



wwPDB X-ray Structure Validation Summary Report ⓘ

Jun 3, 2020 – 11:12 am BST

PDB ID : 5IB8
Title : Structure of T. thermophilus 70S ribosome complex with mRNA, tRNA^{fMet} and near-cognate tRNA^{Lys} with U-G mismatch in the A-site
Authors : Rozov, A.; Demeshkina, N.; Yusupov, M.; Yusupova, G.
Deposited on : 2016-02-22
Resolution : 3.13 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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

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

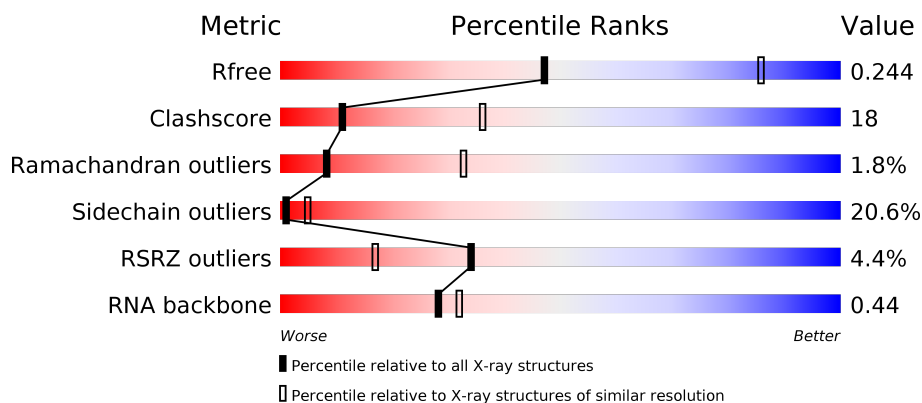
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.13 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1626 (3.18-3.10)
Clashscore	141614	1735 (3.18-3.10)
Ramachandran outliers	138981	1677 (3.18-3.10)
Sidechain outliers	138945	1677 (3.18-3.10)
RSRZ outliers	127900	1588 (3.18-3.10)
RNA backbone	3102	1000 (3.46-2.82)

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

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

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

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Mol	Chain	Length	Quality of chain
15	6I	89	
16	7A	88	
16	7I	88	
17	8A	105	
17	8I	105	
18	9A	88	
18	9I	88	
19	AA	93	
19	AI	93	
20	BA	106	
20	BI	106	
21	1B	27	
21	1F	27	
22	1K	76	
23	2K	77	
23	2L	77	
24	3K	76	
24	3L	76	
25	4K	30	
25	4L	30	
26	14	2917	
26	1H	2917	
27	16	122	
27	1J	122	
28	7I	229	

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



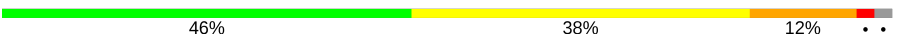
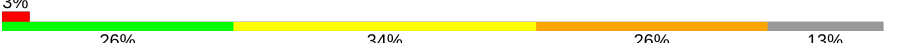
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Mol	Chain	Length	Quality of chain
41	B8	146	
42	85	118	
42	C8	118	
43	95	101	
43	D8	101	
44	A5	113	
44	E8	113	
45	B5	96	
45	F8	96	
46	C5	110	
46	G8	110	
47	D5	206	
47	H8	206	
48	E5	85	
48	I8	85	
49	F5	98	
49	J8	98	
50	G5	72	
50	K8	72	
51	H5	60	
51	L8	60	
52	M8	71	
53	J5	60	
53	N8	60	
54	L5	49	

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

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
57	MG	13	1610	-	-	-	X
57	MG	13	1621	-	-	-	X
57	MG	13	1638	-	-	-	X
57	MG	13	1648	-	-	-	X
57	MG	13	1655	-	-	-	X
57	MG	14	3074	-	-	-	X
57	MG	14	3079	-	-	-	X
57	MG	14	3103	-	-	-	X
57	MG	14	3115	-	-	-	X
57	MG	14	3133	-	-	-	X
57	MG	14	3134	-	-	-	X
57	MG	14	3138	-	-	-	X
57	MG	14	3160	-	-	-	X
57	MG	14	3163	-	-	-	X
57	MG	14	3165	-	-	-	X
57	MG	14	3175	-	-	-	X
57	MG	14	3177	-	-	-	X
57	MG	14	3183	-	-	-	X
57	MG	14	3187	-	-	-	X
57	MG	14	3194	-	-	-	X
57	MG	14	3199	-	-	-	X
57	MG	1G	1609	-	-	-	X
57	MG	1G	1611	-	-	-	X
57	MG	1G	1620	-	-	-	X
57	MG	1H	3077	-	-	-	X
57	MG	1H	3087	-	-	-	X
57	MG	1H	3089	-	-	-	X
57	MG	1H	3142	-	-	-	X
57	MG	1H	3157	-	-	-	X
57	MG	1H	3162	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
57	MG	1H	3167	-	-	-	X
57	MG	1H	3176	-	-	-	X
57	MG	1H	3215	-	-	-	X
57	MG	1H	3237	-	-	-	X
57	MG	1H	3540	-	-	-	X
57	MG	1H	3548	-	-	-	X
57	MG	E5	101	-	-	-	X
57	MG	P8	101	-	-	-	X
58	SF4	32	302	-	-	X	-

2 Entry composition

There are 61 unique types of molecules in this entry. The entry contains 296999 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	1500	Total	C	N	O	P	0	0	0
			32246	14352	5978	10416	1500			
1	1G	1509	Total	C	N	O	P	0	0	0
			32437	14437	6010	10481	1509			

There are 2 discrepancies between the modelled and reference sequences:

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
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			

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

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

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

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

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

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
20	BA	99	Total	C	N	O	S	0	0	0
			762	470	162	128	2			

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
21	1F	23	Total	C	N	O	0	0	0
			199	122	48	29			
21	1B	22	Total	C	N	O	0	0	0
			188	116	44	28			

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

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 tRNA^{fMet}.

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
24	3K	70	Total	C	N	O	P	0	0	0
			1483	664	260	490	69			
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	20	Total	C	N	O	P	0	0	0
			442	198	94	130	20			
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	2831	Total	C	N	O	P	0	0	0
			60991	27142	11416	19602	2831			
26	14	2825	Total	C	N	O	P	0	0	0
			60857	27083	11390	19559	2825			

There are 14 discrepancies between the modelled and reference sequences:

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
28	71	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			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
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			
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			

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
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 L34.

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
56	1L	66	Total	C	N	O	P	0	0	0
			1402	627	244	465	66			

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

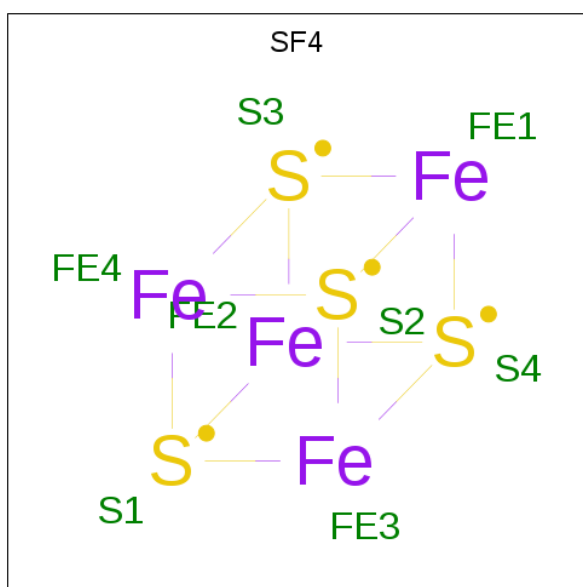
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
57	45	1	Total 1	Mg 1	0	0
57	19	1	Total 1	Mg 1	0	0
57	P8	1	Total 1	Mg 1	0	0
57	32	1	Total 1	Mg 1	0	0
57	2I	1	Total 1	Mg 1	0	0
57	13	141	Total 141	Mg 141	0	0
57	1J	10	Total 10	Mg 10	0	0
57	35	2	Total 2	Mg 2	0	0
57	4L	1	Total 1	Mg 1	0	0
57	16	12	Total 12	Mg 12	0	0
57	42	2	Total 2	Mg 2	0	0
57	B5	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	1	Total 1	Mg 1	0	0
57	Q8	1	Total 1	Mg 1	0	0
57	3I	1	Total 1	Mg 1	0	0
57	I8	2	Total 2	Mg 2	0	0
57	52	1	Total 1	Mg 1	0	0
57	29	1	Total 1	Mg 1	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
57	7A	1	Total 1	Mg 1	0	0
57	2K	3	Total 3	Mg 3	0	0
57	39	1	Total 1	Mg 1	0	0
57	1G	125	Total 125	Mg 125	0	0
57	1H	552	Total 552	Mg 552	0	0
57	E5	2	Total 2	Mg 2	0	0
57	88	3	Total 3	Mg 3	0	0
57	14	460	Total 460	Mg 460	0	0
57	F8	1	Total 1	Mg 1	0	0
57	41	1	Total 1	Mg 1	0	0
57	2L	2	Total 2	Mg 2	0	0

- Molecule 58 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe₄S₄).

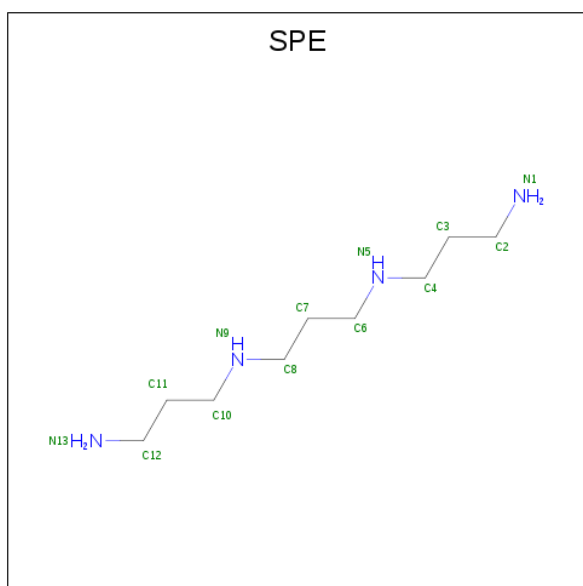


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
58	3E	1	Total	Fe	S	0	0
			8	4	4		
58	32	1	Total	Fe	S	0	0
			8	4	4		

- Molecule 59 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
59	C5	1	Total	Zn	0	0
			1	1		
59	5A	1	Total	Zn	0	0
			1	1		
59	G8	1	Total	Zn	0	0
			1	1		
59	5I	1	Total	Zn	0	0
			1	1		

- Molecule 60 is THERMINE (three-letter code: SPE) (formula: C₉H₂₄N₄).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
60	1G	1	Total	C	N	0	0
			13	9	4		
60	14	1	Total	C	N	0	0
			13	9	4		

- Molecule 61 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
61	13	354	Total 354	O 354	0	0
61	3E	2	Total 2	O 2	0	0
61	4E	3	Total 3	O 3	0	0
61	8E	2	Total 2	O 2	0	0
61	1I	2	Total 2	O 2	0	0
61	3I	2	Total 2	O 2	0	0
61	5I	1	Total 1	O 1	0	0
61	7I	2	Total 2	O 2	0	0
61	BI	3	Total 3	O 3	0	0
61	1K	1	Total 1	O 1	0	0
61	2K	8	Total 8	O 8	0	0
61	3K	1	Total 1	O 1	0	0
61	4K	5	Total 5	O 5	0	0
61	1H	1720	Total 1720	O 1720	0	0
61	16	12	Total 12	O 12	0	0
61	11	10	Total 10	O 10	0	0
61	21	6	Total 6	O 6	0	0
61	31	6	Total 6	O 6	0	0
61	58	2	Total 2	O 2	0	0
61	68	2	Total 2	O 2	0	0
61	78	13	Total 13	O 13	0	0
61	98	1	Total 1	O 1	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
61	B8	1	Total 1	O 1	0	0
61	C8	4	Total 4	O 4	0	0
61	E8	1	Total 1	O 1	0	0
61	F8	3	Total 3	O 3	0	0
61	G8	3	Total 3	O 3	0	0
61	I8	6	Total 6	O 6	0	0
61	J8	5	Total 5	O 5	0	0
61	L8	4	Total 4	O 4	0	0
61	N8	1	Total 1	O 1	0	0
61	Q8	5	Total 5	O 5	0	0
61	1G	364	Total 364	O 364	0	0
61	32	4	Total 4	O 4	0	0
61	42	1	Total 1	O 1	0	0
61	52	4	Total 4	O 4	0	0
61	1A	2	Total 2	O 2	0	0
61	2A	1	Total 1	O 1	0	0
61	4A	2	Total 2	O 2	0	0
61	6A	3	Total 3	O 3	0	0
61	7A	4	Total 4	O 4	0	0
61	9A	2	Total 2	O 2	0	0
61	BA	3	Total 3	O 3	0	0

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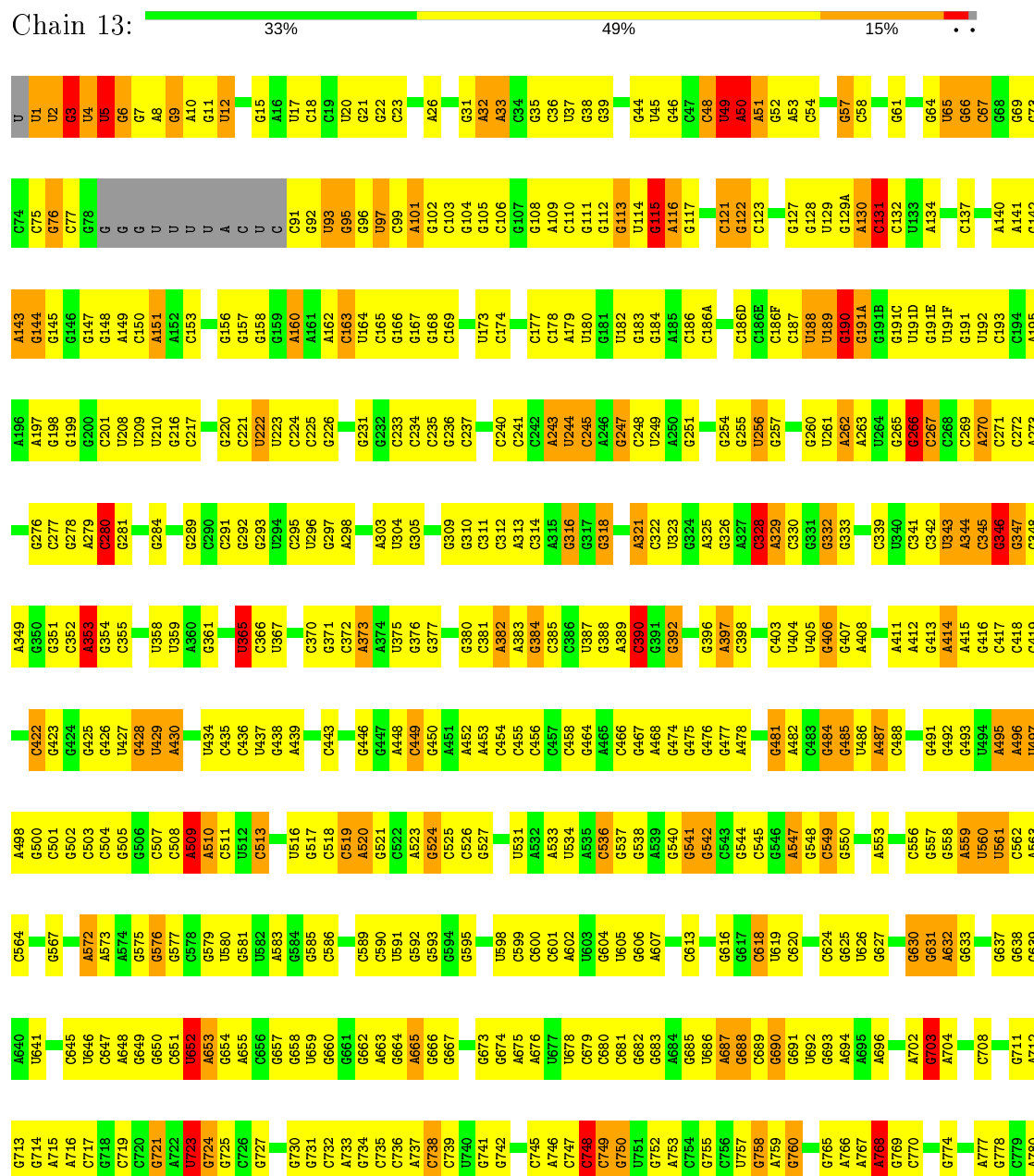
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
61	2L	8	Total 8	O 8	0	0
61	4L	3	Total 3	O 3	0	0
61	14	1303	Total 1303	O 1303	0	0
61	1J	27	Total 27	O 27	0	0
61	19	14	Total 14	O 14	0	0
61	29	6	Total 6	O 6	0	0
61	39	8	Total 8	O 8	0	0
61	15	3	Total 3	O 3	0	0
61	25	8	Total 8	O 8	0	0
61	35	8	Total 8	O 8	0	0
61	55	1	Total 1	O 1	0	0
61	75	1	Total 1	O 1	0	0
61	85	1	Total 1	O 1	0	0
61	B5	1	Total 1	O 1	0	0
61	C5	3	Total 3	O 3	0	0
61	F5	1	Total 1	O 1	0	0
61	H5	1	Total 1	O 1	0	0
61	L5	1	Total 1	O 1	0	0
61	M5	8	Total 8	O 8	0	0

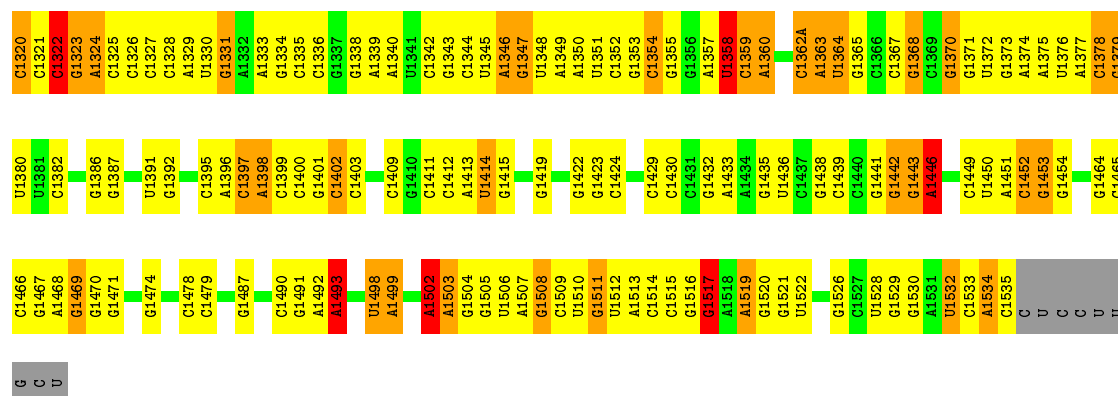
3 Residue-property plots

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

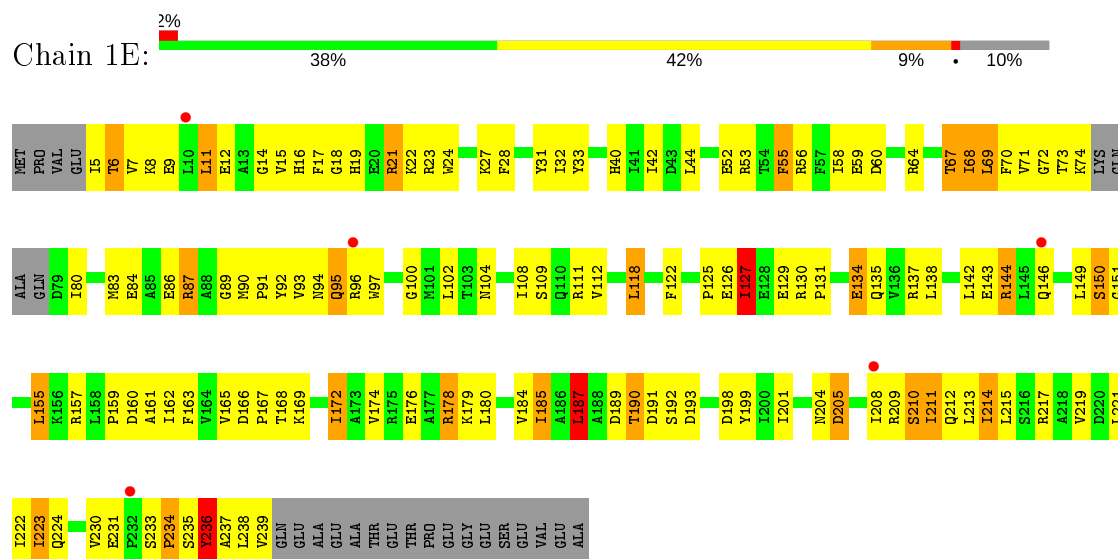
- Molecule 1: 16S ribosomal RNA



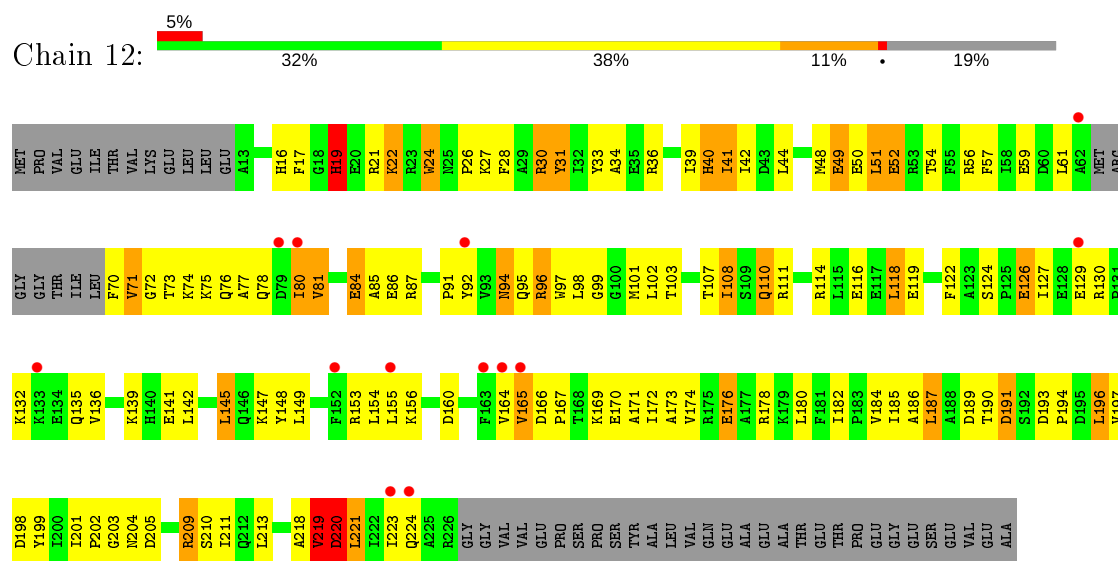
G1255	A1191	A1055	C995	A768	G688	G610	A547	G477	G392	G331
A1256	C1195	U1056	A996	G769	C689	A611	G548	A481	A393	G232
U1257	G1196	G1057	U997	G770	C690	A614	U551	A482	A397	C233
G1258	G1133	G1058	G998	G771	G691	A614	U552	C483	C398	C234
C1259	G1134	C1059	G998A	G776	U692	G616	A553	C484	C398	C235
G1260	U1135	U999	G999	A777	G693	G617	C554	G485	A406	A243
A1261	U1136	U1062	A1000	A778	A694	G618	C555	U486	G407	U244
C1262	G1137	C1063	G1001	G779	A695	G619	C556	A487	A408	U245
G1263	G1138	G1064	G1002	G780	G696	U619	C557	G488	G409	C246
C1264	G1139	U1065	G1003	A780	G697	A621	G558	G491	A410	A247
G1265	C1140	G1066	G1004	G784	G698	A622	U559	G492	G410	G247
A1266	C1141	G1068	U1005	C784	A702	G623	U560	A493	A411	
G1267	G1142	G1069	U1006	A787	A706	G624	U561	A494	A412	A250
A1268	G1143	C1071	C1007	A788	G709	U625	A562	A495	C335	G251
A1269	C1072	G1072	C1008	G791	G710	G626	A563	A496	C336	U252
	U1078	U1078	G1009	U792	G711	G627	U564	A497	C337	
G1272	G1079	G1079	G1010	A793	G712	G628	U565	A498	C341	U255
C1273	C1147	A1080	G1011	U794	G713	G629	U566	G500	U420	U256
G1274	U1148	G1081	G1012	A795	G714	G630	U567	C501	U421	G257
A1275	C1149	G1082	G1013	U801	G717	G631	U568	C502	G422	U261
G1276	U1150	U1083	A1014	A802	G718	A632	U571	C503	G423	A262
C1277	A1151	U1084	A1015	G803	G719	G633	A573	C504	G424	A263
U1278	A1152	G1084	G1016	U804	G720	G634	A574	G505	G425	
A1279	C1153	U1085	G1017	C805	G721	G635	A575	A509	G426	G266
G1280	G1154	G1086	U1018	U806	U722	A640	A576	A510	U427	C267
C1281	C1155	G1088	U1019	C811	U723	A641	G577	C511	U428	
U1282	G1156		U1020	G812	G724	A642	G578	C512	A430	C271
C1283	A1157	G1094	G1021	A816	G725	A643	U580	C513	G433	C272
G1284	C1158	U1095	G1022	C817	G726	U646	U581	C514	U434	A273
C1285	U1159	C1096	G1023	A818	G727	C647	U582	U516	C435	
G1286	G1160	U1097	U1024	G819	G728	G648	U583	G517	C436	G278
A1287	C1161	C1098	G1025	A820	A729	C649	U584	C518	C437	A279
U1288	G1162	U1099	U1026	U821	G730	U651	A582	C519	U438	U358
	C1163	C1100	G1027	C822	G731	U652	G584	A520	G439	U359
G1291	G1164	A1101	C1028A	G825	G735	A653	G585	A523	A440	C360
C1292	C1165	U1102	G1028B	C826	C736	G660	G586	G524	C442	G281
G1293	U1166	C1103	G1029	U827	A737	G661	G587	C525	C443	G286
C1294	A1167	G1104	C1030	A828	C738	G662	G588	C526	C444	
U1295	C1169	A1105	G1031	G829	C739	A663	U591	G527	G445	G289
G1296	A1170	G1106	A1032	U833	U740	G664	G592	C528	G446	G293
C1297	G1171	C1107	G1032A	C834	G741	A665	G593	G529	G447	U296
U1298	C1172	G1108	U1032B	U835	G742	G666	G594	G530	G448	C297
A1299	G1173	C1109	G1033	G836	G743	G667	G595	U531	C449	A298
G1300	U1174	A1110	G1034	U837	U744	G668	U596	A532	G450	G299
U1301	C1175	G1111	C1037	G838	C745	U672	G597	U533	A451	A300
C1302	A1176	C1112	U1037	U841	G746	G673	U598	A534	A452	G301
U1303	G1177	C1113	U1040	C842	G749	A674	G599	A535	C456	G302
G1304	C1178	G1114	A1041	U843	C749	G675	C600	A536	C457	C308
C1305	A1179	C1115	G1042	G844	G750	A676	G601	C537	C458	G309
U1306	U1180	G1116	C1043	U845	U751	U677	A602	G538	G464	
A1307	C1181	G1117	G1044	G846	C754	U678	U603	A539	A465	C312
	G1182	U1121	C1045	G847	G755	C679	U604	G540	G466	A313
G1311	A1183	G1122	U1046	G848	G756	U679	U605	G541	G467	C314
C1312	C1184	A1123	G1047	G849	A759	G683	U606	G542	A468	A315
U1313	G1185	U1124	G1048	G850	G765	A684	A607	C543	G474	G316
G1314	C1186	U1125	U1049	G851	U766	A685	A608	G544	G475	G317
A1315	G1187	U1126	G1050	G852	A767	A686	A609	G545	G476	G318
C1316	U1188	C1127	U1052	G853	A768	A687		G546	G477	
G1317	A1189	G1128	C1053	G854	A769	A688				
A1318	C1190	C1054	C1054	G855	A770	A689				
G1319				G856	A771	A690				



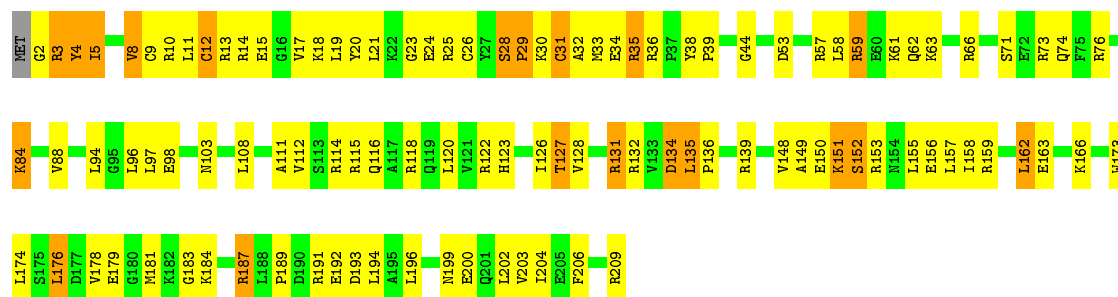
• Molecule 2: 30S ribosomal protein S2



• Molecule 2: 30S ribosomal protein S2

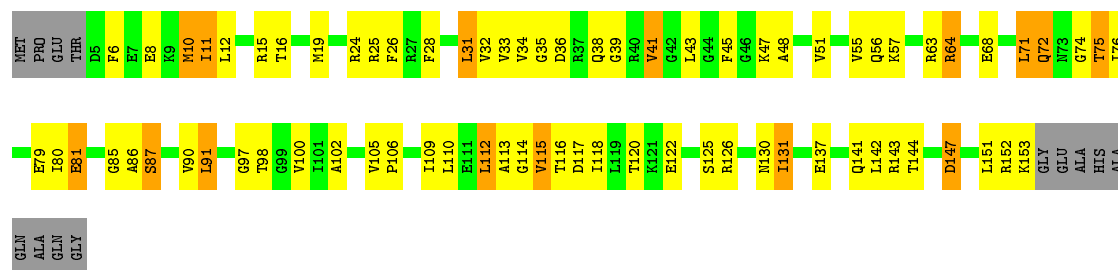


• Molecule 3: 30S ribosomal protein S3



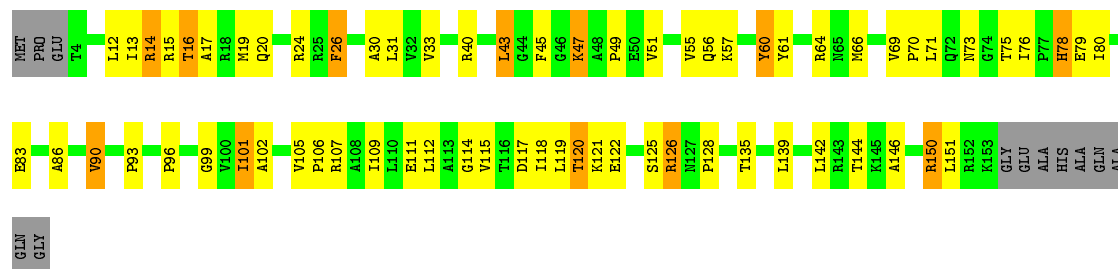
• Molecule 5: 30S ribosomal protein S5

Chain 4E: 46% 37% 9% 8%



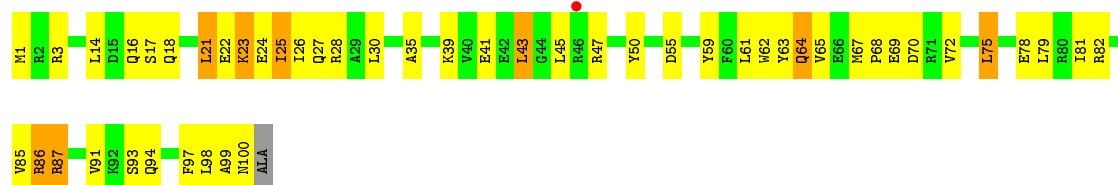
• Molecule 5: 30S ribosomal protein S5

Chain 42: 51% 34% 7% 7%



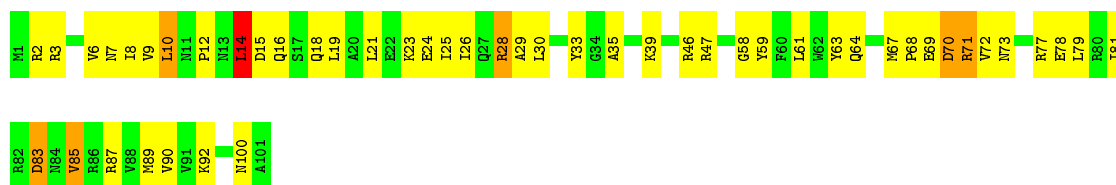
• Molecule 6: 30S ribosomal protein S6

Chain 5E: 50% 41% 8%

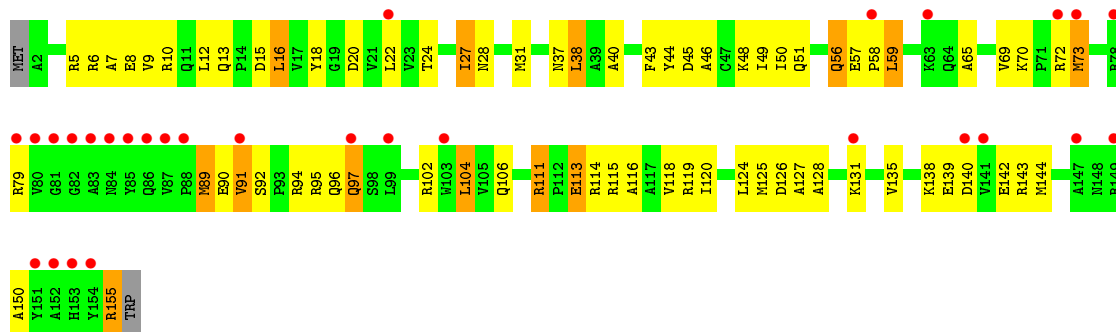


• Molecule 6: 30S ribosomal protein S6

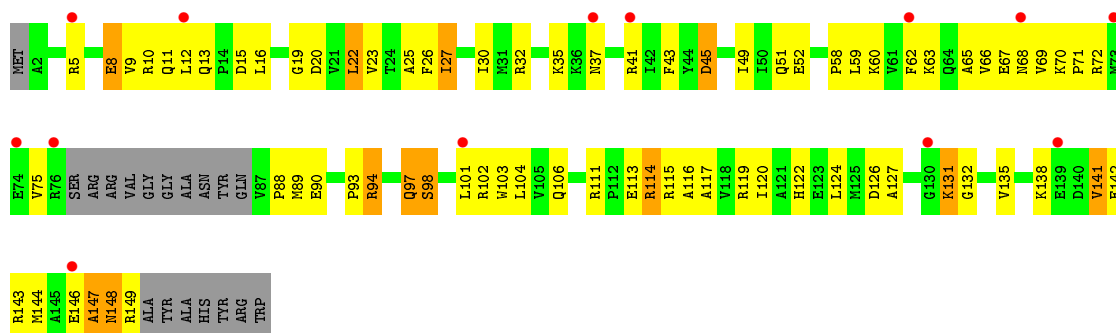
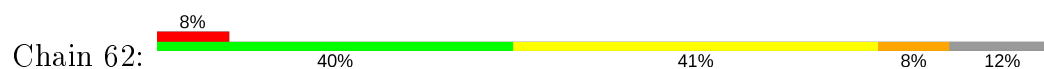
Chain 52: 51% 42% 6%



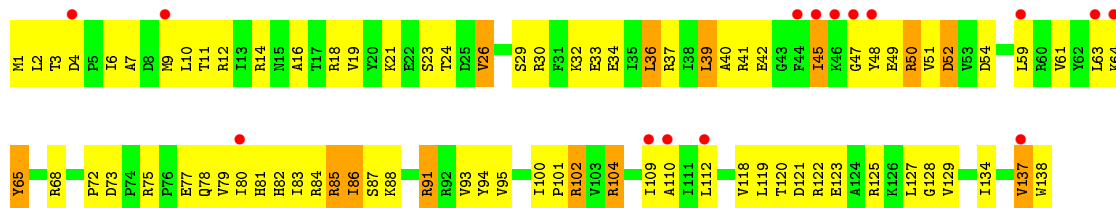
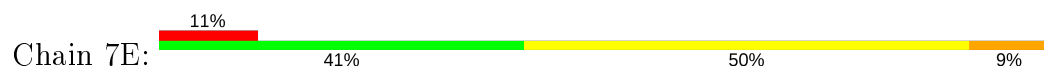
- Molecule 7: 30S ribosomal protein S7



- Molecule 7: 30S ribosomal protein S7



- Molecule 8: 30S ribosomal protein S8



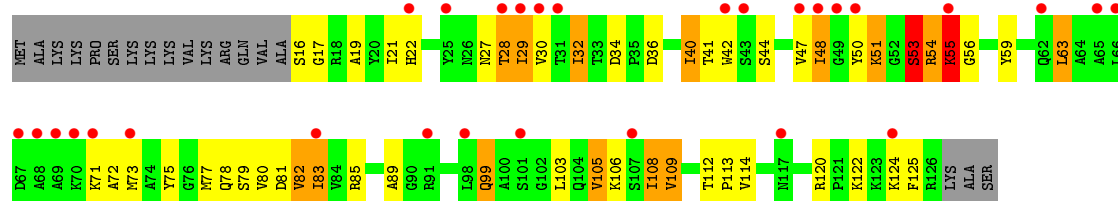
- Molecule 8: 30S ribosomal protein S8



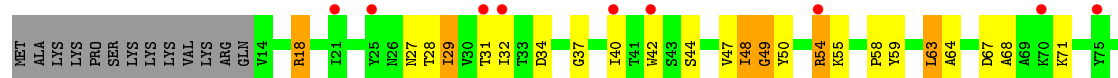




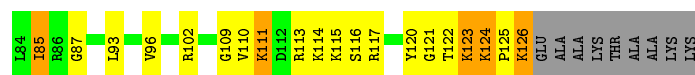
- Molecule 11: 30S ribosomal protein S11



- Molecule 11: 30S ribosomal protein S11



- Molecule 12: 30S ribosomal protein S12

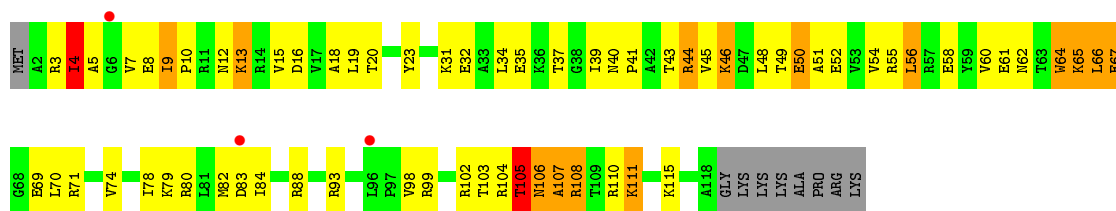


- Molecule 12: 30S ribosomal protein S12

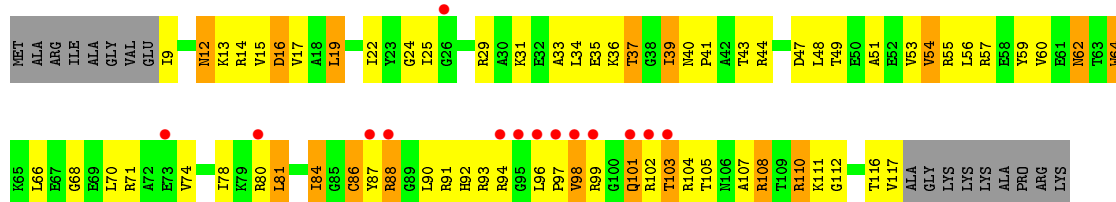


- Molecule 13: 30S ribosomal protein S13

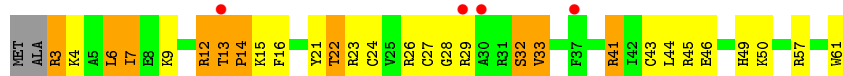




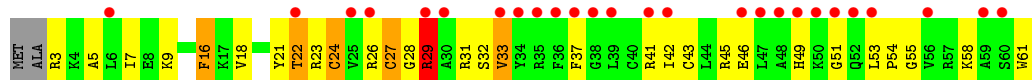
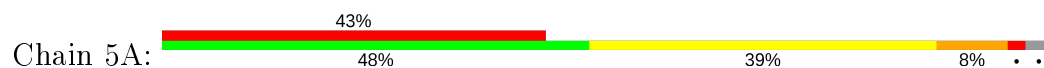
• Molecule 13: 30S ribosomal protein S13



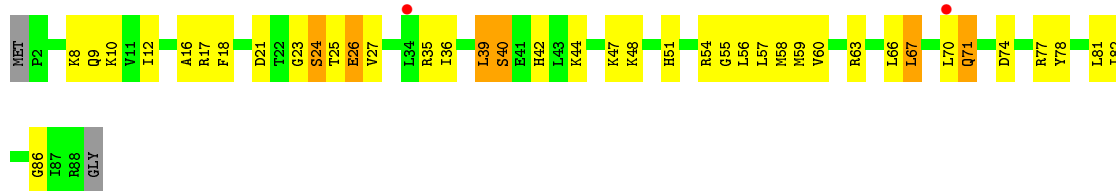
• Molecule 14: 30S ribosomal protein S14 type Z



• Molecule 14: 30S ribosomal protein S14 type Z



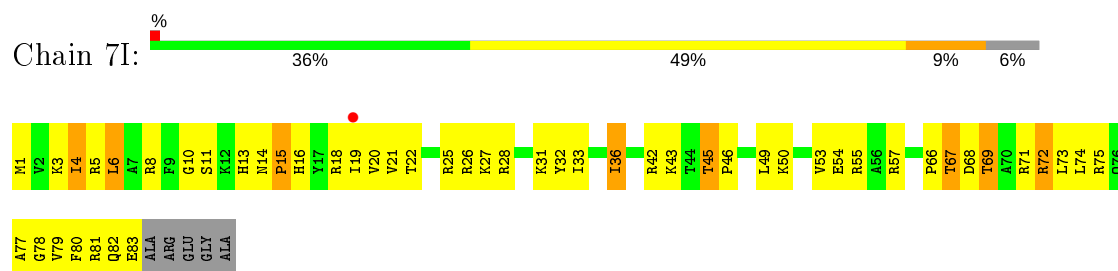
• Molecule 15: 30S ribosomal protein S15



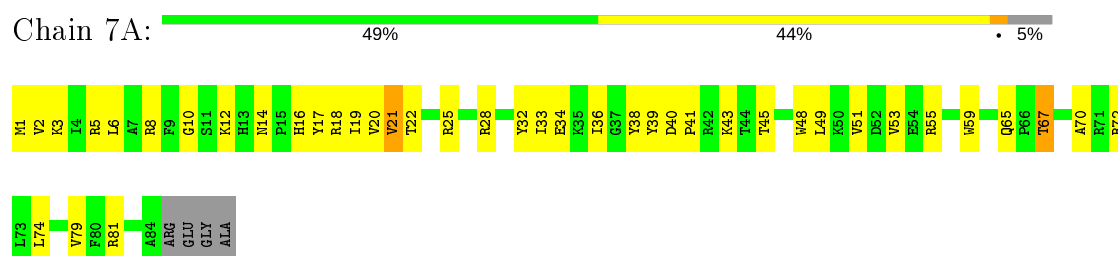
• Molecule 15: 30S ribosomal protein S15



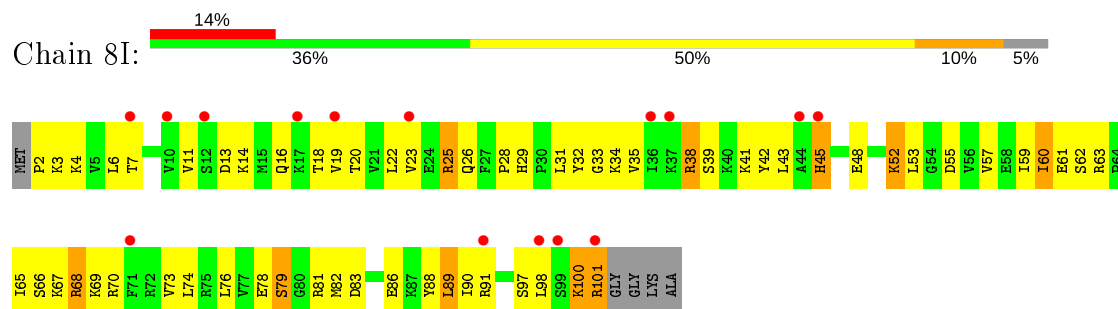
- Molecule 16: 30S ribosomal protein S16



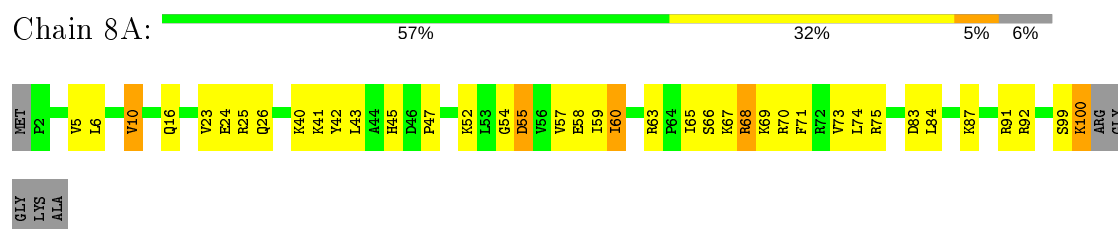
- Molecule 16: 30S ribosomal protein S16



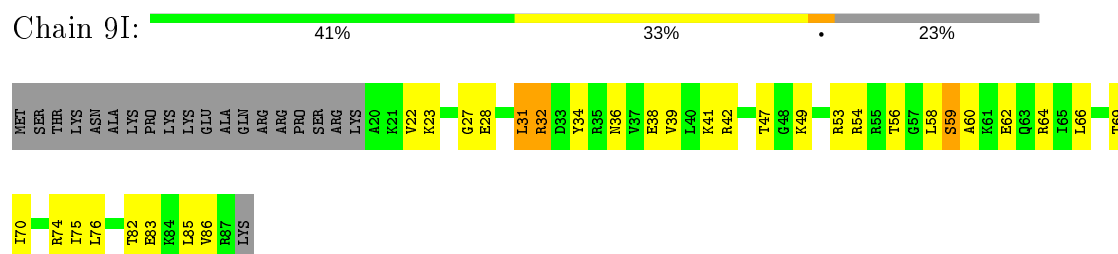
- Molecule 17: 30S ribosomal protein S17



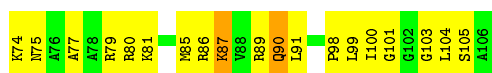
- Molecule 17: 30S ribosomal protein S17



- Molecule 18: 30S ribosomal protein S18



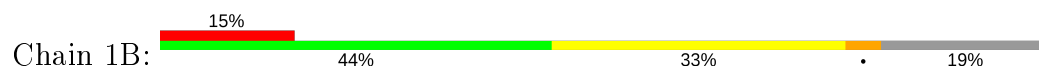
- Chain BA:



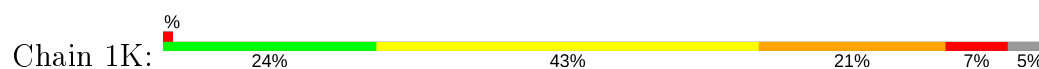
- Molecule 21: 30S ribosomal protein Thx



- Molecule 21: 30S ribosomal protein Thx



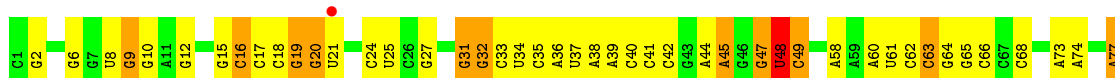
- Molecule 22: tRNA^{Lys}



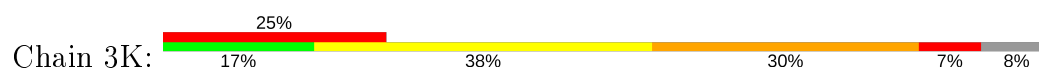
- Molecule 23: tRNA^{fMet}

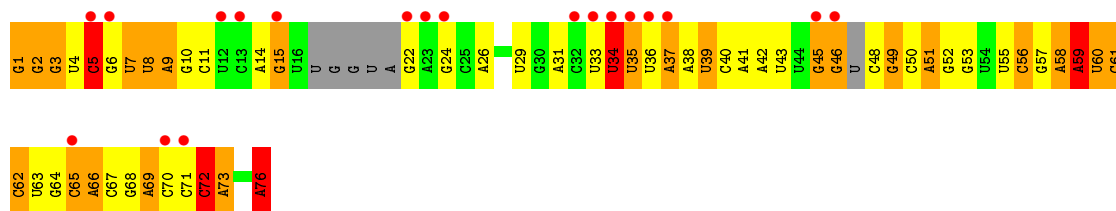


- Molecule 23: tRNA^{fMet}

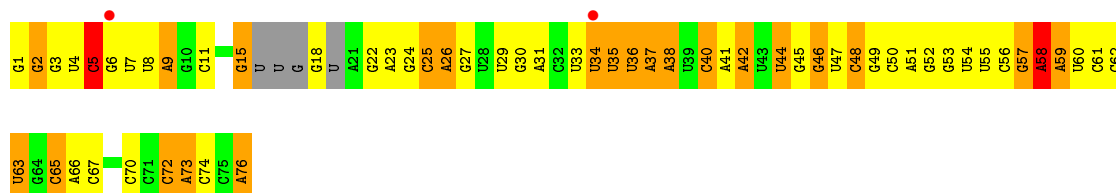
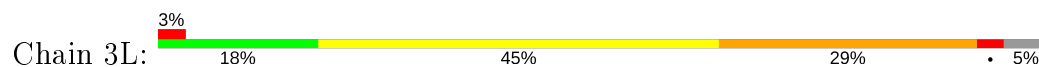


- Molecule 24: tRNA^{Lys}

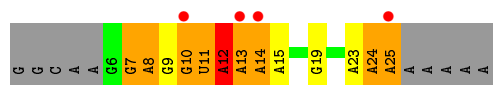




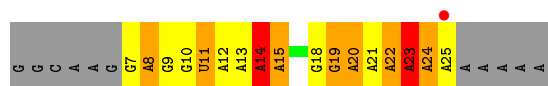
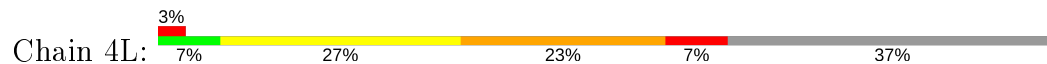
• Molecule 24: tRNA^{Lys}



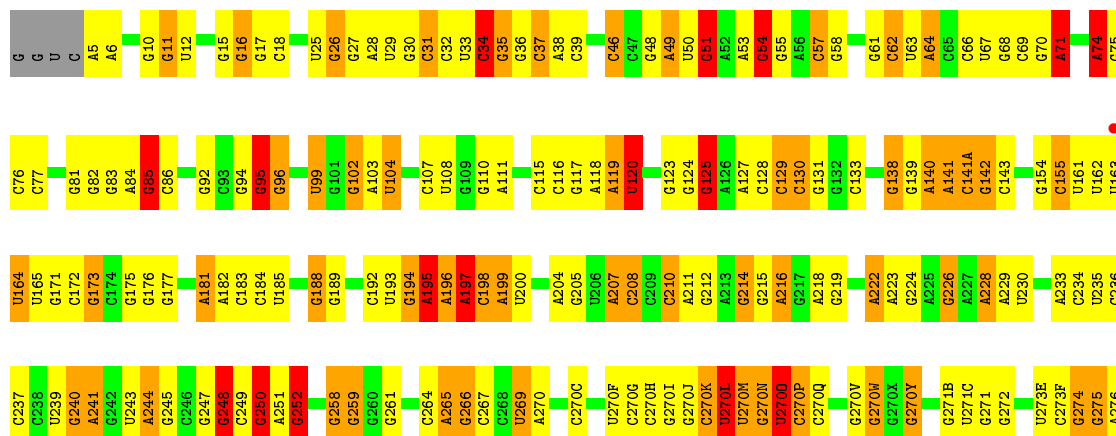
• Molecule 25: mRNA



• Molecule 25: mRNA

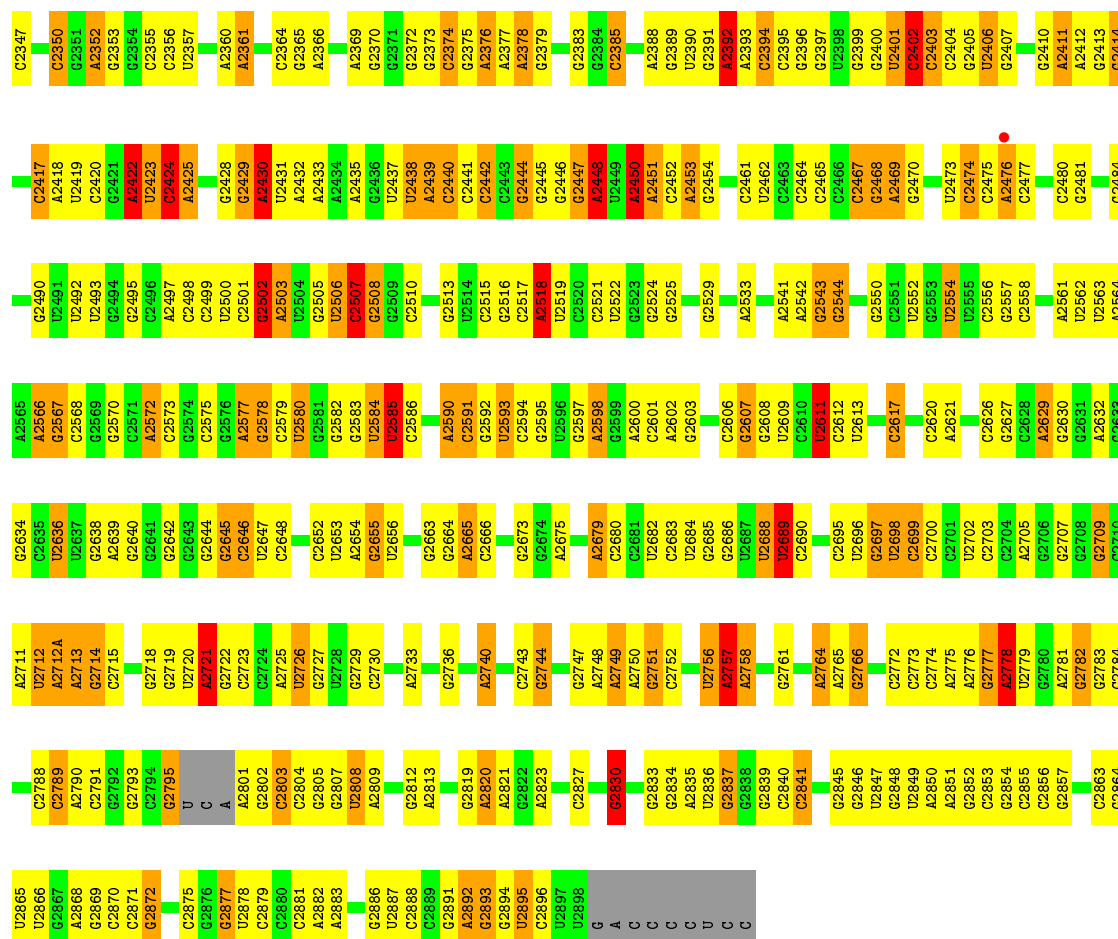


• Molecule 26: 23S ribosomal RNA



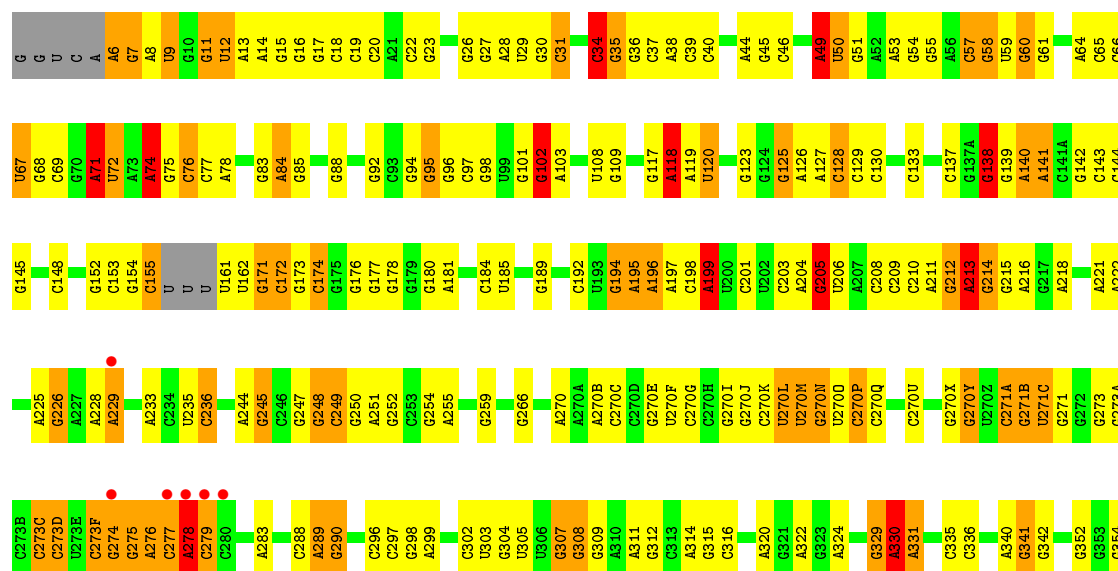






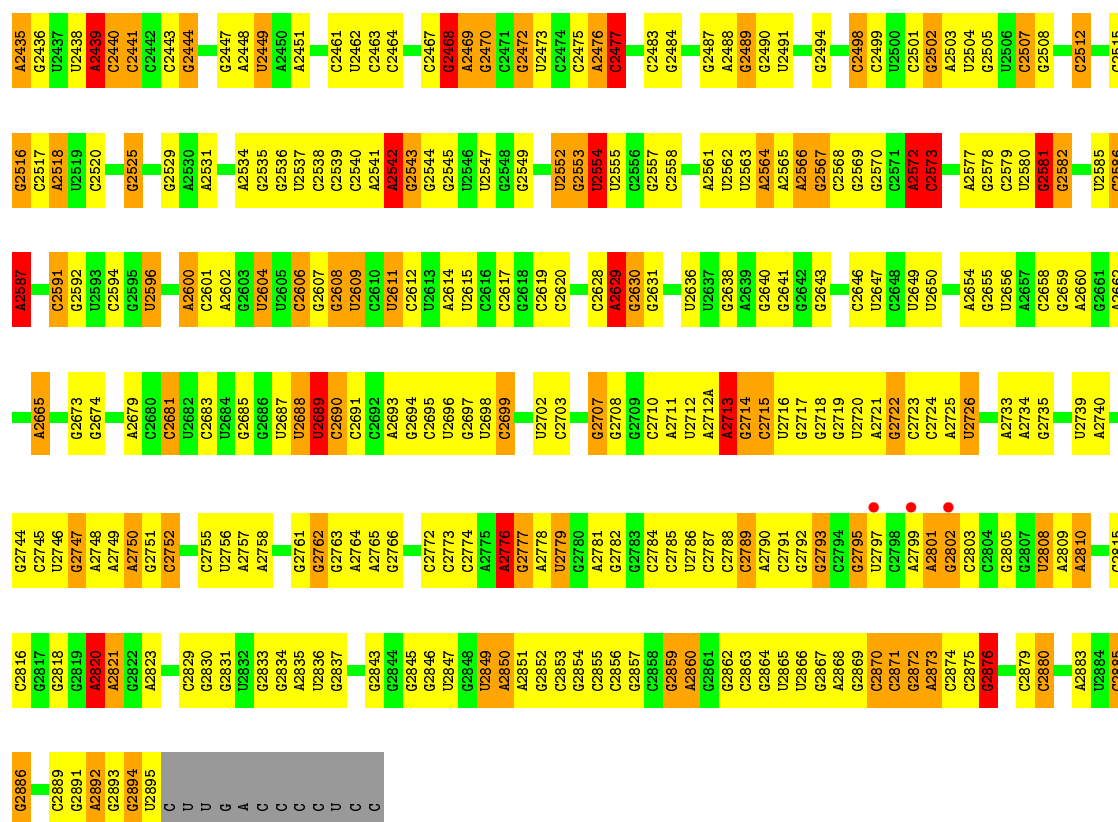
• Molecule 26: 23S ribosomal RNA

Chain 14: 35% 41% 17%

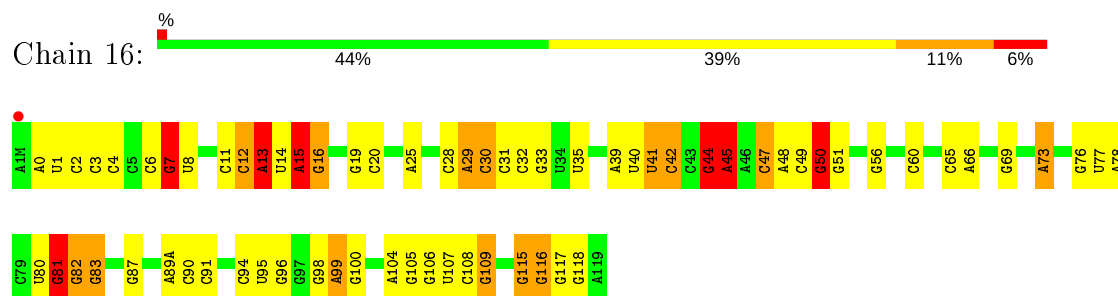


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G1324	G1252	A1174	A	G1037	A973	C898	U833	G768	C692	G649	G582	U504	A432	A359
G1325	A1253	U1175	G	A899	G974	A899	G836	G769	G691	G650	G583	A505	C433	G360
G1326	A1254	C1040	C	C1041	C975	A901	G837	G770	G694	G651	C584	A506	G438	G361
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G1329	C1179	C1180	A	G1044	G978	C904	C840	G776	G697	A654A	U588	C510	G442	A363A
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G1332	G1107	A	G1108	G1047	A981	C909	G845	G779	A699	G654D	C591	A513	C445	U363E
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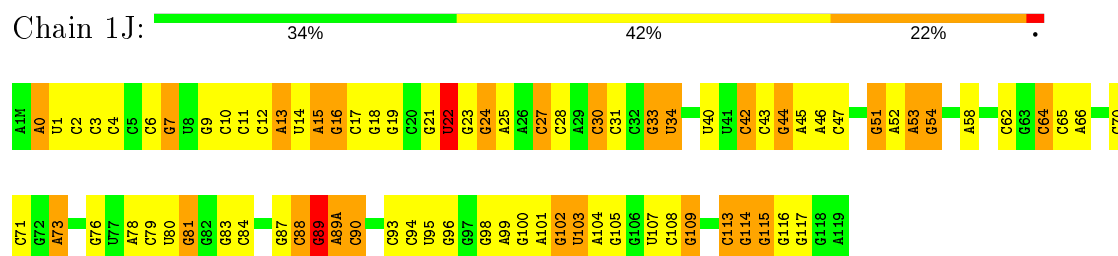
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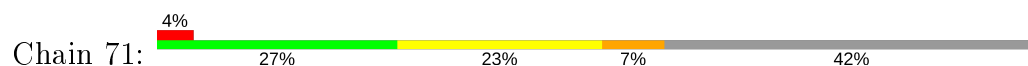
• Molecule 27: 5S ribosomal RNA

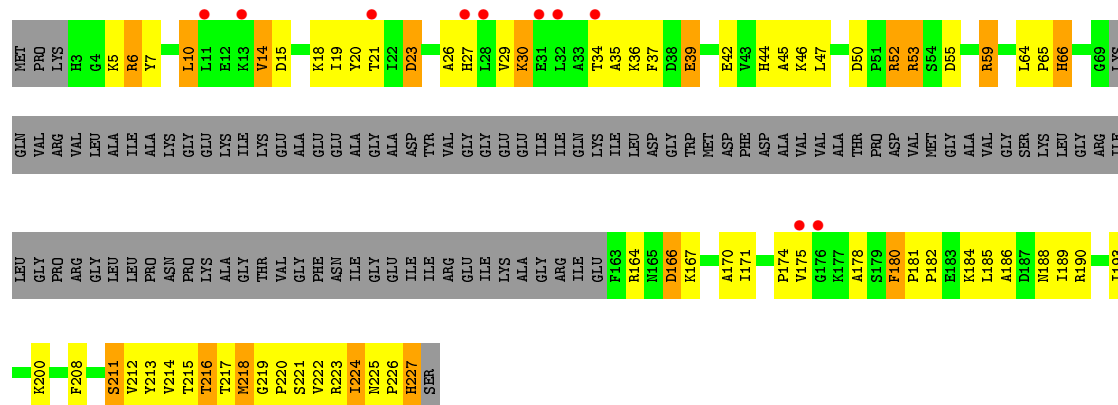


• Molecule 27: 5S ribosomal RNA

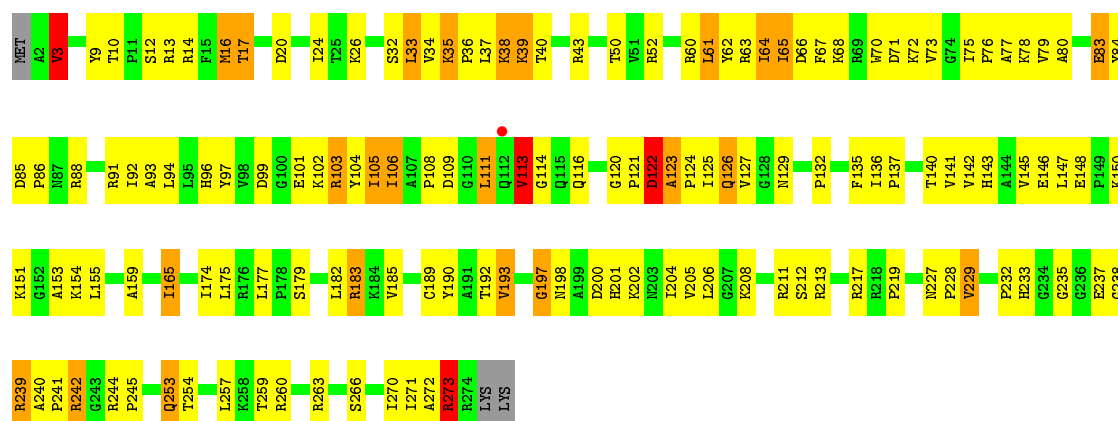


• Molecule 28: 50S ribosomal protein L1

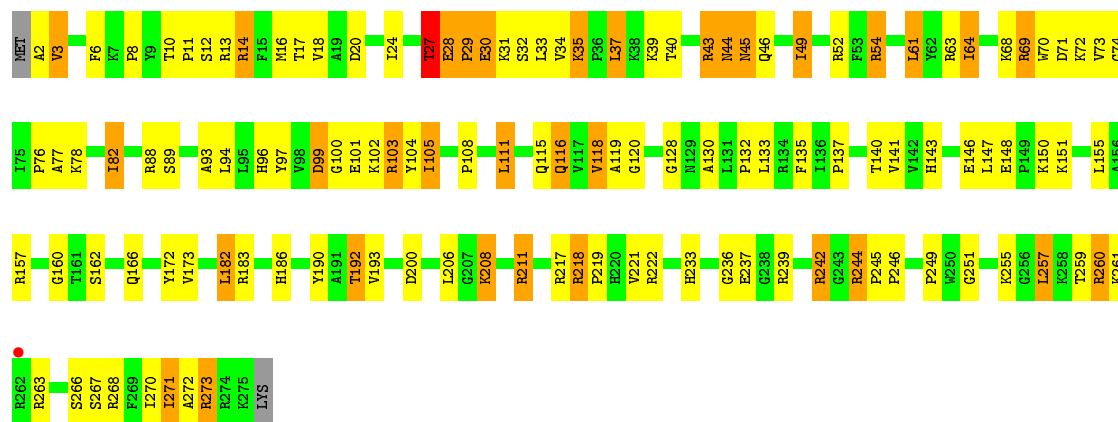




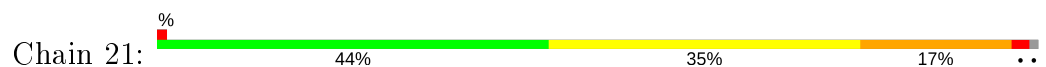
- Molecule 29: 50S ribosomal protein L2

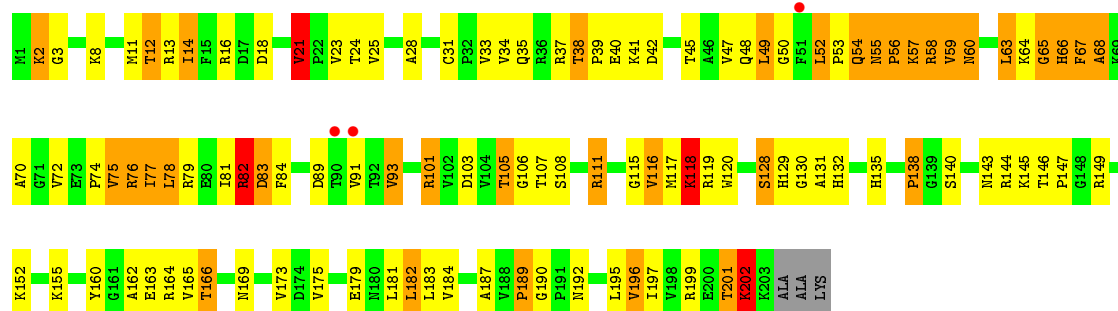


- Molecule 29: 50S ribosomal protein L2

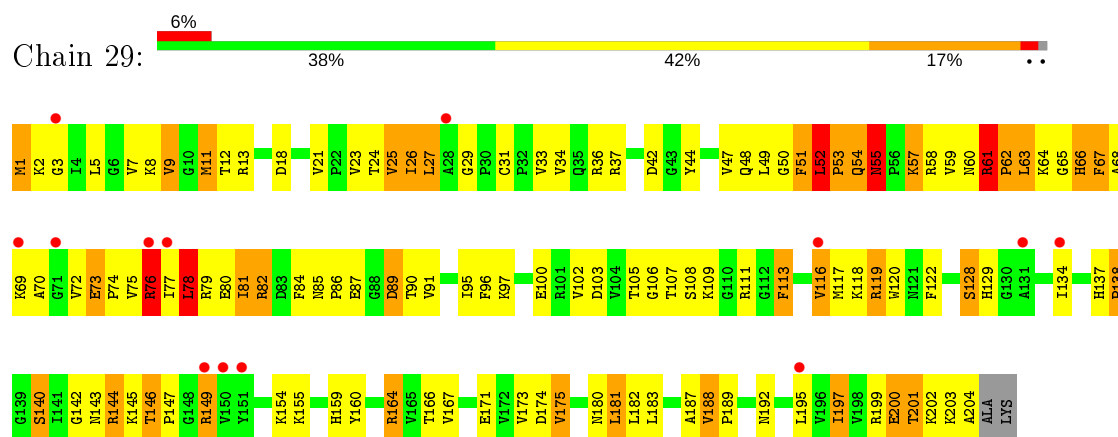


- Molecule 30: 50S ribosomal protein L3

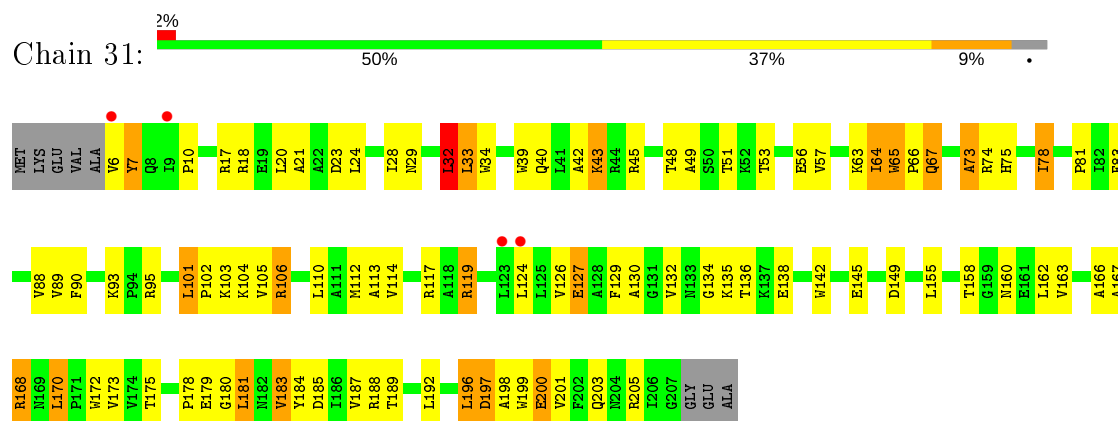




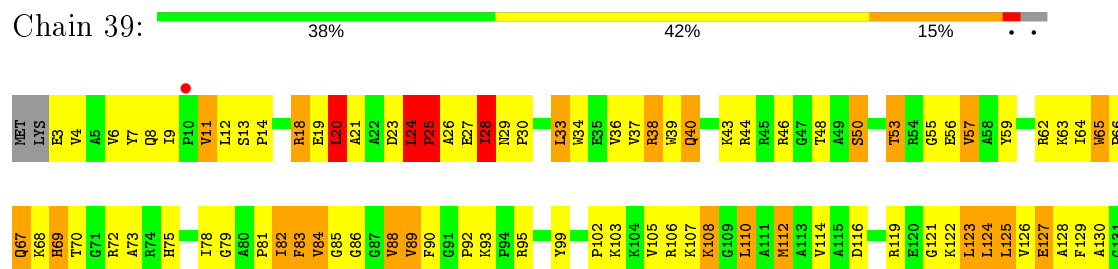
• Molecule 30: 50S ribosomal protein L3



• Molecule 31: 50S ribosomal protein L4

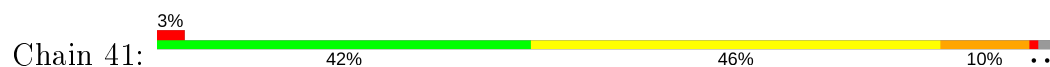


• Molecule 31: 50S ribosomal protein L4

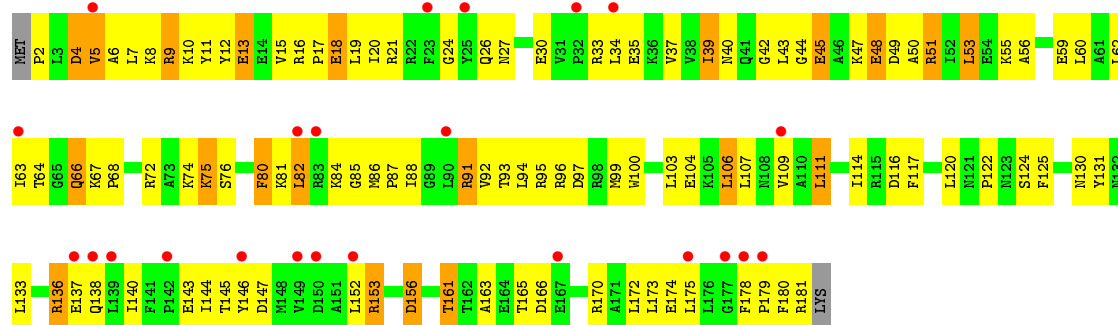




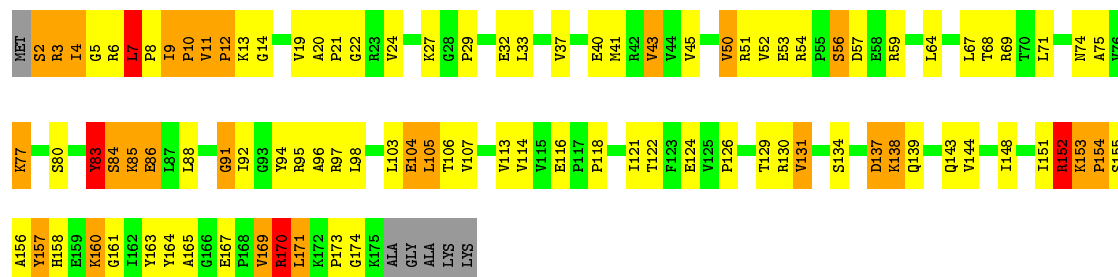
• Molecule 32: 50S ribosomal protein L5



• Molecule 32: 50S ribosomal protein L5



• Molecule 33: 50S ribosomal protein L6



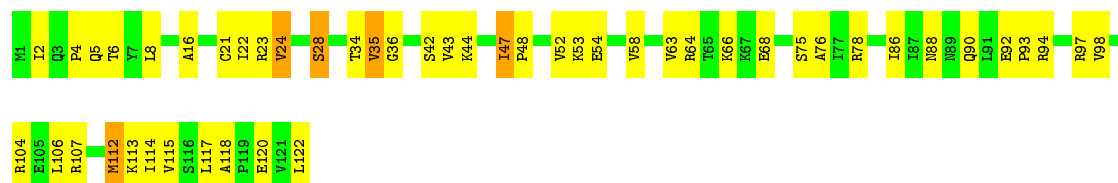
• Molecule 33: 50S ribosomal protein L6





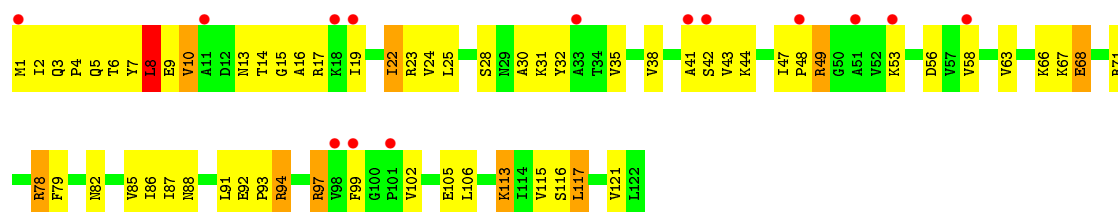
- Molecule 36: 50S ribosomal protein L14

Chain 68: 60% 36%



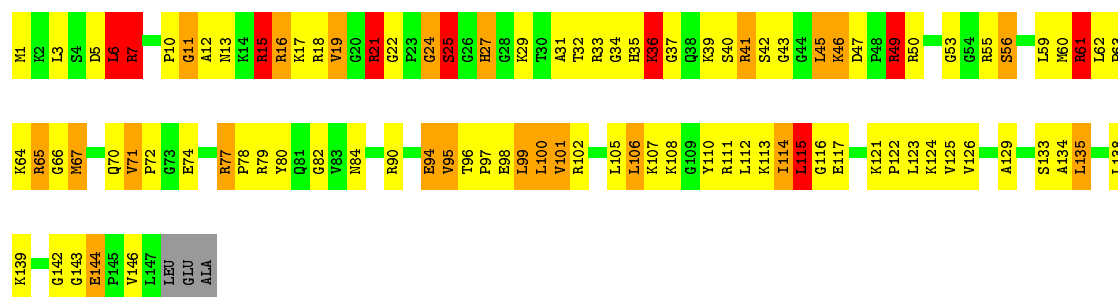
- Molecule 36: 50S ribosomal protein L14

Chain 25: 11% 49% 43% 7%



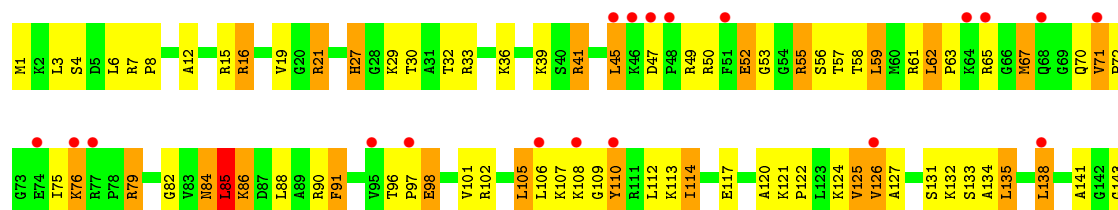
- Molecule 37: 50S ribosomal protein L15

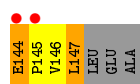
Chain 78: 33% 44% 15% 6%



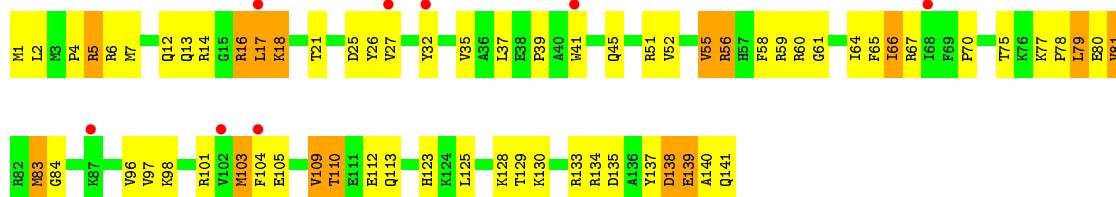
- Molecule 37: 50S ribosomal protein L15

Chain 35: 14% 43% 37% 17%

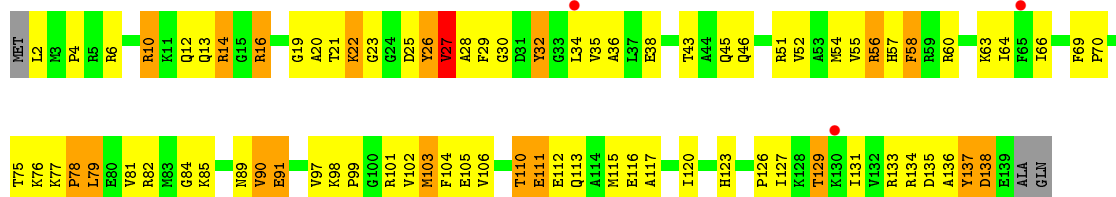
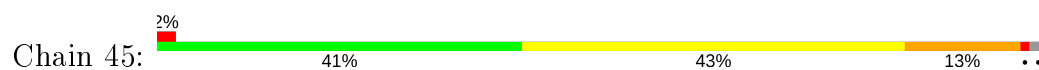




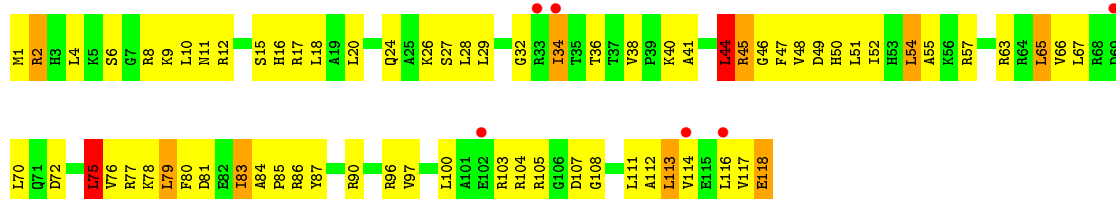
- Molecule 38: 50S ribosomal protein L16



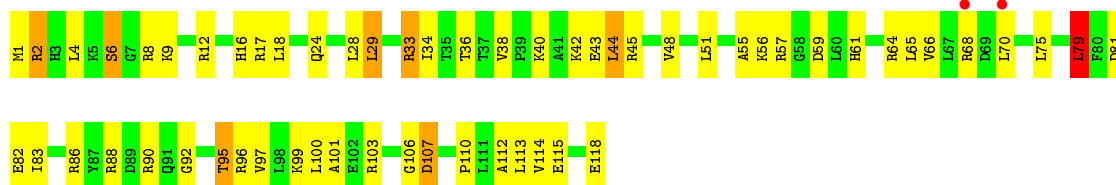
- Molecule 38: 50S ribosomal protein L16



- Molecule 39: 50S ribosomal protein L17

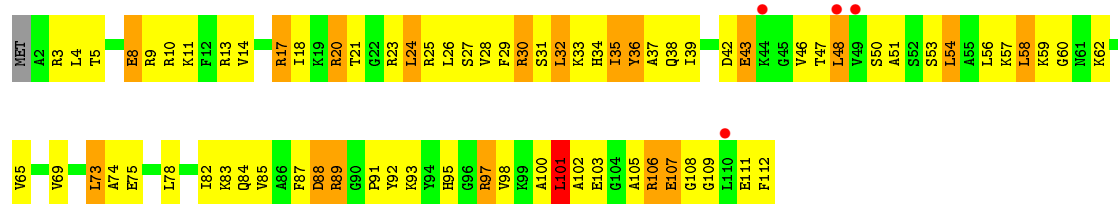


- Molecule 39: 50S ribosomal protein L17

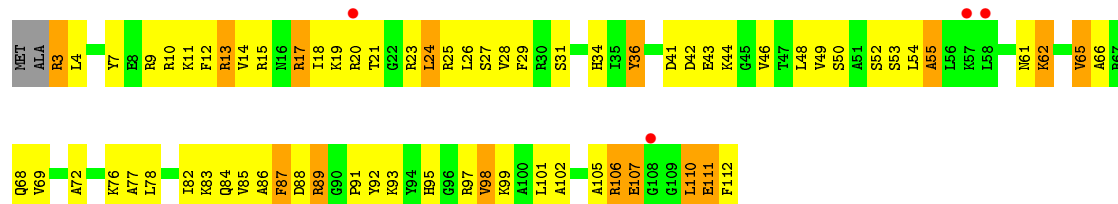


- Molecule 40: 50S ribosomal protein L18

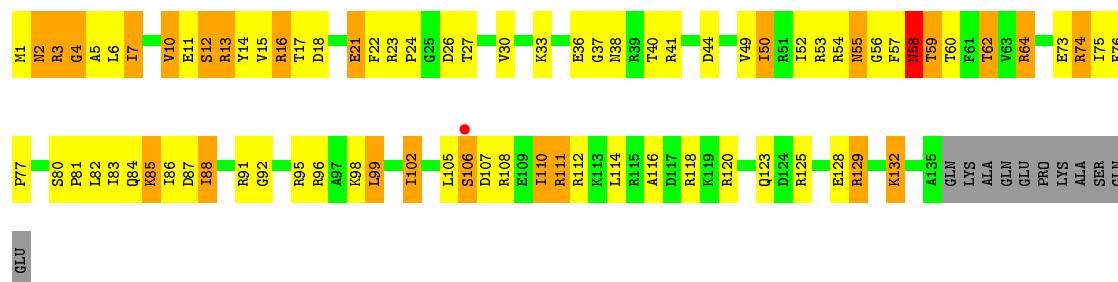




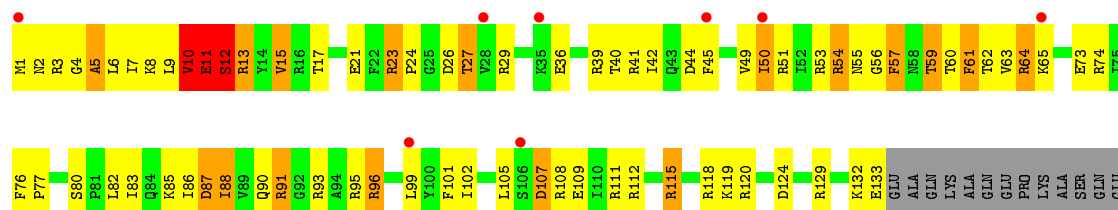
• Molecule 40: 50S ribosomal protein L18



• Molecule 41: 50S ribosomal protein L19

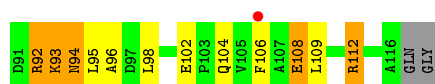


• Molecule 41: 50S ribosomal protein L19



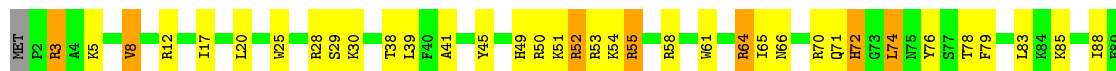
• Molecule 42: 50S ribosomal protein L20





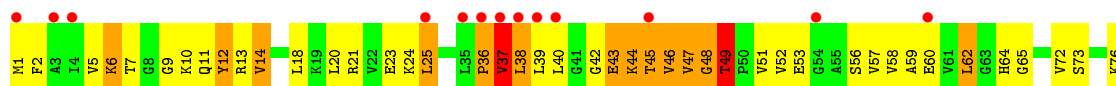
- Molecule 42: 50S ribosomal protein L20

Chain 85: 52% 35% 11% ..



- Molecule 43: 50S ribosomal protein L21

Chain D8: 17% 44% 40% 14% ..



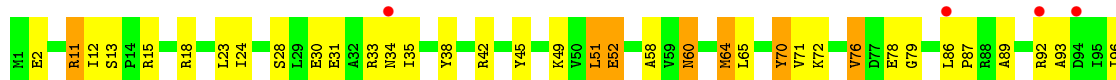
- Molecule 43: 50S ribosomal protein L21

Chain 95: 6% 50% 43% 6% ..



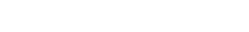
- Molecule 44: 50S ribosomal protein L22

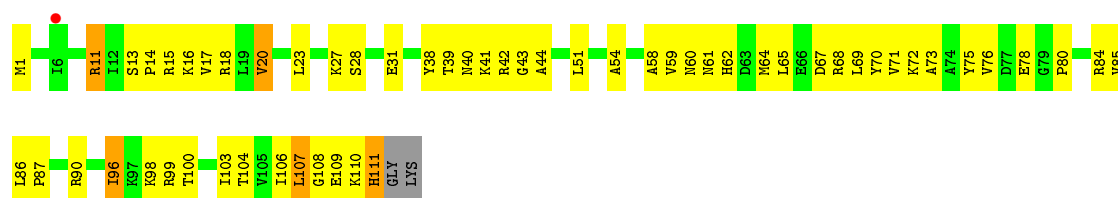
Chain E8: 4% 60% 30% 7% .



- Molecule 44: 50S ribosomal protein L22

Chain A5: 48% 46% . .





- Molecule 45: 50S ribosomal protein L23



- Molecule 45: 50S ribosomal protein L23



- Molecule 46: 50S ribosomal protein L24

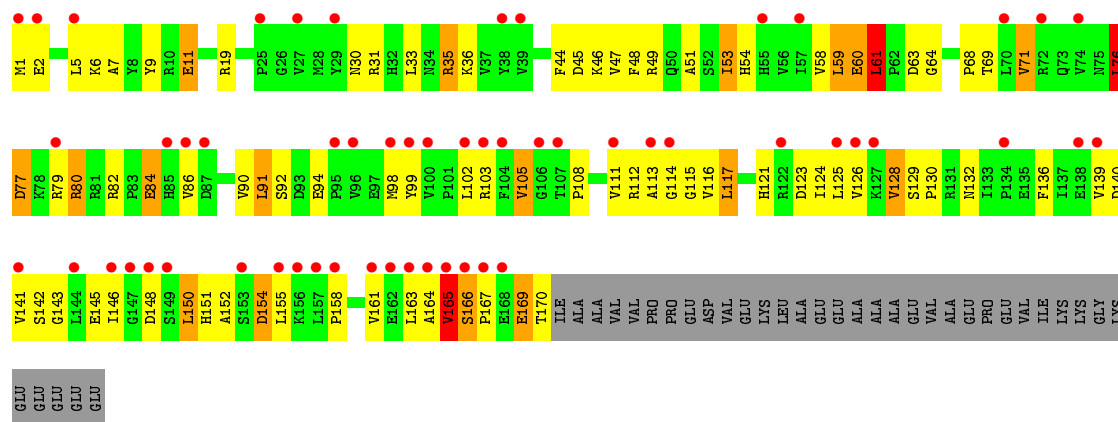


- Molecule 46: 50S ribosomal protein L24

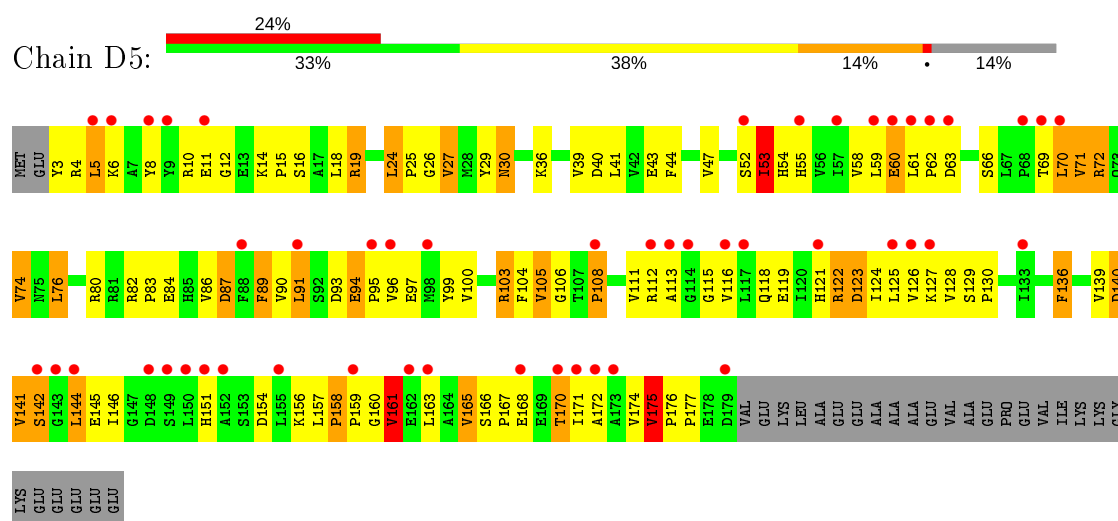


- Molecule 47: 50S ribosomal protein L25

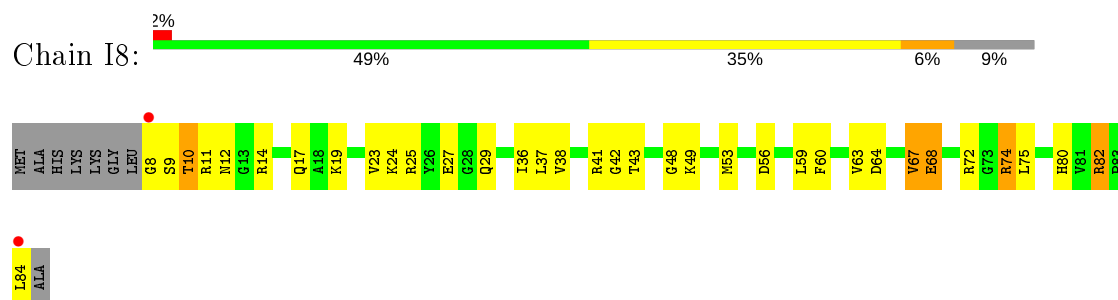




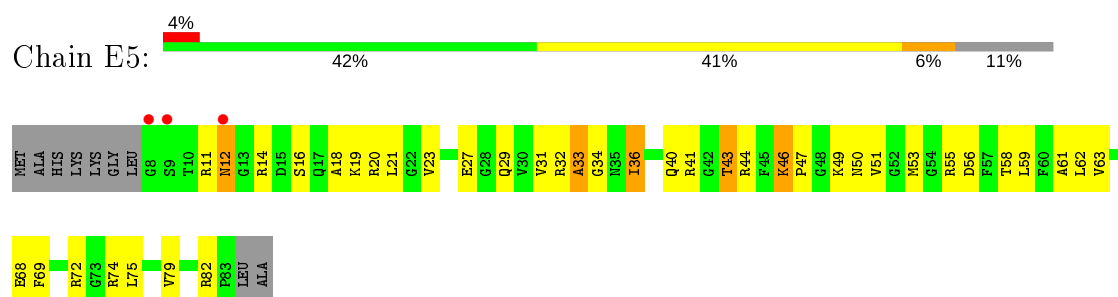
• Molecule 47: 50S ribosomal protein L25



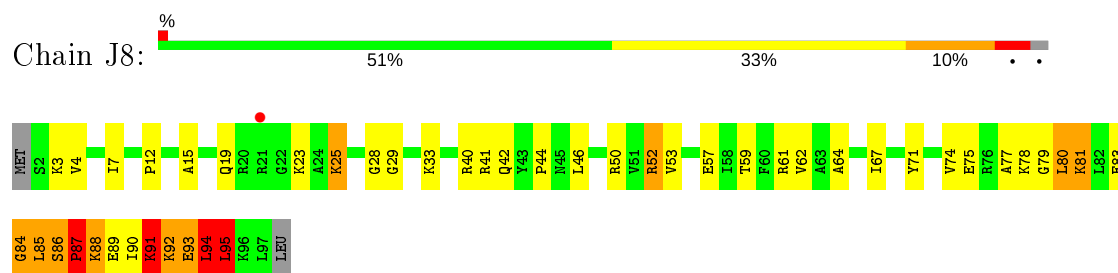
• Molecule 48: 50S ribosomal protein L27



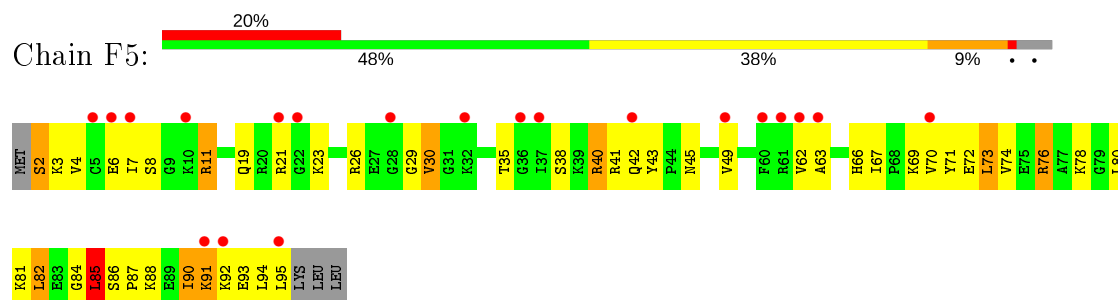
• Molecule 48: 50S ribosomal protein L27



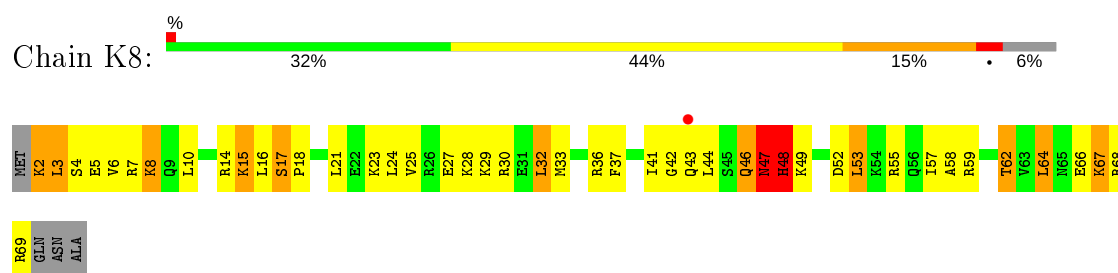
- Molecule 49: 50S ribosomal protein L28



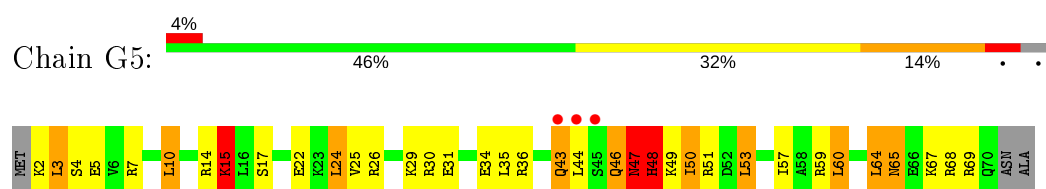
- Molecule 49: 50S ribosomal protein L28



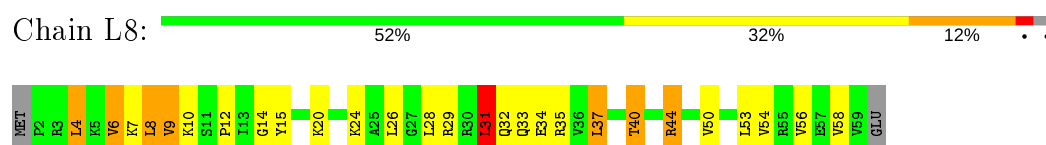
- Molecule 50: 50S ribosomal protein L29



- Molecule 50: 50S ribosomal protein L29



- Molecule 51: 50S ribosomal protein L30

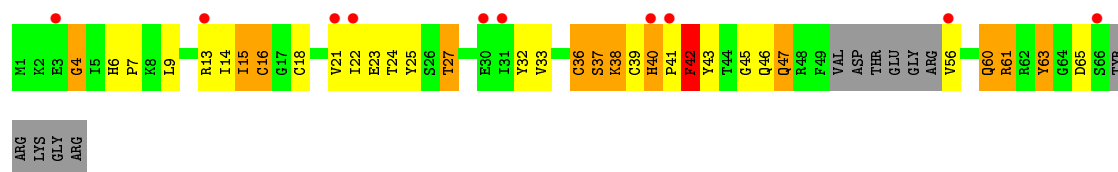


- Molecule 51: 50S ribosomal protein L30





- Molecule 52: 50S ribosomal protein L31



- Molecule 53: 50S ribosomal protein L32



- Molecule 53: 50S ribosomal protein L32



- Molecule 54: 50S ribosomal protein L34



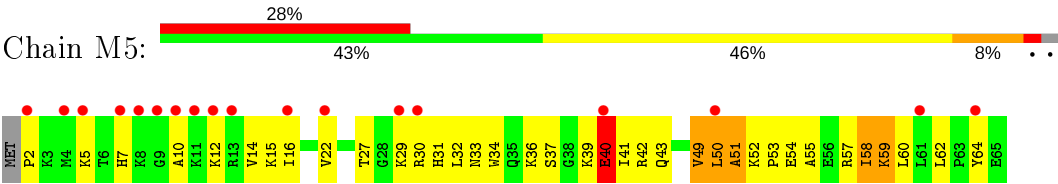
- Molecule 54: 50S ribosomal protein L34



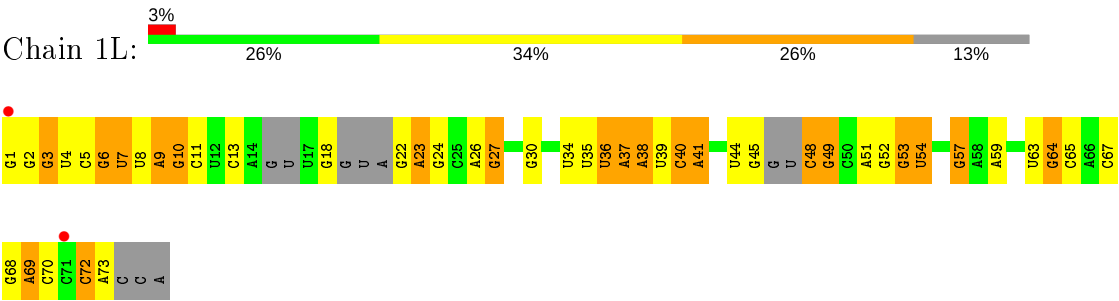
- Molecule 55: 50S ribosomal protein L35



● Molecule 55: 50S ribosomal protein L35



● Molecule 56: tRNA^{Lys}



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	209.15Å 448.16Å 617.80Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	154.45 – 3.13 161.54 – 3.13	Depositor EDS
% Data completeness (in resolution range)	100.0 (154.45-3.13) 90.9 (161.54-3.13)	Depositor EDS
R_{merge}	0.42	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.81 (at 3.13Å)	Xtriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.192 , 0.244 0.192 , 0.244	Depositor DCC
R_{free} test set	2000 reflections (0.20%)	wwPDB-VP
Wilson B-factor (Å ²)	89.4	Xtriage
Anisotropy	0.275	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.27 , 75.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	296999	wwPDB-VP
Average B, all atoms (Å ²)	109.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.50% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: 5MU, OMC, ZN, U8U, H2U, 7MG, SF4, MG, 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	0.67	3/36095 (0.0%)	1.26	206/56332 (0.4%)
1	1G	0.60	2/36309 (0.0%)	1.18	153/56668 (0.3%)
2	12	0.38	0/1727	0.64	2/2326 (0.1%)
2	1E	0.40	0/1908	0.62	2/2573 (0.1%)
3	22	0.47	1/1560 (0.1%)	0.58	0/2104
3	2E	0.44	1/1629 (0.1%)	0.60	1/2195 (0.0%)
4	32	0.41	0/1732	0.60	0/2318
4	3E	0.49	1/1728 (0.1%)	0.64	3/2313 (0.1%)
5	42	0.40	0/1156	0.62	0/1557
5	4E	0.40	0/1158	0.61	0/1559
6	52	0.45	0/855	0.61	1/1154 (0.1%)
6	5E	0.47	0/850	0.61	0/1147
7	62	0.39	0/1122	0.56	0/1500
7	6E	0.40	0/1259	0.51	0/1686
8	72	0.38	0/1127	0.59	0/1517
8	7E	0.40	0/1135	0.61	0/1527
9	82	0.36	0/971	0.62	0/1304
9	8E	0.38	0/1019	0.61	0/1367
10	1A	0.93	2/658 (0.3%)	0.57	0/885
10	1I	0.37	0/762	0.61	0/1027
11	2A	0.40	0/850	0.60	0/1150
11	2I	0.43	0/838	0.62	0/1133
12	3A	0.48	0/963	0.69	1/1290 (0.1%)
12	3I	0.57	0/972	0.76	0/1301
13	4A	0.34	0/889	0.58	0/1192
13	4I	0.46	0/943	0.65	0/1265
14	5A	0.40	0/495	0.66	0/657
14	5I	0.49	0/495	0.74	1/657 (0.2%)
15	6A	0.39	0/740	0.56	0/987
15	6I	0.44	0/740	0.61	0/987
16	7A	0.41	0/721	0.63	0/970
16	7I	0.40	0/716	0.67	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	0.48	0/847	0.66	0/1131
18	9A	0.44	0/549	0.64	0/732
18	9I	0.42	0/554	0.63	0/739
19	AA	0.38	0/520	0.71	0/700
19	AI	0.40	0/676	0.72	1/910 (0.1%)
20	BA	0.37	0/764	0.66	1/1007 (0.1%)
20	BI	0.36	0/748	0.60	1/986 (0.1%)
21	1B	0.37	0/192	0.58	0/252
21	1F	0.43	0/203	0.62	0/266
22	1K	0.57	0/1568	1.21	10/2434 (0.4%)
23	2K	0.73	0/1721	1.30	11/2682 (0.4%)
23	2L	0.67	1/1721 (0.1%)	1.17	4/2682 (0.1%)
24	3K	0.49	0/1654	1.14	11/2570 (0.4%)
24	3L	0.53	0/1705	1.15	12/2650 (0.5%)
25	4K	0.79	0/499	1.32	5/778 (0.6%)
25	4L	0.67	0/473	1.32	3/737 (0.4%)
26	14	0.84	35/68159 (0.1%)	1.43	876/106398 (0.8%)
26	1H	0.99	95/68309 (0.1%)	1.56	1280/106631 (1.2%)
27	16	0.74	0/2928	1.41	33/4568 (0.7%)
27	1J	0.65	0/2928	1.31	16/4568 (0.4%)
28	71	0.30	0/1049	0.54	0/1417
29	11	0.64	1/2170 (0.0%)	0.85	2/2926 (0.1%)
29	19	0.62	1/2175 (0.0%)	0.79	2/2933 (0.1%)
30	21	0.57	0/1579	0.90	5/2131 (0.2%)
30	29	0.56	0/1596	0.82	2/2153 (0.1%)
31	31	0.62	0/1620	0.84	1/2194 (0.0%)
31	39	0.53	1/1637 (0.1%)	0.80	1/2218 (0.0%)
32	41	0.43	0/1481	0.67	0/1994
32	49	0.45	1/1483 (0.1%)	0.62	1/1997 (0.1%)
33	51	0.52	0/1354	0.85	2/1833 (0.1%)
33	59	0.38	0/1320	0.68	2/1787 (0.1%)
34	61	0.43	0/1146	0.71	2/1551 (0.1%)
34	69	0.48	1/1146 (0.1%)	0.68	1/1551 (0.1%)
35	15	0.42	0/1123	0.64	0/1515
35	58	0.51	0/1123	0.76	1/1514 (0.1%)
36	25	0.52	0/942	0.72	1/1269 (0.1%)
36	68	0.57	0/942	0.73	0/1269
37	35	0.52	0/1139	0.78	1/1514 (0.1%)
37	78	0.62	1/1139 (0.1%)	0.96	4/1514 (0.3%)
38	45	0.55	0/1120	0.82	0/1498
38	88	0.61	0/1138	0.90	1/1523 (0.1%)
39	55	0.50	0/981	0.77	1/1312 (0.1%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
39	98	0.48	0/981	0.79	1/1312 (0.1%)
40	65	0.46	0/886	0.75	1/1180 (0.1%)
40	A8	0.53	0/891	0.78	1/1187 (0.1%)
41	75	0.51	0/1123	0.76	1/1500 (0.1%)
41	B8	0.55	0/1133	0.76	1/1514 (0.1%)
42	85	0.46	0/977	0.67	1/1301 (0.1%)
42	C8	0.59	0/968	0.76	1/1289 (0.1%)
43	95	0.46	0/781	0.79	1/1048 (0.1%)
43	D8	0.58	0/785	0.75	1/1052 (0.1%)
44	A5	0.53	0/897	0.69	0/1204
44	E8	0.56	0/886	0.75	0/1189
45	B5	0.56	0/749	0.73	0/1007
45	F8	0.62	0/764	0.80	1/1025 (0.1%)
46	C5	0.64	0/807	0.86	1/1076 (0.1%)
46	G8	0.65	0/796	0.94	2/1062 (0.2%)
47	D5	0.72	1/1443 (0.1%)	0.65	0/1960
47	H8	0.43	0/1395	0.73	2/1890 (0.1%)
48	E5	0.49	0/611	0.73	0/814
48	I8	0.62	0/619	0.81	0/825
49	F5	0.52	0/744	0.84	1/989 (0.1%)
49	J8	0.66	0/754	0.95	3/1003 (0.3%)
50	G5	0.51	0/578	0.70	0/766
50	K8	0.61	0/577	0.93	1/763 (0.1%)
51	H5	0.48	0/464	0.64	0/623
51	L8	0.48	0/464	0.77	1/623 (0.2%)
52	M8	0.45	0/485	0.78	0/652
53	J5	0.49	0/448	0.74	0/606
53	N8	0.59	0/381	0.77	0/516
54	L5	0.52	0/409	0.76	0/540
54	P8	0.67	0/409	0.88	1/540 (0.2%)
55	M5	0.65	0/524	0.85	0/691
55	Q8	0.60	0/524	0.90	1/691 (0.1%)
56	1L	0.47	1/1516 (0.1%)	0.95	1/2350 (0.0%)
All	All	0.74	149/316848 (0.0%)	1.26	2688/474550 (0.6%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
2	12	0	3

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Mol	Chain	#Chirality outliers	#Planarity outliers
2	1E	0	4
4	32	0	5
4	3E	0	1
8	72	0	1
9	82	0	2
9	8E	0	2
10	1A	0	1
11	2A	0	1
12	3A	0	1
12	3I	0	3
13	4I	0	3
14	5A	0	1
16	7I	0	1
19	AA	0	1
19	AI	0	1
20	BA	0	3
20	BI	0	1
29	11	0	4
29	19	0	2
30	21	0	7
30	29	0	5
31	39	0	8
32	49	0	2
33	51	0	6
33	59	0	4
34	61	0	3
34	69	0	4
35	15	0	1
35	58	0	1
37	35	0	1
37	78	0	6
38	45	0	2
38	88	0	1
39	98	0	2
40	65	0	2
40	A8	0	1
41	75	0	3
41	B8	0	3
42	85	0	4
42	C8	0	3
43	D8	0	3
44	A5	0	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
45	B5	0	2
46	C5	0	3
46	G8	0	3
47	D5	0	4
47	H8	0	5
49	F5	0	1
49	J8	0	3
50	G5	0	3
50	K8	0	3
52	M8	0	4
55	M5	0	4
55	Q8	0	2
All	All	0	151

The worst 5 of 149 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
47	D5	94	GLU	C-N	23.32	1.78	1.34
10	1A	38	ILE	C-N	19.43	1.71	1.34
26	1H	2430	A	N9-C4	-14.21	1.29	1.37
26	1H	774	A	N9-C4	-13.66	1.29	1.37
3	22	173	VAL	C-N	12.84	1.58	1.34

The worst 5 of 2688 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	1H	1899	G	N3-C4-N9	-18.59	114.85	126.00
26	1H	1332	G	C5-N7-C8	-17.78	95.41	104.30
26	1H	1332	G	C2-N3-C4	-17.15	103.32	111.90
26	1H	676	A	C2-N3-C4	-16.45	102.38	110.60
26	1H	783	A	C2-N3-C4	-16.44	102.38	110.60

There are no chirality outliers.

5 of 151 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	1E	15	VAL	Peptide
2	1E	234	PRO	Peptide
2	1E	236	TYR	Peptide
2	1E	9	GLU	Peptide
4	3E	29	PRO	Peptide

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	13	32246	0	16276	858	0
1	1G	32437	0	16372	887	2
2	12	1696	0	1730	94	0
2	1E	1874	0	1926	99	0
3	22	1537	0	1603	87	0
3	2E	1605	0	1668	60	0
4	32	1702	0	1765	98	0
4	3E	1698	0	1761	84	0
5	42	1141	0	1198	41	0
5	4E	1142	0	1204	54	0
6	52	842	0	857	34	0
6	5E	837	0	852	34	0
7	62	1110	0	1163	66	0
7	6E	1242	0	1286	54	0
8	72	1107	0	1165	49	0
8	7E	1115	0	1177	69	0
9	82	953	0	983	75	0
9	8E	1000	0	1031	61	0
10	1A	646	0	662	41	0
10	1I	749	0	767	45	0
11	2A	835	0	847	27	0
11	2I	823	0	832	41	0
12	3A	947	0	1033	37	0
12	3I	956	0	1046	33	0
13	4A	879	0	935	67	0
13	4I	933	0	992	51	0
14	5A	486	0	525	34	0
14	5I	486	0	524	28	0
15	6A	729	0	768	27	0
15	6I	729	0	768	31	0
16	7A	705	0	725	29	0
16	7I	700	0	720	49	0
17	8A	823	0	891	32	0
17	8I	834	0	904	62	0
18	9A	544	0	605	23	0
18	9I	549	0	607	23	0
19	AA	510	0	507	34	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
19	AI	661	0	683	38	0
20	BA	762	0	861	40	0
20	BI	746	0	843	45	0
21	1B	188	0	195	11	0
21	1F	199	0	208	12	0
22	1K	1542	0	790	43	0
23	2K	1646	0	843	36	0
23	2L	1646	0	845	32	0
24	3K	1483	0	756	67	0
24	3L	1528	0	778	48	0
25	4K	442	0	219	9	0
25	4L	419	0	208	23	0
26	14	60857	0	30679	1311	1
26	1H	60991	0	30744	1358	1
27	16	2617	0	1328	56	0
27	1J	2617	0	1328	84	0
28	71	1027	0	1043	66	0
29	11	2120	0	2197	121	0
29	19	2125	0	2199	108	0
30	21	1546	0	1602	94	0
30	29	1563	0	1629	110	0
31	31	1585	0	1632	87	0
31	39	1602	0	1649	97	0
32	41	1457	0	1514	76	0
32	49	1459	0	1507	73	0
33	51	1328	0	1396	77	0
33	59	1295	0	1366	74	0
34	61	1131	0	1218	44	0
34	69	1131	0	1218	58	0
35	15	1096	0	1168	56	0
35	58	1096	0	1169	67	0
36	25	932	0	996	48	0
36	68	932	0	996	38	0
37	35	1122	0	1206	75	0
37	78	1122	0	1206	99	0
38	45	1099	0	1154	74	0
38	88	1117	0	1168	55	0
39	55	967	0	1033	47	0
39	98	967	0	1033	51	0
40	65	876	0	938	55	0
40	A8	881	0	943	55	0
41	75	1109	0	1170	63	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
41	B8	1119	0	1177	71	0
42	85	959	0	1019	64	0
42	C8	950	0	1011	55	0
43	95	770	0	838	41	0
43	D8	774	0	849	42	0
44	A5	886	0	948	35	0
44	E8	876	0	941	27	0
45	B5	735	0	785	32	0
45	F8	750	0	814	33	0
46	C5	794	0	885	61	0
46	G8	783	0	869	48	0
47	D5	1411	0	1436	83	0
47	H8	1365	0	1391	60	0
48	E5	603	0	620	40	0
48	I8	611	0	631	32	0
49	F5	737	0	813	43	0
49	J8	747	0	817	35	0
50	G5	576	0	625	33	0
50	K8	575	0	634	45	0
51	H5	459	0	512	15	0
51	L8	459	0	512	22	0
52	M8	475	0	465	34	0
53	J5	434	0	454	23	0
53	N8	369	0	388	21	0
54	L5	401	0	436	21	0
54	P8	401	0	436	13	0
55	M5	516	0	582	28	0
55	Q8	516	0	582	34	0
56	1L	1402	0	715	32	0
57	13	141	0	0	0	0
57	14	460	0	0	0	0
57	16	12	0	0	0	0
57	19	1	0	0	0	0
57	1G	125	0	0	0	0
57	1H	552	0	0	0	0
57	1J	10	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	2I	1	0	0	0	0
57	2K	3	0	0	0	0
57	2L	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
57	31	1	0	0	0	0
57	32	1	0	0	0	0
57	35	2	0	0	0	0
57	39	1	0	0	0	0
57	3I	1	0	0	0	0
57	41	1	0	0	0	0
57	42	2	0	0	0	0
57	45	1	0	0	0	0
57	4L	1	0	0	0	0
57	52	1	0	0	0	0
57	7A	1	0	0	0	0
57	88	3	0	0	0	0
57	B5	1	0	0	0	0
57	E5	2	0	0	0	0
57	F8	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	32	8	0	0	2	0
58	3E	8	0	0	0	0
59	5A	1	0	0	0	0
59	5I	1	0	0	0	0
59	C5	1	0	0	0	0
59	G8	1	0	0	0	0
60	14	13	0	24	0	0
60	1G	13	0	22	3	0
61	11	10	0	0	6	0
61	13	354	0	0	20	0
61	14	1303	0	0	91	0
61	15	3	0	0	0	0
61	16	12	0	0	1	0
61	19	14	0	0	1	0
61	1A	2	0	0	0	0
61	1G	364	0	0	24	0
61	1H	1720	0	0	128	0
61	1I	2	0	0	0	0
61	1J	27	0	0	1	0
61	1K	1	0	0	0	0
61	21	6	0	0	1	0
61	25	8	0	0	0	0
61	29	6	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
61	2A	1	0	0	0	0
61	2K	8	0	0	0	0
61	2L	8	0	0	0	0
61	31	6	0	0	0	0
61	32	4	0	0	1	0
61	35	8	0	0	0	0
61	39	8	0	0	0	0
61	3E	2	0	0	0	0
61	3I	2	0	0	0	0
61	3K	1	0	0	0	0
61	42	1	0	0	0	0
61	4A	2	0	0	0	0
61	4E	3	0	0	2	0
61	4K	5	0	0	0	0
61	4L	3	0	0	0	0
61	52	4	0	0	0	0
61	55	1	0	0	0	0
61	58	2	0	0	0	0
61	5I	1	0	0	0	0
61	68	2	0	0	0	0
61	6A	3	0	0	0	0
61	75	1	0	0	0	0
61	78	13	0	0	4	0
61	7A	4	0	0	0	0
61	7I	2	0	0	0	0
61	85	1	0	0	0	0
61	8E	2	0	0	0	0
61	98	1	0	0	2	0
61	9A	2	0	0	0	0
61	B5	1	0	0	0	0
61	B8	1	0	0	0	0
61	BA	3	0	0	0	0
61	BI	3	0	0	1	0
61	C5	3	0	0	0	0
61	C8	4	0	0	0	0
61	E8	1	0	0	0	0
61	F5	1	0	0	0	0
61	F8	3	0	0	1	0
61	G8	3	0	0	0	0
61	H5	1	0	0	2	0
61	I8	6	0	0	0	0
61	J8	5	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
61	L5	1	0	0	0	0
61	L8	4	0	0	0	0
61	M5	8	0	0	2	0
61	N8	1	0	0	0	0
61	Q8	5	0	0	1	0
All	All	296999	0	196564	8532	2

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 18.

The worst 5 of 8532 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	1.39
47:D5:94:GLU:C	47:D5:95:PRO:N	1.78	1.36
38:45:27:VAL:HB	38:45:28:ALA:HA	1.16	1.08
26:1H:1604:C:OP2	61:1H:3655:HOH:O	1.75	1.04
8:72:12:ARG:HH21	8:72:27:PRO:HD3	1.22	1.02

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

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1G:82:U:O2'	26:14:271(C):U:O4[3_545]	2.14	0.06
26:1H:2137:C:OP1	1:1G:999:U:O2'[4_555]	2.17	0.03

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%)	23 (11%)	7 (3%)	3 18

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	1E	227/256 (89%)	186 (82%)	39 (17%)	2 (1%)	17	50
3	22	191/239 (80%)	172 (90%)	19 (10%)	0	100	100
3	2E	203/239 (85%)	186 (92%)	16 (8%)	1 (0%)	29	63
4	32	206/209 (99%)	180 (87%)	25 (12%)	1 (0%)	29	63
4	3E	205/209 (98%)	193 (94%)	11 (5%)	1 (0%)	29	63
5	42	148/162 (91%)	142 (96%)	5 (3%)	1 (1%)	22	56
5	4E	147/162 (91%)	136 (92%)	10 (7%)	1 (1%)	22	56
6	52	99/101 (98%)	96 (97%)	3 (3%)	0	100	100
6	5E	98/101 (97%)	92 (94%)	6 (6%)	0	100	100
7	62	134/156 (86%)	125 (93%)	8 (6%)	1 (1%)	22	56
7	6E	152/156 (97%)	144 (95%)	8 (5%)	0	100	100
8	72	135/138 (98%)	125 (93%)	8 (6%)	2 (2%)	10	37
8	7E	136/138 (99%)	126 (93%)	9 (7%)	1 (1%)	22	56
9	82	119/128 (93%)	109 (92%)	9 (8%)	1 (1%)	19	53
9	8E	124/128 (97%)	107 (86%)	17 (14%)	0	100	100
10	1A	76/105 (72%)	71 (93%)	5 (7%)	0	100	100
10	1I	92/105 (88%)	83 (90%)	9 (10%)	0	100	100
11	2A	111/129 (86%)	99 (89%)	10 (9%)	2 (2%)	8	33
11	2I	109/129 (84%)	93 (85%)	11 (10%)	5 (5%)	2	13
12	3A	119/132 (90%)	101 (85%)	14 (12%)	4 (3%)	3	18
12	3I	120/132 (91%)	106 (88%)	13 (11%)	1 (1%)	19	53
13	4A	107/126 (85%)	89 (83%)	17 (16%)	1 (1%)	17	50
13	4I	115/126 (91%)	97 (84%)	17 (15%)	1 (1%)	17	50
14	5A	57/61 (93%)	49 (86%)	7 (12%)	1 (2%)	8	33
14	5I	57/61 (93%)	48 (84%)	7 (12%)	2 (4%)	3	18
15	6A	85/89 (96%)	80 (94%)	5 (6%)	0	100	100
15	6I	85/89 (96%)	79 (93%)	6 (7%)	0	100	100
16	7A	82/88 (93%)	76 (93%)	6 (7%)	0	100	100
16	7I	81/88 (92%)	76 (94%)	5 (6%)	0	100	100
17	8A	97/105 (92%)	91 (94%)	6 (6%)	0	100	100
17	8I	98/105 (93%)	93 (95%)	4 (4%)	1 (1%)	15	47

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
18	9A	65/88 (74%)	64 (98%)	1 (2%)	0	100	100
18	9I	66/88 (75%)	63 (96%)	2 (3%)	1 (2%)	10	37
19	AA	59/93 (63%)	49 (83%)	7 (12%)	3 (5%)	2	11
19	AI	80/93 (86%)	69 (86%)	7 (9%)	4 (5%)	2	12
20	BA	97/106 (92%)	79 (81%)	16 (16%)	2 (2%)	7	28
20	BI	95/106 (90%)	83 (87%)	12 (13%)	0	100	100
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	7I	128/229 (56%)	121 (94%)	7 (6%)	0	100	100
29	11	271/276 (98%)	255 (94%)	10 (4%)	6 (2%)	6	27
29	19	272/276 (99%)	248 (91%)	21 (8%)	3 (1%)	14	45
30	21	201/206 (98%)	160 (80%)	28 (14%)	13 (6%)	1	7
30	29	202/206 (98%)	150 (74%)	40 (20%)	12 (6%)	1	9
31	31	200/210 (95%)	177 (88%)	22 (11%)	1 (0%)	29	63
31	39	202/210 (96%)	159 (79%)	36 (18%)	7 (4%)	3	18
32	41	177/182 (97%)	156 (88%)	18 (10%)	3 (2%)	9	34
32	49	178/182 (98%)	155 (87%)	22 (12%)	1 (1%)	25	59
33	51	172/180 (96%)	139 (81%)	23 (13%)	10 (6%)	1	9
33	59	167/180 (93%)	129 (77%)	32 (19%)	6 (4%)	3	18
34	61	143/148 (97%)	123 (86%)	18 (13%)	2 (1%)	11	39
34	69	143/148 (97%)	112 (78%)	28 (20%)	3 (2%)	7	28
35	15	135/140 (96%)	124 (92%)	11 (8%)	0	100	100
35	58	135/140 (96%)	114 (84%)	16 (12%)	5 (4%)	3	17
36	25	120/122 (98%)	110 (92%)	10 (8%)	0	100	100
36	68	120/122 (98%)	115 (96%)	5 (4%)	0	100	100
37	35	145/150 (97%)	120 (83%)	25 (17%)	0	100	100
37	78	145/150 (97%)	113 (78%)	21 (14%)	11 (8%)	1	5
38	45	136/141 (96%)	110 (81%)	23 (17%)	3 (2%)	6	27
38	88	139/141 (99%)	119 (86%)	14 (10%)	6 (4%)	2	14
39	55	116/118 (98%)	110 (95%)	5 (4%)	1 (1%)	17	50
39	98	116/118 (98%)	101 (87%)	15 (13%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
40	65	108/112 (96%)	87 (81%)	19 (18%)	2 (2%)	8	31
40	A8	109/112 (97%)	89 (82%)	19 (17%)	1 (1%)	17	50
41	75	131/146 (90%)	118 (90%)	11 (8%)	2 (2%)	10	37
41	B8	133/146 (91%)	118 (89%)	14 (10%)	1 (1%)	19	53
42	85	114/118 (97%)	107 (94%)	7 (6%)	0	100	100
42	C8	113/118 (96%)	107 (95%)	2 (2%)	4 (4%)	3	18
43	95	98/101 (97%)	81 (83%)	14 (14%)	3 (3%)	4	21
43	D8	98/101 (97%)	87 (89%)	8 (8%)	3 (3%)	4	21
44	A5	109/113 (96%)	101 (93%)	8 (7%)	0	100	100
44	E8	108/113 (96%)	102 (94%)	6 (6%)	0	100	100
45	B5	92/96 (96%)	82 (89%)	8 (9%)	2 (2%)	6	27
45	F8	93/96 (97%)	87 (94%)	6 (6%)	0	100	100
46	C5	102/110 (93%)	74 (72%)	22 (22%)	6 (6%)	1	9
46	G8	101/110 (92%)	83 (82%)	14 (14%)	4 (4%)	3	15
47	D5	175/206 (85%)	133 (76%)	32 (18%)	10 (6%)	1	9
47	H8	168/206 (82%)	136 (81%)	25 (15%)	7 (4%)	3	14
48	E5	74/85 (87%)	65 (88%)	8 (11%)	1 (1%)	11	39
48	I8	75/85 (88%)	67 (89%)	8 (11%)	0	100	100
49	F5	92/98 (94%)	81 (88%)	10 (11%)	1 (1%)	14	45
49	J8	94/98 (96%)	80 (85%)	9 (10%)	5 (5%)	2	11
50	G5	67/72 (93%)	61 (91%)	4 (6%)	2 (3%)	4	21
50	K8	66/72 (92%)	59 (89%)	4 (6%)	3 (4%)	2	13
51	H5	56/60 (93%)	54 (96%)	2 (4%)	0	100	100
51	L8	56/60 (93%)	54 (96%)	2 (4%)	0	100	100
52	M8	56/71 (79%)	39 (70%)	17 (30%)	0	100	100
53	J5	54/60 (90%)	49 (91%)	5 (9%)	0	100	100
53	N8	46/60 (77%)	43 (94%)	3 (6%)	0	100	100
54	L5	45/49 (92%)	42 (93%)	3 (7%)	0	100	100
54	P8	45/49 (92%)	41 (91%)	4 (9%)	0	100	100
55	M5	62/65 (95%)	51 (82%)	11 (18%)	0	100	100
55	Q8	62/65 (95%)	51 (82%)	7 (11%)	4 (6%)	1	7

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	11086/12104 (92%)	9718 (88%)	1167 (10%)	201 (2%)	8 33

5 of 201 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
29	11	239	ARG

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
2	12	179/220 (81%)	144 (80%)	35 (20%)	1 6
2	1E	200/220 (91%)	158 (79%)	42 (21%)	1 5
3	22	154/188 (82%)	123 (80%)	31 (20%)	1 5
3	2E	159/188 (85%)	127 (80%)	32 (20%)	1 5
4	32	180/181 (99%)	152 (84%)	28 (16%)	2 11
4	3E	180/181 (99%)	146 (81%)	34 (19%)	1 6
5	42	114/123 (93%)	88 (77%)	26 (23%)	1 3
5	4E	115/123 (94%)	90 (78%)	25 (22%)	1 4
6	52	90/90 (100%)	78 (87%)	12 (13%)	4 16
6	5E	90/90 (100%)	73 (81%)	17 (19%)	1 6
7	62	114/127 (90%)	91 (80%)	23 (20%)	1 5
7	6E	125/127 (98%)	105 (84%)	20 (16%)	2 10
8	72	118/119 (99%)	101 (86%)	17 (14%)	3 13
8	7E	119/119 (100%)	93 (78%)	26 (22%)	1 4
9	82	92/99 (93%)	73 (79%)	19 (21%)	1 5
9	8E	97/99 (98%)	70 (72%)	27 (28%)	0 1

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
10	1A	71/92 (77%)	54 (76%)	17 (24%)	0	2
10	1I	81/92 (88%)	75 (93%)	6 (7%)	13	40
11	2A	85/99 (86%)	71 (84%)	14 (16%)	2	9
11	2I	84/99 (85%)	66 (79%)	18 (21%)	1	4
12	3A	102/109 (94%)	82 (80%)	20 (20%)	1	6
12	3I	103/109 (94%)	76 (74%)	27 (26%)	0	1
13	4A	90/101 (89%)	68 (76%)	22 (24%)	0	2
13	4I	94/101 (93%)	67 (71%)	27 (29%)	0	1
14	5A	49/50 (98%)	40 (82%)	9 (18%)	1	7
14	5I	49/50 (98%)	39 (80%)	10 (20%)	1	5
15	6A	79/80 (99%)	71 (90%)	8 (10%)	7	26
15	6I	79/80 (99%)	68 (86%)	11 (14%)	3	15
16	7A	72/74 (97%)	64 (89%)	8 (11%)	6	23
16	7I	72/74 (97%)	58 (81%)	14 (19%)	1	6
17	8A	94/97 (97%)	80 (85%)	14 (15%)	3	12
17	8I	95/97 (98%)	80 (84%)	15 (16%)	2	10
18	9A	58/77 (75%)	49 (84%)	9 (16%)	2	11
18	9I	58/77 (75%)	50 (86%)	8 (14%)	3	15
19	AA	56/80 (70%)	43 (77%)	13 (23%)	1	3
19	AI	72/80 (90%)	57 (79%)	15 (21%)	1	5
20	BA	76/82 (93%)	68 (90%)	8 (10%)	7	24
20	BI	75/82 (92%)	67 (89%)	8 (11%)	6	24
21	1B	17/22 (77%)	16 (94%)	1 (6%)	19	48
21	1F	18/22 (82%)	14 (78%)	4 (22%)	1	4
28	7I	108/181 (60%)	87 (81%)	21 (19%)	1	6
29	11	214/218 (98%)	172 (80%)	42 (20%)	1	6
29	19	214/218 (98%)	167 (78%)	47 (22%)	1	4
30	21	162/166 (98%)	124 (76%)	38 (24%)	1	3
30	29	165/166 (99%)	125 (76%)	40 (24%)	0	2
31	31	161/166 (97%)	130 (81%)	31 (19%)	1	6
31	39	163/166 (98%)	123 (76%)	40 (24%)	0	2

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
32	41	153/156 (98%)	120 (78%)	33 (22%)	1	4
32	49	152/156 (97%)	117 (77%)	35 (23%)	1	3
33	51	143/148 (97%)	109 (76%)	34 (24%)	0	2
33	59	140/148 (95%)	101 (72%)	39 (28%)	0	1
34	61	122/124 (98%)	87 (71%)	35 (29%)	0	1
34	69	122/124 (98%)	88 (72%)	34 (28%)	0	1
35	15	116/119 (98%)	91 (78%)	25 (22%)	1	4
35	58	116/119 (98%)	92 (79%)	24 (21%)	1	5
36	25	100/100 (100%)	82 (82%)	18 (18%)	1	7
36	68	100/100 (100%)	89 (89%)	11 (11%)	6	23
37	35	114/116 (98%)	76 (67%)	38 (33%)	0	0
37	78	114/116 (98%)	77 (68%)	37 (32%)	0	0
38	45	109/111 (98%)	82 (75%)	27 (25%)	0	2
38	88	110/111 (99%)	91 (83%)	19 (17%)	2	8
39	55	101/101 (100%)	86 (85%)	15 (15%)	3	12
39	98	101/101 (100%)	79 (78%)	22 (22%)	1	4
40	65	87/88 (99%)	67 (77%)	20 (23%)	1	3
40	A8	87/88 (99%)	61 (70%)	26 (30%)	0	1
41	75	117/127 (92%)	85 (73%)	32 (27%)	0	1
41	B8	117/127 (92%)	84 (72%)	33 (28%)	0	1
42	85	93/94 (99%)	77 (83%)	16 (17%)	2	8
42	C8	92/94 (98%)	80 (87%)	12 (13%)	4	17
43	95	81/82 (99%)	66 (82%)	15 (18%)	1	7
43	D8	82/82 (100%)	54 (66%)	28 (34%)	0	0
44	A5	91/92 (99%)	72 (79%)	19 (21%)	1	5
44	E8	90/92 (98%)	76 (84%)	14 (16%)	2	11
45	B5	74/78 (95%)	58 (78%)	16 (22%)	1	4
45	F8	77/78 (99%)	67 (87%)	10 (13%)	4	17
46	C5	85/91 (93%)	61 (72%)	24 (28%)	0	1
46	G8	84/91 (92%)	67 (80%)	17 (20%)	1	5
47	D5	156/179 (87%)	118 (76%)	38 (24%)	0	2

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
47	H8	151/179 (84%)	128 (85%)	23 (15%)	3	11
48	E5	61/67 (91%)	55 (90%)	6 (10%)	8	27
48	I8	62/67 (92%)	56 (90%)	6 (10%)	8	28
49	F5	79/83 (95%)	64 (81%)	15 (19%)	1	6
49	J8	79/83 (95%)	67 (85%)	12 (15%)	3	11
50	G5	63/67 (94%)	47 (75%)	16 (25%)	0	1
50	K8	64/67 (96%)	47 (73%)	17 (27%)	0	1
51	H5	50/52 (96%)	37 (74%)	13 (26%)	0	1
51	L8	50/52 (96%)	41 (82%)	9 (18%)	1	7
52	M8	52/63 (82%)	38 (73%)	14 (27%)	0	1
53	J5	48/52 (92%)	38 (79%)	10 (21%)	1	5
53	N8	43/52 (83%)	34 (79%)	9 (21%)	1	5
54	L5	38/42 (90%)	31 (82%)	7 (18%)	1	7
54	P8	38/42 (90%)	31 (82%)	7 (18%)	1	7
55	M5	54/55 (98%)	44 (82%)	10 (18%)	1	7
55	Q8	54/55 (98%)	43 (80%)	11 (20%)	1	5
All	All	9354/10012 (93%)	7424 (79%)	1930 (21%)	1	5

5 of 1930 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
47	H8	1	MET
5	42	31	LEU
45	B5	66	LEU
48	I8	67	VAL
55	Q8	62	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 14 such sidechains are listed below:

Mol	Chain	Res	Type
44	E8	40	ASN
55	Q8	31	HIS
30	29	54	GLN
41	B8	58	ASN
29	19	46	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	13	1500/1522 (98%)	349 (23%)	39 (2%)
1	1G	1508/1522 (99%)	354 (23%)	40 (2%)
22	1K	69/76 (90%)	29 (42%)	5 (7%)
23	2K	76/77 (98%)	24 (31%)	2 (2%)
23	2L	76/77 (98%)	20 (26%)	1 (1%)
24	3K	67/76 (88%)	39 (58%)	2 (2%)
24	3L	69/76 (90%)	32 (46%)	2 (2%)
25	4K	19/30 (63%)	11 (57%)	2 (10%)
25	4L	18/30 (60%)	13 (72%)	1 (5%)
26	14	2820/2917 (96%)	664 (23%)	45 (1%)
26	1H	2824/2917 (96%)	601 (21%)	36 (1%)
27	16	121/122 (99%)	22 (18%)	3 (2%)
27	1J	121/122 (99%)	33 (27%)	2 (1%)
56	1L	62/76 (81%)	27 (43%)	4 (6%)
All	All	9350/9640 (96%)	2218 (23%)	184 (1%)

5 of 2218 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	13	2	U
1	13	3	G
1	13	4	U
1	13	5	U
1	13	6	G

5 of 184 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
26	1H	2210	G
1	1G	466	C
26	14	2275	C
26	1H	2756	U
1	1G	87	A

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

18 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	17,24,25	2.61	5 (29%)	19,34,37	1.63	3 (15%)
23	OMC	2K	33	23	15,22,23	2.14	4 (26%)	17,31,34	1.44	3 (17%)
23	OMC	2L	33	23	15,22,23	2.29	4 (26%)	17,31,34	1.23	2 (11%)
22	T6A	1K	37	22	24,34,35	2.66	4 (16%)	24,49,52	3.01	4 (16%)
23	5MU	2K	55	23	15,22,23	2.16	3 (20%)	16,32,35	1.77	2 (12%)
23	PSU	2K	56	23	17,21,22	1.12	2 (11%)	20,30,33	2.99	5 (25%)
23	4SU	2K	8	23	14,21,22	3.01	2 (14%)	15,30,33	1.05	2 (13%)
22	PSU	1K	55	22	17,21,22	1.09	1 (5%)	20,30,33	3.33	6 (30%)
22	H2U	1K	17	22	18,21,22	2.07	4 (22%)	21,30,33	2.18	5 (23%)
56	PSU	1L	55	56	17,21,22	1.06	1 (5%)	20,30,33	3.37	5 (25%)
23	PSU	2L	56	23	17,21,22	1.28	2 (11%)	20,30,33	3.37	6 (30%)
22	PSU	1K	39	22	17,21,22	0.96	1 (5%)	20,30,33	3.22	6 (30%)
56	5MU	1L	54	56	15,22,23	2.18	3 (20%)	16,32,35	1.70	2 (12%)
23	5MU	2L	55	23	15,22,23	2.21	3 (20%)	16,32,35	1.76	2 (12%)
22	5MU	1K	54	22	15,22,23	2.15	3 (20%)	16,32,35	1.81	2 (12%)
23	4SU	2L	8	23	14,21,22	3.44	2 (14%)	15,30,33	1.13	2 (13%)
23	7MG	2K	47	23	22,26,27	3.59	7 (31%)	28,39,42	2.86	12 (42%)
23	7MG	2L	47	23	22,26,27	3.45	7 (31%)	28,39,42	2.66	11 (39%)

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	-	1/7/28/29	0/2/2/2
23	OMC	2K	33	23	-	0/7/27/28	0/2/2/2
23	OMC	2L	33	23	-	0/7/27/28	0/2/2/2
22	T6A	1K	37	22	-	5/15/41/42	0/3/3/3
23	5MU	2K	55	23	-	2/5/25/26	0/2/2/2
23	PSU	2K	56	23	-	0/7/25/26	0/2/2/2
23	4SU	2K	8	23	-	3/5/25/26	0/2/2/2
22	PSU	1K	55	22	-	0/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	H2U	1K	17	22	-	0/7/38/39	0/2/2/2
56	PSU	1L	55	56	-	0/7/25/26	0/2/2/2
23	PSU	2L	56	23	-	0/7/25/26	0/2/2/2
22	PSU	1K	39	22	-	0/7/25/26	0/2/2/2
56	5MU	1L	54	56	-	3/5/25/26	0/2/2/2
23	5MU	2L	55	23	-	0/5/25/26	0/2/2/2
22	5MU	1K	54	22	-	2/5/25/26	0/2/2/2
23	4SU	2L	8	23	-	2/5/25/26	0/2/2/2
23	7MG	2K	47	23	-	4/7/37/38	0/3/3/3
23	7MG	2L	47	23	-	4/7/37/38	0/3/3/3

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	2L	47	7MG	C4-N3	11.37	1.48	1.34
23	2K	47	7MG	C4-N3	10.57	1.47	1.34
23	2L	8	4SU	C5-C4	10.21	1.50	1.38
23	2K	8	4SU	C5-C4	8.88	1.48	1.38
22	1K	37	T6A	C6-N6	7.92	1.50	1.36

The worst 5 of 80 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	1K	39	PSU	N1-C2-N3	-11.20	119.53	128.43
23	2L	56	PSU	N1-C2-N3	-11.12	119.59	128.43
56	1L	55	PSU	N1-C2-N3	-11.05	119.64	128.43
22	1K	37	T6A	C12-N11-C10	10.96	134.45	122.75
22	1K	55	PSU	N1-C2-N3	-10.80	119.85	128.43

There are no chirality outliers.

5 of 26 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
22	1K	37	T6A	C14-C12-N11-C10
22	1K	37	T6A	N11-C12-C14-O14
22	1K	37	T6A	N11-C12-C14-C15
22	1K	37	T6A	C13-C12-C14-O14
22	1K	37	T6A	C13-C12-C14-C15

There are no ring outliers.

9 monomers are involved in 25 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
23	2K	33	OMC	1	0
23	2L	33	OMC	3	0
22	1K	37	T6A	1	0
23	2K	55	5MU	5	0
23	2K	8	4SU	1	0
56	1L	54	5MU	2	0
22	1K	54	5MU	3	0
23	2K	47	7MG	6	0
23	2L	47	7MG	3	0

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 1345 ligands modelled in this entry, 1341 are monoatomic - leaving 4 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	$\# Z > 2$
60	SPE	1G	1725	1	12,12,12	0.41	0	11,11,11	0.73	0
58	SF4	32	302	-	0,12,12	0.00	-	-		
60	SPE	14	3458	-	12,12,12	0.45	0	11,11,11	0.76	0
58	SF4	3E	301	4	0,12,12	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
60	SPE	1G	1725	1	-	5/10/10/10	-
58	SF4	32	302	-	-	-	0/6/5/5

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
60	SPE	14	3458	-	-	5/10/10/10	-
58	SF4	3E	301	4	-	-	0/6/5/5

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

5 of 10 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
60	1G	1725	SPE	C2-C3-C4-N5
60	14	3458	SPE	N9-C10-C11-C12
60	14	3458	SPE	C2-C3-C4-N5
60	14	3458	SPE	C6-C7-C8-N9
60	1G	1725	SPE	C11-C10-N9-C8

There are no ring outliers.

2 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
60	1G	1725	SPE	3	0
58	32	302	SF4	2	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
34	69	1
4	3E	1
47	D5	1
10	1A	1
56	1L	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	1L	72:C	O3'	73:A	P	3.48
1	D5	94:GLU	C	95:PRO	N	1.78
1	1A	38:ILE	C	39:PRO	N	1.71
1	69	79:ILE	C	80:PRO	N	1.17
1	3E	36:ARG	C	37:PRO	N	1.15

6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	13	1500/1522 (98%)	-0.52	0 100 100	67, 111, 176, 243	0
1	1G	1509/1522 (99%)	-0.47	3 (0%) 95 91	76, 123, 193, 253	0
2	12	207/256 (80%)	0.27	13 (6%) 20 9	139, 165, 185, 196	0
2	1E	231/256 (90%)	-0.06	5 (2%) 62 42	118, 145, 172, 180	0
3	22	195/239 (81%)	0.75	27 (13%) 2 1	123, 147, 164, 175	0
3	2E	205/239 (85%)	0.34	12 (5%) 22 10	97, 117, 144, 155	0
4	32	208/209 (99%)	-0.31	0 100 100	104, 123, 142, 149	0
4	3E	207/209 (99%)	-0.20	1 (0%) 91 83	93, 118, 137, 144	0
5	42	150/162 (92%)	-0.23	0 100 100	106, 123, 139, 146	0
5	4E	149/162 (91%)	-0.06	0 100 100	87, 109, 128, 133	0
6	52	101/101 (100%)	-0.42	0 100 100	93, 110, 124, 135	0
6	5E	100/101 (99%)	-0.03	1 (1%) 82 70	92, 111, 127, 135	0
7	62	138/156 (88%)	0.83	13 (9%) 8 3	122, 135, 145, 151	0
7	6E	154/156 (98%)	1.00	29 (18%) 1 0	111, 127, 155, 174	0
8	72	137/138 (99%)	-0.08	2 (1%) 73 56	106, 129, 141, 149	0
8	7E	138/138 (100%)	0.78	15 (10%) 5 2	102, 117, 129, 139	0
9	82	121/128 (94%)	1.39	31 (25%) 0 0	118, 161, 171, 178	0
9	8E	126/128 (98%)	-0.09	2 (1%) 72 53	96, 141, 159, 165	0
10	1A	80/105 (76%)	0.36	11 (13%) 2 1	122, 152, 167, 170	0
10	1I	94/105 (89%)	1.43	26 (27%) 0 0	92, 136, 171, 178	0
11	2A	113/129 (87%)	0.79	13 (11%) 4 2	91, 116, 131, 138	0
11	2I	111/129 (86%)	1.40	29 (26%) 0 0	84, 113, 129, 138	0
12	3A	121/132 (91%)	0.68	18 (14%) 2 1	94, 109, 128, 144	0
12	3I	122/132 (92%)	0.11	3 (2%) 57 37	81, 89, 110, 132	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
13	4A	109/126 (86%)	0.21	14 (12%) 3 1	125, 152, 170, 187	0
13	4I	117/126 (92%)	-0.04	3 (2%) 56 35	97, 125, 138, 145	0
14	5A	59/61 (96%)	2.08	26 (44%) 0 0	131, 146, 164, 167	0
14	5I	59/61 (96%)	0.51	4 (6%) 17 7	92, 106, 121, 129	0
15	6A	87/89 (97%)	-0.54	0 100 100	93, 117, 133, 137	0
15	6I	87/89 (97%)	0.13	2 (2%) 60 40	89, 107, 126, 130	0
16	7A	84/88 (95%)	-0.37	0 100 100	100, 116, 137, 159	0
16	7I	83/88 (94%)	-0.02	1 (1%) 79 64	107, 119, 145, 163	0
17	8A	99/105 (94%)	0.02	0 100 100	100, 112, 125, 131	0
17	8I	100/105 (95%)	1.09	15 (15%) 2 1	95, 114, 124, 128	0
18	9A	67/88 (76%)	-0.23	1 (1%) 73 56	101, 117, 135, 140	0
18	9I	68/88 (77%)	0.03	0 100 100	97, 113, 133, 138	0
19	AA	65/93 (69%)	0.57	9 (13%) 2 1	130, 162, 174, 180	0
19	AI	82/93 (88%)	0.44	7 (8%) 10 4	108, 126, 146, 153	0
20	BA	99/106 (93%)	0.86	17 (17%) 1 1	94, 119, 140, 153	0
20	BI	97/106 (91%)	0.91	21 (21%) 0 0	113, 127, 150, 157	0
21	1B	22/27 (81%)	1.06	4 (18%) 1 0	122, 139, 143, 150	0
21	1F	23/27 (85%)	-0.44	0 100 100	103, 110, 116, 123	0
22	1K	66/76 (86%)	0.03	1 (1%) 73 56	104, 183, 206, 213	0
23	2K	72/77 (93%)	-0.01	2 (2%) 53 31	75, 100, 133, 145	0
23	2L	72/77 (93%)	-0.23	1 (1%) 75 59	85, 120, 153, 162	0
24	3K	70/76 (92%)	1.17	19 (27%) 0 0	82, 225, 245, 249	0
24	3L	72/76 (94%)	-0.01	2 (2%) 53 31	87, 206, 223, 228	0
25	4K	20/30 (66%)	0.71	4 (20%) 1 0	81, 145, 215, 216	0
25	4L	19/30 (63%)	0.13	1 (5%) 26 12	101, 162, 218, 218	0
26	14	2825/2917 (96%)	-0.29	11 (0%) 92 86	62, 91, 198, 251	0
26	1H	2831/2917 (97%)	-0.32	3 (0%) 95 93	51, 79, 176, 251	0
27	16	122/122 (100%)	-0.57	1 (0%) 86 74	76, 98, 118, 204	0
27	1J	122/122 (100%)	-0.76	0 100 100	94, 133, 152, 210	0
28	7I	132/229 (57%)	0.36	10 (7%) 13 5	143, 206, 228, 235	0
29	11	273/276 (98%)	0.12	1 (0%) 92 86	48, 71, 88, 95	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
29	19	274/276 (99%)	0.13	1 (0%) 92 86	56, 80, 94, 111	0
30	21	203/206 (98%)	0.18	3 (1%) 73 56	57, 90, 121, 133	0
30	29	204/206 (99%)	0.40	13 (6%) 19 8	66, 97, 133, 147	0
31	31	202/210 (96%)	0.19	4 (1%) 65 46	51, 82, 114, 134	0
31	39	204/210 (97%)	-0.12	1 (0%) 91 83	64, 105, 148, 175	0
32	41	179/182 (98%)	0.28	6 (3%) 45 24	90, 109, 139, 154	0
32	49	180/182 (98%)	0.59	23 (12%) 3 1	125, 147, 166, 179	0
33	51	174/180 (96%)	-0.31	0 100 100	82, 105, 123, 133	0
33	59	169/180 (93%)	2.49	94 (55%) 0 0	157, 203, 223, 233	0
34	61	145/148 (97%)	0.14	4 (2%) 53 31	82, 128, 147, 153	0
34	69	145/148 (97%)	-0.15	1 (0%) 87 77	91, 129, 149, 154	0
35	15	137/140 (97%)	0.61	12 (8%) 10 4	82, 110, 140, 150	0
35	58	137/140 (97%)	0.31	4 (2%) 51 30	71, 90, 122, 138	0
36	25	122/122 (100%)	1.04	14 (11%) 4 2	74, 90, 108, 120	0
36	68	122/122 (100%)	-0.21	0 100 100	67, 82, 98, 106	0
37	35	147/150 (98%)	0.65	21 (14%) 2 1	64, 106, 141, 158	0
37	78	147/150 (98%)	0.21	0 100 100	58, 84, 106, 114	0
38	45	138/141 (97%)	0.18	3 (2%) 62 42	79, 106, 127, 138	0
38	88	141/141 (100%)	0.62	8 (5%) 23 11	62, 83, 105, 133	0
39	55	118/118 (100%)	0.20	2 (1%) 70 51	68, 85, 100, 113	0
39	98	118/118 (100%)	0.56	6 (5%) 28 13	67, 86, 103, 117	0
40	65	110/112 (98%)	-0.07	4 (3%) 42 22	99, 124, 141, 145	0
40	A8	111/112 (99%)	0.15	4 (3%) 42 22	82, 95, 114, 127	0
41	75	133/146 (91%)	0.72	8 (6%) 21 10	82, 97, 127, 145	0
41	B8	135/146 (92%)	-0.29	1 (0%) 87 77	79, 96, 135, 151	0
42	85	116/118 (98%)	0.03	0 100 100	72, 101, 129, 136	0
42	C8	115/118 (97%)	0.18	2 (1%) 70 51	60, 82, 108, 115	0
43	95	100/101 (99%)	0.55	6 (6%) 21 10	72, 120, 140, 147	0
43	D8	100/101 (99%)	1.15	17 (17%) 1 1	62, 100, 120, 130	0
44	A5	111/113 (98%)	0.15	1 (0%) 84 72	71, 81, 107, 139	0
44	E8	110/113 (97%)	0.27	4 (3%) 42 22	64, 77, 100, 113	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
45	B5	94/96 (97%)	0.84	12 (12%) 3 1	78, 90, 111, 121	0
45	F8	95/96 (98%)	-0.12	0 100 100	59, 74, 98, 108	0
46	C5	104/110 (94%)	1.01	19 (18%) 1 0	92, 119, 152, 158	0
46	G8	103/110 (93%)	-0.38	0 100 100	76, 97, 124, 134	0
47	D5	177/206 (85%)	1.43	50 (28%) 0 0	117, 159, 218, 223	0
47	H8	170/206 (82%)	1.58	56 (32%) 0 0	88, 121, 189, 196	0
48	E5	76/85 (89%)	0.32	3 (3%) 39 20	78, 97, 111, 120	0
48	I8	77/85 (90%)	0.23	2 (2%) 56 35	64, 79, 96, 108	0
49	F5	94/98 (95%)	1.18	20 (21%) 0 0	69, 89, 125, 139	0
49	J8	96/98 (97%)	0.37	1 (1%) 82 70	61, 80, 117, 123	0
50	G5	69/72 (95%)	0.33	3 (4%) 35 17	90, 109, 132, 144	0
50	K8	68/72 (94%)	-0.15	1 (1%) 73 56	68, 84, 105, 129	0
51	H5	58/60 (96%)	0.68	1 (1%) 70 51	81, 101, 126, 136	0
51	L8	58/60 (96%)	0.35	0 100 100	70, 84, 110, 122	0
52	M8	60/71 (84%)	1.13	10 (16%) 1 1	114, 150, 177, 181	0
53	J5	56/60 (93%)	0.13	1 (1%) 68 49	67, 90, 133, 143	0
53	N8	48/60 (80%)	0.27	1 (2%) 63 44	56, 85, 128, 135	0
54	L5	47/49 (95%)	0.46	2 (4%) 35 17	61, 69, 91, 100	0
54	P8	47/49 (95%)	-0.13	0 100 100	54, 59, 77, 89	0
55	M5	64/65 (98%)	1.19	18 (28%) 0 0	76, 86, 101, 117	0
55	Q8	64/65 (98%)	0.22	0 100 100	61, 75, 88, 101	0
56	1L	64/76 (84%)	0.13	2 (3%) 49 27	140, 201, 221, 227	0
All	All	20656/21744 (94%)	0.05	903 (4%) 34 17	48, 105, 181, 253	0

The worst 5 of 903 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
43	D8	37	VAL	14.5
47	H8	113	ALA	10.9
33	59	17	VAL	10.1
33	59	96	ALA	8.5
33	59	95	ARG	8.2

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

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
56	PSU	1L	55	20/21	0.85	0.10	121,135,144,145	0
22	H2U	1K	17	20/21	0.86	0.14	130,139,153,158	0
22	PSU	1K	55	20/21	0.88	0.15	115,126,136,137	0
23	7MG	2K	47	24/25	0.88	0.19	99,108,119,120	0
22	5MU	1K	54	21/22	0.89	0.17	116,121,138,149	0
23	PSU	2L	56	20/21	0.90	0.11	112,122,130,133	0
56	5MU	1L	54	21/22	0.92	0.11	125,136,146,154	0
23	4SU	2K	8	20/21	0.93	0.16	91,99,105,106	0
22	T6A	1K	37	32/33	0.93	0.20	91,108,133,134	0
23	PSU	2K	56	20/21	0.94	0.12	102,108,119,120	0
23	5MU	2K	55	21/22	0.94	0.14	105,112,118,128	0
23	4SU	2L	8	20/21	0.94	0.15	108,116,123,125	0
22	PSU	1K	39	20/21	0.94	0.11	100,119,123,124	0
23	7MG	2L	47	24/25	0.94	0.13	124,131,143,146	0
23	OMC	2L	33	21/22	0.96	0.18	100,107,110,117	0
23	5MU	2L	55	21/22	0.96	0.14	115,126,133,135	0
23	OMC	2K	33	21/22	0.96	0.25	85,89,90,91	0
22	U8U	1K	34	23/24	0.97	0.15	98,105,115,118	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. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
57	MG	14	3456	1/1	0.12	0.16	118,118,118,118	0
57	MG	1H	3347	1/1	0.14	0.12	113,113,113,113	0
57	MG	1H	3176	1/1	0.32	0.41	102,102,102,102	0
57	MG	13	1648	1/1	0.37	0.49	117,117,117,117	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	14	3080	1/1	0.41	0.23	71,71,71,71	0
57	MG	14	3163	1/1	0.44	0.45	104,104,104,104	0
57	MG	1G	1723	1/1	0.45	0.19	127,127,127,127	0
57	MG	14	3074	1/1	0.45	0.59	95,95,95,95	0
57	MG	1G	1620	1/1	0.45	0.63	93,93,93,93	0
57	MG	1H	3452	1/1	0.46	0.10	115,115,115,115	0
57	MG	1H	3534	1/1	0.47	0.11	113,113,113,113	0
57	MG	1H	3493	1/1	0.47	0.16	106,106,106,106	0
57	MG	1G	1629	1/1	0.47	0.19	129,129,129,129	0
57	MG	1H	3421	1/1	0.47	0.38	93,93,93,93	0
57	MG	13	1715	1/1	0.50	0.17	119,119,119,119	0
57	MG	14	3153	1/1	0.50	0.23	123,123,123,123	0
57	MG	14	3199	1/1	0.51	0.55	99,99,99,99	0
57	MG	1H	3197	1/1	0.51	0.38	93,93,93,93	0
57	MG	1H	3525	1/1	0.53	0.19	99,99,99,99	0
57	MG	14	3413	1/1	0.53	0.17	125,125,125,125	0
57	MG	1H	3402	1/1	0.54	0.20	71,71,71,71	0
57	MG	1G	1647	1/1	0.54	0.23	99,99,99,99	0
57	MG	1H	3484	1/1	0.54	0.29	97,97,97,97	0
57	MG	14	3165	1/1	0.54	0.67	97,97,97,97	0
57	MG	1H	3506	1/1	0.54	0.25	103,103,103,103	0
57	MG	1G	1698	1/1	0.54	0.07	138,138,138,138	0
57	MG	14	3453	1/1	0.55	0.20	118,118,118,118	0
57	MG	13	1692	1/1	0.55	0.15	110,110,110,110	0
57	MG	13	1638	1/1	0.55	0.56	103,103,103,103	0
57	MG	13	1728	1/1	0.56	0.09	117,117,117,117	0
57	MG	13	1669	1/1	0.56	0.14	111,111,111,111	0
57	MG	1H	3514	1/1	0.56	0.13	112,112,112,112	0
57	MG	1H	3497	1/1	0.57	0.24	96,96,96,96	0
57	MG	1H	3166	1/1	0.58	0.23	67,67,67,67	0
57	MG	14	3194	1/1	0.58	0.50	84,84,84,84	0
57	MG	14	3135	1/1	0.59	0.38	112,112,112,112	0
57	MG	1H	3013	1/1	0.60	0.18	94,94,94,94	0
57	MG	1G	1711	1/1	0.60	0.06	156,156,156,156	0
57	MG	14	3079	1/1	0.60	0.47	86,86,86,86	0
57	MG	1H	3432	1/1	0.60	0.17	116,116,116,116	0
57	MG	1J	209	1/1	0.60	0.07	131,131,131,131	0
57	MG	1H	3062	1/1	0.60	0.17	64,64,64,64	0
57	MG	14	3177	1/1	0.61	0.46	81,81,81,81	0
57	MG	1H	3167	1/1	0.61	0.48	86,86,86,86	0
57	MG	1H	3489	1/1	0.61	0.15	107,107,107,107	0
57	MG	32	301	1/1	0.62	0.12	137,137,137,137	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	13	1655	1/1	0.62	0.42	83,83,83,83	0
57	MG	14	3355	1/1	0.62	0.20	99,99,99,99	0
57	MG	1H	3177	1/1	0.62	0.20	143,143,143,143	0
57	MG	1G	1702	1/1	0.62	0.08	117,117,117,117	0
57	MG	1H	3180	1/1	0.62	0.34	81,81,81,81	0
57	MG	14	3161	1/1	0.62	0.25	94,94,94,94	0
57	MG	1H	3341	1/1	0.63	0.14	113,113,113,113	0
57	MG	1H	3536	1/1	0.63	0.17	104,104,104,104	0
57	MG	13	1668	1/1	0.63	0.29	112,112,112,112	0
57	MG	14	3333	1/1	0.63	0.19	97,97,97,97	0
57	MG	1H	3371	1/1	0.63	0.15	88,88,88,88	0
57	MG	1H	3210	1/1	0.64	0.34	87,87,87,87	0
57	MG	16	206	1/1	0.64	0.24	83,83,83,83	0
57	MG	14	3429	1/1	0.64	0.31	109,109,109,109	0
57	MG	1H	3365	1/1	0.65	0.10	82,82,82,82	0
57	MG	1H	3071	1/1	0.65	0.25	101,101,101,101	0
57	MG	13	1736	1/1	0.66	0.12	129,129,129,129	0
57	MG	1H	3087	1/1	0.66	0.53	75,75,75,75	0
57	MG	1H	3085	1/1	0.66	0.34	79,79,79,79	0
57	MG	1H	3117	1/1	0.66	0.18	96,96,96,96	0
57	MG	1H	3333	1/1	0.67	0.09	98,98,98,98	0
57	MG	E5	101	1/1	0.67	0.66	99,99,99,99	0
57	MG	1H	3338	1/1	0.67	0.10	99,99,99,99	0
57	MG	1H	3055	1/1	0.67	0.27	62,62,62,62	0
57	MG	1H	3335	1/1	0.67	0.09	83,83,83,83	0
57	MG	1H	3509	1/1	0.67	0.36	114,114,114,114	0
57	MG	1H	3173	1/1	0.67	0.32	77,77,77,77	0
57	MG	1H	3089	1/1	0.67	0.43	88,88,88,88	0
57	MG	13	1667	1/1	0.67	0.15	104,104,104,104	0
57	MG	1H	3422	1/1	0.68	0.11	114,114,114,114	0
57	MG	14	3109	1/1	0.68	0.31	94,94,94,94	0
57	MG	2K	103	1/1	0.68	0.18	88,88,88,88	0
57	MG	1H	3213	1/1	0.68	0.22	83,83,83,83	0
57	MG	1H	3175	1/1	0.68	0.37	73,73,73,73	0
57	MG	13	1683	1/1	0.68	0.12	119,119,119,119	0
57	MG	14	3138	1/1	0.68	0.45	91,91,91,91	0
57	MG	1H	3337	1/1	0.68	0.07	98,98,98,98	0
57	MG	13	1642	1/1	0.69	0.30	95,95,95,95	0
57	MG	13	1666	1/1	0.69	0.24	98,98,98,98	0
57	MG	1H	3481	1/1	0.69	0.15	92,92,92,92	0
57	MG	14	3399	1/1	0.69	0.09	122,122,122,122	0
57	MG	1H	3008	1/1	0.69	0.28	81,81,81,81	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	14	3141	1/1	0.69	0.20	85,85,85,85	0
57	MG	25	301	1/1	0.69	0.20	120,120,120,120	0
57	MG	1H	3433	1/1	0.69	0.10	98,98,98,98	0
57	MG	1G	1609	1/1	0.69	0.65	96,96,96,96	0
57	MG	14	3427	1/1	0.69	0.15	121,121,121,121	0
57	MG	14	3431	1/1	0.69	0.17	107,107,107,107	0
57	MG	14	3103	1/1	0.69	0.53	80,80,80,80	0
57	MG	13	1740	1/1	0.70	0.14	162,162,162,162	0
57	MG	1H	3152	1/1	0.70	0.28	87,87,87,87	0
57	MG	1H	3124	1/1	0.70	0.36	90,90,90,90	0
57	MG	1G	1704	1/1	0.70	0.21	127,127,127,127	0
57	MG	14	3027	1/1	0.70	0.08	85,85,85,85	0
57	MG	13	1719	1/1	0.70	0.07	118,118,118,118	0
57	MG	1G	1638	1/1	0.70	0.34	119,119,119,119	0
57	MG	14	3222	1/1	0.71	0.18	73,73,73,73	0
57	MG	1G	1701	1/1	0.71	0.12	115,115,115,115	0
57	MG	1G	1634	1/1	0.71	0.39	98,98,98,98	0
57	MG	14	3173	1/1	0.71	0.26	90,90,90,90	0
57	MG	1H	3535	1/1	0.71	0.20	110,110,110,110	0
57	MG	14	3133	1/1	0.71	0.93	89,89,89,89	0
57	MG	14	3010	1/1	0.71	0.23	84,84,84,84	0
57	MG	14	3455	1/1	0.72	0.37	115,115,115,115	0
57	MG	1H	3326	1/1	0.72	0.10	109,109,109,109	0
57	MG	1H	3537	1/1	0.72	0.11	112,112,112,112	0
57	MG	14	3423	1/1	0.72	0.18	118,118,118,118	0
57	MG	13	1684	1/1	0.72	0.10	105,105,105,105	0
57	MG	1G	1643	1/1	0.72	0.10	100,100,100,100	0
57	MG	P8	101	1/1	0.72	0.46	76,76,76,76	0
57	MG	14	3446	1/1	0.72	0.07	118,118,118,118	0
57	MG	1H	3408	1/1	0.73	0.10	87,87,87,87	0
57	MG	1H	3241	1/1	0.73	0.20	82,82,82,82	0
57	MG	1H	3459	1/1	0.73	0.16	88,88,88,88	0
57	MG	1H	3169	1/1	0.73	0.27	91,91,91,91	0
57	MG	14	3175	1/1	0.73	0.54	100,100,100,100	0
57	MG	14	3185	1/1	0.73	0.24	93,93,93,93	0
57	MG	13	1610	1/1	0.73	0.56	81,81,81,81	0
57	MG	14	3187	1/1	0.73	0.46	106,106,106,106	0
57	MG	14	3406	1/1	0.73	0.17	121,121,121,121	0
57	MG	1H	3364	1/1	0.73	0.12	85,85,85,85	0
57	MG	14	3377	1/1	0.73	0.12	72,72,72,72	0
57	MG	14	3457	1/1	0.73	0.09	134,134,134,134	0
57	MG	1H	3232	1/1	0.74	0.38	100,100,100,100	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	1H	3519	1/1	0.74	0.16	104,104,104,104	0
57	MG	14	3179	1/1	0.74	0.30	103,103,103,103	0
57	MG	39	301	1/1	0.74	0.17	80,80,80,80	0
57	MG	1H	3552	1/1	0.74	0.22	113,113,113,113	0
57	MG	13	1678	1/1	0.74	0.17	114,114,114,114	0
57	MG	1G	1706	1/1	0.74	0.05	138,138,138,138	0
57	MG	1H	3090	1/1	0.74	0.27	82,82,82,82	0
57	MG	1G	1662	1/1	0.74	0.11	118,118,118,118	0
57	MG	1H	3237	1/1	0.74	0.56	85,85,85,85	0
57	MG	14	3388	1/1	0.74	0.13	72,72,72,72	0
57	MG	1H	3504	1/1	0.74	0.29	104,104,104,104	0
57	MG	1H	3279	1/1	0.75	0.12	68,68,68,68	0
57	MG	13	1654	1/1	0.75	0.34	85,85,85,85	0
57	MG	1H	3050	1/1	0.75	0.35	85,85,85,85	0
57	MG	1G	1712	1/1	0.75	0.29	110,110,110,110	0
57	MG	14	3154	1/1	0.75	0.33	78,78,78,78	0
57	MG	14	3437	1/1	0.75	0.11	111,111,111,111	0
57	MG	1H	3221	1/1	0.75	0.38	81,81,81,81	0
57	MG	14	3301	1/1	0.76	0.11	89,89,89,89	0
57	MG	14	3128	1/1	0.76	0.35	88,88,88,88	0
57	MG	1H	3077	1/1	0.76	0.42	76,76,76,76	0
57	MG	13	1675	1/1	0.76	0.16	91,91,91,91	0
57	MG	14	3115	1/1	0.76	0.45	78,78,78,78	0
57	MG	1G	1684	1/1	0.76	0.07	109,109,109,109	0
57	MG	14	3425	1/1	0.76	0.28	106,106,106,106	0
57	MG	14	3255	1/1	0.76	0.12	110,110,110,110	0
57	MG	14	3144	1/1	0.76	0.40	84,84,84,84	0
57	MG	1H	3086	1/1	0.76	0.29	67,67,67,67	0
57	MG	13	1712	1/1	0.76	0.07	106,106,106,106	0
57	MG	1H	3147	1/1	0.76	0.39	125,125,125,125	0
57	MG	1H	3325	1/1	0.76	0.10	88,88,88,88	0
57	MG	1G	1724	1/1	0.76	0.06	126,126,126,126	0
57	MG	1H	3540	1/1	0.76	0.45	110,110,110,110	0
57	MG	1H	3215	1/1	0.76	0.45	94,94,94,94	0
57	MG	1H	3182	1/1	0.76	0.17	108,108,108,108	0
57	MG	14	3081	1/1	0.76	0.17	79,79,79,79	0
57	MG	14	3341	1/1	0.76	0.32	78,78,78,78	0
57	MG	1J	207	1/1	0.76	0.09	119,119,119,119	0
57	MG	14	3392	1/1	0.76	0.15	98,98,98,98	0
57	MG	88	202	1/1	0.77	0.31	71,71,71,71	0
57	MG	14	3339	1/1	0.77	0.05	106,106,106,106	0
57	MG	1H	3369	1/1	0.77	0.27	90,90,90,90	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	14	3145	1/1	0.77	0.39	71,71,71,71	0
57	MG	14	3198	1/1	0.77	0.30	88,88,88,88	0
57	MG	1H	3181	1/1	0.77	0.35	98,98,98,98	0
57	MG	1H	3510	1/1	0.77	0.07	104,104,104,104	0
57	MG	1G	1720	1/1	0.77	0.10	135,135,135,135	0
57	MG	1H	3411	1/1	0.77	0.17	95,95,95,95	0
57	MG	1H	3498	1/1	0.77	0.08	113,113,113,113	0
57	MG	1H	3227	1/1	0.77	0.20	90,90,90,90	0
57	MG	14	3183	1/1	0.77	0.45	88,88,88,88	0
57	MG	1H	3170	1/1	0.77	0.23	80,80,80,80	0
57	MG	14	3130	1/1	0.77	0.28	92,92,92,92	0
57	MG	13	1723	1/1	0.77	0.12	118,118,118,118	0
57	MG	1H	3208	1/1	0.77	0.19	69,69,69,69	0
57	MG	14	3159	1/1	0.77	0.27	80,80,80,80	0
57	MG	13	1649	1/1	0.78	0.18	83,83,83,83	0
57	MG	1H	3162	1/1	0.78	0.61	92,92,92,92	0
57	MG	13	1629	1/1	0.78	0.31	100,100,100,100	0
57	MG	1H	3235	1/1	0.78	0.22	96,96,96,96	0
57	MG	1J	208	1/1	0.78	0.17	124,124,124,124	0
57	MG	14	3379	1/1	0.78	0.12	107,107,107,107	0
57	MG	1H	3494	1/1	0.78	0.20	87,87,87,87	0
57	MG	14	3300	1/1	0.78	0.08	86,86,86,86	0
57	MG	14	3451	1/1	0.78	0.34	110,110,110,110	0
57	MG	2L	102	1/1	0.78	0.17	126,126,126,126	0
57	MG	14	3087	1/1	0.78	0.18	75,75,75,75	0
57	MG	14	3140	1/1	0.79	0.32	89,89,89,89	0
57	MG	14	3450	1/1	0.79	0.31	116,116,116,116	0
57	MG	14	3124	1/1	0.79	0.35	64,64,64,64	0
57	MG	1H	3399	1/1	0.79	0.07	109,109,109,109	0
57	MG	1G	1605	1/1	0.79	0.32	109,109,109,109	0
57	MG	14	3397	1/1	0.79	0.07	162,162,162,162	0
57	MG	13	1709	1/1	0.79	0.05	128,128,128,128	0
57	MG	14	3158	1/1	0.79	0.26	84,84,84,84	0
57	MG	1G	1611	1/1	0.79	0.62	84,84,84,84	0
57	MG	1H	3415	1/1	0.79	0.13	95,95,95,95	0
57	MG	1H	3543	1/1	0.79	0.12	166,166,166,166	0
57	MG	14	3384	1/1	0.79	0.09	88,88,88,88	0
57	MG	1G	1667	1/1	0.79	0.21	111,111,111,111	0
57	MG	1H	3502	1/1	0.79	0.12	90,90,90,90	0
57	MG	14	3134	1/1	0.79	0.70	99,99,99,99	0
57	MG	14	3351	1/1	0.79	0.10	101,101,101,101	0
57	MG	14	3116	1/1	0.79	0.21	77,77,77,77	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	1H	3142	1/1	0.79	0.48	87,87,87,87	0
57	MG	13	1621	1/1	0.79	0.48	94,94,94,94	0
57	MG	14	3383	1/1	0.79	0.13	91,91,91,91	0
57	MG	13	1735	1/1	0.79	0.13	105,105,105,105	0
57	MG	14	3430	1/1	0.79	0.22	102,102,102,102	0
57	MG	13	1699	1/1	0.79	0.19	114,114,114,114	0
57	MG	14	3375	1/1	0.80	0.39	116,116,116,116	0
57	MG	1H	3401	1/1	0.80	0.14	99,99,99,99	0
57	MG	1H	3217	1/1	0.80	0.39	79,79,79,79	0
57	MG	1H	3551	1/1	0.80	0.11	86,86,86,86	0
57	MG	1H	3456	1/1	0.80	0.15	92,92,92,92	0
57	MG	1J	210	1/1	0.80	0.08	135,135,135,135	0
57	MG	1G	1697	1/1	0.80	0.09	125,125,125,125	0
57	MG	1H	3110	1/1	0.80	0.34	86,86,86,86	0
57	MG	1G	1633	1/1	0.80	0.12	102,102,102,102	0
57	MG	14	3422	1/1	0.80	0.11	104,104,104,104	0
57	MG	13	1734	1/1	0.80	0.10	143,143,143,143	0
57	MG	21	302	1/1	0.80	0.34	85,85,85,85	0
57	MG	13	1727	1/1	0.80	0.07	124,124,124,124	0
57	MG	1H	3048	1/1	0.80	0.14	68,68,68,68	0
57	MG	1H	3042	1/1	0.80	0.28	67,67,67,67	0
57	MG	14	3160	1/1	0.80	0.45	85,85,85,85	0
57	MG	1G	1659	1/1	0.80	0.10	120,120,120,120	0
57	MG	1H	3548	1/1	0.80	0.42	98,98,98,98	0
57	MG	1G	1696	1/1	0.80	0.10	109,109,109,109	0
57	MG	1H	3246	1/1	0.80	0.17	54,54,54,54	0
57	MG	13	1718	1/1	0.80	0.04	130,130,130,130	0
57	MG	14	3008	1/1	0.80	0.15	73,73,73,73	0
57	MG	14	3400	1/1	0.80	0.08	135,135,135,135	0
57	MG	1H	3010	1/1	0.80	0.37	87,87,87,87	0
57	MG	13	1618	1/1	0.80	0.27	72,72,72,72	0
57	MG	13	1700	1/1	0.80	0.06	110,110,110,110	0
57	MG	1G	1650	1/1	0.80	0.23	111,111,111,111	0
57	MG	1H	3513	1/1	0.80	0.14	104,104,104,104	0
57	MG	1H	3157	1/1	0.80	0.45	89,89,89,89	0
57	MG	14	3395	1/1	0.81	0.21	98,98,98,98	0
57	MG	1H	3159	1/1	0.81	0.41	95,95,95,95	0
57	MG	1H	3161	1/1	0.81	0.35	77,77,77,77	0
57	MG	1H	3160	1/1	0.81	0.23	79,79,79,79	0
57	MG	14	3166	1/1	0.81	0.34	95,95,95,95	0
57	MG	14	3137	1/1	0.81	0.34	76,76,76,76	0
57	MG	1H	3436	1/1	0.81	0.10	87,87,87,87	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	52	300	1/1	0.81	0.12	133,133,133,133	0
57	MG	14	3381	1/1	0.81	0.07	136,136,136,136	0
57	MG	1G	1658	1/1	0.81	0.08	97,97,97,97	0
57	MG	14	3324	1/1	0.81	0.09	90,90,90,90	0
57	MG	14	3259	1/1	0.81	0.13	97,97,97,97	0
57	MG	14	3454	1/1	0.81	0.12	108,108,108,108	0
57	MG	1H	3012	1/1	0.81	0.23	81,81,81,81	0
57	MG	16	204	1/1	0.81	0.20	89,89,89,89	0
57	MG	14	3328	1/1	0.81	0.10	95,95,95,95	0
57	MG	1H	3172	1/1	0.81	0.23	64,64,64,64	0
57	MG	1H	3391	1/1	0.81	0.41	90,90,90,90	0
57	MG	14	3267	1/1	0.81	0.07	119,119,119,119	0
57	MG	14	3210	1/1	0.81	0.09	78,78,78,78	0
57	MG	1H	3065	1/1	0.81	0.16	72,72,72,72	0
57	MG	1H	3383	1/1	0.81	0.16	74,74,74,74	0
57	MG	1H	3194	1/1	0.81	0.37	80,80,80,80	0
57	MG	14	3238	1/1	0.81	0.10	67,67,67,67	0
57	MG	1H	3111	1/1	0.81	0.33	94,94,94,94	0
57	MG	14	3448	1/1	0.81	0.10	120,120,120,120	0
57	MG	1J	205	1/1	0.81	0.12	101,101,101,101	0
57	MG	1H	3313	1/1	0.81	0.12	62,62,62,62	0
57	MG	14	3356	1/1	0.81	0.21	78,78,78,78	0
57	MG	1G	1613	1/1	0.81	0.95	93,93,93,93	0
57	MG	1H	3222	1/1	0.81	0.45	86,86,86,86	0
57	MG	13	1641	1/1	0.82	0.45	79,79,79,79	0
57	MG	1H	3060	1/1	0.82	0.54	90,90,90,90	0
57	MG	14	3276	1/1	0.82	0.08	85,85,85,85	0
57	MG	1H	3512	1/1	0.82	0.29	100,100,100,100	0
57	MG	14	3250	1/1	0.82	0.11	84,84,84,84	0
57	MG	14	3428	1/1	0.82	0.05	110,110,110,110	0
57	MG	14	3068	1/1	0.82	0.47	78,78,78,78	0
57	MG	1H	3264	1/1	0.82	0.19	55,55,55,55	0
57	MG	13	1663	1/1	0.82	0.11	77,77,77,77	0
57	MG	14	3114	1/1	0.82	0.18	77,77,77,77	0
57	MG	1J	204	1/1	0.82	0.10	102,102,102,102	0
57	MG	14	3257	1/1	0.82	0.19	118,118,118,118	0
57	MG	1H	3007	1/1	0.82	0.24	57,57,57,57	0
57	MG	14	3162	1/1	0.82	0.26	91,91,91,91	0
57	MG	1H	3403	1/1	0.82	0.07	68,68,68,68	0
57	MG	1H	3531	1/1	0.82	0.13	114,114,114,114	0
57	MG	1H	3492	1/1	0.82	0.16	107,107,107,107	0
57	MG	14	3364	1/1	0.82	0.08	98,98,98,98	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	1H	3533	1/1	0.82	0.33	99,99,99,99	0
57	MG	14	3414	1/1	0.82	0.11	99,99,99,99	0
57	MG	1H	3156	1/1	0.82	0.33	106,106,106,106	0
57	MG	14	3225	1/1	0.82	0.16	79,79,79,79	0
57	MG	14	3009	1/1	0.82	0.28	77,77,77,77	0
57	MG	1H	3477	1/1	0.82	0.18	91,91,91,91	0
57	MG	1H	3107	1/1	0.82	0.35	62,62,62,62	0
57	MG	1G	1664	1/1	0.83	0.14	82,82,82,82	0
57	MG	14	3424	1/1	0.83	0.12	117,117,117,117	0
57	MG	1H	3462	1/1	0.83	0.06	99,99,99,99	0
57	MG	1H	3165	1/1	0.83	0.23	85,85,85,85	0
57	MG	1H	3188	1/1	0.83	0.35	88,88,88,88	0
57	MG	1G	1631	1/1	0.83	0.10	103,103,103,103	0
57	MG	1H	3133	1/1	0.83	0.13	72,72,72,72	0
57	MG	1H	3137	1/1	0.83	0.37	67,67,67,67	0
57	MG	13	1623	1/1	0.83	0.20	70,70,70,70	0
57	MG	1H	3413	1/1	0.83	0.33	93,93,93,93	0
57	MG	1G	1624	1/1	0.83	0.22	103,103,103,103	0
57	MG	13	1720	1/1	0.83	0.06	121,121,121,121	0
57	MG	14	3095	1/1	0.83	0.31	72,72,72,72	0
57	MG	1H	3532	1/1	0.83	0.47	79,79,79,79	0
57	MG	14	3100	1/1	0.83	0.25	77,77,77,77	0
57	MG	1G	1707	1/1	0.83	0.08	115,115,115,115	0
57	MG	1H	3373	1/1	0.83	0.21	79,79,79,79	0
57	MG	14	3360	1/1	0.83	0.16	107,107,107,107	0
57	MG	1H	3091	1/1	0.83	0.64	77,77,77,77	0
57	MG	14	3404	1/1	0.83	0.07	121,121,121,121	0
57	MG	14	3315	1/1	0.83	0.10	83,83,83,83	0
57	MG	14	3025	1/1	0.84	0.24	78,78,78,78	0
57	MG	1H	3528	1/1	0.84	0.12	117,117,117,117	0
57	MG	1H	3103	1/1	0.84	0.15	64,64,64,64	0
57	MG	13	1645	1/1	0.84	0.21	117,117,117,117	0
57	MG	14	3372	1/1	0.84	0.18	112,112,112,112	0
57	MG	14	3439	1/1	0.84	0.24	100,100,100,100	0
57	MG	13	1738	1/1	0.84	0.05	138,138,138,138	0
57	MG	1G	1685	1/1	0.84	0.07	129,129,129,129	0
57	MG	14	3264	1/1	0.84	0.14	88,88,88,88	0
57	MG	1H	3168	1/1	0.84	0.18	89,89,89,89	0
57	MG	1H	3281	1/1	0.84	0.07	85,85,85,85	0
57	MG	1G	1615	1/1	0.84	0.15	89,89,89,89	0
57	MG	1H	3460	1/1	0.84	0.28	85,85,85,85	0
57	MG	14	3117	1/1	0.84	0.34	69,69,69,69	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	1G	1710	1/1	0.84	0.08	113,113,113,113	0
57	MG	14	3373	1/1	0.84	0.19	94,94,94,94	0
57	MG	14	3024	1/1	0.84	0.14	88,88,88,88	0
57	MG	14	3053	1/1	0.84	0.93	82,82,82,82	0
57	MG	13	1617	1/1	0.84	0.37	69,69,69,69	0
57	MG	1H	3501	1/1	0.84	0.07	108,108,108,108	0
57	MG	1H	3056	1/1	0.84	0.47	86,86,86,86	0
57	MG	1H	3412	1/1	0.84	0.07	90,90,90,90	0
57	MG	13	1647	1/1	0.84	0.38	99,99,99,99	0
57	MG	14	3071	1/1	0.84	0.15	82,82,82,82	0
57	MG	1H	3491	1/1	0.84	0.23	100,100,100,100	0
57	MG	1G	1682	1/1	0.84	0.09	123,123,123,123	0
57	MG	2K	101	1/1	0.84	0.13	80,80,80,80	0
57	MG	1G	1612	1/1	0.84	0.11	103,103,103,103	0
57	MG	1H	3418	1/1	0.84	0.15	122,122,122,122	0
57	MG	14	3445	1/1	0.84	0.12	119,119,119,119	0
57	MG	1H	3454	1/1	0.84	0.14	104,104,104,104	0
57	MG	1H	3053	1/1	0.84	0.14	47,47,47,47	0
57	MG	1G	1722	1/1	0.84	0.20	116,116,116,116	0
57	MG	14	3262	1/1	0.84	0.10	104,104,104,104	0
57	MG	1G	1628	1/1	0.84	0.23	123,123,123,123	0
57	MG	1H	3057	1/1	0.84	0.43	71,71,71,71	0
57	MG	14	3211	1/1	0.85	0.09	67,67,67,67	0
57	MG	14	3284	1/1	0.85	0.29	107,107,107,107	0
57	MG	1H	3541	1/1	0.85	0.20	109,109,109,109	0
57	MG	14	3203	1/1	0.85	0.31	95,95,95,95	0
57	MG	1H	3500	1/1	0.85	0.10	90,90,90,90	0
57	MG	14	3089	1/1	0.85	0.23	73,73,73,73	0
57	MG	1H	3014	1/1	0.85	0.42	86,86,86,86	0
57	MG	1H	3475	1/1	0.85	0.05	99,99,99,99	0
57	MG	13	1741	1/1	0.85	0.11	95,95,95,95	0
57	MG	1G	1642	1/1	0.85	0.70	100,100,100,100	0
57	MG	1H	3216	1/1	0.85	0.36	79,79,79,79	0
57	MG	1H	3059	1/1	0.85	0.14	72,72,72,72	0
57	MG	1G	1654	1/1	0.85	0.21	102,102,102,102	0
57	MG	14	3072	1/1	0.85	0.26	88,88,88,88	0
57	MG	13	1646	1/1	0.85	0.52	91,91,91,91	0
57	MG	1H	3488	1/1	0.85	0.19	84,84,84,84	0
57	MG	4L	101	1/1	0.85	0.43	102,102,102,102	0
57	MG	1H	3229	1/1	0.85	0.11	84,84,84,84	0
57	MG	1H	3384	1/1	0.85	0.10	59,59,59,59	0
57	MG	1H	3238	1/1	0.85	0.38	102,102,102,102	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	14	3045	1/1	0.85	0.23	72,72,72,72	0
57	MG	1H	3026	1/1	0.85	0.15	82,82,82,82	0
57	MG	14	3019	1/1	0.85	0.35	131,131,131,131	0
57	MG	1H	3277	1/1	0.85	0.14	79,79,79,79	0
57	MG	14	3204	1/1	0.85	0.13	120,120,120,120	0
57	MG	1H	3455	1/1	0.85	0.08	120,120,120,120	0
57	MG	14	3371	1/1	0.85	0.10	108,108,108,108	0
57	MG	14	3452	1/1	0.85	0.24	122,122,122,122	0
57	MG	1H	3466	1/1	0.85	0.09	103,103,103,103	0
57	MG	1H	3072	1/1	0.85	0.12	60,60,60,60	0
57	MG	1H	3154	1/1	0.85	0.43	67,67,67,67	0
57	MG	1H	3119	1/1	0.85	0.23	79,79,79,79	0
57	MG	1H	3487	1/1	0.85	0.04	108,108,108,108	0
57	MG	13	1725	1/1	0.85	0.05	99,99,99,99	0
57	MG	14	3069	1/1	0.85	0.22	56,56,56,56	0
57	MG	14	3265	1/1	0.85	0.07	100,100,100,100	0
57	MG	1H	3184	1/1	0.85	0.64	100,100,100,100	0
57	MG	1H	3505	1/1	0.85	0.17	112,112,112,112	0
57	MG	42	202	1/1	0.85	0.26	115,115,115,115	0
57	MG	1H	3427	1/1	0.86	0.24	102,102,102,102	0
57	MG	1H	3129	1/1	0.86	0.12	85,85,85,85	0
57	MG	1H	3410	1/1	0.86	0.17	108,108,108,108	0
57	MG	1G	1688	1/1	0.86	0.09	123,123,123,123	0
57	MG	1H	3523	1/1	0.86	0.17	102,102,102,102	0
57	MG	1H	3185	1/1	0.86	0.29	76,76,76,76	0
57	MG	1G	1672	1/1	0.86	0.04	117,117,117,117	0
57	MG	1H	3146	1/1	0.86	0.42	85,85,85,85	0
57	MG	14	3078	1/1	0.86	0.23	88,88,88,88	0
57	MG	1H	3131	1/1	0.86	0.14	101,101,101,101	0
57	MG	14	3380	1/1	0.86	0.12	106,106,106,106	0
57	MG	13	1724	1/1	0.86	0.17	116,116,116,116	0
57	MG	14	3337	1/1	0.86	0.06	116,116,116,116	0
57	MG	14	3345	1/1	0.86	0.15	100,100,100,100	0
57	MG	14	3094	1/1	0.86	0.44	100,100,100,100	0
60	SPE	1G	1725	13/13	0.86	0.09	110,113,117,118	0
57	MG	14	3126	1/1	0.86	0.18	89,89,89,89	0
57	MG	1H	3092	1/1	0.86	0.18	67,67,67,67	0
57	MG	1H	3271	1/1	0.86	0.14	84,84,84,84	0
57	MG	14	3434	1/1	0.86	0.32	110,110,110,110	0
57	MG	88	203	1/1	0.86	0.32	83,83,83,83	0
57	MG	1H	3360	1/1	0.86	0.13	102,102,102,102	0
57	MG	13	1716	1/1	0.86	0.12	116,116,116,116	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	1H	3122	1/1	0.86	0.39	80,80,80,80	0
57	MG	1H	3126	1/1	0.86	0.20	71,71,71,71	0
57	MG	14	3181	1/1	0.86	0.45	91,91,91,91	0
57	MG	14	3367	1/1	0.86	0.10	101,101,101,101	0
57	MG	14	3215	1/1	0.86	0.08	98,98,98,98	0
57	MG	E5	102	1/1	0.86	0.28	68,68,68,68	0
57	MG	1H	3073	1/1	0.86	0.35	84,84,84,84	0
57	MG	14	3306	1/1	0.86	0.17	93,93,93,93	0
57	MG	14	3336	1/1	0.86	0.09	109,109,109,109	0
57	MG	14	3405	1/1	0.86	0.05	118,118,118,118	0
57	MG	13	1650	1/1	0.86	0.38	85,85,85,85	0
57	MG	14	3065	1/1	0.87	0.32	70,70,70,70	0
57	MG	1H	3458	1/1	0.87	0.13	89,89,89,89	0
57	MG	1H	3301	1/1	0.87	0.18	86,86,86,86	0
57	MG	1G	1606	1/1	0.87	0.25	87,87,87,87	0
57	MG	1H	3074	1/1	0.87	0.25	75,75,75,75	0
57	MG	1G	1648	1/1	0.87	0.27	121,121,121,121	0
57	MG	1G	1621	1/1	0.87	0.46	105,105,105,105	0
57	MG	88	201	1/1	0.87	0.20	83,83,83,83	0
57	MG	14	3390	1/1	0.87	0.09	73,73,73,73	0
57	MG	13	1705	1/1	0.87	0.12	108,108,108,108	0
57	MG	14	3143	1/1	0.87	0.31	93,93,93,93	0
57	MG	14	3391	1/1	0.87	0.15	87,87,87,87	0
57	MG	1H	3138	1/1	0.87	0.18	98,98,98,98	0
57	MG	1G	1687	1/1	0.87	0.14	111,111,111,111	0
57	MG	14	3443	1/1	0.87	0.34	115,115,115,115	0
57	MG	1G	1649	1/1	0.87	0.82	96,96,96,96	0
57	MG	1H	3362	1/1	0.87	0.13	78,78,78,78	0
57	MG	31	301	1/1	0.87	0.15	70,70,70,70	0
57	MG	14	3007	1/1	0.87	0.28	61,61,61,61	0
57	MG	1H	3044	1/1	0.87	0.48	80,80,80,80	0
57	MG	13	1627	1/1	0.87	0.17	94,94,94,94	0
57	MG	14	3097	1/1	0.87	0.09	84,84,84,84	0
57	MG	1G	1703	1/1	0.87	0.10	107,107,107,107	0
57	MG	1G	1721	1/1	0.87	0.06	128,128,128,128	0
57	MG	1H	3530	1/1	0.87	0.55	99,99,99,99	0
57	MG	16	210	1/1	0.87	0.36	86,86,86,86	0
57	MG	1G	1718	1/1	0.87	0.10	124,124,124,124	0
57	MG	1H	3354	1/1	0.87	0.17	78,78,78,78	0
57	MG	1H	3158	1/1	0.87	0.24	71,71,71,71	0
57	MG	14	3436	1/1	0.87	0.04	136,136,136,136	0
57	MG	14	3305	1/1	0.87	0.17	64,64,64,64	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	1G	1699	1/1	0.87	0.15	113,113,113,113	0
57	MG	1G	1651	1/1	0.87	0.29	97,97,97,97	0
57	MG	1H	3211	1/1	0.87	0.36	69,69,69,69	0
57	MG	14	3394	1/1	0.87	0.30	91,91,91,91	0
57	MG	1H	3311	1/1	0.87	0.10	91,91,91,91	0
57	MG	14	3359	1/1	0.87	0.10	122,122,122,122	0
57	MG	1H	3346	1/1	0.87	0.10	75,75,75,75	0
57	MG	1H	3093	1/1	0.87	0.31	73,73,73,73	0
57	MG	13	1640	1/1	0.87	0.10	97,97,97,97	0
57	MG	1H	3135	1/1	0.87	0.31	73,73,73,73	0
57	MG	1H	3370	1/1	0.87	0.15	80,80,80,80	0
57	MG	1H	3193	1/1	0.87	0.72	89,89,89,89	0
57	MG	14	3417	1/1	0.87	0.07	117,117,117,117	0
57	MG	1G	1656	1/1	0.87	0.10	89,89,89,89	0
57	MG	1H	3398	1/1	0.88	0.07	86,86,86,86	0
57	MG	1H	3400	1/1	0.88	0.10	79,79,79,79	0
57	MG	14	3314	1/1	0.88	0.19	78,78,78,78	0
57	MG	14	3347	1/1	0.88	0.14	97,97,97,97	0
57	MG	1G	1678	1/1	0.88	0.16	98,98,98,98	0
57	MG	1H	3309	1/1	0.88	0.07	73,73,73,73	0
57	MG	14	3274	1/1	0.88	0.15	62,62,62,62	0
57	MG	1H	3127	1/1	0.88	0.19	69,69,69,69	0
57	MG	1H	3108	1/1	0.88	0.36	68,68,68,68	0
57	MG	14	3073	1/1	0.88	0.43	61,61,61,61	0
57	MG	14	3156	1/1	0.88	0.29	81,81,81,81	0
57	MG	13	1690	1/1	0.88	0.10	117,117,117,117	0
57	MG	14	3196	1/1	0.88	0.46	85,85,85,85	0
57	MG	1H	3542	1/1	0.88	0.07	103,103,103,103	0
57	MG	14	3169	1/1	0.88	0.15	88,88,88,88	0
57	MG	1H	3094	1/1	0.88	0.23	64,64,64,64	0
57	MG	1G	1663	1/1	0.88	0.21	112,112,112,112	0
57	MG	1H	3058	1/1	0.88	0.07	68,68,68,68	0
57	MG	1H	3334	1/1	0.88	0.18	103,103,103,103	0
57	MG	16	209	1/1	0.88	0.07	86,86,86,86	0
57	MG	1H	3068	1/1	0.88	0.22	66,66,66,66	0
57	MG	14	3086	1/1	0.88	0.27	73,73,73,73	0
57	MG	14	3123	1/1	0.88	0.32	75,75,75,75	0
57	MG	1H	3444	1/1	0.88	0.24	72,72,72,72	0
57	MG	1H	3067	1/1	0.88	0.12	55,55,55,55	0
57	MG	1H	3485	1/1	0.88	0.18	102,102,102,102	0
57	MG	1G	1670	1/1	0.88	0.16	109,109,109,109	0
57	MG	14	3047	1/1	0.88	0.12	87,87,87,87	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	2I	303	1/1	0.88	0.12	61,61,61,61	0
57	MG	1H	3490	1/1	0.88	0.08	95,95,95,95	0
57	MG	1H	3141	1/1	0.88	0.15	75,75,75,75	0
57	MG	1H	3299	1/1	0.88	0.19	105,105,105,105	0
57	MG	13	1739	1/1	0.88	0.16	119,119,119,119	0
57	MG	1H	3284	1/1	0.88	0.10	62,62,62,62	0
57	MG	14	3295	1/1	0.88	0.11	88,88,88,88	0
57	MG	1H	3445	1/1	0.88	0.33	87,87,87,87	0
57	MG	1G	1675	1/1	0.88	0.12	86,86,86,86	0
57	MG	14	3148	1/1	0.88	0.18	113,113,113,113	0
57	MG	1H	3434	1/1	0.88	0.14	96,96,96,96	0
57	MG	14	3268	1/1	0.88	0.16	89,89,89,89	0
57	MG	14	3335	1/1	0.88	0.09	94,94,94,94	0
57	MG	14	3243	1/1	0.88	0.18	93,93,93,93	0
57	MG	13	1680	1/1	0.88	0.12	89,89,89,89	0
57	MG	1H	3075	1/1	0.88	0.21	75,75,75,75	0
57	MG	1H	3339	1/1	0.88	0.06	99,99,99,99	0
57	MG	14	3275	1/1	0.88	0.14	85,85,85,85	0
57	MG	1G	1695	1/1	0.88	0.13	126,126,126,126	0
57	MG	1H	3140	1/1	0.88	0.20	90,90,90,90	0
57	MG	1H	3231	1/1	0.88	0.08	103,103,103,103	0
57	MG	13	1662	1/1	0.88	0.43	90,90,90,90	0
57	MG	13	1691	1/1	0.89	0.09	107,107,107,107	0
57	MG	14	3415	1/1	0.89	0.26	93,93,93,93	0
57	MG	14	3270	1/1	0.89	0.19	74,74,74,74	0
57	MG	1H	3243	1/1	0.89	0.10	63,63,63,63	0
57	MG	1H	3463	1/1	0.89	0.12	70,70,70,70	0
57	MG	14	3011	1/1	0.89	0.57	76,76,76,76	0
57	MG	1H	3394	1/1	0.89	0.20	83,83,83,83	0
57	MG	14	3104	1/1	0.89	0.25	89,89,89,89	0
57	MG	13	1653	1/1	0.89	0.12	95,95,95,95	0
57	MG	13	1672	1/1	0.89	0.30	92,92,92,92	0
57	MG	1H	3136	1/1	0.89	0.20	63,63,63,63	0
57	MG	14	3195	1/1	0.89	0.36	98,98,98,98	0
57	MG	14	3113	1/1	0.89	0.34	74,74,74,74	0
57	MG	1G	1652	1/1	0.89	0.18	105,105,105,105	0
57	MG	14	3082	1/1	0.89	0.41	80,80,80,80	0
57	MG	1H	3064	1/1	0.89	0.28	82,82,82,82	0
57	MG	1H	3379	1/1	0.89	0.13	87,87,87,87	0
57	MG	1H	3212	1/1	0.89	0.08	87,87,87,87	0
57	MG	14	3382	1/1	0.89	0.08	116,116,116,116	0
57	MG	1H	3538	1/1	0.89	0.07	107,107,107,107	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	13	1651	1/1	0.89	0.22	118,118,118,118	0
57	MG	13	1656	1/1	0.89	0.27	107,107,107,107	0
57	MG	13	1633	1/1	0.89	0.13	82,82,82,82	0
57	MG	13	1660	1/1	0.89	0.51	91,91,91,91	0
57	MG	1H	3123	1/1	0.89	0.26	68,68,68,68	0
57	MG	14	3421	1/1	0.89	0.23	96,96,96,96	0
57	MG	1H	3270	1/1	0.89	0.14	78,78,78,78	0
57	MG	42	201	1/1	0.89	0.27	107,107,107,107	0
57	MG	14	3167	1/1	0.89	0.07	95,95,95,95	0
57	MG	1H	3187	1/1	0.89	0.28	83,83,83,83	0
57	MG	1H	3196	1/1	0.89	0.22	103,103,103,103	0
57	MG	1H	3308	1/1	0.89	0.14	62,62,62,62	0
57	MG	1H	3420	1/1	0.89	0.22	94,94,94,94	0
57	MG	1H	3473	1/1	0.89	0.13	98,98,98,98	0
57	MG	1J	203	1/1	0.89	0.23	92,92,92,92	0
57	MG	1G	1636	1/1	0.89	0.35	87,87,87,87	0
57	MG	1G	1639	1/1	0.89	0.68	90,90,90,90	0
57	MG	1H	3306	1/1	0.89	0.11	79,79,79,79	0
57	MG	14	3344	1/1	0.89	0.07	104,104,104,104	0
57	MG	14	3102	1/1	0.89	0.28	94,94,94,94	0
57	MG	1H	3385	1/1	0.89	0.19	94,94,94,94	0
57	MG	1H	3358	1/1	0.89	0.07	100,100,100,100	0
57	MG	1G	1693	1/1	0.89	0.10	121,121,121,121	0
57	MG	14	3076	1/1	0.90	0.18	80,80,80,80	0
57	MG	14	3321	1/1	0.90	0.12	89,89,89,89	0
57	MG	1G	1683	1/1	0.90	0.09	132,132,132,132	0
57	MG	14	3438	1/1	0.90	0.13	111,111,111,111	0
57	MG	13	1733	1/1	0.90	0.05	118,118,118,118	0
57	MG	14	3174	1/1	0.90	0.25	78,78,78,78	0
57	MG	35	201	1/1	0.90	0.23	81,81,81,81	0
57	MG	14	3289	1/1	0.90	0.16	89,89,89,89	0
57	MG	1H	3223	1/1	0.90	0.27	79,79,79,79	0
57	MG	41	201	1/1	0.90	0.17	81,81,81,81	0
57	MG	1H	3380	1/1	0.90	0.15	76,76,76,76	0
57	MG	14	3389	1/1	0.90	0.18	72,72,72,72	0
57	MG	14	3018	1/1	0.90	0.24	82,82,82,82	0
57	MG	14	3343	1/1	0.90	0.11	84,84,84,84	0
57	MG	13	1714	1/1	0.90	0.06	94,94,94,94	0
57	MG	1H	3406	1/1	0.90	0.08	95,95,95,95	0
57	MG	1H	3233	1/1	0.90	0.20	94,94,94,94	0
57	MG	13	1601	1/1	0.90	0.32	97,97,97,97	0
57	MG	1H	3218	1/1	0.90	0.32	70,70,70,70	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	14	3263	1/1	0.90	0.13	86,86,86,86	0
57	MG	13	1731	1/1	0.90	0.14	109,109,109,109	0
57	MG	1H	3499	1/1	0.90	0.27	89,89,89,89	0
57	MG	I8	101	1/1	0.90	0.06	95,95,95,95	0
57	MG	1H	3190	1/1	0.90	0.13	73,73,73,73	0
57	MG	1H	3280	1/1	0.90	0.14	47,47,47,47	0
57	MG	1G	1715	1/1	0.90	0.07	110,110,110,110	0
57	MG	45	201	1/1	0.90	0.68	84,84,84,84	0
57	MG	1H	3522	1/1	0.90	0.10	112,112,112,112	0
57	MG	14	3132	1/1	0.90	0.26	90,90,90,90	0
57	MG	13	1614	1/1	0.90	0.31	102,102,102,102	0
57	MG	1H	3155	1/1	0.90	0.27	106,106,106,106	0
57	MG	1H	3495	1/1	0.90	0.08	87,87,87,87	0
57	MG	16	201	1/1	0.90	0.27	73,73,73,73	0
57	MG	14	3409	1/1	0.90	0.11	87,87,87,87	0
57	MG	13	1602	1/1	0.90	0.12	130,130,130,130	0
57	MG	1H	3317	1/1	0.90	0.15	70,70,70,70	0
57	MG	1H	3101	1/1	0.90	0.19	72,72,72,72	0
57	MG	13	1632	1/1	0.90	0.08	95,95,95,95	0
57	MG	14	3444	1/1	0.90	0.48	102,102,102,102	0
57	MG	1H	3547	1/1	0.90	0.06	131,131,131,131	0
57	MG	14	3418	1/1	0.90	0.16	97,97,97,97	0
57	MG	14	3348	1/1	0.90	0.09	102,102,102,102	0
57	MG	1H	3268	1/1	0.90	0.14	70,70,70,70	0
57	MG	1G	1681	1/1	0.90	0.12	131,131,131,131	0
57	MG	1H	3442	1/1	0.90	0.11	107,107,107,107	0
60	SPE	14	3458	13/13	0.90	0.21	92,101,106,108	0
57	MG	14	3152	1/1	0.90	0.37	99,99,99,99	0
57	MG	13	1685	1/1	0.90	0.07	79,79,79,79	0
57	MG	1H	3098	1/1	0.90	0.17	59,59,59,59	0
57	MG	1H	3081	1/1	0.90	0.15	77,77,77,77	0
57	MG	14	3200	1/1	0.90	0.10	86,86,86,86	0
57	MG	1H	3544	1/1	0.90	0.14	105,105,105,105	0
57	MG	14	3020	1/1	0.90	0.21	69,69,69,69	0
57	MG	14	3121	1/1	0.90	0.72	92,92,92,92	0
57	MG	1H	3102	1/1	0.90	0.14	52,52,52,52	0
57	MG	14	3376	1/1	0.90	0.13	82,82,82,82	0
57	MG	14	3092	1/1	0.90	0.21	67,67,67,67	0
57	MG	14	3221	1/1	0.90	0.10	65,65,65,65	0
57	MG	13	1706	1/1	0.90	0.15	88,88,88,88	0
57	MG	13	1689	1/1	0.90	0.22	98,98,98,98	0
57	MG	1H	3023	1/1	0.90	0.30	71,71,71,71	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	14	3291	1/1	0.90	0.16	71,71,71,71	0
57	MG	13	1737	1/1	0.91	0.11	107,107,107,107	0
57	MG	1H	3082	1/1	0.91	0.33	69,69,69,69	0
57	MG	13	1674	1/1	0.91	0.07	105,105,105,105	0
57	MG	1H	3340	1/1	0.91	0.05	109,109,109,109	0
57	MG	14	3046	1/1	0.91	0.20	77,77,77,77	0
57	MG	1H	3143	1/1	0.91	0.25	79,79,79,79	0
57	MG	14	3231	1/1	0.91	0.13	78,78,78,78	0
57	MG	1H	3078	1/1	0.91	0.34	85,85,85,85	0
57	MG	1H	3240	1/1	0.91	0.20	86,86,86,86	0
57	MG	16	207	1/1	0.91	0.10	91,91,91,91	0
57	MG	13	1708	1/1	0.91	0.07	91,91,91,91	0
57	MG	14	3052	1/1	0.91	0.32	59,59,59,59	0
57	MG	14	3374	1/1	0.91	0.10	94,94,94,94	0
57	MG	14	3349	1/1	0.91	0.07	99,99,99,99	0
57	MG	14	3342	1/1	0.91	0.12	105,105,105,105	0
57	MG	1H	3323	1/1	0.91	0.06	78,78,78,78	0
57	MG	13	1639	1/1	0.91	0.44	80,80,80,80	0
57	MG	2K	102	1/1	0.91	0.11	99,99,99,99	0
57	MG	2I	201	1/1	0.91	0.10	97,97,97,97	0
57	MG	1G	1709	1/1	0.91	0.12	119,119,119,119	0
57	MG	14	3296	1/1	0.91	0.10	76,76,76,76	0
57	MG	14	3119	1/1	0.91	0.31	69,69,69,69	0
57	MG	1G	1646	1/1	0.91	0.31	78,78,78,78	0
57	MG	1H	3343	1/1	0.91	0.09	115,115,115,115	0
57	MG	1H	3069	1/1	0.91	0.27	76,76,76,76	0
57	MG	14	3461	1/1	0.91	0.07	108,108,108,108	0
57	MG	1G	1669	1/1	0.91	0.08	114,114,114,114	0
57	MG	1H	3453	1/1	0.91	0.19	82,82,82,82	0
57	MG	14	3233	1/1	0.91	0.11	85,85,85,85	0
57	MG	14	3260	1/1	0.91	0.16	77,77,77,77	0
57	MG	1H	3286	1/1	0.91	0.22	65,65,65,65	0
57	MG	14	3311	1/1	0.91	0.18	84,84,84,84	0
57	MG	14	3363	1/1	0.91	0.05	83,83,83,83	0
57	MG	14	3312	1/1	0.91	0.08	109,109,109,109	0
57	MG	14	3191	1/1	0.91	0.46	76,76,76,76	0
57	MG	1H	3300	1/1	0.91	0.10	73,73,73,73	0
57	MG	1J	206	1/1	0.91	0.07	99,99,99,99	0
57	MG	14	3005	1/1	0.91	0.33	83,83,83,83	0
57	MG	14	3142	1/1	0.91	0.37	98,98,98,98	0
57	MG	14	3186	1/1	0.91	0.13	95,95,95,95	0
57	MG	14	3426	1/1	0.91	0.06	99,99,99,99	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	1G	1635	1/1	0.91	0.30	94,94,94,94	0
57	MG	1H	3545	1/1	0.91	0.46	102,102,102,102	0
57	MG	2I	301	1/1	0.91	0.34	77,77,77,77	0
57	MG	1H	3423	1/1	0.91	0.08	115,115,115,115	0
57	MG	1H	3350	1/1	0.91	0.12	58,58,58,58	0
57	MG	1G	1691	1/1	0.91	0.07	104,104,104,104	0
57	MG	1H	3539	1/1	0.91	0.22	95,95,95,95	0
57	MG	1H	3392	1/1	0.91	0.16	74,74,74,74	0
57	MG	14	3369	1/1	0.91	0.11	90,90,90,90	0
57	MG	1H	3353	1/1	0.91	0.12	62,62,62,62	0
57	MG	1H	3520	1/1	0.91	0.10	88,88,88,88	0
57	MG	13	1707	1/1	0.91	0.06	88,88,88,88	0
57	MG	1H	3030	1/1	0.91	0.17	89,89,89,89	0
57	MG	1H	3342	1/1	0.91	0.10	83,83,83,83	0
57	MG	1G	1716	1/1	0.91	0.14	110,110,110,110	0
57	MG	14	3346	1/1	0.91	0.09	98,98,98,98	0
57	MG	1H	3465	1/1	0.91	0.09	112,112,112,112	0
57	MG	13	1687	1/1	0.91	0.13	89,89,89,89	0
57	MG	1G	1617	1/1	0.91	0.11	89,89,89,89	0
57	MG	14	3170	1/1	0.91	0.25	76,76,76,76	0
57	MG	14	3067	1/1	0.91	0.22	77,77,77,77	0
57	MG	1H	3204	1/1	0.91	0.28	80,80,80,80	0
57	MG	1H	3480	1/1	0.91	0.27	90,90,90,90	0
57	MG	1H	3151	1/1	0.91	0.28	79,79,79,79	0
57	MG	14	3334	1/1	0.91	0.09	83,83,83,83	0
57	MG	1H	3139	1/1	0.91	0.50	90,90,90,90	0
57	MG	14	3411	1/1	0.91	0.07	115,115,115,115	0
57	MG	14	3131	1/1	0.91	0.11	84,84,84,84	0
57	MG	1H	3219	1/1	0.91	0.11	83,83,83,83	0
57	MG	1J	201	1/1	0.91	0.22	97,97,97,97	0
57	MG	1H	3125	1/1	0.91	0.14	79,79,79,79	0
57	MG	16	211	1/1	0.91	0.08	93,93,93,93	0
57	MG	14	3248	1/1	0.91	0.14	76,76,76,76	0
57	MG	1H	3105	1/1	0.91	0.18	78,78,78,78	0
57	MG	1H	3199	1/1	0.92	0.14	81,81,81,81	0
57	MG	1H	3550	1/1	0.92	0.66	111,111,111,111	0
57	MG	1G	1610	1/1	0.92	0.17	84,84,84,84	0
57	MG	14	3038	1/1	0.92	0.27	68,68,68,68	0
57	MG	1H	3387	1/1	0.92	0.08	87,87,87,87	0
57	MG	1H	3191	1/1	0.92	0.30	79,79,79,79	0
57	MG	14	3205	1/1	0.92	0.11	102,102,102,102	0
57	MG	1H	3307	1/1	0.92	0.17	56,56,56,56	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	1H	3192	1/1	0.92	0.25	83,83,83,83	0
57	MG	1G	1692	1/1	0.92	0.07	103,103,103,103	0
57	MG	14	3239	1/1	0.92	0.10	60,60,60,60	0
57	MG	14	3118	1/1	0.92	0.14	96,96,96,96	0
57	MG	1H	3149	1/1	0.92	0.19	81,81,81,81	0
57	MG	1H	3183	1/1	0.92	0.29	75,75,75,75	0
57	MG	1H	3431	1/1	0.92	0.05	102,102,102,102	0
57	MG	1H	3511	1/1	0.92	0.07	113,113,113,113	0
57	MG	1G	1618	1/1	0.92	0.11	91,91,91,91	0
57	MG	1G	1705	1/1	0.92	0.03	117,117,117,117	0
57	MG	14	3370	1/1	0.92	0.14	90,90,90,90	0
57	MG	1H	3404	1/1	0.92	0.67	71,71,71,71	0
57	MG	14	3357	1/1	0.92	0.08	116,116,116,116	0
57	MG	1H	3304	1/1	0.92	0.20	64,64,64,64	0
57	MG	1H	3446	1/1	0.92	0.07	100,100,100,100	0
57	MG	14	3290	1/1	0.92	0.17	71,71,71,71	0
57	MG	13	1670	1/1	0.92	0.60	85,85,85,85	0
57	MG	1G	1660	1/1	0.92	0.12	128,128,128,128	0
57	MG	1H	3228	1/1	0.92	0.15	81,81,81,81	0
57	MG	14	3362	1/1	0.92	0.10	99,99,99,99	0
57	MG	14	3077	1/1	0.92	0.16	85,85,85,85	0
57	MG	13	1665	1/1	0.92	0.19	128,128,128,128	0
57	MG	1H	3203	1/1	0.92	0.24	78,78,78,78	0
57	MG	1H	3443	1/1	0.92	0.08	112,112,112,112	0
57	MG	14	3033	1/1	0.92	0.32	57,57,57,57	0
57	MG	1H	3486	1/1	0.92	0.30	99,99,99,99	0
57	MG	16	202	1/1	0.92	0.27	103,103,103,103	0
57	MG	14	3057	1/1	0.92	0.05	93,93,93,93	0
57	MG	1H	3324	1/1	0.92	0.09	69,69,69,69	0
57	MG	13	1732	1/1	0.92	0.06	108,108,108,108	0
57	MG	1H	3225	1/1	0.92	0.35	74,74,74,74	0
57	MG	14	3217	1/1	0.92	0.09	76,76,76,76	0
57	MG	1G	1632	1/1	0.92	0.25	108,108,108,108	0
57	MG	1H	3249	1/1	0.92	0.14	61,61,61,61	0
57	MG	13	1619	1/1	0.92	0.21	54,54,54,54	0
57	MG	13	1703	1/1	0.92	0.14	71,71,71,71	0
57	MG	1H	3009	1/1	0.92	0.16	82,82,82,82	0
57	MG	14	3386	1/1	0.92	0.12	65,65,65,65	0
57	MG	1H	3508	1/1	0.92	0.11	144,144,144,144	0
57	MG	14	3236	1/1	0.92	0.14	69,69,69,69	0
57	MG	14	3197	1/1	0.92	0.42	92,92,92,92	0
57	MG	1H	3248	1/1	0.92	0.11	57,57,57,57	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	1G	1616	1/1	0.92	0.24	84,84,84,84	0
57	MG	14	3327	1/1	0.92	0.07	108,108,108,108	0
57	MG	1H	3200	1/1	0.92	0.70	82,82,82,82	0
57	MG	13	1682	1/1	0.92	0.05	109,109,109,109	0
57	MG	14	3022	1/1	0.92	0.13	77,77,77,77	0
57	MG	1G	1713	1/1	0.92	0.20	120,120,120,120	0
57	MG	1H	3153	1/1	0.92	0.34	71,71,71,71	0
57	MG	14	3378	1/1	0.92	0.14	101,101,101,101	0
57	MG	1H	3130	1/1	0.92	0.41	97,97,97,97	0
57	MG	1J	202	1/1	0.92	0.20	106,106,106,106	0
57	MG	1H	3474	1/1	0.92	0.09	83,83,83,83	0
57	MG	1H	3397	1/1	0.92	0.14	87,87,87,87	0
57	MG	1H	3043	1/1	0.92	0.15	64,64,64,64	0
57	MG	14	3279	1/1	0.92	0.10	93,93,93,93	0
57	MG	1H	3297	1/1	0.92	0.17	56,56,56,56	0
57	MG	14	3294	1/1	0.92	0.14	66,66,66,66	0
57	MG	1H	3045	1/1	0.92	0.36	63,63,63,63	0
57	MG	1H	3083	1/1	0.92	0.44	80,80,80,80	0
57	MG	14	3237	1/1	0.92	0.12	67,67,67,67	0
57	MG	14	3330	1/1	0.92	0.06	94,94,94,94	0
57	MG	1H	3419	1/1	0.92	0.26	73,73,73,73	0
57	MG	14	3385	1/1	0.92	0.20	82,82,82,82	0
57	MG	14	3023	1/1	0.92	0.34	58,58,58,58	0
57	MG	14	3111	1/1	0.93	0.17	83,83,83,83	0
57	MG	14	3256	1/1	0.93	0.08	99,99,99,99	0
57	MG	14	3252	1/1	0.93	0.14	69,69,69,69	0
57	MG	16	205	1/1	0.93	0.05	84,84,84,84	0
57	MG	1H	3529	1/1	0.93	0.10	110,110,110,110	0
57	MG	14	3441	1/1	0.93	0.14	103,103,103,103	0
57	MG	14	3281	1/1	0.93	0.07	75,75,75,75	0
57	MG	14	3193	1/1	0.93	0.44	96,96,96,96	0
57	MG	14	3352	1/1	0.93	0.11	95,95,95,95	0
57	MG	1G	1680	1/1	0.93	0.14	103,103,103,103	0
57	MG	1H	3114	1/1	0.93	0.16	71,71,71,71	0
57	MG	13	1644	1/1	0.93	0.11	99,99,99,99	0
57	MG	14	3286	1/1	0.93	0.19	58,58,58,58	0
57	MG	1H	3312	1/1	0.93	0.21	69,69,69,69	0
57	MG	14	3449	1/1	0.93	0.06	105,105,105,105	0
57	MG	1H	3296	1/1	0.93	0.16	56,56,56,56	0
57	MG	Q8	101	1/1	0.93	0.23	82,82,82,82	0
57	MG	1H	3116	1/1	0.93	0.21	82,82,82,82	0
57	MG	14	3420	1/1	0.93	0.11	119,119,119,119	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	13	1704	1/1	0.93	0.38	111,111,111,111	0
57	MG	1H	3036	1/1	0.93	0.28	73,73,73,73	0
57	MG	14	3083	1/1	0.93	0.20	58,58,58,58	0
57	MG	1G	1630	1/1	0.93	0.14	132,132,132,132	0
57	MG	1G	1604	1/1	0.93	0.12	132,132,132,132	0
57	MG	13	1661	1/1	0.93	0.17	101,101,101,101	0
57	MG	1H	3100	1/1	0.93	0.27	77,77,77,77	0
57	MG	1H	3461	1/1	0.93	0.08	80,80,80,80	0
57	MG	1H	3450	1/1	0.93	0.06	87,87,87,87	0
57	MG	13	1659	1/1	0.93	0.39	109,109,109,109	0
57	MG	14	3139	1/1	0.93	0.84	88,88,88,88	0
57	MG	14	3054	1/1	0.93	0.28	67,67,67,67	0
57	MG	14	3184	1/1	0.93	0.38	78,78,78,78	0
57	MG	14	3361	1/1	0.93	0.16	87,87,87,87	0
57	MG	14	3309	1/1	0.93	0.13	48,48,48,48	0
57	MG	14	3112	1/1	0.93	0.46	68,68,68,68	0
57	MG	14	3282	1/1	0.93	0.10	82,82,82,82	0
57	MG	14	3228	1/1	0.93	0.25	64,64,64,64	0
57	MG	14	3251	1/1	0.93	0.18	113,113,113,113	0
57	MG	1G	1674	1/1	0.93	0.18	106,106,106,106	0
57	MG	1H	3503	1/1	0.93	0.12	104,104,104,104	0
57	MG	1H	3395	1/1	0.93	0.07	92,92,92,92	0
57	MG	1H	3367	1/1	0.93	0.09	69,69,69,69	0
57	MG	1H	3470	1/1	0.93	0.24	105,105,105,105	0
57	MG	1H	3524	1/1	0.93	0.17	61,61,61,61	0
57	MG	14	3155	1/1	0.93	0.32	83,83,83,83	0
57	MG	1H	3276	1/1	0.93	0.06	80,80,80,80	0
57	MG	13	1622	1/1	0.93	0.05	111,111,111,111	0
57	MG	1H	3267	1/1	0.93	0.05	103,103,103,103	0
57	MG	13	1643	1/1	0.93	0.22	95,95,95,95	0
57	MG	14	3110	1/1	0.93	0.24	85,85,85,85	0
57	MG	1H	3144	1/1	0.93	0.15	71,71,71,71	0
57	MG	13	1637	1/1	0.93	0.18	90,90,90,90	0
57	MG	14	3164	1/1	0.93	0.19	83,83,83,83	0
57	MG	M5	101	1/1	0.93	0.36	81,81,81,81	0
57	MG	14	3288	1/1	0.93	0.20	59,59,59,59	0
57	MG	14	3287	1/1	0.93	0.13	74,74,74,74	0
57	MG	1H	3527	1/1	0.93	0.11	97,97,97,97	0
57	MG	1H	3355	1/1	0.93	0.18	58,58,58,58	0
57	MG	1G	1694	1/1	0.93	0.10	105,105,105,105	0
57	MG	14	3338	1/1	0.93	0.18	112,112,112,112	0
57	MG	1G	1655	1/1	0.93	0.15	90,90,90,90	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	1H	3278	1/1	0.93	0.07	86,86,86,86	0
57	MG	14	3293	1/1	0.93	0.18	70,70,70,70	0
57	MG	14	3307	1/1	0.93	0.15	80,80,80,80	0
57	MG	1H	3469	1/1	0.93	0.05	84,84,84,84	0
57	MG	1G	1622	1/1	0.93	0.16	104,104,104,104	0
57	MG	1H	3517	1/1	0.93	0.29	85,85,85,85	0
57	MG	1G	1686	1/1	0.93	0.08	113,113,113,113	0
57	MG	13	1681	1/1	0.93	0.20	91,91,91,91	0
57	MG	1G	1625	1/1	0.93	0.61	89,89,89,89	0
57	MG	1H	3040	1/1	0.93	0.20	76,76,76,76	0
57	MG	14	3001	1/1	0.94	0.16	51,51,51,51	0
57	MG	14	3031	1/1	0.94	0.24	51,51,51,51	0
57	MG	13	1615	1/1	0.94	0.41	75,75,75,75	0
57	MG	14	3202	1/1	0.94	0.15	106,106,106,106	0
57	MG	1H	3121	1/1	0.94	0.22	89,89,89,89	0
57	MG	1G	1714	1/1	0.94	0.11	126,126,126,126	0
57	MG	14	3412	1/1	0.94	0.16	106,106,106,106	0
57	MG	1H	3049	1/1	0.94	0.27	79,79,79,79	0
57	MG	1H	3262	1/1	0.94	0.14	59,59,59,59	0
57	MG	1H	3189	1/1	0.94	0.27	83,83,83,83	0
57	MG	13	1657	1/1	0.94	0.58	75,75,75,75	0
57	MG	14	3316	1/1	0.94	0.08	100,100,100,100	0
57	MG	1H	3348	1/1	0.94	0.11	66,66,66,66	0
57	MG	1H	3305	1/1	0.94	0.15	72,72,72,72	0
57	MG	1H	3375	1/1	0.94	0.10	80,80,80,80	0
57	MG	14	3442	1/1	0.94	0.08	83,83,83,83	0
57	MG	16	212	1/1	0.94	0.07	78,78,78,78	0
57	MG	14	3004	1/1	0.94	0.35	81,81,81,81	0
57	MG	1G	1679	1/1	0.94	0.17	105,105,105,105	0
57	MG	14	3368	1/1	0.94	0.37	92,92,92,92	0
57	MG	14	3171	1/1	0.94	0.47	86,86,86,86	0
57	MG	14	3176	1/1	0.94	0.52	90,90,90,90	0
57	MG	14	3149	1/1	0.94	0.31	94,94,94,94	0
57	MG	14	3106	1/1	0.94	0.33	79,79,79,79	0
57	MG	14	3433	1/1	0.94	0.11	90,90,90,90	0
57	MG	14	3062	1/1	0.94	0.24	97,97,97,97	0
57	MG	1H	3359	1/1	0.94	0.04	92,92,92,92	0
57	MG	1H	3063	1/1	0.94	0.24	59,59,59,59	0
57	MG	13	1696	1/1	0.94	0.18	114,114,114,114	0
57	MG	14	3034	1/1	0.94	0.28	75,75,75,75	0
57	MG	14	3240	1/1	0.94	0.25	63,63,63,63	0
57	MG	1G	1708	1/1	0.94	0.12	127,127,127,127	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	1H	3150	1/1	0.94	0.34	81,81,81,81	0
57	MG	1G	1637	1/1	0.94	0.38	106,106,106,106	0
57	MG	1H	3035	1/1	0.94	0.36	83,83,83,83	0
57	MG	13	1636	1/1	0.94	0.25	81,81,81,81	0
57	MG	14	3435	1/1	0.94	0.05	122,122,122,122	0
57	MG	1H	3178	1/1	0.94	0.46	80,80,80,80	0
57	MG	1H	3104	1/1	0.94	0.16	68,68,68,68	0
57	MG	1H	3096	1/1	0.94	0.40	83,83,83,83	0
57	MG	14	3227	1/1	0.94	0.17	52,52,52,52	0
57	MG	13	1605	1/1	0.94	0.18	88,88,88,88	0
57	MG	14	3224	1/1	0.94	0.15	76,76,76,76	0
57	MG	14	3447	1/1	0.94	0.07	107,107,107,107	0
57	MG	14	3030	1/1	0.94	0.40	90,90,90,90	0
57	MG	13	1701	1/1	0.94	0.10	124,124,124,124	0
57	MG	1H	3006	1/1	0.94	0.20	77,77,77,77	0
57	MG	1G	1657	1/1	0.94	0.10	114,114,114,114	0
57	MG	14	3157	1/1	0.94	0.13	96,96,96,96	0
57	MG	1H	3260	1/1	0.94	0.07	70,70,70,70	0
57	MG	13	1673	1/1	0.94	0.11	110,110,110,110	0
57	MG	1H	3472	1/1	0.94	0.13	63,63,63,63	0
57	MG	1H	3405	1/1	0.94	0.10	75,75,75,75	0
57	MG	14	3318	1/1	0.94	0.12	65,65,65,65	0
57	MG	1H	3507	1/1	0.94	0.15	90,90,90,90	0
57	MG	1H	3148	1/1	0.94	0.13	88,88,88,88	0
57	MG	14	3407	1/1	0.94	0.18	111,111,111,111	0
57	MG	13	1671	1/1	0.94	0.07	108,108,108,108	0
57	MG	14	3358	1/1	0.94	0.04	78,78,78,78	0
57	MG	14	3229	1/1	0.94	0.11	74,74,74,74	0
57	MG	14	3088	1/1	0.94	0.43	82,82,82,82	0
57	MG	14	3269	1/1	0.94	0.07	104,104,104,104	0
57	MG	1G	1700	1/1	0.94	0.13	107,107,107,107	0
57	MG	13	1628	1/1	0.94	0.59	90,90,90,90	0
57	MG	1H	3274	1/1	0.94	0.12	48,48,48,48	0
57	MG	1H	3272	1/1	0.94	0.13	79,79,79,79	0
57	MG	14	3340	1/1	0.94	0.09	63,63,63,63	0
57	MG	1G	1668	1/1	0.94	0.10	106,106,106,106	0
57	MG	1G	1690	1/1	0.94	0.06	113,113,113,113	0
57	MG	13	1664	1/1	0.94	0.25	91,91,91,91	0
57	MG	1H	3079	1/1	0.94	0.17	85,85,85,85	0
57	MG	1H	3097	1/1	0.94	0.22	43,43,43,43	0
57	MG	14	3402	1/1	0.94	0.07	111,111,111,111	0
57	MG	14	3246	1/1	0.94	0.11	93,93,93,93	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	1H	3526	1/1	0.94	0.20	96,96,96,96	0
57	MG	14	3253	1/1	0.94	0.12	79,79,79,79	0
57	MG	14	3178	1/1	0.94	0.13	83,83,83,83	0
57	MG	14	3129	1/1	0.94	0.21	90,90,90,90	0
57	MG	14	3042	1/1	0.94	0.28	54,54,54,54	0
57	MG	14	3223	1/1	0.94	0.22	61,61,61,61	0
57	MG	13	1717	1/1	0.94	0.09	93,93,93,93	0
57	MG	35	202	1/1	0.94	0.17	80,80,80,80	0
57	MG	14	3232	1/1	0.94	0.11	75,75,75,75	0
57	MG	14	3136	1/1	0.94	0.26	95,95,95,95	0
57	MG	13	1613	1/1	0.94	0.18	94,94,94,94	0
57	MG	F8	101	1/1	0.94	0.14	85,85,85,85	0
57	MG	1H	3435	1/1	0.94	0.30	100,100,100,100	0
57	MG	1H	3314	1/1	0.94	0.15	65,65,65,65	0
57	MG	14	3302	1/1	0.94	0.26	94,94,94,94	0
57	MG	1H	3377	1/1	0.94	0.13	94,94,94,94	0
57	MG	14	3090	1/1	0.94	0.27	77,77,77,77	0
57	MG	1H	3015	1/1	0.94	0.47	77,77,77,77	0
57	MG	14	3297	1/1	0.95	0.08	90,90,90,90	0
57	MG	1H	3424	1/1	0.95	0.15	84,84,84,84	0
57	MG	1G	1602	1/1	0.95	0.32	105,105,105,105	0
57	MG	1G	1719	1/1	0.95	0.09	115,115,115,115	0
57	MG	1H	3417	1/1	0.95	0.04	100,100,100,100	0
57	MG	1H	3426	1/1	0.95	0.17	82,82,82,82	0
57	MG	1H	3327	1/1	0.95	0.14	81,81,81,81	0
57	MG	1G	1623	1/1	0.95	0.12	109,109,109,109	0
57	MG	1H	3482	1/1	0.95	0.10	107,107,107,107	0
57	MG	13	1697	1/1	0.95	0.07	110,110,110,110	0
57	MG	14	3283	1/1	0.95	0.06	105,105,105,105	0
57	MG	1H	3425	1/1	0.95	0.04	81,81,81,81	0
57	MG	1H	3356	1/1	0.95	0.15	79,79,79,79	0
57	MG	1H	3382	1/1	0.95	0.16	43,43,43,43	0
57	MG	1G	1717	1/1	0.95	0.06	126,126,126,126	0
57	MG	14	3285	1/1	0.95	0.11	89,89,89,89	0
57	MG	1H	3438	1/1	0.95	0.07	95,95,95,95	0
57	MG	14	3101	1/1	0.95	0.20	87,87,87,87	0
57	MG	1G	1726	1/1	0.95	0.19	94,94,94,94	0
57	MG	13	1688	1/1	0.95	0.07	96,96,96,96	0
57	MG	1H	3258	1/1	0.95	0.10	56,56,56,56	0
57	MG	1G	1671	1/1	0.95	0.10	101,101,101,101	0
57	MG	1H	3287	1/1	0.95	0.10	76,76,76,76	0
57	MG	1H	3282	1/1	0.95	0.05	54,54,54,54	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	1G	1689	1/1	0.95	0.07	92,92,92,92	0
57	MG	1H	3363	1/1	0.95	0.14	73,73,73,73	0
57	MG	14	3354	1/1	0.95	0.12	80,80,80,80	0
57	MG	1H	3109	1/1	0.95	0.67	79,79,79,79	0
57	MG	13	1730	1/1	0.95	0.07	110,110,110,110	0
57	MG	14	3108	1/1	0.95	0.53	103,103,103,103	0
57	MG	14	3416	1/1	0.95	0.06	87,87,87,87	0
57	MG	14	3266	1/1	0.95	0.10	77,77,77,77	0
57	MG	1G	1644	1/1	0.95	0.15	130,130,130,130	0
57	MG	1H	3515	1/1	0.95	0.12	78,78,78,78	0
57	MG	1H	3396	1/1	0.95	0.17	81,81,81,81	0
57	MG	14	3230	1/1	0.95	0.15	56,56,56,56	0
57	MG	14	3207	1/1	0.95	0.49	70,70,70,70	0
57	MG	14	3012	1/1	0.95	0.32	69,69,69,69	0
57	MG	14	3419	1/1	0.95	0.27	119,119,119,119	0
57	MG	14	3190	1/1	0.95	0.32	89,89,89,89	0
57	MG	14	3206	1/1	0.95	0.27	97,97,97,97	0
57	MG	19	301	1/1	0.95	0.30	61,61,61,61	0
57	MG	1H	3447	1/1	0.95	0.04	98,98,98,98	0
57	MG	1H	3070	1/1	0.95	0.15	51,51,51,51	0
57	MG	1H	3195	1/1	0.95	0.23	85,85,85,85	0
57	MG	29	301	1/1	0.95	0.27	65,65,65,65	0
57	MG	1H	3331	1/1	0.95	0.06	88,88,88,88	0
57	MG	14	3064	1/1	0.95	0.23	99,99,99,99	0
57	MG	1H	3372	1/1	0.95	0.13	66,66,66,66	0
57	MG	1H	3471	1/1	0.95	0.17	83,83,83,83	0
57	MG	1H	3226	1/1	0.95	0.51	92,92,92,92	0
57	MG	1H	3234	1/1	0.95	0.29	84,84,84,84	0
57	MG	1G	1640	1/1	0.95	0.40	80,80,80,80	0
57	MG	14	3059	1/1	0.95	0.20	58,58,58,58	0
57	MG	14	3037	1/1	0.95	0.49	54,54,54,54	0
57	MG	13	1698	1/1	0.95	0.11	93,93,93,93	0
57	MG	1H	3076	1/1	0.95	0.37	75,75,75,75	0
57	MG	1H	3202	1/1	0.95	0.21	80,80,80,80	0
57	MG	14	3245	1/1	0.95	0.16	74,74,74,74	0
57	MG	14	3393	1/1	0.95	0.08	89,89,89,89	0
57	MG	13	1721	1/1	0.95	0.18	77,77,77,77	0
57	MG	14	3258	1/1	0.95	0.05	97,97,97,97	0
57	MG	1H	3046	1/1	0.95	0.17	43,43,43,43	0
57	MG	1H	3236	1/1	0.95	0.16	93,93,93,93	0
57	MG	1H	3293	1/1	0.95	0.10	60,60,60,60	0
57	MG	1H	3113	1/1	0.95	0.16	70,70,70,70	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	1H	3207	1/1	0.95	0.40	77,77,77,77	0
57	MG	1H	3429	1/1	0.95	0.08	87,87,87,87	0
57	MG	1H	3038	1/1	0.95	0.16	61,61,61,61	0
57	MG	1H	3269	1/1	0.95	0.08	83,83,83,83	0
57	MG	1G	1614	1/1	0.95	0.58	91,91,91,91	0
57	MG	1G	1641	1/1	0.95	0.10	115,115,115,115	0
57	MG	1H	3261	1/1	0.95	0.16	61,61,61,61	0
57	MG	3I	201	1/1	0.95	0.24	75,75,75,75	0
57	MG	1H	3174	1/1	0.95	0.31	73,73,73,73	0
57	MG	16	203	1/1	0.95	0.28	84,84,84,84	0
57	MG	1H	3084	1/1	0.95	0.29	77,77,77,77	0
57	MG	1H	3521	1/1	0.95	0.09	65,65,65,65	0
57	MG	13	1722	1/1	0.95	0.18	99,99,99,99	0
57	MG	1H	3390	1/1	0.95	0.13	48,48,48,48	0
57	MG	1H	3239	1/1	0.95	0.09	97,97,97,97	0
57	MG	14	3120	1/1	0.95	0.14	84,84,84,84	0
57	MG	1H	3099	1/1	0.95	0.15	53,53,53,53	0
57	MG	1H	3255	1/1	0.95	0.12	72,72,72,72	0
57	MG	16	208	1/1	0.95	0.26	86,86,86,86	0
57	MG	1H	3549	1/1	0.95	0.15	94,94,94,94	0
57	MG	14	3048	1/1	0.95	0.13	72,72,72,72	0
57	MG	14	3261	1/1	0.95	0.12	64,64,64,64	0
57	MG	14	3350	1/1	0.95	0.09	88,88,88,88	0
57	MG	1H	3310	1/1	0.95	0.06	76,76,76,76	0
57	MG	1H	3468	1/1	0.95	0.05	82,82,82,82	0
57	MG	1H	3004	1/1	0.95	0.25	64,64,64,64	0
57	MG	1G	1666	1/1	0.95	0.18	110,110,110,110	0
57	MG	14	3017	1/1	0.95	0.14	74,74,74,74	0
57	MG	1H	3448	1/1	0.95	0.23	76,76,76,76	0
57	MG	14	3028	1/1	0.95	0.25	67,67,67,67	0
57	MG	1H	3315	1/1	0.95	0.13	61,61,61,61	0
57	MG	14	3249	1/1	0.95	0.05	85,85,85,85	0
57	MG	1G	1601	1/1	0.95	0.20	92,92,92,92	0
57	MG	1H	3483	1/1	0.95	0.06	99,99,99,99	0
57	MG	14	3035	1/1	0.95	0.27	69,69,69,69	0
57	MG	13	1694	1/1	0.95	0.11	92,92,92,92	0
57	MG	14	3278	1/1	0.96	0.13	83,83,83,83	0
59	ZN	G8	201	1/1	0.96	0.09	150,150,150,150	0
57	MG	14	3220	1/1	0.96	0.08	65,65,65,65	0
57	MG	1G	1645	1/1	0.96	0.20	124,124,124,124	0
57	MG	1H	3120	1/1	0.96	0.37	69,69,69,69	0
57	MG	14	3272	1/1	0.96	0.14	71,71,71,71	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	13	1710	1/1	0.96	0.08	73,73,73,73	0
57	MG	14	3002	1/1	0.96	0.35	63,63,63,63	0
57	MG	1H	3386	1/1	0.96	0.21	72,72,72,72	0
57	MG	1H	3018	1/1	0.96	0.34	63,63,63,63	0
57	MG	13	1679	1/1	0.96	0.06	89,89,89,89	0
57	MG	14	3127	1/1	0.96	0.06	70,70,70,70	0
57	MG	13	1625	1/1	0.96	0.23	68,68,68,68	0
57	MG	1H	3332	1/1	0.96	0.10	84,84,84,84	0
57	MG	1H	3316	1/1	0.96	0.07	76,76,76,76	0
57	MG	1H	3374	1/1	0.96	0.07	57,57,57,57	0
57	MG	14	3432	1/1	0.96	0.25	103,103,103,103	0
57	MG	1H	3321	1/1	0.96	0.11	55,55,55,55	0
57	MG	14	3096	1/1	0.96	0.28	84,84,84,84	0
57	MG	14	3322	1/1	0.96	0.14	58,58,58,58	0
57	MG	14	3032	1/1	0.96	0.25	72,72,72,72	0
57	MG	1H	3328	1/1	0.96	0.15	81,81,81,81	0
57	MG	14	3070	1/1	0.96	0.64	66,66,66,66	0
57	MG	1H	3095	1/1	0.96	0.17	76,76,76,76	0
57	MG	1H	3319	1/1	0.96	0.11	58,58,58,58	0
57	MG	14	3401	1/1	0.96	0.20	89,89,89,89	0
57	MG	1H	3298	1/1	0.96	0.06	52,52,52,52	0
57	MG	14	3403	1/1	0.96	0.07	78,78,78,78	0
57	MG	1G	1676	1/1	0.96	0.14	104,104,104,104	0
57	MG	14	3098	1/1	0.96	0.20	63,63,63,63	0
57	MG	14	3026	1/1	0.96	0.06	74,74,74,74	0
57	MG	1H	3290	1/1	0.96	0.09	87,87,87,87	0
57	MG	1H	3368	1/1	0.96	0.06	72,72,72,72	0
57	MG	14	3146	1/1	0.96	0.08	62,62,62,62	0
57	MG	1H	3457	1/1	0.96	0.08	102,102,102,102	0
57	MG	1H	3288	1/1	0.96	0.11	58,58,58,58	0
57	MG	1H	3118	1/1	0.96	0.13	63,63,63,63	0
57	MG	14	3365	1/1	0.96	0.10	93,93,93,93	0
57	MG	14	3061	1/1	0.96	0.35	60,60,60,60	0
57	MG	14	3063	1/1	0.96	0.20	93,93,93,93	0
57	MG	14	3310	1/1	0.96	0.10	71,71,71,71	0
57	MG	14	3058	1/1	0.96	0.24	83,83,83,83	0
57	MG	1G	1627	1/1	0.96	0.13	122,122,122,122	0
57	MG	1H	3253	1/1	0.96	0.12	58,58,58,58	0
57	MG	14	3459	1/1	0.96	0.10	68,68,68,68	0
57	MG	1H	3416	1/1	0.96	0.07	80,80,80,80	0
57	MG	1H	3198	1/1	0.96	0.26	75,75,75,75	0
57	MG	13	1726	1/1	0.96	0.05	107,107,107,107	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	14	3396	1/1	0.96	0.07	71,71,71,71	0
57	MG	1H	3132	1/1	0.96	0.20	55,55,55,55	0
57	MG	1H	3128	1/1	0.96	0.07	66,66,66,66	0
57	MG	1H	3349	1/1	0.96	0.05	61,61,61,61	0
57	MG	1H	3134	1/1	0.96	0.50	77,77,77,77	0
57	MG	13	1616	1/1	0.96	0.30	101,101,101,101	0
57	MG	14	3247	1/1	0.96	0.11	87,87,87,87	0
57	MG	1H	3428	1/1	0.96	0.05	93,93,93,93	0
57	MG	14	3044	1/1	0.96	0.23	71,71,71,71	0
57	MG	1H	3376	1/1	0.96	0.10	71,71,71,71	0
57	MG	1H	3047	1/1	0.96	0.21	64,64,64,64	0
57	MG	1H	3437	1/1	0.96	0.15	76,76,76,76	0
57	MG	1H	3242	1/1	0.96	0.13	50,50,50,50	0
57	MG	14	3325	1/1	0.96	0.08	88,88,88,88	0
57	MG	14	3150	1/1	0.96	0.16	75,75,75,75	0
57	MG	14	3016	1/1	0.96	0.27	69,69,69,69	0
59	ZN	C5	201	1/1	0.96	0.05	167,167,167,167	0
57	MG	1H	3029	1/1	0.96	0.21	59,59,59,59	0
57	MG	1H	3345	1/1	0.96	0.06	85,85,85,85	0
57	MG	13	1677	1/1	0.96	0.13	90,90,90,90	0
57	MG	13	1702	1/1	0.96	0.08	70,70,70,70	0
57	MG	1G	1607	1/1	0.96	0.28	107,107,107,107	0
57	MG	14	3107	1/1	0.96	0.58	94,94,94,94	0
57	MG	14	3075	1/1	0.96	0.28	65,65,65,65	0
57	MG	14	3091	1/1	0.96	0.31	92,92,92,92	0
57	MG	1H	3002	1/1	0.96	0.17	51,51,51,51	0
57	MG	1H	3209	1/1	0.96	0.17	92,92,92,92	0
57	MG	13	1624	1/1	0.96	0.30	83,83,83,83	0
57	MG	14	3308	1/1	0.96	0.13	64,64,64,64	0
57	MG	1H	3220	1/1	0.96	0.22	71,71,71,71	0
57	MG	1H	3080	1/1	0.96	0.17	75,75,75,75	0
57	MG	1H	3163	1/1	0.96	0.18	86,86,86,86	0
57	MG	1H	3414	1/1	0.96	0.07	52,52,52,52	0
57	MG	1H	3366	1/1	0.96	0.12	56,56,56,56	0
57	MG	1H	3171	1/1	0.96	0.18	88,88,88,88	0
57	MG	14	3214	1/1	0.96	0.15	83,83,83,83	0
57	MG	14	3323	1/1	0.96	0.10	84,84,84,84	0
57	MG	14	3182	1/1	0.96	0.26	66,66,66,66	0
57	MG	1H	3031	1/1	0.96	0.33	90,90,90,90	0
57	MG	13	1693	1/1	0.96	0.09	95,95,95,95	0
57	MG	14	3208	1/1	0.96	0.23	63,63,63,63	0
57	MG	1H	3351	1/1	0.96	0.09	66,66,66,66	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	1G	1608	1/1	0.96	0.34	100,100,100,100	0
57	MG	14	3410	1/1	0.96	0.14	107,107,107,107	0
57	MG	13	1611	1/1	0.96	0.24	78,78,78,78	0
57	MG	14	3273	1/1	0.96	0.11	61,61,61,61	0
57	MG	1H	3164	1/1	0.96	0.44	85,85,85,85	0
57	MG	1H	3302	1/1	0.96	0.16	54,54,54,54	0
57	MG	14	3050	1/1	0.96	0.44	87,87,87,87	0
57	MG	14	3298	1/1	0.96	0.07	95,95,95,95	0
57	MG	14	3151	1/1	0.96	0.15	108,108,108,108	0
57	MG	1H	3478	1/1	0.96	0.05	79,79,79,79	0
57	MG	1H	3112	1/1	0.96	0.25	79,79,79,79	0
57	MG	14	3254	1/1	0.96	0.12	87,87,87,87	0
57	MG	14	3066	1/1	0.96	0.25	63,63,63,63	0
57	MG	1H	3516	1/1	0.96	0.09	122,122,122,122	0
57	MG	1G	1653	1/1	0.96	0.07	125,125,125,125	0
57	MG	13	1711	1/1	0.96	0.09	70,70,70,70	0
57	MG	1H	3320	1/1	0.96	0.08	71,71,71,71	0
57	MG	14	3105	1/1	0.96	0.17	92,92,92,92	0
57	MG	14	3049	1/1	0.96	0.19	69,69,69,69	0
57	MG	1H	3407	1/1	0.97	0.07	69,69,69,69	0
57	MG	13	1686	1/1	0.97	0.10	107,107,107,107	0
57	MG	14	3332	1/1	0.97	0.16	63,63,63,63	0
57	MG	14	3056	1/1	0.97	0.37	74,74,74,74	0
57	MG	14	3398	1/1	0.97	0.05	86,86,86,86	0
57	MG	1H	3381	1/1	0.97	0.14	58,58,58,58	0
57	MG	1H	3518	1/1	0.97	0.11	57,57,57,57	0
57	MG	1G	1626	1/1	0.97	0.28	119,119,119,119	0
57	MG	14	3299	1/1	0.97	0.06	63,63,63,63	0
57	MG	14	3099	1/1	0.97	0.55	101,101,101,101	0
57	MG	13	1612	1/1	0.97	0.14	111,111,111,111	0
57	MG	14	3271	1/1	0.97	0.10	67,67,67,67	0
57	MG	1H	3361	1/1	0.97	0.07	53,53,53,53	0
57	MG	14	3320	1/1	0.97	0.15	70,70,70,70	0
57	MG	13	1606	1/1	0.97	0.16	88,88,88,88	0
57	MG	14	3006	1/1	0.97	0.18	78,78,78,78	0
57	MG	14	3085	1/1	0.97	0.23	52,52,52,52	0
57	MG	1H	3016	1/1	0.97	0.35	52,52,52,52	0
57	MG	1H	3254	1/1	0.97	0.14	49,49,49,49	0
57	MG	14	3015	1/1	0.97	0.14	65,65,65,65	0
57	MG	1H	3025	1/1	0.97	0.24	52,52,52,52	0
57	MG	1H	3224	1/1	0.97	0.09	72,72,72,72	0
57	MG	14	3003	1/1	0.97	0.17	68,68,68,68	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	14	3122	1/1	0.97	0.14	90,90,90,90	0
57	MG	1H	3259	1/1	0.97	0.12	59,59,59,59	0
57	MG	1H	3430	1/1	0.97	0.18	94,94,94,94	0
57	MG	B5	101	1/1	0.97	0.10	99,99,99,99	0
57	MG	1H	3352	1/1	0.97	0.08	70,70,70,70	0
57	MG	2L	101	1/1	0.97	0.43	83,83,83,83	0
57	MG	1H	3088	1/1	0.97	0.14	87,87,87,87	0
57	MG	1H	3115	1/1	0.97	0.19	64,64,64,64	0
57	MG	14	3041	1/1	0.97	0.29	66,66,66,66	0
57	MG	14	3277	1/1	0.97	0.06	64,64,64,64	0
57	MG	14	3313	1/1	0.97	0.09	67,67,67,67	0
57	MG	13	1603	1/1	0.97	0.22	92,92,92,92	0
57	MG	1G	1603	1/1	0.97	0.16	91,91,91,91	0
57	MG	14	3353	1/1	0.97	0.10	89,89,89,89	0
57	MG	1H	3303	1/1	0.97	0.11	49,49,49,49	0
57	MG	14	3084	1/1	0.97	0.27	67,67,67,67	0
57	MG	13	1695	1/1	0.97	0.07	91,91,91,91	0
57	MG	1H	3266	1/1	0.97	0.14	92,92,92,92	0
57	MG	1H	3344	1/1	0.97	0.09	60,60,60,60	0
57	MG	1H	3052	1/1	0.97	0.28	58,58,58,58	0
57	MG	1H	3022	1/1	0.97	0.17	56,56,56,56	0
57	MG	1H	3106	1/1	0.97	0.09	73,73,73,73	0
57	MG	14	3055	1/1	0.97	0.25	64,64,64,64	0
57	MG	1H	3252	1/1	0.97	0.07	52,52,52,52	0
57	MG	1H	3464	1/1	0.97	0.17	57,57,57,57	0
57	MG	14	3440	1/1	0.97	0.20	87,87,87,87	0
57	MG	1H	3028	1/1	0.97	0.16	62,62,62,62	0
57	MG	1G	1677	1/1	0.97	0.09	83,83,83,83	0
57	MG	14	3226	1/1	0.97	0.17	54,54,54,54	0
57	MG	1H	3017	1/1	0.97	0.27	56,56,56,56	0
57	MG	1H	3439	1/1	0.97	0.04	76,76,76,76	0
57	MG	14	3242	1/1	0.97	0.11	82,82,82,82	0
57	MG	1H	3250	1/1	0.97	0.10	54,54,54,54	0
57	MG	13	1630	1/1	0.97	0.25	86,86,86,86	0
57	MG	1H	3019	1/1	0.97	0.29	53,53,53,53	0
57	MG	13	1609	1/1	0.97	0.19	88,88,88,88	0
57	MG	14	3303	1/1	0.97	0.11	52,52,52,52	0
57	MG	13	1634	1/1	0.97	0.33	91,91,91,91	0
57	MG	1G	1665	1/1	0.97	0.10	82,82,82,82	0
57	MG	14	3234	1/1	0.97	0.09	62,62,62,62	0
57	MG	13	1607	1/1	0.97	0.23	83,83,83,83	0
57	MG	14	3317	1/1	0.97	0.05	100,100,100,100	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	1H	3020	1/1	0.97	0.24	60,60,60,60	0
57	MG	13	1713	1/1	0.97	0.09	96,96,96,96	0
57	MG	1H	3318	1/1	0.97	0.04	74,74,74,74	0
57	MG	1H	3011	1/1	0.97	0.21	79,79,79,79	0
57	MG	1H	3179	1/1	0.97	0.24	74,74,74,74	0
57	MG	13	1626	1/1	0.97	0.10	96,96,96,96	0
57	MG	14	3036	1/1	0.97	0.28	85,85,85,85	0
57	MG	14	3326	1/1	0.97	0.10	87,87,87,87	0
57	MG	14	3244	1/1	0.97	0.06	68,68,68,68	0
57	MG	1H	3546	1/1	0.97	0.10	105,105,105,105	0
57	MG	1H	3496	1/1	0.97	0.10	89,89,89,89	0
57	MG	1H	3329	1/1	0.97	0.13	53,53,53,53	0
57	MG	14	3125	1/1	0.97	0.10	92,92,92,92	0
57	MG	14	3180	1/1	0.97	0.34	86,86,86,86	0
57	MG	14	3147	1/1	0.97	0.75	86,86,86,86	0
57	MG	1H	3205	1/1	0.97	0.18	71,71,71,71	0
57	MG	1H	3054	1/1	0.97	0.14	63,63,63,63	0
57	MG	14	3331	1/1	0.97	0.14	56,56,56,56	0
57	MG	1H	3051	1/1	0.97	0.29	74,74,74,74	0
57	MG	1G	1673	1/1	0.97	0.11	80,80,80,80	0
57	MG	1H	3037	1/1	0.98	0.11	57,57,57,57	0
57	MG	14	3201	1/1	0.98	0.28	82,82,82,82	0
57	MG	1H	3201	1/1	0.98	0.26	80,80,80,80	0
57	MG	1G	1619	1/1	0.98	0.07	118,118,118,118	0
57	MG	14	3040	1/1	0.98	0.26	80,80,80,80	0
57	MG	14	3292	1/1	0.98	0.06	71,71,71,71	0
57	MG	14	3168	1/1	0.98	0.18	70,70,70,70	0
57	MG	1H	3033	1/1	0.98	0.18	63,63,63,63	0
57	MG	14	3060	1/1	0.98	0.15	65,65,65,65	0
57	MG	14	3213	1/1	0.98	0.12	70,70,70,70	0
57	MG	14	3304	1/1	0.98	0.07	61,61,61,61	0
57	MG	1H	3034	1/1	0.98	0.15	74,74,74,74	0
57	MG	14	3366	1/1	0.98	0.04	99,99,99,99	0
57	MG	1H	3467	1/1	0.98	0.11	74,74,74,74	0
57	MG	14	3021	1/1	0.98	0.37	63,63,63,63	0
57	MG	1H	3066	1/1	0.98	0.23	65,65,65,65	0
57	MG	14	3319	1/1	0.98	0.13	72,72,72,72	0
57	MG	14	3387	1/1	0.98	0.06	83,83,83,83	0
57	MG	14	3043	1/1	0.98	0.70	96,96,96,96	0
57	MG	1H	3024	1/1	0.98	0.17	64,64,64,64	0
57	MG	1H	3289	1/1	0.98	0.11	91,91,91,91	0
59	ZN	5A	101	1/1	0.98	0.09	129,129,129,129	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	13	1729	1/1	0.98	0.08	110,110,110,110	0
57	MG	14	3172	1/1	0.98	0.21	82,82,82,82	0
57	MG	1H	3330	1/1	0.98	0.09	74,74,74,74	0
57	MG	1H	3449	1/1	0.98	0.24	92,92,92,92	0
57	MG	1H	3388	1/1	0.98	0.07	49,49,49,49	0
57	MG	1H	3409	1/1	0.98	0.10	83,83,83,83	0
57	MG	7A	101	1/1	0.98	0.32	110,110,110,110	0
57	MG	14	3013	1/1	0.98	0.30	56,56,56,56	0
57	MG	1H	3244	1/1	0.98	0.11	47,47,47,47	0
57	MG	1H	3001	1/1	0.98	0.23	49,49,49,49	0
57	MG	1H	3479	1/1	0.98	0.05	95,95,95,95	0
57	MG	1H	3206	1/1	0.98	0.34	55,55,55,55	0
57	MG	1H	3393	1/1	0.98	0.10	63,63,63,63	0
57	MG	1H	3027	1/1	0.98	0.17	60,60,60,60	0
57	MG	I8	102	1/1	0.98	0.06	70,70,70,70	0
57	MG	1H	3145	1/1	0.98	0.09	74,74,74,74	0
57	MG	1H	3294	1/1	0.98	0.10	68,68,68,68	0
57	MG	1H	3263	1/1	0.98	0.11	53,53,53,53	0
57	MG	1H	3292	1/1	0.98	0.07	62,62,62,62	0
57	MG	1H	3021	1/1	0.98	0.28	60,60,60,60	0
57	MG	14	3189	1/1	0.98	0.32	81,81,81,81	0
57	MG	14	3219	1/1	0.98	0.14	59,59,59,59	0
57	MG	1H	3273	1/1	0.98	0.16	56,56,56,56	0
57	MG	1H	3265	1/1	0.98	0.11	74,74,74,74	0
57	MG	14	3460	1/1	0.98	0.26	92,92,92,92	0
57	MG	1H	3476	1/1	0.98	0.16	94,94,94,94	0
57	MG	14	3329	1/1	0.98	0.16	93,93,93,93	0
57	MG	14	3188	1/1	0.98	0.23	69,69,69,69	0
57	MG	1H	3440	1/1	0.98	0.05	83,83,83,83	0
57	MG	1H	3039	1/1	0.98	0.17	56,56,56,56	0
57	MG	14	3093	1/1	0.98	0.29	86,86,86,86	0
57	MG	1H	3378	1/1	0.98	0.08	54,54,54,54	0
57	MG	1G	1661	1/1	0.98	0.23	118,118,118,118	0
57	MG	1H	3295	1/1	0.98	0.12	58,58,58,58	0
57	MG	1H	3336	1/1	0.98	0.07	88,88,88,88	0
57	MG	1H	3032	1/1	0.98	0.37	68,68,68,68	0
57	MG	13	1604	1/1	0.98	0.13	79,79,79,79	0
57	MG	1H	3285	1/1	0.98	0.16	69,69,69,69	0
57	MG	13	1652	1/1	0.98	0.18	82,82,82,82	0
57	MG	14	3209	1/1	0.98	0.18	61,61,61,61	0
57	MG	13	1608	1/1	0.98	0.07	93,93,93,93	0
57	MG	1H	3322	1/1	0.98	0.10	59,59,59,59	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	14	3051	1/1	0.98	0.30	70,70,70,70	0
57	MG	13	1631	1/1	0.98	0.35	106,106,106,106	0
57	MG	14	3241	1/1	0.98	0.14	61,61,61,61	0
57	MG	14	3029	1/1	0.98	0.15	80,80,80,80	0
57	MG	14	3280	1/1	0.98	0.16	76,76,76,76	0
57	MG	14	3408	1/1	0.98	0.07	77,77,77,77	0
57	MG	13	1676	1/1	0.99	0.11	67,67,67,67	0
57	MG	1H	3256	1/1	0.99	0.12	48,48,48,48	0
58	SF4	32	302	8/8	0.99	0.20	115,120,128,136	0
57	MG	1H	3257	1/1	0.99	0.16	49,49,49,49	0
57	MG	1H	3061	1/1	0.99	0.38	62,62,62,62	0
57	MG	13	1635	1/1	0.99	0.45	83,83,83,83	0
57	MG	14	3216	1/1	0.99	0.23	62,62,62,62	0
57	MG	14	3235	1/1	0.99	0.09	55,55,55,55	0
57	MG	13	1620	1/1	0.99	0.16	68,68,68,68	0
57	MG	1H	3003	1/1	0.99	0.12	67,67,67,67	0
59	ZN	5I	101	1/1	0.99	0.13	94,94,94,94	0
57	MG	1H	3214	1/1	0.99	0.18	77,77,77,77	0
57	MG	1H	3230	1/1	0.99	0.09	90,90,90,90	0
57	MG	1H	3247	1/1	0.99	0.07	67,67,67,67	0
57	MG	13	1658	1/1	0.99	0.28	83,83,83,83	0
57	MG	1H	3389	1/1	0.99	0.05	63,63,63,63	0
57	MG	1H	3275	1/1	0.99	0.10	72,72,72,72	0
57	MG	1H	3291	1/1	0.99	0.15	57,57,57,57	0
57	MG	14	3014	1/1	0.99	0.36	72,72,72,72	0
57	MG	1H	3441	1/1	0.99	0.07	100,100,100,100	0
57	MG	1H	3245	1/1	0.99	0.11	58,58,58,58	0
58	SF4	3E	301	8/8	0.99	0.21	95,98,106,108	0
57	MG	1H	3357	1/1	0.99	0.11	64,64,64,64	0
57	MG	14	3039	1/1	0.99	0.27	85,85,85,85	0
57	MG	14	3218	1/1	0.99	0.10	55,55,55,55	0
57	MG	1H	3283	1/1	0.99	0.12	59,59,59,59	0
57	MG	1H	3251	1/1	0.99	0.06	49,49,49,49	0
57	MG	1H	3186	1/1	0.99	0.09	56,56,56,56	0
57	MG	14	3212	1/1	0.99	0.11	60,60,60,60	0
57	MG	1H	3041	1/1	0.99	0.27	57,57,57,57	0
57	MG	14	3192	1/1	0.99	0.14	80,80,80,80	0
57	MG	1H	3451	1/1	1.00	0.07	55,55,55,55	0
57	MG	1H	3005	1/1	1.00	0.15	67,67,67,67	0

6.5 Other polymers [i](#)

There are no such residues in this entry.