



# wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 9, 2018 – 11:11 am GMT

PDB ID : 5IB8  
Title : Structure of T. thermophilus 70S ribosome complex with mRNA, tRNA<sup>fMet</sup> and near-cognate tRNA<sup>Lys</sup> 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](mailto:validation@mail.wwpdb.org)

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467  
Mogul : 1.7.3 (157068), CSD as539be (2018)  
Xtriage (Phenix) : 1.13  
EDS : trunk30967  
Percentile statistics : 20171227.v01 (using entries in the PDB archive December 27th 2017)  
Refmac : 5.8.0158  
CCP4 : 7.0 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk30967

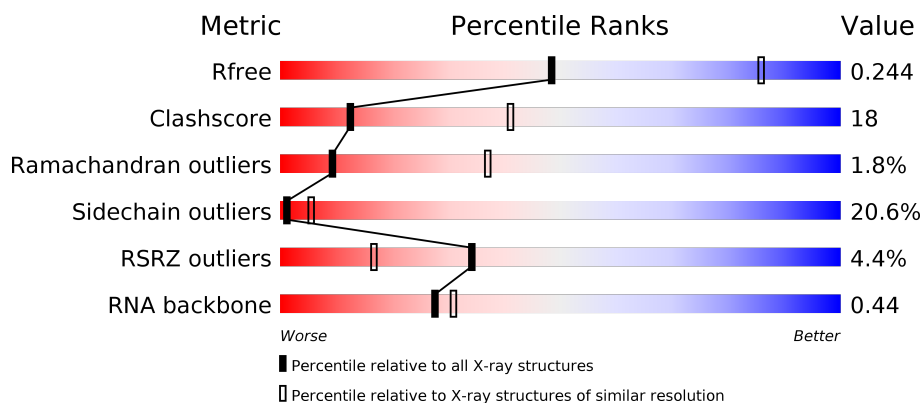
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*


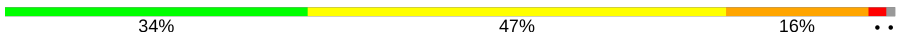
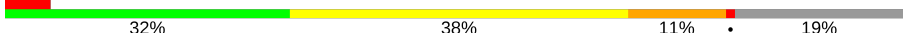

The reported resolution of this entry is 3.13 Å.

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))
$R_{free}$	111664	1371 (3.18-3.10)
Clashscore	122126	1473 (3.18-3.10)
Ramachandran outliers	120053	1429 (3.18-3.10)
Sidechain outliers	120020	1429 (3.18-3.10)
RSRZ outliers	108989	1339 (3.18-3.10)
RNA backbone	2636	1063 (3.50-2.78)

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

Mol	Chain	Length	Quality of chain
1	13	1522	
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	



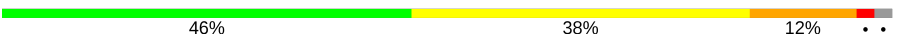
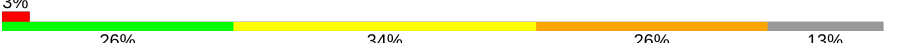
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Mol	Chain	Length	Quality of chain
41	B8	146	
42	85	118	
42	C8	118	
43	95	101	
43	D8	101	
44	A5	113	
44	E8	113	
45	B5	96	
45	F8	96	
46	C5	110	
46	G8	110	
47	D5	206	
47	H8	206	
48	E5	85	
48	I8	85	
49	F5	98	
49	J8	98	
50	G5	72	
50	K8	72	
51	H5	60	
51	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<sup>Lys</sup>.

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<sup>fMet</sup>.

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<sup>Lys</sup>.

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<sup>Lys</sup>.

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).

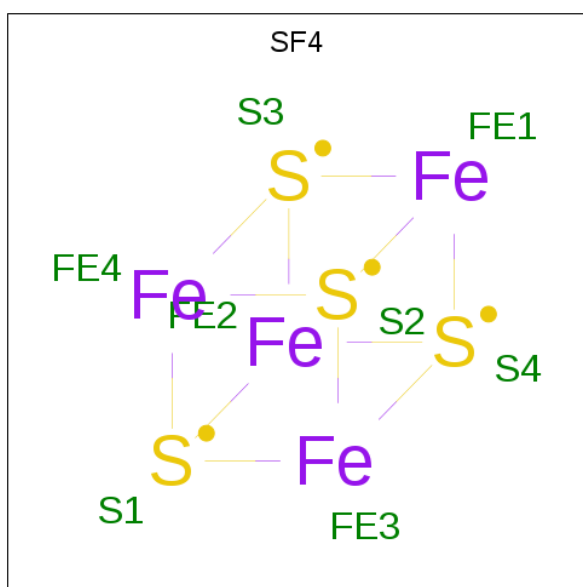
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
57	45	1	Total 1	Mg 1	0	0
57	19	1	Total 1	Mg 1	0	0
57	P8	1	Total 1	Mg 1	0	0
57	32	1	Total 1	Mg 1	0	0
57	2I	1	Total 1	Mg 1	0	0
57	13	141	Total 141	Mg 141	0	0
57	1J	10	Total 10	Mg 10	0	0
57	35	2	Total 2	Mg 2	0	0
57	4L	1	Total 1	Mg 1	0	0
57	16	12	Total 12	Mg 12	0	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:  $\text{Fe}_4\text{S}_4$ ).

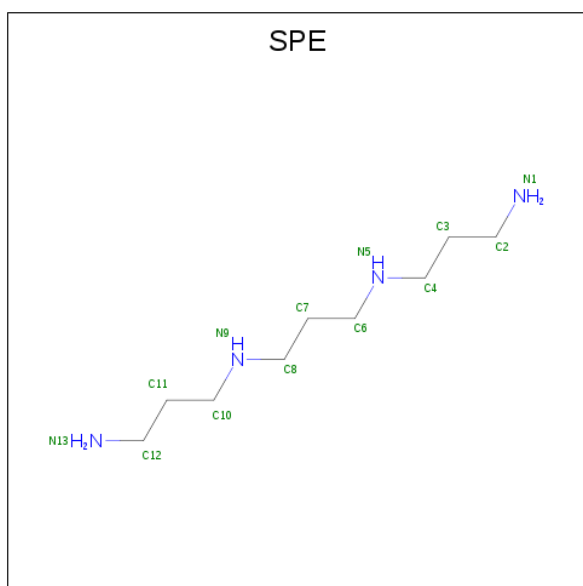


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
58	3E	1	Total	Fe	S	0	0
			8	4	4		
58	32	1	Total	Fe	S	0	0
			8	4	4		

- 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: C<sub>9</sub>H<sub>24</sub>N<sub>4</sub>).



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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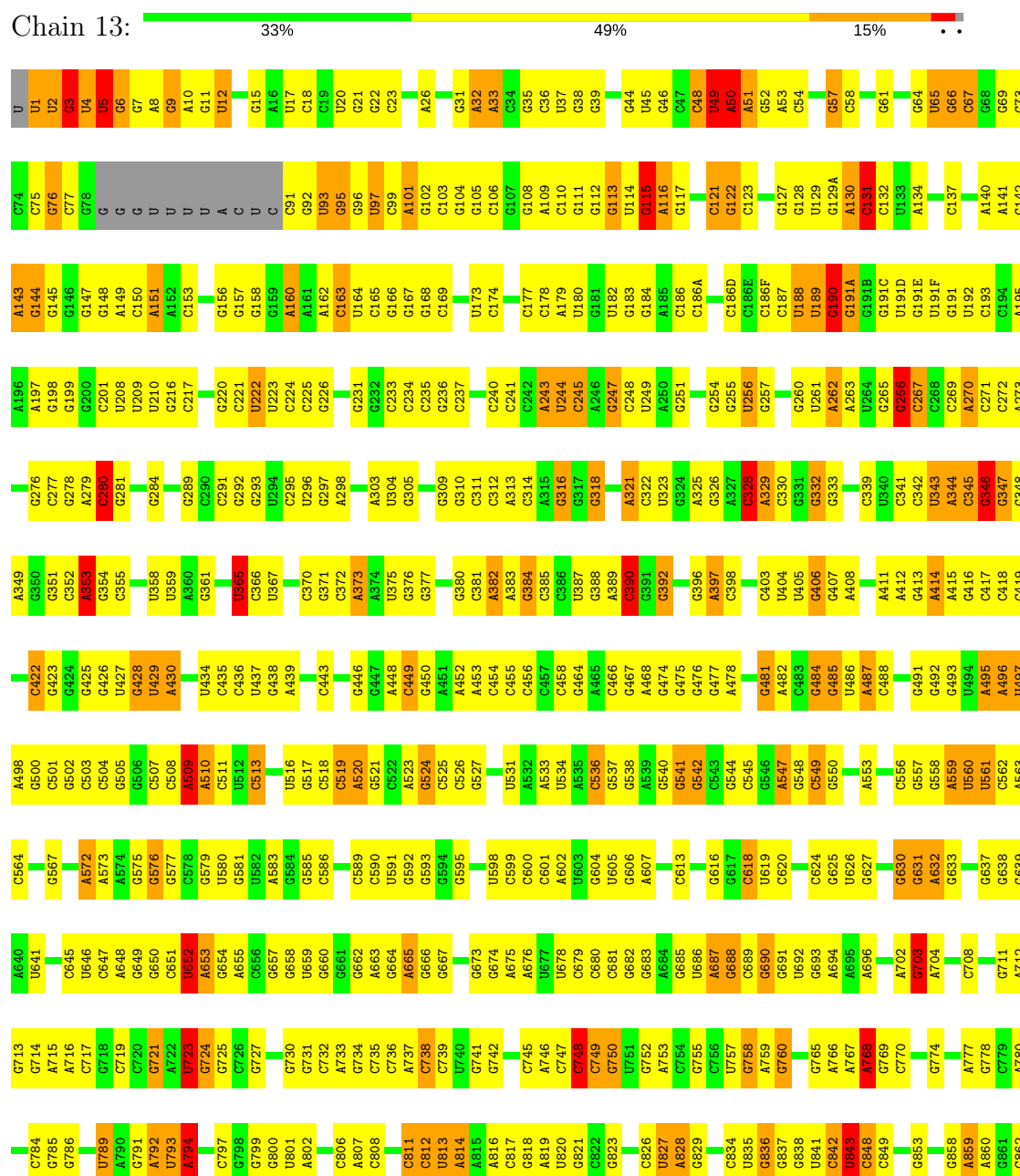
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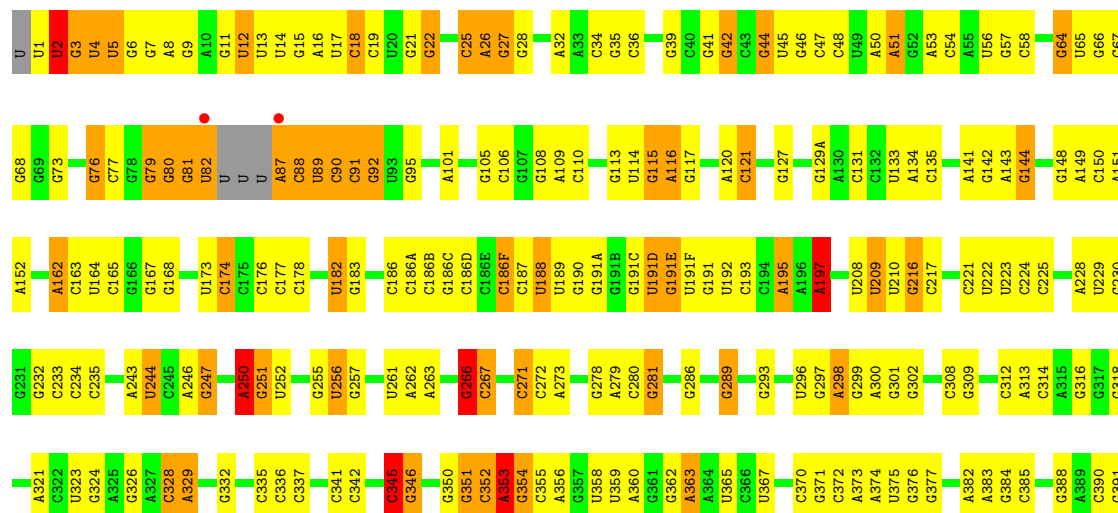
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
61	2L	8	Total 8	O 8	0	0
61	4L	3	Total 3	O 3	0	0
61	14	1303	Total 1303	O 1303	0	0
61	1J	27	Total 27	O 27	0	0
61	19	14	Total 14	O 14	0	0
61	29	6	Total 6	O 6	0	0
61	39	8	Total 8	O 8	0	0
61	15	3	Total 3	O 3	0	0
61	25	8	Total 8	O 8	0	0
61	35	8	Total 8	O 8	0	0
61	55	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

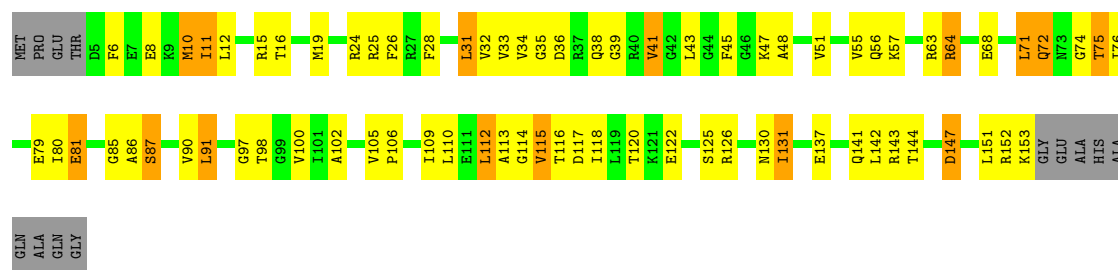




C1466	U1380	G1255	A1191	A1130	A1055	C995	C931	G858	A768	G688	G610	G477	G392
G1467	U1381	A1256	C1195	G1131	U1056	A996	C932	A859	G769	C689	A611	G481	A393
G1468	C1382	U1257	C1196	G1132	G1057	U997	G933	A860	C770	G690	A614	A482	A397
G1469	G1383	G1258	U1196	G1133	G1058	G998	C934	G861	G771	G691	G615	C483	C398
G1470	G1386	A1324	C1259	G1134	C1059	C998A	A935	A862	G776	G692	G616	C484	
G1471	G1387	G1260	G1198	U1135	U1062	U999	C936	U863	A777	U693	G617	G485	G406
		A1261	U1199	U1136	U1063	A1000	A937	A864	G778	A694	G618	G486	G407
G1474	U1391	C1262	C1200	C1137	G1064	G1001	A938	A865	C779		U619	C554	
	G1392	C1263	A1201	G1138	U1065	G1002	G939		C778	U697	U618	C556	A408
C1478	C1395	G1264	G1202	G1139	U1066	G1003	C940	C968	A780	G698	A621	C557	A409
C1479	U1330	G1265	C1203	C1140	U1067	A1004	G941	G869			A622	G491	G410
	A1396	G1266	A1204	C1141	G1068	A1005	U943	U870	C784	A702	G622	C492	A411
G1487	C1397	C1267	U1205	G1142	C1071	C1006	U944	U871			C623	A485	A412
	A1398	A1268	G1206	G1143	G1072	C1007	G944	A872	A706		C624	A486	A414
		A1269	G1207	G1144	G1072	C1008		A873			G625	A487	
C1490	C1399	G1270	C1208	C1145	U1078	C1009	G947	A874	G709	G709	G626	A496	
G1491	C1334	U1271	A1146	G1147	G1079	G1010	C948	C975	A792	G710	G627	U497	
A1492	G1401	G1272	C1209	C1147	U1078	G1011		G876	U793	G711	G628	A498	
A1493	C1402	G1273	U1211	U1148	A1080	C1019	A959	G877	A794	G713	G629	C501	U421
	C1403	U1212	U1212	C1149	G1081	U1020	U952	C977		G714	G630	G502	C422
		A1213	A1213	U1150	G1082	A1014	G953	C978	U801		G631	G567	G423
C1409	C1410	G1214	G1215	A1151	U1083	G1017	U957	C883	A802	C717	G633	G568	
	C1411	G1215	G1216	A1152	G1084	G1018	A958	U884	G803	G718	G634	A572	C419
A1502	C1412	A1280	C1217	G1154	U1085	C1019	A959	G885	U804	C719	G635	A573	U420
A1503	A1413	U1281	C1218	G1155	G1088	U1020	U960		G805			A574	C433
G1505	U1414	C1282	U1219	G1156	G1094	G1021	U961	A889	C811	U723	A640	G575	U434
U1506	G1415	G1283	G1220	A1157	G1095	G1022	C962	G890	U724	G725	U641	G576	C443
A1507	C1347	C1284	G1221	U1158	U1096	G1023	G963	C816	G726	C577	A642	G577	C444
G1508	U1348	A1285	G1222	C1159	C1096	G1024	A964	G894	G727	G578	U646	G579	U435
C1509	C1349	G1286	C1223	G1160	C1097	U1025	A965	G895	G728	U580	C617	G581	C436
U1510	A1350	A1287	G1224	C1161	C1098	G1026	C986	U820	A729	U582	C651	A583	C437
G1511	U1351	A1288	A1225	C1162	C1099	G1027	U967	C999	G821	G730	U652	A584	U438
U1512	C1352	G1291	C1226	C1163	A1100	C1028A	A968	A900	C822	G731	A653	G584	A439
C1513	G1354	U1292	C1228	G1165	A1101	C1028B	C970	G825	G735		G660	G585	A440
C1514	C1355	G1293	A1229	C1166	G1103	G1029	C972	C826	C736		G661	C586	C442
C1515	G1356	G1294	C1230	C1167	G1104	C1030	G973	U827	A737		G662	C587	C445
G1516	A1357	G1295	U1232	A1169	A1105	G1031	A974	A828	C738		A663	G526	C446
		C1296	G1231	A1170	G1106	A1032	G975	G829	C739		G664	G527	G447
		C1297	G1232	C1171	C1107	G1032A	G976	C910	U740	U591	A665	G529	G448
		U1235	U1235	C1172	G1108	G1032B	G977	C912	G741		G666	G530	C449
		A1236	A1236	G1173	C1109	G1033	A978	C913	G742		G667	G531	
		C1237	C1237	G1174	A1110	G1034	U980	A915	C744		G668	A532	G450
		A1238	A1238	G1175	A1111		U981	G837				A533	A451
		U1239	U1239	A1176	C1112	C1037	U982	G838	C748		U672	U534	A452
		G1241	G1241	G1177	C1113		A983	U841	C749		G673	U598	
		A1244	A1244	A1179	G1118	U1040	C984	C842	G750		G674	C599	C456
		C1245	C1245	G1180	G1119	G1042	C985	U843	U751		A675	C600	C457
		U1246	U1246	G1181	G1120	C1043	U986	U844			A676	C601	C458
		G1311	G1311	A1182	U1121	C1044	A987	U845	C754		U677	A602	C459
		U1247	U1247	A1183	U1122	C1045	C988	G851	G755		U678	U603	C464
		C1314	C1314	G1184	A1123	G1046	G987	G852			C679	G604	A465
		U1249	U1249	G1185	G1124	G1047	C989	C924	A759			U605	C466
		A1250	A1250	G1186	U1125	U1048	C990	C925			G683	G606	C467
		C1251	C1251	G1187	U1126		U991	G854			A684	C543	A468
		A1252	A1252	A1188	G1127	U1052	U992	G855	G765		A694	A607	G474
		G1253	G1253	A1189	C1128	C1054	C993	C856	A766			A608	G475
		C1254	C1254	G1190	C1129		A994	C857	A767		A687	A609	G476

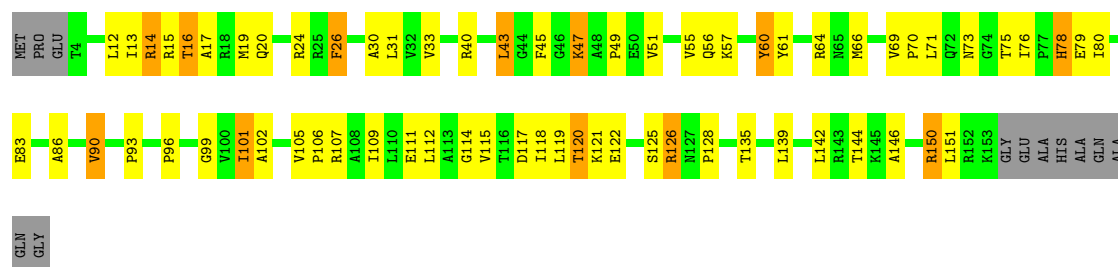






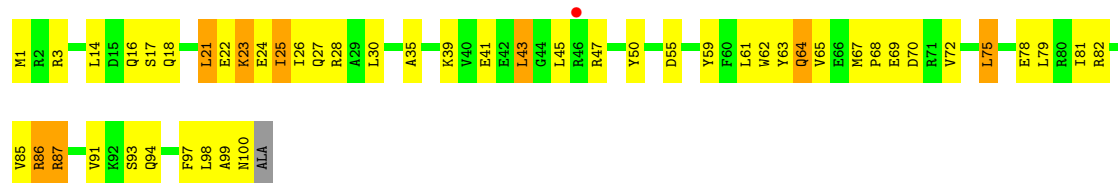
• Molecule 5: 30S ribosomal protein S5

Chain 42: 51% 34% 7% 7%



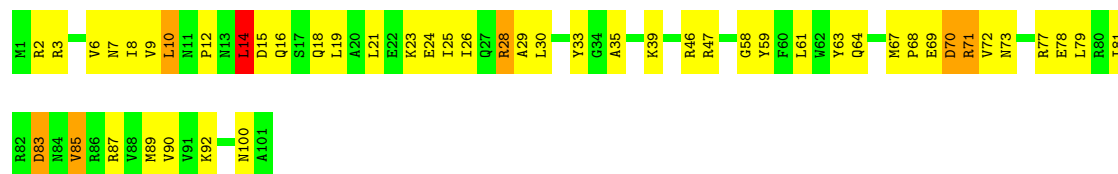
• Molecule 6: 30S ribosomal protein S6

Chain 5E: 50% 41% 8%



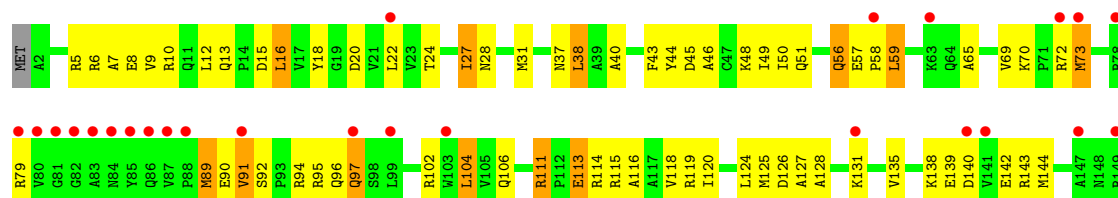
• Molecule 6: 30S ribosomal protein S6

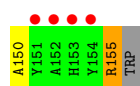
Chain 52: 51% 42% 6%



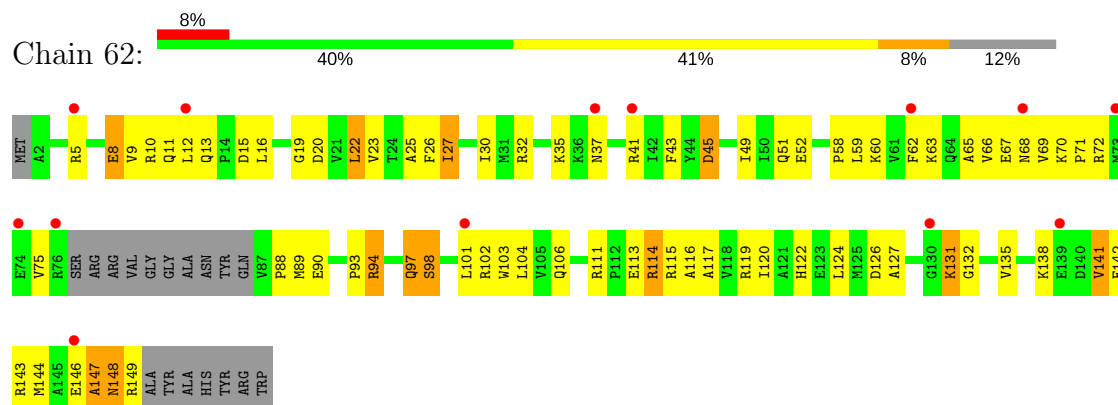
• Molecule 7: 30S ribosomal protein S7

Chain 6E: 19% 53% 38% 8%

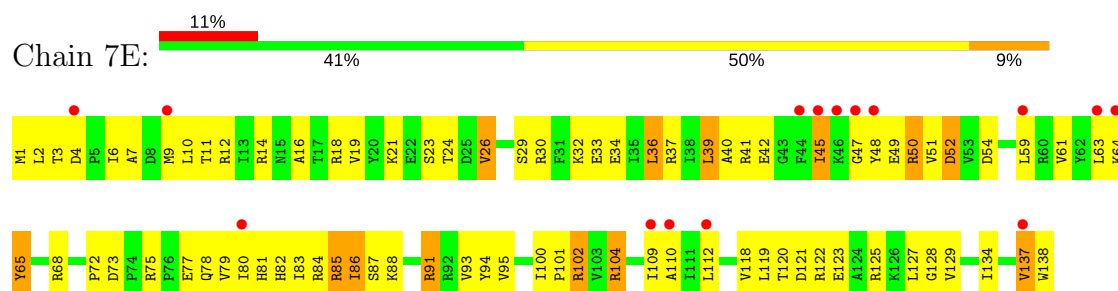




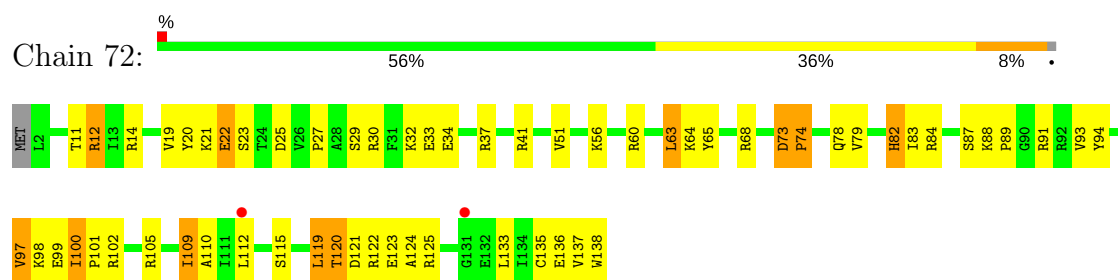
• Molecule 7: 30S ribosomal protein S7



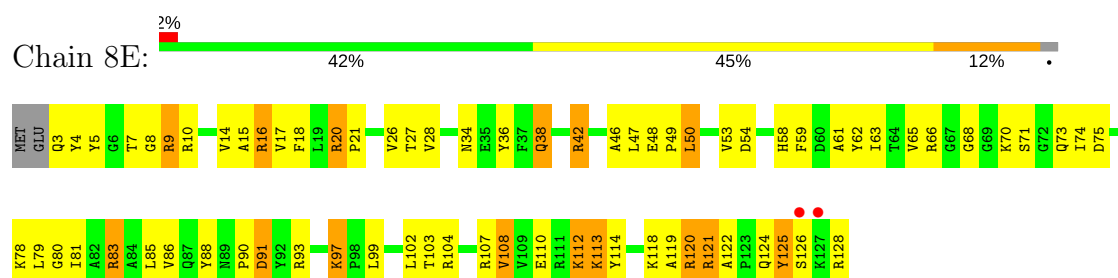
• Molecule 8: 30S ribosomal protein S8



• Molecule 8: 30S ribosomal protein S8

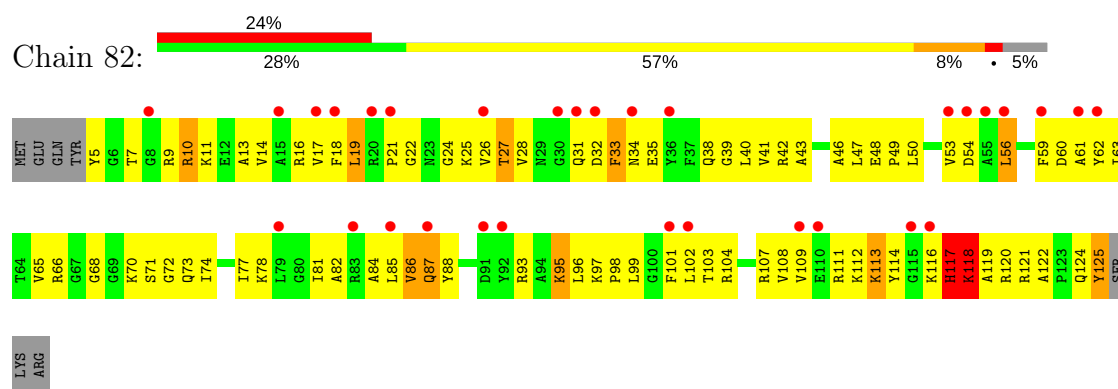


• Molecule 9: 30S ribosomal protein S9

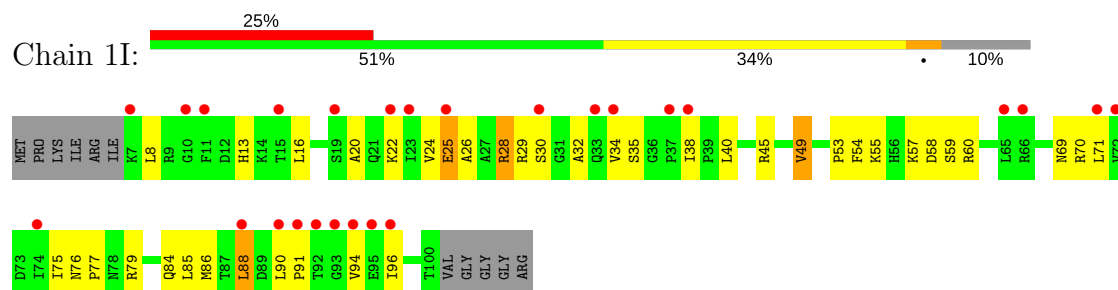


• Molecule 9: 30S ribosomal protein S9

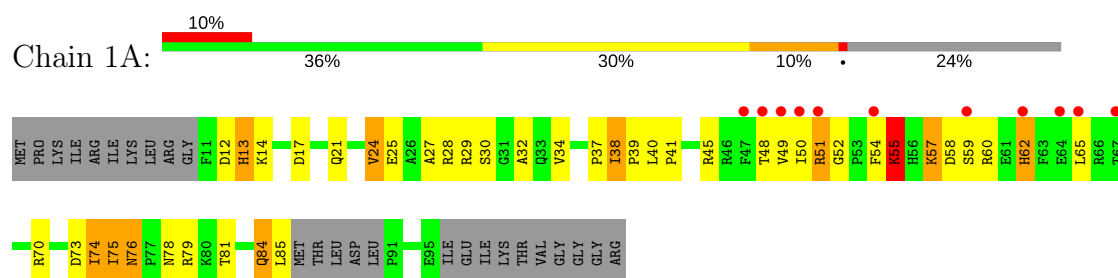




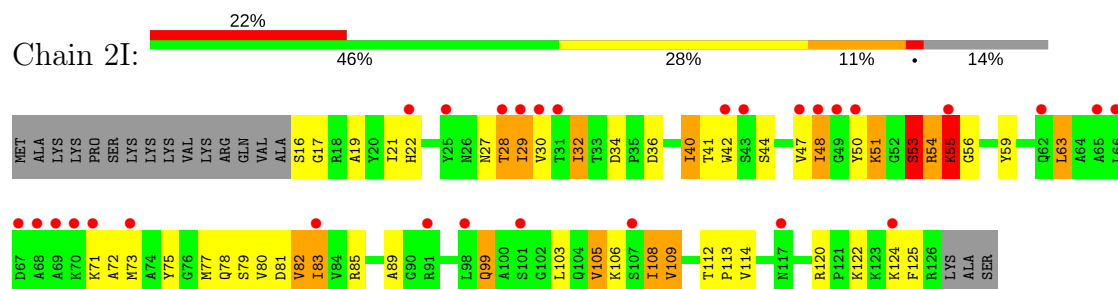
• Molecule 10: 30S ribosomal protein S10



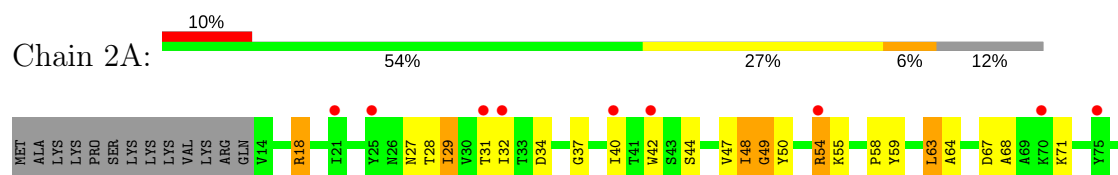
• Molecule 10: 30S ribosomal protein S10



• Molecule 11: 30S ribosomal protein S11

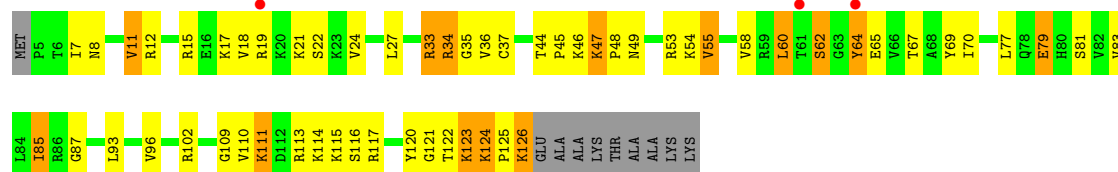


• Molecule 11: 30S ribosomal protein S11

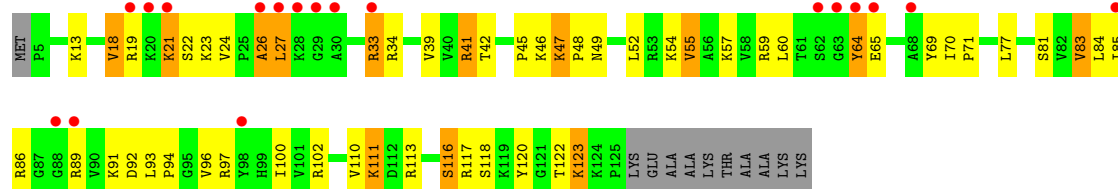




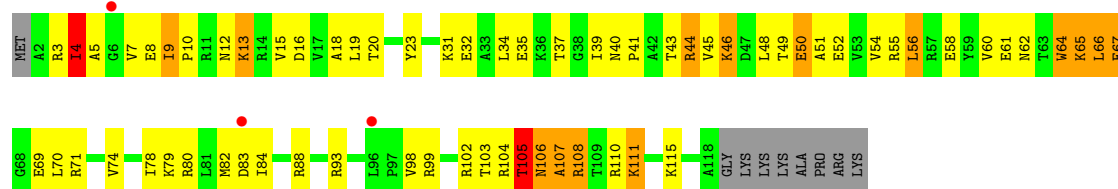
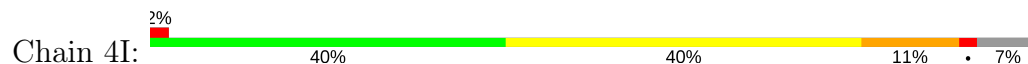
- Molecule 12: 30S ribosomal protein S12



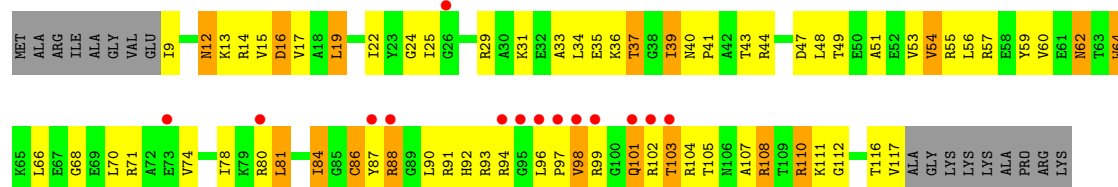
- Molecule 12: 30S ribosomal protein S12



- Molecule 13: 30S ribosomal protein S13

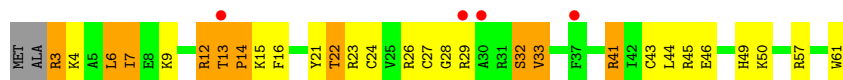


- Molecule 13: 30S ribosomal protein S13

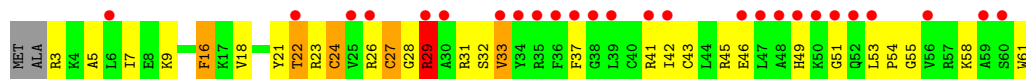
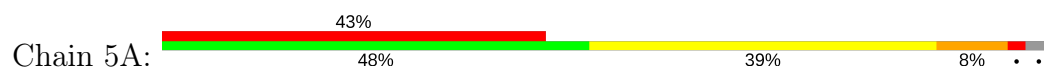


- Molecule 14: 30S ribosomal protein S14 type Z

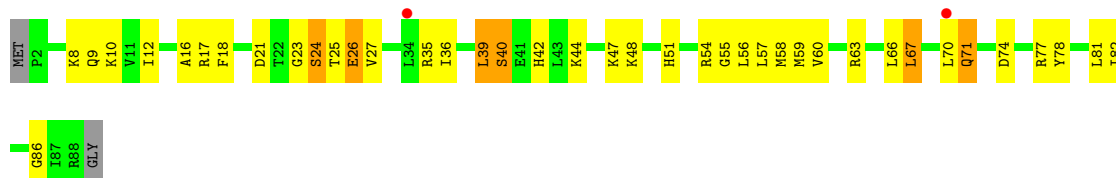




- Molecule 14: 30S ribosomal protein S14 type Z



- Molecule 15: 30S ribosomal protein S15



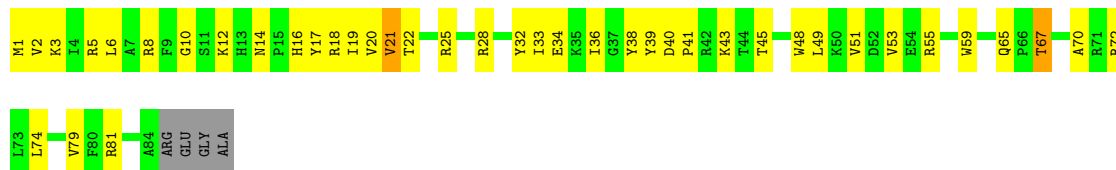
- Molecule 15: 30S ribosomal protein S15



- Molecule 16: 30S ribosomal protein S16

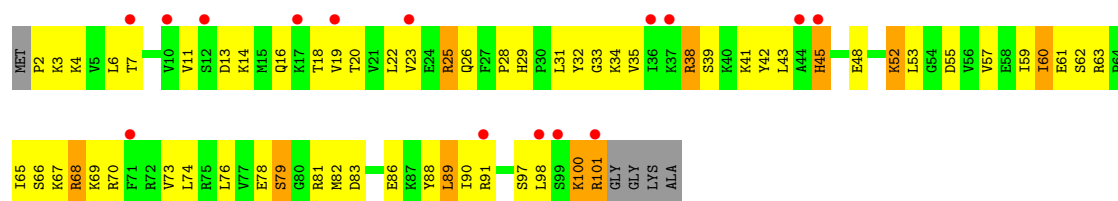


- Molecule 16: 30S ribosomal protein S16



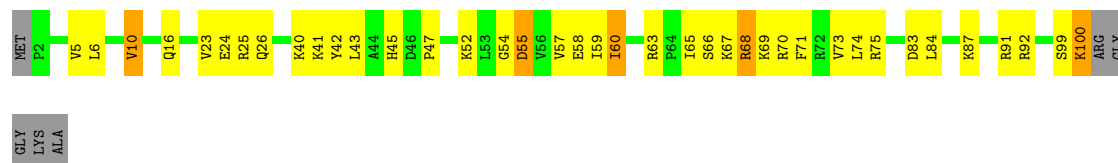
- Molecule 17: 30S ribosomal protein S17





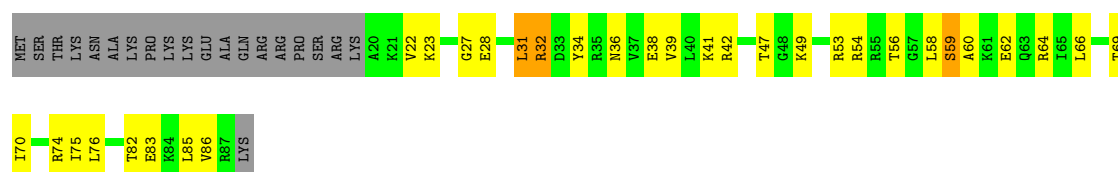
• Molecule 17: 30S ribosomal protein S17

Chain 8A: 57% 32% 5% 6%



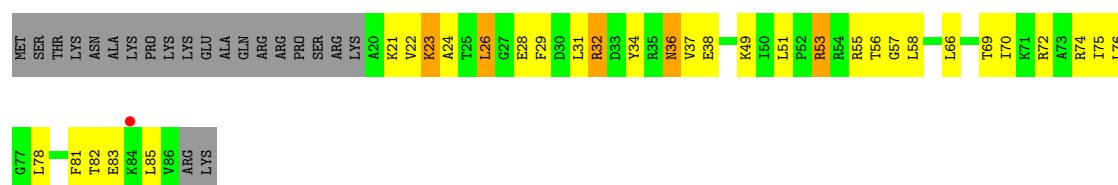
• Molecule 18: 30S ribosomal protein S18

Chain 9I: 41% 33% 23%



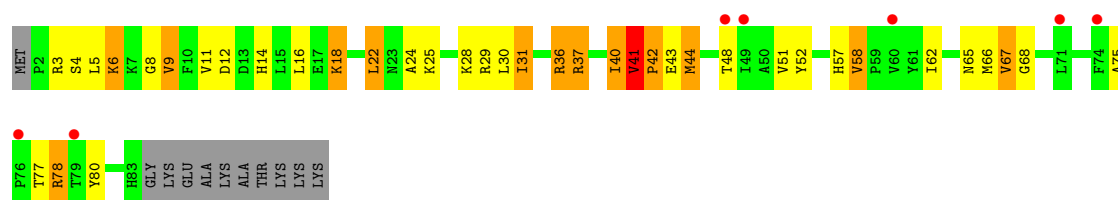
• Molecule 18: 30S ribosomal protein S18

Chain 9A: 40% 31% 6% 24%



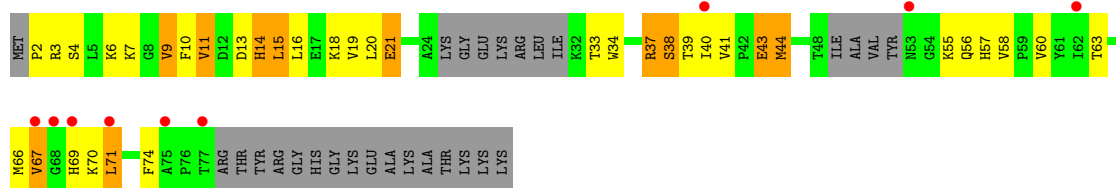
• Molecule 19: 30S ribosomal protein S19

Chain AI: 8% 46% 27% 14% 12%

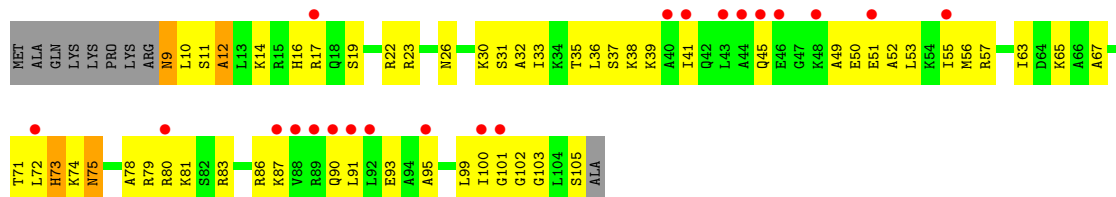
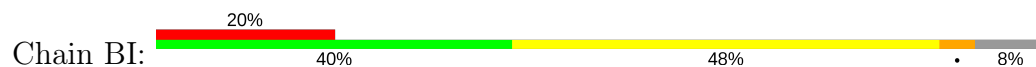


• Molecule 19: 30S ribosomal protein S19

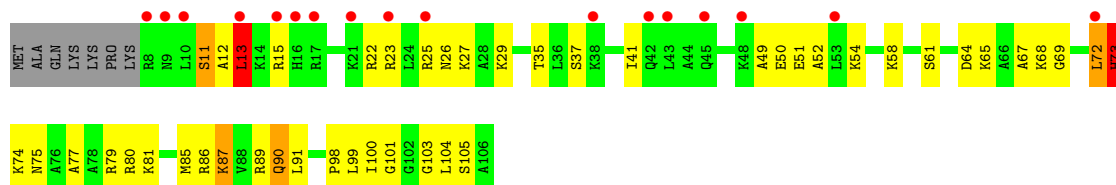
Chain AA: 10% 30% 28% 12% 30%



- Molecule 20: 30S ribosomal protein S20



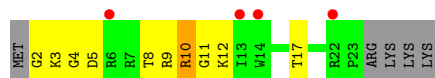
- Molecule 20: 30S ribosomal protein S20



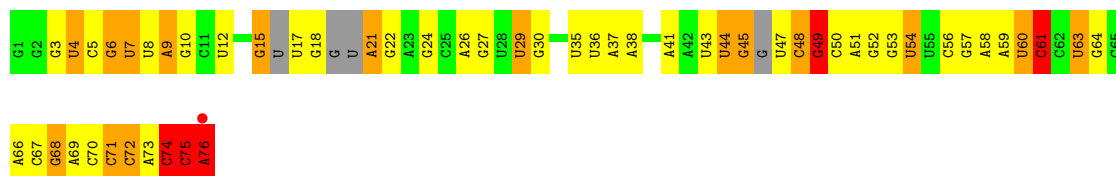
- Molecule 21: 30S ribosomal protein Thx



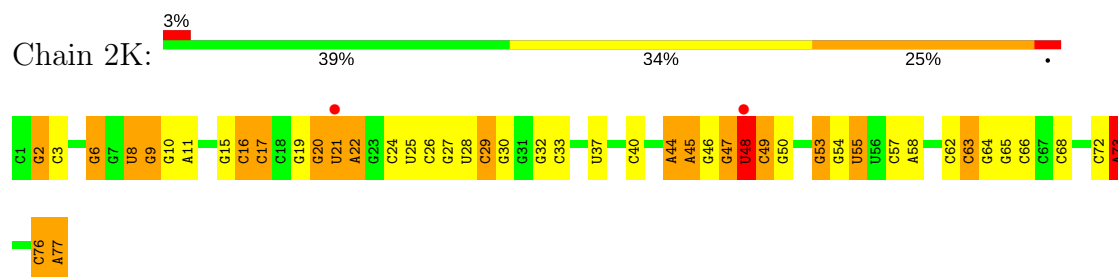
- Molecule 21: 30S ribosomal protein Thx



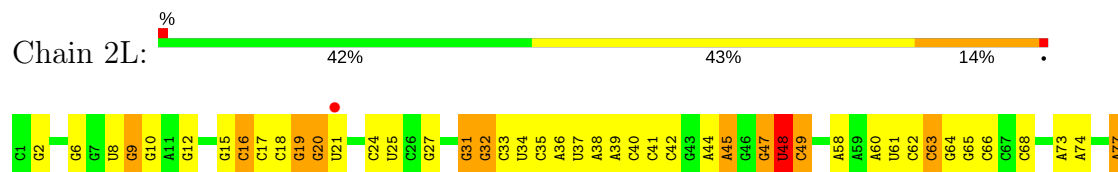
- Molecule 22: tRNA<sup>Lys</sup>



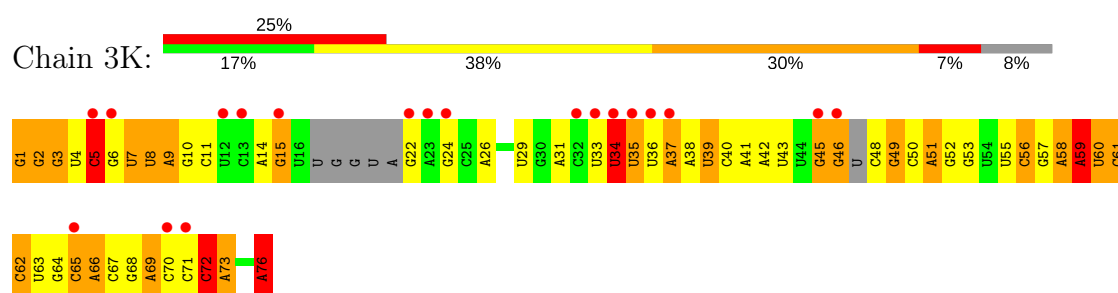
- Molecule 23: tRNA<sup>fMet</sup>



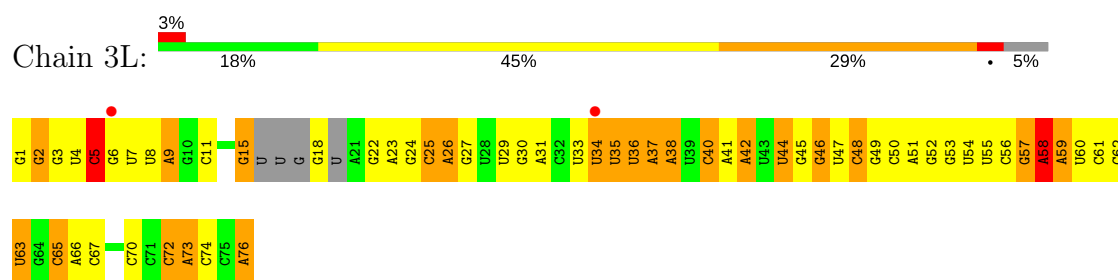
- Molecule 23: tRNA<sup>fMet</sup>



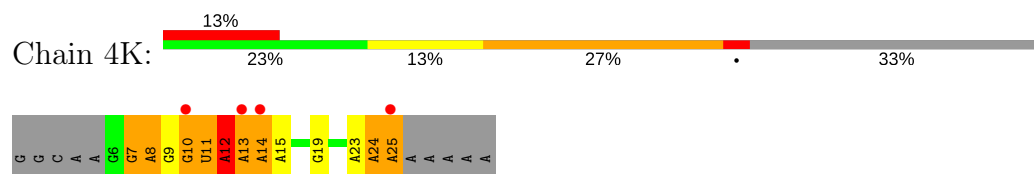
- Molecule 24: tRNA<sup>Lys</sup>



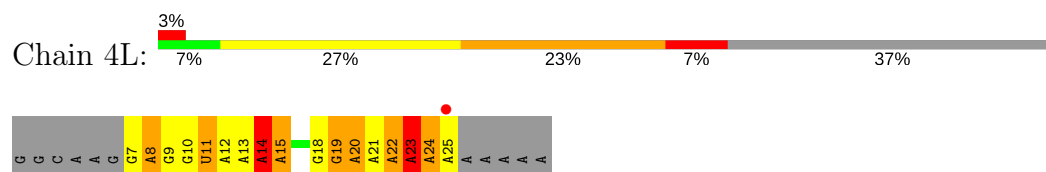
- Molecule 24: tRNA<sup>Lys</sup>



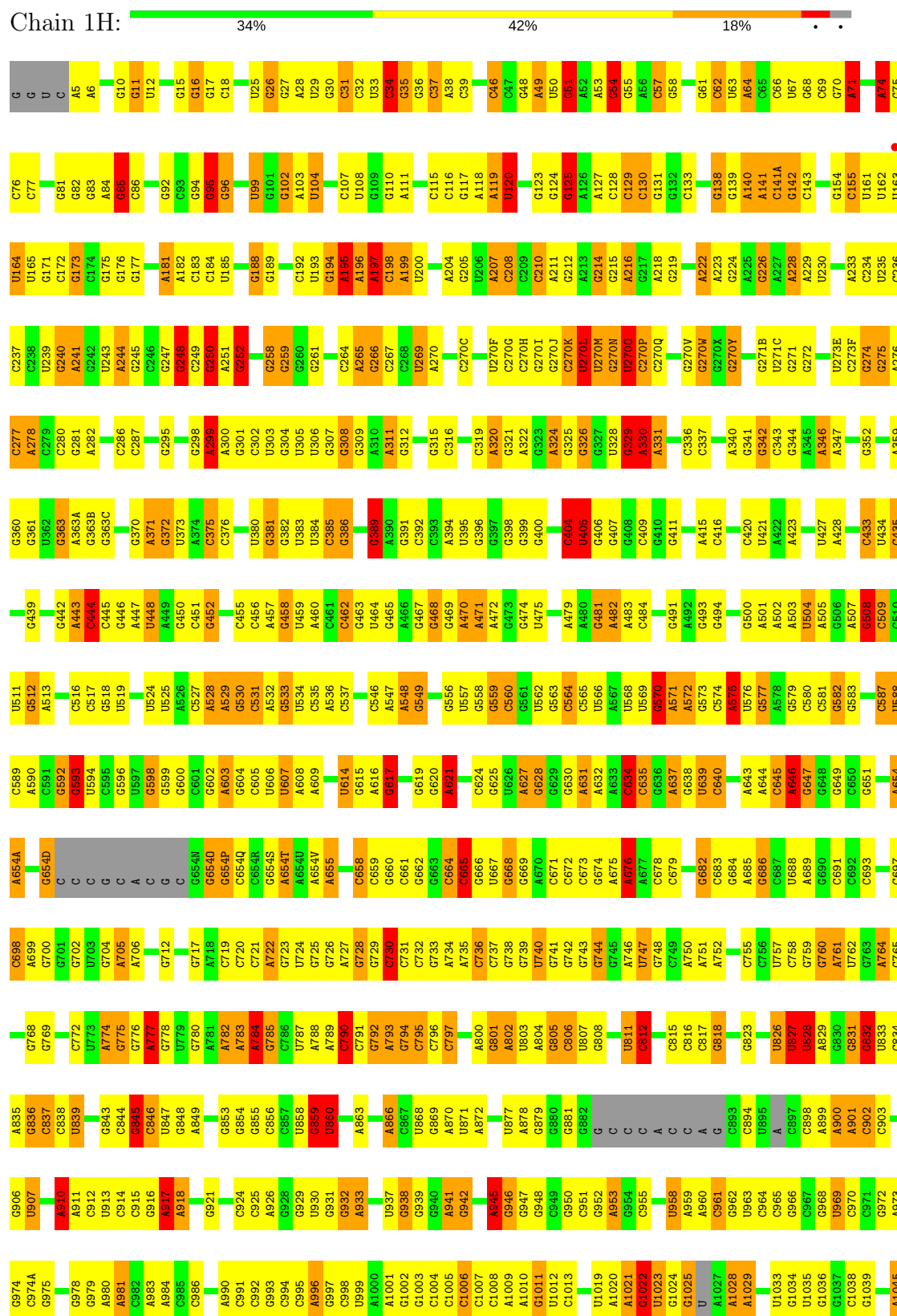
- Molecule 25: mRNA



- Molecule 25: mRNA



● Molecule 26: 23S ribosomal RNA



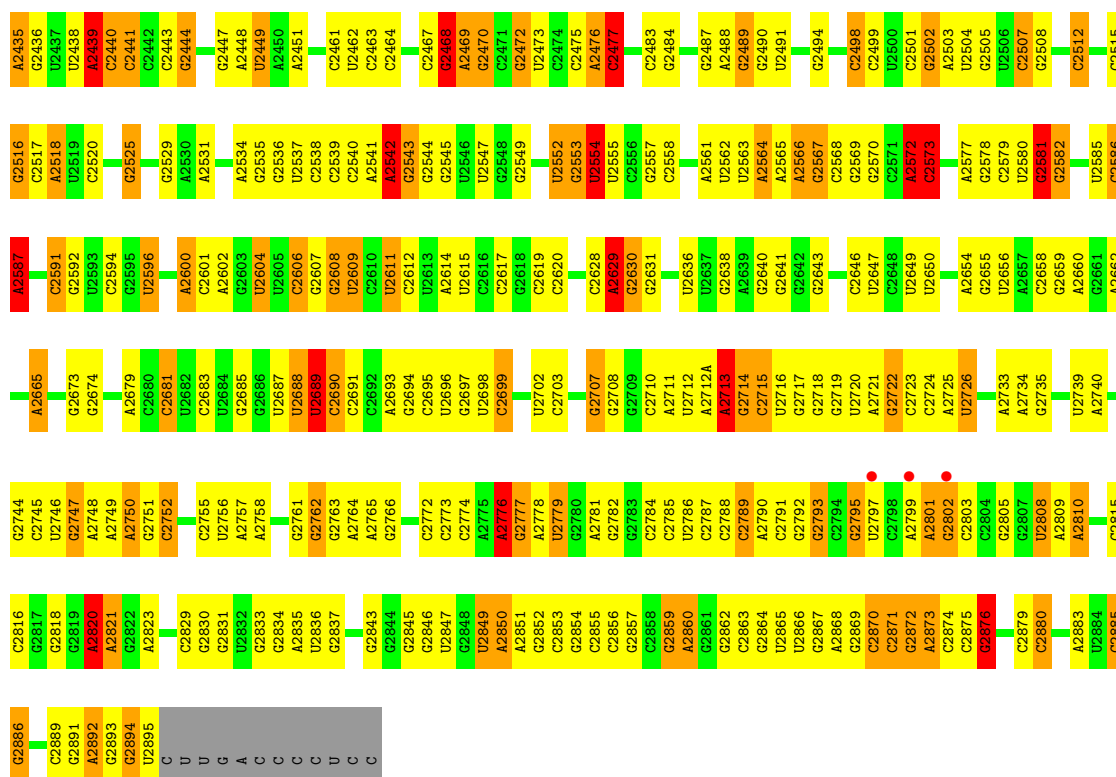
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C2063	U1993		G1828	C1761	G1662	C1598	C1533		C1389		A1246	C1179	U1108	A1048
C2064	A1919	A1919	G1829	A1762		C1599	G1534	G1459	U1390	C1318	A1247	C1180	C1109	C1049
C2065	U1995	C1920	C1830	G1763	A1665	G1601	U1536	A1460	U1391	C1319	G1248	A1181	G1110	A1050
C2066	C1996		G1831	G1764	G1666	C1602	A1536	G1461	A1392	C1320	U1249	A1182	A1111	G1051
C2067	U1926		G1832	C1765	G1667	A1603	C1537		A1393	A1321	G1250	G1183	U1112	C1052
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G2069	G2000	G1929	C1834	C1767	A1669	A1604	C1539	C1467	A1395	U1323	A1253	G1186	G1114	A1054
G2070	A2001	G1930	G1835	U1768	C1670	C1606	U1541	U1396	U1397	G1324	U1254	A1187	G1114	G1055
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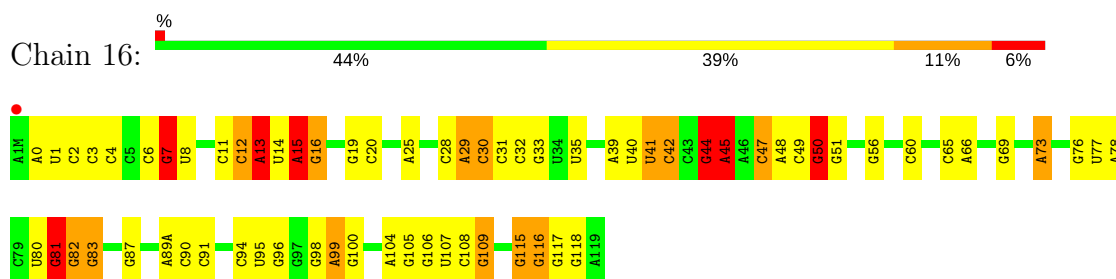




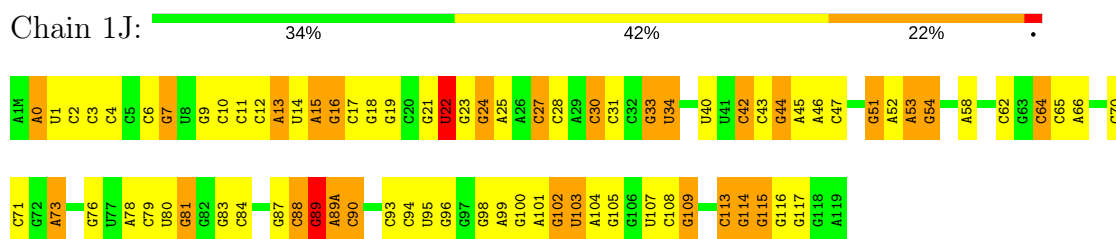
WORLDWIDE  
PDB  
PROTEIN DATA BANK



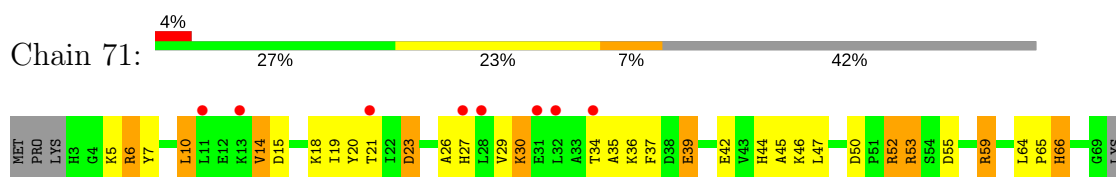
• Molecule 27: 5S ribosomal RNA

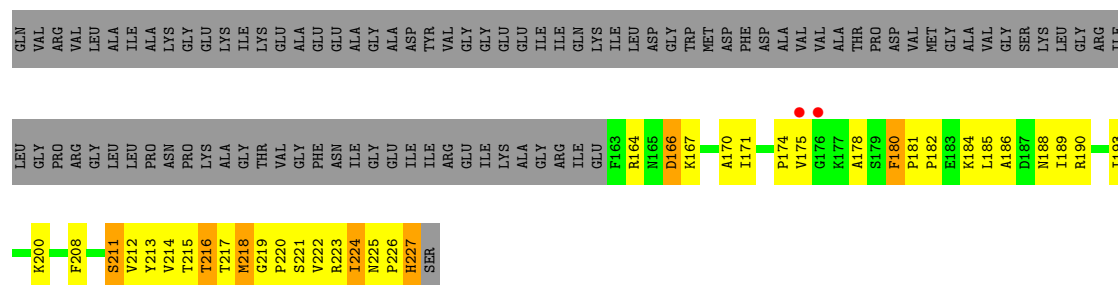


• Molecule 27: 5S ribosomal RNA

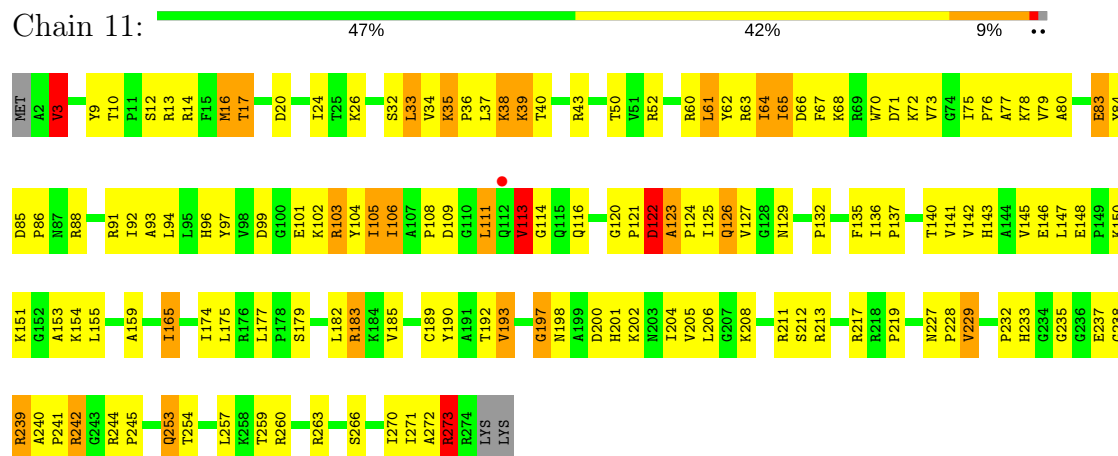


• Molecule 28: 50S ribosomal protein L1

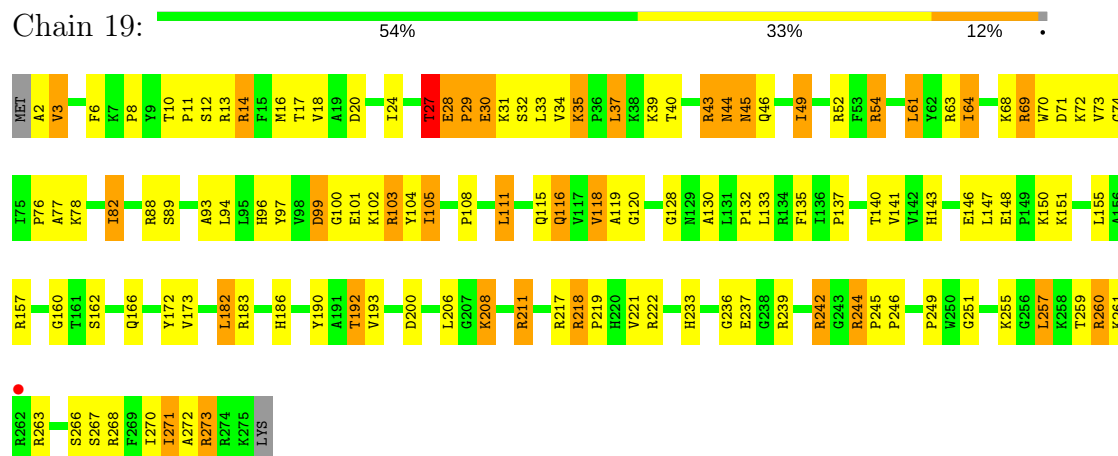




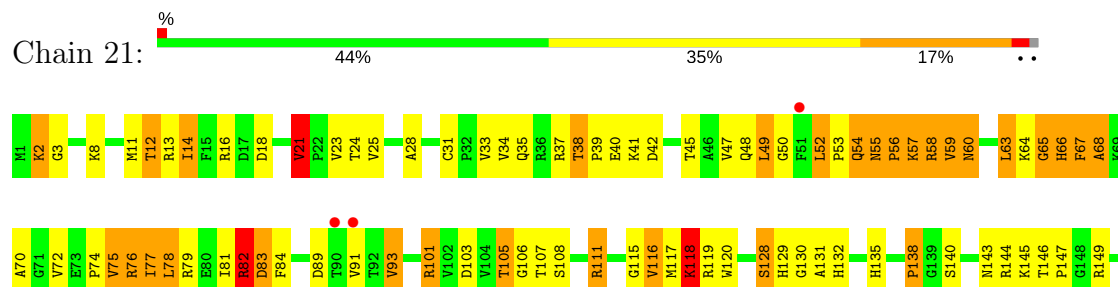
• Molecule 29: 50S ribosomal protein L2

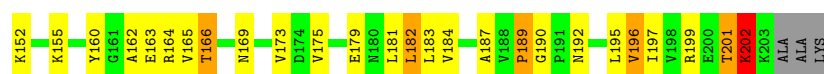


• Molecule 29: 50S ribosomal protein L2

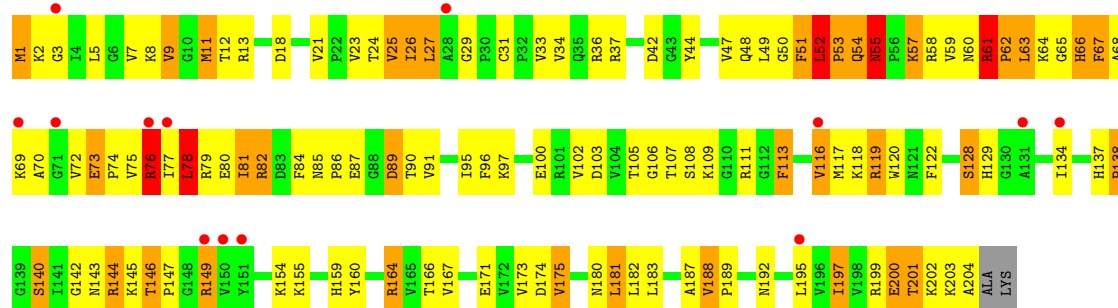


• Molecule 30: 50S ribosomal protein L3

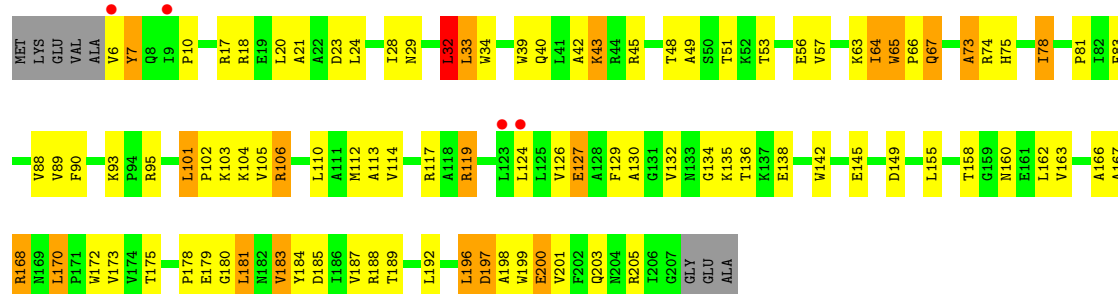




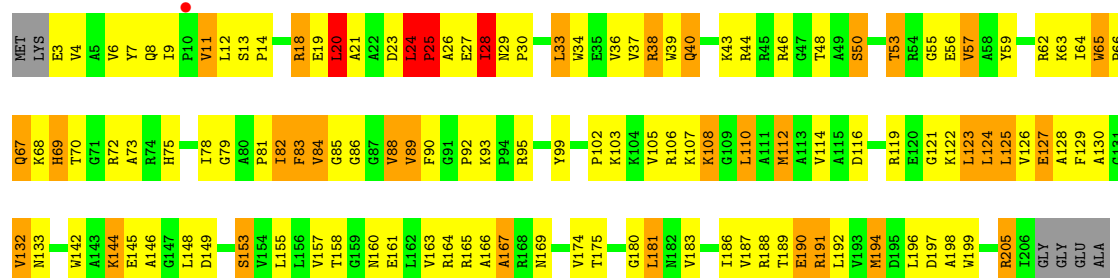
• Molecule 30: 50S ribosomal protein L3



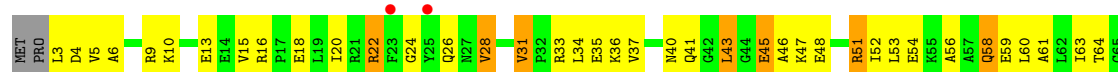
• Molecule 31: 50S ribosomal protein L4

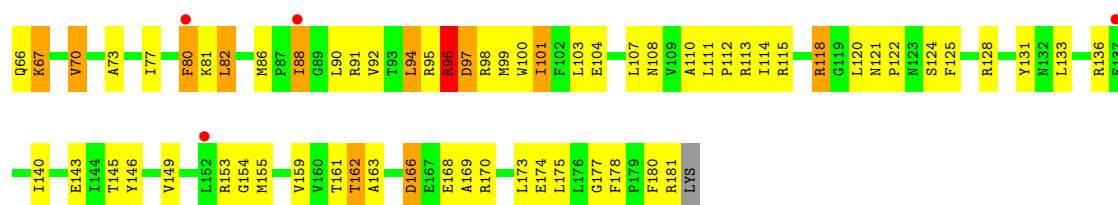


• Molecule 31: 50S ribosomal protein L4

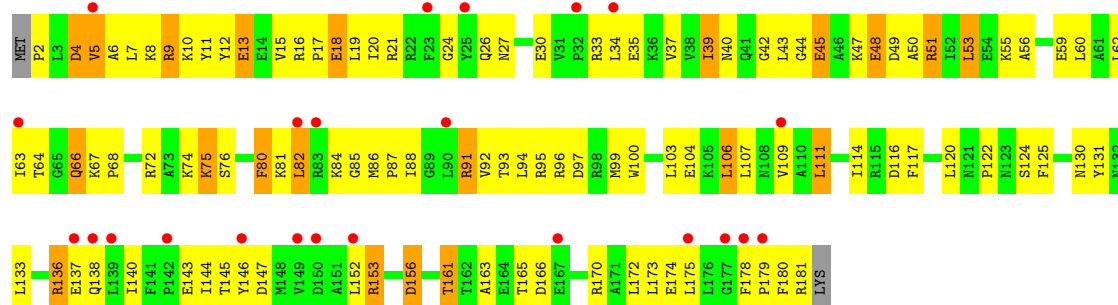


• Molecule 32: 50S ribosomal protein L5

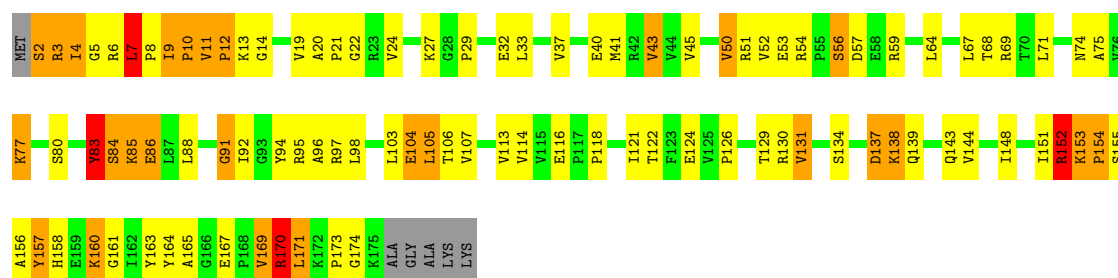


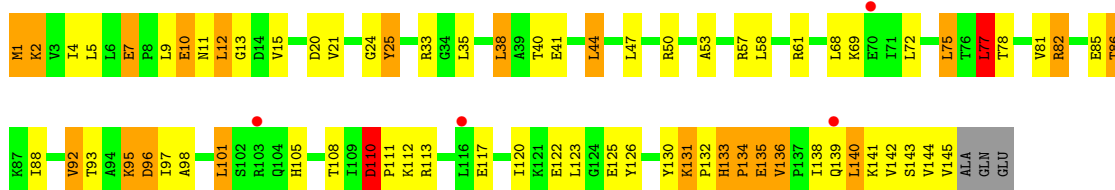


• Molecule 32: 50S ribosomal protein L5

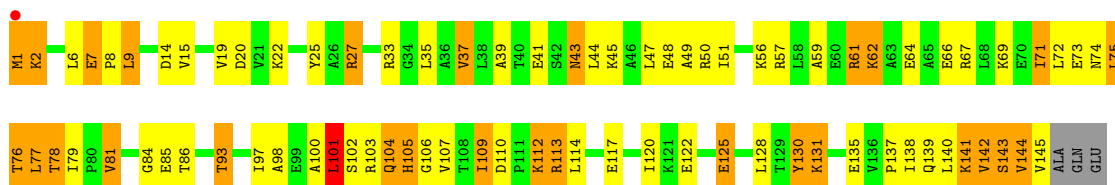
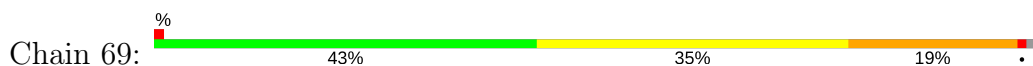


• Molecule 33: 50S ribosomal protein L6

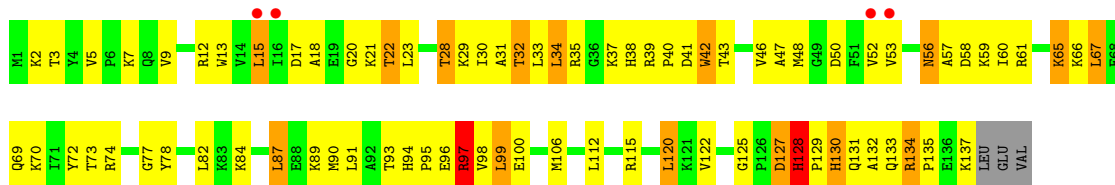




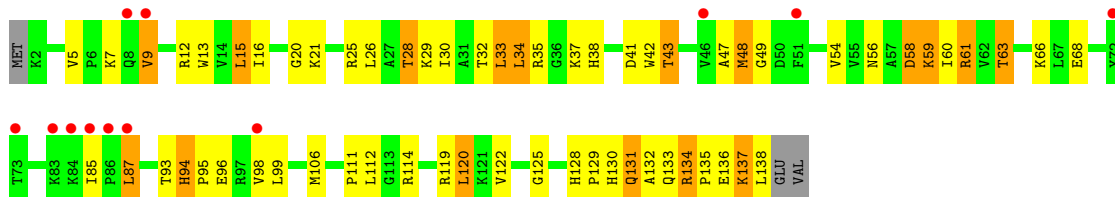
• Molecule 34: 50S ribosomal protein L9



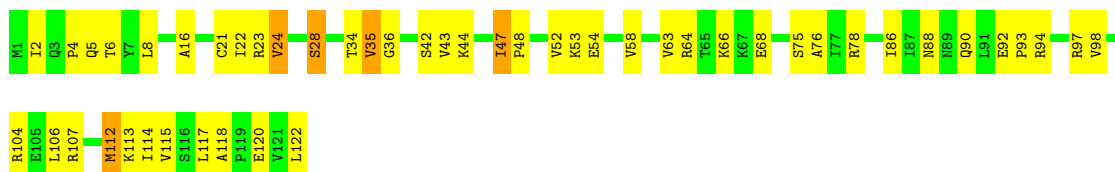
• Molecule 35: 50S ribosomal protein L13



• Molecule 35: 50S ribosomal protein L13



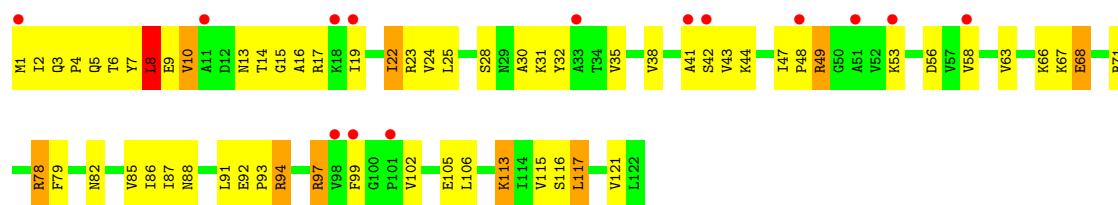
• Molecule 36: 50S ribosomal protein L14



• Molecule 36: 50S ribosomal protein L14

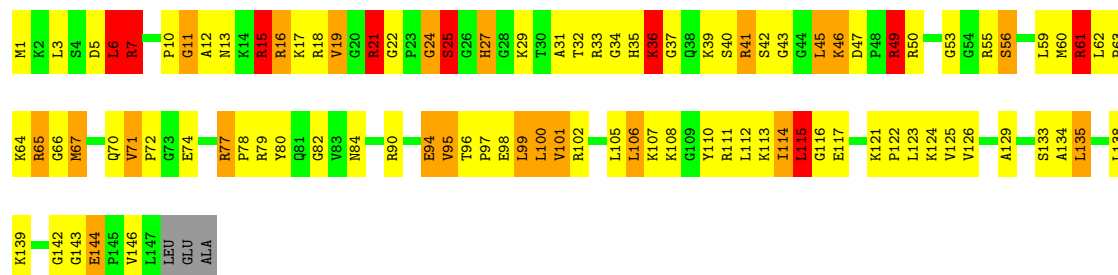






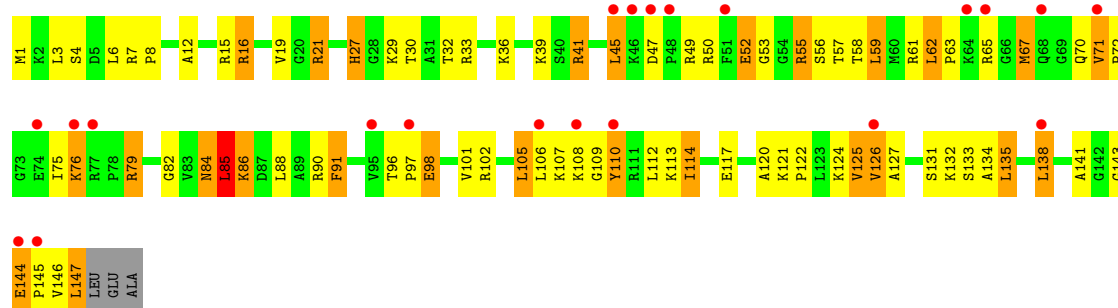
• Molecule 37: 50S ribosomal protein L15

Chain 78: 33% 44% 15% 6%



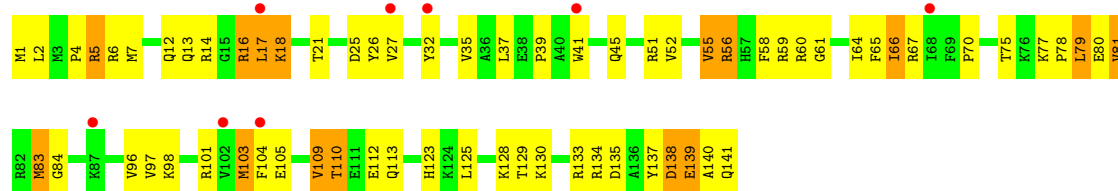
• Molecule 37: 50S ribosomal protein L15

Chain 35: 14% 43% 37% 17%



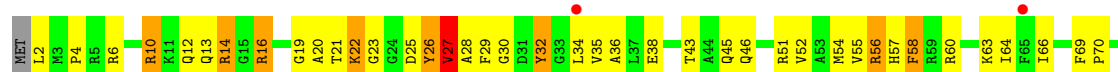
• Molecule 38: 50S ribosomal protein L16

Chain 88: 6% 52% 37% 11%



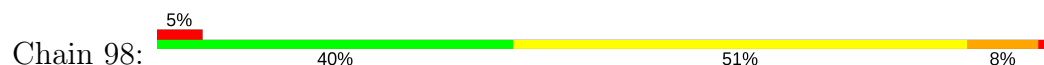
• Molecule 38: 50S ribosomal protein L16

Chain 45: 2% 41% 43% 13%

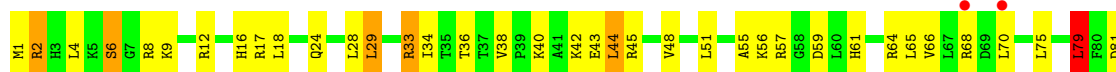




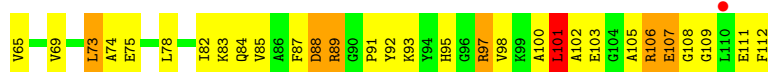
• Molecule 39: 50S ribosomal protein L17



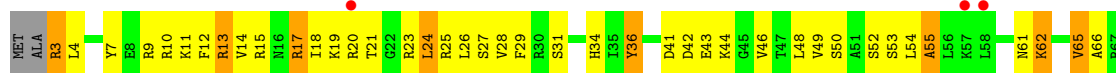
• Molecule 39: 50S ribosomal protein L17



• Molecule 40: 50S ribosomal protein L18

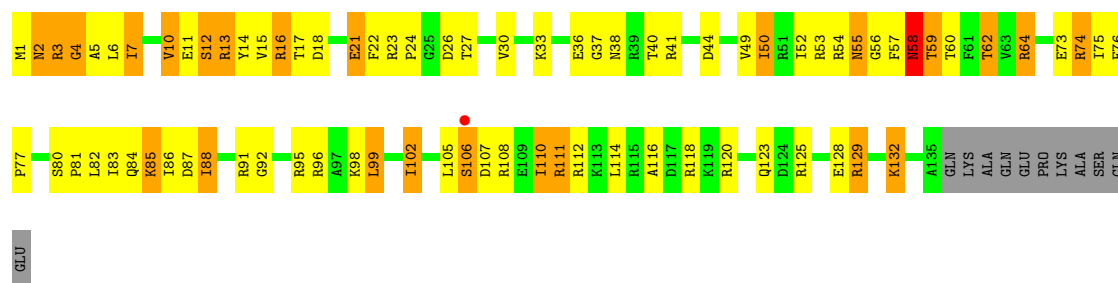


• Molecule 40: 50S ribosomal protein L18

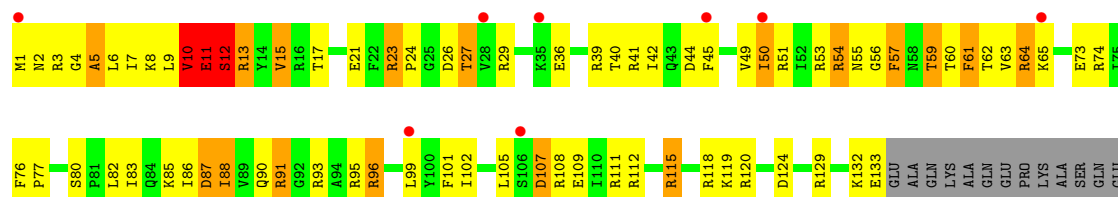


• Molecule 41: 50S ribosomal protein L19

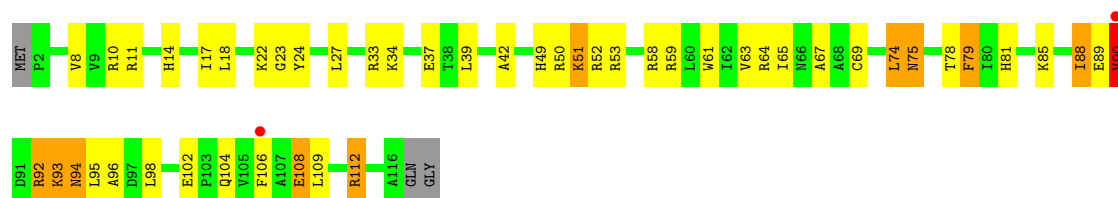




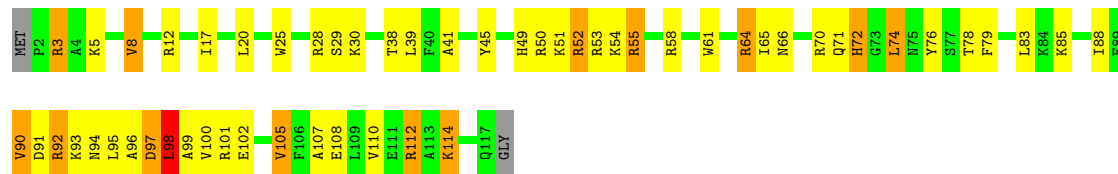
- Molecule 41: 50S ribosomal protein L19



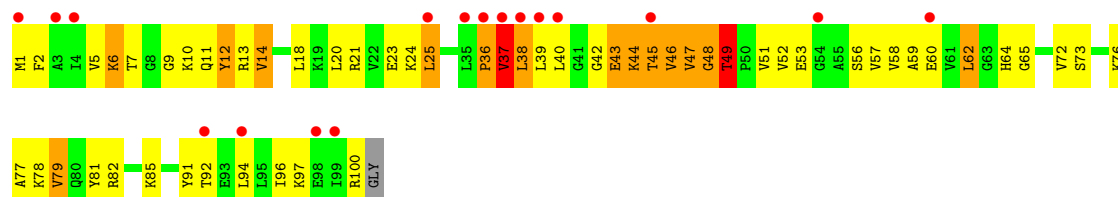
- Molecule 42: 50S ribosomal protein L20



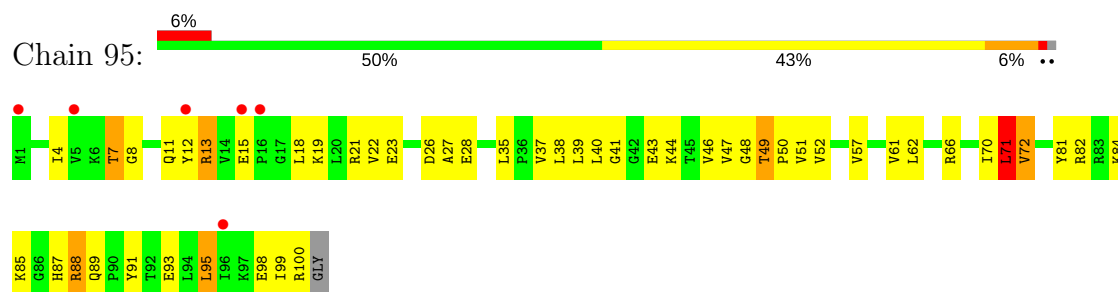
- Molecule 42: 50S ribosomal protein L20



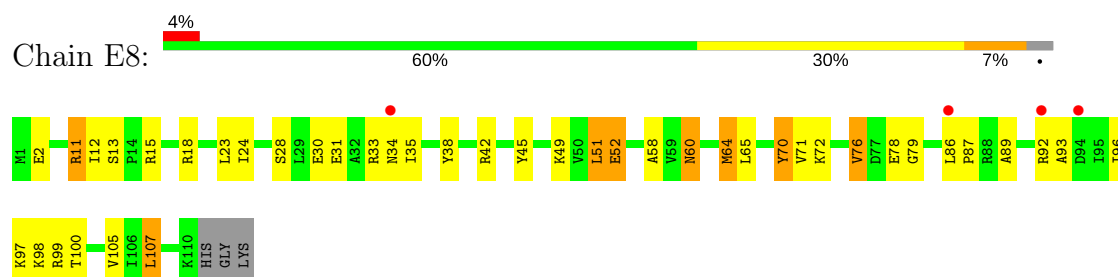
- Molecule 43: 50S ribosomal protein L21



- Molecule 43: 50S ribosomal protein L21



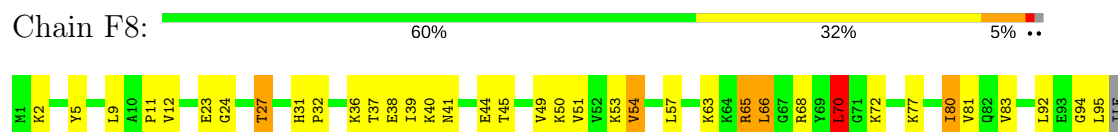
- Molecule 44: 50S ribosomal protein L22



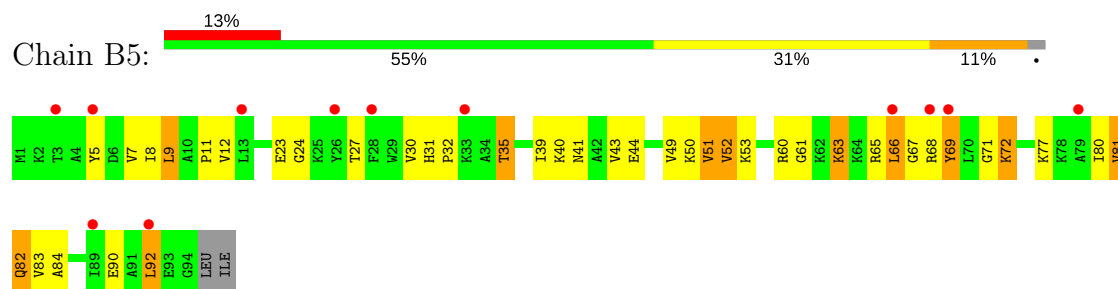
- Molecule 44: 50S ribosomal protein L22



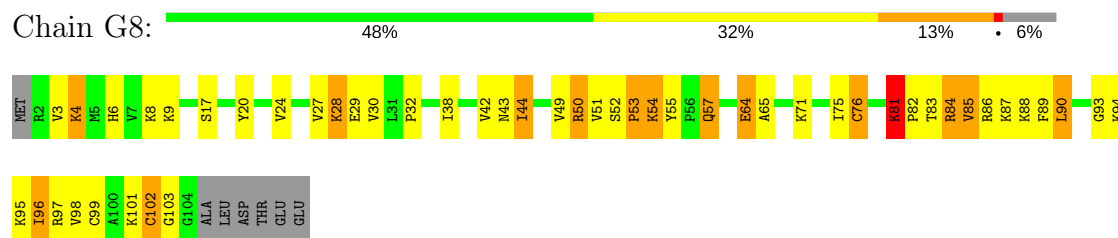
- Molecule 45: 50S ribosomal protein L23



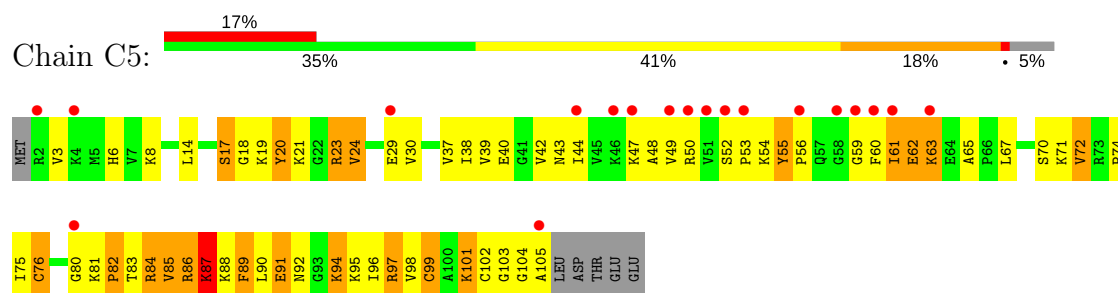
- Molecule 45: 50S ribosomal protein L23



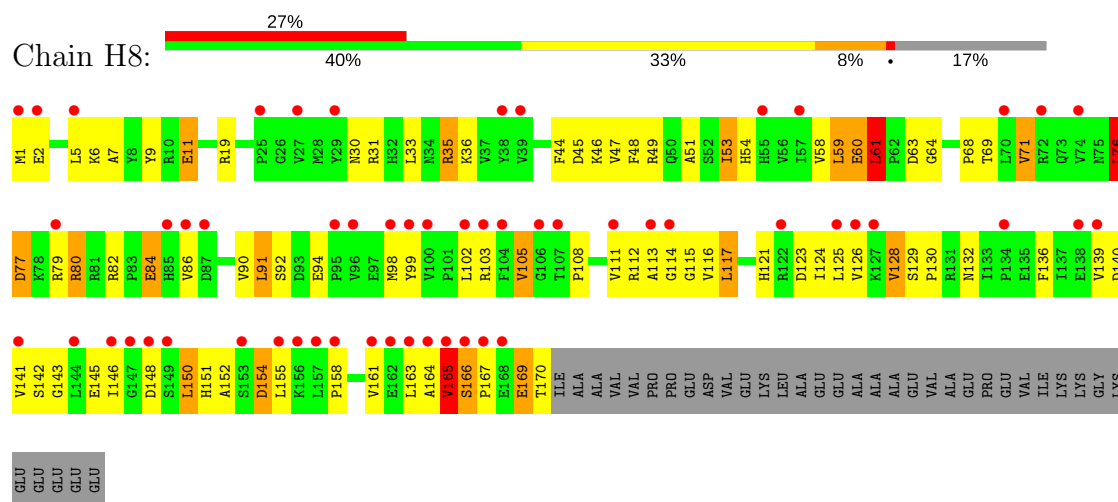
- Molecule 46: 50S ribosomal protein L24



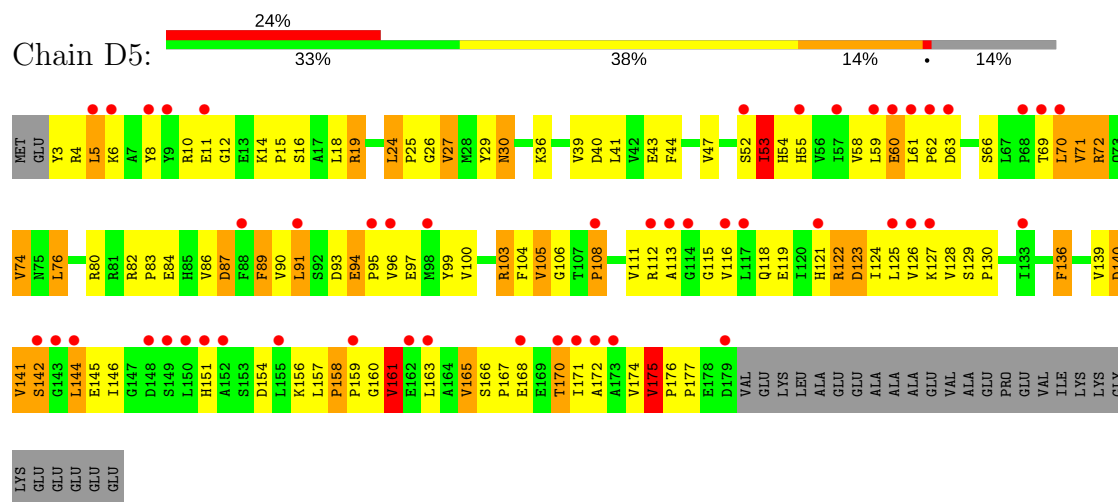
• Molecule 46: 50S ribosomal protein L24



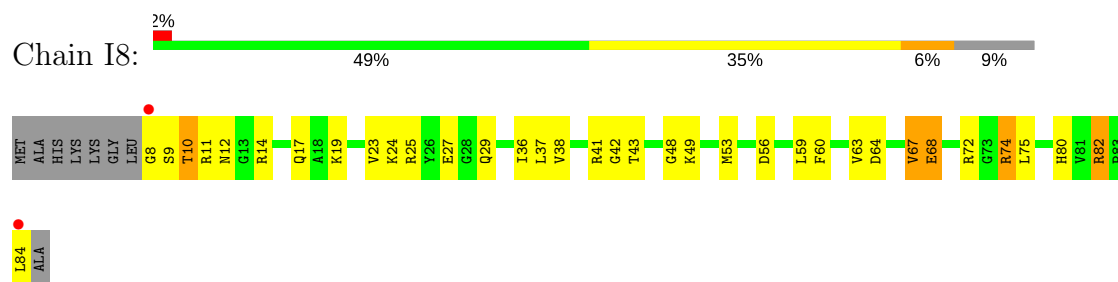
• Molecule 47: 50S ribosomal protein L25



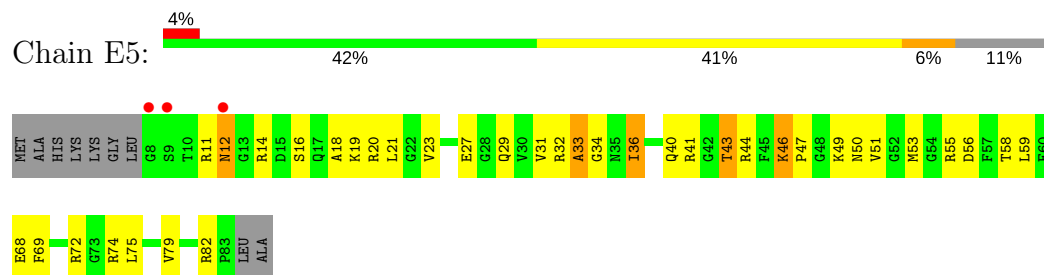
• Molecule 47: 50S ribosomal protein L25



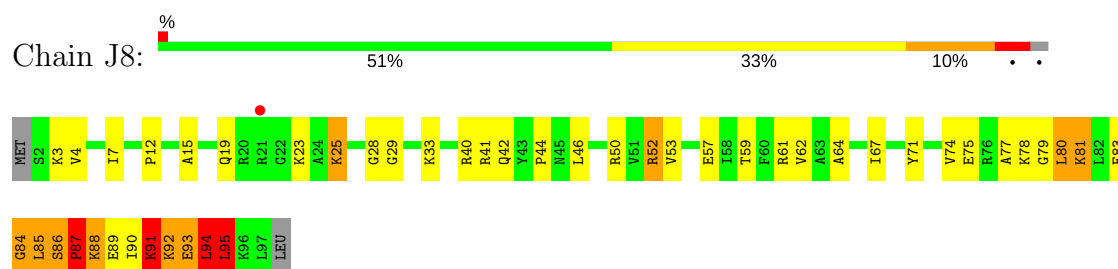
- Molecule 48: 50S ribosomal protein L27



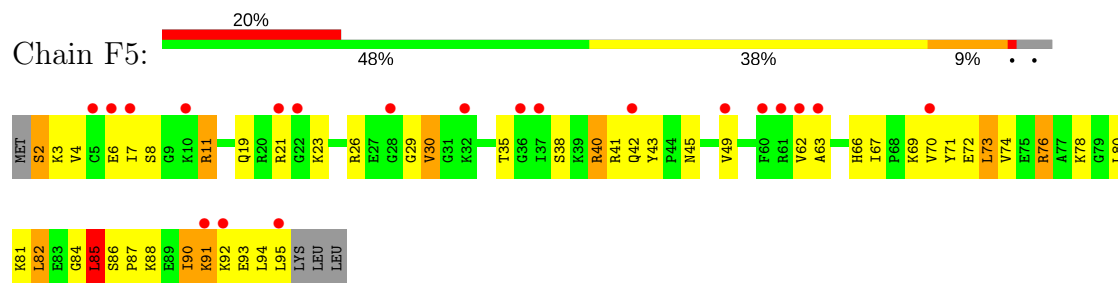
- Molecule 48: 50S ribosomal protein L27



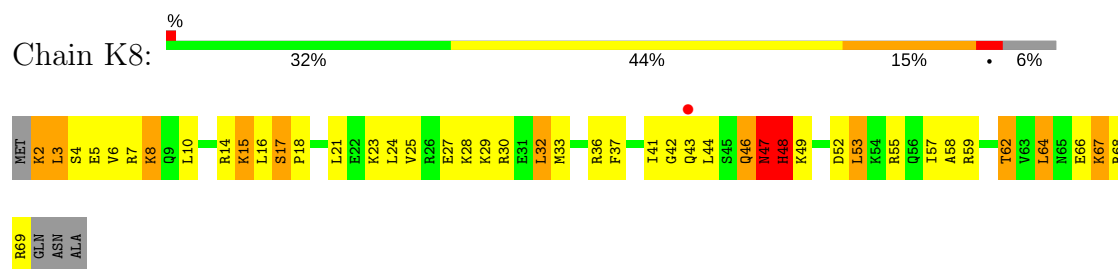
- Molecule 49: 50S ribosomal protein L28



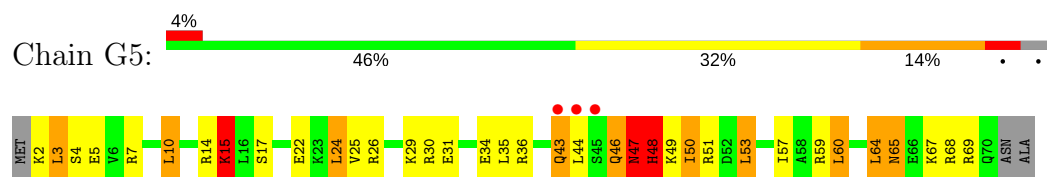
- Molecule 49: 50S ribosomal protein L28



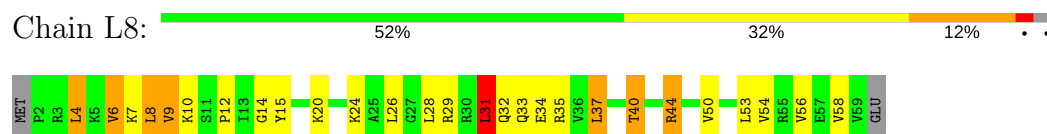
- Molecule 50: 50S ribosomal protein L29



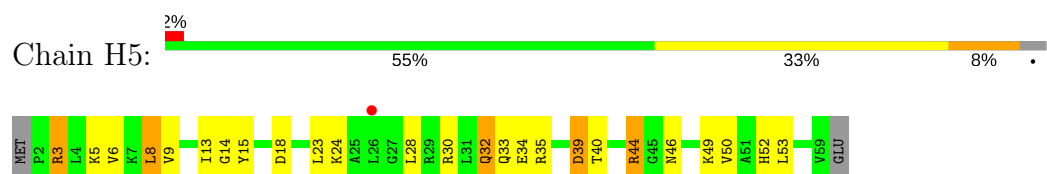
- Molecule 50: 50S ribosomal protein L29



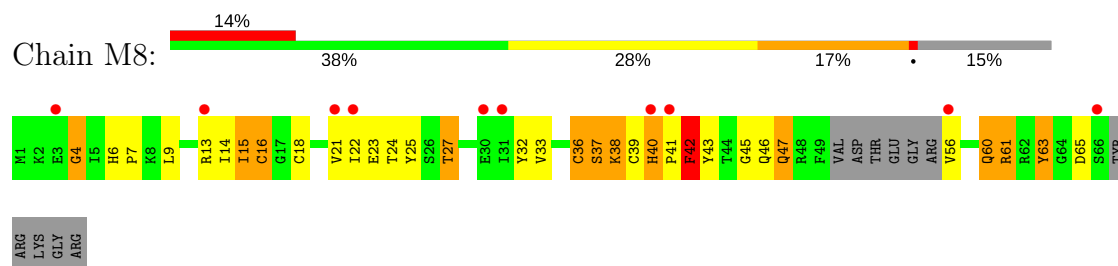
- Molecule 51: 50S ribosomal protein L30



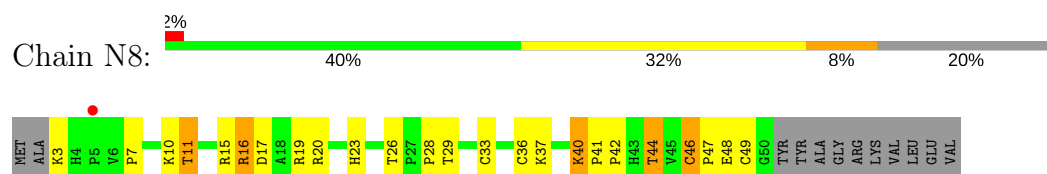
- Molecule 51: 50S ribosomal protein L30



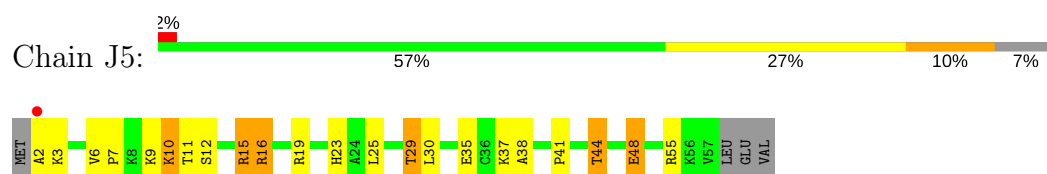
- Molecule 52: 50S ribosomal protein L31



- Molecule 53: 50S ribosomal protein L32



- Molecule 53: 50S ribosomal protein L32



- Molecule 54: 50S ribosomal protein L34





- Molecule 54: 50S ribosomal protein L34



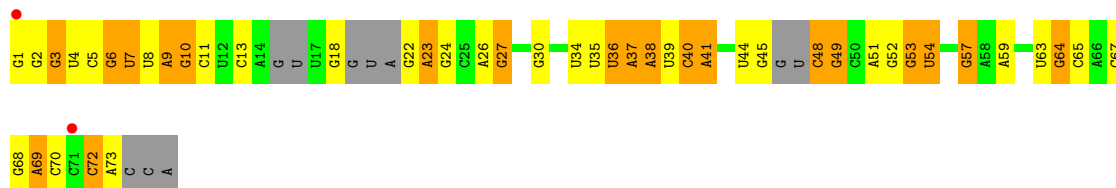
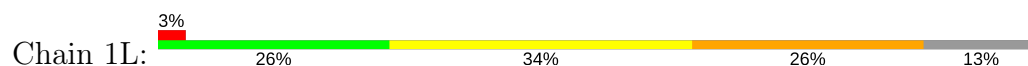
- Molecule 55: 50S ribosomal protein L35



- Molecule 55: 50S ribosomal protein L35



- Molecule 56: tRNA<sup>Lys</sup>





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	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
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	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 <sup>2</sup> )	89.4	Xtriage
Anisotropy	0.275	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.27 , 75.4	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	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 <sup>2</sup> )	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.*

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

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

## 5 Model quality ⓘ

### 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

*Continued on next page...*

*Continued from previous page...*

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%)	<b>4</b> <b>21</b>

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	1E	227/256 (89%)	186 (82%)	39 (17%)	2 (1%)	19	56
3	22	191/239 (80%)	172 (90%)	19 (10%)	0	100	100
3	2E	203/239 (85%)	186 (92%)	16 (8%)	1 (0%)	31	67
4	32	206/209 (99%)	180 (87%)	25 (12%)	1 (0%)	31	67
4	3E	205/209 (98%)	193 (94%)	11 (5%)	1 (0%)	31	67
5	42	148/162 (91%)	142 (96%)	5 (3%)	1 (1%)	24	61
5	4E	147/162 (91%)	136 (92%)	10 (7%)	1 (1%)	24	61
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%)	24	61
7	6E	152/156 (97%)	144 (95%)	8 (5%)	0	100	100
8	72	135/138 (98%)	125 (93%)	8 (6%)	2 (2%)	11	42
8	7E	136/138 (99%)	126 (93%)	9 (7%)	1 (1%)	24	61
9	82	119/128 (93%)	109 (92%)	9 (8%)	1 (1%)	21	58
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%)	9	37
11	2I	109/129 (84%)	93 (85%)	11 (10%)	5 (5%)	2	15
12	3A	119/132 (90%)	101 (85%)	14 (12%)	4 (3%)	4	21
12	3I	120/132 (91%)	106 (88%)	13 (11%)	1 (1%)	21	58
13	4A	107/126 (85%)	89 (83%)	17 (16%)	1 (1%)	19	56
13	4I	115/126 (91%)	97 (84%)	17 (15%)	1 (1%)	19	56
14	5A	57/61 (93%)	49 (86%)	7 (12%)	1 (2%)	9	37
14	5I	57/61 (93%)	48 (84%)	7 (12%)	2 (4%)	4	21
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%)	17	53

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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%)	11	42
19	AA	59/93 (63%)	49 (83%)	7 (12%)	3 (5%)	2	13
19	AI	80/93 (86%)	69 (86%)	7 (9%)	4 (5%)	2	14
20	BA	97/106 (92%)	79 (81%)	16 (16%)	2 (2%)	8	32
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%)	7	31
29	19	272/276 (99%)	248 (91%)	21 (8%)	3 (1%)	16	50
30	21	201/206 (98%)	160 (80%)	28 (14%)	13 (6%)	1	8
30	29	202/206 (98%)	150 (74%)	40 (20%)	12 (6%)	2	10
31	31	200/210 (95%)	177 (88%)	22 (11%)	1 (0%)	31	67
31	39	202/210 (96%)	159 (79%)	36 (18%)	7 (4%)	4	21
32	41	177/182 (97%)	156 (88%)	18 (10%)	3 (2%)	10	39
32	49	178/182 (98%)	155 (87%)	22 (12%)	1 (1%)	27	64
33	51	172/180 (96%)	139 (81%)	23 (13%)	10 (6%)	2	10
33	59	167/180 (93%)	129 (77%)	32 (19%)	6 (4%)	4	20
34	61	143/148 (97%)	123 (86%)	18 (13%)	2 (1%)	12	44
34	69	143/148 (97%)	112 (78%)	28 (20%)	3 (2%)	8	32
35	15	135/140 (96%)	124 (92%)	11 (8%)	0	100	100
35	58	135/140 (96%)	114 (84%)	16 (12%)	5 (4%)	4	20
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	6
38	45	136/141 (96%)	110 (81%)	23 (17%)	3 (2%)	7	31
38	88	139/141 (99%)	119 (86%)	14 (10%)	6 (4%)	3	16
39	55	116/118 (98%)	110 (95%)	5 (4%)	1 (1%)	19	56
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%)	9	35
40	A8	109/112 (97%)	89 (82%)	19 (17%)	1 (1%)	19	56
41	75	131/146 (90%)	118 (90%)	11 (8%)	2 (2%)	11	42
41	B8	133/146 (91%)	118 (89%)	14 (10%)	1 (1%)	21	58
42	85	114/118 (97%)	107 (94%)	7 (6%)	0	100	100
42	C8	113/118 (96%)	107 (95%)	2 (2%)	4 (4%)	4	21
43	95	98/101 (97%)	81 (83%)	14 (14%)	3 (3%)	4	24
43	D8	98/101 (97%)	87 (89%)	8 (8%)	3 (3%)	4	24
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%)	7	31
45	F8	93/96 (97%)	87 (94%)	6 (6%)	0	100	100
46	C5	102/110 (93%)	74 (72%)	22 (22%)	6 (6%)	2	10
46	G8	101/110 (92%)	83 (82%)	14 (14%)	4 (4%)	3	18
47	D5	175/206 (85%)	133 (76%)	32 (18%)	10 (6%)	2	11
47	H8	168/206 (82%)	136 (81%)	25 (15%)	7 (4%)	3	17
48	E5	74/85 (87%)	65 (88%)	8 (11%)	1 (1%)	12	44
48	I8	75/85 (88%)	67 (89%)	8 (11%)	0	100	100
49	F5	92/98 (94%)	81 (88%)	10 (11%)	1 (1%)	16	50
49	J8	94/98 (96%)	80 (85%)	9 (10%)	5 (5%)	2	12
50	G5	67/72 (93%)	61 (91%)	4 (6%)	2 (3%)	5	24
50	K8	66/72 (92%)	59 (89%)	4 (6%)	3 (4%)	3	15
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	8

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	11086/12104 (92%)	9718 (88%)	1167 (10%)	201 (2%)	9 37

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 6
3	2E	159/188 (85%)	127 (80%)	32 (20%)	1 6
4	32	180/181 (99%)	152 (84%)	28 (16%)	3 12
4	3E	180/181 (99%)	146 (81%)	34 (19%)	1 7
5	42	114/123 (93%)	88 (77%)	26 (23%)	1 4
5	4E	115/123 (94%)	90 (78%)	25 (22%)	1 5
6	52	90/90 (100%)	78 (87%)	12 (13%)	4 18
6	5E	90/90 (100%)	73 (81%)	17 (19%)	1 7
7	62	114/127 (90%)	91 (80%)	23 (20%)	1 6
7	6E	125/127 (98%)	105 (84%)	20 (16%)	2 11
8	72	118/119 (99%)	101 (86%)	17 (14%)	3 15
8	7E	119/119 (100%)	93 (78%)	26 (22%)	1 5
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%)	1	3
10	1I	81/92 (88%)	75 (93%)	6 (7%)	15	45
11	2A	85/99 (86%)	71 (84%)	14 (16%)	2	10
11	2I	84/99 (85%)	66 (79%)	18 (21%)	1	5
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%)	1	2
13	4I	94/101 (93%)	67 (71%)	27 (29%)	0	1
14	5A	49/50 (98%)	40 (82%)	9 (18%)	2	8
14	5I	49/50 (98%)	39 (80%)	10 (20%)	1	5
15	6A	79/80 (99%)	71 (90%)	8 (10%)	8	29
15	6I	79/80 (99%)	68 (86%)	11 (14%)	4	16
16	7A	72/74 (97%)	64 (89%)	8 (11%)	7	25
16	7I	72/74 (97%)	58 (81%)	14 (19%)	1	7
17	8A	94/97 (97%)	80 (85%)	14 (15%)	3	13
17	8I	95/97 (98%)	80 (84%)	15 (16%)	3	11
18	9A	58/77 (75%)	49 (84%)	9 (16%)	3	12
18	9I	58/77 (75%)	50 (86%)	8 (14%)	4	17
19	AA	56/80 (70%)	43 (77%)	13 (23%)	1	4
19	AI	72/80 (90%)	57 (79%)	15 (21%)	1	5
20	BA	76/82 (93%)	68 (90%)	8 (10%)	7	27
20	BI	75/82 (92%)	67 (89%)	8 (11%)	7	27
21	1B	17/22 (77%)	16 (94%)	1 (6%)	21	54
21	1F	18/22 (82%)	14 (78%)	4 (22%)	1	4
28	7I	108/181 (60%)	87 (81%)	21 (19%)	1	7
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%)	1	2
31	31	161/166 (97%)	130 (81%)	31 (19%)	1	7
31	39	163/166 (98%)	123 (76%)	40 (24%)	1	2

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
32	41	153/156 (98%)	120 (78%)	33 (22%)	1	5
32	49	152/156 (97%)	117 (77%)	35 (23%)	1	4
33	51	143/148 (97%)	109 (76%)	34 (24%)	1	3
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	5
35	58	116/119 (98%)	92 (79%)	24 (21%)	1	5
36	25	100/100 (100%)	82 (82%)	18 (18%)	2	8
36	68	100/100 (100%)	89 (89%)	11 (11%)	7	26
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	9
39	55	101/101 (100%)	86 (85%)	15 (15%)	3	13
39	98	101/101 (100%)	79 (78%)	22 (22%)	1	5
40	65	87/88 (99%)	67 (77%)	20 (23%)	1	4
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	9
42	C8	92/94 (98%)	80 (87%)	12 (13%)	4	19
43	95	81/82 (99%)	66 (82%)	15 (18%)	2	8
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%)	3	12
45	B5	74/78 (95%)	58 (78%)	16 (22%)	1	5
45	F8	77/78 (99%)	67 (87%)	10 (13%)	4	19
46	C5	85/91 (93%)	61 (72%)	24 (28%)	0	1
46	G8	84/91 (92%)	67 (80%)	17 (20%)	1	6
47	D5	156/179 (87%)	118 (76%)	38 (24%)	1	2

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
47	H8	151/179 (84%)	128 (85%)	23 (15%)	3	13
48	E5	61/67 (91%)	55 (90%)	6 (10%)	9	31
48	I8	62/67 (92%)	56 (90%)	6 (10%)	9	32
49	F5	79/83 (95%)	64 (81%)	15 (19%)	1	7
49	J8	79/83 (95%)	67 (85%)	12 (15%)	3	13
50	G5	63/67 (94%)	47 (75%)	16 (25%)	0	2
50	K8	64/67 (96%)	47 (73%)	17 (27%)	0	1
51	H5	50/52 (96%)	37 (74%)	13 (26%)	0	2
51	L8	50/52 (96%)	41 (82%)	9 (18%)	2	8
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%)	2	8
54	P8	38/42 (90%)	31 (82%)	7 (18%)	2	8
55	M5	54/55 (98%)	44 (82%)	10 (18%)	2	8
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	H2U	1K	17	22	17,21,22	2.27	4 (23%)	21,30,33	2.97	5 (23%)
22	U8U	1K	34	25,22	15,24,25	2.55	4 (26%)	17,34,37	1.58	2 (11%)
22	T6A	1K	37	22	24,34,35	2.61	4 (16%)	23,49,52	3.54	6 (26%)
22	PSU	1K	39	22	16,21,22	1.02	1 (6%)	20,30,33	3.19	6 (30%)
22	5MU	1K	54	22	13,22,23	1.91	3 (23%)	14,32,35	1.91	2 (14%)
22	PSU	1K	55	22	16,21,22	1.13	1 (6%)	20,30,33	3.30	6 (30%)
56	5MU	1L	54	56	13,22,23	1.82	2 (15%)	14,32,35	1.77	2 (14%)
56	PSU	1L	55	56	16,21,22	1.12	1 (6%)	20,30,33	3.34	5 (25%)
23	OMC	2K	33	23	15,22,23	2.08	4 (26%)	19,31,34	1.05	1 (5%)
23	7MG	2K	47	23	20,26,27	3.73	6 (30%)	23,39,42	2.64	9 (39%)
23	5MU	2K	55	23	13,22,23	1.80	2 (15%)	14,32,35	1.84	2 (14%)
23	PSU	2K	56	23	16,21,22	1.16	3 (18%)	20,30,33	2.96	5 (25%)
23	4SU	2K	8	23	13,21,22	2.95	2 (15%)	14,30,33	1.08	2 (14%)
23	OMC	2L	33	23	15,22,23	2.22	4 (26%)	19,31,34	0.83	1 (5%)
23	7MG	2L	47	23	20,26,27	3.62	6 (30%)	23,39,42	2.13	8 (34%)
23	5MU	2L	55	23	13,22,23	1.87	3 (23%)	14,32,35	1.84	2 (14%)
23	PSU	2L	56	23	16,21,22	1.33	2 (12%)	20,30,33	3.33	6 (30%)
23	4SU	2L	8	23	13,21,22	3.35	2 (15%)	14,30,33	1.15	2 (14%)

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	H2U	1K	17	22	-	0/7/38/39	0/2/2/2
22	U8U	1K	34	25,22	-	0/5/28/29	0/2/2/2
22	T6A	1K	37	22	-	0/15/41/42	0/3/3/3
22	PSU	1K	39	22	-	0/7/25/26	0/2/2/2
22	5MU	1K	54	22	-	0/3/25/26	0/2/2/2
22	PSU	1K	55	22	-	0/7/25/26	0/2/2/2
56	5MU	1L	54	56	-	0/3/25/26	0/2/2/2
56	PSU	1L	55	56	-	0/7/25/26	0/2/2/2
23	OMC	2K	33	23	-	0/5/27/28	0/2/2/2

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

The worst 5 of 54 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	2K	47	7MG	C4-N9	-6.96	1.29	1.38
23	2L	47	7MG	C4-N9	-6.25	1.30	1.38
23	2K	47	7MG	C5-C4	-5.65	1.24	1.39
23	2L	47	7MG	C5-C4	-5.44	1.24	1.39
22	1K	17	H2U	C6-N1	-3.88	1.42	1.47

The worst 5 of 72 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	1K	37	T6A	N3-C2-N1	-11.10	119.37	128.86
22	1K	39	PSU	N1-C2-N3	-11.05	119.53	128.41
23	2L	56	PSU	N1-C2-N3	-10.98	119.59	128.41
56	1L	55	PSU	N1-C2-N3	-10.90	119.64	128.41
22	1K	55	PSU	N1-C2-N3	-10.65	119.85	128.41

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

9 monomers are involved in 25 short contacts:

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

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
23	2L	33	OMC	3	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	14	3458	-	12,12,12	0.45	0	11,11,11	0.75	0
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	-	0,24,24	0.00	-
58	SF4	3E	301	4	0,12,12	0.00	-	0,24,24	0.00	-

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
60	SPE	14	3458	-	-	0/10/10/10	0/0/0/0
60	SPE	1G	1725	1	-	0/10/10/10	0/0/0/0
58	SF4	32	302	-	-	0/0/48/48	0/6/5/5
58	SF4	3E	301	4	-	0/0/48/48	0/6/5/5

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

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

### 6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	13	1500/1522 (98%)	-0.52	0 <span>100</span> <span>100</span>	67, 111, 176, 243	0
1	1G	1509/1522 (99%)	-0.47	3 (0%) <span>94</span> <span>91</span>	76, 123, 193, 253	0
2	12	207/256 (80%)	0.27	13 (6%) <span>20</span> <span>8</span>	139, 165, 185, 196	0
2	1E	231/256 (90%)	-0.06	5 (2%) <span>62</span> <span>42</span>	118, 145, 172, 180	0
3	22	195/239 (81%)	0.75	27 (13%) <span>3</span> <span>1</span>	123, 147, 164, 175	0
3	2E	205/239 (85%)	0.34	12 (5%) <span>22</span> <span>9</span>	97, 117, 144, 155	0
4	32	208/209 (99%)	-0.31	0 <span>100</span> <span>100</span>	104, 123, 142, 149	0
4	3E	207/209 (99%)	-0.20	1 (0%) <span>90</span> <span>82</span>	93, 118, 137, 144	0
5	42	150/162 (92%)	-0.23	0 <span>100</span> <span>100</span>	106, 123, 139, 146	0
5	4E	149/162 (91%)	-0.06	0 <span>100</span> <span>100</span>	87, 109, 128, 133	0
6	52	101/101 (100%)	-0.42	0 <span>100</span> <span>100</span>	93, 110, 124, 135	0
6	5E	100/101 (99%)	-0.03	1 (1%) <span>82</span> <span>69</span>	92, 111, 127, 135	0
7	62	138/156 (88%)	0.83	13 (9%) <span>8</span> <span>3</span>	122, 135, 145, 151	0
7	6E	154/156 (98%)	1.00	29 (18%) <span>1</span> <span>0</span>	111, 127, 155, 174	0
8	72	137/138 (99%)	-0.08	2 (1%) <span>73</span> <span>55</span>	106, 129, 141, 149	0
8	7E	138/138 (100%)	0.78	15 (10%) <span>5</span> <span>2</span>	102, 117, 129, 139	0
9	82	121/128 (94%)	1.39	31 (25%) <span>0</span> <span>0</span>	118, 161, 171, 178	0
9	8E	126/128 (98%)	-0.09	2 (1%) <span>72</span> <span>52</span>	96, 141, 159, 165	0
10	1A	80/105 (76%)	0.36	11 (13%) <span>3</span> <span>1</span>	122, 152, 167, 170	0
10	1I	94/105 (89%)	1.43	26 (27%) <span>0</span> <span>0</span>	92, 136, 171, 178	0
11	2A	113/129 (87%)	0.79	13 (11%) <span>5</span> <span>2</span>	91, 116, 131, 138	0
11	2I	111/129 (86%)	1.40	29 (26%) <span>0</span> <span>0</span>	84, 113, 129, 138	0
12	3A	121/132 (91%)	0.68	18 (14%) <span>2</span> <span>1</span>	94, 109, 128, 144	0
12	3I	122/132 (92%)	0.11	3 (2%) <span>57</span> <span>36</span>	81, 89, 110, 132	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	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 63	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 55	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%) 3 1	130, 162, 174, 180	0
19	AI	82/93 (88%)	0.44	7 (8%) 11 4	108, 126, 146, 153	0
20	BA	99/106 (93%)	0.86	17 (17%) 1 0	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 55	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 58	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 11	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 92	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%) 14 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 <sup>2</sup> )	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 55	57, 90, 121, 133	0
30	29	204/206 (99%)	0.40	13 (6%) 19 7	66, 97, 133, 147	0
31	31	202/210 (96%)	0.19	4 (1%) 65 45	51, 82, 114, 134	0
31	39	204/210 (97%)	-0.12	1 (0%) 90 82	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 29	71, 90, 122, 138	0
36	25	122/122 (100%)	1.04	14 (11%) 5 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%) 24 10	62, 83, 105, 133	0
39	55	118/118 (100%)	0.20	2 (1%) 70 50	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%) 22 9	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 50	60, 82, 108, 115	0
43	95	100/101 (99%)	0.55	6 (6%) 22 9	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 71	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 <sup>2</sup> )	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%) 1 0	69, 89, 125, 139	0
49	J8	96/98 (97%)	0.37	1 (1%) 82 69	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 55	68, 84, 105, 129	0
51	H5	58/60 (96%)	0.68	1 (1%) 70 50	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 48	67, 90, 133, 143	0
53	N8	48/60 (80%)	0.27	1 (2%) 63 43	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, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
56	PSU	1L	55	20/21	0.85	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, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
57	MG	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( $\text{\AA}^2$ )	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( $\text{\AA}^2$ )	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( $\text{\AA}^2$ )	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( $\text{\AA}^2$ )	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( $\text{\AA}^2$ )	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( $\text{\AA}^2$ )	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( $\text{\AA}^2$ )	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( $\text{\AA}^2$ )	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( $\text{\AA}^2$ )	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( $\text{\AA}^2$ )	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( $\text{\AA}^2$ )	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( $\text{\AA}^2$ )	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( $\text{\AA}^2$ )	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( $\text{\AA}^2$ )	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( $\text{\AA}^2$ )	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( $\text{\AA}^2$ )	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( $\text{\AA}^2$ )	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( $\text{\AA}^2$ )	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( $\text{\AA}^2$ )	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( $\text{\AA}^2$ )	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( $\text{\AA}^2$ )	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( $\text{\AA}^2$ )	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( $\text{\AA}^2$ )	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( $\text{\AA}^2$ )	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( $\text{\AA}^2$ )	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( $\text{\AA}^2$ )	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( $\text{\AA}^2$ )	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( $\text{\AA}^2$ )	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( $\text{\AA}^2$ )	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( $\text{\AA}^2$ )	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( $\text{\AA}^2$ )	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( $\text{\AA}^2$ )	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.