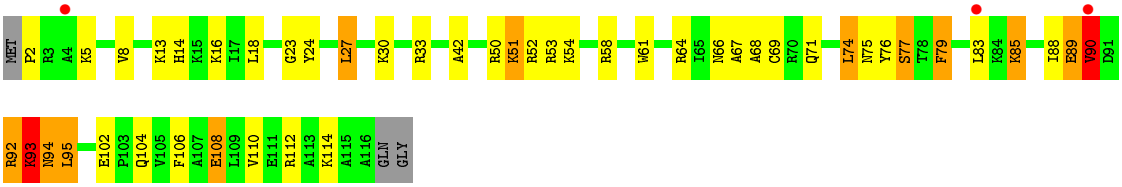
• Molecule 41: 50S ribosomal protein L19

Chain 75:



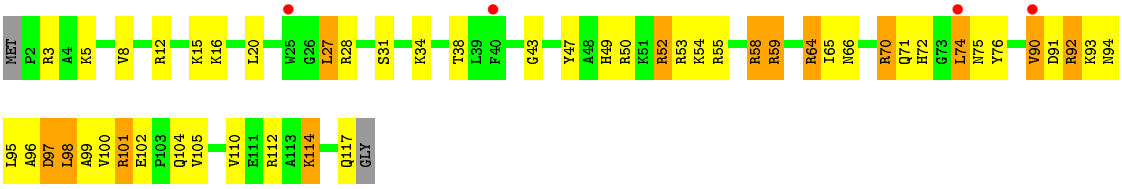
• Molecule 42: 50S ribosomal protein L20

Chain C8:



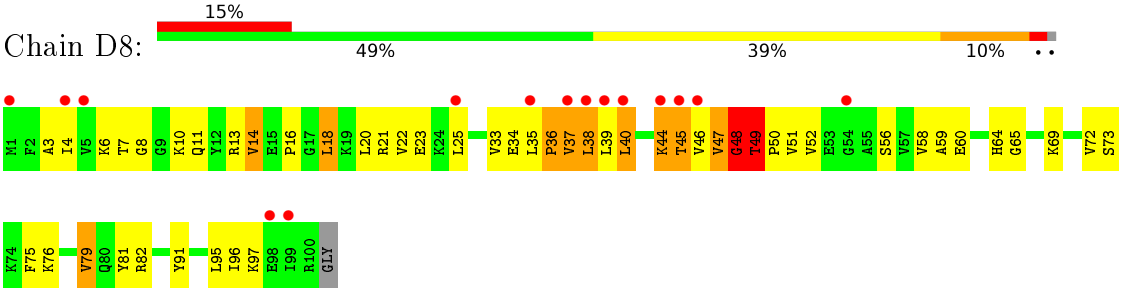
• Molecule 42: 50S ribosomal protein L20

Chain 85:



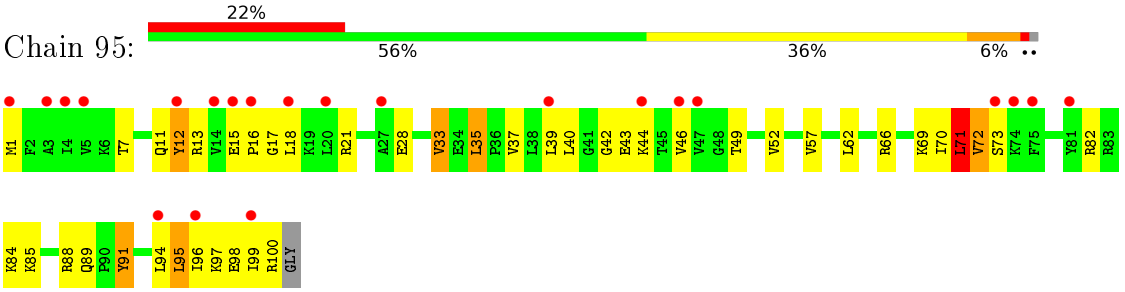
• Molecule 43: 50S ribosomal protein L21

Chain D8:



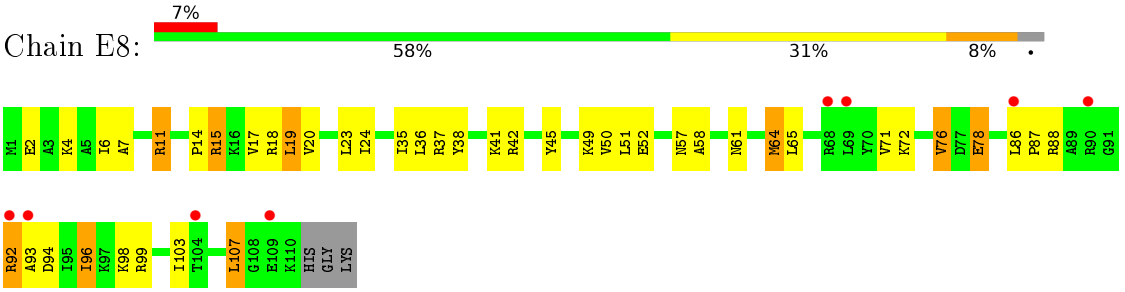
• Molecule 43: 50S ribosomal protein L21

Chain 95:



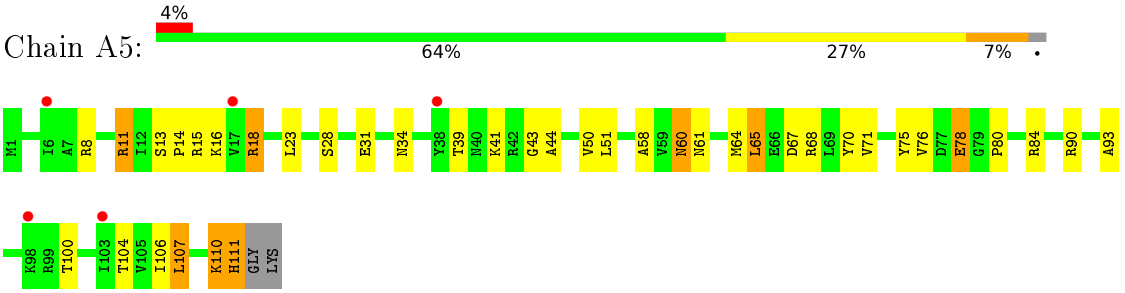
• Molecule 44: 50S ribosomal protein L22

Chain E8:



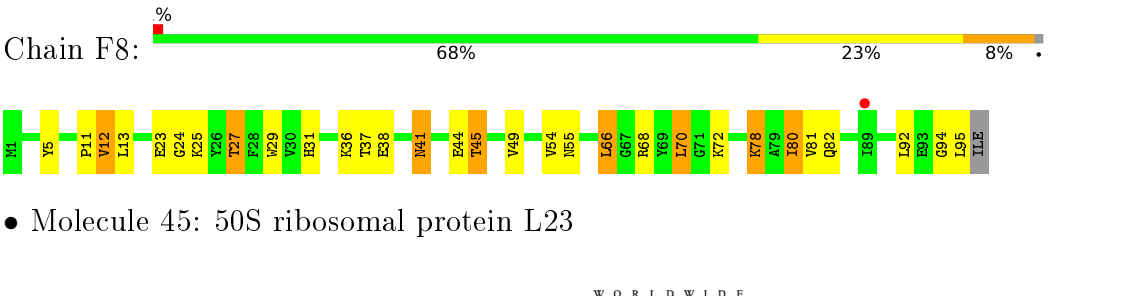
• Molecule 44: 50S ribosomal protein L22

Chain A5:



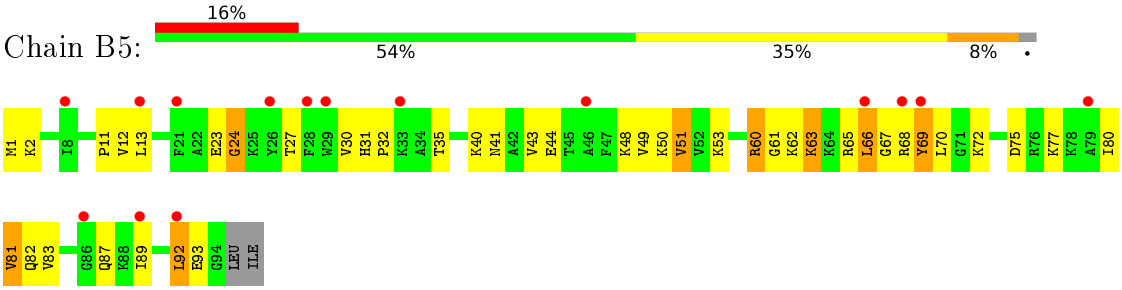
• Molecule 45: 50S ribosomal protein L23

Chain F8:



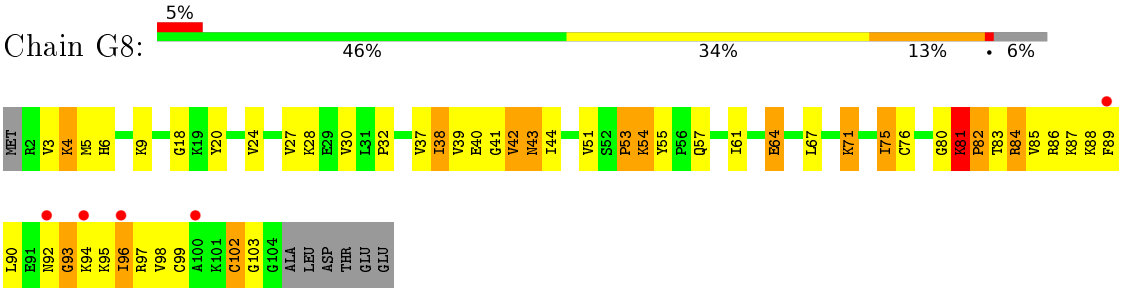
• Molecule 45: 50S ribosomal protein L23

Chain B5:



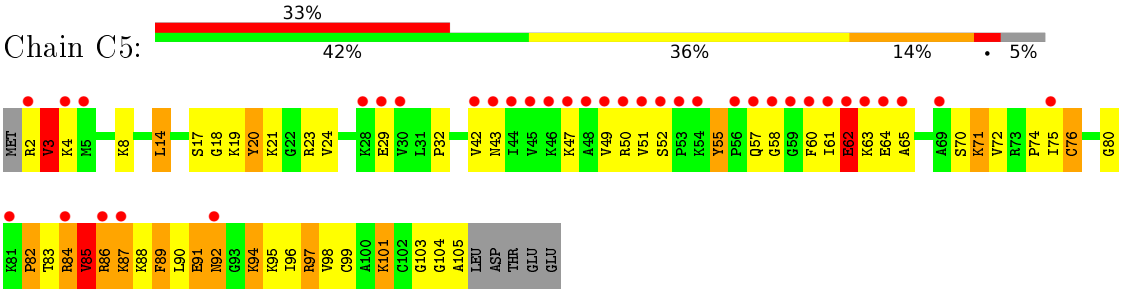
• Molecule 46: 50S ribosomal protein L24

Chain G8:



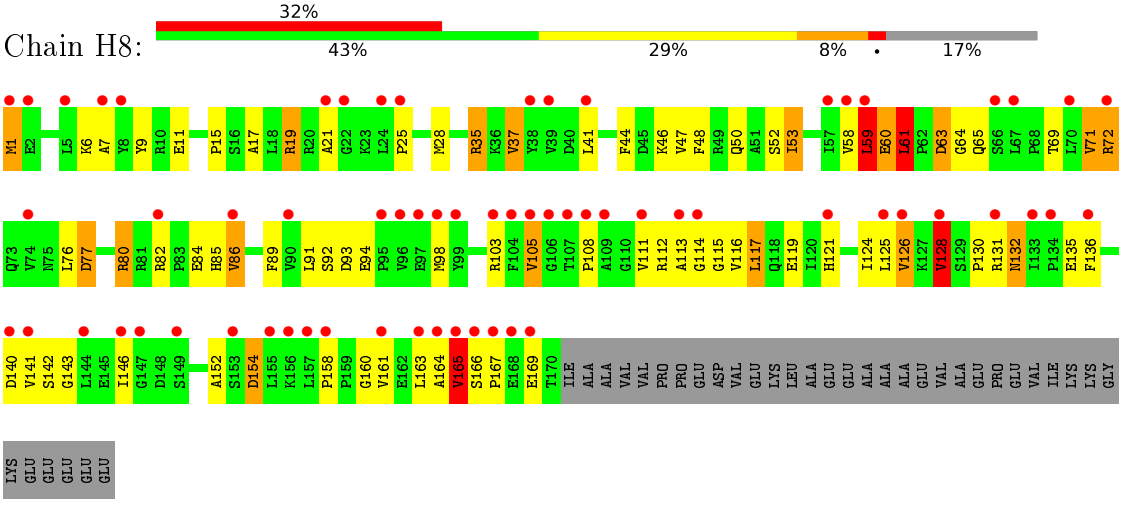
• Molecule 46: 50S ribosomal protein L24

Chain C5:



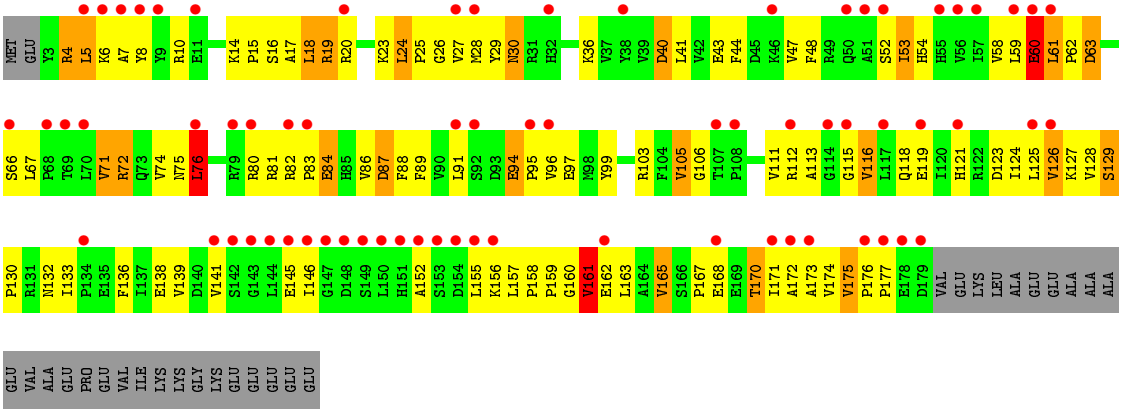
• Molecule 47: 50S ribosomal protein L25

Chain H8:



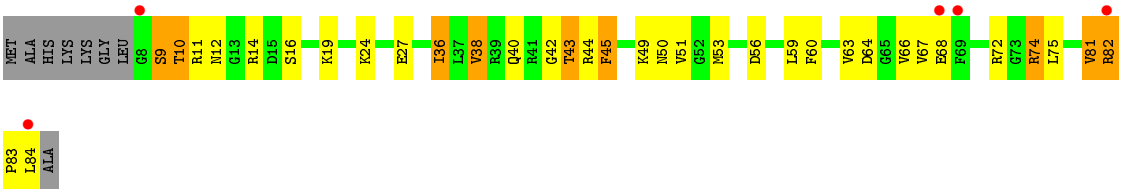
• Molecule 47: 50S ribosomal protein L25

Chain D5:



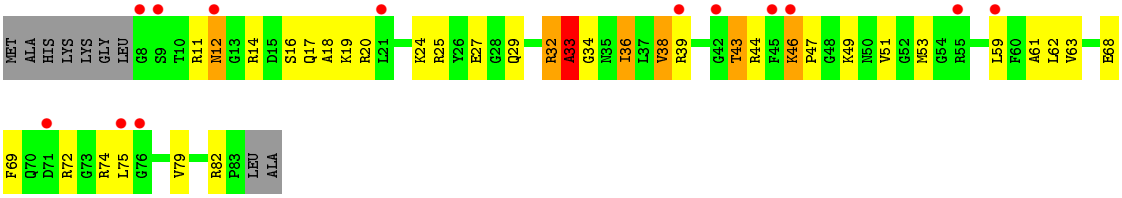
• Molecule 48: 50S ribosomal protein L27

Chain I8:



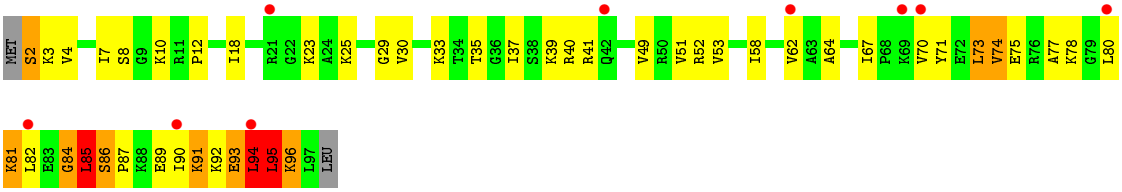
• Molecule 48: 50S ribosomal protein L27

Chain E5:



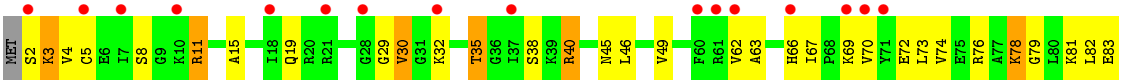
• Molecule 49: 50S ribosomal protein L28

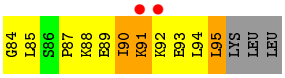
Chain J8:



• Molecule 49: 50S ribosomal protein L28

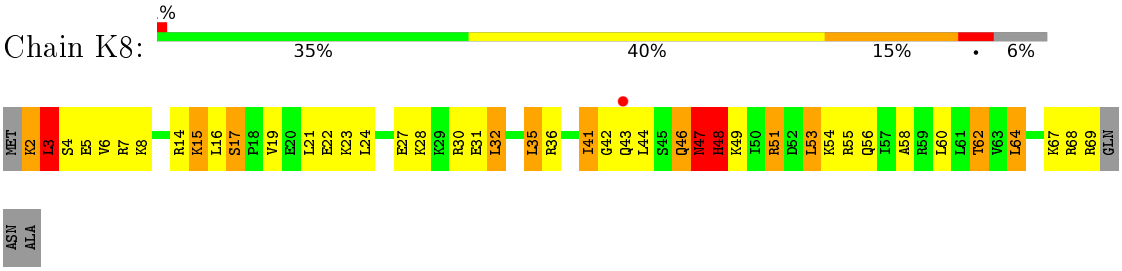
Chain F5:





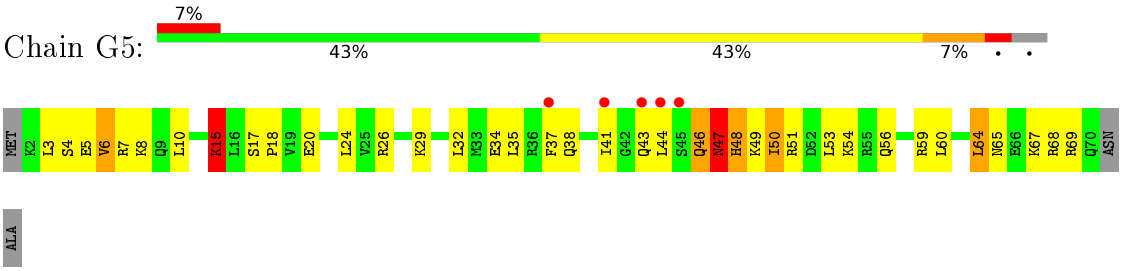
- Molecule 50: 50S ribosomal protein L29

Chain K8:



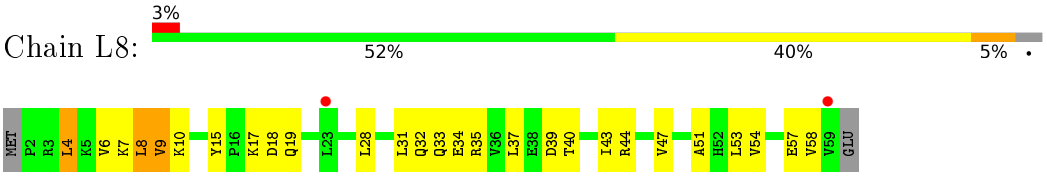
- Molecule 50: 50S ribosomal protein L29

Chain G5:



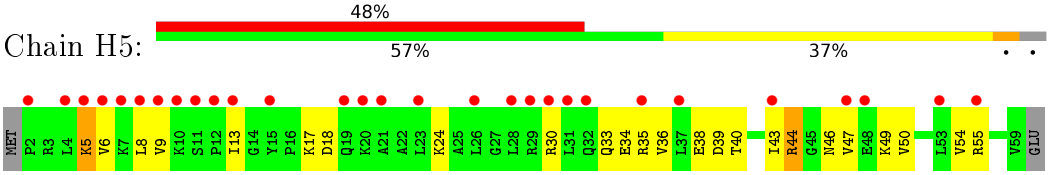
- Molecule 51: 50S ribosomal protein L30

Chain L8:



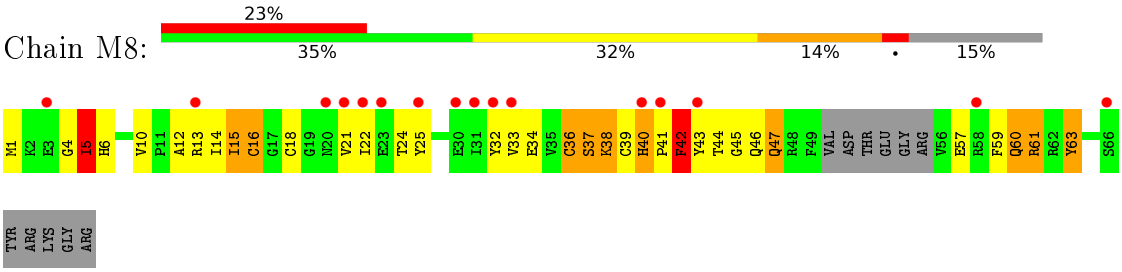
- Molecule 51: 50S ribosomal protein L30

Chain H5:



- Molecule 52: 50S ribosomal protein L31

Chain M8:

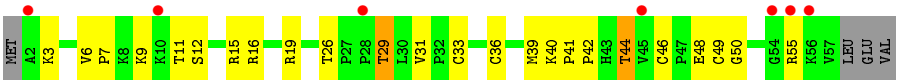


- Molecule 53: 50S ribosomal protein L32

Chain N8:

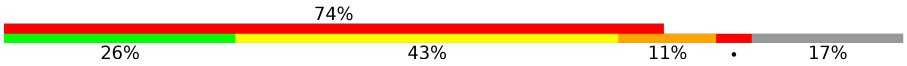
• Molecule 53: 50S ribosomal protein L32

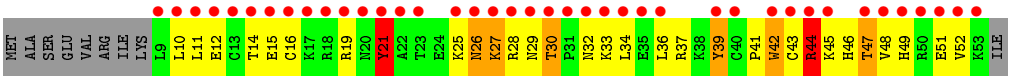
Chain J5:



• Molecule 54: 50S ribosomal protein L33

Chain O8:



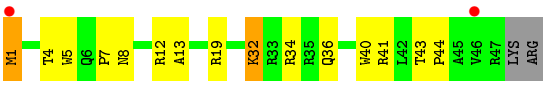


• Molecule 55: 50S ribosomal protein L34

Chain P8:

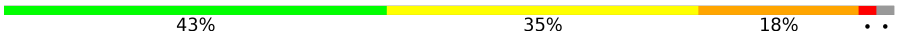
• Molecule 55: 50S ribosomal protein L34

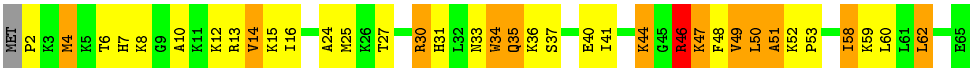
Chain L5:



• Molecule 56: 50S ribosomal protein L35

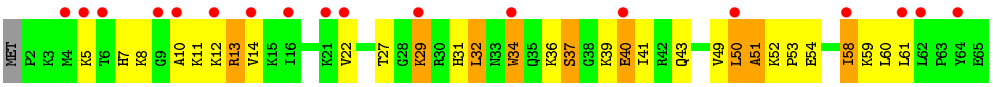
Chain Q8:





• Molecule 56: 50S ribosomal protein L35

Chain M5:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	209.30Å 448.80Å 620.20Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	147.08 – 2.99 161.81 – 2.99	Depositor EDS
% Data completeness (in resolution range)	99.9 (147.08-2.99) 90.8 (161.81-2.99)	Depositor EDS
R_{merge}	0.34	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.76 (at 3.01Å)	Xtriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.202 , 0.241 0.200 , 0.238	Depositor DCC
R_{free} test set	2000 reflections (0.19%)	DCC
Wilson B-factor (Å^2)	82.3	Xtriage
Anisotropy	0.334	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.28 , 75.7	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	297444	wwPDB-VP
Average B, all atoms (Å^2)	104.0	wwPDB-VP

Xtriage'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.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 5MU, OMC, PAR, U8U, MG, SF4, ZN, 7MG, 4SU, T6A, SPE, PSU

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|>5$	RMSZ	#$\|Z\|>5$
1	13	0.70	1/36068 (0.0%)	1.35	292/56287 (0.5%)
1	1G	0.61	0/36282	1.22	170/56623 (0.3%)
2	12	0.37	0/1727	0.61	1/2326 (0.0%)
2	1E	0.40	0/1908	0.63	2/2573 (0.1%)
3	22	0.43	1/1560 (0.1%)	0.56	0/2104
3	2E	0.47	1/1629 (0.1%)	0.62	1/2195 (0.0%)
4	32	0.45	1/1732 (0.1%)	0.64	0/2318
4	3E	0.48	1/1728 (0.1%)	0.62	1/2313 (0.0%)
5	42	0.38	0/1156	0.60	0/1557
5	4E	0.45	0/1158	0.63	0/1559
6	52	0.49	0/855	0.66	1/1154 (0.1%)
6	5E	0.46	0/850	0.61	0/1147
7	62	0.39	0/1122	0.61	0/1500
7	6E	0.39	0/1259	0.54	0/1686
8	72	0.37	0/1127	0.57	0/1517
8	7E	0.41	0/1135	0.64	1/1527 (0.1%)
9	82	0.36	0/971	0.62	0/1304
9	8E	0.39	0/1019	0.61	0/1367
10	1A	1.00	2/658 (0.3%)	0.56	0/885
10	1I	0.40	0/762	0.62	0/1027
11	2A	0.40	0/850	0.61	1/1150 (0.1%)
11	2I	0.47	0/838	0.65	0/1133
12	3A	0.44	0/963	0.66	1/1290 (0.1%)
12	3I	0.63	0/972	0.80	1/1301 (0.1%)
13	4A	0.35	0/889	0.59	0/1192
13	4I	0.50	0/943	0.67	0/1265
14	5A	0.34	0/495	0.65	0/657
14	5I	0.47	0/495	0.69	1/657 (0.2%)
15	6A	0.40	0/740	0.58	0/987
15	6I	0.44	0/740	0.61	0/987
16	7A	0.43	0/721	0.65	0/970
16	7I	0.43	0/716	0.68	0/963

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
17	8A	0.45	0/836	0.59	0/1117
17	8I	0.51	0/836	0.65	0/1117
18	9A	0.46	0/549	0.67	0/732
18	9I	0.42	0/554	0.63	0/739
19	AA	0.38	0/520	0.67	0/700
19	AI	0.42	0/676	0.72	0/910
20	BA	0.35	0/764	0.67	1/1007 (0.1%)
20	BI	0.50	1/748 (0.1%)	0.63	0/986
21	1B	0.40	0/192	0.61	0/252
21	1F	0.42	0/203	0.71	0/266
22	1K	0.56	0/1589	1.11	6/2464 (0.2%)
23	2K	0.77	0/1721	1.42	16/2682 (0.6%)
23	2L	0.66	1/1721 (0.1%)	1.22	7/2682 (0.3%)
24	1L	0.39	0/1560	0.96	3/2418 (0.1%)
24	3K	0.52	0/1654	1.19	13/2570 (0.5%)
24	3L	0.52	0/1705	1.12	9/2650 (0.3%)
25	4K	0.74	0/473	1.15	0/735
25	4L	0.69	0/473	1.29	3/737 (0.4%)
26	14	0.84	45/68181 (0.1%)	1.54	1291/106432 (1.2%)
26	1H	1.01	117/68997 (0.2%)	1.75	2061/107696 (1.9%)
27	16	0.83	0/2928	1.57	59/4568 (1.3%)
27	1J	0.70	0/2928	1.37	32/4568 (0.7%)
28	71	0.29	0/1049	0.54	0/1417
29	11	0.66	1/2170 (0.0%)	0.90	4/2926 (0.1%)
29	19	0.64	1/2175 (0.0%)	0.85	2/2933 (0.1%)
30	21	0.57	0/1579	0.92	3/2131 (0.1%)
30	29	0.53	0/1596	0.80	3/2153 (0.1%)
31	31	0.63	1/1620 (0.1%)	0.90	3/2194 (0.1%)
31	39	0.51	0/1637	0.80	1/2218 (0.0%)
32	41	0.47	0/1481	0.68	0/1994
32	49	0.38	0/1483	0.63	1/1997 (0.1%)
33	51	0.53	0/1354	0.86	4/1833 (0.2%)
33	59	0.35	0/1320	0.69	3/1787 (0.2%)
34	61	0.41	0/1146	0.71	1/1551 (0.1%)
34	69	0.41	0/1146	0.70	1/1551 (0.1%)
35	15	0.41	0/1123	0.61	0/1515
35	58	0.52	0/1123	0.75	0/1514
36	25	0.48	0/942	0.71	1/1269 (0.1%)
36	68	0.55	0/942	0.76	2/1269 (0.2%)
37	35	0.53	0/1139	0.83	2/1514 (0.1%)
37	78	0.61	0/1139	1.04	8/1514 (0.5%)
38	45	0.61	2/1120 (0.2%)	0.81	0/1498
38	88	0.69	0/1138	0.92	1/1523 (0.1%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
39	55	0.51	0/981	0.83	0/1312
39	98	0.49	0/981	0.81	1/1312 (0.1%)
40	65	0.47	0/886	0.83	3/1180 (0.3%)
40	A8	0.59	0/891	0.83	2/1187 (0.2%)
41	75	0.51	0/1123	0.74	2/1500 (0.1%)
41	B8	0.58	0/1133	0.83	2/1514 (0.1%)
42	85	0.50	0/977	0.67	0/1301
42	C8	0.61	0/968	0.82	2/1289 (0.2%)
43	95	0.47	0/781	0.76	0/1048
43	D8	0.53	0/785	0.74	1/1052 (0.1%)
44	A5	0.55	0/897	0.77	1/1204 (0.1%)
44	E8	0.57	0/886	0.81	0/1189
45	B5	0.57	0/749	0.71	0/1007
45	F8	0.64	0/764	0.80	1/1025 (0.1%)
46	C5	0.52	0/807	0.81	1/1076 (0.1%)
46	G8	0.65	0/796	0.95	2/1062 (0.2%)
47	D5	0.54	1/1443 (0.1%)	0.64	1/1960 (0.1%)
47	H8	0.44	0/1395	0.73	1/1890 (0.1%)
48	E5	0.52	0/611	0.77	0/814
48	I8	0.76	1/619 (0.2%)	0.94	1/825 (0.1%)
49	F5	0.52	0/744	0.90	1/989 (0.1%)
49	J8	0.69	0/754	0.96	4/1003 (0.4%)
50	G5	0.53	0/578	0.73	0/766
50	K8	0.69	0/577	1.02	3/763 (0.4%)
51	H5	0.46	0/464	0.64	0/623
51	L8	0.50	0/464	0.73	0/623
52	M8	0.47	0/485	0.83	0/652
53	J5	0.58	0/448	0.76	0/606
53	N8	0.61	0/381	0.83	1/516 (0.2%)
54	O8	0.63	1/396 (0.3%)	0.90	1/529 (0.2%)
55	L5	0.57	0/409	0.78	0/540
55	P8	0.75	0/409	0.98	2/540 (0.4%)
56	M5	0.65	0/524	0.87	1/691 (0.1%)
56	Q8	0.69	0/524	1.02	3/691 (0.4%)
All	All	0.76	179/317928 (0.1%)	1.36	4051/476129 (0.9%)

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

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Mol	Chain	#Chirality outliers	#Planarity outliers
2	1E	0	4
4	32	0	2
9	82	0	1
9	8E	0	2
10	1A	0	1
11	2A	0	1
12	3A	0	1
12	3I	0	2
13	4A	0	1
13	4I	0	1
14	5A	0	1
19	AA	0	2
19	AI	0	1
20	BA	0	2
29	11	0	5
29	19	0	3
30	21	0	8
30	29	0	5
31	39	0	7
32	41	0	1
32	49	0	2
33	51	0	5
33	59	0	1
34	61	0	3
34	69	0	4
35	58	0	1
37	35	0	2
37	78	0	6
38	45	0	2
38	88	0	4
39	55	0	1
39	98	0	2
40	65	0	1
40	A8	0	2
41	75	0	3
41	B8	0	3
42	85	0	4
42	C8	0	2
43	D8	0	3
44	A5	0	1
45	B5	0	2
46	C5	0	2

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Mol	Chain	#Chirality outliers	#Planarity outliers
46	G8	0	5
47	D5	0	3
47	H8	0	6
48	E5	0	2
48	I8	0	1
49	F5	0	1
49	J8	0	1
50	G5	0	2
50	K8	0	2
52	M8	0	3
54	O8	0	1
55	P8	0	1
56	M5	0	2
56	Q8	0	3
All	All	0	145

The worst 5 of 179 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	1A	38	ILE	C-N	19.47	1.71	1.34
47	D5	94	GLU	C-N	14.46	1.61	1.34
10	1A	76	ASN	C-N	14.15	1.61	1.34
26	1H	774	A	N9-C4	-13.65	1.29	1.37
26	14	783	A	N9-C4	-12.02	1.30	1.37

The worst 5 of 4051 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	1H	1899	G	N3-C4-N9	-23.89	111.67	126.00
26	1H	945	A	C6-C5-N7	-20.89	117.67	132.30
26	1H	945	A	N1-C6-N6	20.76	131.05	118.60
26	1H	1899	G	N3-C4-C5	20.42	138.81	128.60
26	1H	2430	A	C2-N3-C4	-20.30	100.45	110.60

There are no chirality outliers.

5 of 145 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	1E	15	VAL	Peptide
2	1E	194	PRO	Peptide
2	1E	234	PRO	Peptide

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Mol	Chain	Res	Type	Group
2	1E	236	TYR	Peptide
9	8E	4	TYR	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	32223	0	16267	692	0
1	1G	32414	0	16360	752	0
2	12	1696	0	1730	89	0
2	1E	1874	0	1926	95	0
3	22	1537	0	1603	84	0
3	2E	1605	0	1668	54	0
4	32	1702	0	1765	93	0
4	3E	1698	0	1759	84	0
5	42	1141	0	1199	40	0
5	4E	1142	0	1204	40	0
6	52	842	0	857	19	0
6	5E	837	0	852	34	0
7	62	1110	0	1163	53	0
7	6E	1242	0	1286	51	0
8	72	1107	0	1165	49	0
8	7E	1115	0	1177	46	0
9	82	953	0	983	62	0
9	8E	1000	0	1031	63	0
10	1A	646	0	662	45	0
10	1I	749	0	767	42	0
11	2A	835	0	847	25	0
11	2I	823	0	833	29	0
12	3A	947	0	1033	45	0
12	3I	956	0	1046	35	0
13	4A	879	0	935	46	0
13	4I	933	0	992	57	0
14	5A	486	0	525	35	0
14	5I	486	0	524	29	0
15	6A	729	0	768	26	0
15	6I	729	0	768	23	0
16	7A	705	0	725	23	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
16	7I	700	0	720	45	0
17	8A	823	0	891	22	0
17	8I	823	0	891	34	0
18	9A	544	0	605	19	0
18	9I	549	0	607	21	0
19	AA	510	0	507	21	0
19	AI	661	0	683	43	0
20	BA	762	0	861	43	0
20	BI	746	0	843	44	0
21	1B	188	0	195	8	0
21	1F	199	0	208	9	0
22	1K	1542	0	790	25	0
23	2K	1646	0	845	18	0
23	2L	1646	0	845	25	0
24	1L	1401	0	713	22	0
24	3K	1483	0	756	50	0
24	3L	1528	0	778	42	0
25	4K	420	0	209	7	0
25	4L	419	0	208	17	0
26	14	60877	0	30690	1171	0
26	1H	61609	0	31058	1189	0
27	16	2617	0	1328	50	0
27	1J	2617	0	1328	76	0
28	71	1027	0	1043	57	0
29	11	2120	0	2197	100	0
29	19	2125	0	2199	105	0
30	21	1546	0	1602	86	0
30	29	1563	0	1629	93	0
31	31	1585	0	1632	70	0
31	39	1602	0	1649	88	0
32	41	1457	0	1514	68	0
32	49	1459	0	1507	65	0
33	51	1328	0	1396	64	0
33	59	1295	0	1366	58	0
34	61	1131	0	1218	36	0
34	69	1131	0	1218	49	0
35	15	1096	0	1168	47	0
35	58	1096	0	1169	48	0
36	25	932	0	996	46	0
36	68	932	0	996	41	0
37	35	1122	0	1206	75	0
37	78	1122	0	1206	80	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
38	45	1099	0	1154	73	0
38	88	1117	0	1168	58	0
39	55	967	0	1033	42	0
39	98	967	0	1033	45	0
40	65	876	0	938	63	0
40	A8	881	0	943	54	0
41	75	1109	0	1170	61	0
41	B8	1119	0	1177	72	0
42	85	959	0	1019	40	0
42	C8	950	0	1011	58	0
43	95	770	0	838	32	0
43	D8	774	0	849	40	0
44	A5	886	0	948	23	0
44	E8	876	0	941	30	0
45	B5	735	0	785	30	0
45	F8	750	0	814	19	0
46	C5	794	0	885	52	0
46	G8	783	0	869	49	0
47	D5	1411	0	1436	82	0
47	H8	1365	0	1391	57	0
48	E5	603	0	620	33	0
48	I8	611	0	631	34	0
49	F5	737	0	813	32	0
49	J8	747	0	817	42	0
50	G5	576	0	625	27	0
50	K8	575	0	634	42	0
51	H5	459	0	512	11	0
51	L8	459	0	512	13	0
52	M8	475	0	465	34	0
53	J5	434	0	454	22	0
53	N8	369	0	388	21	0
54	O8	389	0	404	26	0
55	L5	401	0	436	10	0
55	P8	401	0	436	11	0
56	M5	516	0	582	25	0
56	Q8	516	0	582	37	0
57	13	140	0	0	0	0
57	14	435	0	0	0	0
57	16	11	0	0	0	0
57	19	1	0	0	0	0
57	1G	102	0	0	0	0
57	1H	525	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
57	1J	8	0	0	0	0
57	21	3	0	0	0	0
57	25	1	0	0	0	0
57	29	1	0	0	0	0
57	2K	2	0	0	0	0
57	2L	2	0	0	0	0
57	31	2	0	0	0	0
57	32	1	0	0	0	0
57	35	1	0	0	0	0
57	39	2	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	2	0	0	0	0
57	4I	1	0	0	0	0
57	4L	1	0	0	0	0
57	52	1	0	0	0	0
57	5I	1	0	0	0	0
57	78	1	0	0	0	0
57	7A	1	0	0	0	0
57	88	3	0	0	0	0
57	C5	1	0	0	0	0
57	E5	1	0	0	0	0
57	I8	2	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	42	0	43	0	0
58	1G	42	0	45	1	0
59	32	8	0	0	3	0
59	3E	8	0	0	1	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	14	26	0	45	8	0
61	1G	13	0	24	0	0
62	11	17	0	0	4	0
62	13	320	0	0	12	0
62	14	1144	0	0	65	0
62	15	1	0	0	0	0
62	16	12	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
62	19	15	0	0	3	0
62	1A	1	0	0	0	0
62	1F	1	0	0	0	0
62	1G	317	0	0	21	0
62	1H	1470	0	0	90	0
62	1I	2	0	0	0	0
62	1J	12	0	0	1	0
62	1K	2	0	0	0	0
62	21	7	0	0	1	0
62	25	6	0	0	0	0
62	29	4	0	0	0	0
62	2K	8	0	0	1	0
62	2L	6	0	0	0	0
62	31	5	0	0	0	0
62	32	1	0	0	0	0
62	35	8	0	0	1	0
62	39	5	0	0	1	0
62	3I	2	0	0	0	0
62	41	1	0	0	0	0
62	4E	3	0	0	0	0
62	4K	5	0	0	0	0
62	4L	6	0	0	0	0
62	52	4	0	0	0	0
62	55	3	0	0	0	0
62	58	2	0	0	0	0
62	5I	2	0	0	0	0
62	6A	2	0	0	0	0
62	6I	3	0	0	0	0
62	78	10	0	0	0	0
62	7A	5	0	0	0	0
62	7I	1	0	0	0	0
62	85	2	0	0	0	0
62	8E	2	0	0	0	0
62	9A	2	0	0	0	0
62	A5	1	0	0	0	0
62	B5	1	0	0	0	0
62	B8	1	0	0	0	0
62	BA	2	0	0	0	0
62	BI	2	0	0	1	0
62	C5	3	0	0	0	0
62	C8	3	0	0	0	0
62	F5	1	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
62	F8	2	0	0	0	0
62	G8	2	0	0	0	0
62	H5	2	0	0	1	0
62	I8	6	0	0	1	0
62	J8	4	0	0	0	0
62	L8	3	0	0	1	0
62	M5	9	0	0	1	0
62	P8	1	0	0	0	0
62	Q8	5	0	0	2	0
All	All	297444	0	197360	7486	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 16.

The worst 5 of 7486 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)
10:1A:38:ILE:C	10:1A:39:PRO:N	1.71	1.44
38:45:27:VAL:HB	38:45:28:ALA:HA	1.19	1.13
29:11:182:LEU:H	29:11:272:ALA:HB3	1.23	1.02
37:78:63:PRO:HB2	56:Q8:30:ARG:HH21	1.23	1.01
26:1H:1496:A:H8	26:1H:1577:C:HO2'	1.00	0.99

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%)	173 (85%)	25 (12%)	5 (2%)	7 34
2	1E	227/256 (89%)	185 (82%)	39 (17%)	3 (1%)	15 53

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	22	191/239 (80%)	171 (90%)	20 (10%)	0	100	100
3	2E	203/239 (85%)	186 (92%)	17 (8%)	0	100	100
4	32	206/209 (99%)	184 (89%)	21 (10%)	1 (0%)	34	76
4	3E	205/209 (98%)	192 (94%)	12 (6%)	1 (0%)	34	76
5	42	148/162 (91%)	141 (95%)	7 (5%)	0	100	100
5	4E	147/162 (91%)	141 (96%)	5 (3%)	1 (1%)	26	70
6	52	99/101 (98%)	96 (97%)	3 (3%)	0	100	100
6	5E	98/101 (97%)	94 (96%)	4 (4%)	0	100	100
7	62	134/156 (86%)	123 (92%)	10 (8%)	1 (1%)	26	70
7	6E	152/156 (97%)	144 (95%)	8 (5%)	0	100	100
8	72	135/138 (98%)	125 (93%)	8 (6%)	2 (2%)	13	50
8	7E	136/138 (99%)	125 (92%)	10 (7%)	1 (1%)	26	70
9	82	119/128 (93%)	109 (92%)	9 (8%)	1 (1%)	24	66
9	8E	124/128 (97%)	108 (87%)	16 (13%)	0	100	100
10	1A	76/105 (72%)	71 (93%)	5 (7%)	0	100	100
10	1I	92/105 (88%)	85 (92%)	7 (8%)	0	100	100
11	2A	111/129 (86%)	101 (91%)	8 (7%)	2 (2%)	11	45
11	2I	109/129 (84%)	94 (86%)	12 (11%)	3 (3%)	6	30
12	3A	119/132 (90%)	100 (84%)	15 (13%)	4 (3%)	5	25
12	3I	120/132 (91%)	107 (89%)	12 (10%)	1 (1%)	24	66
13	4A	107/126 (85%)	88 (82%)	18 (17%)	1 (1%)	21	64
13	4I	115/126 (91%)	96 (84%)	18 (16%)	1 (1%)	21	64
14	5A	57/61 (93%)	48 (84%)	8 (14%)	1 (2%)	11	45
14	5I	57/61 (93%)	48 (84%)	7 (12%)	2 (4%)	4	24
15	6A	85/89 (96%)	81 (95%)	4 (5%)	0	100	100
15	6I	85/89 (96%)	77 (91%)	8 (9%)	0	100	100
16	7A	82/88 (93%)	76 (93%)	6 (7%)	0	100	100
16	7I	81/88 (92%)	77 (95%)	4 (5%)	0	100	100
17	8A	97/105 (92%)	90 (93%)	7 (7%)	0	100	100
17	8I	97/105 (92%)	92 (95%)	4 (4%)	1 (1%)	19	61
18	9A	65/88 (74%)	62 (95%)	3 (5%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
18	9I	66/88 (75%)	64 (97%)	1 (2%)	1 (2%)	13 50
19	AA	59/93 (63%)	49 (83%)	8 (14%)	2 (3%)	5 25
19	AI	80/93 (86%)	68 (85%)	9 (11%)	3 (4%)	4 22
20	BA	97/106 (92%)	83 (86%)	13 (13%)	1 (1%)	19 61
20	BI	95/106 (90%)	84 (88%)	10 (10%)	1 (1%)	17 58
21	1B	20/27 (74%)	19 (95%)	1 (5%)	0	100 100
21	1F	21/27 (78%)	20 (95%)	1 (5%)	0	100 100
28	71	128/229 (56%)	120 (94%)	8 (6%)	0	100 100
29	11	271/276 (98%)	249 (92%)	17 (6%)	5 (2%)	11 45
29	19	272/276 (99%)	246 (90%)	23 (8%)	3 (1%)	17 58
30	21	201/206 (98%)	158 (79%)	33 (16%)	10 (5%)	3 15
30	29	202/206 (98%)	149 (74%)	42 (21%)	11 (5%)	2 14
31	31	200/210 (95%)	181 (90%)	17 (8%)	2 (1%)	19 61
31	39	202/210 (96%)	162 (80%)	34 (17%)	6 (3%)	5 29
32	41	177/182 (97%)	156 (88%)	18 (10%)	3 (2%)	11 46
32	49	178/182 (98%)	155 (87%)	22 (12%)	1 (1%)	30 72
33	51	172/180 (96%)	141 (82%)	20 (12%)	11 (6%)	2 9
33	59	167/180 (93%)	129 (77%)	32 (19%)	6 (4%)	4 24
34	61	143/148 (97%)	122 (85%)	19 (13%)	2 (1%)	14 51
34	69	143/148 (97%)	111 (78%)	29 (20%)	3 (2%)	9 40
35	15	135/140 (96%)	122 (90%)	13 (10%)	0	100 100
35	58	135/140 (96%)	114 (84%)	17 (13%)	4 (3%)	5 29
36	25	120/122 (98%)	112 (93%)	8 (7%)	0	100 100
36	68	120/122 (98%)	115 (96%)	5 (4%)	0	100 100
37	35	145/150 (97%)	119 (82%)	26 (18%)	0	100 100
37	78	145/150 (97%)	114 (79%)	22 (15%)	9 (6%)	2 10
38	45	136/141 (96%)	115 (85%)	19 (14%)	2 (2%)	13 50
38	88	139/141 (99%)	116 (84%)	18 (13%)	5 (4%)	4 24
39	55	116/118 (98%)	110 (95%)	5 (4%)	1 (1%)	21 64
39	98	116/118 (98%)	104 (90%)	11 (10%)	1 (1%)	21 64
40	65	108/112 (96%)	89 (82%)	16 (15%)	3 (3%)	6 30

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
40	A8	109/112 (97%)	90 (83%)	19 (17%)	0	100 100
41	75	131/146 (90%)	117 (89%)	12 (9%)	2 (2%)	13 50
41	B8	133/146 (91%)	118 (89%)	15 (11%)	0	100 100
42	85	114/118 (97%)	104 (91%)	9 (8%)	1 (1%)	21 64
42	C8	113/118 (96%)	104 (92%)	6 (5%)	3 (3%)	6 32
43	95	98/101 (97%)	80 (82%)	15 (15%)	3 (3%)	5 28
43	D8	98/101 (97%)	88 (90%)	6 (6%)	4 (4%)	3 20
44	A5	109/113 (96%)	101 (93%)	7 (6%)	1 (1%)	21 64
44	E8	108/113 (96%)	100 (93%)	8 (7%)	0	100 100
45	B5	92/96 (96%)	84 (91%)	6 (6%)	2 (2%)	8 38
45	F8	93/96 (97%)	88 (95%)	5 (5%)	0	100 100
46	C5	102/110 (93%)	74 (72%)	21 (21%)	7 (7%)	1 7
46	G8	101/110 (92%)	81 (80%)	16 (16%)	4 (4%)	4 21
47	D5	175/206 (85%)	136 (78%)	31 (18%)	8 (5%)	3 18
47	H8	168/206 (82%)	136 (81%)	25 (15%)	7 (4%)	3 20
48	E5	74/85 (87%)	66 (89%)	6 (8%)	2 (3%)	6 32
48	I8	75/85 (88%)	67 (89%)	7 (9%)	1 (1%)	15 53
49	F5	92/98 (94%)	79 (86%)	12 (13%)	1 (1%)	17 58
49	J8	94/98 (96%)	83 (88%)	9 (10%)	2 (2%)	9 40
50	G5	67/72 (93%)	61 (91%)	4 (6%)	2 (3%)	5 29
50	K8	66/72 (92%)	60 (91%)	3 (4%)	3 (4%)	3 18
51	H5	56/60 (93%)	53 (95%)	3 (5%)	0	100 100
51	L8	56/60 (93%)	54 (96%)	2 (4%)	0	100 100
52	M8	56/71 (79%)	40 (71%)	15 (27%)	1 (2%)	11 45
53	J5	54/60 (90%)	50 (93%)	4 (7%)	0	100 100
53	N8	46/60 (77%)	43 (94%)	3 (6%)	0	100 100
54	O8	43/54 (80%)	30 (70%)	12 (28%)	1 (2%)	8 36
55	L5	45/49 (92%)	42 (93%)	3 (7%)	0	100 100
55	P8	45/49 (92%)	42 (93%)	3 (7%)	0	100 100
56	M5	62/65 (95%)	52 (84%)	9 (14%)	1 (2%)	12 48
56	Q8	62/65 (95%)	53 (86%)	7 (11%)	2 (3%)	5 27

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	11128/12158 (92%)	9762 (88%)	1180 (11%)	186 (2%)	11 46

5 of 186 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
11	2I	55	LYS
12	3I	48	PRO
18	9I	22	VAL
19	AI	41	VAL
30	21	83	ASP

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%)	143 (80%)	36 (20%)	1 8
2	1E	200/220 (91%)	154 (77%)	46 (23%)	1 5
3	22	154/188 (82%)	128 (83%)	26 (17%)	2 13
3	2E	159/188 (85%)	131 (82%)	28 (18%)	2 12
4	32	180/181 (99%)	151 (84%)	29 (16%)	3 14
4	3E	180/181 (99%)	146 (81%)	34 (19%)	2 10
5	42	114/123 (93%)	87 (76%)	27 (24%)	1 4
5	4E	115/123 (94%)	93 (81%)	22 (19%)	2 10
6	52	90/90 (100%)	74 (82%)	16 (18%)	2 11
6	5E	90/90 (100%)	80 (89%)	10 (11%)	8 29
7	62	114/127 (90%)	88 (77%)	26 (23%)	1 5
7	6E	125/127 (98%)	105 (84%)	20 (16%)	3 15
8	72	118/119 (99%)	101 (86%)	17 (14%)	4 18
8	7E	119/119 (100%)	99 (83%)	20 (17%)	2 13
9	82	92/99 (93%)	73 (79%)	19 (21%)	1 7
9	8E	97/99 (98%)	75 (77%)	22 (23%)	1 5

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
10	1A	71/92 (77%)	51 (72%)	20 (28%)	0 2
10	1I	81/92 (88%)	73 (90%)	8 (10%)	10 35
11	2A	85/99 (86%)	67 (79%)	18 (21%)	1 6
11	2I	84/99 (85%)	70 (83%)	14 (17%)	3 13
12	3A	102/109 (94%)	79 (78%)	23 (22%)	1 5
12	3I	103/109 (94%)	91 (88%)	12 (12%)	7 27
13	4A	90/101 (89%)	68 (76%)	22 (24%)	1 4
13	4I	94/101 (93%)	74 (79%)	20 (21%)	1 6
14	5A	49/50 (98%)	41 (84%)	8 (16%)	3 14
14	5I	49/50 (98%)	36 (74%)	13 (26%)	0 3
15	6A	79/80 (99%)	71 (90%)	8 (10%)	9 34
15	6I	79/80 (99%)	65 (82%)	14 (18%)	2 11
16	7A	72/74 (97%)	61 (85%)	11 (15%)	3 16
16	7I	72/74 (97%)	58 (81%)	14 (19%)	2 9
17	8A	94/97 (97%)	82 (87%)	12 (13%)	5 23
17	8I	94/97 (97%)	82 (87%)	12 (13%)	5 23
18	9A	58/77 (75%)	47 (81%)	11 (19%)	2 10
18	9I	58/77 (75%)	49 (84%)	9 (16%)	3 16
19	AA	56/80 (70%)	47 (84%)	9 (16%)	3 14
19	AI	72/80 (90%)	61 (85%)	11 (15%)	3 16
20	BA	76/82 (93%)	66 (87%)	10 (13%)	5 22
20	BI	75/82 (92%)	61 (81%)	14 (19%)	2 10
21	1B	17/22 (77%)	16 (94%)	1 (6%)	24 63
21	1F	18/22 (82%)	14 (78%)	4 (22%)	1 5
28	71	108/181 (60%)	87 (81%)	21 (19%)	2 9
29	11	214/218 (98%)	173 (81%)	41 (19%)	2 10
29	19	214/218 (98%)	171 (80%)	43 (20%)	1 8
30	21	162/166 (98%)	118 (73%)	44 (27%)	0 2
30	29	165/166 (99%)	135 (82%)	30 (18%)	2 11
31	31	161/166 (97%)	128 (80%)	33 (20%)	1 7
31	39	163/166 (98%)	126 (77%)	37 (23%)	1 5

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
32	41	153/156 (98%)	126 (82%)	27 (18%)	2 12
32	49	152/156 (97%)	125 (82%)	27 (18%)	2 11
33	51	143/148 (97%)	106 (74%)	37 (26%)	0 3
33	59	140/148 (95%)	106 (76%)	34 (24%)	1 4
34	61	122/124 (98%)	86 (70%)	36 (30%)	0 2
34	69	122/124 (98%)	89 (73%)	33 (27%)	0 3
35	15	116/119 (98%)	90 (78%)	26 (22%)	1 5
35	58	116/119 (98%)	87 (75%)	29 (25%)	1 3
36	25	100/100 (100%)	76 (76%)	24 (24%)	1 4
36	68	100/100 (100%)	90 (90%)	10 (10%)	9 34
37	35	114/116 (98%)	82 (72%)	32 (28%)	0 2
37	78	114/116 (98%)	78 (68%)	36 (32%)	0 1
38	45	109/111 (98%)	88 (81%)	21 (19%)	2 9
38	88	110/111 (99%)	90 (82%)	20 (18%)	2 11
39	55	101/101 (100%)	80 (79%)	21 (21%)	1 7
39	98	101/101 (100%)	72 (71%)	29 (29%)	0 2
40	65	87/88 (99%)	61 (70%)	26 (30%)	0 2
40	A8	87/88 (99%)	66 (76%)	21 (24%)	1 4
41	75	117/127 (92%)	95 (81%)	22 (19%)	2 10
41	B8	117/127 (92%)	83 (71%)	34 (29%)	0 2
42	85	93/94 (99%)	73 (78%)	20 (22%)	1 6
42	C8	92/94 (98%)	76 (83%)	16 (17%)	2 12
43	95	81/82 (99%)	68 (84%)	13 (16%)	3 15
43	D8	82/82 (100%)	63 (77%)	19 (23%)	1 5
44	A5	91/92 (99%)	74 (81%)	17 (19%)	2 10
44	E8	90/92 (98%)	73 (81%)	17 (19%)	2 10
45	B5	74/78 (95%)	56 (76%)	18 (24%)	1 4
45	F8	77/78 (99%)	64 (83%)	13 (17%)	2 13
46	C5	85/91 (93%)	63 (74%)	22 (26%)	0 3
46	G8	84/91 (92%)	66 (79%)	18 (21%)	1 6
47	D5	156/179 (87%)	124 (80%)	32 (20%)	1 7

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
47	H8	151/179 (84%)	124 (82%)	27 (18%)	2 11
48	E5	61/67 (91%)	55 (90%)	6 (10%)	10 36
48	I8	62/67 (92%)	53 (86%)	9 (14%)	4 18
49	F5	79/83 (95%)	63 (80%)	16 (20%)	1 7
49	J8	79/83 (95%)	67 (85%)	12 (15%)	3 16
50	G5	63/67 (94%)	46 (73%)	17 (27%)	0 3
50	K8	64/67 (96%)	43 (67%)	21 (33%)	0 1
51	H5	50/52 (96%)	38 (76%)	12 (24%)	1 4
51	L8	50/52 (96%)	40 (80%)	10 (20%)	1 8
52	M8	52/63 (82%)	38 (73%)	14 (27%)	0 3
53	J5	48/52 (92%)	41 (85%)	7 (15%)	4 18
53	N8	43/52 (83%)	34 (79%)	9 (21%)	1 7
54	O8	44/52 (85%)	29 (66%)	15 (34%)	0 1
55	L5	38/42 (90%)	32 (84%)	6 (16%)	3 15
55	P8	38/42 (90%)	31 (82%)	7 (18%)	2 10
56	M5	54/55 (98%)	43 (80%)	11 (20%)	1 7
56	Q8	54/55 (98%)	44 (82%)	10 (18%)	2 10
All	All	9397/10064 (93%)	7493 (80%)	1904 (20%)	1 7

5 of 1904 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
47	H8	82	ARG
4	32	150	GLU
45	B5	27	THR
49	J8	73	LEU
55	P8	8	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 13 such sidechains are listed below:

Mol	Chain	Res	Type
2	12	40	HIS
5	42	78	HIS
40	65	95	HIS
2	12	19	HIS

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Mol	Chain	Res	Type
29	19	253	GLN

5.3.3 RNA

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	13	1497/1522 (98%)	331 (22%)	33 (2%)
1	1G	1506/1522 (98%)	352 (23%)	33 (2%)
22	1K	68/76 (89%)	27 (39%)	4 (5%)
23	2K	76/77 (98%)	21 (27%)	2 (2%)
23	2L	76/77 (98%)	15 (19%)	2 (2%)
24	1L	61/76 (80%)	24 (39%)	2 (3%)
24	3K	67/76 (88%)	37 (55%)	2 (2%)
24	3L	69/76 (90%)	30 (43%)	2 (2%)
25	4K	17/30 (56%)	9 (52%)	1 (5%)
25	4L	18/30 (60%)	12 (66%)	1 (5%)
26	14	2821/2917 (96%)	675 (23%)	42 (1%)
26	1H	2850/2917 (97%)	630 (22%)	52 (1%)
27	16	121/122 (99%)	24 (19%)	1 (0%)
27	1J	121/122 (99%)	32 (26%)	3 (2%)
All	All	9368/9640 (97%)	2219 (23%)	180 (1%)

5 of 2219 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	13	2	U
1	13	5	U
1	13	6	G
1	13	7	G
1	13	9	G

5 of 180 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
26	1H	1858	G
1	1G	250	A
26	14	2308	G
26	1H	1992	G
26	1H	2481	G

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
22	U8U	1K	34	25,22	15,24,25	2.57	4 (26%)	17,34,37	1.85	2 (11%)
22	T6A	1K	37	22	23,34,35	2.47	4 (17%)	26,49,52	3.42	7 (26%)
22	PSU	1K	39	22	15,21,22	0.96	1 (6%)	16,30,33	2.02	4 (25%)
22	5MU	1K	54	22	13,22,23	1.73	2 (15%)	16,32,35	1.78	2 (12%)
22	PSU	1K	55	22	15,21,22	1.13	1 (6%)	16,30,33	2.29	3 (18%)
23	OMC	2K	33	23	15,22,23	2.22	4 (26%)	20,31,34	1.82	3 (15%)
23	7MG	2K	47	23	20,26,27	3.34	6 (30%)	23,39,42	2.29	5 (21%)
23	5MU	2K	55	23	13,22,23	1.69	2 (15%)	16,32,35	1.53	2 (12%)
23	PSU	2K	56	23	15,21,22	1.04	1 (6%)	16,30,33	1.87	3 (18%)
23	4SU	2K	8	23	12,21,22	3.01	2 (16%)	15,30,33	0.76	1 (6%)
23	OMC	2L	33	23	15,22,23	2.29	4 (26%)	20,31,34	1.11	2 (10%)
23	7MG	2L	47	23	20,26,27	3.42	5 (25%)	23,39,42	2.27	6 (26%)
23	5MU	2L	55	23	13,22,23	1.71	2 (15%)	16,32,35	1.50	1 (6%)
23	PSU	2L	56	23	15,21,22	1.10	1 (6%)	16,30,33	1.97	3 (18%)
23	4SU	2L	8	23	12,21,22	3.40	2 (16%)	15,30,33	0.92	1 (6%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	U8U	1K	34	25,22	-	0/5/28/29	0/2/2/2
22	T6A	1K	37	22	-	0/15/41/42	0/3/3/3
22	PSU	1K	39	22	-	0/7/25/26	0/2/2/2
22	5MU	1K	54	22	-	0/3/25/26	0/2/2/2
22	PSU	1K	55	22	-	0/7/25/26	0/2/2/2
23	OMC	2K	33	23	-	0/5/27/28	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
23	7MG	2K	47	23	-	0/7/37/38	0/3/3/3
23	5MU	2K	55	23	-	0/3/25/26	0/2/2/2
23	PSU	2K	56	23	-	0/7/25/26	0/2/2/2
23	4SU	2K	8	23	-	0/3/25/26	0/2/2/2
23	OMC	2L	33	23	-	0/5/27/28	0/2/2/2
23	7MG	2L	47	23	-	0/7/37/38	0/3/3/3
23	5MU	2L	55	23	-	0/3/25/26	0/2/2/2
23	PSU	2L	56	23	-	0/7/25/26	0/2/2/2
23	4SU	2L	8	23	-	0/3/25/26	0/2/2/2

The worst 5 of 41 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	2K	47	7MG	C5-C4	-5.57	1.24	1.39
23	2L	47	7MG	C5-C4	-5.28	1.25	1.39
22	1K	34	U8U	C2-S2	-3.90	1.58	1.66
23	2K	55	5MU	C4-N3	-2.85	1.27	1.33
22	1K	37	T6A	C5-C4	-2.82	1.34	1.40

The worst 5 of 45 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	1K	37	T6A	N3-C2-N1	-11.74	119.65	128.87
23	2K	47	7MG	C5-C4-N3	-7.75	118.84	126.74
23	2L	47	7MG	C5-C4-N3	-7.35	119.25	126.74
22	1K	34	U8U	C5-C4-N3	-6.24	119.59	125.19
22	1K	37	T6A	C13-C12-N11	-5.21	103.39	113.40

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

7 monomers are involved in 13 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
22	1K	37	T6A	1	0
22	1K	54	5MU	1	0
23	2K	33	OMC	1	0
23	2K	47	7MG	2	0
23	2K	55	5MU	3	0
23	2L	33	OMC	3	0
23	2L	55	5MU	2	0

5.5 Carbohydrates (i)

There are no carbohydrates in this entry.

5.6 Ligand geometry (i)

Of 1269 ligands modelled in this entry, 1262 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	PAR	13	1741	1	45,45,45	0.67	0	60,67,67	1.42	9 (15%)
61	SPE	14	3436	-	12,12,12	0.44	0	11,11,11	0.64	0
61	SPE	14	3437	26	12,12,12	0.82	0	11,11,11	1.16	1 (9%)
58	PAR	1G	1702	-	45,45,45	0.66	1 (2%)	60,67,67	1.36	7 (11%)
61	SPE	1G	1703	-	12,12,12	0.37	0	11,11,11	0.73	0
59	SF4	32	302	4	0,12,12	0.00	-	0,24,24	0.00	-
59	SF4	3E	301	4	0,12,12	0.00	-	0,24,24	0.00	-

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
58	PAR	13	1741	1	-	0/18/94/94	0/4/4/4
61	SPE	14	3436	-	-	0/10/10/10	0/0/0/0
61	SPE	14	3437	26	-	0/10/10/10	0/0/0/0
58	PAR	1G	1702	-	-	0/18/94/94	0/4/4/4
61	SPE	1G	1703	-	-	0/10/10/10	0/0/0/0
59	SF4	32	302	4	-	0/0/48/48	0/6/5/5
59	SF4	3E	301	4	-	0/0/48/48	0/6/5/5

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
58	1G	1702	PAR	C24-N24	-2.19	1.43	1.47

The worst 5 of 17 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
58	1G	1702	PAR	C14-O33-C33	-3.33	109.14	118.00
58	1G	1702	PAR	C13-O52-C52	-3.07	109.84	118.00
58	13	1741	PAR	O33-C14-O54	-3.01	102.86	110.69
61	14	3437	SPE	C6-N5-C4	-2.79	103.68	113.35
58	13	1741	PAR	C14-O33-C33	-2.70	110.83	118.00

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5 monomers are involved in 13 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
61	14	3436	SPE	2	0
61	14	3437	SPE	6	0
58	1G	1702	PAR	1	0
59	32	302	SF4	3	0
59	3E	301	SF4	1	0

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
10	1A	2
26	1H	1
4	3E	1
47	D5	1
24	1L	1

The worst 5 of 6 chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	1H	1055:G	O3'	1059:G	P	14.13
1	1L	72:C	O3'	73:A	P	3.25
1	1A	38:ILE	C	39:PRO	N	1.71

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Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	1A	76:ASN	C	77:PRO	N	1.61
1	D5	94:GLU	C	95:PRO	N	1.61

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	13	1499/1522 (98%)	-0.23	1 (0%) 95 90	57, 100, 176, 247	0
1	1G	1508/1522 (99%)	-0.17	10 (0%) 89 70	71, 119, 192, 267	0
2	12	207/256 (80%)	0.76	26 (12%) 5 2	131, 164, 184, 192	0
2	1E	231/256 (90%)	0.24	12 (5%) 31 12	112, 143, 169, 174	0
3	22	195/239 (81%)	1.21	50 (25%) 1 1	135, 160, 173, 178	0
3	2E	205/239 (85%)	0.67	22 (10%) 8 3	88, 111, 143, 151	0
4	32	208/209 (99%)	0.65	14 (6%) 21 7	92, 113, 136, 142	0
4	3E	207/209 (99%)	0.31	12 (5%) 26 10	84, 108, 132, 144	0
5	42	150/162 (92%)	0.49	11 (7%) 18 6	108, 128, 148, 160	0
5	4E	149/162 (91%)	0.30	4 (2%) 58 28	82, 103, 121, 131	0
6	52	101/101 (100%)	0.02	0 100 100	85, 104, 121, 132	0
6	5E	100/101 (99%)	0.52	7 (7%) 19 7	85, 105, 120, 132	0
7	62	138/156 (88%)	1.18	33 (23%) 1 1	116, 130, 141, 147	0
7	6E	154/156 (98%)	1.23	36 (23%) 1 1	102, 120, 150, 171	0
8	72	137/138 (99%)	0.73	15 (10%) 7 3	100, 131, 142, 149	0
8	7E	138/138 (100%)	1.07	29 (21%) 1 1	93, 110, 122, 134	0
9	82	121/128 (94%)	1.87	50 (41%) 0 0	116, 163, 174, 182	0
9	8E	126/128 (98%)	0.24	5 (3%) 42 17	87, 138, 157, 163	0
10	1A	80/105 (76%)	1.02	22 (27%) 1 0	133, 156, 169, 174	0
10	1I	94/105 (89%)	1.42	28 (29%) 1 0	81, 131, 168, 173	0
11	2A	113/129 (87%)	1.33	27 (23%) 1 1	84, 109, 124, 135	0
11	2I	111/129 (86%)	1.14	25 (22%) 1 1	72, 107, 123, 133	0
12	3A	121/132 (91%)	1.72	45 (37%) 0 0	90, 112, 135, 151	0
12	3I	122/132 (92%)	0.72	15 (12%) 5 2	66, 76, 102, 135	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
13	4A	109/126 (86%)	0.85	26 (23%) 1 1	123, 150, 180, 194	0
13	4I	117/126 (92%)	0.31	4 (3%) 49 21	88, 116, 131, 138	0
14	5A	59/61 (96%)	3.89	41 (69%) 0 0	137, 158, 180, 183	0
14	5I	59/61 (96%)	0.83	8 (13%) 4 1	81, 96, 114, 122	0
15	6A	87/89 (97%)	0.13	3 (3%) 49 21	84, 113, 128, 131	0
15	6I	87/89 (97%)	0.35	3 (3%) 49 21	80, 98, 113, 123	0
16	7A	84/88 (95%)	0.26	2 (2%) 62 32	92, 105, 129, 155	0
16	7I	83/88 (94%)	1.13	20 (24%) 1 1	96, 111, 137, 155	0
17	8A	99/105 (94%)	1.30	27 (27%) 1 0	97, 113, 130, 135	0
17	8I	99/105 (94%)	1.10	18 (18%) 2 1	89, 106, 115, 124	0
18	9A	67/88 (76%)	0.35	4 (5%) 25 9	92, 112, 132, 138	0
18	9I	68/88 (77%)	0.20	2 (2%) 55 26	88, 107, 131, 135	0
19	AA	65/93 (69%)	1.17	13 (20%) 1 1	162, 178, 187, 192	0
19	AI	82/93 (88%)	0.24	3 (3%) 45 19	96, 117, 138, 151	0
20	BA	99/106 (93%)	1.15	18 (18%) 2 1	90, 114, 140, 152	0
20	BI	97/106 (91%)	1.36	27 (27%) 1 0	106, 119, 145, 151	0
21	1B	22/27 (81%)	1.72	8 (36%) 0 0	127, 141, 145, 148	0
21	1F	23/27 (85%)	0.24	0 100 100	92, 99, 107, 115	0
22	1K	67/76 (88%)	0.54	5 (7%) 17 6	90, 193, 226, 233	0
23	2K	72/77 (93%)	0.03	1 (1%) 78 51	67, 92, 124, 140	0
23	2L	72/77 (93%)	0.07	0 100 100	80, 116, 152, 163	0
24	1L	66/76 (86%)	1.06	11 (16%) 2 1	145, 224, 245, 249	0
24	3K	70/76 (92%)	0.91	10 (14%) 4 1	76, 229, 251, 253	0
24	3L	72/76 (94%)	0.16	3 (4%) 40 16	85, 220, 238, 240	0
25	4K	19/30 (63%)	0.97	4 (21%) 1 1	71, 140, 219, 219	0
25	4L	19/30 (63%)	1.35	3 (15%) 3 1	98, 158, 230, 230	0
26	14	2826/2917 (96%)	-0.06	17 (0%) 90 73	50, 85, 199, 264	0
26	1H	2860/2917 (98%)	-0.10	7 (0%) 95 87	40, 69, 186, 257	0
27	16	122/122 (100%)	-0.35	1 (0%) 87 67	61, 88, 107, 197	0
27	1J	122/122 (100%)	-0.45	0 100 100	85, 119, 145, 205	0
28	71	132/229 (57%)	0.80	20 (15%) 3 1	146, 210, 235, 243	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
29	11	273/276 (98%)	0.46	5 (1%) 71 43	41, 63, 79, 93	0
29	19	274/276 (99%)	0.59	7 (2%) 59 29	47, 73, 88, 107	0
30	21	203/206 (98%)	0.63	10 (4%) 33 13	48, 84, 120, 130	0
30	29	204/206 (99%)	1.03	39 (19%) 2 1	60, 95, 134, 149	0
31	31	202/210 (96%)	0.62	9 (4%) 37 15	46, 76, 112, 127	0
31	39	204/210 (97%)	0.56	14 (6%) 20 7	57, 101, 148, 177	0
32	41	179/182 (98%)	0.77	21 (11%) 6 2	79, 100, 134, 146	0
32	49	180/182 (98%)	1.22	48 (26%) 1 0	117, 138, 156, 174	0
33	51	174/180 (96%)	0.30	5 (2%) 55 26	77, 102, 119, 130	0
33	59	169/180 (93%)	2.48	92 (54%) 0 0	152, 196, 220, 233	0
34	61	145/148 (97%)	0.52	17 (11%) 6 2	76, 131, 149, 157	0
34	69	145/148 (97%)	0.46	12 (8%) 14 5	86, 122, 149, 156	0
35	15	137/140 (97%)	1.16	25 (18%) 2 1	81, 108, 135, 151	0
35	58	137/140 (97%)	0.86	18 (13%) 5 2	63, 85, 121, 138	0
36	25	122/122 (100%)	0.91	14 (11%) 6 2	69, 88, 105, 117	0
36	68	122/122 (100%)	0.39	3 (2%) 61 30	56, 72, 90, 99	0
37	35	147/150 (98%)	0.86	21 (14%) 4 1	58, 102, 135, 152	0
37	78	147/150 (98%)	0.57	10 (6%) 20 7	47, 80, 104, 115	0
38	45	138/141 (97%)	0.95	27 (19%) 1 1	76, 105, 124, 155	0
38	88	141/141 (100%)	0.71	10 (7%) 19 7	54, 75, 95, 123	0
39	55	118/118 (100%)	0.59	6 (5%) 32 12	65, 80, 97, 112	0
39	98	118/118 (100%)	0.81	12 (10%) 9 3	60, 78, 94, 106	0
40	65	110/112 (98%)	1.06	22 (20%) 1 1	89, 112, 132, 137	0
40	A8	111/112 (99%)	1.09	18 (16%) 3 1	72, 85, 105, 116	0
41	75	133/146 (91%)	0.40	7 (5%) 30 12	80, 96, 128, 151	0
41	B8	135/146 (92%)	0.14	5 (3%) 45 19	67, 84, 128, 139	0
42	85	116/118 (98%)	0.54	4 (3%) 49 21	63, 96, 127, 134	0
42	C8	115/118 (97%)	0.31	3 (2%) 59 29	53, 77, 102, 108	0
43	95	100/101 (99%)	1.08	22 (22%) 1 1	65, 116, 135, 142	0
43	D8	100/101 (99%)	0.89	15 (15%) 3 1	53, 101, 119, 126	0
44	A5	111/113 (98%)	0.79	5 (4%) 37 15	57, 75, 101, 137	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
44	E8	110/113 (97%)	0.49	8 (7%) 18 6	53, 70, 94, 106	0
45	B5	94/96 (97%)	1.09	15 (15%) 3 1	68, 83, 104, 118	0
45	F8	95/96 (98%)	0.21	1 (1%) 82 58	49, 66, 97, 110	0
46	C5	104/110 (94%)	2.12	36 (34%) 0 0	92, 118, 156, 164	0
46	G8	103/110 (93%)	0.26	5 (4%) 33 13	73, 95, 122, 130	0
47	D5	177/206 (85%)	1.81	70 (39%) 0 0	108, 148, 226, 236	0
47	H8	170/206 (82%)	1.81	65 (38%) 0 0	80, 116, 202, 210	0
48	E5	76/85 (89%)	1.15	13 (17%) 2 1	66, 88, 102, 115	0
48	I8	77/85 (90%)	0.58	5 (6%) 22 8	54, 69, 91, 102	0
49	F5	94/98 (95%)	1.20	18 (19%) 2 1	60, 83, 122, 136	0
49	J8	96/98 (97%)	0.85	9 (9%) 11 4	51, 71, 126, 138	0
50	G5	69/72 (95%)	0.44	5 (7%) 18 7	81, 104, 124, 138	0
50	K8	68/72 (94%)	0.12	1 (1%) 76 49	59, 79, 96, 120	0
51	H5	58/60 (96%)	2.04	29 (50%) 0 0	77, 99, 122, 135	0
51	L8	58/60 (96%)	0.54	2 (3%) 49 21	60, 77, 103, 110	0
52	M8	60/71 (84%)	1.54	16 (26%) 1 0	102, 143, 168, 171	0
53	J5	56/60 (93%)	0.72	7 (12%) 5 2	58, 85, 131, 141	0
53	N8	48/60 (80%)	0.35	0 100 100	46, 78, 119, 127	0
54	O8	45/54 (83%)	4.56	40 (88%) 0 0	117, 153, 171, 177	0
55	L5	47/49 (95%)	0.47	2 (4%) 39 16	47, 60, 87, 97	0
55	P8	47/49 (95%)	0.09	1 (2%) 67 36	42, 50, 72, 87	0
56	M5	64/65 (98%)	1.47	18 (28%) 1 0	68, 80, 97, 117	0
56	Q8	64/65 (98%)	0.36	0 100 100	51, 65, 80, 98	0
All	All	20730/21798 (95%)	0.42	1700 (8%) 14 5	40, 99, 184, 267	0

The worst 5 of 1700 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
46	C5	59	GLY	14.7
14	5A	38	GLY	12.9
33	59	96	ALA	12.6
46	C5	49	VAL	12.1
52	M8	40	HIS	11.7

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

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
22	PSU	1K	55	20/21	0.87	0.16	-	107,127,140,145	0
23	OMC	2K	33	21/22	0.96	0.21	-	73,79,82,94	0
23	4SU	2K	8	20/21	0.94	0.17	-	89,95,101,103	0
23	7MG	2L	47	24/25	0.92	0.14	-	118,128,137,141	0
23	OMC	2L	33	21/22	0.90	0.19	-	94,103,107,109	0
22	5MU	1K	54	21/22	0.92	0.16	-	104,125,133,143	0
23	5MU	2K	55	21/22	0.95	0.14	-	98,105,112,114	0
23	4SU	2L	8	20/21	0.88	0.16	-	107,118,124,125	0
23	7MG	2K	47	24/25	0.94	0.15	-	96,101,113,116	0
22	U8U	1K	34	23/24	0.96	0.17	-	83,98,108,110	0
22	PSU	1K	39	20/21	0.93	0.21	-	94,112,118,120	0
23	PSU	2L	56	20/21	0.91	0.10	-	109,121,126,126	0
22	T6A	1K	37	32/33	0.94	0.20	-	81,92,114,116	0
23	PSU	2K	56	20/21	0.92	0.12	-	91,101,110,117	0
23	5MU	2L	55	21/22	0.94	0.14	-	115,122,127,130	0

6.3 Carbohydrates (i)

There are no carbohydrates in this entry.

6.4 Ligands (i)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
57	MG	1H	3205	1/1	0.62	0.60	117.16	79,79,79,79	0
57	MG	1H	3151	1/1	0.92	0.55	58.39	80,80,80,80	0
57	MG	13	1627	1/1	0.84	0.48	53.46	71,71,71,71	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
57	MG	14	3208	1/1	0.61	0.95	39.77	88,88,88,88	0
57	MG	1H	3009	1/1	0.94	0.54	36.07	71,71,71,71	0
57	MG	1G	1614	1/1	0.90	0.60	34.55	88,88,88,88	0
57	MG	14	3117	1/1	0.85	0.47	32.77	64,64,64,64	0
57	MG	1H	3130	1/1	0.70	0.47	31.50	63,63,63,63	0
57	MG	14	3136	1/1	0.95	0.46	30.42	92,92,92,92	0
57	MG	14	3064	1/1	0.65	0.48	29.88	63,63,63,63	0
57	MG	14	3016	1/1	0.96	0.38	25.60	74,74,74,74	0
57	MG	14	3203	1/1	0.89	0.53	23.30	79,79,79,79	0
57	MG	1H	3188	1/1	0.96	0.41	22.29	49,49,49,49	0
57	MG	14	3048	1/1	0.97	0.47	20.80	51,51,51,51	0
57	MG	1H	3061	1/1	0.85	0.28	19.51	53,53,53,53	0
57	MG	14	3035	1/1	0.94	0.41	19.15	58,58,58,58	0
57	MG	13	1601	1/1	0.98	0.42	18.90	80,80,80,80	0
57	MG	14	3088	1/1	0.87	0.49	18.86	87,87,87,87	0
57	MG	14	3090	1/1	0.91	0.35	17.94	86,86,86,86	0
57	MG	14	3126	1/1	0.95	0.28	17.89	72,72,72,72	0
57	MG	1H	3187	1/1	0.98	0.42	17.89	44,44,44,44	0
57	MG	1H	3041	1/1	0.94	0.28	17.49	51,51,51,51	0
57	MG	14	3046	1/1	0.94	0.45	17.39	79,79,79,79	0
57	MG	14	3142	1/1	0.80	0.29	15.82	80,80,80,80	0
57	MG	1H	3098	1/1	0.89	0.41	15.63	46,46,46,46	0
57	MG	14	3198	1/1	0.83	0.43	15.02	81,81,81,81	0
57	MG	13	1669	1/1	0.73	0.53	14.98	95,95,95,95	0
57	MG	1H	3143	1/1	0.95	0.37	14.68	50,50,50,50	0
57	MG	1H	3172	1/1	0.73	0.30	14.52	83,83,83,83	0
57	MG	1H	3079	1/1	0.66	0.34	14.30	63,63,63,63	0
57	MG	1H	3015	1/1	0.98	0.31	13.81	51,51,51,51	0
57	MG	13	1654	1/1	0.85	0.41	13.77	101,101,101,101	0
57	MG	1H	3165	1/1	0.88	0.29	13.72	64,64,64,64	0
57	MG	1H	3078	1/1	0.92	0.28	13.54	58,58,58,58	0
57	MG	14	3072	1/1	0.82	0.27	13.49	94,94,94,94	0
57	MG	1H	3074	1/1	0.81	0.38	13.21	64,64,64,64	0
57	MG	13	1628	1/1	0.82	0.32	12.83	91,91,91,91	0
57	MG	13	1624	1/1	0.95	0.32	12.09	59,59,59,59	0
57	MG	14	3205	1/1	0.94	0.45	12.03	59,59,59,59	0
57	MG	14	3034	1/1	0.98	0.49	11.19	40,40,40,40	0
57	MG	13	1614	1/1	0.96	0.34	10.95	84,84,84,84	0
57	MG	14	3118	1/1	0.74	0.44	10.73	61,61,61,61	0
57	MG	1H	3076	1/1	0.93	0.24	10.25	72,72,72,72	0
57	MG	1G	1636	1/1	0.80	0.33	10.22	90,90,90,90	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
57	MG	1H	3066	1/1	0.83	0.26	10.06	60,60,60,60	0
57	MG	1H	3029	1/1	0.96	0.32	10.02	77,77,77,77	0
57	MG	1H	3056	1/1	0.97	0.31	9.95	49,49,49,49	0
57	MG	14	3122	1/1	0.67	0.37	9.89	75,75,75,75	0
57	MG	14	3030	1/1	0.95	0.36	9.78	57,57,57,57	0
57	MG	1H	3321	1/1	0.90	0.46	9.62	86,86,86,86	0
57	MG	1H	3178	1/1	0.84	0.43	9.48	63,63,63,63	0
57	MG	1H	3181	1/1	0.89	0.24	9.42	65,65,65,65	0
57	MG	19	301	1/1	0.79	0.42	9.18	48,48,48,48	0
57	MG	1H	3105	1/1	0.78	0.23	8.86	72,72,72,72	0
57	MG	1H	3186	1/1	0.97	0.26	8.62	62,62,62,62	0
57	MG	14	3134	1/1	0.78	0.33	8.45	85,85,85,85	0
57	MG	14	3179	1/1	0.95	0.32	8.43	77,77,77,77	0
57	MG	13	1668	1/1	0.70	0.29	8.26	66,66,66,66	0
57	MG	1H	3175	1/1	0.94	0.29	8.15	64,64,64,64	0
61	SPE	14	3437	13/13	0.82	0.29	8.02	59,68,73,74	0
57	MG	1H	3040	1/1	0.97	0.31	7.97	44,44,44,44	0
57	MG	14	3114	1/1	0.64	0.22	7.95	70,70,70,70	0
57	MG	1H	3108	1/1	0.87	0.24	7.76	64,64,64,64	0
57	MG	13	1629	1/1	0.89	0.21	7.61	72,72,72,72	0
57	MG	14	3181	1/1	0.73	0.30	7.46	75,75,75,75	0
57	MG	16	202	1/1	0.89	0.23	7.44	82,82,82,82	0
57	MG	13	1670	1/1	0.83	0.30	7.44	82,82,82,82	0
57	MG	14	3124	1/1	0.93	0.18	7.39	97,97,97,97	0
57	MG	14	3089	1/1	0.96	0.24	7.31	54,54,54,54	0
57	MG	1H	3045	1/1	0.98	0.28	6.97	46,46,46,46	0
57	MG	14	3107	1/1	0.84	0.36	6.81	54,54,54,54	0
57	MG	13	1645	1/1	0.91	0.28	6.80	92,92,92,92	0
57	MG	1H	3203	1/1	0.78	0.24	6.70	74,74,74,74	0
57	MG	14	3108	1/1	0.80	0.28	6.49	72,72,72,72	0
57	MG	14	3171	1/1	0.97	0.34	6.48	56,56,56,56	0
57	MG	16	203	1/1	0.75	0.21	6.41	82,82,82,82	0
57	MG	2L	101	1/1	0.93	0.40	6.35	91,91,91,91	0
57	MG	14	3248	1/1	0.95	0.29	6.28	47,47,47,47	0
57	MG	1H	3085	1/1	0.69	0.28	6.26	70,70,70,70	0
57	MG	14	3031	1/1	0.96	0.28	6.17	73,73,73,73	0
57	MG	1H	3200	1/1	0.95	0.26	6.13	71,71,71,71	0
57	MG	1H	3212	1/1	0.88	0.27	6.11	65,65,65,65	0
57	MG	14	3151	1/1	0.74	0.29	6.10	70,70,70,70	0
57	MG	1H	3121	1/1	0.99	0.24	5.84	39,39,39,39	0
57	MG	14	3099	1/1	0.84	0.18	5.82	78,78,78,78	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
57	MG	14	3097	1/1	0.94	0.26	5.65	97,97,97,97	0
57	MG	14	3023	1/1	0.73	0.27	5.52	76,76,76,76	0
57	MG	14	3028	1/1	0.95	0.33	5.41	45,45,45,45	0
57	MG	1H	3167	1/1	0.92	0.53	5.31	98,98,98,98	0
57	MG	13	1636	1/1	0.95	0.28	5.29	74,74,74,74	0
57	MG	14	3054	1/1	0.94	0.25	5.13	79,79,79,79	0
57	MG	1H	3011	1/1	0.97	0.30	5.08	56,56,56,56	0
57	MG	14	3125	1/1	0.87	0.21	5.02	81,81,81,81	0
57	MG	14	3092	1/1	0.95	0.26	5.01	66,66,66,66	0
57	MG	1H	3102	1/1	0.92	0.21	4.89	60,60,60,60	0
57	MG	1H	3042	1/1	0.96	0.26	4.75	65,65,65,65	0
61	SPE	14	3436	13/13	0.75	0.25	4.68	83,88,93,94	0
57	MG	1H	3221	1/1	0.89	0.24	4.55	73,73,73,73	0
57	MG	14	3042	1/1	0.90	0.19	4.49	65,65,65,65	0
57	MG	1H	3082	1/1	0.88	0.28	4.48	71,71,71,71	0
57	MG	14	3145	1/1	0.94	0.21	4.44	90,90,90,90	0
57	MG	1H	3002	1/1	0.86	0.21	4.41	48,48,48,48	0
57	MG	14	3059	1/1	0.96	0.23	4.36	89,89,89,89	0
57	MG	14	3007	1/1	0.80	0.26	4.20	60,60,60,60	0
57	MG	13	1633	1/1	0.94	0.22	4.15	73,73,73,73	0
57	MG	14	3100	1/1	0.76	0.27	4.08	71,71,71,71	0
57	MG	14	3062	1/1	0.95	0.25	4.04	59,59,59,59	0
57	MG	14	3070	1/1	0.89	0.22	4.03	52,52,52,52	0
57	MG	1H	3264	1/1	0.97	0.25	3.98	50,50,50,50	0
57	MG	1H	3133	1/1	0.86	0.23	3.81	55,55,55,55	0
57	MG	1H	3034	1/1	0.92	0.21	3.56	46,46,46,46	0
57	MG	14	3139	1/1	0.78	0.31	3.47	68,68,68,68	0
57	MG	14	3074	1/1	0.81	0.27	3.39	69,69,69,69	0
57	MG	14	3015	1/1	0.91	0.29	3.35	63,63,63,63	0
57	MG	1H	3235	1/1	0.86	0.20	3.32	71,71,71,71	0
57	MG	14	3224	1/1	0.92	0.24	3.12	45,45,45,45	0
57	MG	1H	3140	1/1	0.84	0.20	3.10	54,54,54,54	0
57	MG	14	3077	1/1	0.86	0.22	3.09	52,52,52,52	0
57	MG	14	3076	1/1	0.87	0.45	3.09	81,81,81,81	0
57	MG	14	3233	1/1	0.93	0.26	2.99	65,65,65,65	0
57	MG	14	3236	1/1	0.88	0.28	2.99	44,44,44,44	0
57	MG	14	3008	1/1	0.60	0.21	2.91	77,77,77,77	0
57	MG	14	3061	1/1	0.85	0.31	2.91	61,61,61,61	0
57	MG	13	1635	1/1	0.88	0.24	2.90	81,81,81,81	0
57	MG	13	1659	1/1	0.85	0.15	2.84	126,126,126,126	0
57	MG	13	1661	1/1	0.78	0.19	2.69	90,90,90,90	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
57	MG	14	3014	1/1	0.97	0.25	2.67	59,59,59,59	0
57	MG	14	3080	1/1	0.76	0.25	2.58	68,68,68,68	0
57	MG	1H	3013	1/1	0.90	0.27	2.50	40,40,40,40	0
57	MG	1H	3067	1/1	0.93	0.21	2.50	58,58,58,58	0
57	MG	14	3194	1/1	0.96	0.22	2.43	80,80,80,80	0
57	MG	14	3191	1/1	0.98	0.27	2.28	67,67,67,67	0
57	MG	14	3119	1/1	0.90	0.20	2.24	81,81,81,81	0
57	MG	1H	3059	1/1	0.99	0.27	2.20	56,56,56,56	0
57	MG	13	1623	1/1	0.96	0.22	2.14	76,76,76,76	0
57	MG	14	3237	1/1	0.91	0.26	2.08	51,51,51,51	0
57	MG	1H	3193	1/1	0.91	0.26	1.97	61,61,61,61	0
57	MG	1H	3275	1/1	0.96	0.18	1.95	57,57,57,57	0
57	MG	1H	3080	1/1	0.86	0.17	1.83	80,80,80,80	0
58	PAR	13	1741	42/42	0.95	0.24	1.83	64,71,75,82	0
57	MG	13	1607	1/1	0.99	0.20	1.81	72,72,72,72	0
57	MG	13	1646	1/1	0.95	0.17	1.58	71,71,71,71	0
57	MG	4I	200	1/1	0.70	0.23	1.54	95,95,95,95	0
57	MG	13	1641	1/1	0.90	0.19	1.50	81,81,81,81	0
57	MG	14	3086	1/1	0.97	0.23	1.45	56,56,56,56	0
57	MG	1H	3022	1/1	0.96	0.19	1.43	49,49,49,49	0
57	MG	14	3231	1/1	0.97	0.23	1.41	55,55,55,55	0
57	MG	14	3040	1/1	0.98	0.25	1.24	68,68,68,68	0
57	MG	14	3235	1/1	0.98	0.24	1.16	48,48,48,48	0
57	MG	1H	3090	1/1	0.97	0.21	1.08	42,42,42,42	0
57	MG	14	3041	1/1	0.92	0.20	0.98	55,55,55,55	0
57	MG	14	3290	1/1	0.95	0.22	0.97	59,59,59,59	0
57	MG	1H	3092	1/1	0.92	0.24	0.93	61,61,61,61	0
57	MG	1H	3134	1/1	0.83	0.14	0.89	57,57,57,57	0
57	MG	13	1692	1/1	0.96	0.18	0.85	72,72,72,72	0
58	PAR	1G	1702	42/42	0.94	0.22	0.77	83,92,100,103	0
57	MG	14	3288	1/1	0.95	0.20	0.73	49,49,49,49	0
57	MG	1H	3417	1/1	0.92	0.18	0.72	83,83,83,83	0
57	MG	1G	1622	1/1	0.98	0.20	0.71	125,125,125,125	0
57	MG	1H	3117	1/1	0.91	0.18	0.70	60,60,60,60	0
57	MG	14	3087	1/1	0.95	0.27	0.66	76,76,76,76	0
57	MG	1G	1633	1/1	0.98	0.21	0.56	118,118,118,118	0
57	MG	14	3005	1/1	0.84	0.26	0.54	54,54,54,54	0
57	MG	1H	3170	1/1	0.79	0.34	0.46	80,80,80,80	0
57	MG	13	1606	1/1	0.97	0.25	0.42	72,72,72,72	0
57	MG	1G	1644	1/1	0.74	0.20	0.42	106,106,106,106	0
57	MG	14	3216	1/1	0.98	0.21	0.36	52,52,52,52	0
57	MG	42	201	1/1	0.90	0.21	0.35	120,120,120,120	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
57	MG	14	3045	1/1	0.97	0.20	0.22	53,53,53,53	0
57	MG	14	3111	1/1	0.85	0.19	0.22	58,58,58,58	0
57	MG	1H	3300	1/1	0.93	0.19	0.21	62,62,62,62	0
57	MG	13	1642	1/1	0.94	0.13	0.19	103,103,103,103	0
57	MG	1G	1649	1/1	0.88	0.14	0.19	113,113,113,113	0
57	MG	1G	1607	1/1	0.98	0.20	0.18	86,86,86,86	0
57	MG	14	3217	1/1	0.96	0.20	0.10	56,56,56,56	0
57	MG	1H	3208	1/1	0.96	0.15	0.10	72,72,72,72	0
57	MG	1H	3294	1/1	0.90	0.16	0.06	54,54,54,54	0
57	MG	1H	3114	1/1	0.94	0.15	0.00	71,71,71,71	0
57	MG	1H	3039	1/1	0.95	0.20	-0.04	33,33,33,33	0
57	MG	1H	3027	1/1	0.97	0.19	-0.05	52,52,52,52	0
57	MG	1H	3525	1/1	0.84	0.22	-0.06	68,68,68,68	0
57	MG	1H	3397	1/1	0.92	0.19	-0.11	51,51,51,51	0
57	MG	1H	3365	1/1	0.94	0.16	-0.13	67,67,67,67	0
57	MG	13	1648	1/1	0.98	0.16	-0.14	67,67,67,67	0
57	MG	1H	3021	1/1	0.94	0.17	-0.16	49,49,49,49	0
57	MG	1H	3323	1/1	0.96	0.17	-0.19	57,57,57,57	0
57	MG	1G	1615	1/1	0.87	0.21	-0.21	86,86,86,86	0
57	MG	14	3029	1/1	0.94	0.21	-0.22	57,57,57,57	0
57	MG	52	201	1/1	0.79	0.16	-0.23	129,129,129,129	0
57	MG	14	3155	1/1	0.82	0.16	-0.24	78,78,78,78	0
57	MG	1H	3259	1/1	0.94	0.17	-0.28	54,54,54,54	0
57	MG	1H	3313	1/1	0.94	0.17	-0.30	47,47,47,47	0
57	MG	1G	1685	1/1	0.93	0.14	-0.31	110,110,110,110	0
59	SF4	3E	301	8/8	0.99	0.21	-0.33	82,91,95,98	0
57	MG	1H	3433	1/1	0.85	0.14	-0.34	72,72,72,72	0
57	MG	1G	1704	1/1	0.80	0.20	-0.35	84,84,84,84	0
57	MG	1G	1604	1/1	0.91	0.17	-0.35	127,127,127,127	0
57	MG	1H	3263	1/1	0.96	0.19	-0.36	46,46,46,46	0
57	MG	14	3390	1/1	0.87	0.22	-0.41	94,94,94,94	0
57	MG	88	201	1/1	0.93	0.19	-0.45	76,76,76,76	0
57	MG	13	1672	1/1	0.91	0.15	-0.47	88,88,88,88	0
57	MG	13	1657	1/1	0.90	0.15	-0.47	68,68,68,68	0
57	MG	13	1602	1/1	0.97	0.14	-0.52	120,120,120,120	0
57	MG	16	206	1/1	0.85	0.12	-0.52	77,77,77,77	0
57	MG	39	301	1/1	0.91	0.18	-0.61	89,89,89,89	0
57	MG	13	1700	1/1	0.88	0.12	-0.63	102,102,102,102	0
57	MG	1H	3215	1/1	0.89	0.13	-0.63	63,63,63,63	0
57	MG	14	3081	1/1	0.97	0.15	-0.64	56,56,56,56	0
59	SF4	32	302	8/8	0.99	0.18	-0.72	100,109,118,124	0
57	MG	14	3105	1/1	0.94	0.14	-0.75	73,73,73,73	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
57	MG	1H	3415	1/1	0.75	0.14	-0.77	72,72,72,72	0
57	MG	1H	3285	1/1	0.94	0.14	-0.80	55,55,55,55	0
57	MG	14	3395	1/1	0.67	0.10	-0.82	118,118,118,118	0
57	MG	14	3261	1/1	0.96	0.17	-0.84	59,59,59,59	0
57	MG	14	3027	1/1	0.96	0.14	-0.86	66,66,66,66	0
57	MG	1H	3020	1/1	0.82	0.14	-0.93	73,73,73,73	0
57	MG	1G	1678	1/1	0.58	0.11	-0.96	111,111,111,111	0
57	MG	13	1663	1/1	0.97	0.10	-0.99	107,107,107,107	0
57	MG	14	3113	1/1	0.92	0.18	-1.00	52,52,52,52	0
57	MG	1H	3273	1/1	0.97	0.14	-1.02	78,78,78,78	0
60	ZN	5I	102	1/1	0.99	0.13	-1.02	86,86,86,86	0
57	MG	1H	3297	1/1	0.96	0.14	-1.02	49,49,49,49	0
57	MG	13	1612	1/1	0.92	0.12	-1.05	86,86,86,86	0
57	MG	1H	3210	1/1	0.98	0.18	-1.05	56,56,56,56	0
57	MG	1H	3303	1/1	0.90	0.17	-1.05	48,48,48,48	0
57	MG	14	3268	1/1	0.87	0.15	-1.07	82,82,82,82	0
57	MG	1G	1638	1/1	0.95	0.14	-1.11	127,127,127,127	0
57	MG	13	1618	1/1	0.90	0.20	-1.13	48,48,48,48	0
57	MG	1G	1684	1/1	0.94	0.06	-1.16	96,96,96,96	0
57	MG	1G	1603	1/1	0.96	0.14	-1.16	88,88,88,88	0
57	MG	1H	3279	1/1	0.94	0.15	-1.17	48,48,48,48	0
57	MG	14	3249	1/1	0.93	0.15	-1.18	52,52,52,52	0
57	MG	1H	3262	1/1	0.97	0.18	-1.20	43,43,43,43	0
57	MG	1G	1666	1/1	0.94	0.14	-1.20	100,100,100,100	0
57	MG	14	3310	1/1	0.96	0.15	-1.22	54,54,54,54	0
57	MG	1H	3055	1/1	0.81	0.18	-1.25	48,48,48,48	0
57	MG	1H	3023	1/1	0.92	0.17	-1.26	50,50,50,50	0
57	MG	45	201	1/1	0.95	0.13	-1.28	101,101,101,101	0
57	MG	13	1691	1/1	0.94	0.12	-1.31	92,92,92,92	0
57	MG	1H	3492	1/1	0.86	0.15	-1.32	78,78,78,78	0
57	MG	14	3083	1/1	0.91	0.15	-1.33	72,72,72,72	0
57	MG	41	201	1/1	0.81	0.12	-1.35	69,69,69,69	0
57	MG	1H	3047	1/1	0.95	0.15	-1.37	55,55,55,55	0
57	MG	21	301	1/1	0.94	0.14	-1.38	59,59,59,59	0
57	MG	1H	3386	1/1	0.81	0.18	-1.42	42,42,42,42	0
60	ZN	5A	101	1/1	0.98	0.09	-1.43	146,146,146,146	0
57	MG	13	1680	1/1	0.96	0.16	-1.45	64,64,64,64	0
57	MG	1H	3116	1/1	0.91	0.16	-1.46	53,53,53,53	0
57	MG	13	1733	1/1	0.85	0.12	-1.46	101,101,101,101	0
57	MG	14	3378	1/1	0.93	0.13	-1.49	92,92,92,92	0
57	MG	14	3238	1/1	0.94	0.20	-1.50	50,50,50,50	0
57	MG	1H	3335	1/1	0.96	0.14	-1.51	48,48,48,48	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
57	MG	1H	3036	1/1	0.97	0.16	-1.56	37,37,37,37	0
57	MG	1H	3312	1/1	0.92	0.15	-1.57	44,44,44,44	0
57	MG	13	1682	1/1	0.92	0.11	-1.58	93,93,93,93	0
57	MG	14	3349	1/1	0.90	0.13	-1.59	83,83,83,83	0
57	MG	13	1631	1/1	0.90	0.09	-1.66	78,78,78,78	0
57	MG	14	3156	1/1	0.77	0.17	-1.67	87,87,87,87	0
57	MG	1H	3509	1/1	0.89	0.12	-1.69	47,47,47,47	0
57	MG	1H	3281	1/1	0.98	0.15	-1.71	61,61,61,61	0
57	MG	14	3230	1/1	0.83	0.17	-1.72	63,63,63,63	0
57	MG	14	3025	1/1	0.86	0.12	-1.74	80,80,80,80	0
57	MG	1H	3298	1/1	0.83	0.11	-1.75	51,51,51,51	0
57	MG	1H	3305	1/1	0.96	0.14	-1.76	63,63,63,63	0
57	MG	1H	3336	1/1	0.90	0.14	-1.81	62,62,62,62	0
57	MG	1H	3228	1/1	0.91	0.15	-1.81	60,60,60,60	0
57	MG	1G	1619	1/1	0.91	0.10	-1.82	102,102,102,102	0
57	MG	1G	1617	1/1	0.95	0.12	-1.85	116,116,116,116	0
57	MG	14	3287	1/1	0.96	0.11	-1.86	88,88,88,88	0
57	MG	14	3254	1/1	0.86	0.10	-1.87	77,77,77,77	0
57	MG	5I	101	1/1	0.83	0.10	-1.89	79,79,79,79	0
57	MG	14	3245	1/1	0.90	0.14	-1.97	63,63,63,63	0
57	MG	14	3121	1/1	0.90	0.12	-2.00	61,61,61,61	0
57	MG	14	3270	1/1	0.97	0.13	-2.01	67,67,67,67	0
57	MG	14	3272	1/1	0.95	0.09	-2.03	71,71,71,71	0
57	MG	14	3020	1/1	0.92	0.12	-2.06	75,75,75,75	0
57	MG	1H	3155	1/1	0.93	0.15	-2.12	55,55,55,55	0
57	MG	14	3295	1/1	0.82	0.10	-2.13	60,60,60,60	0
57	MG	14	3262	1/1	0.82	0.14	-2.15	83,83,83,83	0
57	MG	1H	3222	1/1	0.82	0.14	-2.19	69,69,69,69	0
61	SPE	1G	1703	13/13	0.88	0.09	-2.22	90,107,113,114	0
57	MG	14	3387	1/1	0.67	0.14	-2.22	83,83,83,83	0
60	ZN	C5	202	1/1	0.85	0.06	-2.22	165,165,165,165	0
57	MG	M5	101	1/1	0.93	0.18	-2.23	88,88,88,88	0
57	MG	Q8	300	1/1	0.92	0.12	-2.24	80,80,80,80	0
57	MG	14	3018	1/1	0.94	0.14	-2.28	44,44,44,44	0
57	MG	14	3150	1/1	0.94	0.12	-2.36	63,63,63,63	0
57	MG	1G	1667	1/1	0.86	0.11	-2.39	103,103,103,103	0
57	MG	1H	3325	1/1	0.99	0.15	-2.40	46,46,46,46	0
57	MG	1H	3491	1/1	0.94	0.10	-2.42	70,70,70,70	0
57	MG	13	1683	1/1	0.87	0.05	-2.43	93,93,93,93	0
57	MG	1H	3267	1/1	0.73	0.10	-2.44	56,56,56,56	0
57	MG	13	1714	1/1	0.74	0.09	-2.44	122,122,122,122	0
57	MG	78	201	1/1	0.86	0.10	-2.45	66,66,66,66	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
57	MG	14	3321	1/1	0.94	0.08	-2.48	69,69,69,69	0
57	MG	14	3309	1/1	0.91	0.14	-2.49	55,55,55,55	0
57	MG	1H	3194	1/1	0.85	0.10	-2.52	63,63,63,63	0
57	MG	1H	3257	1/1	0.95	0.14	-2.56	43,43,43,43	0
57	MG	14	3373	1/1	0.86	0.12	-2.57	65,65,65,65	0
57	MG	14	3293	1/1	0.97	0.10	-2.60	63,63,63,63	0
57	MG	1H	3469	1/1	0.94	0.15	-2.61	58,58,58,58	0
57	MG	1H	3094	1/1	0.92	0.15	-2.64	33,33,33,33	0
57	MG	14	3322	1/1	0.98	0.14	-2.67	58,58,58,58	0
57	MG	14	3211	1/1	0.74	0.09	-2.69	81,81,81,81	0
57	MG	14	3410	1/1	0.93	0.06	-2.71	85,85,85,85	0
57	MG	14	3296	1/1	0.90	0.12	-2.72	72,72,72,72	0
57	MG	14	3056	1/1	0.99	0.11	-2.73	54,54,54,54	0
57	MG	1H	3107	1/1	0.94	0.12	-2.73	60,60,60,60	0
57	MG	1H	3400	1/1	0.96	0.12	-2.77	53,53,53,53	0
57	MG	1G	1647	1/1	0.85	0.10	-2.79	97,97,97,97	0
57	MG	14	3159	1/1	0.88	0.11	-2.81	79,79,79,79	0
57	MG	1H	3138	1/1	0.91	0.14	-2.84	54,54,54,54	0
57	MG	14	3427	1/1	0.84	0.08	-2.88	65,65,65,65	0
57	MG	14	3116	1/1	0.96	0.13	-3.03	88,88,88,88	0
57	MG	1G	1632	1/1	0.79	0.09	-3.04	91,91,91,91	0
57	MG	1H	3051	1/1	0.92	0.11	-3.04	60,60,60,60	0
57	MG	13	1698	1/1	0.92	0.11	-3.08	83,83,83,83	0
57	MG	14	3354	1/1	0.90	0.14	-3.09	60,60,60,60	0
57	MG	1H	3381	1/1	0.95	0.11	-3.11	74,74,74,74	0
57	MG	1H	3046	1/1	0.86	0.13	-3.12	33,33,33,33	0
57	MG	1G	1672	1/1	0.97	0.12	-3.17	110,110,110,110	0
57	MG	1H	3361	1/1	0.97	0.07	-3.17	52,52,52,52	0
57	MG	1H	3278	1/1	0.98	0.09	-3.18	75,75,75,75	0
57	MG	1H	3115	1/1	0.90	0.10	-3.19	61,61,61,61	0
57	MG	1H	3331	1/1	0.90	0.12	-3.19	70,70,70,70	0
57	MG	14	3302	1/1	0.92	0.11	-3.29	58,58,58,58	0
57	MG	14	3283	1/1	0.95	0.07	-3.31	68,68,68,68	0
57	MG	1H	3431	1/1	0.82	0.09	-3.33	98,98,98,98	0
57	MG	1H	3307	1/1	0.96	0.14	-3.37	44,44,44,44	0
57	MG	13	1703	1/1	0.95	0.13	-3.44	70,70,70,70	0
57	MG	1H	3269	1/1	0.95	0.16	-3.46	41,41,41,41	0
57	MG	14	3324	1/1	0.96	0.15	-3.46	48,48,48,48	0
57	MG	14	3282	1/1	0.89	0.06	-3.54	90,90,90,90	0
57	MG	1H	3369	1/1	0.96	0.08	-3.67	44,44,44,44	0
57	MG	1H	3031	1/1	0.99	0.14	-3.67	51,51,51,51	0
57	MG	1H	3028	1/1	0.93	0.10	-3.69	67,67,67,67	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
57	MG	1H	3280	1/1	0.98	0.15	-3.72	36,36,36,36	0
57	MG	14	3251	1/1	0.91	0.09	-3.72	80,80,80,80	0
57	MG	1H	3371	1/1	0.89	0.10	-3.74	56,56,56,56	0
57	MG	14	3280	1/1	0.96	0.14	-3.89	61,61,61,61	0
57	MG	13	1718	1/1	0.94	0.09	-3.90	90,90,90,90	0
57	MG	14	3229	1/1	0.98	0.13	-3.93	59,59,59,59	0
57	MG	1H	3355	1/1	0.95	0.09	-4.11	59,59,59,59	0
57	MG	1H	3364	1/1	0.97	0.09	-4.12	44,44,44,44	0
57	MG	14	3220	1/1	0.93	0.12	-4.17	54,54,54,54	0
57	MG	14	3307	1/1	0.90	0.15	-4.21	66,66,66,66	0
57	MG	1H	3356	1/1	0.94	0.11	-4.21	54,54,54,54	0
57	MG	14	3275	1/1	0.87	0.10	-4.31	65,65,65,65	0
57	MG	14	3091	1/1	0.81	0.09	-4.33	78,78,78,78	0
57	MG	13	1617	1/1	0.88	0.14	-4.45	51,51,51,51	0
57	MG	14	3315	1/1	0.95	0.12	-4.48	68,68,68,68	0
57	MG	1H	3252	1/1	0.98	0.09	-4.48	65,65,65,65	0
57	MG	1H	3199	1/1	0.96	0.12	-4.48	61,61,61,61	0
57	MG	1H	3427	1/1	0.91	0.10	-4.49	67,67,67,67	0
57	MG	1H	3330	1/1	0.95	0.10	-4.51	71,71,71,71	0
57	MG	1G	1646	1/1	0.88	0.10	-4.54	86,86,86,86	0
57	MG	14	3253	1/1	0.97	0.07	-4.55	58,58,58,58	0
57	MG	1H	3299	1/1	0.92	0.13	-4.55	48,48,48,48	0
57	MG	16	204	1/1	0.88	0.06	-4.64	59,59,59,59	0
57	MG	1H	3304	1/1	0.97	0.10	-4.72	58,58,58,58	0
57	MG	14	3244	1/1	0.94	0.15	-4.76	54,54,54,54	0
57	MG	1H	3093	1/1	0.91	0.09	-4.77	56,56,56,56	0
57	MG	1H	3477	1/1	0.87	0.14	-4.78	83,83,83,83	0
57	MG	1H	3104	1/1	0.91	0.13	-4.85	43,43,43,43	0
57	MG	14	3289	1/1	0.92	0.13	-4.88	74,74,74,74	0
57	MG	1H	3239	1/1	0.94	0.10	-4.99	67,67,67,67	0
57	MG	1H	3302	1/1	0.98	0.13	-5.00	51,51,51,51	0
57	MG	1H	3437	1/1	0.97	0.09	-5.01	92,92,92,92	0
57	MG	14	3305	1/1	0.98	0.12	-5.04	49,49,49,49	0
57	MG	1G	1657	1/1	0.84	0.06	-5.17	121,121,121,121	0
57	MG	1G	1652	1/1	0.91	0.15	-5.19	81,81,81,81	0
57	MG	14	3242	1/1	0.99	0.10	-5.21	62,62,62,62	0
57	MG	1G	1651	1/1	0.97	0.11	-5.22	76,76,76,76	0
57	MG	1H	3392	1/1	0.86	0.15	-5.23	48,48,48,48	0
57	MG	1G	1606	1/1	0.85	0.13	-5.28	73,73,73,73	0
57	MG	1H	3470	1/1	0.81	0.08	-5.31	83,83,83,83	0
57	MG	1G	1645	1/1	0.93	0.14	-5.32	81,81,81,81	0
57	MG	1H	3048	1/1	0.93	0.13	-5.40	45,45,45,45	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
57	MG	1H	3272	1/1	0.96	0.09	-5.47	63,63,63,63	0
57	MG	14	3250	1/1	0.93	0.08	-5.56	79,79,79,79	0
57	MG	14	3388	1/1	0.89	0.07	-5.60	85,85,85,85	0
57	MG	1H	3248	1/1	0.96	0.11	-5.67	44,44,44,44	0
57	MG	1H	3465	1/1	0.96	0.09	-5.76	67,67,67,67	0
57	MG	14	3247	1/1	0.95	0.09	-5.89	52,52,52,52	0
57	MG	13	1621	1/1	0.98	0.09	-6.11	85,85,85,85	0
57	MG	14	3392	1/1	0.91	0.07	-6.22	63,63,63,63	0
57	MG	1H	3290	1/1	0.96	0.12	-6.25	55,55,55,55	0
57	MG	14	3389	1/1	0.84	0.07	-6.44	93,93,93,93	0
57	MG	14	3240	1/1	0.96	0.11	-6.57	73,73,73,73	0
57	MG	1H	3334	1/1	0.90	0.10	-6.58	77,77,77,77	0
57	MG	14	3218	1/1	0.94	0.09	-6.61	65,65,65,65	0
57	MG	14	3024	1/1	0.89	0.07	-6.63	81,81,81,81	0
57	MG	14	3317	1/1	0.93	0.08	-6.66	82,82,82,82	0
57	MG	14	3380	1/1	0.85	0.08	-6.77	78,78,78,78	0
57	MG	14	3400	1/1	0.92	0.05	-6.92	108,108,108,108	0
57	MG	1H	3265	1/1	0.97	0.08	-7.32	46,46,46,46	0
57	MG	13	1689	1/1	0.96	0.07	-7.41	88,88,88,88	0
57	MG	1H	3246	1/1	0.89	0.09	-7.44	55,55,55,55	0
57	MG	1H	3398	1/1	0.98	0.07	-7.55	78,78,78,78	0
57	MG	1H	3387	1/1	0.96	0.10	-7.68	33,33,33,33	0
57	MG	1J	204	1/1	0.89	0.09	-7.69	89,89,89,89	0
57	MG	14	3375	1/1	0.97	0.07	-7.70	93,93,93,93	0
57	MG	1H	3450	1/1	1.00	0.06	-7.73	44,44,44,44	0
57	MG	1H	3474	1/1	0.94	0.09	-8.12	93,93,93,93	0
57	MG	1H	3245	1/1	0.94	0.11	-8.20	47,47,47,47	0
57	MG	14	3368	1/1	0.83	0.09	-8.36	88,88,88,88	0
57	MG	14	3267	1/1	0.84	0.06	-8.46	82,82,82,82	0
57	MG	1H	3466	1/1	0.97	0.05	-8.55	72,72,72,72	0
57	MG	1H	3375	1/1	0.87	0.10	-8.87	79,79,79,79	0
57	MG	13	1715	1/1	0.94	0.06	-9.54	76,76,76,76	0
57	MG	1H	3289	1/1	0.95	0.12	-9.55	59,59,59,59	0
57	MG	1H	3393	1/1	0.93	0.11	-9.98	50,50,50,50	0
57	MG	1H	3378	1/1	0.93	0.09	-10.02	50,50,50,50	0
57	MG	1H	3461	1/1	0.96	0.06	-10.21	45,45,45,45	0
57	MG	1H	3284	1/1	0.95	0.07	-10.66	83,83,83,83	0
57	MG	14	3065	1/1	0.95	0.10	-10.76	47,47,47,47	0
57	MG	1H	3421	1/1	0.80	0.06	-12.06	82,82,82,82	0
57	MG	13	1638	1/1	0.92	0.07	-12.51	85,85,85,85	0
57	MG	1H	3418	1/1	0.92	0.10	-12.61	46,46,46,46	0
57	MG	13	1732	1/1	0.84	0.08	-12.70	114,114,114,114	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
57	MG	14	3225	1/1	0.83	0.07	-12.89	73,73,73,73	0
57	MG	1H	3064	1/1	0.92	0.07	-12.92	51,51,51,51	0
57	MG	1H	3485	1/1	0.83	0.06	-15.92	77,77,77,77	0
57	MG	13	1701	1/1	0.91	0.12	-	108,108,108,108	0
57	MG	14	3022	1/1	0.90	0.13	-	81,81,81,81	0
57	MG	1G	1689	1/1	0.91	0.06	-	116,116,116,116	0
57	MG	1J	202	1/1	0.86	0.28	-	92,92,92,92	0
57	MG	1H	3156	1/1	0.83	0.15	-	83,83,83,83	0
57	MG	1G	1668	1/1	0.74	0.09	-	124,124,124,124	0
57	MG	1H	3318	1/1	0.96	0.15	-	59,59,59,59	0
57	MG	1H	3254	1/1	0.98	0.08	-	46,46,46,46	0
57	MG	1H	3128	1/1	0.85	0.42	-	85,85,85,85	0
57	MG	1H	3410	1/1	0.88	0.10	-	83,83,83,83	0
57	MG	14	3279	1/1	0.90	0.08	-	58,58,58,58	0
57	MG	14	3102	1/1	0.96	0.56	-	85,85,85,85	0
57	MG	14	3415	1/1	0.93	0.15	-	103,103,103,103	0
57	MG	1H	3301	1/1	0.91	0.17	-	45,45,45,45	0
57	MG	14	3271	1/1	0.80	0.06	-	94,94,94,94	0
57	MG	1H	3489	1/1	0.85	0.32	-	73,73,73,73	0
57	MG	14	3146	1/1	0.80	0.28	-	75,75,75,75	0
57	MG	14	3342	1/1	0.78	0.09	-	113,113,113,113	0
57	MG	1H	3024	1/1	0.96	0.24	-	83,83,83,83	0
57	MG	1H	3050	1/1	0.59	0.38	-	72,72,72,72	0
57	MG	1H	3166	1/1	0.96	0.43	-	78,78,78,78	0
57	MG	1H	3348	1/1	0.87	0.10	-	111,111,111,111	0
57	MG	14	3206	1/1	0.98	0.27	-	85,85,85,85	0
57	MG	14	3384	1/1	0.63	0.14	-	78,78,78,78	0
57	MG	14	3053	1/1	0.95	0.07	-	95,95,95,95	0
57	MG	14	3416	1/1	0.87	0.13	-	102,102,102,102	0
57	MG	1H	3004	1/1	0.67	0.50	-	89,89,89,89	0
57	MG	14	3311	1/1	0.93	0.11	-	67,67,67,67	0
57	MG	1H	3270	1/1	0.91	0.15	-	50,50,50,50	0
57	MG	1H	3380	1/1	0.98	0.18	-	55,55,55,55	0
57	MG	13	1603	1/1	0.98	0.24	-	74,74,74,74	0
57	MG	1H	3382	1/1	0.97	0.09	-	49,49,49,49	0
57	MG	1H	3484	1/1	0.90	0.09	-	105,105,105,105	0
57	MG	14	3137	1/1	0.86	0.53	-	99,99,99,99	0
57	MG	1G	1605	1/1	0.81	0.39	-	104,104,104,104	0
57	MG	1H	3332	1/1	0.80	0.16	-	102,102,102,102	0
57	MG	1H	3315	1/1	0.97	0.10	-	63,63,63,63	0
57	MG	1G	1620	1/1	0.93	0.19	-	91,91,91,91	0
57	MG	14	3379	1/1	0.77	0.14	-	84,84,84,84	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
57	MG	14	3210	1/1	0.88	0.29	-	91,91,91,91	0
57	MG	1H	3184	1/1	0.94	0.24	-	70,70,70,70	0
57	MG	14	3209	1/1	0.87	0.17	-	83,83,83,83	0
57	MG	1H	3373	1/1	0.84	0.09	-	80,80,80,80	0
57	MG	13	1679	1/1	0.57	0.30	-	99,99,99,99	0
57	MG	1H	3512	1/1	0.86	0.13	-	87,87,87,87	0
57	MG	13	1637	1/1	0.74	0.32	-	74,74,74,74	0
57	MG	14	3371	1/1	0.93	0.10	-	107,107,107,107	0
57	MG	14	3075	1/1	0.82	0.16	-	73,73,73,73	0
57	MG	13	1613	1/1	0.88	0.13	-	87,87,87,87	0
57	MG	1H	3457	1/1	0.86	0.16	-	84,84,84,84	0
57	MG	1H	3120	1/1	0.60	0.18	-	88,88,88,88	0
57	MG	2L	102	1/1	0.88	0.18	-	132,132,132,132	0
57	MG	14	3286	1/1	0.85	0.11	-	73,73,73,73	0
57	MG	1G	1686	1/1	0.57	0.13	-	106,106,106,106	0
57	MG	14	3133	1/1	0.81	1.00	-	88,88,88,88	0
57	MG	1H	3359	1/1	0.98	0.17	-	44,44,44,44	0
57	MG	14	3278	1/1	0.83	0.09	-	102,102,102,102	0
57	MG	14	3012	1/1	0.96	0.32	-	57,57,57,57	0
57	MG	1H	3196	1/1	0.76	0.38	-	77,77,77,77	0
57	MG	14	3068	1/1	0.93	0.41	-	53,53,53,53	0
57	MG	1H	3122	1/1	0.91	0.09	-	52,52,52,52	0
57	MG	1H	3456	1/1	0.82	0.06	-	94,94,94,94	0
57	MG	1G	1637	1/1	0.80	0.16	-	103,103,103,103	0
57	MG	1H	3319	1/1	0.98	0.18	-	57,57,57,57	0
57	MG	14	3325	1/1	0.98	0.04	-	79,79,79,79	0
57	MG	1G	1612	1/1	0.90	0.15	-	106,106,106,106	0
57	MG	14	3033	1/1	0.94	0.33	-	80,80,80,80	0
57	MG	1H	3225	1/1	0.72	0.43	-	71,71,71,71	0
57	MG	13	1686	1/1	0.92	0.17	-	76,76,76,76	0
57	MG	1H	3463	1/1	0.96	0.09	-	81,81,81,81	0
57	MG	14	3393	1/1	0.32	0.08	-	165,165,165,165	0
57	MG	1H	3032	1/1	0.99	0.25	-	47,47,47,47	0
57	MG	1H	3467	1/1	0.95	0.03	-	84,84,84,84	0
57	MG	14	3346	1/1	0.89	0.08	-	99,99,99,99	0
57	MG	14	3433	1/1	0.64	0.26	-	114,114,114,114	0
57	MG	13	1647	1/1	0.79	0.47	-	88,88,88,88	0
57	MG	13	1704	1/1	0.32	0.13	-	106,106,106,106	0
57	MG	14	3197	1/1	0.76	0.61	-	77,77,77,77	0
57	MG	14	3098	1/1	0.76	0.35	-	77,77,77,77	0
57	MG	1H	3189	1/1	0.92	0.35	-	68,68,68,68	0
57	MG	14	3228	1/1	0.98	0.14	-	56,56,56,56	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
57	MG	1H	3110	1/1	0.95	0.23	-	79,79,79,79	0
57	MG	14	3320	1/1	0.95	0.09	-	53,53,53,53	0
57	MG	14	3110	1/1	0.70	0.24	-	69,69,69,69	0
57	MG	14	3147	1/1	0.98	0.40	-	69,69,69,69	0
57	MG	1H	3423	1/1	0.67	0.18	-	84,84,84,84	0
57	MG	1H	3197	1/1	0.82	0.51	-	77,77,77,77	0
57	MG	13	1729	1/1	0.68	0.11	-	110,110,110,110	0
57	MG	13	1666	1/1	0.94	0.20	-	85,85,85,85	0
57	MG	14	3148	1/1	0.89	0.39	-	85,85,85,85	0
57	MG	1H	3434	1/1	0.79	0.17	-	95,95,95,95	0
57	MG	13	1609	1/1	0.97	0.15	-	70,70,70,70	0
57	MG	14	3421	1/1	0.79	0.10	-	97,97,97,97	0
57	MG	14	3093	1/1	0.97	0.42	-	84,84,84,84	0
57	MG	14	3312	1/1	0.86	0.16	-	92,92,92,92	0
57	MG	14	3085	1/1	0.94	0.25	-	88,88,88,88	0
57	MG	1H	3035	1/1	0.94	0.11	-	40,40,40,40	0
57	MG	1H	3202	1/1	0.91	0.45	-	73,73,73,73	0
57	MG	13	1710	1/1	0.86	0.07	-	96,96,96,96	0
57	MG	14	3327	1/1	0.90	0.09	-	82,82,82,82	0
57	MG	1H	3328	1/1	0.97	0.13	-	47,47,47,47	0
57	MG	1H	3081	1/1	0.19	0.45	-	83,83,83,83	0
57	MG	14	3345	1/1	0.82	0.16	-	99,99,99,99	0
57	MG	14	3339	1/1	0.80	0.10	-	107,107,107,107	0
57	MG	1H	3180	1/1	0.34	0.42	-	90,90,90,90	0
57	MG	1H	3148	1/1	0.85	0.37	-	83,83,83,83	0
57	MG	14	3017	1/1	0.68	0.34	-	119,119,119,119	0
57	MG	1H	3216	1/1	0.69	0.27	-	82,82,82,82	0
57	MG	14	3376	1/1	0.65	0.23	-	102,102,102,102	0
57	MG	13	1719	1/1	0.89	0.04	-	81,81,81,81	0
57	MG	14	3187	1/1	0.79	0.25	-	117,117,117,117	0
57	MG	1H	3389	1/1	0.77	0.14	-	88,88,88,88	0
57	MG	14	3260	1/1	0.90	0.11	-	106,106,106,106	0
57	MG	13	1656	1/1	0.90	0.38	-	74,74,74,74	0
57	MG	13	1608	1/1	0.96	0.08	-	76,76,76,76	0
57	MG	1H	3514	1/1	0.95	0.05	-	98,98,98,98	0
57	MG	14	3409	1/1	0.72	0.22	-	88,88,88,88	0
57	MG	1H	3075	1/1	0.73	0.29	-	76,76,76,76	0
57	MG	1H	3404	1/1	0.90	0.13	-	71,71,71,71	0
57	MG	1G	1663	1/1	0.80	0.23	-	98,98,98,98	0
57	MG	1G	1624	1/1	0.91	0.13	-	95,95,95,95	0
57	MG	1H	3411	1/1	0.97	0.07	-	63,63,63,63	0
57	MG	1H	3296	1/1	0.88	0.08	-	91,91,91,91	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
57	MG	14	3258	1/1	0.77	0.07	-	79,79,79,79	0
57	MG	14	3274	1/1	0.77	0.05	-	85,85,85,85	0
57	MG	1H	3100	1/1	0.92	0.54	-	68,68,68,68	0
57	MG	13	1722	1/1	0.90	0.09	-	87,87,87,87	0
57	MG	14	3213	1/1	0.84	0.70	-	87,87,87,87	0
57	MG	1H	3125	1/1	0.81	0.20	-	56,56,56,56	0
57	MG	1G	1693	1/1	0.80	0.07	-	129,129,129,129	0
57	MG	14	3109	1/1	0.71	0.43	-	67,67,67,67	0
57	MG	1H	3096	1/1	0.95	0.14	-	64,64,64,64	0
57	MG	14	3177	1/1	0.87	0.45	-	101,101,101,101	0
57	MG	14	3383	1/1	0.91	0.07	-	90,90,90,90	0
57	MG	1G	1654	1/1	0.86	0.30	-	108,108,108,108	0
57	MG	1H	3065	1/1	0.68	0.53	-	65,65,65,65	0
57	MG	14	3140	1/1	0.96	0.13	-	51,51,51,51	0
57	MG	1G	1631	1/1	0.96	0.56	-	92,92,92,92	0
57	MG	13	1693	1/1	0.96	0.07	-	85,85,85,85	0
57	MG	1G	1630	1/1	0.91	0.37	-	72,72,72,72	0
57	MG	1H	3142	1/1	0.88	0.29	-	68,68,68,68	0
57	MG	14	3004	1/1	0.97	0.28	-	63,63,63,63	0
57	MG	13	1725	1/1	0.90	0.04	-	115,115,115,115	0
57	MG	13	1734	1/1	0.97	0.10	-	94,94,94,94	0
57	MG	1H	3471	1/1	0.96	0.12	-	90,90,90,90	0
57	MG	1H	3340	1/1	0.92	0.05	-	76,76,76,76	0
57	MG	14	3172	1/1	0.88	0.39	-	77,77,77,77	0
57	MG	14	3246	1/1	0.95	0.13	-	61,61,61,61	0
57	MG	14	3164	1/1	0.71	0.33	-	78,78,78,78	0
57	MG	14	3372	1/1	0.96	0.12	-	86,86,86,86	0
57	MG	1H	3311	1/1	0.98	0.08	-	53,53,53,53	0
57	MG	14	3407	1/1	0.69	0.12	-	123,123,123,123	0
57	MG	14	3047	1/1	0.98	0.34	-	65,65,65,65	0
57	MG	1G	1626	1/1	0.94	0.19	-	83,83,83,83	0
57	MG	1H	3072	1/1	0.95	0.20	-	58,58,58,58	0
57	MG	1G	1613	1/1	0.93	0.76	-	89,89,89,89	0
57	MG	14	3168	1/1	0.78	0.24	-	89,89,89,89	0
57	MG	14	3170	1/1	0.85	0.59	-	81,81,81,81	0
57	MG	14	3397	1/1	0.90	0.17	-	96,96,96,96	0
57	MG	1H	3220	1/1	0.82	0.45	-	89,89,89,89	0
57	MG	1H	3445	1/1	0.18	0.12	-	92,92,92,92	0
57	MG	1H	3480	1/1	0.89	0.07	-	87,87,87,87	0
57	MG	1H	3038	1/1	0.82	0.32	-	50,50,50,50	0
57	MG	14	3352	1/1	0.93	0.07	-	82,82,82,82	0
57	MG	1H	3448	1/1	0.97	0.07	-	80,80,80,80	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
57	MG	1H	3077	1/1	0.92	0.42	-	80,80,80,80	0
57	MG	14	3291	1/1	0.72	0.21	-	85,85,85,85	0
57	MG	1H	3498	1/1	0.86	0.20	-	98,98,98,98	0
57	MG	14	3323	1/1	0.85	0.11	-	81,81,81,81	0
57	MG	14	3006	1/1	0.85	0.32	-	75,75,75,75	0
57	MG	14	3396	1/1	0.91	0.03	-	126,126,126,126	0
57	MG	14	3408	1/1	0.86	0.13	-	92,92,92,92	0
57	MG	1H	3037	1/1	0.90	0.54	-	75,75,75,75	0
57	MG	13	1687	1/1	0.94	0.06	-	103,103,103,103	0
57	MG	13	1658	1/1	0.89	0.25	-	82,82,82,82	0
57	MG	1H	3360	1/1	0.99	0.09	-	78,78,78,78	0
57	MG	1H	3493	1/1	0.95	0.04	-	101,101,101,101	0
57	MG	14	3180	1/1	0.91	0.41	-	91,91,91,91	0
57	MG	14	3021	1/1	0.95	0.35	-	38,38,38,38	0
57	MG	1H	3422	1/1	0.69	0.33	-	65,65,65,65	0
57	MG	14	3169	1/1	0.90	0.31	-	85,85,85,85	0
57	MG	14	3195	1/1	0.95	0.25	-	78,78,78,78	0
57	MG	14	3239	1/1	0.97	0.17	-	77,77,77,77	0
57	MG	1H	3227	1/1	0.72	0.28	-	72,72,72,72	0
57	MG	13	1675	1/1	0.81	0.47	-	101,101,101,101	0
57	MG	1H	3234	1/1	0.68	0.20	-	79,79,79,79	0
57	MG	1H	3174	1/1	0.86	0.23	-	55,55,55,55	0
57	MG	14	3204	1/1	0.83	0.22	-	72,72,72,72	0
57	MG	1H	3306	1/1	0.98	0.09	-	75,75,75,75	0
57	MG	14	3026	1/1	0.97	0.29	-	56,56,56,56	0
57	MG	1H	3501	1/1	0.92	0.06	-	90,90,90,90	0
57	MG	14	3183	1/1	0.81	0.30	-	103,103,103,103	0
57	MG	1G	1642	1/1	0.55	0.28	-	99,99,99,99	0
57	MG	13	1717	1/1	0.92	0.11	-	99,99,99,99	0
57	MG	1H	3508	1/1	0.90	0.10	-	117,117,117,117	0
57	MG	1H	3129	1/1	0.78	0.20	-	76,76,76,76	0
57	MG	2K	101	1/1	0.91	0.11	-	100,100,100,100	0
57	MG	1H	3062	1/1	0.90	0.13	-	38,38,38,38	0
57	MG	14	3192	1/1	0.95	0.28	-	74,74,74,74	0
57	MG	1H	3157	1/1	0.54	0.38	-	89,89,89,89	0
57	MG	14	3049	1/1	0.86	1.18	-	83,83,83,83	0
57	MG	1G	1623	1/1	0.94	0.21	-	115,115,115,115	0
57	MG	14	3009	1/1	0.90	0.34	-	57,57,57,57	0
57	MG	1H	3443	1/1	0.86	0.10	-	75,75,75,75	0
57	MG	13	1632	1/1	0.96	0.22	-	78,78,78,78	0
57	MG	13	1655	1/1	0.89	0.50	-	82,82,82,82	0
57	MG	14	3357	1/1	0.92	0.08	-	105,105,105,105	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
57	MG	1H	3345	1/1	0.92	0.06	-	102,102,102,102	0
57	MG	13	1738	1/1	0.64	0.09	-	133,133,133,133	0
57	MG	13	1676	1/1	0.77	0.47	-	93,93,93,93	0
57	MG	1H	3049	1/1	0.83	0.25	-	62,62,62,62	0
57	MG	13	1713	1/1	0.88	0.08	-	86,86,86,86	0
57	MG	14	3165	1/1	0.86	0.66	-	77,77,77,77	0
57	MG	14	3332	1/1	0.65	0.09	-	102,102,102,102	0
57	MG	14	3106	1/1	0.94	0.41	-	57,57,57,57	0
57	MG	16	207	1/1	0.92	0.33	-	74,74,74,74	0
57	MG	1H	3266	1/1	0.94	0.08	-	54,54,54,54	0
57	MG	1H	3123	1/1	0.77	0.37	-	65,65,65,65	0
57	MG	14	3223	1/1	0.89	0.10	-	87,87,87,87	0
57	MG	1G	1653	1/1	0.95	0.11	-	97,97,97,97	0
57	MG	1H	3482	1/1	0.85	0.09	-	94,94,94,94	0
57	MG	1H	3366	1/1	0.94	0.17	-	68,68,68,68	0
57	MG	1H	3060	1/1	0.99	0.16	-	35,35,35,35	0
57	MG	14	3010	1/1	0.94	0.24	-	57,57,57,57	0
57	MG	14	3423	1/1	0.90	0.07	-	120,120,120,120	0
57	MG	1J	201	1/1	0.90	0.29	-	73,73,73,73	0
57	MG	14	3037	1/1	0.97	0.26	-	65,65,65,65	0
57	MG	13	1667	1/1	0.93	0.67	-	89,89,89,89	0
57	MG	1H	3261	1/1	0.93	0.08	-	63,63,63,63	0
57	MG	1H	3344	1/1	0.95	0.08	-	103,103,103,103	0
57	MG	14	3273	1/1	0.88	0.09	-	86,86,86,86	0
57	MG	13	1706	1/1	0.77	0.08	-	117,117,117,117	0
57	MG	14	3414	1/1	0.84	0.12	-	97,97,97,97	0
57	MG	1H	3012	1/1	0.97	0.41	-	58,58,58,58	0
57	MG	14	3094	1/1	0.93	0.65	-	73,73,73,73	0
57	MG	1H	3163	1/1	0.78	0.44	-	91,91,91,91	0
57	MG	1G	1635	1/1	0.71	0.20	-	105,105,105,105	0
57	MG	1H	3154	1/1	0.53	0.23	-	58,58,58,58	0
57	MG	1G	1687	1/1	0.90	0.08	-	111,111,111,111	0
57	MG	16	201	1/1	0.84	0.25	-	62,62,62,62	0
57	MG	14	3178	1/1	0.92	0.73	-	78,78,78,78	0
57	MG	14	3330	1/1	0.71	0.14	-	94,94,94,94	0
57	MG	1H	3468	1/1	0.93	0.24	-	82,82,82,82	0
57	MG	E5	101	1/1	0.60	0.58	-	89,89,89,89	0
57	MG	1H	3226	1/1	0.74	0.31	-	71,71,71,71	0
57	MG	1H	3083	1/1	0.81	0.84	-	83,83,83,83	0
57	MG	1H	3523	1/1	0.83	0.11	-	82,82,82,82	0
57	MG	14	3363	1/1	0.95	0.09	-	107,107,107,107	0
57	MG	13	1716	1/1	0.94	0.10	-	71,71,71,71	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
57	MG	14	3153	1/1	0.84	0.59	-	90,90,90,90	0
57	MG	1G	1629	1/1	0.88	0.52	-	85,85,85,85	0
57	MG	13	1684	1/1	0.89	0.08	-	85,85,85,85	0
57	MG	1H	3444	1/1	0.74	0.11	-	74,74,74,74	0
57	MG	1G	1655	1/1	0.93	0.12	-	110,110,110,110	0
57	MG	14	3308	1/1	0.97	0.10	-	94,94,94,94	0
57	MG	14	3411	1/1	0.87	0.04	-	105,105,105,105	0
57	MG	14	3292	1/1	0.94	0.12	-	74,74,74,74	0
57	MG	1G	1694	1/1	0.79	0.12	-	113,113,113,113	0
57	MG	1H	3233	1/1	0.95	0.07	-	93,93,93,93	0
57	MG	13	1696	1/1	0.88	0.05	-	93,93,93,93	0
57	MG	14	3207	1/1	0.71	0.37	-	70,70,70,70	0
57	MG	1H	3006	1/1	0.72	0.28	-	74,74,74,74	0
60	ZN	G8	201	1/1	0.92	0.14	-	139,139,139,139	0
57	MG	1H	3118	1/1	0.75	0.15	-	69,69,69,69	0
57	MG	14	3422	1/1	0.52	0.24	-	108,108,108,108	0
57	MG	14	3430	1/1	0.61	0.18	-	107,107,107,107	0
57	MG	1G	1634	1/1	0.79	0.72	-	85,85,85,85	0
57	MG	1H	3005	1/1	0.86	0.21	-	68,68,68,68	0
57	MG	14	3078	1/1	0.96	0.29	-	56,56,56,56	0
57	MG	14	3394	1/1	0.96	0.05	-	91,91,91,91	0
57	MG	14	3173	1/1	0.70	0.45	-	79,79,79,79	0
57	MG	1H	3231	1/1	0.91	0.49	-	66,66,66,66	0
57	MG	1H	3016	1/1	0.98	0.19	-	44,44,44,44	0
57	MG	1H	3101	1/1	0.86	0.41	-	78,78,78,78	0
57	MG	1H	3250	1/1	0.95	0.18	-	41,41,41,41	0
57	MG	1G	1661	1/1	0.97	0.08	-	95,95,95,95	0
57	MG	1H	3368	1/1	0.80	0.12	-	69,69,69,69	0
57	MG	1H	3291	1/1	0.99	0.13	-	59,59,59,59	0
57	MG	13	1625	1/1	0.94	0.16	-	82,82,82,82	0
57	MG	1H	3391	1/1	0.80	0.13	-	89,89,89,89	0
57	MG	1G	1700	1/1	0.93	0.06	-	109,109,109,109	0
57	MG	13	1727	1/1	0.76	0.13	-	90,90,90,90	0
57	MG	13	1711	1/1	0.80	0.16	-	74,74,74,74	0
57	MG	13	1673	1/1	0.68	0.40	-	84,84,84,84	0
57	MG	14	3319	1/1	0.90	0.07	-	95,95,95,95	0
57	MG	1H	3363	1/1	0.77	0.12	-	96,96,96,96	0
57	MG	1H	3310	1/1	0.91	0.18	-	70,70,70,70	0
57	MG	14	3050	1/1	0.94	0.20	-	57,57,57,57	0
57	MG	1H	3145	1/1	0.56	0.53	-	80,80,80,80	0
57	MG	13	1651	1/1	0.87	0.29	-	98,98,98,98	0
57	MG	14	3052	1/1	0.97	0.23	-	54,54,54,54	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
57	MG	14	3297	1/1	0.91	0.17	-	71,71,71,71	0
57	MG	1J	207	1/1	0.79	0.15	-	97,97,97,97	0
57	MG	1H	3113	1/1	0.48	0.26	-	81,81,81,81	0
57	MG	1H	3438	1/1	0.93	0.04	-	62,62,62,62	0
57	MG	1H	3058	1/1	0.85	0.17	-	60,60,60,60	0
57	MG	13	1615	1/1	0.88	0.24	-	88,88,88,88	0
57	MG	14	3424	1/1	0.88	0.09	-	109,109,109,109	0
57	MG	14	3039	1/1	0.91	0.71	-	89,89,89,89	0
57	MG	14	3182	1/1	0.96	0.35	-	74,74,74,74	0
57	MG	1G	1695	1/1	0.86	0.23	-	107,107,107,107	0
57	MG	1G	1671	1/1	0.72	0.17	-	112,112,112,112	0
57	MG	1H	3146	1/1	0.92	0.16	-	52,52,52,52	0
57	MG	1H	3001	1/1	0.87	0.39	-	84,84,84,84	0
57	MG	1H	3183	1/1	0.96	0.21	-	70,70,70,70	0
57	MG	3I	201	1/1	0.92	0.24	-	60,60,60,60	0
57	MG	14	3043	1/1	0.93	0.29	-	71,71,71,71	0
57	MG	1H	3008	1/1	0.87	0.39	-	82,82,82,82	0
57	MG	14	3386	1/1	0.82	0.09	-	74,74,74,74	0
57	MG	1H	3238	1/1	0.94	0.34	-	80,80,80,80	0
57	MG	1H	3274	1/1	0.84	0.14	-	97,97,97,97	0
57	MG	1H	3160	1/1	0.93	0.18	-	71,71,71,71	0
57	MG	1H	3333	1/1	0.98	0.13	-	77,77,77,77	0
57	MG	1H	3276	1/1	0.94	0.10	-	78,78,78,78	0
57	MG	14	3264	1/1	0.71	0.14	-	93,93,93,93	0
57	MG	1G	1669	1/1	0.81	0.09	-	105,105,105,105	0
57	MG	1H	3019	1/1	0.95	0.23	-	32,32,32,32	0
57	MG	1H	3505	1/1	0.90	0.14	-	100,100,100,100	0
57	MG	13	1740	1/1	0.86	0.06	-	98,98,98,98	0
57	MG	1H	3292	1/1	0.98	0.21	-	43,43,43,43	0
57	MG	1H	3449	1/1	0.94	0.10	-	80,80,80,80	0
57	MG	32	301	1/1	0.85	0.47	-	113,113,113,113	0
57	MG	1G	1625	1/1	0.89	0.08	-	99,99,99,99	0
57	MG	1H	3214	1/1	0.96	0.47	-	77,77,77,77	0
57	MG	1H	3379	1/1	0.88	0.09	-	73,73,73,73	0
57	MG	35	201	1/1	0.69	0.22	-	75,75,75,75	0
57	MG	1H	3401	1/1	0.81	0.09	-	64,64,64,64	0
57	MG	1H	3244	1/1	0.90	0.42	-	74,74,74,74	0
57	MG	1G	1602	1/1	0.92	0.33	-	106,106,106,106	0
57	MG	1H	3374	1/1	0.76	0.11	-	83,83,83,83	0
57	MG	1H	3412	1/1	0.87	0.10	-	75,75,75,75	0
57	MG	1H	3518	1/1	0.78	0.11	-	96,96,96,96	0
57	MG	14	3284	1/1	0.93	0.14	-	72,72,72,72	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
57	MG	1H	3152	1/1	0.98	0.41	-	70,70,70,70	0
57	MG	14	3135	1/1	0.66	0.32	-	79,79,79,79	0
57	MG	14	3252	1/1	0.72	0.18	-	90,90,90,90	0
57	MG	13	1616	1/1	0.87	0.48	-	74,74,74,74	0
57	MG	14	3333	1/1	0.92	0.17	-	50,50,50,50	0
57	MG	1G	1688	1/1	0.79	0.24	-	113,113,113,113	0
57	MG	1H	3095	1/1	0.92	0.17	-	70,70,70,70	0
57	MG	1H	3502	1/1	0.85	0.18	-	141,141,141,141	0
57	MG	1H	3453	1/1	0.83	0.12	-	93,93,93,93	0
57	MG	14	3115	1/1	0.40	0.78	-	87,87,87,87	0
57	MG	14	3360	1/1	0.92	0.07	-	96,96,96,96	0
57	MG	14	3167	1/1	0.88	0.32	-	78,78,78,78	0
57	MG	14	3266	1/1	0.65	0.08	-	107,107,107,107	0
57	MG	14	3011	1/1	0.91	0.18	-	44,44,44,44	0
57	MG	14	3435	1/1	0.70	0.20	-	92,92,92,92	0
57	MG	1H	3426	1/1	0.96	0.05	-	74,74,74,74	0
57	MG	14	3001	1/1	0.89	0.17	-	57,57,57,57	0
57	MG	1G	1696	1/1	0.91	0.07	-	128,128,128,128	0
57	MG	13	1736	1/1	0.96	0.12	-	101,101,101,101	0
57	MG	1H	3451	1/1	0.65	0.08	-	102,102,102,102	0
57	MG	1H	3516	1/1	0.77	0.14	-	102,102,102,102	0
57	MG	1H	3342	1/1	0.96	0.06	-	86,86,86,86	0
57	MG	14	3129	1/1	0.88	0.42	-	118,118,118,118	0
57	MG	1H	3161	1/1	0.83	0.38	-	67,67,67,67	0
57	MG	14	3269	1/1	0.94	0.05	-	78,78,78,78	0
57	MG	1H	3068	1/1	0.95	0.40	-	72,72,72,72	0
57	MG	1H	3124	1/1	0.92	0.21	-	61,61,61,61	0
57	MG	1H	3464	1/1	0.96	0.08	-	63,63,63,63	0
57	MG	13	1685	1/1	0.64	0.16	-	90,90,90,90	0
57	MG	1H	3191	1/1	0.82	0.27	-	58,58,58,58	0
57	MG	1H	3256	1/1	0.89	0.13	-	47,47,47,47	0
57	MG	1H	3223	1/1	0.82	0.43	-	85,85,85,85	0
57	MG	C5	201	1/1	0.65	0.10	-	113,113,113,113	0
57	MG	14	3158	1/1	0.90	0.24	-	66,66,66,66	0
57	MG	14	3084	1/1	0.87	0.27	-	79,79,79,79	0
57	MG	1G	1679	1/1	0.88	0.09	-	94,94,94,94	0
57	MG	13	1728	1/1	0.83	0.05	-	117,117,117,117	0
57	MG	14	3347	1/1	0.64	0.10	-	88,88,88,88	0
57	MG	1H	3413	1/1	0.97	0.10	-	78,78,78,78	0
57	MG	1H	3258	1/1	0.96	0.11	-	47,47,47,47	0
57	MG	1H	3159	1/1	0.95	0.13	-	80,80,80,80	0
57	MG	13	1678	1/1	0.01	0.16	-	112,112,112,112	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
57	MG	1G	1608	1/1	0.92	0.37	-	93,93,93,93	0
57	MG	1H	3017	1/1	0.95	0.29	-	62,62,62,62	0
57	MG	1H	3271	1/1	0.86	0.19	-	51,51,51,51	0
57	MG	1H	3481	1/1	0.85	0.11	-	103,103,103,103	0
57	MG	13	1702	1/1	0.98	0.13	-	85,85,85,85	0
57	MG	1H	3007	1/1	0.59	0.31	-	81,81,81,81	0
57	MG	14	3328	1/1	0.85	0.08	-	81,81,81,81	0
57	MG	1G	1662	1/1	0.92	0.13	-	91,91,91,91	0
57	MG	1H	3211	1/1	0.66	0.46	-	78,78,78,78	0
57	MG	1H	3206	1/1	0.78	0.56	-	93,93,93,93	0
57	MG	1H	3287	1/1	0.96	0.08	-	71,71,71,71	0
57	MG	13	1735	1/1	0.91	0.07	-	100,100,100,100	0
57	MG	1H	3018	1/1	0.97	0.18	-	41,41,41,41	0
57	MG	1H	3277	1/1	0.77	0.16	-	71,71,71,71	0
57	MG	1H	3144	1/1	0.80	0.60	-	102,102,102,102	0
57	MG	14	3374	1/1	0.89	0.12	-	92,92,92,92	0
57	MG	13	1626	1/1	0.90	0.33	-	84,84,84,84	0
57	MG	1H	3500	1/1	0.62	0.14	-	94,94,94,94	0
57	MG	1H	3179	1/1	0.95	0.14	-	80,80,80,80	0
57	MG	14	3299	1/1	0.89	0.11	-	79,79,79,79	0
57	MG	13	1721	1/1	0.95	0.17	-	106,106,106,106	0
57	MG	21	302	1/1	0.86	0.25	-	72,72,72,72	0
57	MG	1H	3370	1/1	0.92	0.08	-	68,68,68,68	0
57	MG	14	3428	1/1	0.77	0.29	-	119,119,119,119	0
57	MG	14	3127	1/1	0.56	1.03	-	87,87,87,87	0
57	MG	1G	1698	1/1	0.96	0.10	-	123,123,123,123	0
57	MG	13	1652	1/1	0.96	0.62	-	71,71,71,71	0
57	MG	39	302	1/1	0.82	0.20	-	74,74,74,74	0
57	MG	1H	3137	1/1	0.86	0.43	-	70,70,70,70	0
57	MG	13	1730	1/1	0.88	0.09	-	94,94,94,94	0
57	MG	13	1660	1/1	0.74	0.23	-	88,88,88,88	0
57	MG	14	3051	1/1	0.93	0.27	-	61,61,61,61	0
57	MG	1H	3424	1/1	0.89	0.04	-	101,101,101,101	0
57	MG	1H	3406	1/1	0.84	0.08	-	85,85,85,85	0
57	MG	1H	3503	1/1	0.64	0.12	-	91,91,91,91	0
57	MG	1G	1628	1/1	0.90	0.31	-	113,113,113,113	0
57	MG	14	3101	1/1	0.96	0.33	-	87,87,87,87	0
57	MG	1H	3218	1/1	0.94	0.21	-	37,37,37,37	0
57	MG	14	3256	1/1	0.84	0.13	-	83,83,83,83	0
57	MG	1H	3164	1/1	0.85	0.41	-	69,69,69,69	0
57	MG	1H	3003	1/1	0.77	0.37	-	65,65,65,65	0
57	MG	14	3355	1/1	0.56	0.10	-	104,104,104,104	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
57	MG	14	3227	1/1	0.90	0.15	-	58,58,58,58	0
57	MG	14	3193	1/1	0.90	0.13	-	45,45,45,45	0
57	MG	1H	3376	1/1	0.83	0.15	-	66,66,66,66	0
57	MG	14	3277	1/1	0.68	0.16	-	84,84,84,84	0
57	MG	14	3382	1/1	0.78	0.12	-	66,66,66,66	0
57	MG	14	3334	1/1	0.95	0.10	-	60,60,60,60	0
57	MG	1H	3241	1/1	0.78	0.22	-	58,58,58,58	0
57	MG	1H	3475	1/1	0.94	0.12	-	97,97,97,97	0
57	MG	14	3103	1/1	0.76	0.43	-	96,96,96,96	0
57	MG	1H	3053	1/1	0.76	0.46	-	75,75,75,75	0
57	MG	1G	1621	1/1	0.85	0.42	-	82,82,82,82	0
57	MG	14	3335	1/1	0.93	0.08	-	81,81,81,81	0
57	MG	1H	3462	1/1	0.93	0.10	-	94,94,94,94	0
57	MG	1H	3317	1/1	0.96	0.07	-	66,66,66,66	0
57	MG	1H	3192	1/1	0.87	0.34	-	75,75,75,75	0
57	MG	1H	3416	1/1	0.90	0.06	-	89,89,89,89	0
57	MG	13	1634	1/1	0.94	0.36	-	75,75,75,75	0
57	MG	14	3337	1/1	0.92	0.14	-	104,104,104,104	0
57	MG	1H	3385	1/1	0.98	0.15	-	25,25,25,25	0
57	MG	1H	3182	1/1	0.95	0.57	-	60,60,60,60	0
57	MG	1H	3479	1/1	0.76	0.10	-	83,83,83,83	0
57	MG	1H	3513	1/1	0.86	0.15	-	53,53,53,53	0
57	MG	1H	3507	1/1	0.94	0.08	-	57,57,57,57	0
57	MG	1H	3497	1/1	0.79	0.10	-	107,107,107,107	0
57	MG	1H	3436	1/1	0.93	0.10	-	70,70,70,70	0
57	MG	14	3138	1/1	0.71	0.67	-	78,78,78,78	0
57	MG	14	3316	1/1	0.90	0.13	-	69,69,69,69	0
57	MG	1G	1690	1/1	0.80	0.06	-	117,117,117,117	0
57	MG	1H	3139	1/1	0.95	0.35	-	71,71,71,71	0
57	MG	14	3234	1/1	0.96	0.18	-	57,57,57,57	0
57	MG	14	3257	1/1	0.78	0.16	-	69,69,69,69	0
57	MG	13	1650	1/1	0.85	0.40	-	75,75,75,75	0
57	MG	1H	3253	1/1	0.92	0.08	-	42,42,42,42	0
57	MG	1H	3033	1/1	0.96	0.25	-	70,70,70,70	0
57	MG	14	3358	1/1	0.90	0.15	-	86,86,86,86	0
57	MG	31	301	1/1	0.69	0.13	-	63,63,63,63	0
57	MG	1H	3504	1/1	0.83	0.07	-	109,109,109,109	0
57	MG	1H	3520	1/1	0.54	0.10	-	105,105,105,105	0
57	MG	1H	3521	1/1	0.87	0.12	-	82,82,82,82	0
57	MG	13	1665	1/1	0.85	0.69	-	82,82,82,82	0
57	MG	1H	3026	1/1	0.94	0.39	-	55,55,55,55	0
57	MG	1H	3476	1/1	0.74	0.21	-	82,82,82,82	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
57	MG	1H	3487	1/1	0.68	0.11	-	85,85,85,85	0
57	MG	1H	3106	1/1	0.81	0.23	-	87,87,87,87	0
57	MG	14	3343	1/1	0.84	0.06	-	80,80,80,80	0
57	MG	1H	3044	1/1	0.98	0.36	-	67,67,67,67	0
57	MG	14	3255	1/1	0.86	0.13	-	79,79,79,79	0
57	MG	1H	3324	1/1	0.96	0.08	-	70,70,70,70	0
57	MG	1H	3405	1/1	0.80	0.09	-	66,66,66,66	0
57	MG	14	3032	1/1	0.97	0.41	-	64,64,64,64	0
57	MG	1J	203	1/1	0.95	0.26	-	73,73,73,73	0
57	MG	1H	3428	1/1	0.70	0.09	-	89,89,89,89	0
57	MG	1G	1639	1/1	0.90	0.54	-	78,78,78,78	0
57	MG	14	3298	1/1	0.82	0.11	-	86,86,86,86	0
57	MG	1H	3293	1/1	0.93	0.14	-	73,73,73,73	0
57	MG	14	3412	1/1	0.82	0.10	-	97,97,97,97	0
57	MG	1H	3446	1/1	0.93	0.06	-	98,98,98,98	0
57	MG	1H	3111	1/1	0.79	0.61	-	79,79,79,79	0
57	MG	14	3221	1/1	0.82	0.20	-	62,62,62,62	0
57	MG	14	3176	1/1	0.67	0.20	-	82,82,82,82	0
57	MG	14	3367	1/1	0.94	0.08	-	106,106,106,106	0
57	MG	14	3301	1/1	0.98	0.04	-	85,85,85,85	0
57	MG	1H	3442	1/1	0.65	0.09	-	103,103,103,103	0
57	MG	13	1622	1/1	0.86	0.26	-	63,63,63,63	0
57	MG	14	3079	1/1	0.93	0.30	-	48,48,48,48	0
57	MG	14	3069	1/1	0.80	0.46	-	86,86,86,86	0
57	MG	14	3338	1/1	0.93	0.05	-	107,107,107,107	0
57	MG	1H	3511	1/1	0.68	0.16	-	101,101,101,101	0
57	MG	1H	3329	1/1	0.80	0.08	-	85,85,85,85	0
57	MG	14	3265	1/1	0.94	0.07	-	91,91,91,91	0
57	MG	13	1697	1/1	0.91	0.07	-	84,84,84,84	0
57	MG	1H	3224	1/1	0.80	0.33	-	85,85,85,85	0
57	MG	14	3401	1/1	0.86	0.15	-	110,110,110,110	0
57	MG	1H	3394	1/1	0.85	0.11	-	49,49,49,49	0
57	MG	14	3163	1/1	0.51	0.38	-	93,93,93,93	0
57	MG	1G	1616	1/1	0.95	0.13	-	94,94,94,94	0
57	MG	1H	3384	1/1	0.87	0.08	-	67,67,67,67	0
57	MG	1H	3337	1/1	0.94	0.05	-	86,86,86,86	0
57	MG	1G	1658	1/1	0.95	0.06	-	104,104,104,104	0
57	MG	14	3128	1/1	0.74	0.41	-	89,89,89,89	0
57	MG	1H	3063	1/1	0.76	0.27	-	100,100,100,100	0
57	MG	14	3362	1/1	0.94	0.06	-	114,114,114,114	0
57	MG	14	3353	1/1	0.95	0.08	-	83,83,83,83	0
57	MG	1H	3236	1/1	0.83	0.31	-	67,67,67,67	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
57	MG	14	3157	1/1	0.85	0.32	-	92,92,92,92	0
57	MG	1H	3213	1/1	0.87	0.29	-	71,71,71,71	0
57	MG	1H	3362	1/1	0.88	0.13	-	100,100,100,100	0
57	MG	1G	1683	1/1	0.82	0.13	-	121,121,121,121	0
57	MG	1H	3515	1/1	0.88	0.19	-	58,58,58,58	0
57	MG	P8	101	1/1	0.73	0.56	-	71,71,71,71	0
57	MG	1H	3171	1/1	0.73	0.38	-	73,73,73,73	0
57	MG	1H	3488	1/1	0.77	0.28	-	105,105,105,105	0
57	MG	1H	3052	1/1	0.95	0.18	-	59,59,59,59	0
57	MG	1H	3103	1/1	0.90	0.32	-	61,61,61,61	0
57	MG	14	3226	1/1	0.97	0.16	-	51,51,51,51	0
57	MG	1H	3494	1/1	0.92	0.08	-	72,72,72,72	0
57	MG	1H	3354	1/1	0.97	0.17	-	60,60,60,60	0
57	MG	14	3403	1/1	0.87	0.12	-	84,84,84,84	0
57	MG	14	3417	1/1	0.73	0.12	-	108,108,108,108	0
57	MG	1H	3388	1/1	0.66	0.13	-	55,55,55,55	0
57	MG	1H	3247	1/1	0.97	0.14	-	36,36,36,36	0
57	MG	16	209	1/1	0.91	0.47	-	76,76,76,76	0
57	MG	1H	3069	1/1	0.88	0.41	-	69,69,69,69	0
57	MG	1H	3286	1/1	0.96	0.12	-	40,40,40,40	0
57	MG	1J	206	1/1	0.86	0.24	-	94,94,94,94	0
57	MG	1H	3414	1/1	0.76	0.14	-	105,105,105,105	0
57	MG	14	3067	1/1	0.78	0.23	-	78,78,78,78	0
57	MG	1G	1670	1/1	0.81	0.06	-	134,134,134,134	0
57	MG	1H	3341	1/1	0.81	0.12	-	78,78,78,78	0
57	MG	14	3044	1/1	0.96	0.18	-	57,57,57,57	0
57	MG	14	3419	1/1	0.85	0.06	-	110,110,110,110	0
57	MG	14	3359	1/1	0.91	0.08	-	93,93,93,93	0
57	MG	25	201	1/1	0.91	0.05	-	115,115,115,115	0
57	MG	14	3214	1/1	0.83	0.70	-	80,80,80,80	0
57	MG	13	1694	1/1	0.88	0.14	-	82,82,82,82	0
57	MG	1H	3496	1/1	0.67	0.16	-	89,89,89,89	0
57	MG	13	1695	1/1	0.90	0.10	-	106,106,106,106	0
57	MG	14	3434	1/1	0.66	0.12	-	110,110,110,110	0
57	MG	1H	3185	1/1	0.91	0.48	-	64,64,64,64	0
57	MG	1G	1659	1/1	0.87	0.04	-	115,115,115,115	0
57	MG	14	3161	1/1	0.71	0.42	-	78,78,78,78	0
57	MG	1H	3372	1/1	0.94	0.08	-	89,89,89,89	0
57	MG	14	3144	1/1	0.89	0.32	-	102,102,102,102	0
57	MG	1H	3054	1/1	0.95	0.35	-	52,52,52,52	0
57	MG	1H	3229	1/1	0.83	0.50	-	90,90,90,90	0
57	MG	14	3344	1/1	0.66	0.09	-	93,93,93,93	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
57	MG	1H	3030	1/1	0.94	0.10	-	39,39,39,39	0
57	MG	16	205	1/1	0.73	0.18	-	69,69,69,69	0
57	MG	1H	3168	1/1	0.72	0.49	-	80,80,80,80	0
57	MG	13	1640	1/1	0.90	0.28	-	92,92,92,92	0
57	MG	14	3073	1/1	0.74	0.31	-	78,78,78,78	0
57	MG	1H	3407	1/1	0.83	0.09	-	72,72,72,72	0
57	MG	13	1644	1/1	0.94	0.45	-	85,85,85,85	0
57	MG	14	3241	1/1	0.89	0.05	-	78,78,78,78	0
57	MG	14	3071	1/1	0.93	0.19	-	74,74,74,74	0
57	MG	13	1707	1/1	0.92	0.10	-	56,56,56,56	0
57	MG	1H	3308	1/1	0.81	0.14	-	50,50,50,50	0
57	MG	14	3196	1/1	0.85	0.51	-	71,71,71,71	0
57	MG	16	210	1/1	0.93	0.11	-	73,73,73,73	0
57	MG	14	3385	1/1	0.70	0.16	-	67,67,67,67	0
57	MG	14	3399	1/1	0.85	0.09	-	123,123,123,123	0
57	MG	1H	3322	1/1	0.98	0.06	-	58,58,58,58	0
57	MG	14	3381	1/1	0.79	0.31	-	79,79,79,79	0
57	MG	14	3130	1/1	0.85	0.24	-	66,66,66,66	0
57	MG	14	3058	1/1	0.95	0.34	-	84,84,84,84	0
57	MG	1H	3510	1/1	0.94	0.14	-	39,39,39,39	0
57	MG	14	3404	1/1	0.82	0.16	-	97,97,97,97	0
57	MG	14	3038	1/1	0.94	0.21	-	52,52,52,52	0
57	MG	14	3285	1/1	0.81	0.06	-	108,108,108,108	0
57	MG	1H	3314	1/1	0.87	0.08	-	68,68,68,68	0
57	MG	14	3013	1/1	0.98	0.23	-	47,47,47,47	0
57	MG	1H	3351	1/1	0.91	0.09	-	68,68,68,68	0
57	MG	13	1726	1/1	0.87	0.08	-	74,74,74,74	0
57	MG	1G	1692	1/1	0.90	0.12	-	101,101,101,101	0
57	MG	14	3188	1/1	0.91	0.50	-	72,72,72,72	0
57	MG	1G	1691	1/1	0.84	0.05	-	133,133,133,133	0
57	MG	16	208	1/1	0.70	0.39	-	85,85,85,85	0
57	MG	1H	3087	1/1	0.92	0.20	-	71,71,71,71	0
57	MG	1H	3349	1/1	0.98	0.12	-	50,50,50,50	0
57	MG	1H	3435	1/1	0.90	0.06	-	62,62,62,62	0
57	MG	14	3131	1/1	0.81	0.28	-	64,64,64,64	0
57	MG	1H	3316	1/1	0.95	0.07	-	78,78,78,78	0
57	MG	14	3189	1/1	0.95	0.33	-	51,51,51,51	0
57	MG	14	3215	1/1	0.84	1.26	-	86,86,86,86	0
57	MG	1G	1610	1/1	0.84	0.23	-	91,91,91,91	0
57	MG	14	3212	1/1	0.70	0.32	-	75,75,75,75	0
57	MG	1G	1641	1/1	0.85	0.59	-	103,103,103,103	0
57	MG	14	3418	1/1	0.84	0.07	-	90,90,90,90	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
57	MG	1H	3169	1/1	0.97	0.45	-	91,91,91,91	0
57	MG	1H	3399	1/1	0.96	0.06	-	73,73,73,73	0
57	MG	1H	3409	1/1	0.90	0.07	-	85,85,85,85	0
57	MG	1G	1697	1/1	0.81	0.09	-	128,128,128,128	0
57	MG	14	3402	1/1	0.89	0.08	-	78,78,78,78	0
57	MG	1G	1674	1/1	0.83	0.08	-	107,107,107,107	0
57	MG	1H	3367	1/1	0.82	0.08	-	66,66,66,66	0
57	MG	1H	3396	1/1	0.74	0.22	-	59,59,59,59	0
57	MG	1H	3429	1/1	0.90	0.10	-	88,88,88,88	0
57	MG	1G	1643	1/1	0.90	0.54	-	83,83,83,83	0
57	MG	14	3003	1/1	0.83	0.27	-	78,78,78,78	0
57	MG	1J	205	1/1	0.82	0.16	-	73,73,73,73	0
57	MG	14	3340	1/1	0.94	0.09	-	107,107,107,107	0
57	MG	1H	3352	1/1	0.77	0.12	-	57,57,57,57	0
57	MG	14	3331	1/1	0.93	0.20	-	90,90,90,90	0
57	MG	14	3391	1/1	0.83	0.23	-	99,99,99,99	0
57	MG	14	3219	1/1	0.96	0.10	-	57,57,57,57	0
57	MG	13	1619	1/1	0.98	0.21	-	52,52,52,52	0
57	MG	13	1639	1/1	0.93	0.58	-	70,70,70,70	0
57	MG	1H	3237	1/1	0.57	0.46	-	81,81,81,81	0
57	MG	14	3123	1/1	0.94	0.28	-	83,83,83,83	0
57	MG	1H	3153	1/1	0.77	0.44	-	77,77,77,77	0
57	MG	1H	3499	1/1	0.68	0.09	-	112,112,112,112	0
57	MG	14	3066	1/1	0.98	0.57	-	61,61,61,61	0
57	MG	14	3300	1/1	0.95	0.09	-	89,89,89,89	0
57	MG	14	3160	1/1	0.89	0.18	-	65,65,65,65	0
57	MG	1H	3204	1/1	0.66	0.20	-	91,91,91,91	0
57	MG	14	3425	1/1	0.85	0.12	-	91,91,91,91	0
57	MG	1H	3135	1/1	0.71	0.49	-	79,79,79,79	0
57	MG	1H	3440	1/1	0.96	0.09	-	92,92,92,92	0
57	MG	1H	3010	1/1	0.89	0.37	-	39,39,39,39	0
57	MG	1H	3402	1/1	0.96	0.05	-	85,85,85,85	0
57	MG	1H	3243	1/1	0.76	0.17	-	82,82,82,82	0
57	MG	14	3406	1/1	0.72	0.12	-	101,101,101,101	0
57	MG	14	3175	1/1	0.79	0.21	-	88,88,88,88	0
57	MG	1H	3158	1/1	0.92	0.17	-	71,71,71,71	0
57	MG	1H	3209	1/1	0.92	0.60	-	76,76,76,76	0
57	MG	1H	3338	1/1	0.96	0.11	-	66,66,66,66	0
57	MG	1H	3014	1/1	0.96	0.17	-	53,53,53,53	0
57	MG	1H	3472	1/1	0.95	0.04	-	83,83,83,83	0
57	MG	1H	3132	1/1	0.91	0.23	-	65,65,65,65	0
57	MG	1G	1673	1/1	0.34	0.14	-	115,115,115,115	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
57	MG	13	1705	1/1	0.96	0.17	-	97,97,97,97	0
57	MG	1H	3295	1/1	0.94	0.09	-	89,89,89,89	0
57	MG	1H	3089	1/1	0.78	0.20	-	38,38,38,38	0
57	MG	14	3002	1/1	0.97	0.37	-	57,57,57,57	0
57	MG	13	1690	1/1	0.96	0.05	-	70,70,70,70	0
57	MG	1H	3455	1/1	0.87	0.15	-	76,76,76,76	0
57	MG	1G	1648	1/1	0.89	0.16	-	115,115,115,115	0
57	MG	1H	3232	1/1	0.93	0.22	-	48,48,48,48	0
57	MG	1H	3126	1/1	0.88	0.43	-	86,86,86,86	0
57	MG	1H	3326	1/1	0.95	0.10	-	62,62,62,62	0
57	MG	1G	1665	1/1	0.95	0.05	-	91,91,91,91	0
57	MG	14	3259	1/1	0.92	0.10	-	71,71,71,71	0
57	MG	1H	3357	1/1	0.94	0.12	-	52,52,52,52	0
57	MG	1H	3255	1/1	0.98	0.08	-	49,49,49,49	0
57	MG	13	1604	1/1	0.96	0.15	-	62,62,62,62	0
57	MG	14	3143	1/1	0.88	0.17	-	57,57,57,57	0
57	MG	14	3199	1/1	0.97	0.38	-	76,76,76,76	0
57	MG	13	1664	1/1	0.80	0.46	-	78,78,78,78	0
57	MG	1H	3136	1/1	0.84	0.41	-	116,116,116,116	0
57	MG	1H	3420	1/1	0.84	0.12	-	69,69,69,69	0
57	MG	14	3365	1/1	0.93	0.13	-	78,78,78,78	0
57	MG	1G	1609	1/1	0.49	0.87	-	92,92,92,92	0
57	MG	1G	1681	1/1	0.93	0.06	-	96,96,96,96	0
57	MG	14	3364	1/1	0.96	0.07	-	92,92,92,92	0
57	MG	13	1708	1/1	0.90	0.16	-	65,65,65,65	0
57	MG	13	1671	1/1	0.66	0.51	-	79,79,79,79	0
57	MG	1H	3230	1/1	0.60	0.36	-	82,82,82,82	0
57	MG	1H	3043	1/1	0.81	0.40	-	75,75,75,75	0
57	MG	1H	3071	1/1	0.83	0.22	-	79,79,79,79	0
57	MG	1H	3217	1/1	0.75	0.64	-	82,82,82,82	0
57	MG	1H	3219	1/1	0.92	0.20	-	71,71,71,71	0
57	MG	1H	3478	1/1	0.93	0.05	-	101,101,101,101	0
57	MG	14	3431	1/1	0.88	0.25	-	116,116,116,116	0
57	MG	13	1720	1/1	0.91	0.15	-	109,109,109,109	0
57	MG	14	3201	1/1	0.91	0.20	-	88,88,88,88	0
57	MG	1H	3309	1/1	0.78	0.23	-	54,54,54,54	0
57	MG	14	3185	1/1	0.73	0.41	-	86,86,86,86	0
57	MG	14	3019	1/1	0.98	0.35	-	57,57,57,57	0
57	MG	14	3096	1/1	0.96	0.20	-	65,65,65,65	0
57	MG	14	3377	1/1	0.47	0.10	-	131,131,131,131	0
57	MG	14	3329	1/1	0.95	0.06	-	105,105,105,105	0
57	MG	1H	3408	1/1	0.82	0.12	-	67,67,67,67	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
57	MG	14	3154	1/1	0.58	0.40	-	95,95,95,95	0
57	MG	1H	3403	1/1	0.93	0.07	-	99,99,99,99	0
57	MG	14	3162	1/1	0.94	0.40	-	74,74,74,74	0
57	MG	14	3351	1/1	0.95	0.11	-	78,78,78,78	0
57	MG	88	203	1/1	0.83	0.33	-	79,79,79,79	0
57	MG	1H	3441	1/1	0.94	0.06	-	105,105,105,105	0
57	MG	14	3082	1/1	0.96	0.49	-	79,79,79,79	0
57	MG	14	3366	1/1	0.73	0.23	-	82,82,82,82	0
57	MG	13	1737	1/1	0.73	0.11	-	99,99,99,99	0
57	MG	14	3370	1/1	0.95	0.06	-	97,97,97,97	0
57	MG	1H	3086	1/1	0.89	0.18	-	53,53,53,53	0
57	MG	14	3243	1/1	0.83	0.15	-	58,58,58,58	0
57	MG	1H	3522	1/1	0.75	0.14	-	110,110,110,110	0
57	MG	13	1681	1/1	0.94	0.14	-	59,59,59,59	0
57	MG	1H	3119	1/1	0.82	0.39	-	83,83,83,83	0
57	MG	13	1677	1/1	0.91	0.47	-	77,77,77,77	0
57	MG	1H	3486	1/1	0.81	0.07	-	95,95,95,95	0
57	MG	1H	3177	1/1	0.70	0.90	-	82,82,82,82	0
57	MG	1H	3524	1/1	0.92	0.18	-	81,81,81,81	0
57	MG	21	303	1/1	0.97	0.09	-	46,46,46,46	0
57	MG	1H	3447	1/1	0.91	0.24	-	70,70,70,70	0
57	MG	1H	3439	1/1	0.97	0.07	-	67,67,67,67	0
57	MG	14	3200	1/1	0.87	0.15	-	89,89,89,89	0
57	MG	1G	1627	1/1	0.98	0.41	-	87,87,87,87	0
57	MG	1G	1682	1/1	0.72	0.05	-	123,123,123,123	0
57	MG	14	3174	1/1	0.95	0.08	-	89,89,89,89	0
57	MG	14	3055	1/1	0.99	0.30	-	60,60,60,60	0
57	MG	1H	3395	1/1	0.75	0.14	-	68,68,68,68	0
57	MG	13	1605	1/1	0.97	0.20	-	71,71,71,71	0
57	MG	1H	3084	1/1	0.84	0.20	-	62,62,62,62	0
57	MG	14	3104	1/1	0.94	0.18	-	78,78,78,78	0
57	MG	14	3341	1/1	0.98	0.12	-	66,66,66,66	0
57	MG	1H	3483	1/1	0.84	0.17	-	91,91,91,91	0
57	MG	14	3190	1/1	0.92	0.37	-	59,59,59,59	0
57	MG	1G	1680	1/1	0.79	0.07	-	123,123,123,123	0
57	MG	29	301	1/1	0.98	0.35	-	58,58,58,58	0
57	MG	14	3348	1/1	0.78	0.11	-	96,96,96,96	0
57	MG	1H	3097	1/1	0.98	0.06	-	65,65,65,65	0
57	MG	1H	3149	1/1	0.89	0.24	-	55,55,55,55	0
57	MG	88	202	1/1	0.90	0.32	-	66,66,66,66	0
57	MG	13	1611	1/1	0.95	0.24	-	70,70,70,70	0
57	MG	1H	3473	1/1	0.94	0.14	-	95,95,95,95	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
57	MG	1H	3347	1/1	0.83	0.10	-	67,67,67,67	0
57	MG	14	3306	1/1	0.92	0.08	-	58,58,58,58	0
57	MG	1H	3346	1/1	0.85	0.10	-	92,92,92,92	0
57	MG	1H	3195	1/1	0.72	0.31	-	55,55,55,55	0
57	MG	1H	3150	1/1	0.61	0.70	-	98,98,98,98	0
57	MG	1H	3242	1/1	0.85	0.47	-	90,90,90,90	0
57	MG	14	3326	1/1	0.78	0.09	-	77,77,77,77	0
57	MG	1H	3490	1/1	0.90	0.07	-	89,89,89,89	0
57	MG	14	3036	1/1	0.95	0.27	-	85,85,85,85	0
57	MG	I8	102	1/1	0.95	0.05	-	62,62,62,62	0
57	MG	14	3263	1/1	0.90	0.08	-	71,71,71,71	0
57	MG	45	202	1/1	0.91	0.44	-	64,64,64,64	0
57	MG	14	3314	1/1	0.96	0.16	-	69,69,69,69	0
57	MG	1H	3430	1/1	0.93	0.08	-	73,73,73,73	0
57	MG	13	1649	1/1	0.82	0.42	-	75,75,75,75	0
57	MG	14	3281	1/1	0.95	0.16	-	69,69,69,69	0
57	MG	14	3057	1/1	0.90	0.25	-	49,49,49,49	0
57	MG	14	3095	1/1	0.91	0.18	-	62,62,62,62	0
57	MG	14	3112	1/1	0.93	0.20	-	83,83,83,83	0
57	MG	1H	3283	1/1	0.94	0.15	-	71,71,71,71	0
57	MG	1H	3091	1/1	0.99	0.15	-	41,41,41,41	0
57	MG	1H	3454	1/1	0.54	0.07	-	111,111,111,111	0
57	MG	14	3413	1/1	0.88	0.15	-	107,107,107,107	0
57	MG	14	3313	1/1	0.91	0.05	-	105,105,105,105	0
57	MG	14	3152	1/1	0.66	0.17	-	78,78,78,78	0
57	MG	16	211	1/1	0.97	0.11	-	73,73,73,73	0
57	MG	14	3120	1/1	0.90	0.18	-	78,78,78,78	0
57	MG	1H	3358	1/1	0.94	0.18	-	45,45,45,45	0
57	MG	14	3294	1/1	0.98	0.05	-	75,75,75,75	0
57	MG	14	3063	1/1	0.84	0.24	-	67,67,67,67	0
57	MG	13	1712	1/1	0.88	0.07	-	89,89,89,89	0
57	MG	1H	3327	1/1	0.98	0.08	-	50,50,50,50	0
57	MG	1H	3506	1/1	0.84	0.08	-	106,106,106,106	0
57	MG	1H	3268	1/1	0.90	0.17	-	59,59,59,59	0
57	MG	1H	3459	1/1	0.95	0.13	-	75,75,75,75	0
57	MG	I8	101	1/1	0.86	0.09	-	85,85,85,85	0
57	MG	1H	3057	1/1	0.88	0.38	-	75,75,75,75	0
57	MG	1H	3519	1/1	0.92	0.18	-	116,116,116,116	0
57	MG	13	1630	1/1	0.99	0.34	-	96,96,96,96	0
57	MG	1H	3339	1/1	0.61	0.12	-	106,106,106,106	0
57	MG	1H	3141	1/1	0.59	0.29	-	83,83,83,83	0
57	MG	14	3276	1/1	0.79	0.10	-	120,120,120,120	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
57	MG	1H	3460	1/1	0.89	0.06	-	96,96,96,96	0
57	MG	1G	1650	1/1	0.93	0.16	-	101,101,101,101	0
57	MG	1H	3173	1/1	0.94	0.22	-	59,59,59,59	0
57	MG	14	3426	1/1	0.65	0.16	-	104,104,104,104	0
57	MG	1G	1676	1/1	0.89	0.09	-	93,93,93,93	0
57	MG	1H	3260	1/1	0.95	0.19	-	42,42,42,42	0
57	MG	1J	208	1/1	0.65	0.10	-	103,103,103,103	0
57	MG	1H	3383	1/1	0.86	0.10	-	68,68,68,68	0
57	MG	13	1620	1/1	0.88	0.52	-	86,86,86,86	0
57	MG	1G	1611	1/1	0.87	0.65	-	76,76,76,76	0
57	MG	1H	3432	1/1	0.92	0.11	-	93,93,93,93	0
57	MG	1H	3390	1/1	0.92	0.20	-	64,64,64,64	0
57	MG	1H	3353	1/1	0.97	0.14	-	48,48,48,48	0
57	MG	1H	3201	1/1	0.82	0.74	-	104,104,104,104	0
57	MG	14	3184	1/1	0.83	0.26	-	78,78,78,78	0
57	MG	1H	3249	1/1	0.96	0.13	-	63,63,63,63	0
57	MG	14	3303	1/1	0.92	0.07	-	74,74,74,74	0
57	MG	1H	3088	1/1	0.90	0.42	-	80,80,80,80	0
57	MG	1H	3070	1/1	0.96	0.34	-	75,75,75,75	0
57	MG	1H	3320	1/1	0.86	0.08	-	58,58,58,58	0
57	MG	14	3356	1/1	0.98	0.06	-	75,75,75,75	0
57	MG	14	3336	1/1	0.87	0.09	-	94,94,94,94	0
57	MG	1G	1664	1/1	0.89	0.05	-	80,80,80,80	0
57	MG	1H	3112	1/1	0.96	0.26	-	55,55,55,55	0
57	MG	1H	3377	1/1	0.95	0.09	-	76,76,76,76	0
57	MG	14	3432	1/1	0.76	0.13	-	116,116,116,116	0
57	MG	14	3232	1/1	0.94	0.14	-	66,66,66,66	0
57	MG	13	1674	1/1	0.74	0.36	-	92,92,92,92	0
57	MG	1H	3425	1/1	0.92	0.07	-	64,64,64,64	0
57	MG	1H	3288	1/1	0.94	0.08	-	54,54,54,54	0
57	MG	14	3186	1/1	0.90	0.16	-	108,108,108,108	0
57	MG	13	1610	1/1	0.87	0.38	-	82,82,82,82	0
57	MG	1G	1699	1/1	0.75	0.07	-	133,133,133,133	0
57	MG	1H	3240	1/1	0.86	0.38	-	73,73,73,73	0
57	MG	1H	3198	1/1	0.79	0.23	-	79,79,79,79	0
57	MG	1H	3350	1/1	0.80	0.11	-	74,74,74,74	0
57	MG	13	1688	1/1	0.95	0.10	-	109,109,109,109	0
57	MG	14	3202	1/1	0.81	0.49	-	84,84,84,84	0
57	MG	1H	3517	1/1	0.83	0.07	-	91,91,91,91	0
57	MG	1G	1701	1/1	0.92	0.03	-	111,111,111,111	0
57	MG	1G	1660	1/1	0.92	0.14	-	74,74,74,74	0
57	MG	14	3132	1/1	0.61	0.44	-	82,82,82,82	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
57	MG	14	3318	1/1	0.85	0.12	-	89,89,89,89	0
57	MG	1H	3099	1/1	0.94	0.44	-	56,56,56,56	0
57	MG	13	1723	1/1	0.66	0.07	-	128,128,128,128	0
57	MG	14	3149	1/1	0.92	0.28	-	72,72,72,72	0
57	MG	1G	1640	1/1	0.92	0.39	-	108,108,108,108	0
57	MG	1H	3190	1/1	0.91	0.38	-	91,91,91,91	0
57	MG	1H	3343	1/1	0.93	0.07	-	78,78,78,78	0
57	MG	1H	3109	1/1	0.90	0.31	-	59,59,59,59	0
57	MG	1H	3073	1/1	0.92	0.21	-	66,66,66,66	0
57	MG	1H	3282	1/1	0.95	0.04	-	71,71,71,71	0
57	MG	1H	3025	1/1	0.96	0.35	-	75,75,75,75	0
57	MG	31	302	1/1	0.95	0.16	-	77,77,77,77	0
57	MG	14	3398	1/1	0.76	0.14	-	76,76,76,76	0
57	MG	2K	102	1/1	0.95	0.17	-	78,78,78,78	0
57	MG	1H	3131	1/1	0.94	0.50	-	83,83,83,83	0
57	MG	1H	3495	1/1	0.96	0.05	-	97,97,97,97	0
57	MG	13	1643	1/1	0.59	0.23	-	101,101,101,101	0
57	MG	1H	3162	1/1	0.83	0.29	-	60,60,60,60	0
57	MG	1G	1601	1/1	0.97	0.20	-	77,77,77,77	0
57	MG	14	3304	1/1	0.94	0.10	-	74,74,74,74	0
57	MG	1H	3127	1/1	0.90	0.12	-	91,91,91,91	0
57	MG	1G	1656	1/1	0.87	0.08	-	100,100,100,100	0
57	MG	1H	3176	1/1	0.83	0.14	-	83,83,83,83	0
57	MG	13	1724	1/1	0.84	0.11	-	117,117,117,117	0
57	MG	13	1662	1/1	0.69	0.50	-	89,89,89,89	0
57	MG	1H	3147	1/1	0.84	0.39	-	84,84,84,84	0
57	MG	14	3350	1/1	0.39	0.16	-	101,101,101,101	0
57	MG	1H	3207	1/1	0.96	0.24	-	92,92,92,92	0
57	MG	14	3420	1/1	0.90	0.07	-	107,107,107,107	0
57	MG	1G	1618	1/1	0.77	0.69	-	78,78,78,78	0
57	MG	13	1709	1/1	0.54	0.26	-	99,99,99,99	0
57	MG	14	3141	1/1	0.92	0.28	-	95,95,95,95	0
57	MG	14	3369	1/1	0.91	0.10	-	91,91,91,91	0
57	MG	14	3361	1/1	0.92	0.05	-	79,79,79,79	0
57	MG	1H	3419	1/1	0.70	0.15	-	86,86,86,86	0
57	MG	13	1653	1/1	0.94	0.33	-	73,73,73,73	0
57	MG	14	3166	1/1	0.65	0.46	-	79,79,79,79	0
57	MG	13	1739	1/1	0.59	0.06	-	121,121,121,121	0
57	MG	13	1699	1/1	0.96	0.09	-	83,83,83,83	0
57	MG	4L	101	1/1	0.74	0.32	-	131,131,131,131	0
57	MG	1H	3452	1/1	0.88	0.10	-	72,72,72,72	0
57	MG	7A	101	1/1	0.73	0.26	-	114,114,114,114	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
57	MG	1H	3251	1/1	0.91	0.16	-	48,48,48,48	0
57	MG	14	3405	1/1	0.90	0.07	-	108,108,108,108	0
57	MG	1G	1675	1/1	0.76	0.08	-	103,103,103,103	0
57	MG	1H	3458	1/1	0.73	0.10	-	82,82,82,82	0
57	MG	14	3222	1/1	0.98	0.20	-	59,59,59,59	0
57	MG	14	3060	1/1	0.77	0.30	-	98,98,98,98	0
57	MG	1G	1677	1/1	0.93	0.17	-	92,92,92,92	0
57	MG	13	1731	1/1	0.88	0.05	-	112,112,112,112	0
57	MG	14	3429	1/1	0.67	0.30	-	95,95,95,95	0

6.5 Other polymers (i)

There are no such residues in this entry.