



wwPDB X-ray Structure Validation Summary Report ⓘ

Jun 17, 2026 – 03:16 pm BST

PDB ID : 5IBB / pdb_00005ibb
Title : Structure of T. thermophilus 70S ribosome complex with mRNA, tRNA^{fMet} and cognate tRNA^{Val} in the A-site
Authors : Rozov, A.; Demeshkina, N.; Yusupov, M.; Yusupova, G.
Deposited on : 2016-02-22
Resolution : 2.96 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

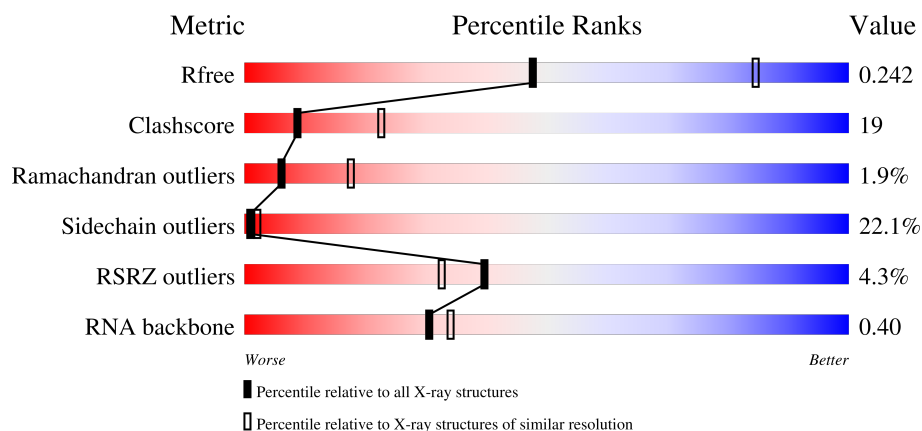
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.96 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1130 (2.98-2.94)
Clashscore	190562	1157 (2.98-2.94)
Ramachandran outliers	187476	1101 (2.98-2.94)
Sidechain outliers	187428	1101 (2.98-2.94)
RSRZ outliers	180081	1130 (2.98-2.94)
RNA backbone	3983	1046 (3.16-2.76)

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

Mol	Chain	Length	Quality of chain
1	13	1522	0% 42% 43% 13% .
1	1G	1522	2% 44% 43% 11% .
2	12	256	9% 30% 36% 12% . 19%
2	1E	256	4% 29% 48% 14% 8%

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

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

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

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
57	MG	13	1653	-	-	-	X
57	MG	13	1660	-	-	-	X
57	MG	13	1671	-	-	-	X
57	MG	13	1676	-	-	-	X
57	MG	13	1685	-	-	-	X
57	MG	13	1687	-	-	-	X
57	MG	13	1690	-	-	-	X
57	MG	14	3157	-	-	-	X
57	MG	14	3178	-	-	-	X
57	MG	14	3214	-	-	-	X
57	MG	1G	1624	-	-	-	X
57	MG	1G	1630	-	-	-	X
57	MG	1G	1648	-	-	-	X
57	MG	1H	3008	-	-	-	X
57	MG	1H	3087	-	-	-	X
57	MG	1H	3097	-	-	-	X
57	MG	1H	3120	-	-	-	X
57	MG	1H	3133	-	-	-	X
57	MG	1H	3188	-	-	-	X
57	MG	1H	3224	-	-	-	X
57	MG	1H	3239	-	-	-	X
57	MG	1H	3248	-	-	-	X
57	MG	1H	3250	-	-	-	X
57	MG	1H	3260	-	-	-	X
57	MG	1H	3269	-	-	-	X
57	MG	1H	3274	-	-	-	X
57	MG	1H	3285	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
57	MG	4E	201	-	-	-	X
57	MG	J8	101	-	-	-	X
59	SF4	3E	301	-	-	X	-

2 Entry composition

There are 61 unique types of molecules in this entry. The entry contains 296743 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	13	1496	Total	C	N	O	P	0	0	0
			32157	14313	5960	10388	1496			
1	1G	1506	Total	C	N	O	P	0	0	0
			32371	14409	6001	10456	1505			

There are 2 discrepancies between the modelled and reference sequences:

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
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	149	Total	C	N	O	S	0	0	0
			1139	721	216	198	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	140	Total	C	N	O	S	0	0	0
			1120	695	223	196	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	95	Total	C	N	O	S	0	0	0
			754	471	148	134	1			
10	1A	80	Total	C	N	O		0	0	0
			646	403	129	114				

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

- Molecule 22 is a RNA chain called tRNAVal.

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

- Molecule 23 is a RNA chain called tRNAfMet.

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

- Molecule 24 is a RNA chain called tRNAVal.

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

- Molecule 25 is a RNA chain called mRNA.

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

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

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

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	133	Total	C	N	O	S	0	0	0
			1033	651	194	187	1			
28	79	57	Total	C	N	O		0	0	0
			456	283	91	82				

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

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

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

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

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

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

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

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

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

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

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

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

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
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	138	Total	C	N	O	S	0	0	0
			1104	712	206	182	4			

- 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	139	Total	C	N	O	S	0	0	0
			1104	705	209	184	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	136	Total	C	N	O	S	0	0	0
			1124	700	231	192	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
			743	482	134	126	1			
45	B5	94	Total	C	N	O	S	0	0	0
			735	477	133	125				

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

- Molecule 56 is a RNA chain called tRNAVal.

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

- Molecule 57 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

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

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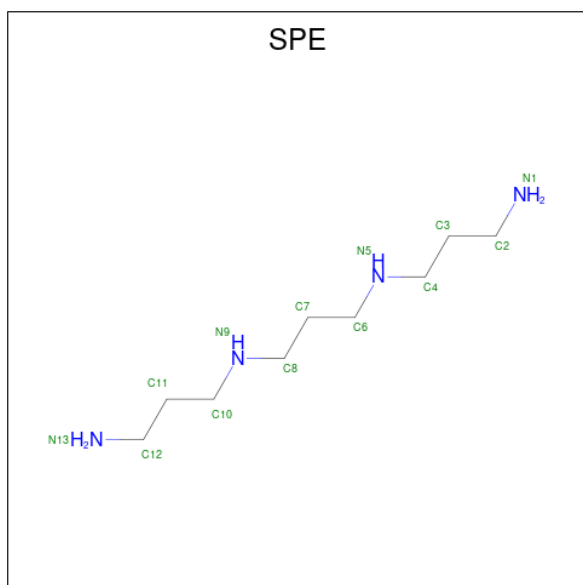
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
57	J8	1	Total 1	Mg 1	0	0
57	L8	1	Total 1	Mg 1	0	0
57	P8	1	Total 1	Mg 1	0	0
57	Q8	1	Total 1	Mg 1	0	0
57	1G	133	Total 133	Mg 133	0	0
57	42	1	Total 1	Mg 1	0	0
57	3A	1	Total 1	Mg 1	0	0
57	4A	1	Total 1	Mg 1	0	0
57	9A	1	Total 1	Mg 1	0	0
57	2L	3	Total 3	Mg 3	0	0
57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

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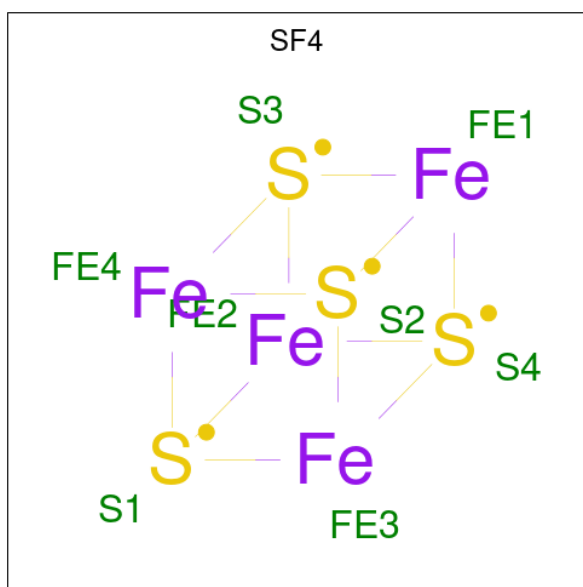
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
57	E5	1	Total	Mg	0	0
			1	1		
57	M5	1	Total	Mg	0	0
			1	1		

- Molecule 58 is THERMINE (CCD ID: SPE) (formula: $C_9H_{24}N_4$).



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

- Molecule 59 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe_4S_4).



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

- Molecule 60 is ZINC ION (CCD ID: ZN) (formula: Zn).

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

- Molecule 61 is water.

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

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

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

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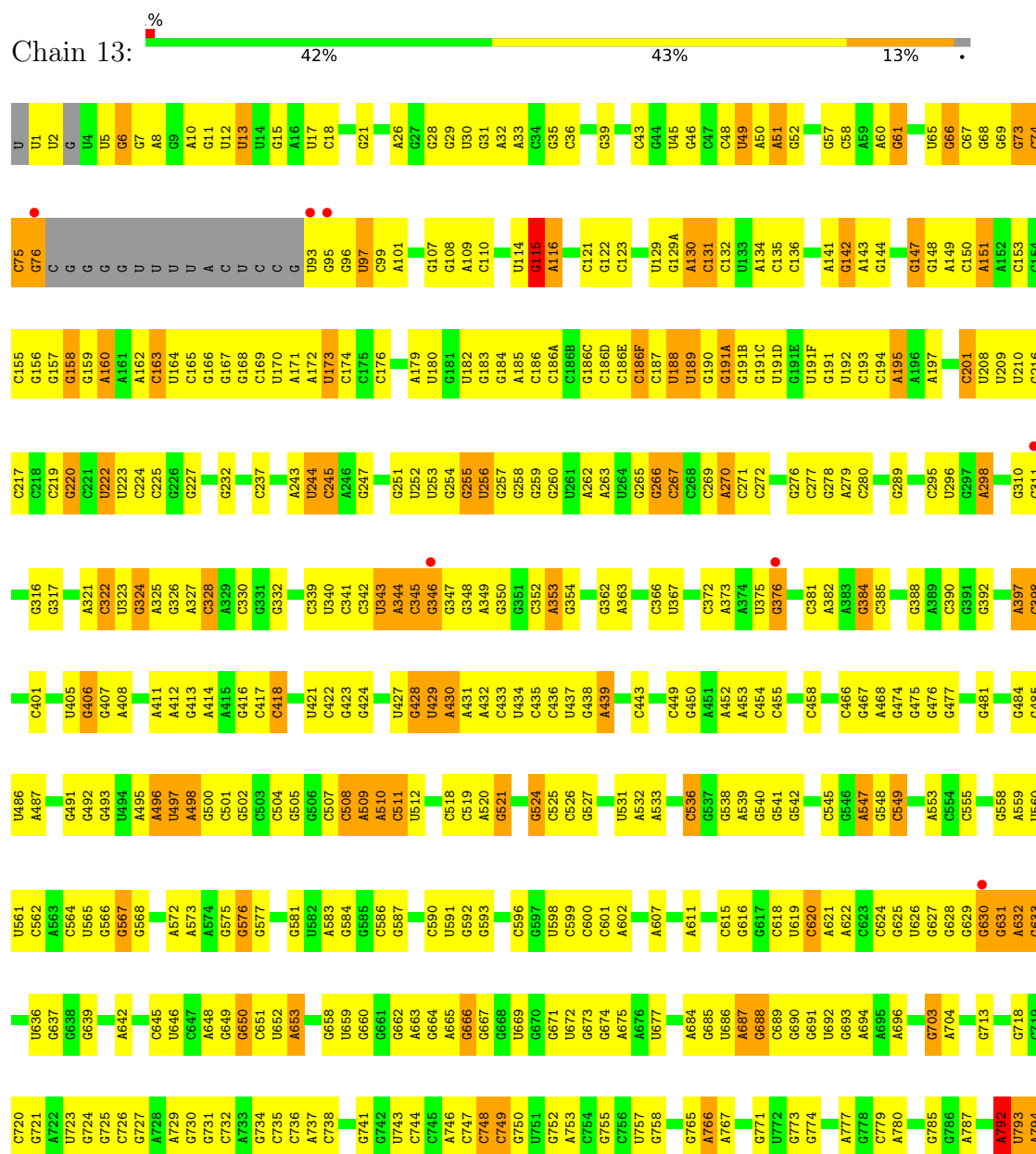
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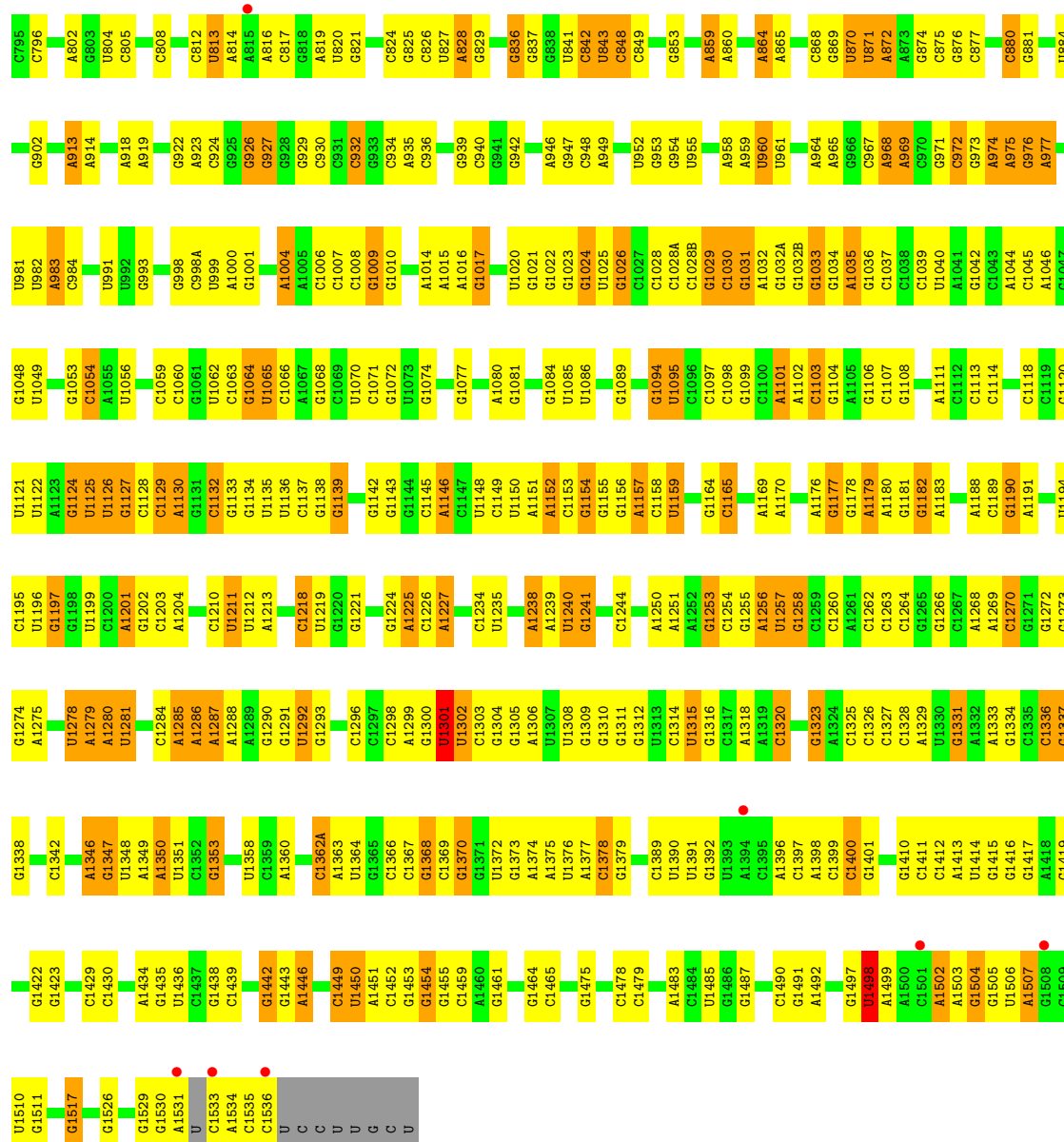
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
61	45	3	Total	O	0	0
			3	3		
61	55	1	Total	O	0	0
			1	1		
61	75	1	Total	O	0	0
			1	1		
61	85	1	Total	O	0	0
			1	1		
61	A5	1	Total	O	0	0
			1	1		
61	C5	3	Total	O	0	0
			3	3		
61	E5	5	Total	O	0	0
			5	5		
61	F5	3	Total	O	0	0
			3	3		
61	H5	1	Total	O	0	0
			1	1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

3 Residue-property plots

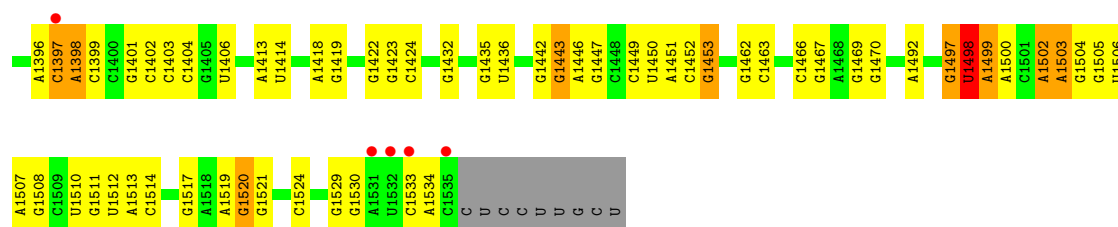
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

- Molecule 1: 16S ribosomal RNA

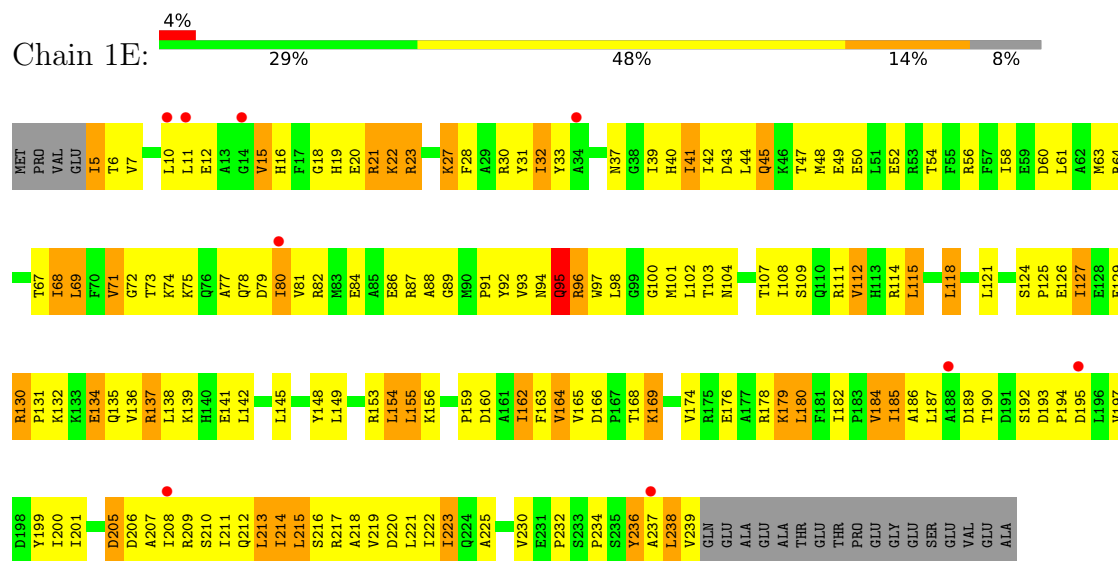




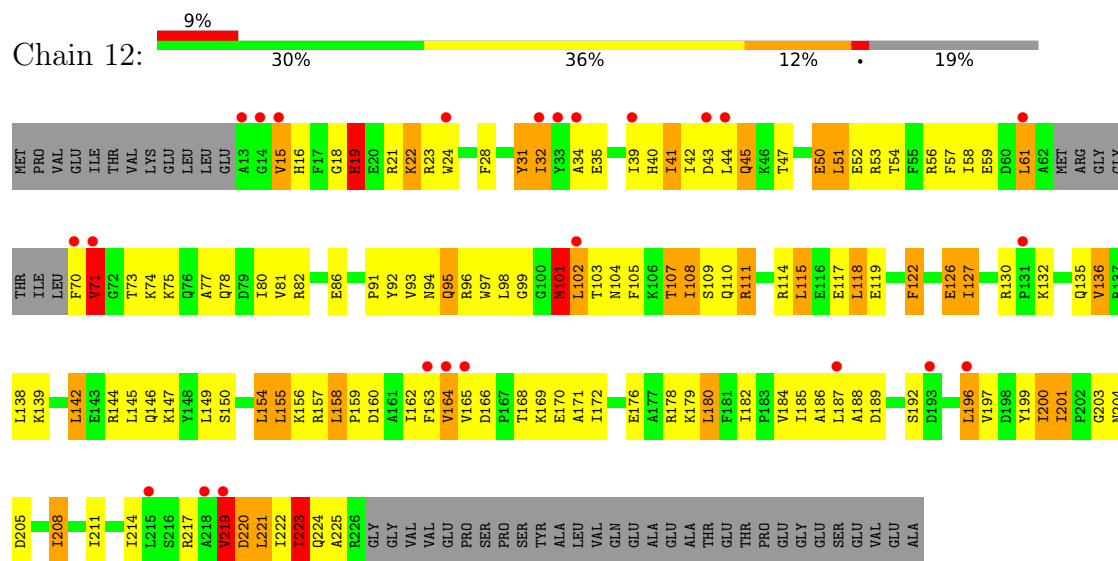
C1328	C1329	U1330	G1331	A1332	A1333	A1334	G1335	C1336	G1337	G1338	A1339	A1340	U1341	C1342	G1343	A1346	G1347	U1348	A1349	A1350	U1351	C1352	G1353	G1356	A1357	U1358	C1359	U1360	C1362A	A1363	U1364	C1367	G1368	C1369	G1370	U1371	U1372	G1373	A1374	A1375	U1376	A1377	C1378	G1379	U1380	U1381	C1382	G1386	C1387	C1388	C1389	U1390	A1391	C1392					
C1259	C1260	A1268	A1269	G1272	G1273	G1274	A1275	G1276	C1277	U1278	A1279	A1280	C1281	C1282	G1283	C1284	A1285	A1286	A1287	A1288	A1289	C1290	G1291	U1292	C1296	C1297	C1298	A1299	G1300	U1301	U1302	C1303	G1304	G1305	A1306	U1307	U1308	G1309	G1310	G1311	G1312	U1313	C1314	U1315	G1316	C1317	A1318	A1319	C1320	C1321	C1322	A1324	C1325	C1326	C1327				
G1190	A1191	C1192	G1193	U1194	C1195	U1196	G1197	U1199	C1200	A1201	G1202	C1203	A1204	U1205	G1206	G1207	C1208	C1209	C1210	U1211	U1212	A1213	C1214	G1215	C1216	C1217	G1218	U1219	G1220	G1221	G1222	C1223	G1224	C1225	A1226	A1227	C1228	U1232	U1235	A1238	A1239	U1240	G1241	A1245	C1246	C1249	A1250	A1251	G1255	A1256	U1257	G1258							
U1126	G1127	C1128	C1129	A1130	G1131	C1132	G1133	G1134	U1135	U1136	G1137	G1138	G1139	C1140	C1141	G1142	G1143	G1144	C1145	A1146	U1147	U1148	C1149	U1150	A1151	A1152	C1153	G1154	G1155	G1156	A1157	C1158	U1159	G1160	C1161	U1094	U1095	C1098	A1169	G1170	G1171	C1172	G1173	G1174	A1175	A1176	G1177	G1178	A1179	A1180	G1181	G1182	A1183	G1184	G1185	G1186	G1187	A1188	C1189
A1046	G1047	G1048	C1051	U1052	G1053	C1054	A1055	U1056	G1057	G1058	C1059	C1060	U0991	U0992	G0993	A0996	U0997	G0998	U0999	A1000	G1001	G1002	G1003	A1004	A1005	C1006	C1007	C1008	G1009	A1014	A1015	A1016	G1017	C1018	C1019	U1020	G1021	U1022	G1023	G1024	U1025	G1026	C1027	C1028	A1101	A1102	A1105	G1106	C1107	G1108	C1109	C1112	C1116	G1117	C1118	C1119	A1123	G1124	U1125
A0913	A0914	A0915	A0918	A0919	U0920	U0921	G0922	A0923	G0926	G0927	C0931	C0932	G0933	C0934	A0935	C0936	G0937	A0938	G0939	C0940	G0941	G0942	U0943	G0944	A0945	A0946	G0947	C0948	A0949	U0950	G0951	U0952	G0953	U0957	A0958	A0959	U0960	U0961	C0962	G0963	A0964	A0965	G0966	C0967	A0968	A0969	C0970	C0971	G0972	C0973	A0974	A0975	G0976	A0977	A0978				
A0792	U0793	A0794	G0800	U0804	C0805	C0808	G0809	C0810	C0811	C0812	U0813	A0814	A0815	A0816	C0817	G0818	U0820	G0821	C0822	C0826	U0827	A0828	G0829	G0836	C0842	U0843	C0848	G0851	G0855	C0856	C0857	G0858	A0859	C0860	G0861	G0865	G0867	G0868	G0869	G0870	G0871	G0872	A0873	G0878	G0889	C0890	G0891	G0895	C0896	A0900									
C0701	A0702	A0706	C0707	G0710	G0711	A0712	G0713	C0717	G0718	C0719	G0720	A0722	U0723	G0724	G0730	G0731	A0735	C0736	G0737	C0738	G0741	U0742	U0743	C0744	C0745	A0746	C0747	C0748	C0749	G0750	U0751	G0752	C0756	U0757	G0758	A0759	G0765	G0767	G0768	C0778	C0779	A0780	C0784	A0787															
U0605	G0606	A0607	A0608	A0614	G0617	G0618	U0619	C0620	A0621	A0622	C0624	U0626	G0628	G0629	G0630	A0631	A0632	G0633	A0640	G0650	C0651	U0652	A0653	G0660	G0661	G0664	A0665	G0666	G0667	G0668	G0673	G0674	U0677	G0683	A0684	G0685	U0686	A0687	C0689	G0690	G0691	U0692	G0693	A0694	A0695														
G0530	U0531	A0532	A0533	U0534	A0535	C0536	G0537	G0538	A0539	C0540	G0541	G0542	C0543	G0544	C0545	G0546	A0547	G0550	C0554	C0555	C0556	G0557	G0558	A0559	U0560	U0561	C0562	A0563	C0564	G0567	G0568	A0572	A0573	G0576	U0580	G0581	U0582	A0583	G0584	G0587	G0588	C0589	C0590	C0591	G0592	C0599	C0600	C0601	A0602	G0604									
A0437	G0438	A0439	A0440	C0442	G0445	G0446	A0448	A0452	A0453	C0456	C0457	C0458	G0464	A0465	C0466	G0467	A0468	G0474	G0475	G0476	G0477	A0478	G0481	A0482	C0483	C0484	G0485	U0486	C0489	G0490	A0496	U0497	C0503	C0504	G0505	A0509	C0510	U0512	C0513	C0518	C0519	A0520	G0521	C0526	G0527	U0534	C0535	C0536											
A0353	G0354	C0355	A0356	U0357	G0358	U0359	G0362	A0363	A0364	U0365	C0366	U0367	G0371	C0372	A0373	A0374	U0375	G0377	G0384	C0385	G0388	A0389	C0390	C0391	G0392	A0393	G0396	C0397	C0398	U0405	G0406	A0407	A0408	G0409	A0410	A0411	A0412	A0413	C0422	G0423	G0426	U0427	C0428	U0429	A0430	U0434	C0435	C0436											
A0250	G0251	U0256	G0257	G0258	G0259	G0260	U0261	A0262	A0263	G0266	C0267	C0268	C0269	A0270	C0271	C0272	A0273	A0274	C0277	G0278	A0279	C0280	A0281	G0282	G0289	G0297	A0298	G0299	A0300	G0309	G0310	A0313	C0314	A0315	G0316	A0321	C0322	C0328	A0329	G0332	A0344	C0345	G0346	G0347	G0350	G0351	C0352												



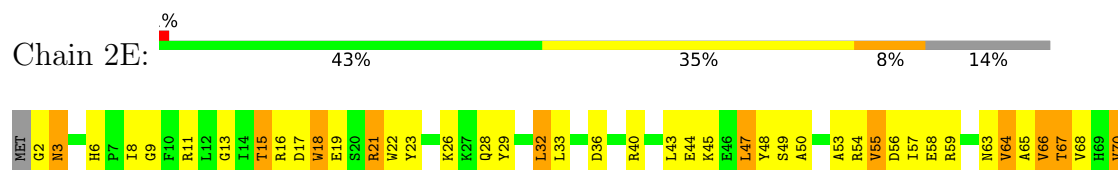
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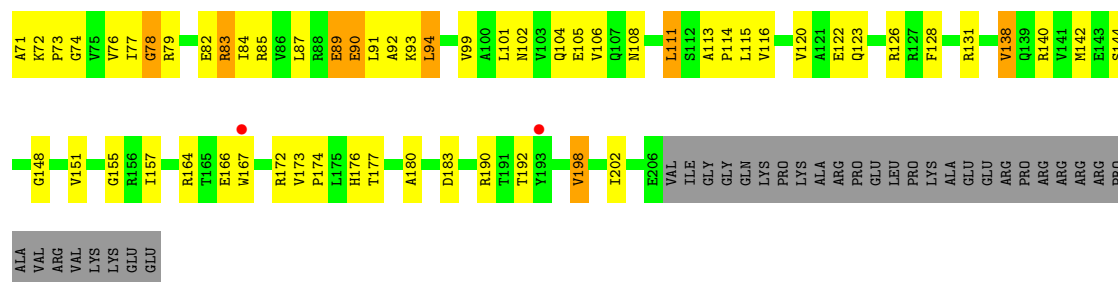


• Molecule 2: 30S ribosomal protein S2

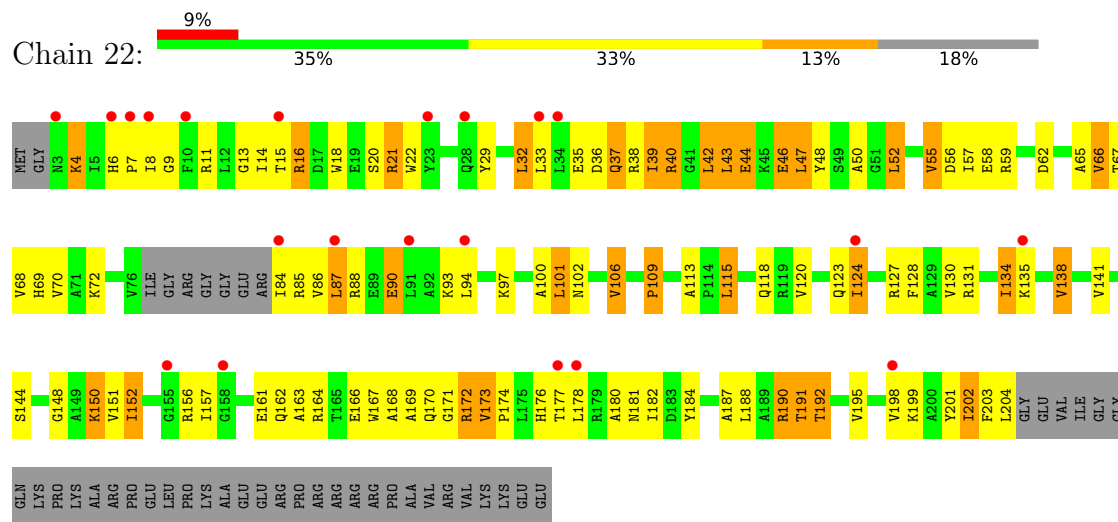


• Molecule 3: 30S ribosomal protein S3

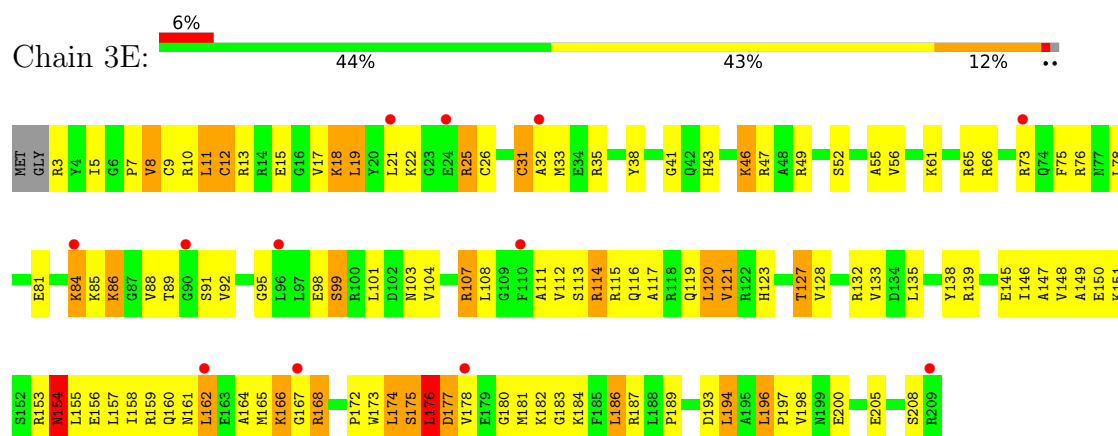




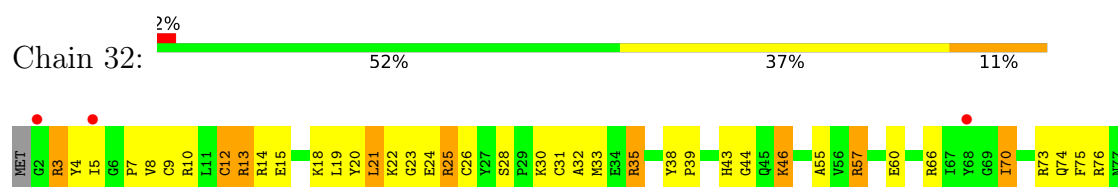
• Molecule 3: 30S ribosomal protein S3

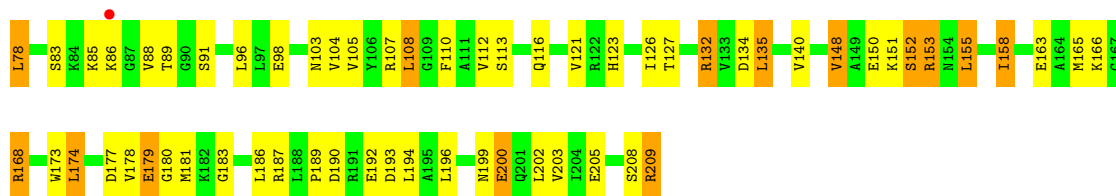


• Molecule 4: 30S ribosomal protein S4



• Molecule 4: 30S ribosomal protein S4

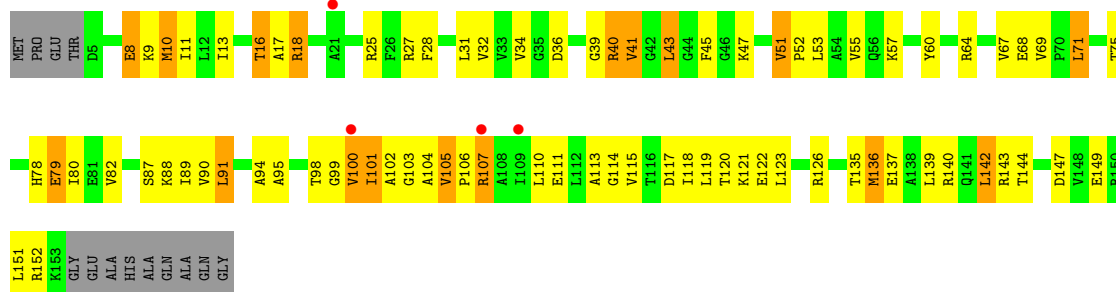




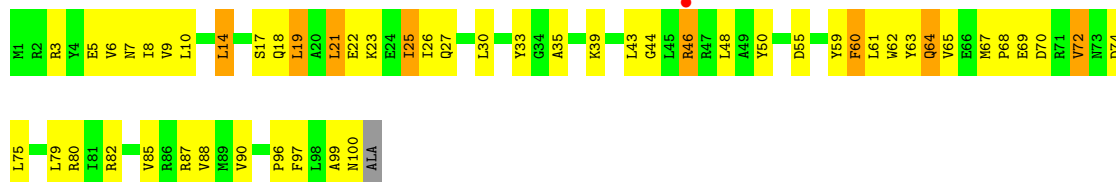
• Molecule 5: 30S ribosomal protein S5



• Molecule 5: 30S ribosomal protein S5



• Molecule 6: 30S ribosomal protein S6

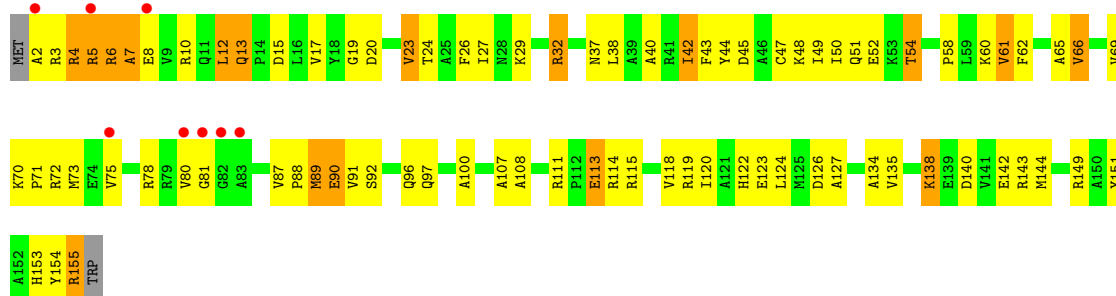


• Molecule 6: 30S ribosomal protein S6

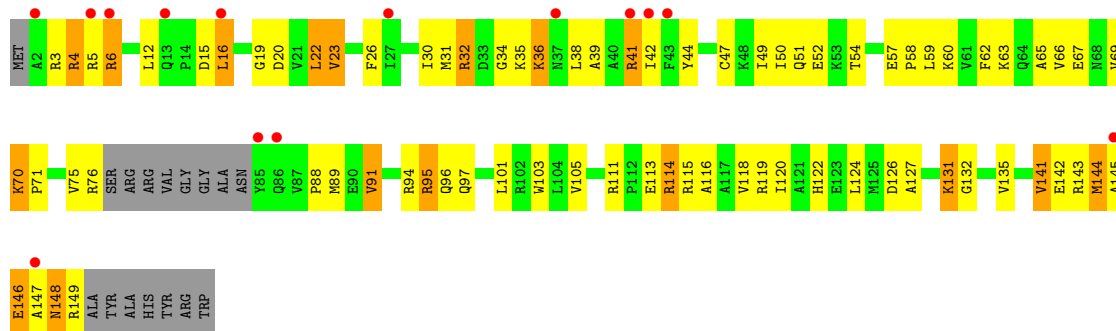




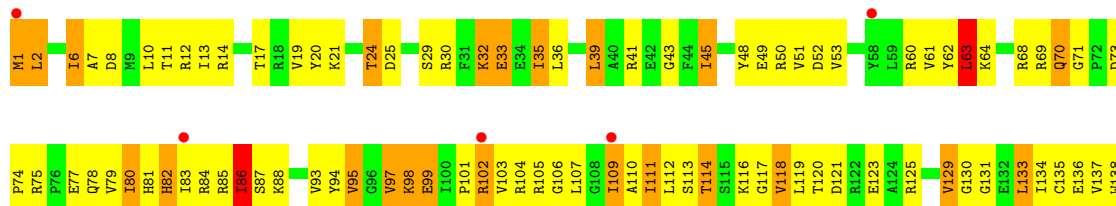
- Molecule 7: 30S ribosomal protein S7



- Molecule 7: 30S ribosomal protein S7

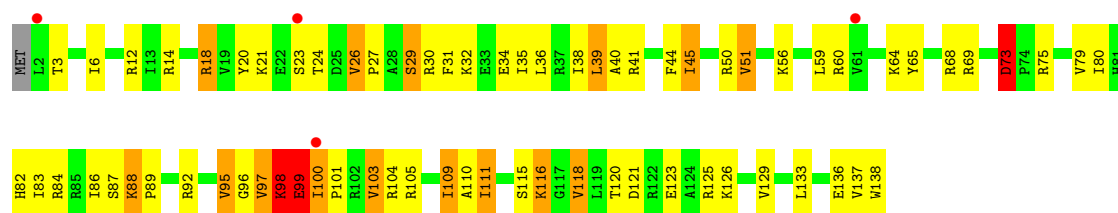


- Molecule 8: 30S ribosomal protein S8

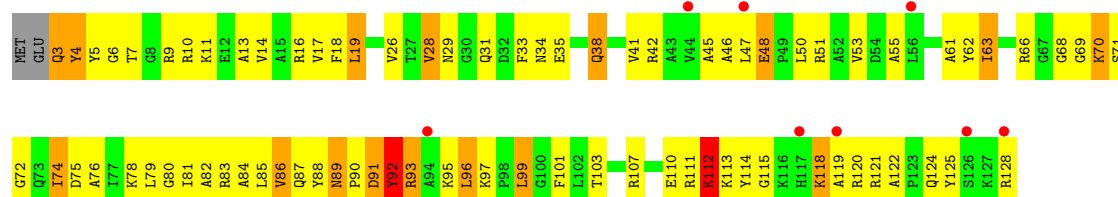


- Molecule 8: 30S ribosomal protein S8

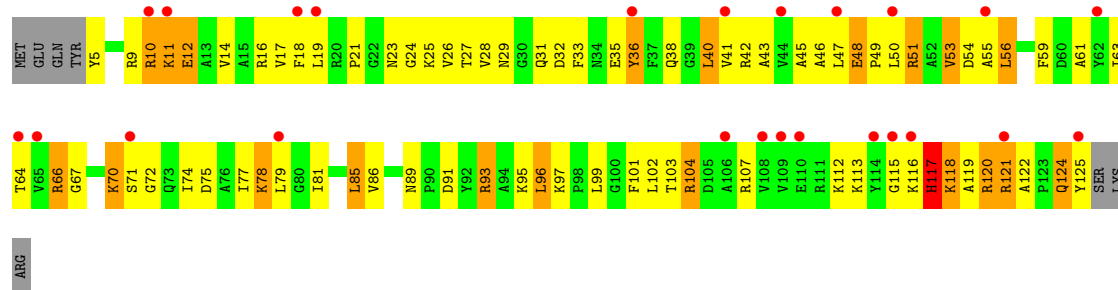




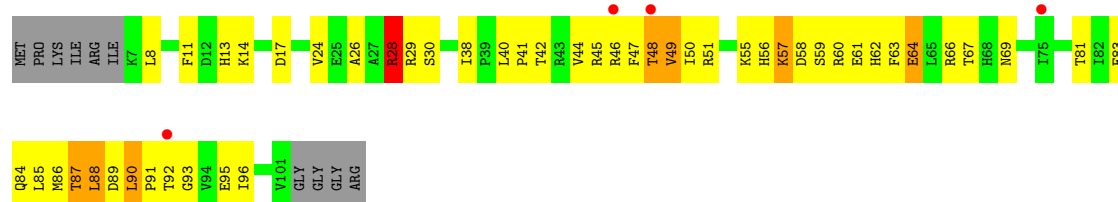
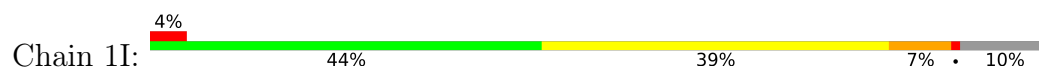
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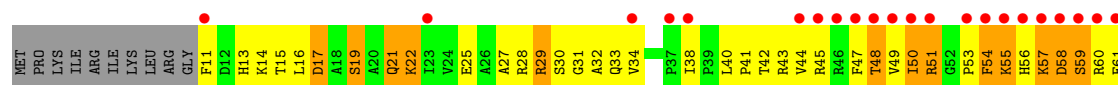
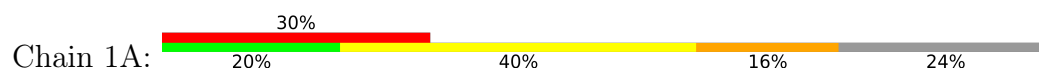
• Molecule 9: 30S ribosomal protein S9

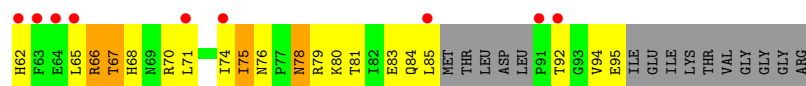


• Molecule 10: 30S ribosomal protein S10

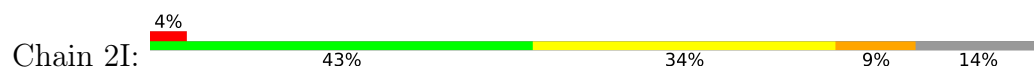


• Molecule 10: 30S ribosomal protein S10

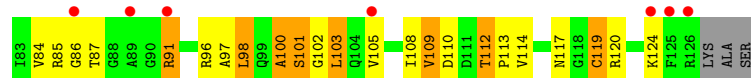
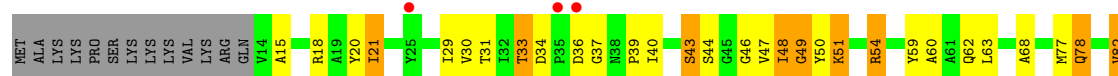




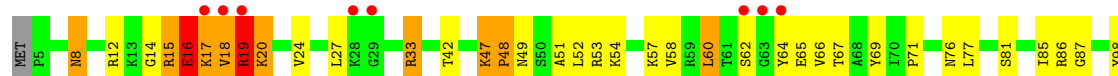
- Molecule 11: 30S ribosomal protein S11



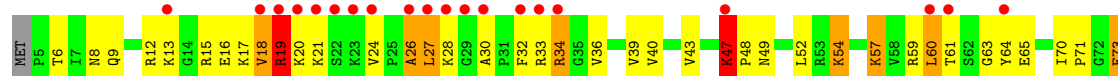
- Molecule 11: 30S ribosomal protein S11



- Molecule 12: 30S ribosomal protein S12

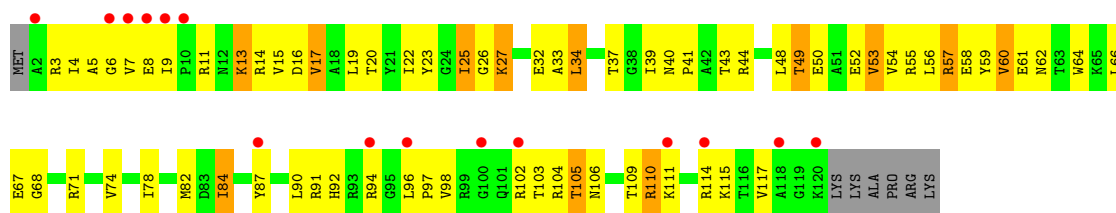


- Molecule 12: 30S ribosomal protein S12

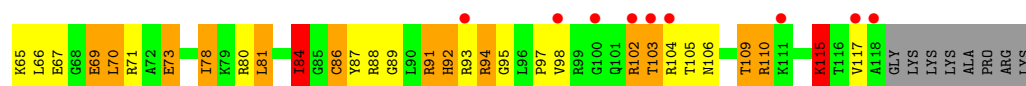


- Molecule 13: 30S ribosomal protein S13

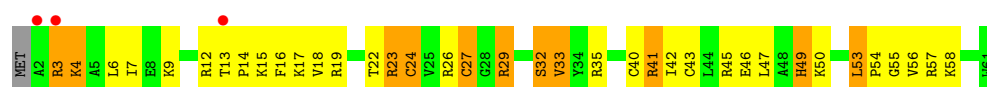




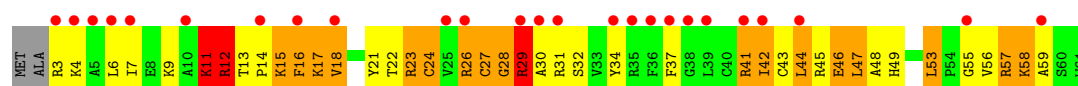
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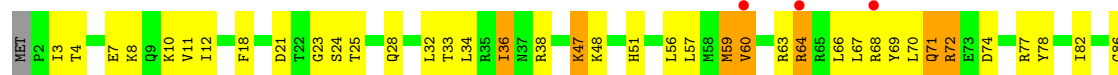
• Molecule 14: 30S ribosomal protein S14 type Z



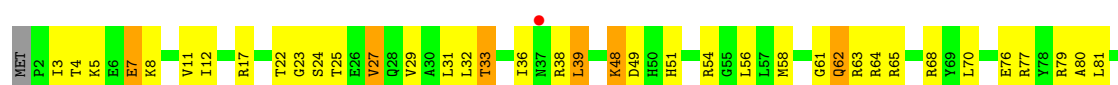
• Molecule 14: 30S ribosomal protein S14 type Z



• Molecule 15: 30S ribosomal protein S15

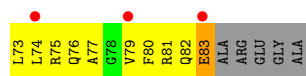
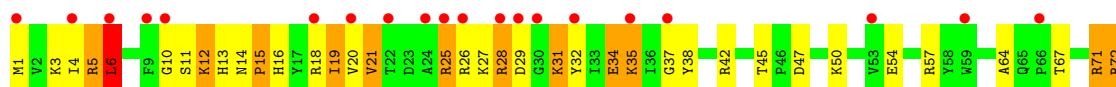


• Molecule 15: 30S ribosomal protein S15

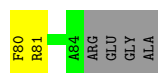
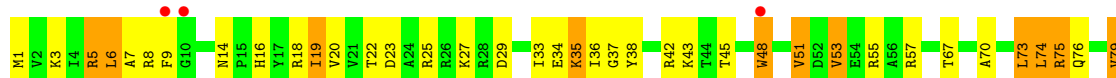




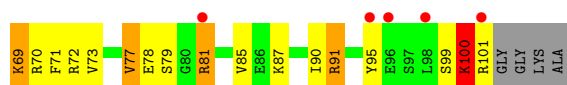
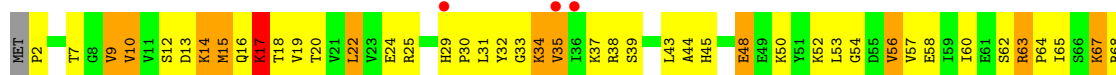
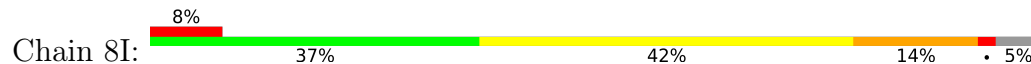
• Molecule 16: 30S ribosomal protein S16



• Molecule 16: 30S ribosomal protein S16



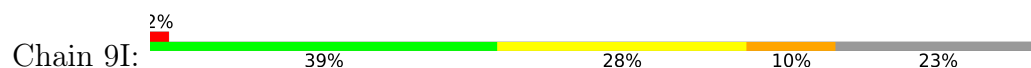
• Molecule 17: 30S ribosomal protein S17

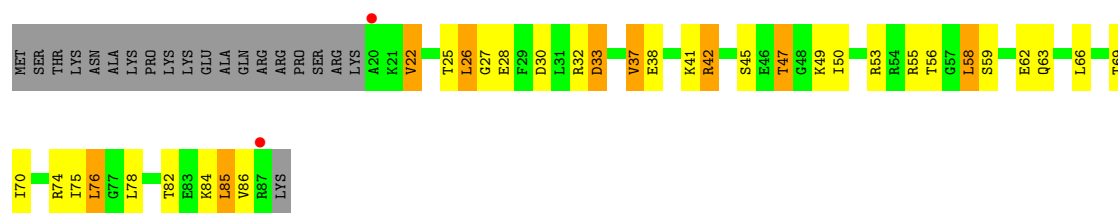


• Molecule 17: 30S ribosomal protein S17

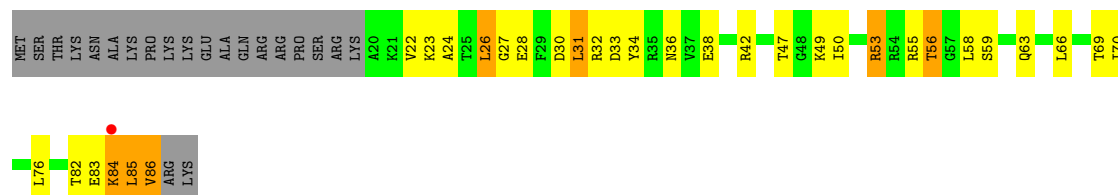


• Molecule 18: 30S ribosomal protein S18

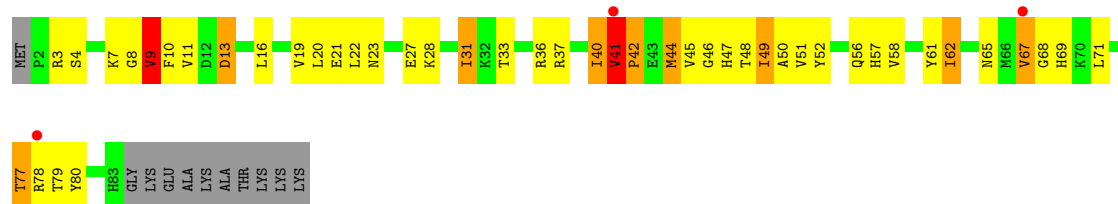




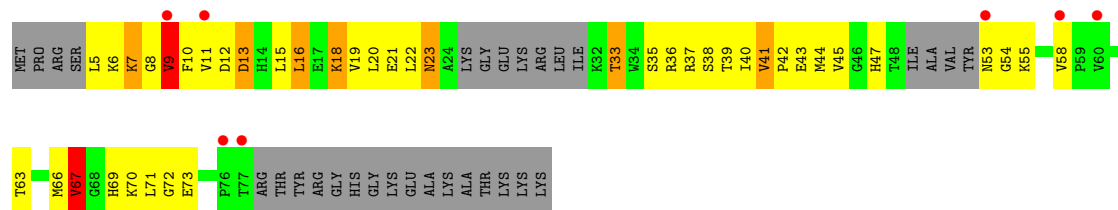
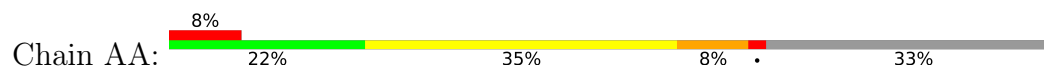
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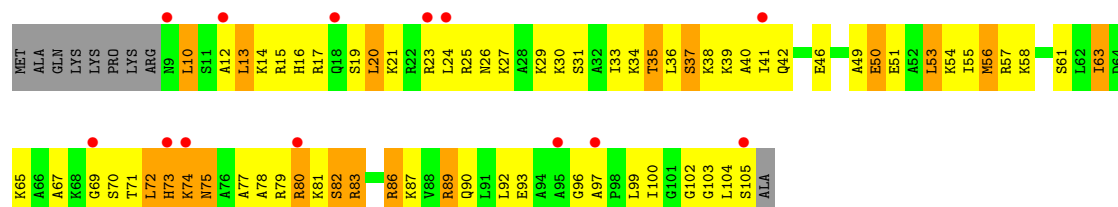
• Molecule 19: 30S ribosomal protein S19



• Molecule 19: 30S ribosomal protein S19

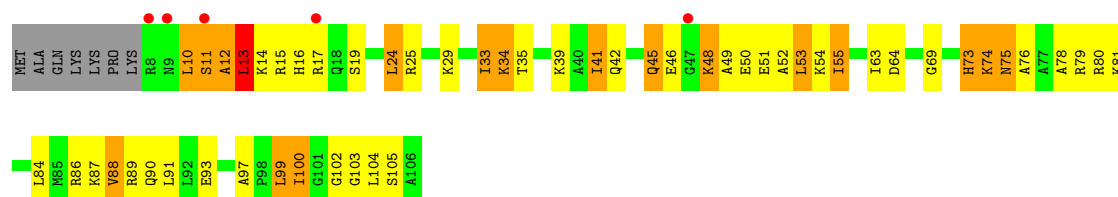


• Molecule 20: 30S ribosomal protein S20



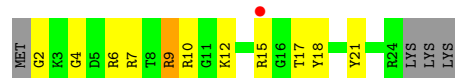
- Molecule 20: 30S ribosomal protein S20

Chain BA: 



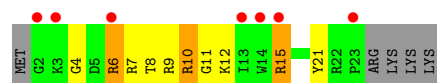
- Molecule 21: 30S ribosomal protein Thx

Chain 1F: 

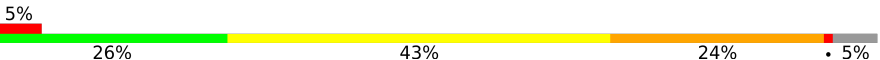


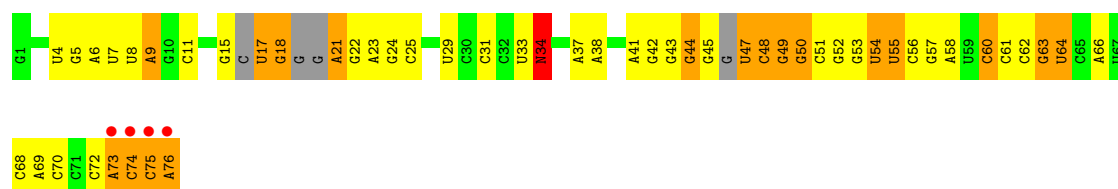
- Molecule 21: 30S ribosomal protein Thx

Chain 1B: 



- Molecule 22: tRNAVal

Chain 1K: 



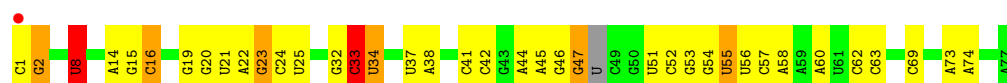
- Molecule 23: tRNAfMet

Chain 2K: 

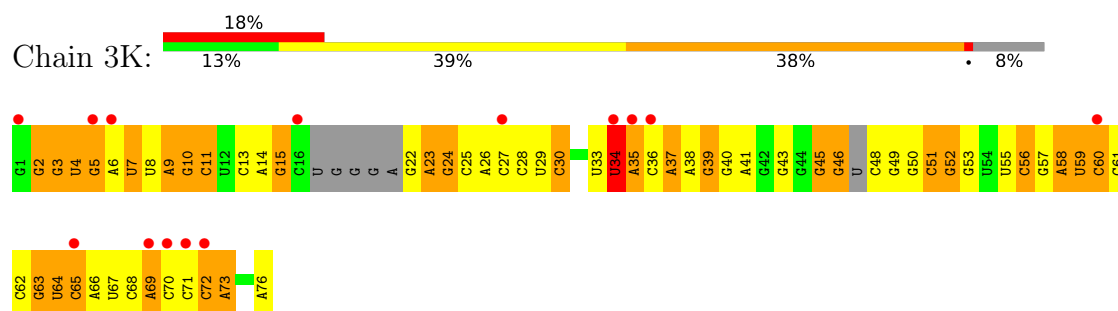


- Molecule 23: tRNAfMet

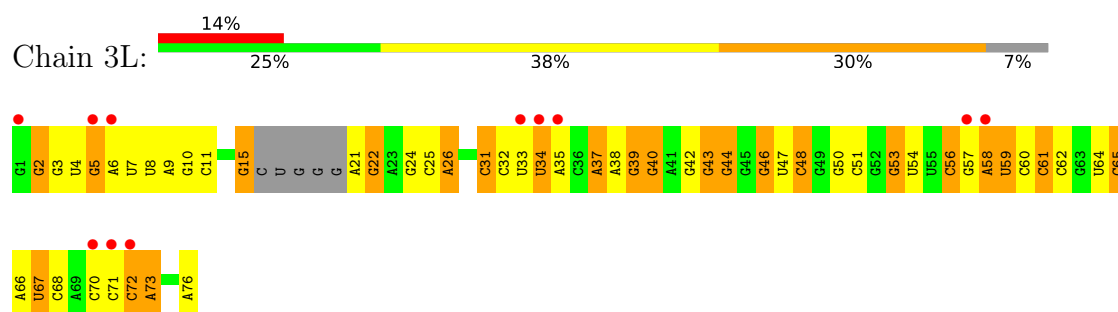
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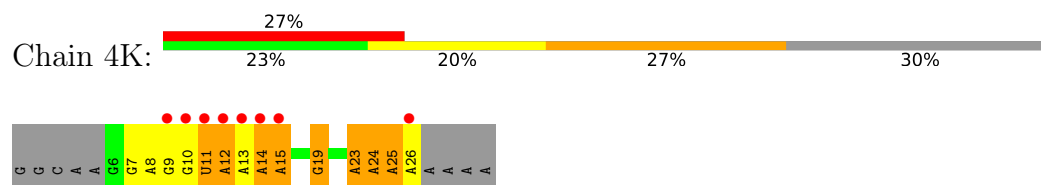
- Molecule 24: tRNAVal



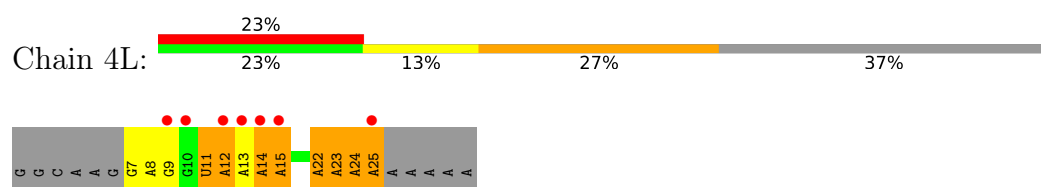
- Molecule 24: tRNAVal



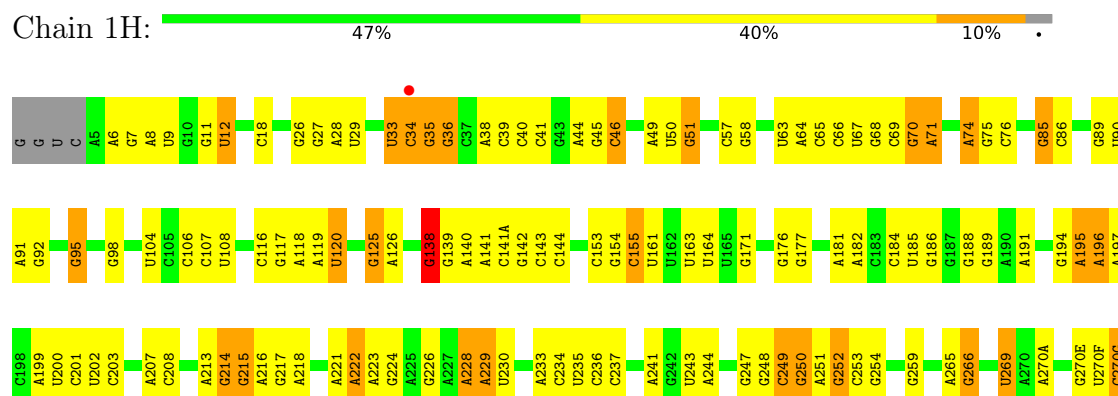
- Molecule 25: mRNA



- Molecule 25: mRNA



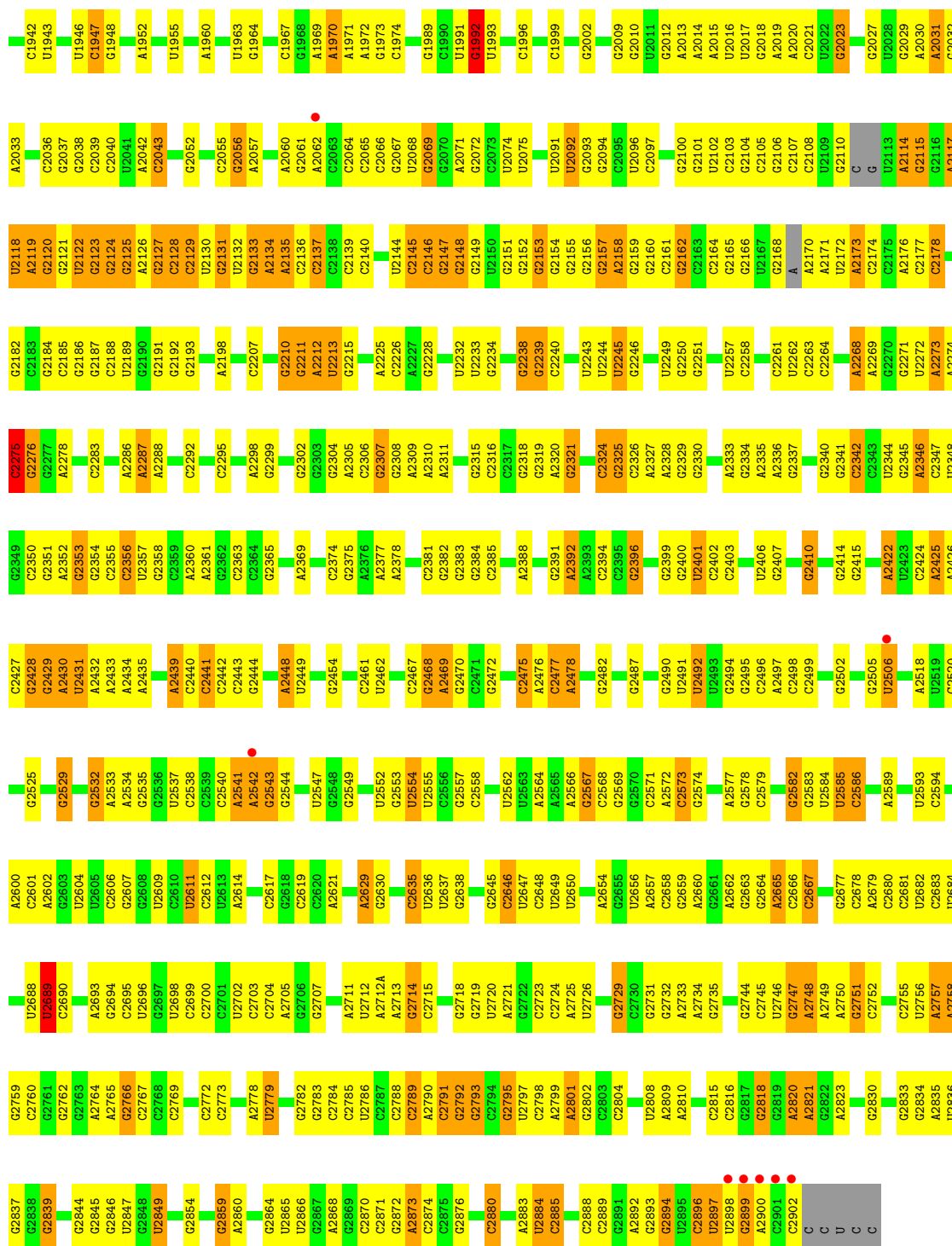
- Molecule 26: 23S ribosomal RNA





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U1864	C1781	A1577		A1577	U1673	A1577	C1781	U1864	G785
	C1782	C1577	A1490	C1577	G1674	A1577	C1782		A788
A1871	A1783	U1578	A1490	U1578	G1675	A1578	A1783	A1871	
A1872	A1784	C1582	C1493	C1582	G1676	A1582	A1784	A1872	G792
G1878	A1785	A1583	A1494	A1583	G1677	A1583	A1785	G1878	A793
	A1786	A1584	A1495	A1584	G1678	A1584	A1786		G796
G1883	A1787	A1585	A1496	A1585	C1686	A1585	A1787	G1883	C797
A1884	C1788	A1586	A1497	A1586	G1687	A1586	C1788	A1884	
	A1789	A1587	U1497	A1587	G1688	A1587	A1789		G801
G1888	A1790	A1588	C1501	A1588	U1689	A1588	A1790	G1888	G802
A1889	C1791	A1589	A1508	A1589	G1690	A1589	C1791	A1889	G805
A1890	U1794	C1589	C1509	C1589	G1691	A1590	U1794	A1890	
G1891	G1795	G1595	A1510	G1595	G1692	A1595	G1795	G1891	
	U1796	C1598	C1515	C1598	G1693	A1598	U1796		U811
C1895	C1797	U1602	U1516	U1602	G1694	A1602	C1797	C1895	C812
G1899	U1798	C1607	G1517	C1607	G1695	A1607	U1798	G1899	U813
A1900	G1799	A1608	C1518	A1608	G1696	A1608	G1799	A1900	C814
A1901	C1800	A1609	G1519	A1609	G1697	A1609	C1800	A1901	C815
C1902	G1801	A1610	U1520	A1610	G1698	A1610	G1801	C1902	C816
			G1521		G1699				C817
C1905	U1805		G1522		G1700		U1805	C1905	C818
G1906	U1808	G1613	G1435	G1613	G1701	G1613	U1808	G1906	A819
	A1809	A1614	G1436	A1614	G1702	A1614	A1809		A820
C1914	A1810	C1615	A1444	C1615	G1703	A1615	A1810	C1914	A821
U1915	G1811	A1616	A1445	A1616	G1704	A1616	G1811	U1915	U822
A1916		C1617	C1446	C1617	G1705	C1617		A1916	G823
	U1923	A1618	G1447	A1618	G1706	A1618	U1923		A824
		G1619	G1448	G1619	G1707	A1619			
A1927	G1817	G1628	C1532	G1628	G1708	A1628	A1927	A1927	U827
A1928	U1818	U1629	C1533	U1629	G1709	A1629	A1928	A1928	U828
G1929	A1819	G1635	G1534	G1635	G1710	A1635	G1929	G1929	A829
U1931	A1821	C1636	U1535	C1636	G1711	A1636	U1931	U1931	G830
A1932		C1637	C1536	C1637	G1712	A1637	A1932	A1932	G831
G1933	G1826	C1638	G1537	C1638	G1713	A1638	G1933	G1933	U833
	C1827	A1639	G1538	A1639	G1714	A1639			C838
A1936	G1828	U1639	G1539	U1639	C1754	A1639	A1936	A1936	U839
A1937	A1829	C1640	C1458	C1640	A1755	A1640	A1937	A1937	C840
A1938	C1830	A1641	G1459	A1641	G1756	A1641	A1938	A1938	A841
U1939		G1642	A1460	A1642	U1757	A1642	U1939	U1939	G843

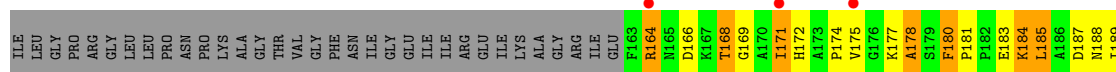
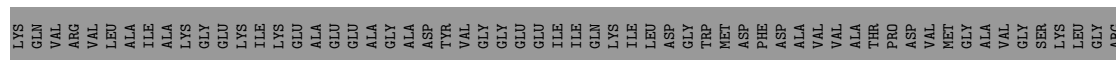
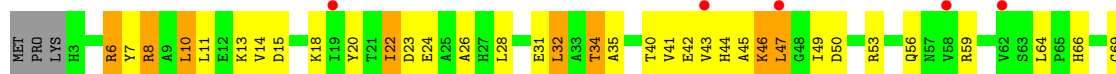
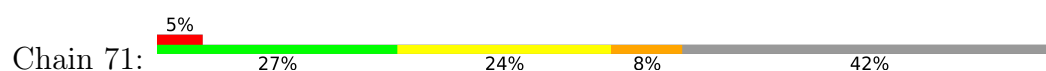




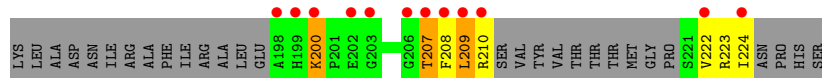
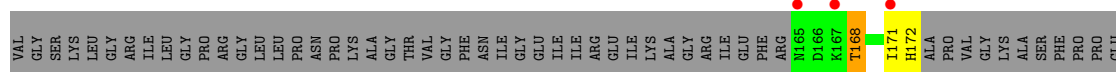
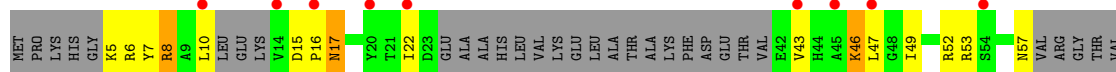
• Molecule 27: 5S ribosomal RNA



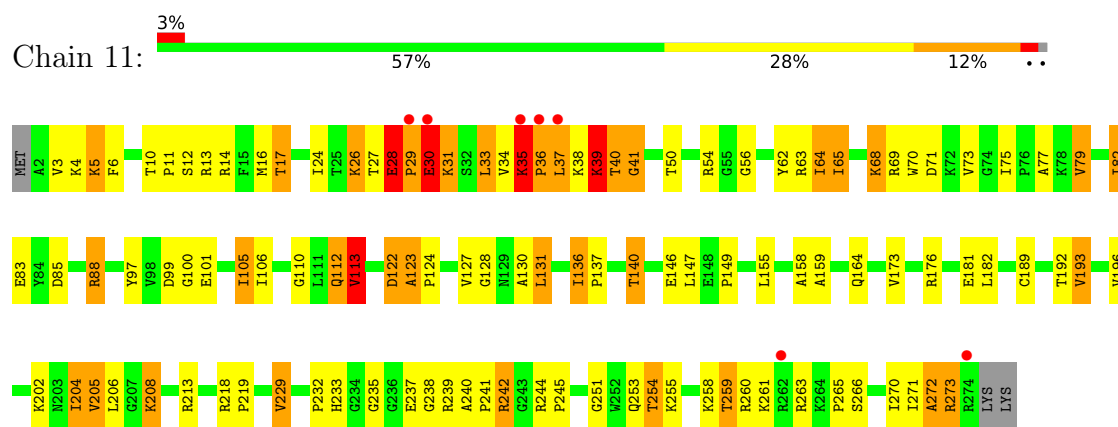
• Molecule 28: 50S ribosomal protein L1



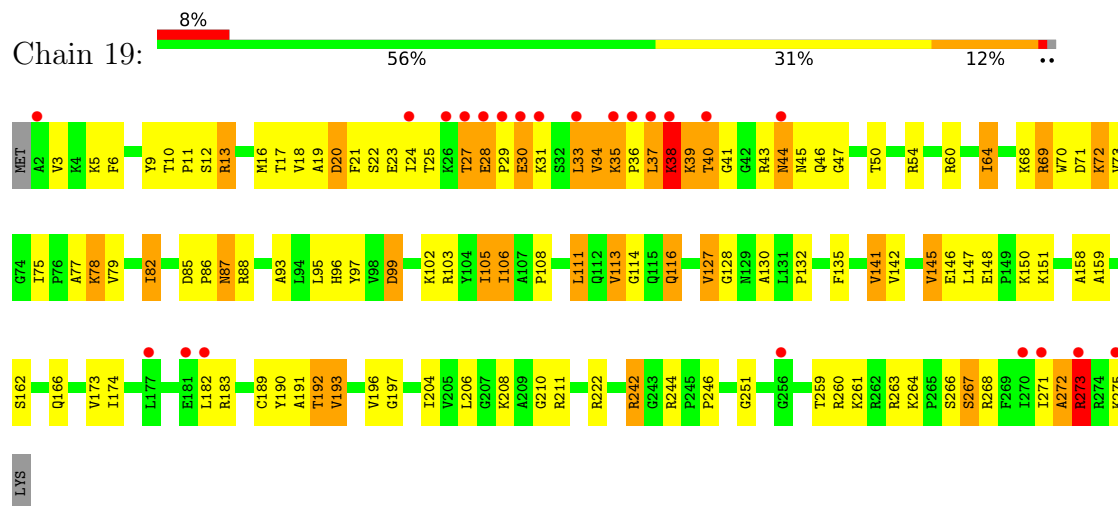
• Molecule 28: 50S ribosomal protein L1



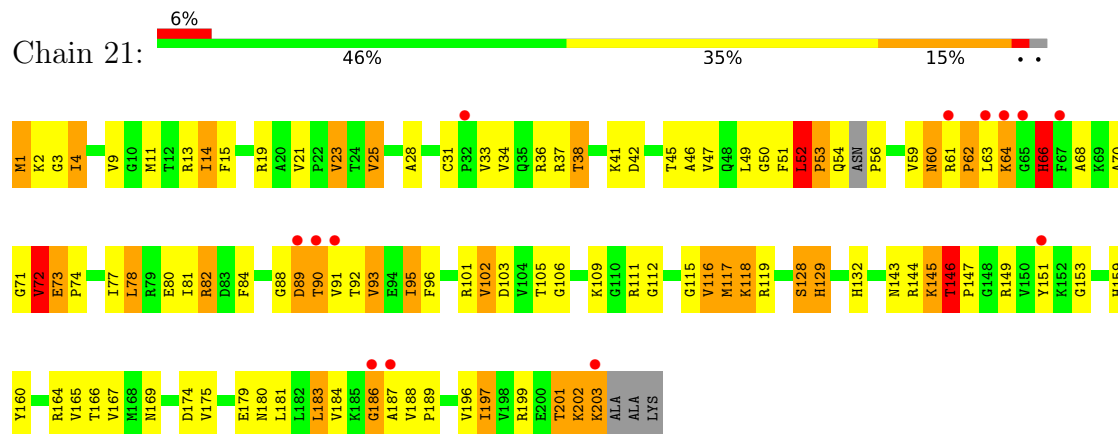
• Molecule 29: 50S ribosomal protein L2



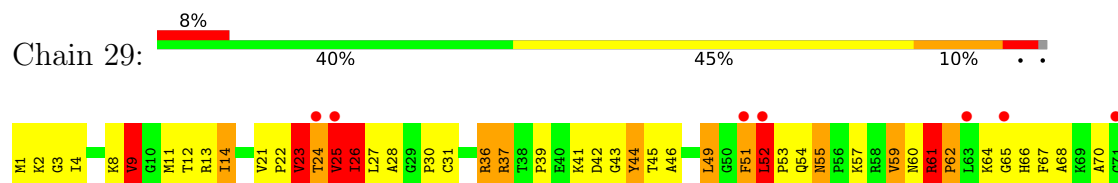
- Molecule 29: 50S ribosomal protein L2

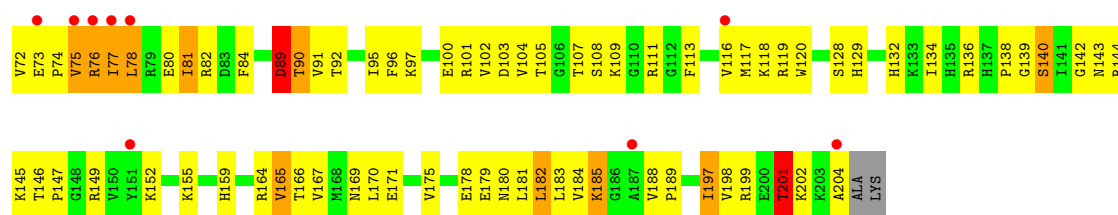


- Molecule 30: 50S ribosomal protein L3

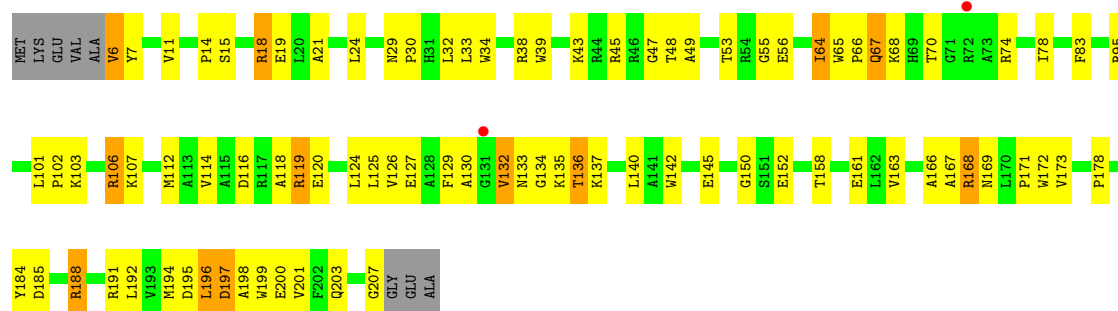


- Molecule 30: 50S ribosomal protein L3

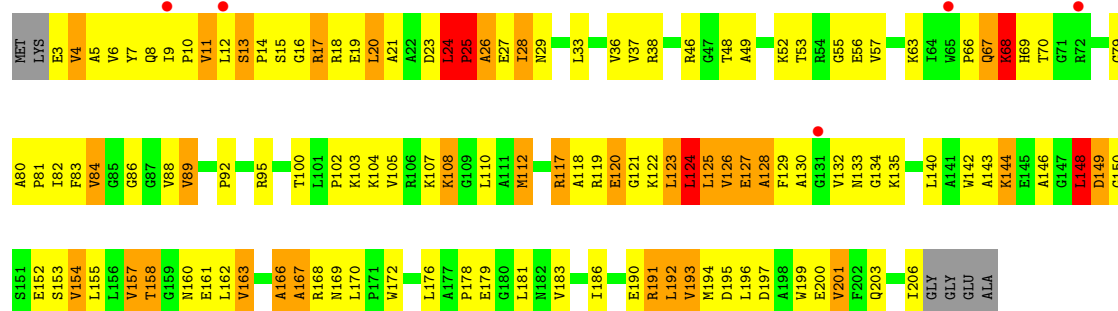




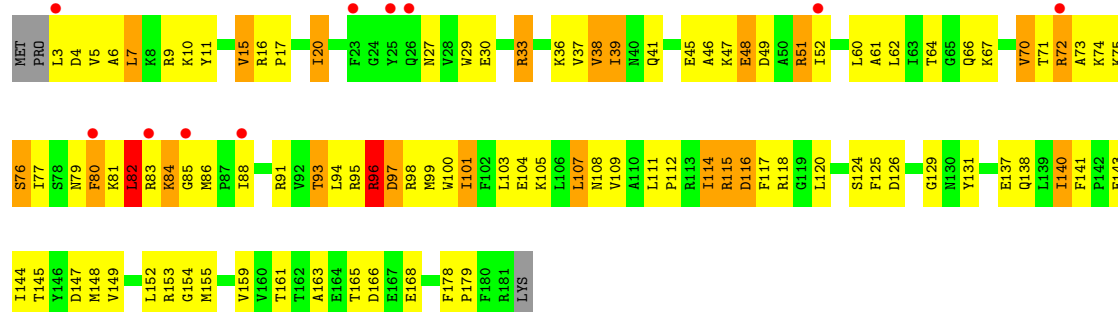
• Molecule 31: 50S ribosomal protein L4



• Molecule 31: 50S ribosomal protein L4

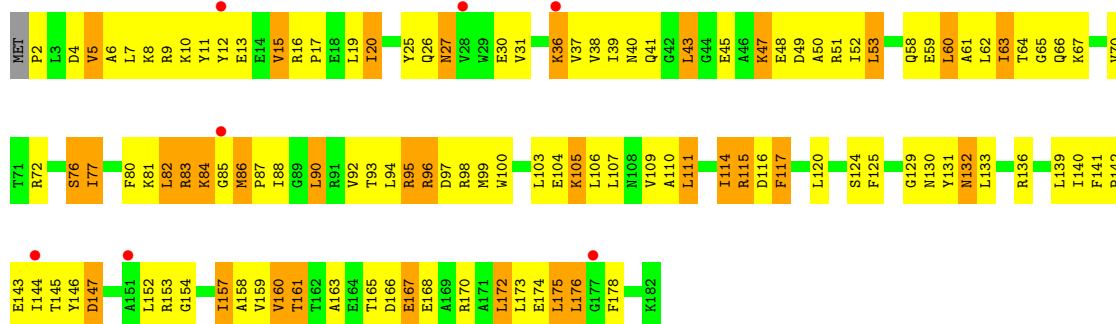


• Molecule 32: 50S ribosomal protein L5



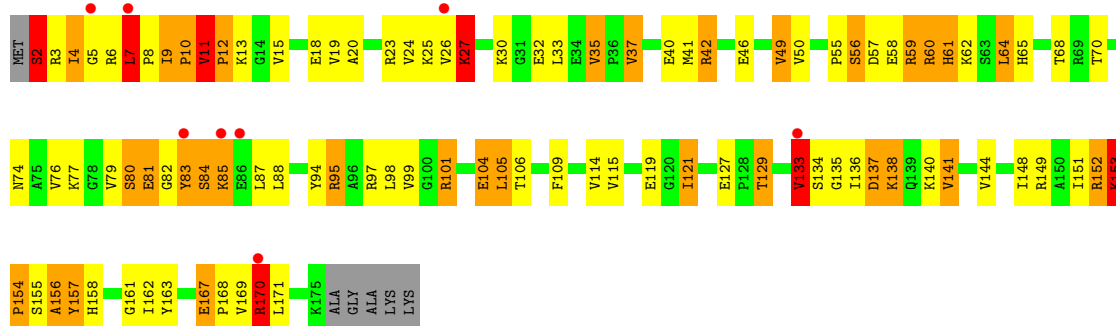
• Molecule 32: 50S ribosomal protein L5

Chain 49: 



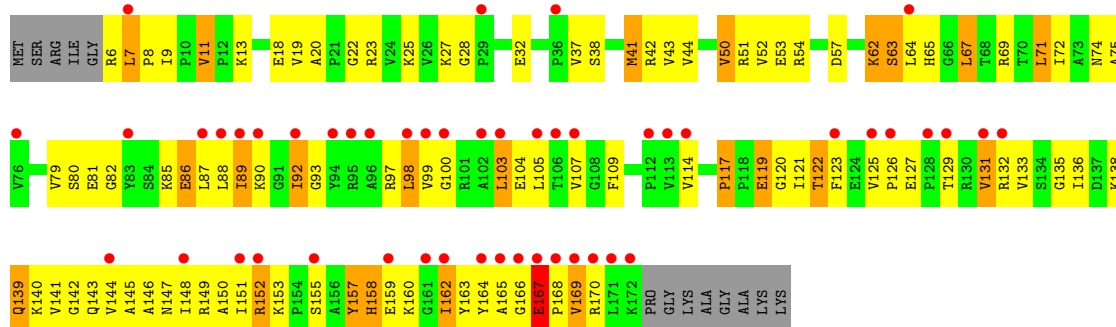
• Molecule 33: 50S ribosomal protein L6

Chain 51: 



• Molecule 33: 50S ribosomal protein L6

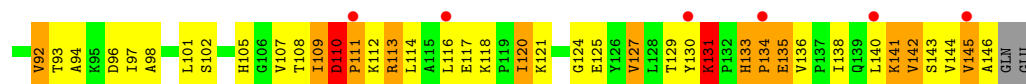
Chain 59: 



• Molecule 34: 50S ribosomal protein L9

Chain 61: 

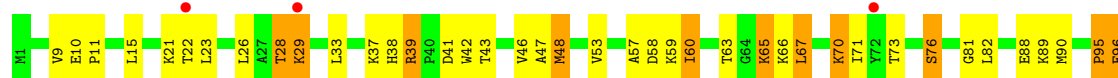




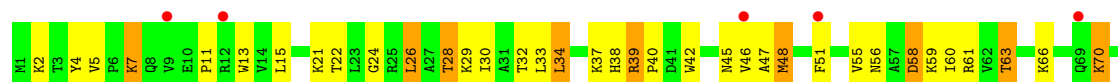
- Molecule 34: 50S ribosomal protein L9



- Molecule 35: 50S ribosomal protein L13



- Molecule 35: 50S ribosomal protein L13

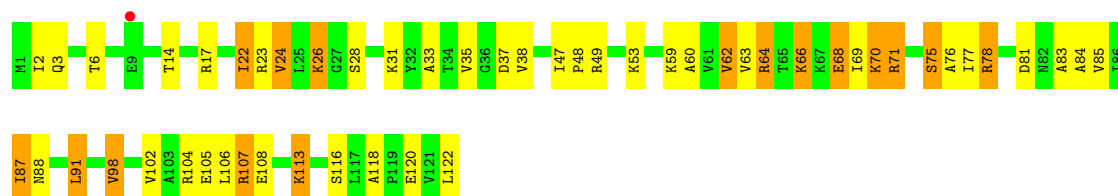


- Molecule 36: 50S ribosomal protein L14

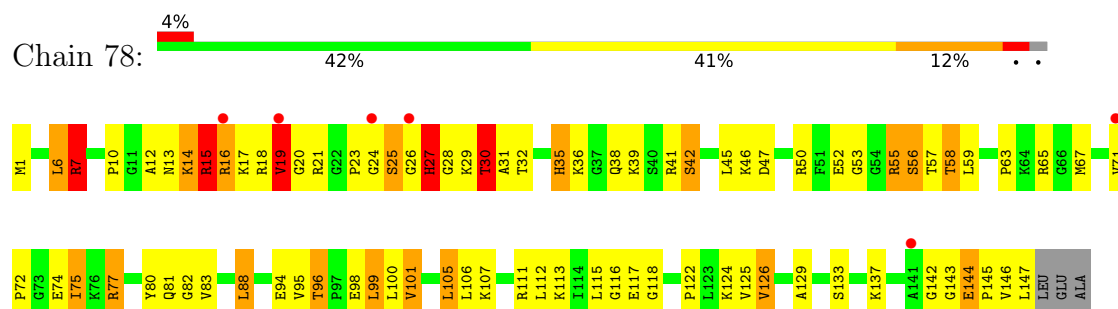


- Molecule 36: 50S ribosomal protein L14

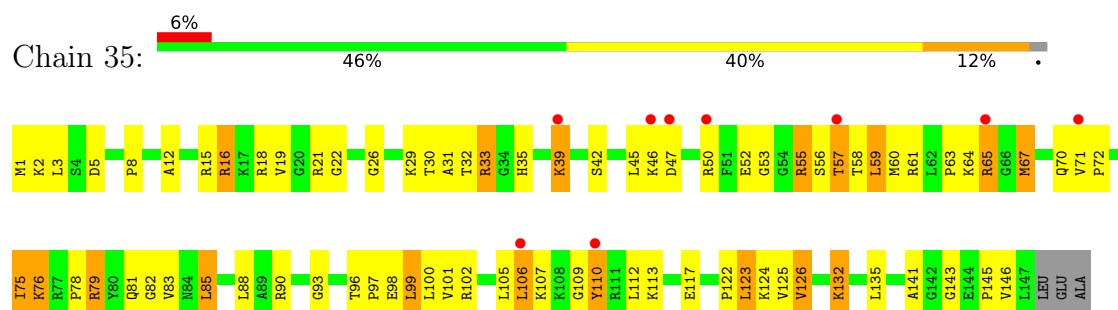




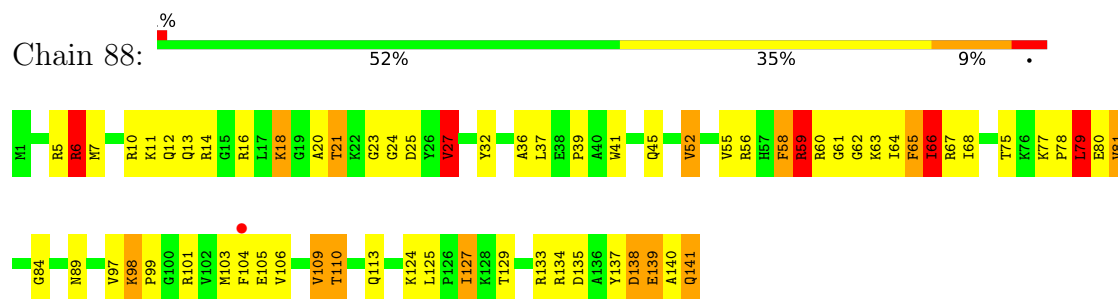
• Molecule 37: 50S ribosomal protein L15



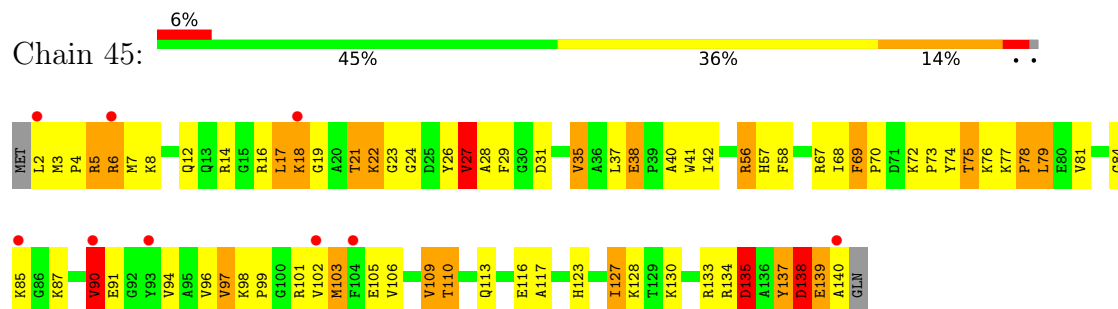
• Molecule 37: 50S ribosomal protein L15



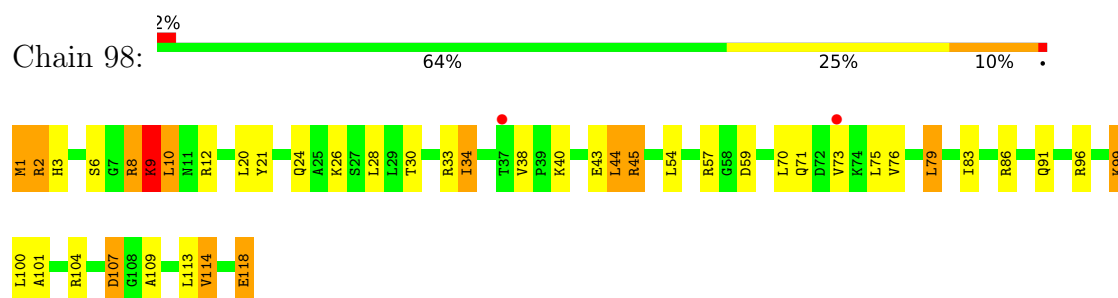
• Molecule 38: 50S ribosomal protein L16



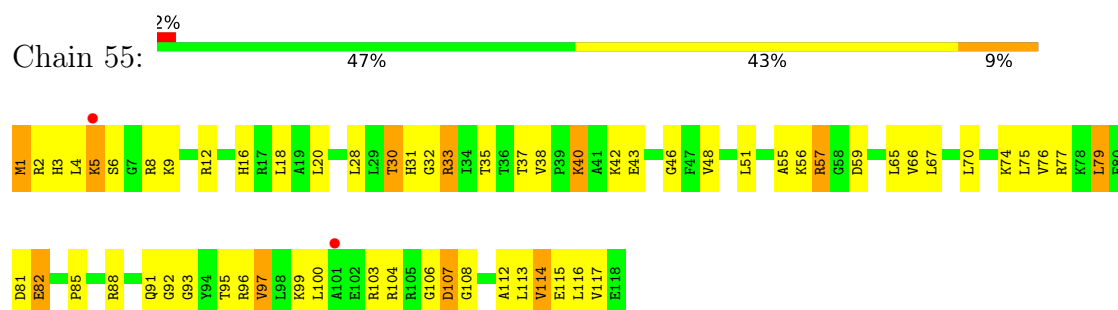
• Molecule 38: 50S ribosomal protein L16



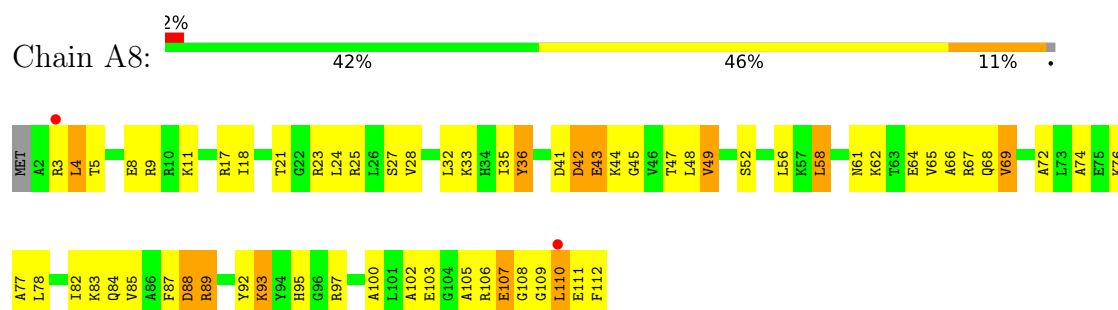
- Molecule 39: 50S ribosomal protein L17



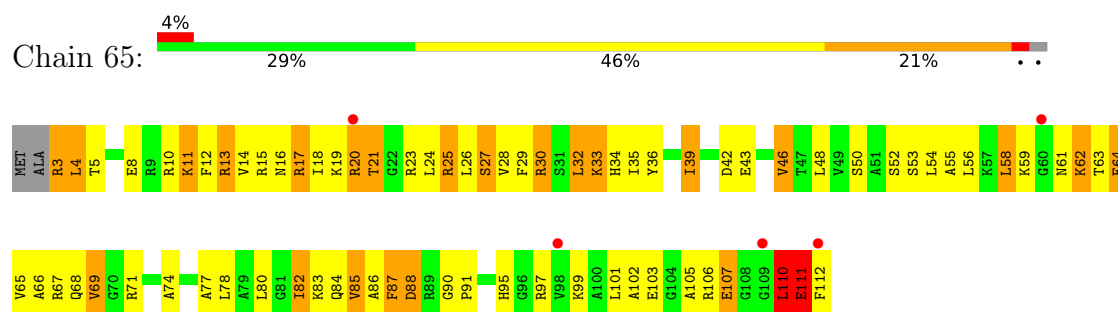
- Molecule 39: 50S ribosomal protein L17



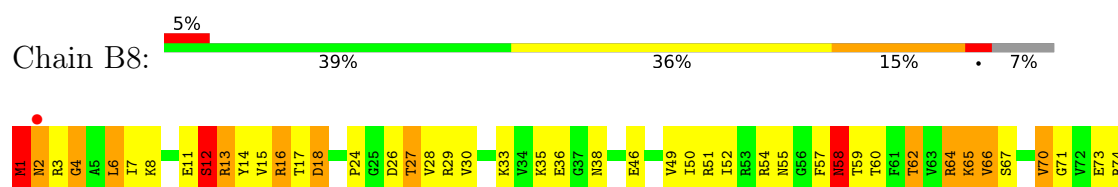
- Molecule 40: 50S ribosomal protein L18



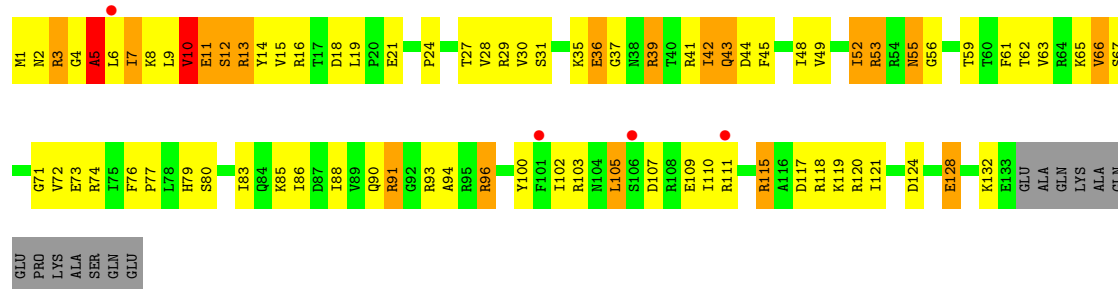
- Molecule 40: 50S ribosomal protein L18



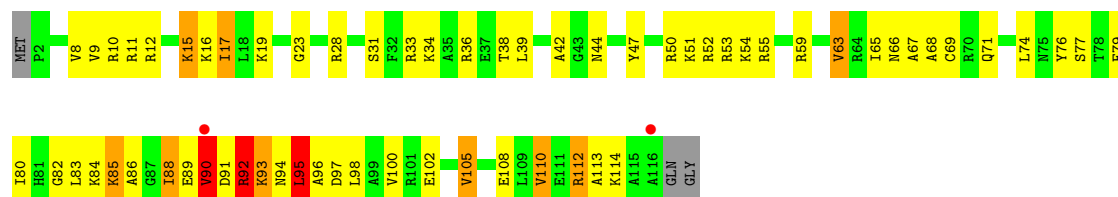
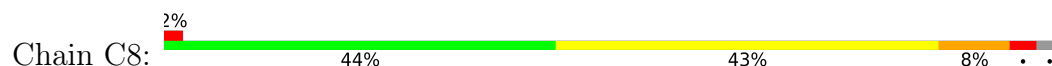
- Molecule 41: 50S ribosomal protein L19



- Molecule 41: 50S ribosomal protein L19



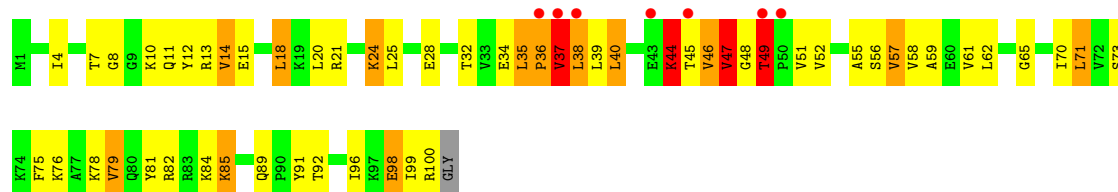
- Molecule 42: 50S ribosomal protein L20



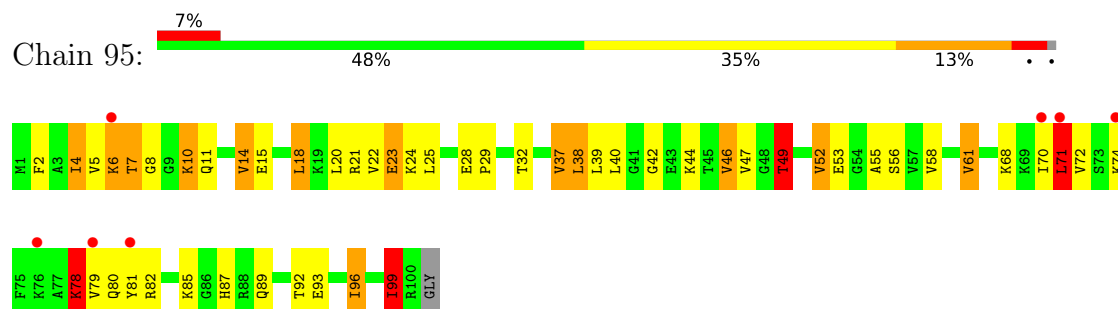
- Molecule 42: 50S ribosomal protein L20



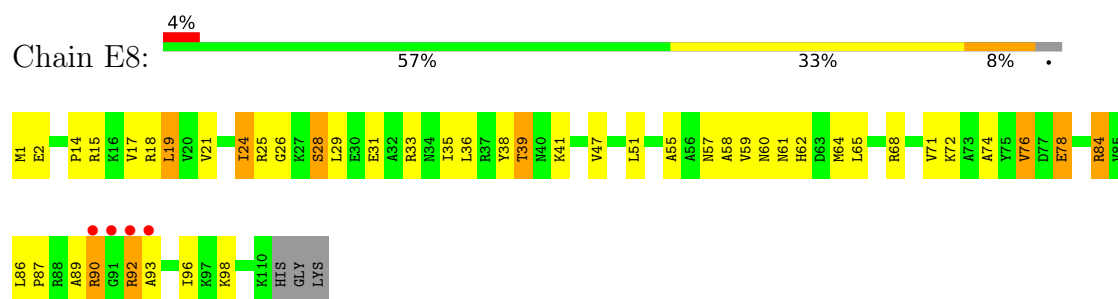
- Molecule 43: 50S ribosomal protein L21



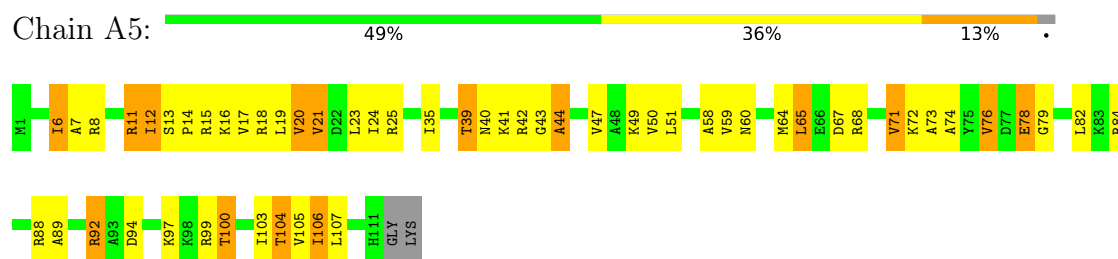
- Molecule 43: 50S ribosomal protein L21



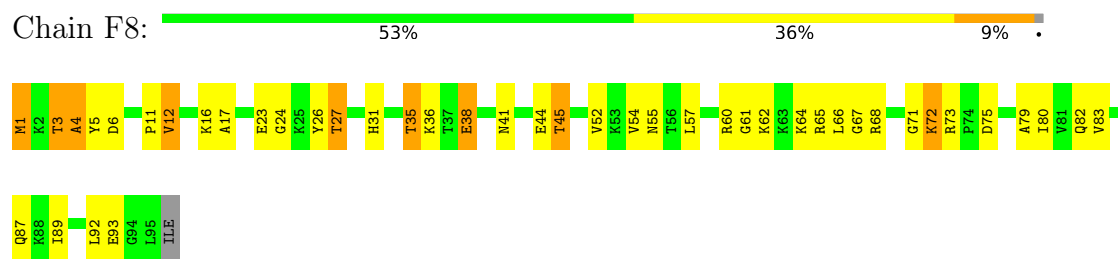
- Molecule 44: 50S ribosomal protein L22



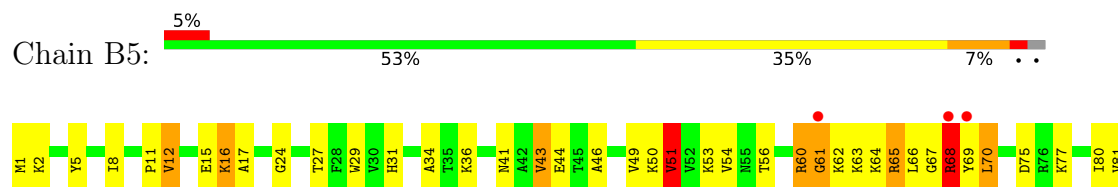
- Molecule 44: 50S ribosomal protein L22

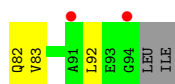


- Molecule 45: 50S ribosomal protein L23

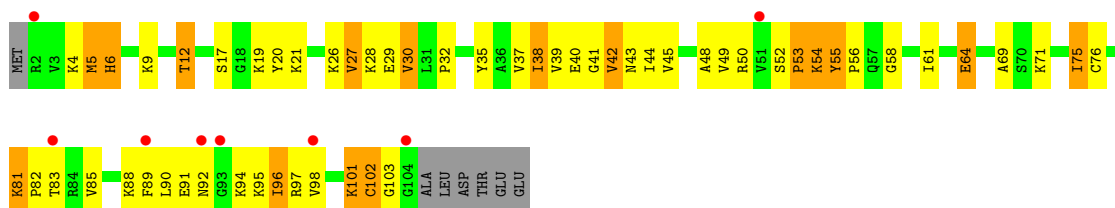
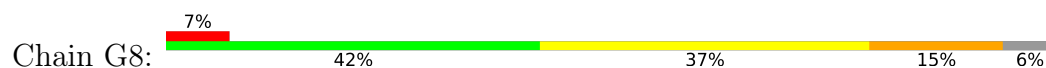


- Molecule 45: 50S ribosomal protein L23

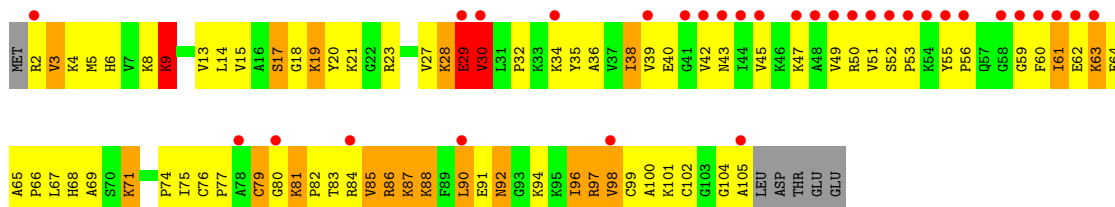




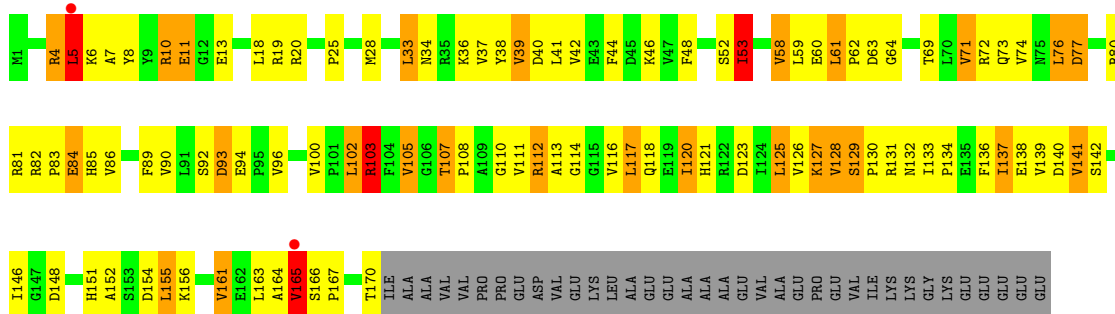
- Molecule 46: 50S ribosomal protein L24



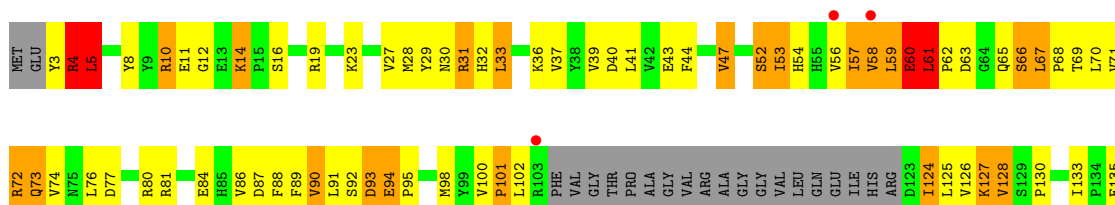
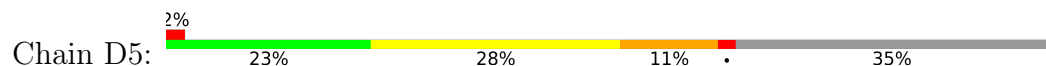
- Molecule 46: 50S ribosomal protein L24

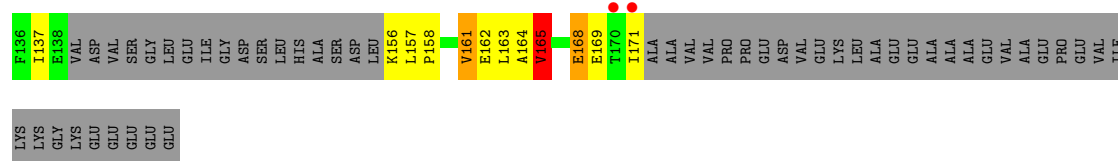


- Molecule 47: 50S ribosomal protein L25

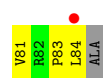


- Molecule 47: 50S ribosomal protein L25

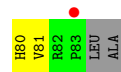
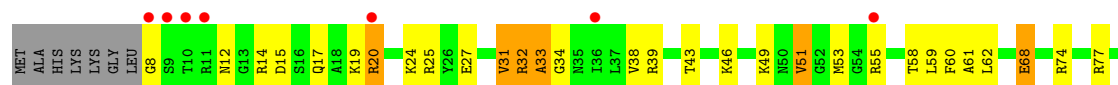




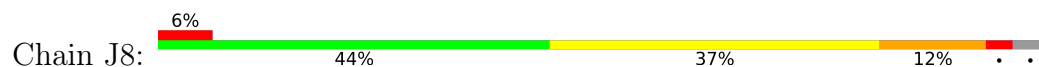
- Molecule 48: 50S ribosomal protein L27



- Molecule 48: 50S ribosomal protein L27



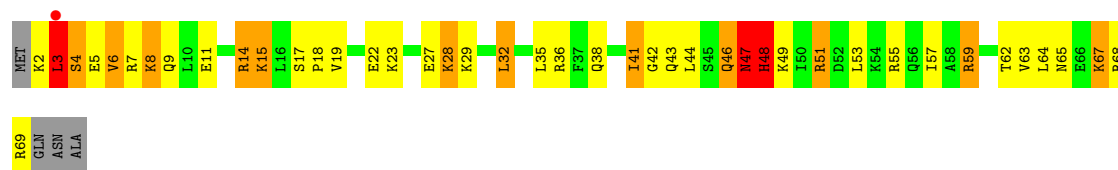
- Molecule 49: 50S ribosomal protein L28



- Molecule 49: 50S ribosomal protein L28



- Molecule 50: 50S ribosomal protein L29



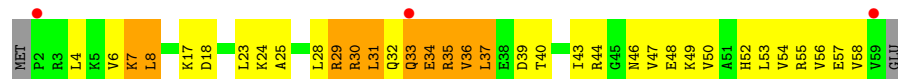
- Molecule 50: 50S ribosomal protein L29



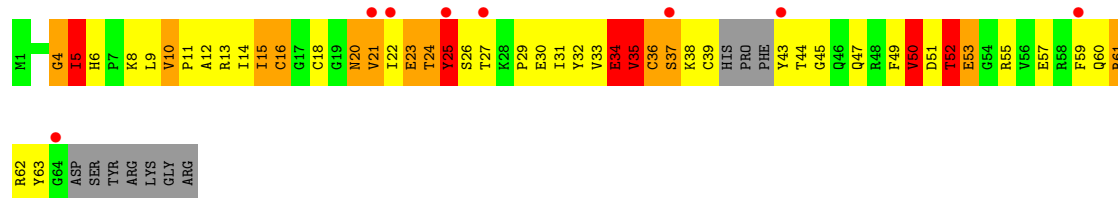
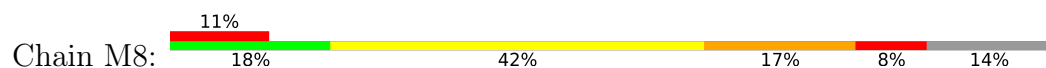
- Molecule 51: 50S ribosomal protein L30



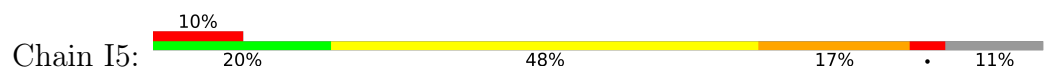
- Molecule 51: 50S ribosomal protein L30

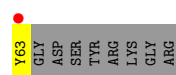


- Molecule 52: 50S ribosomal protein L31



- Molecule 52: 50S ribosomal protein L31

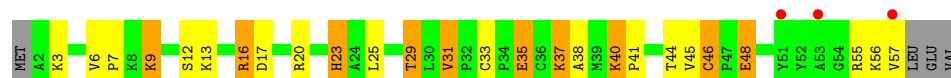




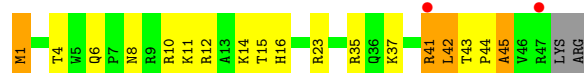
- Molecule 53: 50S ribosomal protein L32



- Molecule 53: 50S ribosomal protein L32



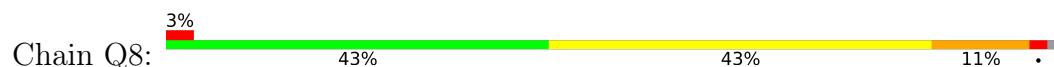
- Molecule 54: 50S ribosomal protein L34



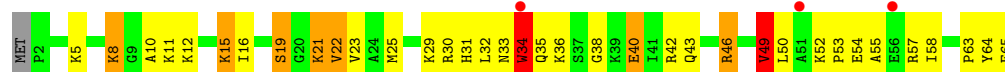
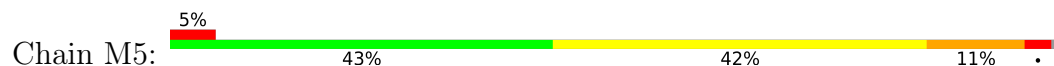
- Molecule 54: 50S ribosomal protein L34



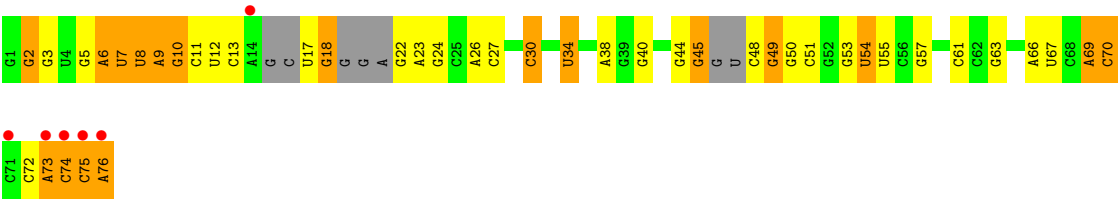
- Molecule 55: 50S ribosomal protein L35



- Molecule 55: 50S ribosomal protein L35



- Molecule 56: tRNAVal



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	209.50Å 448.90Å 620.80Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	146.68 – 2.96 146.68 – 2.96	Depositor EDS
% Data completeness (in resolution range)	99.8 (146.68-2.96) 89.3 (146.68-2.96)	Depositor EDS
R_{merge}	0.44	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.84 (at 2.96Å)	Xtriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.201 , 0.243 0.203 , 0.242	Depositor DCC
R_{free} test set	2000 reflections (0.17%)	wwPDB-VP
Wilson B-factor (Å ²)	75.4	Xtriage
Anisotropy	0.336	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.27 , 50.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	296743	wwPDB-VP
Average B, all atoms (Å ²)	97.0	wwPDB-VP

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

¹Intensities estimated from amplitudes.

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

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

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	0.38	0/35994	0.64	10/56171 (0.0%)
1	1G	0.34	0/36236	0.59	3/56555 (0.0%)
2	12	0.37	0/1727	0.76	0/2326
2	1E	0.36	0/1936	0.70	0/2611
3	22	0.52	1/1560 (0.1%)	0.62	0/2104
3	2E	0.43	1/1629 (0.1%)	0.66	0/2195
4	32	0.38	0/1732	0.69	0/2318
4	3E	0.42	0/1728	0.76	2/2313 (0.1%)
5	42	0.39	0/1155	0.67	0/1555
5	4E	0.40	0/1158	0.68	0/1559
6	52	0.40	0/855	0.60	0/1154
6	5E	0.41	0/850	0.65	0/1147
7	62	0.37	0/1132	0.71	2/1514 (0.1%)
7	6E	0.39	0/1259	0.60	0/1686
8	72	0.36	0/1127	0.65	0/1517
8	7E	0.38	0/1135	0.72	0/1527
9	82	0.35	0/971	0.79	0/1304
9	8E	0.39	0/1019	0.80	0/1367
10	1A	0.64	1/658 (0.2%)	0.75	2/885 (0.2%)
10	1I	0.40	0/767	0.78	2/1034 (0.2%)
11	2A	0.39	0/850	0.67	0/1150
11	2I	0.41	0/838	0.73	0/1133
12	3A	0.50	0/972	0.78	0/1301
12	3I	0.54	0/972	0.90	0/1301
13	4A	0.39	0/903	0.75	0/1211
13	4I	0.45	0/952	0.76	0/1277
14	5A	0.42	0/495	1.01	4/657 (0.6%)
14	5I	0.51	0/500	0.90	1/664 (0.2%)
15	6A	0.40	0/740	0.62	0/987
15	6I	0.43	0/740	0.69	0/987
16	7A	0.39	0/721	0.74	0/970
16	7I	0.44	0/716	0.78	1/963 (0.1%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
17	8A	0.38	0/836	0.64	0/1117
17	8I	0.48	0/847	0.82	0/1131
18	9A	0.42	0/549	0.76	0/732
18	9I	0.41	0/554	0.72	0/739
19	AA	0.39	0/490	0.88	3/662 (0.5%)
19	AI	0.39	0/676	0.90	3/910 (0.3%)
20	BA	0.36	0/764	0.77	3/1007 (0.3%)
20	BI	0.50	1/748 (0.1%)	0.81	0/986
21	1B	0.41	0/192	0.65	0/252
21	1F	0.40	0/203	0.68	0/266
22	1K	0.35	0/1595	0.52	0/2475
23	2K	0.44	1/1721 (0.1%)	0.65	0/2682
23	2L	0.38	0/1698	0.60	0/2644
24	3K	0.33	0/1663	0.55	1/2585 (0.0%)
24	3L	0.32	0/1689	0.51	0/2628
25	4K	0.41	0/520	0.60	0/808
25	4L	0.36	0/470	0.62	0/732
26	14	0.44	0/67798	0.70	15/105832 (0.0%)
26	1H	0.51	0/68537	0.76	22/106989 (0.0%)
27	16	0.44	0/2928	0.72	0/4568
27	1J	0.40	0/2928	0.66	0/4568
28	71	0.28	0/1055	0.61	0/1425
28	79	0.30	0/459	0.56	0/608
29	11	0.68	1/2170 (0.0%)	1.10	20/2926 (0.7%)
29	19	0.58	0/2175	0.97	7/2933 (0.2%)
30	21	0.59	0/1537	1.11	11/2081 (0.5%)
30	29	0.53	0/1596	0.98	7/2153 (0.3%)
31	31	0.52	0/1620	0.81	0/2194
31	39	0.51	0/1637	0.99	5/2218 (0.2%)
32	41	0.44	0/1481	0.80	0/1994
32	49	0.37	0/1492	0.77	1/2008 (0.0%)
33	51	0.52	0/1354	1.08	8/1833 (0.4%)
33	59	0.37	0/1308	0.77	2/1771 (0.1%)
34	61	0.44	0/1151	0.85	6/1558 (0.4%)
34	69	0.41	0/1146	0.81	3/1551 (0.2%)
35	15	0.41	0/1131	0.77	0/1525
35	58	0.50	0/1123	0.83	5/1514 (0.3%)
36	25	0.44	0/942	0.74	0/1269
36	68	0.50	0/942	0.83	0/1269
37	35	0.52	0/1139	0.96	2/1514 (0.1%)
37	78	0.65	0/1139	1.12	9/1514 (0.6%)
38	45	0.62	3/1125 (0.3%)	0.94	1/1505 (0.1%)
38	88	0.67	0/1138	0.97	2/1523 (0.1%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
39	55	0.48	0/981	0.75	0/1312
39	98	0.50	0/981	0.85	2/1312 (0.2%)
40	65	0.48	0/886	0.87	1/1180 (0.1%)
40	A8	0.49	0/891	0.79	0/1187
41	75	0.48	0/1123	0.93	4/1500 (0.3%)
41	B8	0.53	1/1138 (0.1%)	0.94	4/1521 (0.3%)
42	85	0.54	1/977 (0.1%)	0.79	1/1301 (0.1%)
42	C8	0.51	0/968	0.80	0/1289
43	95	0.46	0/781	0.87	0/1048
43	D8	0.51	0/785	0.92	2/1052 (0.2%)
44	A5	0.51	0/897	0.80	0/1204
44	E8	0.55	0/886	0.83	0/1189
45	B5	0.49	0/749	0.85	0/1007
45	F8	0.56	0/757	0.85	2/1017 (0.2%)
46	C5	0.56	0/807	1.06	0/1076
46	G8	0.63	0/790	1.09	4/1055 (0.4%)
47	D5	0.50	2/1103 (0.2%)	0.90	7/1494 (0.5%)
47	H8	0.47	1/1395 (0.1%)	0.82	1/1890 (0.1%)
48	E5	0.56	0/611	0.84	0/814
48	I8	0.53	0/619	0.98	3/825 (0.4%)
49	F5	0.50	0/744	1.08	6/989 (0.6%)
49	J8	0.56	0/744	1.00	3/989 (0.3%)
50	G5	0.47	0/578	0.88	2/766 (0.3%)
50	K8	0.63	0/577	0.94	1/763 (0.1%)
51	H5	0.44	0/464	0.71	0/623
51	L8	0.44	0/464	0.72	0/623
52	I5	0.42	0/527	0.97	0/709
52	M8	0.48	0/486	1.07	6/652 (0.9%)
53	J5	0.46	0/448	0.82	0/606
53	N8	0.54	0/451	0.83	1/610 (0.2%)
54	L5	0.60	0/409	0.78	0/540
54	P8	0.75	0/409	0.99	3/540 (0.6%)
55	M5	0.60	0/524	1.04	4/691 (0.6%)
55	Q8	0.68	0/524	1.13	3/691 (0.4%)
56	1L	0.30	0/1592	0.46	0/2472
All	All	0.45	14/317359 (0.0%)	0.73	223/475179 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
2	12	0	5
2	1E	0	3
3	22	0	1
3	2E	0	1
4	32	0	2
4	3E	0	2
7	6E	0	1
8	72	0	2
8	7E	0	1
9	82	0	1
9	8E	0	2
10	1I	0	2
11	2A	0	2
12	3I	0	6
13	4A	0	4
13	4I	0	2
14	5A	0	5
14	5I	0	1
16	7I	0	1
17	8I	0	1
18	9I	0	1
19	AA	0	1
19	AI	0	1
20	BA	0	2
28	71	0	1
29	11	0	3
29	19	0	4
30	21	0	5
30	29	0	3
31	31	0	1
31	39	0	9
32	41	0	3
32	49	0	3
33	51	0	7
33	59	0	2
34	61	0	3
34	69	0	5
35	58	0	1
36	68	0	1
37	35	0	5
37	78	0	4
38	45	0	3
38	88	0	4

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

The worst 5 of 14 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	22	173	VAL	C-N	16.01	1.71	1.33
10	1A	38	ILE	C-N	12.34	1.62	1.33
42	85	96	ALA	CA-C	9.11	1.65	1.52
20	BI	97	ALA	C-N	8.59	1.53	1.33
3	2E	173	VAL	C-N	8.24	1.53	1.33

The worst 5 of 223 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	11	39	LYS	CA-C-N	9.98	139.66	121.70
29	11	39	LYS	C-N-CA	9.98	139.66	121.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	11	30	GLU	N-CA-C	-9.61	90.34	110.80
29	19	38	LYS	CA-C-N	9.42	139.53	121.54
29	19	38	LYS	C-N-CA	9.42	139.53	121.54

There are no chirality outliers.

5 of 180 planarity outliers are listed below:

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

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	13	32157	0	16234	741	0
1	1G	32371	0	16342	719	0
2	12	1696	0	1730	129	0
2	1E	1902	0	1949	160	0
3	22	1537	0	1603	118	0
3	2E	1605	0	1668	79	0
4	32	1702	0	1764	96	0
4	3E	1698	0	1760	130	0
5	42	1139	0	1202	89	0
5	4E	1142	0	1204	71	0
6	52	842	0	857	28	0
6	5E	837	0	852	41	0
7	62	1120	0	1167	89	0
7	6E	1242	0	1286	81	0
8	72	1107	0	1165	65	0
8	7E	1115	0	1177	94	0
9	82	953	0	983	107	0
9	8E	1000	0	1031	101	0
10	1A	646	0	662	81	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
10	1I	754	0	769	45	0
11	2A	835	0	847	44	0
11	2I	823	0	832	35	0
12	3A	956	0	1046	64	0
12	3I	956	0	1046	39	0
13	4A	893	0	946	73	0
13	4I	942	0	997	77	0
14	5A	486	0	525	66	0
14	5I	491	0	532	49	0
15	6A	729	0	768	32	0
15	6I	729	0	768	38	0
16	7A	705	0	725	59	0
16	7I	700	0	720	78	0
17	8A	823	0	891	32	0
17	8I	834	0	904	82	0
18	9A	544	0	605	26	0
18	9I	549	0	607	34	0
19	AA	481	0	468	40	0
19	AI	661	0	683	55	0
20	BA	762	0	861	48	0
20	BI	746	0	843	99	0
21	1B	188	0	195	12	0
21	1F	199	0	208	19	0
22	1K	1540	0	787	25	0
23	2K	1646	0	843	25	0
23	2L	1626	0	836	27	0
24	3K	1491	0	761	58	0
24	3L	1513	0	770	34	0
25	4K	462	0	230	12	0
25	4L	417	0	207	12	0
26	14	60535	0	30516	1089	0
26	1H	61195	0	30847	1155	0
27	16	2617	0	1328	53	0
27	1J	2617	0	1328	89	0
28	71	1033	0	1048	71	0
28	79	456	0	460	20	0
29	11	2120	0	2197	115	0
29	19	2125	0	2199	99	0
30	21	1505	0	1526	90	0
30	29	1563	0	1629	139	0
31	31	1585	0	1632	66	0
31	39	1602	0	1649	123	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
32	41	1457	0	1514	104	0
32	49	1468	0	1520	116	0
33	51	1328	0	1396	110	0
33	59	1283	0	1352	89	0
34	61	1136	0	1223	75	0
34	69	1131	0	1218	64	0
35	15	1104	0	1180	60	0
35	58	1096	0	1169	56	0
36	25	932	0	996	43	0
36	68	932	0	996	40	0
37	35	1122	0	1206	77	0
37	78	1122	0	1206	91	0
38	45	1104	0	1159	88	0
38	88	1117	0	1168	68	0
39	55	967	0	1033	46	0
39	98	967	0	1033	35	0
40	65	876	0	938	100	0
40	A8	881	0	943	59	0
41	75	1109	0	1170	75	0
41	B8	1124	0	1179	77	0
42	85	959	0	1019	60	0
42	C8	950	0	1011	83	0
43	95	770	0	838	48	0
43	D8	774	0	849	57	0
44	A5	886	0	948	38	0
44	E8	876	0	941	44	0
45	B5	735	0	785	37	0
45	F8	743	0	794	31	0
46	C5	794	0	886	84	0
46	G8	777	0	857	42	0
47	D5	1079	0	1088	87	0
47	H8	1365	0	1391	108	0
48	E5	603	0	620	36	0
48	I8	611	0	631	24	0
49	F5	737	0	813	44	0
49	J8	737	0	813	58	0
50	G5	576	0	625	35	0
50	K8	575	0	634	43	0
51	H5	459	0	512	40	0
51	L8	459	0	512	18	0
52	I5	515	0	514	48	0
52	M8	479	0	475	53	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
53	J5	434	0	454	26	0
53	N8	437	0	460	21	0
54	L5	401	0	436	14	0
54	P8	401	0	436	10	0
55	M5	516	0	582	32	0
55	Q8	516	0	582	31	0
56	1L	1469	0	752	36	0
57	11	2	0	0	0	0
57	13	148	0	0	0	0
57	14	445	0	0	0	0
57	16	11	0	0	0	0
57	19	1	0	0	0	0
57	1G	133	0	0	0	0
57	1H	548	0	0	0	0
57	1J	7	0	0	0	0
57	21	2	0	0	0	0
57	25	2	0	0	0	0
57	29	2	0	0	0	0
57	2K	4	0	0	0	0
57	2L	3	0	0	0	0
57	31	2	0	0	0	0
57	35	2	0	0	0	0
57	39	2	0	0	0	0
57	3A	1	0	0	0	0
57	3I	1	0	0	0	0
57	41	1	0	0	0	0
57	42	1	0	0	0	0
57	45	1	0	0	0	0
57	4A	1	0	0	0	0
57	4E	1	0	0	0	0
57	4K	2	0	0	0	0
57	4L	2	0	0	0	0
57	5E	1	0	0	0	0
57	5I	1	0	0	0	0
57	68	2	0	0	0	0
57	78	1	0	0	0	0
57	88	3	0	0	0	0
57	9A	1	0	0	0	0
57	B5	1	0	0	0	0
57	C5	1	0	0	0	0
57	E5	1	0	0	0	0
57	F8	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
57	I8	1	0	0	0	0
57	J8	1	0	0	0	0
57	L8	1	0	0	0	0
57	M5	1	0	0	0	0
57	P8	1	0	0	0	0
57	Q8	1	0	0	0	0
58	13	13	0	22	3	0
58	14	26	0	46	11	0
58	1G	13	0	24	0	0
58	1J	13	0	24	1	0
59	32	8	0	0	1	0
59	3E	8	0	0	3	0
60	5A	1	0	0	0	0
60	5I	1	0	0	0	0
60	C5	1	0	0	0	0
60	G8	1	0	0	0	0
61	11	16	0	0	6	0
61	13	304	0	0	17	0
61	14	1135	0	0	56	0
61	16	15	0	0	1	0
61	19	8	0	0	0	0
61	1G	391	0	0	17	0
61	1H	1133	0	0	85	0
61	1I	2	0	0	0	0
61	1J	18	0	0	1	0
61	1K	1	0	0	0	0
61	21	8	0	0	0	0
61	22	1	0	0	0	0
61	25	11	0	0	1	0
61	29	6	0	0	0	0
61	2I	1	0	0	0	0
61	2K	6	0	0	0	0
61	31	4	0	0	0	0
61	35	9	0	0	4	0
61	39	6	0	0	0	0
61	3A	1	0	0	0	0
61	3E	1	0	0	0	0
61	3I	2	0	0	0	0
61	3K	1	0	0	0	0
61	42	1	0	0	0	0
61	45	3	0	0	0	0
61	4E	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
61	4K	11	0	0	0	0
61	4L	14	0	0	1	0
61	52	3	0	0	0	0
61	55	1	0	0	0	0
61	58	1	0	0	0	0
61	5I	2	0	0	0	0
61	75	1	0	0	0	0
61	78	11	0	0	5	0
61	7A	1	0	0	0	0
61	7I	2	0	0	1	0
61	85	1	0	0	0	0
61	98	2	0	0	0	0
61	9A	3	0	0	3	0
61	A5	1	0	0	0	0
61	A8	3	0	0	1	0
61	B8	1	0	0	0	0
61	BA	2	0	0	0	0
61	C5	3	0	0	0	0
61	E5	5	0	0	0	0
61	E8	1	0	0	0	0
61	F5	3	0	0	0	0
61	F8	1	0	0	0	0
61	H5	1	0	0	0	0
61	I8	6	0	0	1	0
61	K8	1	0	0	0	0
61	L8	1	0	0	1	0
61	M5	7	0	0	1	0
61	P8	1	0	0	0	0
61	Q8	5	0	0	1	0
All	All	296743	0	197188	8943	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 19.

The worst 5 of 8943 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:22:173:VAL:C	3:22:174:PRO:N	1.71	1.45
4:3E:25:ARG:NH1	59:3E:301:SF4:S3	2.12	1.23
19:AI:3:ARG:HE	19:AI:9:VAL:HG11	1.07	1.14
44:E8:89:ALA:O	44:E8:92:ARG:NH1	1.81	1.12

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

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	12	203/256 (79%)	172 (85%)	25 (12%)	6 (3%)	3	9
2	1E	231/256 (90%)	188 (81%)	41 (18%)	2 (1%)	14	34
3	22	191/239 (80%)	167 (87%)	24 (13%)	0	100	100
3	2E	203/239 (85%)	181 (89%)	22 (11%)	0	100	100
4	32	206/209 (99%)	183 (89%)	22 (11%)	1 (0%)	24	49
4	3E	205/209 (98%)	190 (93%)	15 (7%)	0	100	100
5	42	147/162 (91%)	140 (95%)	7 (5%)	0	100	100
5	4E	147/162 (91%)	140 (95%)	6 (4%)	1 (1%)	18	40
6	52	99/101 (98%)	97 (98%)	2 (2%)	0	100	100
6	5E	98/101 (97%)	93 (95%)	5 (5%)	0	100	100
7	62	136/156 (87%)	123 (90%)	13 (10%)	0	100	100
7	6E	152/156 (97%)	140 (92%)	12 (8%)	0	100	100
8	72	135/138 (98%)	125 (93%)	7 (5%)	3 (2%)	5	15
8	7E	136/138 (99%)	124 (91%)	11 (8%)	1 (1%)	18	40
9	82	119/128 (93%)	101 (85%)	17 (14%)	1 (1%)	16	37
9	8E	124/128 (97%)	101 (82%)	19 (15%)	4 (3%)	3	8
10	1A	76/105 (72%)	70 (92%)	6 (8%)	0	100	100
10	1I	93/105 (89%)	82 (88%)	10 (11%)	1 (1%)	11	29
11	2A	111/129 (86%)	102 (92%)	7 (6%)	2 (2%)	6	19

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
11	2I	109/129 (84%)	98 (90%)	10 (9%)	1 (1%)	14	34
12	3A	120/132 (91%)	101 (84%)	14 (12%)	5 (4%)	2	5
12	3I	120/132 (91%)	106 (88%)	11 (9%)	3 (2%)	4	13
13	4A	109/126 (86%)	98 (90%)	9 (8%)	2 (2%)	6	19
13	4I	117/126 (93%)	97 (83%)	20 (17%)	0	100	100
14	5A	57/61 (93%)	48 (84%)	8 (14%)	1 (2%)	6	19
14	5I	58/61 (95%)	48 (83%)	8 (14%)	2 (3%)	3	7
15	6A	85/89 (96%)	83 (98%)	2 (2%)	0	100	100
15	6I	85/89 (96%)	81 (95%)	4 (5%)	0	100	100
16	7A	82/88 (93%)	76 (93%)	5 (6%)	1 (1%)	10	28
16	7I	81/88 (92%)	79 (98%)	2 (2%)	0	100	100
17	8A	97/105 (92%)	91 (94%)	6 (6%)	0	100	100
17	8I	98/105 (93%)	89 (91%)	7 (7%)	2 (2%)	6	16
18	9A	65/88 (74%)	61 (94%)	4 (6%)	0	100	100
18	9I	66/88 (75%)	62 (94%)	3 (4%)	1 (2%)	8	23
19	AA	56/93 (60%)	49 (88%)	5 (9%)	2 (4%)	2	6
19	AI	80/93 (86%)	67 (84%)	8 (10%)	5 (6%)	1	2
20	BA	97/106 (92%)	85 (88%)	10 (10%)	2 (2%)	5	16
20	BI	95/106 (90%)	82 (86%)	13 (14%)	0	100	100
21	1B	20/27 (74%)	19 (95%)	1 (5%)	0	100	100
21	1F	21/27 (78%)	19 (90%)	2 (10%)	0	100	100
28	7I	129/229 (56%)	116 (90%)	12 (9%)	1 (1%)	16	37
28	79	45/229 (20%)	40 (89%)	4 (9%)	1 (2%)	5	15
29	11	271/276 (98%)	241 (89%)	21 (8%)	9 (3%)	3	7
29	19	272/276 (99%)	243 (89%)	25 (9%)	4 (2%)	8	23
30	21	200/206 (97%)	154 (77%)	37 (18%)	9 (4%)	2	4
30	29	202/206 (98%)	155 (77%)	35 (17%)	12 (6%)	1	2
31	31	200/210 (95%)	179 (90%)	18 (9%)	3 (2%)	8	23
31	39	202/210 (96%)	159 (79%)	35 (17%)	8 (4%)	2	5
32	41	177/182 (97%)	156 (88%)	18 (10%)	3 (2%)	7	20
32	49	179/182 (98%)	159 (89%)	19 (11%)	1 (1%)	21	45

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
33	51	172/180 (96%)	138 (80%)	23 (13%)	11 (6%)	1	2
33	59	165/180 (92%)	129 (78%)	30 (18%)	6 (4%)	2	6
34	61	144/148 (97%)	120 (83%)	21 (15%)	3 (2%)	5	16
34	69	143/148 (97%)	113 (79%)	27 (19%)	3 (2%)	5	16
35	15	136/140 (97%)	124 (91%)	11 (8%)	1 (1%)	18	40
35	58	135/140 (96%)	115 (85%)	17 (13%)	3 (2%)	5	15
36	25	120/122 (98%)	114 (95%)	6 (5%)	0	100	100
36	68	120/122 (98%)	116 (97%)	4 (3%)	0	100	100
37	35	145/150 (97%)	117 (81%)	27 (19%)	1 (1%)	18	40
37	78	145/150 (97%)	116 (80%)	21 (14%)	8 (6%)	1	3
38	45	137/141 (97%)	115 (84%)	19 (14%)	3 (2%)	5	15
38	88	139/141 (99%)	121 (87%)	12 (9%)	6 (4%)	2	4
39	55	116/118 (98%)	109 (94%)	6 (5%)	1 (1%)	14	34
39	98	116/118 (98%)	107 (92%)	7 (6%)	2 (2%)	7	20
40	65	108/112 (96%)	91 (84%)	16 (15%)	1 (1%)	14	34
40	A8	109/112 (97%)	92 (84%)	15 (14%)	2 (2%)	6	19
41	75	131/146 (90%)	120 (92%)	8 (6%)	3 (2%)	5	14
41	B8	134/146 (92%)	120 (90%)	12 (9%)	2 (2%)	8	23
42	85	114/118 (97%)	102 (90%)	12 (10%)	0	100	100
42	C8	113/118 (96%)	105 (93%)	3 (3%)	5 (4%)	2	4
43	95	98/101 (97%)	81 (83%)	14 (14%)	3 (3%)	3	8
43	D8	98/101 (97%)	88 (90%)	8 (8%)	2 (2%)	6	16
44	A5	109/113 (96%)	103 (94%)	5 (5%)	1 (1%)	14	34
44	E8	108/113 (96%)	100 (93%)	8 (7%)	0	100	100
45	B5	92/96 (96%)	81 (88%)	9 (10%)	2 (2%)	5	15
45	F8	93/96 (97%)	87 (94%)	5 (5%)	1 (1%)	11	29
46	C5	102/110 (93%)	71 (70%)	24 (24%)	7 (7%)	1	1
46	G8	101/110 (92%)	82 (81%)	15 (15%)	4 (4%)	2	5
47	D5	127/206 (62%)	102 (80%)	21 (16%)	4 (3%)	3	8
47	H8	168/206 (82%)	132 (79%)	32 (19%)	4 (2%)	4	13
48	E5	74/85 (87%)	66 (89%)	7 (10%)	1 (1%)	9	24

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
48	I8	75/85 (88%)	68 (91%)	6 (8%)	1 (1%)	9	26
49	F5	92/98 (94%)	80 (87%)	11 (12%)	1 (1%)	11	29
49	J8	92/98 (94%)	86 (94%)	4 (4%)	2 (2%)	5	15
50	G5	67/72 (93%)	62 (92%)	2 (3%)	3 (4%)	2	4
50	K8	66/72 (92%)	60 (91%)	3 (4%)	3 (4%)	2	4
51	H5	56/60 (93%)	55 (98%)	1 (2%)	0	100	100
51	L8	56/60 (93%)	51 (91%)	5 (9%)	0	100	100
52	I5	61/71 (86%)	28 (46%)	28 (46%)	5 (8%)	0	1
52	M8	57/71 (80%)	39 (68%)	13 (23%)	5 (9%)	0	1
53	J5	54/60 (90%)	50 (93%)	4 (7%)	0	100	100
53	N8	54/60 (90%)	49 (91%)	5 (9%)	0	100	100
54	L5	45/49 (92%)	42 (93%)	3 (7%)	0	100	100
54	P8	45/49 (92%)	43 (96%)	2 (4%)	0	100	100
55	M5	62/65 (95%)	54 (87%)	6 (10%)	2 (3%)	3	8
55	Q8	62/65 (95%)	52 (84%)	7 (11%)	3 (5%)	2	3
All	All	11163/12404 (90%)	9756 (87%)	1192 (11%)	215 (2%)	6	17

5 of 215 Ramachandran outliers are listed below:

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

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	12	179/220 (81%)	136 (76%)	43 (24%)	1	1

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	1E	202/220 (92%)	152 (75%)	50 (25%)	1	1
3	22	154/188 (82%)	115 (75%)	39 (25%)	0	1
3	2E	159/188 (85%)	123 (77%)	36 (23%)	1	2
4	32	180/181 (99%)	151 (84%)	29 (16%)	2	7
4	3E	180/181 (99%)	141 (78%)	39 (22%)	1	2
5	42	114/123 (93%)	85 (75%)	29 (25%)	0	1
5	4E	115/123 (94%)	88 (76%)	27 (24%)	1	1
6	52	90/90 (100%)	78 (87%)	12 (13%)	4	12
6	5E	90/90 (100%)	80 (89%)	10 (11%)	6	17
7	62	114/127 (90%)	88 (77%)	26 (23%)	1	2
7	6E	125/127 (98%)	100 (80%)	25 (20%)	1	3
8	72	118/119 (99%)	92 (78%)	26 (22%)	1	2
8	7E	119/119 (100%)	84 (71%)	35 (29%)	0	0
9	82	92/99 (93%)	63 (68%)	29 (32%)	0	0
9	8E	97/99 (98%)	76 (78%)	21 (22%)	1	2
10	1A	71/92 (77%)	50 (70%)	21 (30%)	0	0
10	1I	81/92 (88%)	65 (80%)	16 (20%)	1	3
11	2A	85/99 (86%)	65 (76%)	20 (24%)	1	1
11	2I	84/99 (85%)	67 (80%)	17 (20%)	1	3
12	3A	103/109 (94%)	83 (81%)	20 (19%)	1	3
12	3I	103/109 (94%)	90 (87%)	13 (13%)	4	13
13	4A	91/101 (90%)	63 (69%)	28 (31%)	0	0
13	4I	94/101 (93%)	73 (78%)	21 (22%)	1	2
14	5A	49/50 (98%)	29 (59%)	20 (41%)	0	0
14	5I	49/50 (98%)	36 (74%)	13 (26%)	0	1
15	6A	79/80 (99%)	69 (87%)	10 (13%)	4	13
15	6I	79/80 (99%)	69 (87%)	10 (13%)	4	13
16	7A	72/74 (97%)	60 (83%)	12 (17%)	2	6
16	7I	72/74 (97%)	58 (81%)	14 (19%)	1	3
17	8A	94/97 (97%)	76 (81%)	18 (19%)	1	3
17	8I	95/97 (98%)	71 (75%)	24 (25%)	0	1

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
18	9A	58/77 (75%)	43 (74%)	15 (26%)	0	1
18	9I	58/77 (75%)	42 (72%)	16 (28%)	0	0
19	AA	52/80 (65%)	40 (77%)	12 (23%)	1	2
19	AI	72/80 (90%)	60 (83%)	12 (17%)	2	6
20	BA	76/82 (93%)	56 (74%)	20 (26%)	0	1
20	BI	75/82 (92%)	54 (72%)	21 (28%)	0	0
21	1B	17/22 (77%)	13 (76%)	4 (24%)	1	1
21	1F	18/22 (82%)	15 (83%)	3 (17%)	2	6
28	71	109/181 (60%)	85 (78%)	24 (22%)	1	2
28	79	48/181 (26%)	34 (71%)	14 (29%)	0	0
29	11	214/218 (98%)	177 (83%)	37 (17%)	2	5
29	19	214/218 (98%)	175 (82%)	39 (18%)	2	4
30	21	155/166 (93%)	119 (77%)	36 (23%)	1	2
30	29	165/166 (99%)	138 (84%)	27 (16%)	2	7
31	31	161/166 (97%)	135 (84%)	26 (16%)	2	7
31	39	163/166 (98%)	126 (77%)	37 (23%)	1	2
32	41	153/156 (98%)	125 (82%)	28 (18%)	2	4
32	49	153/156 (98%)	113 (74%)	40 (26%)	0	1
33	51	143/148 (97%)	102 (71%)	41 (29%)	0	0
33	59	139/148 (94%)	108 (78%)	31 (22%)	1	2
34	61	122/124 (98%)	98 (80%)	24 (20%)	1	3
34	69	122/124 (98%)	93 (76%)	29 (24%)	1	1
35	15	117/119 (98%)	95 (81%)	22 (19%)	1	4
35	58	116/119 (98%)	97 (84%)	19 (16%)	2	7
36	25	100/100 (100%)	75 (75%)	25 (25%)	0	1
36	68	100/100 (100%)	87 (87%)	13 (13%)	4	12
37	35	114/116 (98%)	87 (76%)	27 (24%)	1	1
37	78	114/116 (98%)	89 (78%)	25 (22%)	1	2
38	45	109/111 (98%)	81 (74%)	28 (26%)	0	1
38	88	110/111 (99%)	91 (83%)	19 (17%)	2	5
39	55	101/101 (100%)	82 (81%)	19 (19%)	1	4

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
39	98	101/101 (100%)	85 (84%)	16 (16%)	2	8
40	65	87/88 (99%)	54 (62%)	33 (38%)	0	0
40	A8	87/88 (99%)	72 (83%)	15 (17%)	2	5
41	75	117/127 (92%)	92 (79%)	25 (21%)	1	2
41	B8	117/127 (92%)	86 (74%)	31 (26%)	0	1
42	85	93/94 (99%)	75 (81%)	18 (19%)	1	3
42	C8	92/94 (98%)	77 (84%)	15 (16%)	2	7
43	95	81/82 (99%)	57 (70%)	24 (30%)	0	0
43	D8	82/82 (100%)	58 (71%)	24 (29%)	0	0
44	A5	91/92 (99%)	71 (78%)	20 (22%)	1	2
44	E8	90/92 (98%)	76 (84%)	14 (16%)	2	8
45	B5	74/78 (95%)	58 (78%)	16 (22%)	1	2
45	F8	75/78 (96%)	63 (84%)	12 (16%)	2	8
46	C5	85/91 (93%)	61 (72%)	24 (28%)	0	0
46	G8	83/91 (91%)	65 (78%)	18 (22%)	1	2
47	D5	118/179 (66%)	87 (74%)	31 (26%)	0	1
47	H8	151/179 (84%)	110 (73%)	41 (27%)	0	0
48	E5	61/67 (91%)	54 (88%)	7 (12%)	5	16
48	I8	62/67 (92%)	46 (74%)	16 (26%)	0	1
49	F5	79/83 (95%)	62 (78%)	17 (22%)	1	2
49	J8	79/83 (95%)	60 (76%)	19 (24%)	1	1
50	G5	63/67 (94%)	41 (65%)	22 (35%)	0	0
50	K8	64/67 (96%)	46 (72%)	18 (28%)	0	0
51	H5	50/52 (96%)	35 (70%)	15 (30%)	0	0
51	L8	50/52 (96%)	39 (78%)	11 (22%)	1	2
52	I5	57/63 (90%)	41 (72%)	16 (28%)	0	0
52	M8	52/63 (82%)	32 (62%)	20 (38%)	0	0
53	J5	48/52 (92%)	35 (73%)	13 (27%)	0	0
53	N8	49/52 (94%)	39 (80%)	10 (20%)	1	3
54	L5	38/42 (90%)	31 (82%)	7 (18%)	1	4
54	P8	38/42 (90%)	32 (84%)	6 (16%)	2	8

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
55	M5	54/55 (98%)	43 (80%)	11 (20%)	1	3
55	Q8	54/55 (98%)	45 (83%)	9 (17%)	2	6
All	All	9419/10256 (92%)	7339 (78%)	2080 (22%)	1	2

5 of 2080 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
42	85	100	VAL
45	B5	54	VAL
42	85	95	LEU
42	C8	8	VAL
41	B8	49	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 58 such sidechains are listed below:

Mol	Chain	Res	Type
50	K8	46	GLN
44	A5	40	ASN
11	2A	117	ASN
43	95	80	GLN
32	49	130	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	13	1493/1522 (98%)	349 (23%)	34 (2%)
1	1G	1505/1522 (98%)	326 (21%)	33 (2%)
22	1K	70/76 (92%)	38 (54%)	4 (5%)
23	2K	76/77 (98%)	20 (26%)	1 (1%)
23	2L	75/77 (97%)	10 (13%)	2 (2%)
24	3K	67/76 (88%)	37 (55%)	3 (4%)
24	3L	69/76 (90%)	32 (46%)	1 (1%)
25	4K	20/30 (66%)	13 (65%)	2 (10%)
25	4L	18/30 (60%)	10 (55%)	2 (11%)
26	14	2804/2917 (96%)	643 (22%)	37 (1%)
26	1H	2836/2917 (97%)	594 (20%)	43 (1%)
27	16	121/122 (99%)	24 (19%)	0
27	1J	121/122 (99%)	34 (28%)	2 (1%)
56	1L	65/76 (85%)	24 (36%)	2 (3%)

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Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
All	All	9340/9640 (96%)	2154 (23%)	166 (1%)

5 of 2154 RNA backbone outliers are listed below:

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

5 of 166 RNA pucker outliers are listed below:

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

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
23	OMC	2K	33	23	19,22,23	1.81	3 (15%)	26,31,34	1.09	3 (11%)
23	5MU	2L	55	23	19,22,23	3.93	5 (26%)	28,32,35	3.04	9 (32%)
56	PSU	1L	55	56	18,21,22	1.38	1 (5%)	22,30,33	1.51	4 (18%)
23	PSU	2L	56	23	18,21,22	1.14	1 (5%)	22,30,33	1.58	2 (9%)
22	CM0	1K	34	22	22,26,27	3.97	7 (31%)	28,37,40	1.54	4 (14%)
23	7MG	2L	47	23	22,26,27	2.83	8 (36%)	29,39,42	3.00	10 (34%)
23	7MG	2K	47	23	22,26,27	3.09	6 (27%)	29,39,42	2.81	11 (37%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
22	6MZ	1K	37	22	22,25,26	3.00	5 (22%)	30,36,39	2.61	11 (36%)
23	4SU	2K	8	23	18,21,22	1.91	3 (16%)	26,30,33	2.56	4 (15%)
23	4SU	2L	8	23	18,21,22	1.94	3 (16%)	26,30,33	2.59	4 (15%)
23	OMC	2L	33	23	19,22,23	1.80	4 (21%)	26,31,34	1.03	1 (3%)
23	5MU	2K	55	23,57	19,22,23	3.85	5 (26%)	28,32,35	3.22	8 (28%)
56	5MU	1L	54	56	19,22,23	3.87	5 (26%)	28,32,35	3.17	9 (32%)
22	H2U	1K	17	22	18,21,22	2.13	4 (22%)	21,30,33	2.38	5 (23%)
23	PSU	2K	56	23	18,21,22	1.16	2 (11%)	22,30,33	2.02	4 (18%)
22	5MU	1K	54	22	19,22,23	3.90	5 (26%)	28,32,35	2.99	7 (25%)
22	PSU	1K	55	22	18,21,22	1.36	1 (5%)	22,30,33	1.75	4 (18%)

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

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

The worst 5 of 68 bond length outliers are listed below:

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

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

The worst 5 of 100 bond angle outliers are listed below:

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

There are no chirality outliers.

5 of 16 torsion outliers are listed below:

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

There are no ring outliers.

13 monomers are involved in 21 short contacts:

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

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

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

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

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
58	SPE	14	3445	26	-	6/10/10/10	-
58	SPE	14	3446	-	-	5/10/10/10	-
59	SF4	32	301	4	-	-	0/6/5/5
58	SPE	1G	1733	-	-	4/10/10/10	-
58	SPE	1J	208	-	-	5/10/10/10	-
59	SF4	3E	301	4	-	-	0/6/5/5
58	SPE	13	1748	1	-	7/10/10/10	-

There are no bond length outliers.

All (2) bond angle outliers are listed below:

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

There are no chirality outliers.

5 of 27 torsion outliers are listed below:

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

There are no ring outliers.

6 monomers are involved in 19 short contacts:

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

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

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

All chain breaks are listed below:

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

6 Fit of model and data ⓘ

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, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	13	1496/1522 (98%)	-0.14	14 (0%) 81 76	57, 98, 164, 235	0
1	1G	1506/1522 (98%)	-0.01	24 (1%) 70 63	68, 105, 166, 238	0
2	12	207/256 (80%)	0.92	24 (11%) 9 8	121, 148, 168, 185	0
2	1E	235/256 (91%)	0.61	9 (3%) 44 36	108, 135, 160, 171	0
3	22	195/239 (81%)	0.94	21 (10%) 11 10	113, 131, 152, 164	0
3	2E	205/239 (85%)	0.30	2 (0%) 79 74	85, 107, 142, 149	0
4	32	208/209 (99%)	0.38	4 (1%) 66 58	84, 101, 123, 132	0
4	3E	207/209 (99%)	0.64	12 (5%) 29 24	77, 103, 125, 132	0
5	42	149/162 (91%)	0.62	4 (2%) 56 48	91, 111, 128, 149	0
5	4E	149/162 (91%)	0.50	3 (2%) 65 57	79, 98, 118, 135	0
6	52	101/101 (100%)	0.01	0 100 100	81, 97, 110, 131	0
6	5E	100/101 (99%)	0.20	1 (1%) 79 74	83, 99, 113, 123	0
7	62	140/156 (89%)	0.54	14 (10%) 12 11	103, 119, 131, 138	0
7	6E	154/156 (98%)	0.36	8 (5%) 33 28	98, 113, 138, 162	0
8	72	137/138 (99%)	0.65	4 (2%) 53 46	90, 114, 125, 128	0
8	7E	138/138 (100%)	0.66	5 (3%) 46 38	87, 102, 113, 120	0
9	82	121/128 (94%)	1.48	24 (19%) 3 3	101, 144, 160, 164	0
9	8E	126/128 (98%)	0.76	8 (6%) 26 22	84, 133, 153, 157	0
10	1A	80/105 (76%)	1.70	31 (38%) 1 0	111, 138, 152, 156	0
10	1I	95/105 (90%)	0.58	4 (4%) 40 33	80, 127, 155, 159	0
11	2A	113/129 (87%)	0.60	10 (8%) 15 14	78, 103, 117, 120	0
11	2I	111/129 (86%)	0.54	5 (4%) 38 31	70, 99, 115, 125	0
12	3A	122/132 (92%)	1.01	20 (16%) 4 4	74, 91, 116, 132	0
12	3I	122/132 (92%)	0.31	9 (7%) 20 18	65, 76, 103, 112	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
13	4A	111/126 (88%)	0.66	10 (9%) 15 13	102, 129, 143, 152	0
13	4I	119/126 (94%)	0.66	15 (12%) 8 7	87, 111, 129, 139	0
14	5A	59/61 (96%)	2.04	25 (42%) 0 0	118, 129, 141, 142	0
14	5I	60/61 (98%)	0.67	3 (5%) 34 28	83, 97, 112, 119	0
15	6A	87/89 (97%)	0.01	1 (1%) 78 73	79, 100, 115, 117	0
15	6I	87/89 (97%)	0.19	3 (3%) 48 41	75, 94, 109, 116	0
16	7A	84/88 (95%)	0.47	3 (3%) 46 38	85, 98, 119, 145	0
16	7I	83/88 (94%)	1.37	23 (27%) 1 1	91, 107, 132, 147	0
17	8A	99/105 (94%)	0.50	5 (5%) 33 28	89, 100, 117, 120	0
17	8I	100/105 (95%)	0.65	8 (8%) 18 16	81, 98, 108, 115	0
18	9A	67/88 (76%)	0.35	1 (1%) 72 65	87, 101, 125, 129	0
18	9I	68/88 (77%)	0.33	2 (2%) 53 46	85, 100, 125, 128	0
19	AA	62/93 (66%)	1.13	7 (11%) 10 9	118, 142, 155, 158	0
19	AI	82/93 (88%)	0.42	3 (3%) 45 37	95, 110, 128, 136	0
20	BA	99/106 (93%)	0.54	5 (5%) 33 28	85, 104, 128, 140	0
20	BI	97/106 (91%)	1.04	13 (13%) 7 7	103, 117, 138, 145	0
21	1B	22/27 (81%)	1.44	7 (31%) 1 1	110, 116, 124, 134	0
21	1F	23/27 (85%)	0.40	1 (4%) 40 32	90, 98, 106, 108	0
22	1K	67/76 (88%)	0.54	4 (5%) 27 23	80, 167, 196, 203	0
23	2K	72/77 (93%)	0.15	1 (1%) 73 67	68, 89, 116, 129	0
23	2L	71/77 (92%)	0.20	1 (1%) 73 67	78, 100, 132, 145	0
24	3K	70/76 (92%)	1.26	14 (20%) 3 3	71, 198, 222, 224	0
24	3L	71/76 (93%)	0.86	11 (15%) 5 5	78, 191, 215, 218	0
25	4K	21/30 (70%)	1.37	8 (38%) 1 0	69, 129, 212, 213	0
25	4L	19/30 (63%)	1.35	7 (36%) 1 1	85, 144, 210, 210	0
26	14	2810/2917 (96%)	-0.36	18 (0%) 85 82	54, 81, 180, 237	0
26	1H	2841/2917 (97%)	-0.49	10 (0%) 88 86	44, 70, 166, 244	0
27	16	122/122 (100%)	-0.45	0 100 100	65, 87, 105, 180	0
27	1J	122/122 (100%)	-0.07	3 (2%) 58 50	79, 106, 125, 185	0
28	71	133/229 (58%)	0.76	11 (8%) 17 15	136, 194, 219, 229	0
28	79	57/229 (24%)	1.92	24 (42%) 0 0	136, 178, 198, 205	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
29	11	273/276 (98%)	0.12	7 (2%) 57 49	44, 62, 78, 94	0
29	19	274/276 (99%)	0.44	23 (8%) 17 15	50, 72, 87, 102	0
30	21	202/206 (98%)	0.45	13 (6%) 25 21	49, 82, 115, 123	0
30	29	204/206 (99%)	0.56	16 (7%) 19 17	57, 88, 124, 135	0
31	31	202/210 (96%)	0.00	2 (0%) 79 74	46, 75, 108, 123	0
31	39	204/210 (97%)	0.26	5 (2%) 58 50	57, 95, 139, 164	0
32	41	179/182 (98%)	0.57	10 (5%) 30 25	75, 95, 124, 138	0
32	49	181/182 (99%)	0.55	7 (3%) 43 35	99, 118, 142, 156	0
33	51	174/180 (96%)	0.46	8 (4%) 37 31	76, 99, 116, 128	0
33	59	167/180 (92%)	1.65	49 (29%) 1 1	123, 190, 216, 225	0
34	61	146/148 (98%)	0.43	6 (4%) 41 34	75, 119, 134, 148	0
34	69	145/148 (97%)	0.60	10 (6%) 23 19	80, 115, 138, 144	0
35	15	138/140 (98%)	1.00	12 (8%) 16 14	76, 98, 124, 139	0
35	58	137/140 (97%)	0.54	6 (4%) 39 32	64, 84, 113, 134	0
36	25	122/122 (100%)	0.27	1 (0%) 82 78	68, 81, 97, 107	0
36	68	122/122 (100%)	0.12	1 (0%) 82 78	57, 72, 87, 93	0
37	35	147/150 (98%)	0.53	9 (6%) 27 22	58, 93, 121, 133	0
37	78	147/150 (98%)	0.23	6 (4%) 41 34	46, 77, 98, 106	0
38	45	139/141 (98%)	0.45	9 (6%) 25 21	70, 94, 112, 126	0
38	88	141/141 (100%)	-0.02	1 (0%) 84 80	57, 74, 97, 117	0
39	55	118/118 (100%)	0.17	2 (1%) 69 62	61, 77, 92, 109	0
39	98	118/118 (100%)	0.27	2 (1%) 69 62	58, 76, 94, 104	0
40	65	110/112 (98%)	0.66	5 (4%) 38 31	82, 100, 119, 130	0
40	A8	111/112 (99%)	0.17	2 (1%) 67 59	73, 86, 104, 112	0
41	75	133/146 (91%)	0.48	4 (3%) 52 45	76, 88, 117, 142	0
41	B8	136/146 (93%)	0.36	8 (5%) 28 23	66, 83, 121, 152	0
42	85	116/118 (98%)	0.46	4 (3%) 48 41	65, 91, 116, 123	0
42	C8	115/118 (97%)	0.32	2 (1%) 69 62	57, 75, 96, 106	0
43	95	100/101 (99%)	0.73	7 (7%) 22 19	65, 108, 126, 132	0
43	D8	100/101 (99%)	0.53	7 (7%) 22 19	56, 92, 111, 125	0
44	A5	111/113 (98%)	0.11	0 100 100	62, 73, 95, 128	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
44	E8	110/113 (97%)	0.18	4 (3%) 46 38	57, 69, 90, 101	0
45	B5	94/96 (97%)	0.57	5 (5%) 32 27	66, 80, 103, 111	0
45	F8	95/96 (98%)	0.24	0 100 100	50, 66, 91, 99	0
46	C5	104/110 (94%)	1.62	32 (30%) 1 1	84, 110, 143, 150	0
46	G8	103/110 (93%)	0.62	8 (7%) 19 17	74, 91, 118, 125	0
47	D5	133/206 (64%)	0.51	5 (3%) 44 36	93, 123, 150, 159	0
47	H8	170/206 (82%)	0.28	2 (1%) 76 71	77, 112, 191, 198	0
48	E5	76/85 (89%)	0.61	8 (10%) 11 10	58, 82, 94, 108	0
48	I8	77/85 (90%)	0.22	4 (5%) 33 28	54, 70, 87, 98	0
49	F5	94/98 (95%)	0.70	7 (7%) 20 18	61, 76, 117, 123	0
49	J8	94/98 (95%)	0.56	6 (6%) 25 21	49, 70, 115, 135	0
50	G5	69/72 (95%)	0.46	3 (4%) 40 32	77, 96, 113, 130	0
50	K8	68/72 (94%)	0.06	1 (1%) 72 65	60, 76, 94, 124	0
51	H5	58/60 (96%)	0.56	3 (5%) 33 28	73, 90, 118, 123	0
51	L8	58/60 (96%)	0.21	1 (1%) 69 62	59, 75, 94, 101	0
52	I5	63/71 (88%)	0.77	7 (11%) 10 9	132, 174, 191, 195	0
52	M8	61/71 (85%)	1.07	8 (13%) 7 7	96, 137, 167, 174	0
53	J5	56/60 (93%)	0.44	3 (5%) 31 26	57, 81, 130, 140	0
53	N8	56/60 (93%)	0.48	7 (12%) 8 7	50, 83, 145, 155	0
54	L5	47/49 (95%)	0.17	4 (8%) 16 15	51, 61, 82, 96	0
54	P8	47/49 (95%)	-0.10	2 (4%) 40 32	44, 53, 68, 89	0
55	M5	64/65 (98%)	0.62	3 (4%) 36 30	64, 76, 89, 114	0
55	Q8	64/65 (98%)	0.23	2 (3%) 51 44	52, 64, 78, 91	0
56	1L	67/76 (88%)	0.70	6 (8%) 15 13	98, 180, 207, 210	0
All	All	20742/22044 (94%)	0.18	882 (4%) 40 32	44, 93, 167, 244	0

The worst 5 of 882 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
33	59	131	VAL	9.3
14	5A	38	GLY	8.5
9	82	115	GLY	7.7
30	29	76	ARG	7.3
10	1A	63	PHE	7.2

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

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
22	H2U	1K	17	20/21	0.71	0.09	119,145,154,154	0
23	7MG	2L	47	24/25	0.72	0.15	92,112,117,118	0
56	PSU	1L	55	20/21	0.73	0.10	118,133,146,147	0
22	PSU	1K	55	20/21	0.76	0.11	102,116,131,132	0
56	5MU	1L	54	21/22	0.83	0.08	117,124,131,143	0
23	OMC	2L	33	21/22	0.83	0.16	83,94,97,100	0
23	PSU	2L	56	20/21	0.87	0.09	105,114,120,120	0
22	5MU	1K	54	21/22	0.87	0.07	100,106,117,129	0
23	PSU	2K	56	20/21	0.87	0.08	93,98,106,114	0
23	5MU	2L	55	21/22	0.88	0.08	111,115,122,127	0
23	5MU	2K	55	21/22	0.89	0.10	99,102,106,113	0
23	4SU	2L	8	20/21	0.90	0.08	104,106,109,112	0
23	4SU	2K	8	20/21	0.94	0.10	84,88,92,94	0
23	7MG	2K	47	24/25	0.94	0.09	90,98,109,111	0
22	CM0	1K	34	25/26	0.94	0.10	72,89,106,107	0
23	OMC	2K	33	21/22	0.96	0.12	72,79,82,89	0
22	6MZ	1K	37	23/24	0.98	0.06	61,79,86,90	0

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
57	MG	1G	1653	1/1	0.11	0.35	103,103,103,103	0
57	MG	14	3189	1/1	0.48	0.27	85,85,85,85	0
57	MG	1G	1604	1/1	0.49	0.40	103,103,103,103	0
57	MG	1H	3322	1/1	0.51	0.29	100,100,100,100	0
57	MG	1H	3235	1/1	0.51	0.26	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	1630	1/1	0.52	0.43	106,106,106,106	0
57	MG	13	1690	1/1	0.55	0.44	100,100,100,100	0
57	MG	1H	3104	1/1	0.55	0.31	88,88,88,88	0
57	MG	1H	3233	1/1	0.55	0.25	110,110,110,110	0
57	MG	14	3173	1/1	0.56	0.27	98,98,98,98	0
57	MG	1H	3227	1/1	0.57	0.22	79,79,79,79	0
57	MG	1H	3283	1/1	0.57	0.26	146,146,146,146	0
57	MG	1H	3247	1/1	0.58	0.33	101,101,101,101	0
57	MG	1H	3058	1/1	0.58	0.31	77,77,77,77	0
57	MG	1H	3120	1/1	0.59	0.41	96,96,96,96	0
57	MG	13	1645	1/1	0.59	0.20	78,78,78,78	0
57	MG	1H	3006	1/1	0.59	0.17	71,71,71,71	0
57	MG	14	3225	1/1	0.59	0.20	95,95,95,95	0
57	MG	14	3031	1/1	0.60	0.30	86,86,86,86	0
57	MG	1G	1644	1/1	0.61	0.37	107,107,107,107	0
57	MG	1G	1615	1/1	0.61	0.37	91,91,91,91	0
57	MG	1H	3155	1/1	0.61	0.32	91,91,91,91	0
57	MG	1G	1650	1/1	0.62	0.22	114,114,114,114	0
57	MG	1H	3248	1/1	0.62	0.43	96,96,96,96	0
57	MG	13	1646	1/1	0.63	0.37	97,97,97,97	0
57	MG	1H	3206	1/1	0.64	0.31	91,91,91,91	0
57	MG	1H	3205	1/1	0.65	0.22	90,90,90,90	0
57	MG	1G	1710	1/1	0.65	0.20	102,102,102,102	0
57	MG	1H	3118	1/1	0.65	0.27	83,83,83,83	0
57	MG	1H	3224	1/1	0.65	0.40	90,90,90,90	0
57	MG	13	1654	1/1	0.65	0.11	113,113,113,113	0
57	MG	13	1660	1/1	0.65	0.52	96,96,96,96	0
57	MG	14	3110	1/1	0.66	0.36	72,72,72,72	0
57	MG	13	1653	1/1	0.66	0.46	94,94,94,94	0
57	MG	13	1677	1/1	0.67	0.40	92,92,92,92	0
57	MG	2K	103	1/1	0.67	0.30	89,89,89,89	0
57	MG	1H	3260	1/1	0.68	0.45	98,98,98,98	0
57	MG	1H	3188	1/1	0.68	0.53	95,95,95,95	0
57	MG	14	3166	1/1	0.68	0.38	82,82,82,82	0
57	MG	1H	3246	1/1	0.68	0.23	72,72,72,72	0
57	MG	13	1686	1/1	0.68	0.31	104,104,104,104	0
57	MG	14	3224	1/1	0.68	0.23	113,113,113,113	0
57	MG	1H	3077	1/1	0.68	0.18	56,56,56,56	0
57	MG	1H	3161	1/1	0.69	0.36	93,93,93,93	0
57	MG	13	1687	1/1	0.69	0.41	82,82,82,82	0
57	MG	14	3190	1/1	0.69	0.27	79,79,79,79	0
57	MG	1H	3217	1/1	0.69	0.35	80,80,80,80	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	0.69	0.37	88,88,88,88	0
57	MG	13	1635	1/1	0.70	0.21	99,99,99,99	0
57	MG	14	3158	1/1	0.70	0.34	76,76,76,76	0
57	MG	1H	3295	1/1	0.70	0.17	70,70,70,70	0
57	MG	1G	1623	1/1	0.70	0.38	75,75,75,75	0
57	MG	14	3229	1/1	0.70	0.33	90,90,90,90	0
57	MG	1G	1608	1/1	0.71	0.17	111,111,111,111	0
57	MG	14	3101	1/1	0.71	0.29	90,90,90,90	0
57	MG	13	1668	1/1	0.71	0.21	121,121,121,121	0
57	MG	1H	3115	1/1	0.71	0.40	84,84,84,84	0
57	MG	1H	3282	1/1	0.71	0.32	89,89,89,89	0
57	MG	13	1656	1/1	0.71	0.31	87,87,87,87	0
57	MG	1H	3061	1/1	0.71	0.27	76,76,76,76	0
57	MG	1H	3321	1/1	0.71	0.37	90,90,90,90	0
57	MG	13	1622	1/1	0.71	0.38	74,74,74,74	0
57	MG	1H	3218	1/1	0.71	0.23	81,81,81,81	0
57	MG	14	3030	1/1	0.71	0.34	89,89,89,89	0
57	MG	1J	201	1/1	0.71	0.30	86,86,86,86	0
57	MG	1G	1635	1/1	0.72	0.24	102,102,102,102	0
57	MG	13	1603	1/1	0.72	0.23	116,116,116,116	0
57	MG	13	1682	1/1	0.72	0.34	85,85,85,85	0
57	MG	1H	3296	1/1	0.72	0.34	81,81,81,81	0
57	MG	1H	3276	1/1	0.72	0.33	90,90,90,90	0
57	MG	14	3217	1/1	0.72	0.16	77,77,77,77	0
57	MG	1G	1617	1/1	0.72	0.29	86,86,86,86	0
57	MG	13	1670	1/1	0.72	0.21	100,100,100,100	0
57	MG	1G	1624	1/1	0.72	0.41	76,76,76,76	0
57	MG	16	201	1/1	0.72	0.25	83,83,83,83	0
57	MG	29	301	1/1	0.72	0.29	75,75,75,75	0
57	MG	39	302	1/1	0.72	0.25	67,67,67,67	0
57	MG	14	3174	1/1	0.73	0.25	83,83,83,83	0
57	MG	1H	3274	1/1	0.73	0.43	83,83,83,83	0
57	MG	14	3023	1/1	0.73	0.36	82,82,82,82	0
57	MG	14	3214	1/1	0.73	0.45	93,93,93,93	0
57	MG	14	3216	1/1	0.73	0.20	106,106,106,106	0
57	MG	13	1614	1/1	0.73	0.29	88,88,88,88	0
57	MG	14	3220	1/1	0.73	0.32	73,73,73,73	0
57	MG	1H	3080	1/1	0.73	0.39	103,103,103,103	0
57	MG	1H	3170	1/1	0.73	0.27	79,79,79,79	0
57	MG	1H	3183	1/1	0.73	0.21	73,73,73,73	0
57	MG	14	3394	1/1	0.73	0.14	63,63,63,63	0
57	MG	1H	3185	1/1	0.73	0.36	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	13	1678	1/1	0.73	0.26	94,94,94,94	0
57	MG	1G	1661	1/1	0.73	0.29	99,99,99,99	0
57	MG	14	3199	1/1	0.74	0.28	68,68,68,68	0
57	MG	13	1636	1/1	0.74	0.25	103,103,103,103	0
57	MG	13	1669	1/1	0.74	0.33	92,92,92,92	0
57	MG	14	3138	1/1	0.74	0.30	86,86,86,86	0
57	MG	1H	3008	1/1	0.74	0.44	75,75,75,75	0
57	MG	14	3164	1/1	0.74	0.24	80,80,80,80	0
57	MG	1G	1680	1/1	0.74	0.19	91,91,91,91	0
57	MG	14	3226	1/1	0.74	0.39	83,83,83,83	0
57	MG	13	1683	1/1	0.74	0.27	72,72,72,72	0
57	MG	4E	201	1/1	0.74	0.46	85,85,85,85	0
57	MG	14	3177	1/1	0.74	0.28	82,82,82,82	0
57	MG	2K	102	1/1	0.74	0.31	92,92,92,92	0
57	MG	1G	1647	1/1	0.74	0.30	102,102,102,102	0
57	MG	1H	3239	1/1	0.75	0.41	92,92,92,92	0
57	MG	1H	3315	1/1	0.75	0.31	99,99,99,99	0
57	MG	14	3014	1/1	0.75	0.19	62,62,62,62	0
57	MG	1G	1629	1/1	0.75	0.36	97,97,97,97	0
57	MG	J8	101	1/1	0.75	0.46	79,79,79,79	0
57	MG	13	1675	1/1	0.75	0.21	104,104,104,104	0
57	MG	14	3035	1/1	0.75	0.34	79,79,79,79	0
57	MG	14	3097	1/1	0.75	0.38	90,90,90,90	0
57	MG	1H	3269	1/1	0.76	0.43	86,86,86,86	0
57	MG	14	3178	1/1	0.76	0.48	92,92,92,92	0
57	MG	1H	3523	1/1	0.76	0.21	84,84,84,84	0
57	MG	13	1649	1/1	0.76	0.20	72,72,72,72	0
57	MG	13	1662	1/1	0.76	0.15	76,76,76,76	0
57	MG	14	3058	1/1	0.76	0.21	83,83,83,83	0
57	MG	14	3081	1/1	0.76	0.36	81,81,81,81	0
57	MG	13	1625	1/1	0.76	0.36	93,93,93,93	0
57	MG	1H	3078	1/1	0.76	0.26	79,79,79,79	0
57	MG	1G	1652	1/1	0.76	0.36	94,94,94,94	0
57	MG	1H	3286	1/1	0.76	0.33	87,87,87,87	0
57	MG	1H	3133	1/1	0.76	0.43	78,78,78,78	0
57	MG	1H	3010	1/1	0.76	0.23	78,78,78,78	0
57	MG	1H	3086	1/1	0.76	0.29	66,66,66,66	0
57	MG	14	3170	1/1	0.76	0.29	87,87,87,87	0
57	MG	1G	1712	1/1	0.76	0.10	142,142,142,142	0
57	MG	1H	3103	1/1	0.76	0.33	82,82,82,82	0
57	MG	1H	3212	1/1	0.77	0.18	65,65,65,65	0
57	MG	14	3198	1/1	0.77	0.24	86,86,86,86	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	1H	3535	1/1	0.77	0.18	93,93,93,93	0
57	MG	1H	3214	1/1	0.77	0.36	86,86,86,86	0
57	MG	16	206	1/1	0.77	0.27	77,77,77,77	0
57	MG	2L	103	1/1	0.77	0.28	75,75,75,75	0
57	MG	1H	3094	1/1	0.77	0.36	68,68,68,68	0
57	MG	1H	3095	1/1	0.77	0.25	69,69,69,69	0
57	MG	1H	3125	1/1	0.77	0.25	63,63,63,63	0
57	MG	13	1679	1/1	0.77	0.33	86,86,86,86	0
57	MG	13	1676	1/1	0.77	0.41	92,92,92,92	0
57	MG	1H	3031	1/1	0.77	0.36	74,74,74,74	0
57	MG	14	3063	1/1	0.77	0.23	52,52,52,52	0
57	MG	14	3074	1/1	0.77	0.24	81,81,81,81	0
57	MG	14	3077	1/1	0.77	0.27	84,84,84,84	0
57	MG	35	201	1/1	0.77	0.21	86,86,86,86	0
57	MG	13	1671	1/1	0.78	0.40	91,91,91,91	0
57	MG	14	3218	1/1	0.78	0.18	84,84,84,84	0
57	MG	1H	3250	1/1	0.78	0.45	93,93,93,93	0
57	MG	13	1606	1/1	0.78	0.26	77,77,77,77	0
57	MG	14	3104	1/1	0.78	0.24	84,84,84,84	0
57	MG	1H	3171	1/1	0.78	0.33	90,90,90,90	0
57	MG	14	3057	1/1	0.78	0.34	84,84,84,84	0
57	MG	1G	1648	1/1	0.78	0.40	79,79,79,79	0
57	MG	3A	201	1/1	0.78	0.27	77,77,77,77	0
57	MG	14	3210	1/1	0.78	0.17	80,80,80,80	0
57	MG	1H	3325	1/1	0.78	0.32	88,88,88,88	0
57	MG	1H	3182	1/1	0.78	0.27	90,90,90,90	0
58	SPE	1J	208	13/13	0.78	0.17	94,98,105,105	0
57	MG	14	3053	1/1	0.79	0.12	72,72,72,72	0
57	MG	1G	1632	1/1	0.79	0.15	99,99,99,99	0
57	MG	1H	3097	1/1	0.79	0.43	83,83,83,83	0
57	MG	14	3060	1/1	0.79	0.36	56,56,56,56	0
57	MG	1H	3087	1/1	0.79	0.41	79,79,79,79	0
57	MG	1H	3285	1/1	0.79	0.45	96,96,96,96	0
57	MG	1H	3124	1/1	0.79	0.35	73,73,73,73	0
57	MG	1G	1649	1/1	0.79	0.36	89,89,89,89	0
57	MG	14	3291	1/1	0.79	0.14	90,90,90,90	0
57	MG	1H	3207	1/1	0.79	0.38	87,87,87,87	0
57	MG	14	3025	1/1	0.79	0.35	80,80,80,80	0
57	MG	13	1624	1/1	0.79	0.19	93,93,93,93	0
57	MG	1H	3105	1/1	0.79	0.28	79,79,79,79	0
57	MG	13	1685	1/1	0.79	0.42	91,91,91,91	0
57	MG	14	3157	1/1	0.79	0.48	89,89,89,89	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	14	3085	1/1	0.80	0.44	81,81,81,81	0
57	MG	1H	3122	1/1	0.80	0.22	67,67,67,67	0
57	MG	1G	1609	1/1	0.80	0.40	96,96,96,96	0
57	MG	14	3103	1/1	0.80	0.37	75,75,75,75	0
57	MG	1G	1613	1/1	0.80	0.36	83,83,83,83	0
57	MG	1H	3112	1/1	0.80	0.23	79,79,79,79	0
57	MG	14	3112	1/1	0.80	0.32	99,99,99,99	0
57	MG	14	3124	1/1	0.80	0.30	82,82,82,82	0
57	MG	14	3032	1/1	0.80	0.29	80,80,80,80	0
57	MG	1H	3180	1/1	0.80	0.35	88,88,88,88	0
57	MG	1H	3450	1/1	0.80	0.16	59,59,59,59	0
57	MG	1H	3198	1/1	0.80	0.26	108,108,108,108	0
57	MG	1H	3216	1/1	0.80	0.32	89,89,89,89	0
57	MG	1H	3266	1/1	0.80	0.32	89,89,89,89	0
57	MG	14	3061	1/1	0.80	0.38	56,56,56,56	0
57	MG	1H	3027	1/1	0.80	0.27	84,84,84,84	0
57	MG	14	3175	1/1	0.80	0.17	107,107,107,107	0
57	MG	1H	3302	1/1	0.80	0.32	81,81,81,81	0
57	MG	1H	3245	1/1	0.80	0.28	78,78,78,78	0
57	MG	1G	1607	1/1	0.80	0.26	92,92,92,92	0
57	MG	13	1726	1/1	0.81	0.14	103,103,103,103	0
57	MG	1H	3091	1/1	0.81	0.38	77,77,77,77	0
57	MG	4K	101	1/1	0.81	0.28	86,86,86,86	0
57	MG	1H	3312	1/1	0.81	0.22	94,94,94,94	0
57	MG	13	1688	1/1	0.81	0.33	72,72,72,72	0
57	MG	1H	3317	1/1	0.81	0.41	83,83,83,83	0
57	MG	14	3194	1/1	0.81	0.33	87,87,87,87	0
57	MG	1H	3134	1/1	0.81	0.22	44,44,44,44	0
57	MG	14	3082	1/1	0.81	0.30	90,90,90,90	0
57	MG	14	3206	1/1	0.81	0.23	101,101,101,101	0
57	MG	1G	1620	1/1	0.81	0.30	79,79,79,79	0
57	MG	14	3212	1/1	0.81	0.37	94,94,94,94	0
57	MG	14	3213	1/1	0.81	0.31	76,76,76,76	0
57	MG	14	3095	1/1	0.81	0.29	74,74,74,74	0
57	MG	1H	3145	1/1	0.81	0.30	62,62,62,62	0
57	MG	4L	101	1/1	0.81	0.10	110,110,110,110	0
57	MG	14	3007	1/1	0.81	0.36	72,72,72,72	0
57	MG	14	3013	1/1	0.81	0.30	63,63,63,63	0
57	MG	1H	3149	1/1	0.81	0.30	86,86,86,86	0
57	MG	1H	3270	1/1	0.81	0.31	61,61,61,61	0
57	MG	1H	3189	1/1	0.81	0.28	78,78,78,78	0
57	MG	1H	3232	1/1	0.81	0.37	85,85,85,85	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	1H	3036	1/1	0.81	0.31	70,70,70,70	0
57	MG	14	3295	1/1	0.81	0.21	90,90,90,90	0
57	MG	16	203	1/1	0.81	0.16	78,78,78,78	0
57	MG	14	3423	1/1	0.81	0.30	92,92,92,92	0
57	MG	14	3159	1/1	0.81	0.34	93,93,93,93	0
57	MG	1H	3202	1/1	0.81	0.35	82,82,82,82	0
57	MG	14	3042	1/1	0.81	0.26	69,69,69,69	0
57	MG	1H	3157	1/1	0.81	0.13	73,73,73,73	0
57	MG	13	1651	1/1	0.81	0.39	97,97,97,97	0
57	MG	14	3134	1/1	0.82	0.16	71,71,71,71	0
57	MG	13	1616	1/1	0.82	0.25	82,82,82,82	0
57	MG	14	3141	1/1	0.82	0.19	76,76,76,76	0
57	MG	14	3145	1/1	0.82	0.15	85,85,85,85	0
57	MG	1H	3259	1/1	0.82	0.32	92,92,92,92	0
57	MG	1H	3313	1/1	0.82	0.21	74,74,74,74	0
57	MG	1H	3012	1/1	0.82	0.23	84,84,84,84	0
57	MG	13	1707	1/1	0.82	0.16	92,92,92,92	0
57	MG	1H	3067	1/1	0.82	0.26	62,62,62,62	0
57	MG	1G	1659	1/1	0.82	0.24	72,72,72,72	0
57	MG	14	3223	1/1	0.82	0.32	87,87,87,87	0
57	MG	14	3172	1/1	0.82	0.29	82,82,82,82	0
57	MG	1H	3200	1/1	0.82	0.32	73,73,73,73	0
57	MG	13	1630	1/1	0.82	0.33	87,87,87,87	0
57	MG	1H	3340	1/1	0.82	0.17	70,70,70,70	0
57	MG	14	3176	1/1	0.82	0.19	69,69,69,69	0
57	MG	1H	3377	1/1	0.82	0.17	75,75,75,75	0
57	MG	1G	1715	1/1	0.82	0.15	119,119,119,119	0
57	MG	14	3411	1/1	0.82	0.16	93,93,93,93	0
57	MG	1G	1643	1/1	0.82	0.25	83,83,83,83	0
57	MG	2L	102	1/1	0.82	0.49	90,90,90,90	0
57	MG	1J	204	1/1	0.82	0.20	88,88,88,88	0
57	MG	14	3191	1/1	0.82	0.17	82,82,82,82	0
57	MG	14	3193	1/1	0.82	0.27	95,95,95,95	0
57	MG	1H	3300	1/1	0.82	0.22	87,87,87,87	0
57	MG	14	3131	1/1	0.82	0.28	70,70,70,70	0
57	MG	14	3128	1/1	0.83	0.24	88,88,88,88	0
57	MG	13	1659	1/1	0.83	0.46	85,85,85,85	0
57	MG	1H	3141	1/1	0.83	0.22	66,66,66,66	0
57	MG	14	3136	1/1	0.83	0.17	127,127,127,127	0
57	MG	1G	1619	1/1	0.83	0.31	86,86,86,86	0
57	MG	14	3008	1/1	0.83	0.35	90,90,90,90	0
57	MG	14	3064	1/1	0.83	0.23	62,62,62,62	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	14	3151	1/1	0.83	0.33	87,87,87,87	0
57	MG	14	3068	1/1	0.83	0.24	64,64,64,64	0
57	MG	1H	3144	1/1	0.83	0.26	64,64,64,64	0
57	MG	13	1627	1/1	0.83	0.28	85,85,85,85	0
57	MG	14	3222	1/1	0.83	0.29	88,88,88,88	0
57	MG	1G	1657	1/1	0.83	0.26	82,82,82,82	0
57	MG	14	3024	1/1	0.83	0.22	77,77,77,77	0
57	MG	1H	3320	1/1	0.83	0.33	80,80,80,80	0
57	MG	14	3027	1/1	0.83	0.27	76,76,76,76	0
57	MG	1H	3287	1/1	0.83	0.29	78,78,78,78	0
57	MG	14	3100	1/1	0.83	0.21	61,61,61,61	0
57	MG	1H	3289	1/1	0.83	0.29	78,78,78,78	0
57	MG	14	3386	1/1	0.83	0.14	93,93,93,93	0
57	MG	13	1618	1/1	0.83	0.28	60,60,60,60	0
57	MG	1H	3204	1/1	0.83	0.36	81,81,81,81	0
57	MG	14	3106	1/1	0.83	0.45	94,94,94,94	0
57	MG	13	1633	1/1	0.83	0.22	87,87,87,87	0
57	MG	1J	202	1/1	0.83	0.13	84,84,84,84	0
57	MG	1J	203	1/1	0.83	0.26	91,91,91,91	0
57	MG	1H	3434	1/1	0.83	0.15	68,68,68,68	0
57	MG	14	3115	1/1	0.83	0.21	48,48,48,48	0
57	MG	14	3192	1/1	0.83	0.34	82,82,82,82	0
57	MG	14	3117	1/1	0.83	0.17	58,58,58,58	0
57	MG	1H	3088	1/1	0.83	0.22	61,61,61,61	0
57	MG	14	3171	1/1	0.84	0.10	57,57,57,57	0
57	MG	1G	1654	1/1	0.84	0.37	94,94,94,94	0
57	MG	1H	3261	1/1	0.84	0.30	77,77,77,77	0
57	MG	1H	3265	1/1	0.84	0.22	77,77,77,77	0
57	MG	1H	3220	1/1	0.84	0.18	89,89,89,89	0
57	MG	1H	3316	1/1	0.84	0.39	89,89,89,89	0
57	MG	14	3070	1/1	0.84	0.34	82,82,82,82	0
57	MG	1G	1707	1/1	0.84	0.17	108,108,108,108	0
57	MG	14	3187	1/1	0.84	0.25	90,90,90,90	0
57	MG	1G	1614	1/1	0.84	0.27	82,82,82,82	0
57	MG	1H	3126	1/1	0.84	0.15	75,75,75,75	0
57	MG	1G	1714	1/1	0.84	0.15	99,99,99,99	0
57	MG	1H	3128	1/1	0.84	0.18	79,79,79,79	0
57	MG	14	3087	1/1	0.84	0.21	58,58,58,58	0
57	MG	42	201	1/1	0.84	0.17	116,116,116,116	0
57	MG	1H	3272	1/1	0.84	0.36	80,80,80,80	0
57	MG	14	3099	1/1	0.84	0.26	77,77,77,77	0
57	MG	14	3200	1/1	0.84	0.34	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	3132	1/1	0.84	0.23	88,88,88,88	0
57	MG	14	3208	1/1	0.84	0.25	78,78,78,78	0
57	MG	13	1648	1/1	0.84	0.20	77,77,77,77	0
57	MG	14	3211	1/1	0.84	0.44	85,85,85,85	0
57	MG	1H	3172	1/1	0.84	0.29	84,84,84,84	0
57	MG	14	3004	1/1	0.84	0.15	73,73,73,73	0
57	MG	1H	3364	1/1	0.84	0.10	72,72,72,72	0
57	MG	1H	3100	1/1	0.84	0.16	62,62,62,62	0
57	MG	1H	3240	1/1	0.84	0.26	67,67,67,67	0
57	MG	14	3114	1/1	0.84	0.35	63,63,63,63	0
57	MG	1H	3449	1/1	0.84	0.21	80,80,80,80	0
57	MG	14	3116	1/1	0.84	0.27	66,66,66,66	0
57	MG	14	3018	1/1	0.84	0.25	78,78,78,78	0
57	MG	14	3021	1/1	0.84	0.21	76,76,76,76	0
57	MG	14	3126	1/1	0.84	0.28	75,75,75,75	0
57	MG	1G	1633	1/1	0.84	0.20	89,89,89,89	0
57	MG	14	3228	1/1	0.84	0.40	86,86,86,86	0
57	MG	13	1623	1/1	0.84	0.34	80,80,80,80	0
57	MG	1G	1637	1/1	0.84	0.14	113,113,113,113	0
57	MG	1G	1640	1/1	0.84	0.12	92,92,92,92	0
57	MG	14	3298	1/1	0.84	0.13	56,56,56,56	0
57	MG	14	3029	1/1	0.84	0.25	73,73,73,73	0
57	MG	14	3388	1/1	0.84	0.14	89,89,89,89	0
57	MG	1H	3210	1/1	0.84	0.14	83,83,83,83	0
57	MG	14	3396	1/1	0.84	0.18	109,109,109,109	0
57	MG	1H	3070	1/1	0.84	0.26	56,56,56,56	0
57	MG	14	3147	1/1	0.84	0.10	69,69,69,69	0
57	MG	13	1647	1/1	0.84	0.33	91,91,91,91	0
57	MG	14	3155	1/1	0.84	0.20	80,80,80,80	0
57	MG	1H	3106	1/1	0.84	0.17	68,68,68,68	0
57	MG	14	3040	1/1	0.84	0.18	72,72,72,72	0
57	MG	1H	3108	1/1	0.84	0.23	69,69,69,69	0
57	MG	31	301	1/1	0.84	0.11	63,63,63,63	0
57	MG	1H	3190	1/1	0.84	0.30	75,75,75,75	0
57	MG	1H	3311	1/1	0.84	0.24	93,93,93,93	0
57	MG	14	3009	1/1	0.85	0.24	68,68,68,68	0
57	MG	1H	3127	1/1	0.85	0.27	84,84,84,84	0
57	MG	1H	3184	1/1	0.85	0.36	93,93,93,93	0
57	MG	2K	101	1/1	0.85	0.22	63,63,63,63	0
57	MG	1H	3186	1/1	0.85	0.37	94,94,94,94	0
57	MG	1H	3066	1/1	0.85	0.21	65,65,65,65	0
57	MG	1H	3504	1/1	0.85	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	3509	1/1	0.85	0.16	88,88,88,88	0
57	MG	13	1626	1/1	0.85	0.29	67,67,67,67	0
57	MG	1H	3018	1/1	0.85	0.28	55,55,55,55	0
57	MG	1H	3238	1/1	0.85	0.28	87,87,87,87	0
57	MG	14	3120	1/1	0.85	0.27	75,75,75,75	0
57	MG	14	3122	1/1	0.85	0.23	84,84,84,84	0
57	MG	16	202	1/1	0.85	0.29	78,78,78,78	0
57	MG	1H	3196	1/1	0.85	0.14	56,56,56,56	0
57	MG	1H	3073	1/1	0.85	0.34	59,59,59,59	0
57	MG	13	1661	1/1	0.85	0.20	92,92,92,92	0
57	MG	68	202	1/1	0.85	0.22	83,83,83,83	0
57	MG	14	3043	1/1	0.85	0.30	83,83,83,83	0
57	MG	88	202	1/1	0.85	0.30	72,72,72,72	0
57	MG	14	3056	1/1	0.85	0.20	80,80,80,80	0
57	MG	1H	3297	1/1	0.85	0.16	78,78,78,78	0
57	MG	13	1634	1/1	0.85	0.26	78,78,78,78	0
57	MG	14	3148	1/1	0.85	0.15	63,63,63,63	0
57	MG	14	3150	1/1	0.85	0.34	81,81,81,81	0
57	MG	1G	1675	1/1	0.85	0.12	107,107,107,107	0
57	MG	14	3154	1/1	0.85	0.15	87,87,87,87	0
57	MG	14	3230	1/1	0.85	0.26	81,81,81,81	0
57	MG	1G	1605	1/1	0.85	0.30	82,82,82,82	0
57	MG	1H	3203	1/1	0.85	0.33	74,74,74,74	0
57	MG	1H	3303	1/1	0.85	0.29	76,76,76,76	0
57	MG	1H	3033	1/1	0.85	0.21	73,73,73,73	0
57	MG	1H	3034	1/1	0.85	0.24	72,72,72,72	0
57	MG	1H	3252	1/1	0.85	0.38	81,81,81,81	0
57	MG	1H	3117	1/1	0.85	0.26	54,54,54,54	0
57	MG	1H	3035	1/1	0.85	0.28	80,80,80,80	0
57	MG	13	1667	1/1	0.85	0.41	96,96,96,96	0
57	MG	14	3083	1/1	0.85	0.39	87,87,87,87	0
57	MG	1H	3089	1/1	0.85	0.21	66,66,66,66	0
57	MG	14	3086	1/1	0.85	0.22	64,64,64,64	0
57	MG	1H	3038	1/1	0.85	0.35	65,65,65,65	0
57	MG	1H	3268	1/1	0.85	0.42	92,92,92,92	0
57	MG	1H	3048	1/1	0.85	0.13	43,43,43,43	0
57	MG	14	3181	1/1	0.85	0.25	81,81,81,81	0
57	MG	13	1673	1/1	0.85	0.37	80,80,80,80	0
57	MG	1H	3197	1/1	0.86	0.33	80,80,80,80	0
57	MG	1H	3069	1/1	0.86	0.23	60,60,60,60	0
57	MG	1H	3199	1/1	0.86	0.19	78,78,78,78	0
57	MG	1G	1662	1/1	0.86	0.42	94,94,94,94	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	1H	3256	1/1	0.86	0.24	67,67,67,67	0
57	MG	1H	3309	1/1	0.86	0.24	74,74,74,74	0
57	MG	1H	3004	1/1	0.86	0.31	79,79,79,79	0
57	MG	14	3293	1/1	0.86	0.13	72,72,72,72	0
57	MG	1H	3016	1/1	0.86	0.21	47,47,47,47	0
57	MG	1H	3284	1/1	0.86	0.20	71,71,71,71	0
57	MG	1G	1611	1/1	0.86	0.38	77,77,77,77	0
57	MG	14	3168	1/1	0.86	0.16	87,87,87,87	0
57	MG	13	1650	1/1	0.86	0.39	85,85,85,85	0
57	MG	13	1643	1/1	0.86	0.33	86,86,86,86	0
57	MG	1H	3537	1/1	0.86	0.15	61,61,61,61	0
57	MG	14	3033	1/1	0.86	0.40	75,75,75,75	0
57	MG	1H	3191	1/1	0.86	0.18	72,72,72,72	0
57	MG	14	3215	1/1	0.86	0.10	72,72,72,72	0
57	MG	1H	3267	1/1	0.86	0.37	68,68,68,68	0
57	MG	1G	1651	1/1	0.86	0.24	105,105,105,105	0
57	MG	1H	3292	1/1	0.86	0.19	84,84,84,84	0
57	MG	14	3046	1/1	0.86	0.37	76,76,76,76	0
57	MG	1H	3221	1/1	0.86	0.27	64,64,64,64	0
57	MG	1H	3002	1/1	0.86	0.44	82,82,82,82	0
57	MG	14	3207	1/1	0.87	0.32	85,85,85,85	0
57	MG	14	3006	1/1	0.87	0.28	79,79,79,79	0
57	MG	88	203	1/1	0.87	0.26	76,76,76,76	0
57	MG	1H	3223	1/1	0.87	0.20	80,80,80,80	0
57	MG	14	3076	1/1	0.87	0.18	89,89,89,89	0
57	MG	1H	3055	1/1	0.87	0.20	60,60,60,60	0
57	MG	14	3012	1/1	0.87	0.31	60,60,60,60	0
57	MG	1H	3324	1/1	0.87	0.24	66,66,66,66	0
57	MG	1H	3098	1/1	0.87	0.36	78,78,78,78	0
57	MG	1H	3290	1/1	0.87	0.18	87,87,87,87	0
57	MG	1H	3291	1/1	0.87	0.23	78,78,78,78	0
57	MG	1H	3263	1/1	0.87	0.42	91,91,91,91	0
57	MG	1H	3402	1/1	0.87	0.11	79,79,79,79	0
57	MG	13	1631	1/1	0.87	0.25	78,78,78,78	0
57	MG	1H	3059	1/1	0.87	0.27	72,72,72,72	0
57	MG	1H	3153	1/1	0.87	0.24	82,82,82,82	0
57	MG	13	1601	1/1	0.87	0.27	74,74,74,74	0
57	MG	13	1607	1/1	0.87	0.29	80,80,80,80	0
57	MG	1H	3019	1/1	0.87	0.19	61,61,61,61	0
57	MG	1G	1622	1/1	0.87	0.41	85,85,85,85	0
57	MG	14	3261	1/1	0.87	0.12	67,67,67,67	0
57	MG	1H	3307	1/1	0.87	0.44	72,72,72,72	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	14	3039	1/1	0.87	0.27	65,65,65,65	0
57	MG	1H	3271	1/1	0.87	0.14	77,77,77,77	0
57	MG	1H	3192	1/1	0.87	0.33	76,76,76,76	0
57	MG	13	1604	1/1	0.87	0.24	77,77,77,77	0
57	MG	14	3185	1/1	0.87	0.18	76,76,76,76	0
57	MG	14	3391	1/1	0.87	0.12	103,103,103,103	0
57	MG	1G	1631	1/1	0.87	0.17	82,82,82,82	0
57	MG	14	3047	1/1	0.87	0.21	81,81,81,81	0
57	MG	14	3409	1/1	0.87	0.12	95,95,95,95	0
57	MG	1H	3131	1/1	0.87	0.25	75,75,75,75	0
57	MG	1H	3042	1/1	0.87	0.28	67,67,67,67	0
57	MG	14	3428	1/1	0.87	0.12	109,109,109,109	0
57	MG	14	3435	1/1	0.87	0.11	93,93,93,93	0
57	MG	14	3443	1/1	0.87	0.18	92,92,92,92	0
57	MG	14	3447	1/1	0.87	0.40	69,69,69,69	0
57	MG	4A	201	1/1	0.87	0.22	96,96,96,96	0
57	MG	1G	1634	1/1	0.87	0.17	93,93,93,93	0
57	MG	1H	3072	1/1	0.87	0.33	72,72,72,72	0
57	MG	13	1605	1/1	0.87	0.23	70,70,70,70	0
57	MG	14	3002	1/1	0.87	0.34	68,68,68,68	0
57	MG	1H	3222	1/1	0.87	0.26	64,64,64,64	0
57	MG	14	3204	1/1	0.87	0.36	80,80,80,80	0
57	MG	14	3140	1/1	0.87	0.23	89,89,89,89	0
57	MG	14	3195	1/1	0.88	0.31	78,78,78,78	0
57	MG	68	201	1/1	0.88	0.24	78,78,78,78	0
57	MG	1H	3306	1/1	0.88	0.14	70,70,70,70	0
57	MG	13	1632	1/1	0.88	0.45	90,90,90,90	0
57	MG	1H	3150	1/1	0.88	0.31	67,67,67,67	0
57	MG	13	1613	1/1	0.88	0.26	81,81,81,81	0
57	MG	P8	101	1/1	0.88	0.27	71,71,71,71	0
57	MG	14	3038	1/1	0.88	0.16	69,69,69,69	0
57	MG	1H	3093	1/1	0.88	0.34	71,71,71,71	0
57	MG	1H	3231	1/1	0.88	0.23	67,67,67,67	0
57	MG	1H	3009	1/1	0.88	0.34	77,77,77,77	0
57	MG	1H	3158	1/1	0.88	0.37	71,71,71,71	0
57	MG	14	3133	1/1	0.88	0.15	58,58,58,58	0
57	MG	1H	3273	1/1	0.88	0.14	69,69,69,69	0
57	MG	1H	3234	1/1	0.88	0.33	76,76,76,76	0
57	MG	14	3137	1/1	0.88	0.20	68,68,68,68	0
57	MG	13	1663	1/1	0.88	0.41	90,90,90,90	0
57	MG	1H	3279	1/1	0.88	0.36	76,76,76,76	0
57	MG	14	3221	1/1	0.88	0.17	91,91,91,91	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	1H	3281	1/1	0.88	0.19	67,67,67,67	0
57	MG	1H	3096	1/1	0.88	0.14	53,53,53,53	0
57	MG	1G	1723	1/1	0.88	0.19	94,94,94,94	0
57	MG	13	1629	1/1	0.88	0.19	56,56,56,56	0
57	MG	13	1672	1/1	0.88	0.46	86,86,86,86	0
57	MG	1H	3242	1/1	0.88	0.14	74,74,74,74	0
57	MG	14	3066	1/1	0.88	0.24	59,59,59,59	0
57	MG	14	3067	1/1	0.88	0.26	69,69,69,69	0
57	MG	13	1736	1/1	0.88	0.12	104,104,104,104	0
57	MG	13	1743	1/1	0.88	0.07	153,153,153,153	0
57	MG	1H	3130	1/1	0.88	0.40	87,87,87,87	0
57	MG	14	3162	1/1	0.88	0.21	67,67,67,67	0
57	MG	14	3075	1/1	0.88	0.37	89,89,89,89	0
57	MG	1G	1626	1/1	0.88	0.25	68,68,68,68	0
57	MG	1H	3211	1/1	0.88	0.38	79,79,79,79	0
57	MG	1H	3052	1/1	0.88	0.21	50,50,50,50	0
57	MG	1H	3022	1/1	0.88	0.19	41,41,41,41	0
57	MG	1H	3519	1/1	0.88	0.17	83,83,83,83	0
57	MG	1H	3294	1/1	0.88	0.14	90,90,90,90	0
57	MG	1H	3056	1/1	0.88	0.44	73,73,73,73	0
57	MG	1H	3107	1/1	0.88	0.26	72,72,72,72	0
57	MG	14	3092	1/1	0.88	0.37	81,81,81,81	0
57	MG	14	3093	1/1	0.88	0.22	79,79,79,79	0
57	MG	1H	3005	1/1	0.88	0.40	74,74,74,74	0
57	MG	14	3015	1/1	0.88	0.22	73,73,73,73	0
57	MG	14	3016	1/1	0.88	0.28	63,63,63,63	0
57	MG	1H	3219	1/1	0.88	0.36	82,82,82,82	0
57	MG	1H	3109	1/1	0.88	0.27	79,79,79,79	0
57	MG	1H	3029	1/1	0.88	0.18	63,63,63,63	0
57	MG	16	207	1/1	0.88	0.10	84,84,84,84	0
57	MG	14	3105	1/1	0.88	0.26	73,73,73,73	0
57	MG	16	208	1/1	0.88	0.32	79,79,79,79	0
57	MG	35	202	1/1	0.88	0.33	84,84,84,84	0
58	SPE	13	1748	13/13	0.88	0.14	60,77,82,87	0
58	SPE	1G	1733	13/13	0.88	0.15	98,101,104,105	0
57	MG	1H	3304	1/1	0.88	0.37	85,85,85,85	0
57	MG	1H	3114	1/1	0.89	0.31	67,67,67,67	0
57	MG	13	1637	1/1	0.89	0.14	79,79,79,79	0
57	MG	1H	3373	1/1	0.89	0.11	89,89,89,89	0
57	MG	14	3118	1/1	0.89	0.08	73,73,73,73	0
57	MG	14	3201	1/1	0.89	0.55	95,95,95,95	0
57	MG	1H	3262	1/1	0.89	0.19	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	1H	3380	1/1	0.89	0.11	59,59,59,59	0
57	MG	1H	3194	1/1	0.89	0.36	71,71,71,71	0
57	MG	14	3050	1/1	0.89	0.29	77,77,77,77	0
57	MG	1H	3415	1/1	0.89	0.13	72,72,72,72	0
57	MG	1H	3152	1/1	0.89	0.18	51,51,51,51	0
57	MG	1H	3448	1/1	0.89	0.11	86,86,86,86	0
57	MG	13	1680	1/1	0.89	0.44	84,84,84,84	0
57	MG	1H	3092	1/1	0.89	0.08	74,74,74,74	0
57	MG	1H	3464	1/1	0.89	0.10	48,48,48,48	0
57	MG	14	3062	1/1	0.89	0.40	71,71,71,71	0
57	MG	14	3139	1/1	0.89	0.33	84,84,84,84	0
57	MG	2L	101	1/1	0.89	0.29	77,77,77,77	0
57	MG	1H	3017	1/1	0.89	0.22	53,53,53,53	0
57	MG	1H	3301	1/1	0.89	0.20	70,70,70,70	0
57	MG	1G	1625	1/1	0.89	0.12	98,98,98,98	0
57	MG	5I	101	1/1	0.89	0.12	80,80,80,80	0
57	MG	14	3069	1/1	0.89	0.21	93,93,93,93	0
57	MG	1H	3521	1/1	0.89	0.18	86,86,86,86	0
57	MG	14	3153	1/1	0.89	0.22	65,65,65,65	0
57	MG	14	3072	1/1	0.89	0.13	57,57,57,57	0
57	MG	14	3005	1/1	0.89	0.16	50,50,50,50	0
57	MG	14	3156	1/1	0.89	0.13	71,71,71,71	0
57	MG	13	1641	1/1	0.89	0.24	68,68,68,68	0
57	MG	1H	3524	1/1	0.89	0.16	96,96,96,96	0
57	MG	1H	3164	1/1	0.89	0.15	64,64,64,64	0
57	MG	14	3161	1/1	0.89	0.30	79,79,79,79	0
57	MG	1H	3037	1/1	0.89	0.26	71,71,71,71	0
57	MG	14	3351	1/1	0.89	0.10	104,104,104,104	0
57	MG	14	3380	1/1	0.89	0.10	85,85,85,85	0
57	MG	14	3381	1/1	0.89	0.19	74,74,74,74	0
57	MG	1H	3020	1/1	0.89	0.15	47,47,47,47	0
57	MG	1H	3308	1/1	0.89	0.20	56,56,56,56	0
57	MG	14	3167	1/1	0.89	0.20	76,76,76,76	0
57	MG	1H	3021	1/1	0.89	0.27	63,63,63,63	0
57	MG	16	205	1/1	0.89	0.10	66,66,66,66	0
57	MG	14	3405	1/1	0.89	0.10	91,91,91,91	0
57	MG	1G	1642	1/1	0.89	0.21	82,82,82,82	0
57	MG	14	3089	1/1	0.89	0.35	79,79,79,79	0
57	MG	14	3421	1/1	0.89	0.15	98,98,98,98	0
57	MG	14	3090	1/1	0.89	0.25	65,65,65,65	0
57	MG	14	3017	1/1	0.89	0.33	60,60,60,60	0
57	MG	1H	3043	1/1	0.89	0.24	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	1H	3278	1/1	0.89	0.23	83,83,83,83	0
57	MG	1H	3209	1/1	0.89	0.21	52,52,52,52	0
57	MG	1H	3314	1/1	0.89	0.20	88,88,88,88	0
57	MG	14	3179	1/1	0.89	0.23	71,71,71,71	0
57	MG	1H	3074	1/1	0.89	0.28	73,73,73,73	0
57	MG	1H	3044	1/1	0.89	0.44	81,81,81,81	0
57	MG	1J	206	1/1	0.89	0.11	109,109,109,109	0
57	MG	88	201	1/1	0.89	0.23	78,78,78,78	0
57	MG	13	1642	1/1	0.89	0.17	72,72,72,72	0
57	MG	1H	3051	1/1	0.89	0.30	76,76,76,76	0
57	MG	1H	3082	1/1	0.89	0.34	76,76,76,76	0
57	MG	13	1602	1/1	0.89	0.29	78,78,78,78	0
57	MG	1H	3028	1/1	0.89	0.25	62,62,62,62	0
58	SPE	14	3445	13/13	0.89	0.18	70,76,79,79	0
58	SPE	14	3446	13/13	0.89	0.24	68,79,87,89	0
57	MG	13	1620	1/1	0.89	0.20	57,57,57,57	0
57	MG	14	3078	1/1	0.90	0.37	64,64,64,64	0
57	MG	1H	3208	1/1	0.90	0.33	78,78,78,78	0
57	MG	13	1681	1/1	0.90	0.10	68,68,68,68	0
57	MG	13	1608	1/1	0.90	0.13	71,71,71,71	0
57	MG	13	1710	1/1	0.90	0.09	82,82,82,82	0
57	MG	13	1628	1/1	0.90	0.29	79,79,79,79	0
57	MG	1H	3244	1/1	0.90	0.35	77,77,77,77	0
57	MG	1G	1658	1/1	0.90	0.17	84,84,84,84	0
57	MG	1H	3085	1/1	0.90	0.39	75,75,75,75	0
57	MG	14	3091	1/1	0.90	0.32	66,66,66,66	0
57	MG	1H	3515	1/1	0.90	0.09	98,98,98,98	0
57	MG	13	1619	1/1	0.90	0.11	53,53,53,53	0
57	MG	14	3094	1/1	0.90	0.31	70,70,70,70	0
57	MG	1H	3310	1/1	0.90	0.51	87,87,87,87	0
57	MG	14	3165	1/1	0.90	0.25	74,74,74,74	0
57	MG	1H	3165	1/1	0.90	0.17	59,59,59,59	0
57	MG	1G	1696	1/1	0.90	0.09	91,91,91,91	0
57	MG	1G	1618	1/1	0.90	0.35	89,89,89,89	0
57	MG	1H	3168	1/1	0.90	0.12	80,80,80,80	0
57	MG	1H	3529	1/1	0.90	0.24	78,78,78,78	0
57	MG	1G	1621	1/1	0.90	0.32	86,86,86,86	0
57	MG	1H	3531	1/1	0.90	0.17	76,76,76,76	0
57	MG	14	3365	1/1	0.90	0.12	96,96,96,96	0
57	MG	14	3045	1/1	0.90	0.24	61,61,61,61	0
57	MG	14	3107	1/1	0.90	0.18	65,65,65,65	0
57	MG	1H	3068	1/1	0.90	0.36	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	1G	1729	1/1	0.90	0.09	104,104,104,104	0
57	MG	14	3113	1/1	0.90	0.21	57,57,57,57	0
57	MG	13	1610	1/1	0.90	0.33	73,73,73,73	0
57	MG	1H	3542	1/1	0.90	0.16	90,90,90,90	0
57	MG	14	3401	1/1	0.90	0.17	85,85,85,85	0
57	MG	14	3402	1/1	0.90	0.07	118,118,118,118	0
57	MG	14	3182	1/1	0.90	0.08	82,82,82,82	0
57	MG	1H	3253	1/1	0.90	0.37	71,71,71,71	0
57	MG	13	1665	1/1	0.90	0.44	88,88,88,88	0
57	MG	1H	3257	1/1	0.90	0.18	51,51,51,51	0
57	MG	14	3119	1/1	0.90	0.24	79,79,79,79	0
57	MG	1H	3258	1/1	0.90	0.33	84,84,84,84	0
57	MG	14	3434	1/1	0.90	0.08	115,115,115,115	0
57	MG	1H	3288	1/1	0.90	0.27	77,77,77,77	0
57	MG	1H	3173	1/1	0.90	0.49	89,89,89,89	0
57	MG	14	3003	1/1	0.90	0.28	54,54,54,54	0
57	MG	1H	3201	1/1	0.90	0.40	88,88,88,88	0
57	MG	14	3196	1/1	0.90	0.23	68,68,68,68	0
57	MG	1H	3176	1/1	0.90	0.14	62,62,62,62	0
57	MG	1H	3148	1/1	0.90	0.22	80,80,80,80	0
57	MG	1G	1639	1/1	0.90	0.17	103,103,103,103	0
57	MG	1H	3293	1/1	0.90	0.31	46,46,46,46	0
57	MG	14	3203	1/1	0.90	0.46	93,93,93,93	0
57	MG	25	201	1/1	0.90	0.07	118,118,118,118	0
57	MG	1H	3228	1/1	0.90	0.25	70,70,70,70	0
57	MG	1H	3053	1/1	0.90	0.35	66,66,66,66	0
57	MG	13	1612	1/1	0.90	0.24	76,76,76,76	0
57	MG	1H	3151	1/1	0.90	0.14	59,59,59,59	0
57	MG	13	1689	1/1	0.90	0.37	85,85,85,85	0
57	MG	1G	1602	1/1	0.90	0.17	81,81,81,81	0
57	MG	14	3146	1/1	0.90	0.14	51,51,51,51	0
57	MG	1H	3213	1/1	0.91	0.33	77,77,77,77	0
57	MG	13	1727	1/1	0.91	0.11	90,90,90,90	0
57	MG	13	1733	1/1	0.91	0.10	106,106,106,106	0
57	MG	1H	3323	1/1	0.91	0.21	75,75,75,75	0
57	MG	13	1609	1/1	0.91	0.20	71,71,71,71	0
57	MG	1H	3243	1/1	0.91	0.21	79,79,79,79	0
57	MG	1H	3547	1/1	0.91	0.23	61,61,61,61	0
57	MG	14	3282	1/1	0.91	0.10	105,105,105,105	0
57	MG	1H	3110	1/1	0.91	0.21	65,65,65,65	0
57	MG	14	3071	1/1	0.91	0.17	63,63,63,63	0
57	MG	1H	3179	1/1	0.91	0.28	67,67,67,67	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	14	3073	1/1	0.91	0.20	48,48,48,48	0
57	MG	14	3307	1/1	0.91	0.11	72,72,72,72	0
57	MG	14	3324	1/1	0.91	0.12	66,66,66,66	0
57	MG	14	3127	1/1	0.91	0.29	62,62,62,62	0
57	MG	14	3355	1/1	0.91	0.08	107,107,107,107	0
57	MG	1H	3111	1/1	0.91	0.50	73,73,73,73	0
57	MG	14	3130	1/1	0.91	0.31	70,70,70,70	0
57	MG	14	3019	1/1	0.91	0.10	53,53,53,53	0
57	MG	16	204	1/1	0.91	0.30	70,70,70,70	0
57	MG	1H	3129	1/1	0.91	0.32	69,69,69,69	0
57	MG	1G	1691	1/1	0.91	0.12	99,99,99,99	0
57	MG	1H	3154	1/1	0.91	0.16	66,66,66,66	0
57	MG	1G	1698	1/1	0.91	0.09	105,105,105,105	0
57	MG	1G	1701	1/1	0.91	0.08	101,101,101,101	0
57	MG	13	1737	1/1	0.91	0.12	98,98,98,98	0
57	MG	14	3404	1/1	0.91	0.12	100,100,100,100	0
57	MG	1H	3251	1/1	0.91	0.19	77,77,77,77	0
57	MG	1H	3421	1/1	0.91	0.09	99,99,99,99	0
57	MG	3I	302	1/1	0.91	0.18	73,73,73,73	0
57	MG	14	3419	1/1	0.91	0.08	110,110,110,110	0
57	MG	1H	3422	1/1	0.91	0.09	101,101,101,101	0
57	MG	1G	1717	1/1	0.91	0.09	99,99,99,99	0
57	MG	14	3202	1/1	0.91	0.18	83,83,83,83	0
57	MG	14	3431	1/1	0.91	0.11	60,60,60,60	0
57	MG	14	3149	1/1	0.91	0.31	71,71,71,71	0
57	MG	1H	3429	1/1	0.91	0.09	56,56,56,56	0
57	MG	14	3441	1/1	0.91	0.13	102,102,102,102	0
57	MG	13	1711	1/1	0.91	0.13	102,102,102,102	0
57	MG	14	3152	1/1	0.91	0.41	86,86,86,86	0
57	MG	14	3041	1/1	0.91	0.51	76,76,76,76	0
57	MG	1H	3011	1/1	0.91	0.16	73,73,73,73	0
57	MG	1H	3001	1/1	0.91	0.25	61,61,61,61	0
57	MG	1H	3229	1/1	0.91	0.25	64,64,64,64	0
57	MG	1H	3230	1/1	0.91	0.22	87,87,87,87	0
57	MG	1H	3162	1/1	0.91	0.32	68,68,68,68	0
57	MG	13	1745	1/1	0.91	0.07	111,111,111,111	0
57	MG	14	3160	1/1	0.91	0.42	92,92,92,92	0
57	MG	13	1640	1/1	0.91	0.29	77,77,77,77	0
57	MG	1H	3121	1/1	0.91	0.51	80,80,80,80	0
57	MG	B5	101	1/1	0.91	0.11	85,85,85,85	0
57	MG	14	3219	1/1	0.91	0.26	54,54,54,54	0
57	MG	1G	1645	1/1	0.91	0.12	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	3064	1/1	0.91	0.22	63,63,63,63	0
57	MG	1H	3237	1/1	0.91	0.21	73,73,73,73	0
57	MG	1G	1610	1/1	0.91	0.18	69,69,69,69	0
57	MG	1G	1685	1/1	0.92	0.09	91,91,91,91	0
57	MG	1G	1689	1/1	0.92	0.10	89,89,89,89	0
57	MG	1H	3147	1/1	0.92	0.23	64,64,64,64	0
57	MG	1H	3350	1/1	0.92	0.10	57,57,57,57	0
57	MG	1H	3352	1/1	0.92	0.07	84,84,84,84	0
57	MG	14	3227	1/1	0.92	0.24	76,76,76,76	0
57	MG	14	3037	1/1	0.92	0.22	57,57,57,57	0
57	MG	14	3163	1/1	0.92	0.41	84,84,84,84	0
57	MG	1H	3298	1/1	0.92	0.11	83,83,83,83	0
57	MG	14	3246	1/1	0.92	0.10	72,72,72,72	0
57	MG	14	3256	1/1	0.92	0.08	54,54,54,54	0
57	MG	1H	3370	1/1	0.92	0.09	59,59,59,59	0
57	MG	13	1666	1/1	0.92	0.19	78,78,78,78	0
57	MG	13	1639	1/1	0.92	0.14	73,73,73,73	0
57	MG	1G	1713	1/1	0.92	0.11	113,113,113,113	0
57	MG	1G	1627	1/1	0.92	0.24	77,77,77,77	0
57	MG	14	3296	1/1	0.92	0.09	62,62,62,62	0
57	MG	1G	1628	1/1	0.92	0.34	76,76,76,76	0
57	MG	14	3109	1/1	0.92	0.42	74,74,74,74	0
57	MG	14	3313	1/1	0.92	0.10	87,87,87,87	0
57	MG	1H	3175	1/1	0.92	0.12	64,64,64,64	0
57	MG	14	3331	1/1	0.92	0.10	79,79,79,79	0
57	MG	14	3111	1/1	0.92	0.39	86,86,86,86	0
57	MG	13	1657	1/1	0.92	0.41	80,80,80,80	0
57	MG	1G	1725	1/1	0.92	0.08	113,113,113,113	0
57	MG	14	3378	1/1	0.92	0.07	86,86,86,86	0
57	MG	14	3052	1/1	0.92	0.40	79,79,79,79	0
57	MG	1H	3083	1/1	0.92	0.35	71,71,71,71	0
57	MG	14	3054	1/1	0.92	0.13	49,49,49,49	0
57	MG	21	301	1/1	0.92	0.20	62,62,62,62	0
57	MG	14	3390	1/1	0.92	0.13	108,108,108,108	0
57	MG	1H	3084	1/1	0.92	0.32	68,68,68,68	0
57	MG	1H	3280	1/1	0.92	0.22	68,68,68,68	0
57	MG	1H	3181	1/1	0.92	0.12	94,94,94,94	0
57	MG	1G	1636	1/1	0.92	0.09	91,91,91,91	0
57	MG	1H	3255	1/1	0.92	0.28	73,73,73,73	0
57	MG	14	3125	1/1	0.92	0.30	70,70,70,70	0
57	MG	1H	3113	1/1	0.92	0.26	64,64,64,64	0
57	MG	13	1715	1/1	0.92	0.07	114,114,114,114	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	1G	1641	1/1	0.92	0.09	88,88,88,88	0
57	MG	14	3413	1/1	0.92	0.17	81,81,81,81	0
57	MG	1H	3023	1/1	0.92	0.15	72,72,72,72	0
57	MG	1H	3156	1/1	0.92	0.13	66,66,66,66	0
57	MG	14	3422	1/1	0.92	0.14	100,100,100,100	0
57	MG	1H	3484	1/1	0.92	0.09	84,84,84,84	0
57	MG	14	3426	1/1	0.92	0.06	126,126,126,126	0
57	MG	1H	3498	1/1	0.92	0.13	85,85,85,85	0
57	MG	14	3135	1/1	0.92	0.18	69,69,69,69	0
57	MG	1H	3500	1/1	0.92	0.10	93,93,93,93	0
57	MG	1H	3071	1/1	0.92	0.23	57,57,57,57	0
57	MG	14	3010	1/1	0.92	0.14	50,50,50,50	0
57	MG	1H	3508	1/1	0.92	0.08	84,84,84,84	0
57	MG	14	3444	1/1	0.92	0.17	85,85,85,85	0
57	MG	14	3205	1/1	0.92	0.23	79,79,79,79	0
57	MG	13	1658	1/1	0.92	0.39	75,75,75,75	0
57	MG	1H	3062	1/1	0.92	0.13	40,40,40,40	0
57	MG	14	3142	1/1	0.92	0.19	76,76,76,76	0
57	MG	14	3209	1/1	0.92	0.20	65,65,65,65	0
57	MG	1H	3137	1/1	0.92	0.18	57,57,57,57	0
57	MG	19	301	1/1	0.92	0.21	57,57,57,57	0
57	MG	1H	3163	1/1	0.92	0.13	74,74,74,74	0
57	MG	1G	1612	1/1	0.92	0.17	82,82,82,82	0
57	MG	1H	3139	1/1	0.92	0.09	54,54,54,54	0
57	MG	1H	3241	1/1	0.92	0.09	64,64,64,64	0
57	MG	14	3084	1/1	0.92	0.28	87,87,87,87	0
57	MG	1H	3527	1/1	0.92	0.07	107,107,107,107	0
57	MG	13	1674	1/1	0.92	0.27	92,92,92,92	0
57	MG	1H	3065	1/1	0.92	0.16	50,50,50,50	0
57	MG	1H	3123	1/1	0.92	0.30	65,65,65,65	0
57	MG	1G	1678	1/1	0.92	0.10	73,73,73,73	0
57	MG	1H	3331	1/1	0.92	0.10	53,53,53,53	0
57	MG	14	3268	1/1	0.93	0.19	86,86,86,86	0
57	MG	1H	3024	1/1	0.93	0.09	51,51,51,51	0
57	MG	14	3284	1/1	0.93	0.07	72,72,72,72	0
57	MG	14	3051	1/1	0.93	0.20	72,72,72,72	0
57	MG	1H	3026	1/1	0.93	0.27	52,52,52,52	0
57	MG	1H	3045	1/1	0.93	0.13	42,42,42,42	0
57	MG	1H	3090	1/1	0.93	0.21	77,77,77,77	0
57	MG	13	1747	1/1	0.93	0.08	110,110,110,110	0
57	MG	1G	1638	1/1	0.93	0.15	93,93,93,93	0
57	MG	1H	3451	1/1	0.93	0.08	83,83,83,83	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	1H	3167	1/1	0.93	0.08	60,60,60,60	0
57	MG	14	3184	1/1	0.93	0.18	72,72,72,72	0
57	MG	14	3346	1/1	0.93	0.07	92,92,92,92	0
57	MG	1H	3473	1/1	0.93	0.08	76,76,76,76	0
57	MG	14	3352	1/1	0.93	0.10	84,84,84,84	0
57	MG	14	3353	1/1	0.93	0.08	90,90,90,90	0
57	MG	1H	3479	1/1	0.93	0.10	75,75,75,75	0
57	MG	14	3188	1/1	0.93	0.43	76,76,76,76	0
57	MG	14	3369	1/1	0.93	0.08	92,92,92,92	0
57	MG	14	3376	1/1	0.93	0.14	78,78,78,78	0
57	MG	1H	3480	1/1	0.93	0.11	53,53,53,53	0
57	MG	1H	3483	1/1	0.93	0.10	103,103,103,103	0
57	MG	14	3065	1/1	0.93	0.21	60,60,60,60	0
57	MG	1G	1603	1/1	0.93	0.18	79,79,79,79	0
57	MG	1G	1646	1/1	0.93	0.08	83,83,83,83	0
57	MG	1H	3014	1/1	0.93	0.18	43,43,43,43	0
57	MG	1H	3254	1/1	0.93	0.42	75,75,75,75	0
57	MG	1H	3226	1/1	0.93	0.32	60,60,60,60	0
57	MG	1H	3169	1/1	0.93	0.40	82,82,82,82	0
57	MG	1H	3015	1/1	0.93	0.22	65,65,65,65	0
57	MG	13	1749	1/1	0.93	0.10	78,78,78,78	0
57	MG	1H	3513	1/1	0.93	0.12	80,80,80,80	0
57	MG	1H	3032	1/1	0.93	0.11	56,56,56,56	0
57	MG	1H	3119	1/1	0.93	0.18	62,62,62,62	0
57	MG	13	1730	1/1	0.93	0.09	81,81,81,81	0
57	MG	1H	3522	1/1	0.93	0.10	91,91,91,91	0
57	MG	14	3415	1/1	0.93	0.06	101,101,101,101	0
57	MG	14	3144	1/1	0.93	0.17	56,56,56,56	0
57	MG	1G	1660	1/1	0.93	0.24	75,75,75,75	0
57	MG	1H	3057	1/1	0.93	0.15	72,72,72,72	0
57	MG	5E	201	1/1	0.93	0.19	75,75,75,75	0
57	MG	13	1684	1/1	0.93	0.24	74,74,74,74	0
57	MG	14	3022	1/1	0.93	0.19	44,44,44,44	0
57	MG	1H	3349	1/1	0.93	0.14	67,67,67,67	0
57	MG	1H	3236	1/1	0.93	0.27	70,70,70,70	0
57	MG	1H	3101	1/1	0.93	0.10	65,65,65,65	0
57	MG	14	3436	1/1	0.93	0.15	96,96,96,96	0
57	MG	14	3438	1/1	0.93	0.11	101,101,101,101	0
57	MG	1G	1686	1/1	0.93	0.06	107,107,107,107	0
57	MG	14	3442	1/1	0.93	0.24	75,75,75,75	0
57	MG	1H	3081	1/1	0.93	0.09	55,55,55,55	0
57	MG	1H	3299	1/1	0.93	0.11	78,78,78,78	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	1G	1695	1/1	0.93	0.07	112,112,112,112	0
57	MG	1H	3060	1/1	0.93	0.20	51,51,51,51	0
57	MG	13	1652	1/1	0.93	0.20	68,68,68,68	0
57	MG	14	3096	1/1	0.93	0.18	50,50,50,50	0
57	MG	1G	1700	1/1	0.93	0.07	109,109,109,109	0
57	MG	1H	3379	1/1	0.93	0.09	58,58,58,58	0
57	MG	1G	1702	1/1	0.93	0.07	95,95,95,95	0
57	MG	13	1664	1/1	0.93	0.17	69,69,69,69	0
57	MG	39	301	1/1	0.93	0.17	95,95,95,95	0
57	MG	1G	1709	1/1	0.93	0.09	87,87,87,87	0
57	MG	13	1702	1/1	0.93	0.07	107,107,107,107	0
57	MG	1G	1711	1/1	0.93	0.10	108,108,108,108	0
57	MG	1H	3187	1/1	0.93	0.38	81,81,81,81	0
57	MG	1H	3418	1/1	0.93	0.08	86,86,86,86	0
57	MG	14	3231	1/1	0.93	0.44	80,80,80,80	0
57	MG	14	3244	1/1	0.93	0.10	58,58,58,58	0
57	MG	13	1611	1/1	0.93	0.12	85,85,85,85	0
57	MG	1H	3159	1/1	0.93	0.13	74,74,74,74	0
57	MG	14	3049	1/1	0.93	0.19	57,57,57,57	0
57	MG	14	3048	1/1	0.94	0.13	67,67,67,67	0
57	MG	13	1732	1/1	0.94	0.07	118,118,118,118	0
57	MG	11	301	1/1	0.94	0.25	60,60,60,60	0
57	MG	13	1655	1/1	0.94	0.16	65,65,65,65	0
57	MG	1G	1664	1/1	0.94	0.10	73,73,73,73	0
57	MG	1G	1666	1/1	0.94	0.07	103,103,103,103	0
57	MG	14	3370	1/1	0.94	0.21	87,87,87,87	0
57	MG	1H	3025	1/1	0.94	0.19	48,48,48,48	0
57	MG	1H	3003	1/1	0.94	0.36	65,65,65,65	0
57	MG	1H	3138	1/1	0.94	0.24	41,41,41,41	0
57	MG	1G	1681	1/1	0.94	0.10	96,96,96,96	0
57	MG	1G	1684	1/1	0.94	0.06	120,120,120,120	0
57	MG	14	3387	1/1	0.94	0.06	89,89,89,89	0
57	MG	13	1617	1/1	0.94	0.41	78,78,78,78	0
57	MG	1H	3365	1/1	0.94	0.09	62,62,62,62	0
57	MG	3I	201	1/1	0.94	0.20	64,64,64,64	0
57	MG	14	3393	1/1	0.94	0.08	118,118,118,118	0
57	MG	13	1615	1/1	0.94	0.13	73,73,73,73	0
57	MG	1H	3264	1/1	0.94	0.08	59,59,59,59	0
57	MG	13	1728	1/1	0.94	0.06	112,112,112,112	0
57	MG	Q8	101	1/1	0.94	0.17	81,81,81,81	0
57	MG	14	3020	1/1	0.94	0.25	61,61,61,61	0
57	MG	1H	3146	1/1	0.94	0.25	58,58,58,58	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	1H	3388	1/1	0.94	0.09	58,58,58,58	0
57	MG	14	3169	1/1	0.94	0.09	53,53,53,53	0
57	MG	1H	3397	1/1	0.94	0.08	58,58,58,58	0
57	MG	1H	3046	1/1	0.94	0.13	49,49,49,49	0
57	MG	14	3418	1/1	0.94	0.06	101,101,101,101	0
57	MG	14	3123	1/1	0.94	0.29	60,60,60,60	0
57	MG	1H	3166	1/1	0.94	0.23	56,56,56,56	0
57	MG	14	3026	1/1	0.94	0.15	69,69,69,69	0
57	MG	1H	3047	1/1	0.94	0.22	55,55,55,55	0
57	MG	14	3424	1/1	0.94	0.13	94,94,94,94	0
57	MG	14	3028	1/1	0.94	0.22	61,61,61,61	0
57	MG	14	3427	1/1	0.94	0.14	92,92,92,92	0
57	MG	1H	3526	1/1	0.94	0.07	113,113,113,113	0
57	MG	14	3429	1/1	0.94	0.07	99,99,99,99	0
57	MG	14	3430	1/1	0.94	0.10	88,88,88,88	0
57	MG	1H	3249	1/1	0.94	0.16	68,68,68,68	0
57	MG	14	3079	1/1	0.94	0.18	61,61,61,61	0
57	MG	14	3232	1/1	0.94	0.10	56,56,56,56	0
57	MG	14	3236	1/1	0.94	0.08	70,70,70,70	0
57	MG	14	3437	1/1	0.94	0.06	107,107,107,107	0
57	MG	14	3132	1/1	0.94	0.19	78,78,78,78	0
57	MG	13	1638	1/1	0.94	0.09	78,78,78,78	0
57	MG	14	3254	1/1	0.94	0.07	52,52,52,52	0
57	MG	1H	3425	1/1	0.94	0.09	74,74,74,74	0
57	MG	1H	3318	1/1	0.94	0.13	54,54,54,54	0
57	MG	14	3186	1/1	0.94	0.15	74,74,74,74	0
57	MG	14	3274	1/1	0.94	0.07	81,81,81,81	0
57	MG	14	3279	1/1	0.94	0.16	83,83,83,83	0
57	MG	14	3280	1/1	0.94	0.08	97,97,97,97	0
57	MG	14	3281	1/1	0.94	0.07	95,95,95,95	0
57	MG	1J	205	1/1	0.94	0.08	87,87,87,87	0
57	MG	1H	3431	1/1	0.94	0.08	60,60,60,60	0
57	MG	1H	3049	1/1	0.94	0.27	69,69,69,69	0
57	MG	1H	3436	1/1	0.94	0.08	65,65,65,65	0
57	MG	1H	3440	1/1	0.94	0.11	61,61,61,61	0
57	MG	13	1746	1/1	0.94	0.05	119,119,119,119	0
57	MG	13	1731	1/1	0.94	0.07	90,90,90,90	0
57	MG	1H	3275	1/1	0.94	0.26	67,67,67,67	0
57	MG	14	3143	1/1	0.94	0.26	54,54,54,54	0
57	MG	1G	1656	1/1	0.94	0.19	66,66,66,66	0
57	MG	C5	201	1/1	0.94	0.09	103,103,103,103	0
57	MG	1H	3193	1/1	0.94	0.43	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	14	3327	1/1	0.94	0.07	100,100,100,100	0
57	MG	1H	3458	1/1	0.94	0.11	82,82,82,82	0
57	MG	14	3335	1/1	0.94	0.11	63,63,63,63	0
57	MG	1H	3116	1/1	0.94	0.12	82,82,82,82	0
57	MG	14	3044	1/1	0.95	0.28	48,48,48,48	0
57	MG	13	1695	1/1	0.95	0.07	82,82,82,82	0
57	MG	14	3374	1/1	0.95	0.07	83,83,83,83	0
57	MG	9A	101	1/1	0.95	0.07	115,115,115,115	0
57	MG	1H	3452	1/1	0.95	0.07	75,75,75,75	0
57	MG	13	1723	1/1	0.95	0.07	83,83,83,83	0
57	MG	1H	3174	1/1	0.95	0.05	37,37,37,37	0
57	MG	1H	3079	1/1	0.95	0.17	45,45,45,45	0
57	MG	1H	3140	1/1	0.95	0.07	40,40,40,40	0
57	MG	1H	3374	1/1	0.95	0.09	86,86,86,86	0
57	MG	1H	3482	1/1	0.95	0.08	102,102,102,102	0
57	MG	13	1740	1/1	0.95	0.05	132,132,132,132	0
57	MG	14	3055	1/1	0.95	0.19	50,50,50,50	0
57	MG	1H	3160	1/1	0.95	0.36	68,68,68,68	0
57	MG	1H	3050	1/1	0.95	0.16	54,54,54,54	0
57	MG	41	201	1/1	0.95	0.09	62,62,62,62	0
57	MG	14	3059	1/1	0.95	0.16	70,70,70,70	0
57	MG	13	1741	1/1	0.95	0.06	110,110,110,110	0
57	MG	1H	3502	1/1	0.95	0.06	90,90,90,90	0
57	MG	14	3011	1/1	0.95	0.23	51,51,51,51	0
57	MG	1H	3395	1/1	0.95	0.06	84,84,84,84	0
57	MG	14	3412	1/1	0.95	0.07	101,101,101,101	0
57	MG	13	1742	1/1	0.95	0.06	98,98,98,98	0
57	MG	1G	1688	1/1	0.95	0.07	89,89,89,89	0
57	MG	14	3121	1/1	0.95	0.14	55,55,55,55	0
57	MG	1H	3401	1/1	0.95	0.11	63,63,63,63	0
57	MG	F8	101	1/1	0.95	0.14	86,86,86,86	0
57	MG	1H	3319	1/1	0.95	0.11	56,56,56,56	0
57	MG	14	3239	1/1	0.95	0.07	59,59,59,59	0
57	MG	14	3243	1/1	0.95	0.07	82,82,82,82	0
57	MG	L8	101	1/1	0.95	0.33	86,86,86,86	0
57	MG	1G	1697	1/1	0.95	0.06	110,110,110,110	0
57	MG	14	3180	1/1	0.95	0.11	65,65,65,65	0
57	MG	13	1724	1/1	0.95	0.06	73,73,73,73	0
57	MG	1H	3517	1/1	0.95	0.16	87,87,87,87	0
57	MG	14	3183	1/1	0.95	0.30	65,65,65,65	0
57	MG	14	3432	1/1	0.95	0.10	103,103,103,103	0
57	MG	14	3129	1/1	0.95	0.51	75,75,75,75	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	1H	3040	1/1	0.95	0.15	36,36,36,36	0
57	MG	1H	3007	1/1	0.95	0.05	58,58,58,58	0
57	MG	1H	3225	1/1	0.95	0.19	74,74,74,74	0
57	MG	13	1699	1/1	0.95	0.07	102,102,102,102	0
57	MG	1H	3428	1/1	0.95	0.10	68,68,68,68	0
57	MG	1H	3030	1/1	0.95	0.27	75,75,75,75	0
57	MG	1H	3330	1/1	0.95	0.07	47,47,47,47	0
57	MG	14	3294	1/1	0.95	0.06	114,114,114,114	0
57	MG	14	3080	1/1	0.95	0.19	51,51,51,51	0
57	MG	1H	3432	1/1	0.95	0.09	56,56,56,56	0
57	MG	1H	3305	1/1	0.95	0.27	71,71,71,71	0
57	MG	14	3303	1/1	0.95	0.10	70,70,70,70	0
57	MG	1H	3533	1/1	0.95	0.08	44,44,44,44	0
57	MG	14	3308	1/1	0.95	0.09	58,58,58,58	0
57	MG	1H	3339	1/1	0.95	0.08	43,43,43,43	0
57	MG	1J	207	1/1	0.95	0.06	92,92,92,92	0
57	MG	1G	1719	1/1	0.95	0.09	119,119,119,119	0
57	MG	14	3034	1/1	0.95	0.13	48,48,48,48	0
57	MG	1G	1722	1/1	0.95	0.08	101,101,101,101	0
57	MG	14	3332	1/1	0.95	0.08	80,80,80,80	0
57	MG	13	1644	1/1	0.95	0.07	82,82,82,82	0
57	MG	1G	1724	1/1	0.95	0.07	94,94,94,94	0
57	MG	14	3349	1/1	0.95	0.06	105,105,105,105	0
57	MG	1H	3348	1/1	0.95	0.07	49,49,49,49	0
57	MG	1G	1728	1/1	0.95	0.05	114,114,114,114	0
57	MG	M5	101	1/1	0.95	0.11	86,86,86,86	0
57	MG	13	1735	1/1	0.95	0.06	111,111,111,111	0
57	MG	1H	3135	1/1	0.95	0.12	42,42,42,42	0
57	MG	14	3362	1/1	0.95	0.06	97,97,97,97	0
57	MG	1G	1655	1/1	0.95	0.13	70,70,70,70	0
57	MG	14	3367	1/1	0.95	0.06	99,99,99,99	0
60	ZN	G8	201	1/1	0.95	0.14	131,131,131,131	0
57	MG	1H	3516	1/1	0.96	0.11	79,79,79,79	0
57	MG	14	3342	1/1	0.96	0.07	82,82,82,82	0
57	MG	14	3197	1/1	0.96	0.15	78,78,78,78	0
57	MG	14	3348	1/1	0.96	0.06	101,101,101,101	0
57	MG	1H	3357	1/1	0.96	0.12	62,62,62,62	0
57	MG	1G	1606	1/1	0.96	0.07	84,84,84,84	0
57	MG	1H	3518	1/1	0.96	0.12	101,101,101,101	0
57	MG	1H	3099	1/1	0.96	0.34	84,84,84,84	0
57	MG	1H	3520	1/1	0.96	0.07	97,97,97,97	0
57	MG	1H	3178	1/1	0.96	0.14	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	1H	3369	1/1	0.96	0.15	54,54,54,54	0
57	MG	13	1744	1/1	0.96	0.10	90,90,90,90	0
57	MG	14	3368	1/1	0.96	0.07	74,74,74,74	0
57	MG	1H	3372	1/1	0.96	0.07	76,76,76,76	0
57	MG	1G	1668	1/1	0.96	0.09	95,95,95,95	0
57	MG	14	3373	1/1	0.96	0.07	97,97,97,97	0
57	MG	1G	1674	1/1	0.96	0.08	78,78,78,78	0
57	MG	4K	102	1/1	0.96	0.07	93,93,93,93	0
57	MG	1H	3443	1/1	0.96	0.06	53,53,53,53	0
57	MG	1H	3528	1/1	0.96	0.10	96,96,96,96	0
57	MG	1H	3444	1/1	0.96	0.06	73,73,73,73	0
57	MG	14	3383	1/1	0.96	0.11	92,92,92,92	0
57	MG	1G	1683	1/1	0.96	0.05	113,113,113,113	0
57	MG	1H	3530	1/1	0.96	0.10	98,98,98,98	0
57	MG	1H	3447	1/1	0.96	0.09	66,66,66,66	0
57	MG	1H	3532	1/1	0.96	0.06	103,103,103,103	0
57	MG	1H	3102	1/1	0.96	0.29	66,66,66,66	0
57	MG	14	3392	1/1	0.96	0.05	112,112,112,112	0
57	MG	1H	3041	1/1	0.96	0.13	51,51,51,51	0
57	MG	1H	3327	1/1	0.96	0.06	65,65,65,65	0
57	MG	1H	3540	1/1	0.96	0.07	81,81,81,81	0
57	MG	14	3397	1/1	0.96	0.04	109,109,109,109	0
57	MG	13	1706	1/1	0.96	0.06	103,103,103,103	0
57	MG	1H	3544	1/1	0.96	0.11	84,84,84,84	0
57	MG	1H	3142	1/1	0.96	0.09	64,64,64,64	0
57	MG	1H	3548	1/1	0.96	0.10	70,70,70,70	0
57	MG	1H	3389	1/1	0.96	0.08	68,68,68,68	0
57	MG	14	3410	1/1	0.96	0.04	116,116,116,116	0
57	MG	1H	3459	1/1	0.96	0.10	64,64,64,64	0
57	MG	1G	1703	1/1	0.96	0.06	113,113,113,113	0
57	MG	1G	1704	1/1	0.96	0.04	107,107,107,107	0
57	MG	14	3098	1/1	0.96	0.40	62,62,62,62	0
57	MG	14	3416	1/1	0.96	0.07	89,89,89,89	0
57	MG	1H	3391	1/1	0.96	0.08	50,50,50,50	0
57	MG	1G	1708	1/1	0.96	0.05	140,140,140,140	0
57	MG	14	3420	1/1	0.96	0.09	96,96,96,96	0
57	MG	1H	3468	1/1	0.96	0.08	68,68,68,68	0
57	MG	14	3102	1/1	0.96	0.14	73,73,73,73	0
57	MG	14	3238	1/1	0.96	0.07	66,66,66,66	0
57	MG	1H	3469	1/1	0.96	0.05	93,93,93,93	0
57	MG	14	3241	1/1	0.96	0.06	100,100,100,100	0
57	MG	1H	3332	1/1	0.96	0.08	50,50,50,50	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	1H	3474	1/1	0.96	0.06	82,82,82,82	0
57	MG	1H	3334	1/1	0.96	0.10	42,42,42,42	0
57	MG	14	3251	1/1	0.96	0.08	63,63,63,63	0
57	MG	16	211	1/1	0.96	0.12	99,99,99,99	0
57	MG	14	3108	1/1	0.96	0.48	77,77,77,77	0
57	MG	1H	3399	1/1	0.96	0.07	54,54,54,54	0
57	MG	1H	3481	1/1	0.96	0.06	80,80,80,80	0
57	MG	13	1700	1/1	0.96	0.06	86,86,86,86	0
57	MG	1G	1720	1/1	0.96	0.05	106,106,106,106	0
57	MG	1G	1721	1/1	0.96	0.06	107,107,107,107	0
57	MG	14	3439	1/1	0.96	0.07	99,99,99,99	0
57	MG	14	3440	1/1	0.96	0.07	98,98,98,98	0
57	MG	13	1734	1/1	0.96	0.04	100,100,100,100	0
57	MG	1H	3409	1/1	0.96	0.06	55,55,55,55	0
57	MG	14	3283	1/1	0.96	0.08	71,71,71,71	0
57	MG	1H	3488	1/1	0.96	0.07	88,88,88,88	0
57	MG	14	3287	1/1	0.96	0.06	73,73,73,73	0
57	MG	14	3288	1/1	0.96	0.07	77,77,77,77	0
57	MG	1H	3493	1/1	0.96	0.06	102,102,102,102	0
57	MG	1G	1726	1/1	0.96	0.05	113,113,113,113	0
57	MG	1H	3496	1/1	0.96	0.08	98,98,98,98	0
57	MG	1H	3410	1/1	0.96	0.06	106,106,106,106	0
57	MG	1G	1731	1/1	0.96	0.06	114,114,114,114	0
57	MG	1H	3343	1/1	0.96	0.06	44,44,44,44	0
57	MG	14	3299	1/1	0.96	0.09	58,58,58,58	0
57	MG	1H	3417	1/1	0.96	0.05	74,74,74,74	0
57	MG	14	3305	1/1	0.96	0.07	78,78,78,78	0
57	MG	14	3306	1/1	0.96	0.08	86,86,86,86	0
57	MG	13	1691	1/1	0.96	0.07	65,65,65,65	0
57	MG	25	202	1/1	0.96	0.07	110,110,110,110	0
57	MG	1H	3075	1/1	0.96	0.11	61,61,61,61	0
57	MG	13	1705	1/1	0.96	0.16	83,83,83,83	0
57	MG	14	3316	1/1	0.96	0.06	90,90,90,90	0
57	MG	14	3317	1/1	0.96	0.07	64,64,64,64	0
57	MG	E5	101	1/1	0.96	0.07	100,100,100,100	0
57	MG	14	3319	1/1	0.96	0.06	78,78,78,78	0
57	MG	14	3322	1/1	0.96	0.07	64,64,64,64	0
57	MG	1H	3512	1/1	0.96	0.09	97,97,97,97	0
57	MG	1H	3013	1/1	0.96	0.20	37,37,37,37	0
57	MG	1H	3426	1/1	0.96	0.09	76,76,76,76	0
57	MG	4L	102	1/1	0.96	0.15	108,108,108,108	0
57	MG	14	3334	1/1	0.96	0.07	94,94,94,94	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	14	3347	1/1	0.97	0.04	101,101,101,101	0
57	MG	1H	3503	1/1	0.97	0.10	47,47,47,47	0
57	MG	1H	3326	1/1	0.97	0.06	47,47,47,47	0
57	MG	1H	3430	1/1	0.97	0.06	61,61,61,61	0
57	MG	1G	1601	1/1	0.97	0.10	70,70,70,70	0
57	MG	13	1693	1/1	0.97	0.05	84,84,84,84	0
57	MG	14	3001	1/1	0.97	0.07	52,52,52,52	0
57	MG	14	3356	1/1	0.97	0.06	67,67,67,67	0
57	MG	14	3357	1/1	0.97	0.05	96,96,96,96	0
57	MG	14	3358	1/1	0.97	0.05	88,88,88,88	0
57	MG	1H	3510	1/1	0.97	0.05	70,70,70,70	0
57	MG	1H	3329	1/1	0.97	0.07	50,50,50,50	0
57	MG	14	3366	1/1	0.97	0.12	98,98,98,98	0
57	MG	1H	3433	1/1	0.97	0.09	61,61,61,61	0
57	MG	1G	1663	1/1	0.97	0.12	76,76,76,76	0
57	MG	13	1716	1/1	0.97	0.05	55,55,55,55	0
57	MG	13	1719	1/1	0.97	0.05	71,71,71,71	0
57	MG	14	3371	1/1	0.97	0.07	90,90,90,90	0
57	MG	14	3372	1/1	0.97	0.11	79,79,79,79	0
57	MG	1H	3439	1/1	0.97	0.05	95,95,95,95	0
57	MG	1G	1670	1/1	0.97	0.13	88,88,88,88	0
57	MG	14	3375	1/1	0.97	0.04	84,84,84,84	0
57	MG	1G	1672	1/1	0.97	0.09	92,92,92,92	0
57	MG	1H	3039	1/1	0.97	0.14	40,40,40,40	0
57	MG	1H	3441	1/1	0.97	0.06	44,44,44,44	0
57	MG	1G	1676	1/1	0.97	0.05	100,100,100,100	0
57	MG	14	3382	1/1	0.97	0.06	72,72,72,72	0
57	MG	1H	3442	1/1	0.97	0.12	69,69,69,69	0
57	MG	1H	3054	1/1	0.97	0.17	37,37,37,37	0
57	MG	1H	3336	1/1	0.97	0.06	50,50,50,50	0
57	MG	1H	3445	1/1	0.97	0.06	44,44,44,44	0
57	MG	14	3389	1/1	0.97	0.14	94,94,94,94	0
57	MG	14	3088	1/1	0.97	0.07	53,53,53,53	0
57	MG	1H	3338	1/1	0.97	0.08	63,63,63,63	0
57	MG	1H	3525	1/1	0.97	0.12	134,134,134,134	0
57	MG	14	3235	1/1	0.97	0.09	65,65,65,65	0
57	MG	1H	3215	1/1	0.97	0.33	69,69,69,69	0
57	MG	1H	3390	1/1	0.97	0.07	68,68,68,68	0
57	MG	1H	3177	1/1	0.97	0.45	77,77,77,77	0
57	MG	14	3398	1/1	0.97	0.07	99,99,99,99	0
57	MG	14	3400	1/1	0.97	0.06	76,76,76,76	0
57	MG	1H	3392	1/1	0.97	0.10	52,52,52,52	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	1G	1692	1/1	0.97	0.06	105,105,105,105	0
57	MG	14	3403	1/1	0.97	0.09	83,83,83,83	0
57	MG	1G	1694	1/1	0.97	0.07	94,94,94,94	0
57	MG	1H	3063	1/1	0.97	0.13	53,53,53,53	0
57	MG	14	3407	1/1	0.97	0.05	83,83,83,83	0
57	MG	14	3408	1/1	0.97	0.04	111,111,111,111	0
57	MG	14	3248	1/1	0.97	0.05	57,57,57,57	0
57	MG	1H	3455	1/1	0.97	0.05	42,42,42,42	0
57	MG	1H	3344	1/1	0.97	0.04	46,46,46,46	0
57	MG	13	1621	1/1	0.97	0.10	56,56,56,56	0
57	MG	14	3257	1/1	0.97	0.06	69,69,69,69	0
57	MG	1G	1699	1/1	0.97	0.07	93,93,93,93	0
57	MG	14	3262	1/1	0.97	0.07	66,66,66,66	0
57	MG	14	3417	1/1	0.97	0.08	89,89,89,89	0
57	MG	1H	3462	1/1	0.97	0.06	53,53,53,53	0
57	MG	14	3272	1/1	0.97	0.06	78,78,78,78	0
57	MG	14	3273	1/1	0.97	0.10	70,70,70,70	0
57	MG	2K	104	1/1	0.97	0.10	89,89,89,89	0
57	MG	14	3275	1/1	0.97	0.06	74,74,74,74	0
57	MG	1H	3539	1/1	0.97	0.07	45,45,45,45	0
57	MG	1H	3465	1/1	0.97	0.07	63,63,63,63	0
57	MG	14	3425	1/1	0.97	0.11	91,91,91,91	0
57	MG	1H	3467	1/1	0.97	0.05	85,85,85,85	0
57	MG	14	3036	1/1	0.97	0.14	47,47,47,47	0
57	MG	13	1729	1/1	0.97	0.10	73,73,73,73	0
57	MG	1H	3404	1/1	0.97	0.05	65,65,65,65	0
57	MG	1H	3471	1/1	0.97	0.06	73,73,73,73	0
57	MG	1H	3472	1/1	0.97	0.14	62,62,62,62	0
57	MG	14	3289	1/1	0.97	0.05	90,90,90,90	0
57	MG	1H	3405	1/1	0.97	0.06	46,46,46,46	0
57	MG	14	3292	1/1	0.97	0.05	85,85,85,85	0
57	MG	1H	3277	1/1	0.97	0.30	82,82,82,82	0
57	MG	1H	3477	1/1	0.97	0.05	83,83,83,83	0
57	MG	1H	3353	1/1	0.97	0.11	64,64,64,64	0
57	MG	1H	3414	1/1	0.97	0.06	95,95,95,95	0
57	MG	14	3297	1/1	0.97	0.08	66,66,66,66	0
57	MG	1G	1716	1/1	0.97	0.05	92,92,92,92	0
57	MG	1H	3354	1/1	0.97	0.07	73,73,73,73	0
57	MG	14	3301	1/1	0.97	0.07	117,117,117,117	0
57	MG	14	3302	1/1	0.97	0.12	86,86,86,86	0
57	MG	1G	1718	1/1	0.97	0.07	91,91,91,91	0
57	MG	1H	3356	1/1	0.97	0.05	75,75,75,75	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	1H	3136	1/1	0.97	0.11	45,45,45,45	0
57	MG	1H	3420	1/1	0.97	0.06	102,102,102,102	0
57	MG	1H	3487	1/1	0.97	0.08	72,72,72,72	0
57	MG	14	3310	1/1	0.97	0.06	64,64,64,64	0
57	MG	14	3312	1/1	0.97	0.05	80,80,80,80	0
57	MG	1H	3360	1/1	0.97	0.10	76,76,76,76	0
57	MG	1H	3489	1/1	0.97	0.06	69,69,69,69	0
57	MG	1H	3491	1/1	0.97	0.14	62,62,62,62	0
57	MG	1H	3195	1/1	0.97	0.07	59,59,59,59	0
57	MG	14	3320	1/1	0.97	0.05	46,46,46,46	0
57	MG	1H	3495	1/1	0.97	0.05	94,94,94,94	0
57	MG	14	3323	1/1	0.97	0.05	83,83,83,83	0
57	MG	78	201	1/1	0.97	0.10	57,57,57,57	0
57	MG	1G	1730	1/1	0.97	0.08	94,94,94,94	0
57	MG	14	3330	1/1	0.97	0.06	64,64,64,64	0
57	MG	1H	3076	1/1	0.97	0.09	39,39,39,39	0
57	MG	1G	1734	1/1	0.97	0.10	84,84,84,84	0
57	MG	1H	3366	1/1	0.97	0.07	63,63,63,63	0
57	MG	1H	3427	1/1	0.97	0.05	66,66,66,66	0
57	MG	14	3337	1/1	0.97	0.05	57,57,57,57	0
57	MG	14	3338	1/1	0.97	0.07	81,81,81,81	0
57	MG	1H	3501	1/1	0.97	0.07	75,75,75,75	0
57	MG	14	3343	1/1	0.97	0.05	87,87,87,87	0
57	MG	1H	3368	1/1	0.97	0.08	59,59,59,59	0
57	MG	14	3379	1/1	0.98	0.07	99,99,99,99	0
57	MG	1H	3463	1/1	0.98	0.06	48,48,48,48	0
57	MG	1H	3396	1/1	0.98	0.05	64,64,64,64	0
57	MG	13	1718	1/1	0.98	0.04	88,88,88,88	0
57	MG	14	3285	1/1	0.98	0.09	79,79,79,79	0
57	MG	14	3384	1/1	0.98	0.05	88,88,88,88	0
57	MG	14	3385	1/1	0.98	0.08	80,80,80,80	0
57	MG	14	3286	1/1	0.98	0.04	93,93,93,93	0
57	MG	13	1697	1/1	0.98	0.05	78,78,78,78	0
57	MG	1G	1682	1/1	0.98	0.05	105,105,105,105	0
57	MG	1H	3400	1/1	0.98	0.04	59,59,59,59	0
57	MG	14	3290	1/1	0.98	0.06	66,66,66,66	0
57	MG	13	1720	1/1	0.98	0.04	100,100,100,100	0
57	MG	1H	3371	1/1	0.98	0.05	56,56,56,56	0
57	MG	13	1722	1/1	0.98	0.04	77,77,77,77	0
57	MG	1G	1687	1/1	0.98	0.04	95,95,95,95	0
57	MG	1H	3435	1/1	0.98	0.04	60,60,60,60	0
57	MG	1H	3333	1/1	0.98	0.10	67,67,67,67	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	1G	1690	1/1	0.98	0.05	114,114,114,114	0
57	MG	14	3399	1/1	0.98	0.12	95,95,95,95	0
57	MG	1H	3476	1/1	0.98	0.05	68,68,68,68	0
57	MG	1H	3437	1/1	0.98	0.07	46,46,46,46	0
57	MG	14	3300	1/1	0.98	0.10	73,73,73,73	0
57	MG	1G	1693	1/1	0.98	0.06	84,84,84,84	0
57	MG	1H	3478	1/1	0.98	0.08	78,78,78,78	0
57	MG	1H	3438	1/1	0.98	0.05	50,50,50,50	0
57	MG	14	3406	1/1	0.98	0.05	90,90,90,90	0
57	MG	14	3304	1/1	0.98	0.05	68,68,68,68	0
57	MG	1H	3407	1/1	0.98	0.07	77,77,77,77	0
57	MG	1H	3408	1/1	0.98	0.05	69,69,69,69	0
57	MG	13	1738	1/1	0.98	0.05	70,70,70,70	0
57	MG	1H	3143	1/1	0.98	0.08	66,66,66,66	0
57	MG	1H	3411	1/1	0.98	0.06	80,80,80,80	0
57	MG	14	3311	1/1	0.98	0.05	68,68,68,68	0
57	MG	14	3414	1/1	0.98	0.12	100,100,100,100	0
57	MG	1H	3486	1/1	0.98	0.06	89,89,89,89	0
57	MG	1H	3378	1/1	0.98	0.05	65,65,65,65	0
57	MG	14	3314	1/1	0.98	0.08	83,83,83,83	0
57	MG	1H	3534	1/1	0.98	0.08	92,92,92,92	0
57	MG	13	1739	1/1	0.98	0.03	92,92,92,92	0
57	MG	1G	1705	1/1	0.98	0.05	124,124,124,124	0
57	MG	1H	3536	1/1	0.98	0.05	60,60,60,60	0
57	MG	1H	3446	1/1	0.98	0.06	60,60,60,60	0
57	MG	14	3234	1/1	0.98	0.06	56,56,56,56	0
57	MG	1H	3416	1/1	0.98	0.04	89,89,89,89	0
57	MG	14	3325	1/1	0.98	0.10	52,52,52,52	0
57	MG	1H	3492	1/1	0.98	0.04	83,83,83,83	0
57	MG	14	3328	1/1	0.98	0.09	56,56,56,56	0
57	MG	1H	3541	1/1	0.98	0.05	67,67,67,67	0
57	MG	1H	3358	1/1	0.98	0.05	40,40,40,40	0
57	MG	14	3240	1/1	0.98	0.04	62,62,62,62	0
57	MG	1H	3543	1/1	0.98	0.07	70,70,70,70	0
57	MG	1H	3386	1/1	0.98	0.04	48,48,48,48	0
57	MG	1H	3545	1/1	0.98	0.03	116,116,116,116	0
57	MG	13	1708	1/1	0.98	0.07	95,95,95,95	0
57	MG	14	3339	1/1	0.98	0.04	49,49,49,49	0
57	MG	14	3341	1/1	0.98	0.05	91,91,91,91	0
57	MG	14	3247	1/1	0.98	0.07	60,60,60,60	0
57	MG	1H	3362	1/1	0.98	0.05	56,56,56,56	0
57	MG	14	3344	1/1	0.98	0.07	88,88,88,88	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	14	3250	1/1	0.98	0.05	76,76,76,76	0
57	MG	1H	3363	1/1	0.98	0.05	47,47,47,47	0
57	MG	14	3252	1/1	0.98	0.07	62,62,62,62	0
57	MG	1H	3453	1/1	0.98	0.10	58,58,58,58	0
57	MG	14	3255	1/1	0.98	0.06	52,52,52,52	0
57	MG	1H	3424	1/1	0.98	0.04	100,100,100,100	0
57	MG	1H	3456	1/1	0.98	0.05	41,41,41,41	0
57	MG	14	3260	1/1	0.98	0.05	55,55,55,55	0
57	MG	1G	1667	1/1	0.98	0.09	90,90,90,90	0
57	MG	13	1694	1/1	0.98	0.04	94,94,94,94	0
57	MG	14	3263	1/1	0.98	0.04	56,56,56,56	0
57	MG	14	3359	1/1	0.98	0.04	86,86,86,86	0
57	MG	14	3360	1/1	0.98	0.07	94,94,94,94	0
57	MG	14	3264	1/1	0.98	0.06	52,52,52,52	0
57	MG	29	302	1/1	0.98	0.04	52,52,52,52	0
57	MG	14	3363	1/1	0.98	0.05	102,102,102,102	0
57	MG	14	3364	1/1	0.98	0.08	85,85,85,85	0
57	MG	14	3265	1/1	0.98	0.06	52,52,52,52	0
57	MG	14	3267	1/1	0.98	0.04	86,86,86,86	0
57	MG	1G	1669	1/1	0.98	0.08	99,99,99,99	0
57	MG	14	3271	1/1	0.98	0.07	72,72,72,72	0
57	MG	13	1717	1/1	0.98	0.06	53,53,53,53	0
57	MG	1G	1671	1/1	0.98	0.06	86,86,86,86	0
57	MG	1G	1727	1/1	0.98	0.04	93,93,93,93	0
57	MG	1H	3461	1/1	0.98	0.05	48,48,48,48	0
57	MG	14	3276	1/1	0.98	0.05	95,95,95,95	0
57	MG	14	3277	1/1	0.98	0.06	59,59,59,59	0
57	MG	1G	1673	1/1	0.98	0.06	71,71,71,71	0
57	MG	1H	3328	1/1	0.98	0.06	46,46,46,46	0
57	MG	14	3377	1/1	0.98	0.05	64,64,64,64	0
57	MG	1H	3511	1/1	0.98	0.04	92,92,92,92	0
57	MG	I8	101	1/1	0.99	0.06	69,69,69,69	0
57	MG	14	3242	1/1	0.99	0.05	44,44,44,44	0
57	MG	1H	3341	1/1	0.99	0.07	48,48,48,48	0
57	MG	1H	3342	1/1	0.99	0.04	42,42,42,42	0
57	MG	14	3245	1/1	0.99	0.06	56,56,56,56	0
57	MG	14	3395	1/1	0.99	0.05	91,91,91,91	0
57	MG	14	3315	1/1	0.99	0.09	86,86,86,86	0
57	MG	1H	3381	1/1	0.99	0.05	48,48,48,48	0
57	MG	1H	3382	1/1	0.99	0.09	54,54,54,54	0
57	MG	14	3318	1/1	0.99	0.04	75,75,75,75	0
57	MG	1G	1706	1/1	0.99	0.04	79,79,79,79	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	14	3249	1/1	0.99	0.06	60,60,60,60	0
57	MG	14	3321	1/1	0.99	0.05	64,64,64,64	0
57	MG	1H	3413	1/1	0.99	0.04	59,59,59,59	0
57	MG	1H	3384	1/1	0.99	0.02	61,61,61,61	0
57	MG	1H	3385	1/1	0.99	0.04	77,77,77,77	0
57	MG	14	3253	1/1	0.99	0.09	53,53,53,53	0
57	MG	14	3326	1/1	0.99	0.04	60,60,60,60	0
57	MG	13	1701	1/1	0.99	0.08	69,69,69,69	0
57	MG	1H	3485	1/1	0.99	0.03	83,83,83,83	0
57	MG	14	3329	1/1	0.99	0.03	60,60,60,60	0
57	MG	1H	3387	1/1	0.99	0.04	53,53,53,53	0
57	MG	13	1698	1/1	0.99	0.03	94,94,94,94	0
57	MG	14	3258	1/1	0.99	0.03	71,71,71,71	0
57	MG	14	3333	1/1	0.99	0.05	66,66,66,66	0
57	MG	14	3259	1/1	0.99	0.05	63,63,63,63	0
57	MG	1H	3419	1/1	0.99	0.04	78,78,78,78	0
57	MG	14	3336	1/1	0.99	0.09	65,65,65,65	0
57	MG	1H	3346	1/1	0.99	0.05	53,53,53,53	0
57	MG	1H	3490	1/1	0.99	0.03	65,65,65,65	0
57	MG	1H	3347	1/1	0.99	0.07	56,56,56,56	0
57	MG	14	3340	1/1	0.99	0.06	69,69,69,69	0
57	MG	1H	3538	1/1	0.99	0.11	58,58,58,58	0
57	MG	1H	3367	1/1	0.99	0.05	56,56,56,56	0
57	MG	14	3266	1/1	0.99	0.04	72,72,72,72	0
57	MG	1G	1665	1/1	0.99	0.10	78,78,78,78	0
57	MG	14	3345	1/1	0.99	0.07	83,83,83,83	0
57	MG	1H	3454	1/1	0.99	0.02	48,48,48,48	0
57	MG	14	3269	1/1	0.99	0.03	63,63,63,63	0
57	MG	1H	3494	1/1	0.99	0.05	98,98,98,98	0
57	MG	1H	3423	1/1	0.99	0.04	66,66,66,66	0
57	MG	14	3350	1/1	0.99	0.04	61,61,61,61	0
57	MG	13	1709	1/1	0.99	0.06	69,69,69,69	0
57	MG	14	3433	1/1	0.99	0.04	69,69,69,69	0
57	MG	1H	3497	1/1	0.99	0.03	79,79,79,79	0
57	MG	1H	3457	1/1	0.99	0.03	45,45,45,45	0
57	MG	14	3354	1/1	0.99	0.04	73,73,73,73	0
57	MG	1H	3546	1/1	0.99	0.03	41,41,41,41	0
57	MG	1H	3393	1/1	0.99	0.03	69,69,69,69	0
57	MG	14	3278	1/1	0.99	0.05	80,80,80,80	0
57	MG	1H	3394	1/1	0.99	0.05	74,74,74,74	0
57	MG	1H	3460	1/1	0.99	0.03	48,48,48,48	0
57	MG	13	1704	1/1	0.99	0.05	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	14	3361	1/1	0.99	0.04	80,80,80,80	0
57	MG	1G	1732	1/1	0.99	0.04	114,114,114,114	0
57	MG	1G	1677	1/1	0.99	0.07	97,97,97,97	0
57	MG	13	1696	1/1	0.99	0.07	83,83,83,83	0
57	MG	1G	1679	1/1	0.99	0.05	93,93,93,93	0
57	MG	1H	3505	1/1	0.99	0.04	79,79,79,79	0
57	MG	1H	3506	1/1	0.99	0.06	61,61,61,61	0
57	MG	1H	3507	1/1	0.99	0.05	74,74,74,74	0
57	MG	13	1712	1/1	0.99	0.08	101,101,101,101	0
57	MG	1H	3398	1/1	0.99	0.06	61,61,61,61	0
57	MG	16	209	1/1	0.99	0.06	68,68,68,68	0
57	MG	16	210	1/1	0.99	0.04	78,78,78,78	0
57	MG	13	1713	1/1	0.99	0.04	65,65,65,65	0
57	MG	1H	3466	1/1	0.99	0.03	89,89,89,89	0
57	MG	1H	3337	1/1	0.99	0.07	44,44,44,44	0
57	MG	21	302	1/1	0.99	0.03	46,46,46,46	0
57	MG	13	1714	1/1	0.99	0.06	100,100,100,100	0
57	MG	1H	3514	1/1	0.99	0.07	76,76,76,76	0
57	MG	1H	3375	1/1	0.99	0.07	48,48,48,48	0
57	MG	45	201	1/1	0.99	0.14	74,74,74,74	0
57	MG	1H	3470	1/1	0.99	0.07	73,73,73,73	0
57	MG	14	3233	1/1	0.99	0.10	54,54,54,54	0
57	MG	1H	3403	1/1	0.99	0.04	50,50,50,50	0
57	MG	1H	3376	1/1	0.99	0.04	45,45,45,45	0
57	MG	13	1725	1/1	0.99	0.06	90,90,90,90	0
57	MG	14	3237	1/1	0.99	0.06	56,56,56,56	0
57	MG	1H	3406	1/1	0.99	0.04	46,46,46,46	0
57	MG	1H	3475	1/1	0.99	0.04	83,83,83,83	0
57	MG	13	1692	1/1	0.99	0.05	61,61,61,61	0
59	SF4	3E	301	8/8	0.99	0.03	86,90,100,103	0
59	SF4	32	301	8/8	0.99	0.04	90,99,108,116	0
60	ZN	5I	102	1/1	0.99	0.03	98,98,98,98	0
57	MG	14	3309	1/1	0.99	0.05	71,71,71,71	0
60	ZN	5A	101	1/1	0.99	0.04	123,123,123,123	0
60	ZN	C5	202	1/1	0.99	0.06	151,151,151,151	0
57	MG	14	3270	1/1	1.00	0.03	65,65,65,65	0
57	MG	1H	3412	1/1	1.00	0.03	51,51,51,51	0
57	MG	1H	3335	1/1	1.00	0.03	53,53,53,53	0
57	MG	1H	3361	1/1	1.00	0.02	74,74,74,74	0
57	MG	11	302	1/1	1.00	0.05	47,47,47,47	0
57	MG	1H	3345	1/1	1.00	0.04	51,51,51,51	0
57	MG	1H	3355	1/1	1.00	0.05	67,67,67,67	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	13	1721	1/1	1.00	0.07	62,62,62,62	0
57	MG	1H	3351	1/1	1.00	0.04	59,59,59,59	0
57	MG	1H	3499	1/1	1.00	0.02	52,52,52,52	0
57	MG	13	1703	1/1	1.00	0.07	66,66,66,66	0
57	MG	1H	3383	1/1	1.00	0.02	53,53,53,53	0
57	MG	1H	3359	1/1	1.00	0.04	60,60,60,60	0

6.5 Other polymers [i](#)

There are no such residues in this entry.