



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 17, 2026 – 09:19 PM UTC

PDB ID : 5EL4 / pdb_00005el4
Title : Structure of T. thermophilus 70S ribosome complex with mRNA and tRNA^{Lys} in the A-site with a U-U mismatch in the first position
Authors : Rozov, A.; Demeshkina, N.; Khusainov, I.; Yusupov, M.; Yusupova, G.
Deposited on : 2015-11-04
Resolution : 3.15 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	:	2022.3.0, CSD as543be (2022)
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

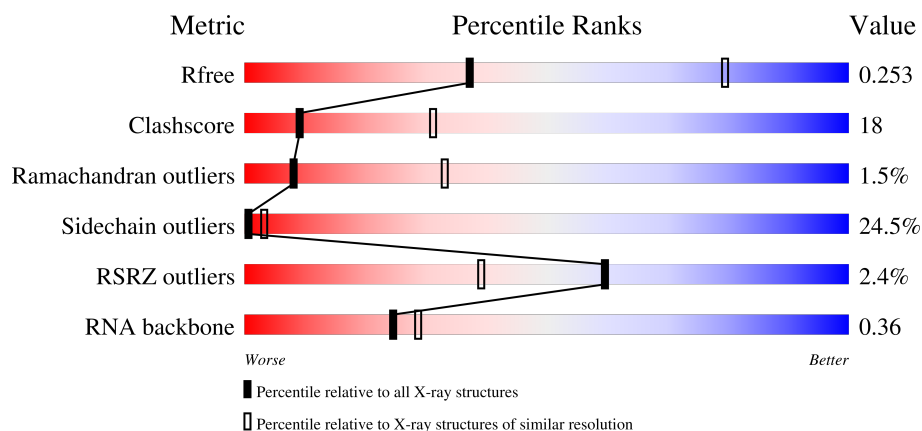
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.15 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	2361 (3.20-3.12)
Clashscore	190562	2486 (3.20-3.12)
Ramachandran outliers	187476	2405 (3.20-3.12)
Sidechain outliers	187428	2404 (3.20-3.12)
RSRZ outliers	180081	2361 (3.20-3.12)
RNA backbone	3983	1113 (3.42-2.90)

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	38% 45% 15% •
1	1G	1522	2% 37% 47% 15% •
2	12	256	28% 36% 15% • 19%
2	1E	256	39% 39% 12% 10%

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

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Mol	Chain	Length	Quality of chain
15	6I	89	
16	7A	88	
16	7I	88	
17	8A	105	
17	8I	105	
18	9A	88	
18	9I	88	
19	AA	93	
19	AI	93	
20	BA	106	
20	BI	106	
21	1B	27	
21	1F	27	
22	1K	76	
23	2K	77	
23	2L	77	
24	3K	76	
25	4K	27	
25	4L	27	
26	14	2917	
26	1H	2917	
27	16	122	
27	1J	122	
28	7I	229	
29	11	276	

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Mol	Chain	Length	Quality of chain
29	19	276	
30	21	206	
30	29	206	
31	31	210	
31	39	210	
32	41	182	
32	49	182	
33	51	180	
33	59	180	
34	61	148	
34	69	148	
35	15	140	
35	58	140	
36	25	122	
36	68	122	
37	35	150	
37	78	150	
38	45	141	
38	88	141	
39	55	118	
39	98	118	
40	65	112	
40	A8	112	
41	75	146	
41	B8	146	

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Mol	Chain	Length	Quality of chain
42	85	118	
42	C8	118	
43	95	101	
43	D8	101	
44	A5	113	
44	E8	113	
45	B5	96	
45	F8	96	
46	C5	110	
46	G8	110	
47	D5	206	
47	H8	206	
48	E5	85	
48	I8	85	
49	F5	98	
49	J8	98	
50	G5	72	
50	K8	72	
51	H5	60	
51	L8	60	
52	M8	71	
53	J5	60	
53	N8	60	
54	L5	49	
54	P8	49	

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Mol	Chain	Length	Quality of chain
55	M5	65	
55	Q8	65	
56	1L	76	
57	3L	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
58	MG	14	3068	-	-	-	X
58	MG	14	3102	-	-	-	X
58	MG	14	3226	-	-	-	X
58	MG	14	3277	-	-	-	X
58	MG	1H	3317	-	-	-	X
58	MG	1H	3318	-	-	-	X

2 Entry composition

There are 61 unique types of molecules in this entry. The entry contains 294304 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	1507	Total	C	N	O	P	0	0	0
			32391	14418	6004	10463	1506			

There are 6 discrepancies between the modelled and reference sequences:

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	1E	231	Total	C	N	O	S	0	0	0
			1874	1199	334	336	5			
2	12	208	Total	C	N	O	S	0	0	0
			1711	1094	307	306	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	194	Total	C	N	O	S	0	0	0
			1529	967	296	265	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	3E	208	Total	C	N	O	S	0	0	0
			1702	1066	339	290	7			
4	32	208	Total	C	N	O	S	0	0	0
			1702	1066	339	290	7			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	4E	149	Total	C	N	O	S	0	0	0
			1142	722	216	200	4			
5	42	147	Total	C	N	O	S	0	0	0
			1123	709	214	196	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	149	Total	C	N	O	S	0	0	0
			1214	754	244	210	6			
7	62	138	Total	C	N	O	S	0	0	0
			1110	689	221	194	6			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	7E	138	Total	C	N	O	S	0	0	0
			1115	705	215	192	3			
8	72	138	Total	C	N	O	S	0	0	0
			1115	705	215	192	3			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	8E	127	Total	C	N	O		0	0	0
			1005	637	197	171				

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
9	82	124	Total	C	N	O	0	0	0
			983	624	190	169			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	1I	91	Total	C	N	O	S	0	0	0
			734	459	144	130	1			
10	1A	78	Total	C	N	O		0	0	0
			626	388	126	112				

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	3I	122	Total	C	N	O	S	0	0	0
			956	603	193	159	1			
12	3A	121	Total	C	N	O	S	0	0	0
			947	597	191	158	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	4I	116	Total	C	N	O	S	0	0	0
			928	574	191	161	2			
13	4A	110	Total	C	N	O	S	0	0	0
			888	549	182	155	2			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
14	5I	61	Total	C	N	O	S	0	0	0
			496	315	105	72	4			
14	5A	57	Total	C	N	O	S	0	0	0
			466	297	97	68	4			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
15	6I	88	Total	C	N	O	S	0	0	0
			733	459	147	125	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	80	Total	C	N	O	S	0	0	0
			671	427	132	111	1			
16	7A	84	Total	C	N	O	S	0	0	0
			705	446	140	118	1			

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

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

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
18	9I	67	Total	C	N	O	0	0	0
			544	349	104	91			
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	80	Total	C	N	O	S	0	0	0
			643	411	118	112	2			
19	AA	60	Total	C	N	O	S	0	0	0
			471	300	83	86	2			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
20	BI	97	Total	C	N	O	S	0	0	0
			746	461	157	126	2			
20	BA	98	Total	C	N	O	S	0	0	0
			757	467	161	127	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	24	Total	C	N	O		0	0	0
			208	128	50	30				

- Molecule 22 is a RNA chain called tRNA-Lys.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
22	1K	69	Total	C	N	O	P	S	0	0	0
			1477	662	257	488	69	1			

- Molecule 23 is a RNA chain called tRNA-fMet.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
23	2K	77	Total	C	N	O	P	S	0	0	0
			1646	735	297	536	77	1			
23	2L	76	Total	C	N	O	P	S	0	0	0
			1626	726	295	528	76	1			

- Molecule 24 is a RNA chain called tRNA-Lys.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
24	3K	76	Total	C	N	O	P	0	0	0
			1611	721	281	534	75			

- Molecule 25 is a RNA chain called mRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
25	4K	20	Total	C	N	O	P	0	0	0
			439	197	91	131	20			
25	4L	17	Total	C	N	O	P	0	0	0
			373	167	76	113	17			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
26	1H	2833	Total 61028	C 27159	N 11418	O 19618	P 2833	0	0	0
26	14	2861	Total 61630	C 27429	N 11535	O 19806	P 2860	0	0	0

There are 14 discrepancies between the modelled and reference sequences:

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
28	71	133	Total 1033	C 651	N 194	O 187	S 1	0	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
71	19	ILE	VAL	conflict	UNP Q5SLP7
71	27	HIS	ARG	conflict	UNP Q5SLP7

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
30	21	204	Total	C	N	O	S	0	0	0
			1563	988	299	270	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	205	Total	C	N	O	S	0	0	0
			1606	1024	300	280	2			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
32	41	180	Total	C	N	O	S	0	0	0
			1464	936	266	258	4			
32	49	180	Total	C	N	O	S	0	0	0
			1464	936	266	258	4			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
33	51	173	Total	C	N	O	S	0	0	0
			1327	842	249	235	1			
33	59	69	Total	C	N	O		0	0	0
			539	339	109	91				

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
35	58	138	Total	C	N	O	S	0	0	0
			1104	712	206	182	4			
35	15	137	Total	C	N	O	S	0	0	0
			1096	707	205	181	3			

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
37	78	147	Total	C	N	O	S	0	0	0
			1122	698	229	192	3			
37	35	148	Total	C	N	O	S	0	0	0
			1130	704	230	193	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
			1113	709	210	187	7			
38	45	138	Total	C	N	O	S	0	0	0
			1099	702	208	183	6			

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
41	B8	134	Total	C	N	O	S	0	0	0
			1118	696	229	192	1			
41	75	136	Total	C	N	O	S	0	0	0
			1132	704	232	195	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	99	Total	C	N	O	S	0	0	0
			763	493	137	132	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
44	E8	112	Total	C	N	O	S	0	0	0
			890	560	175	153	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	96	Total	C	N	O		0	0	0
			751	489	135	127				
45	B5	94	Total	C	N	O	S	0	0	0
			738	479	133	125	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
46	G8	103	Total	C	N	O	S	0	0	0
			783	504	148	126	5			
46	C5	104	Total	C	N	O	S	0	0	0
			794	510	152	127	5			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
47	H8	148	Total	C	N	O	S	0	0	0
			1222	781	221	217	3			
47	D5	126	Total	C	N	O	S	0	0	0
			1034	667	187	178	2			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
48	I8	78	Total	C	N	O	S	0	0	0
			616	381	130	104	1			
48	E5	78	Total	C	N	O	S	0	0	0
			616	381	130	104	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
			571	355	115	100	1			
50	G5	69	Total	C	N	O	S	0	0	0
			573	355	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	S	0	0	0
			459	293	89	77				
51	H5	58	Total	C	N	O	S	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	47	Total	C	N	O	S	0	0	0
			366	234	61	66	5			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
53	N8	49	Total	C	N	O	S	0	0	0
			381	238	76	62	5			
53	J5	56	Total	C	N	O	S	0	0	0
			434	272	87	70	5			

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

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

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

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

- Molecule 56 is a RNA chain called tRNA-Lys.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
56	1L	74	Total	C	N	O	P	0	0	0
			1570	702	271	523	74			

- Molecule 57 is a RNA chain called tRNA-Lys.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
57	3L	74	Total	C	N	O	P	0	0	0
			1571	703	277	518	73			

- Molecule 58 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

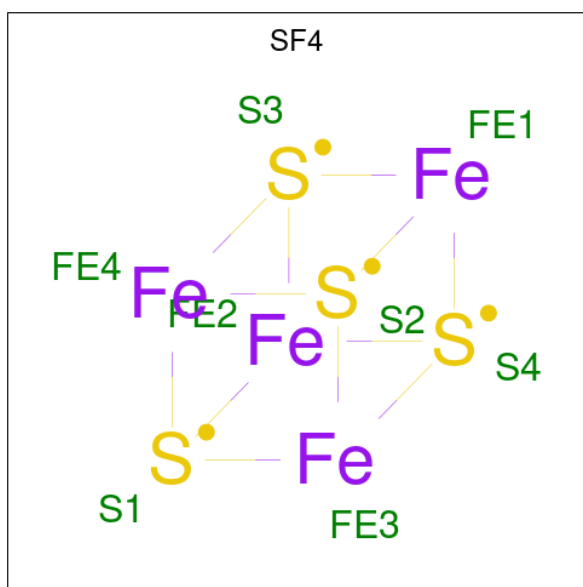
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
58	13	142	Total	Mg	0	0
			142	142		
58	1I	1	Total	Mg	0	0
			1	1		
58	2I	1	Total	Mg	0	0
			1	1		
58	3I	1	Total	Mg	0	0
			1	1		
58	4I	1	Total	Mg	0	0
			1	1		
58	5I	1	Total	Mg	0	0
			1	1		
58	7I	1	Total	Mg	0	0
			1	1		
58	1K	1	Total	Mg	0	0
			1	1		
58	2K	2	Total	Mg	0	0
			2	2		
58	4K	1	Total	Mg	0	0
			1	1		
58	1H	495	Total	Mg	0	0
			495	495		
58	16	11	Total	Mg	0	0
			11	11		
58	11	1	Total	Mg	0	0
			1	1		
58	21	2	Total	Mg	0	0
			2	2		
58	41	1	Total	Mg	0	0
			1	1		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
58	78	1	Total 1	Mg 1	0	0
58	88	3	Total 3	Mg 3	0	0
58	I8	1	Total 1	Mg 1	0	0
58	J8	1	Total 1	Mg 1	0	0
58	N8	1	Total 1	Mg 1	0	0
58	P8	1	Total 1	Mg 1	0	0
58	Q8	1	Total 1	Mg 1	0	0
58	1G	95	Total 95	Mg 95	0	0
58	2L	2	Total 2	Mg 2	0	0
58	3L	1	Total 1	Mg 1	0	0
58	14	421	Total 421	Mg 421	0	0
58	1J	6	Total 6	Mg 6	0	0
58	19	1	Total 1	Mg 1	0	0
58	29	3	Total 3	Mg 3	0	0
58	39	2	Total 2	Mg 2	0	0
58	25	1	Total 1	Mg 1	0	0
58	45	3	Total 3	Mg 3	0	0
58	E5	1	Total 1	Mg 1	0	0

- Molecule 59 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe₄S₄).



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	207	Total	O	0	0
			207	207		
61	3E	2	Total	O	0	0
			2	2		
61	4E	2	Total	O	0	0
			2	2		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
61	8E	1	Total 1	O 1	0	0
61	1I	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	6I	1	Total 1	O 1	0	0
61	4K	4	Total 4	O 4	0	0
61	1H	819	Total 819	O 819	0	0
61	16	22	Total 22	O 22	0	0
61	11	9	Total 9	O 9	0	0
61	21	6	Total 6	O 6	0	0
61	31	4	Total 4	O 4	0	0
61	78	1	Total 1	O 1	0	0
61	B8	1	Total 1	O 1	0	0
61	C8	3	Total 3	O 3	0	0
61	F8	1	Total 1	O 1	0	0
61	I8	5	Total 5	O 5	0	0
61	J8	2	Total 2	O 2	0	0
61	L8	3	Total 3	O 3	0	0
61	1G	117	Total 117	O 117	0	0
61	32	2	Total 2	O 2	0	0
61	2A	1	Total 1	O 1	0	0

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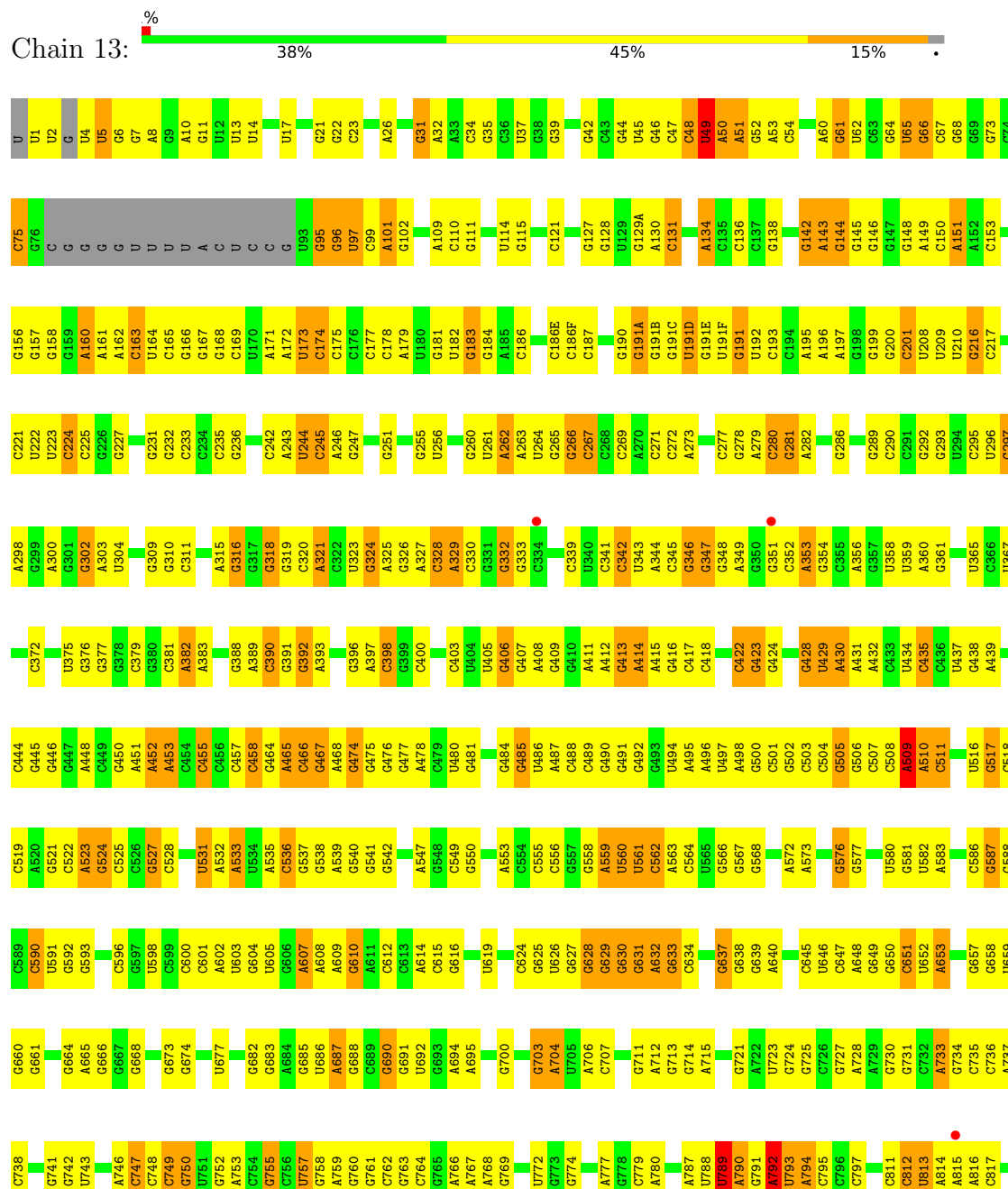
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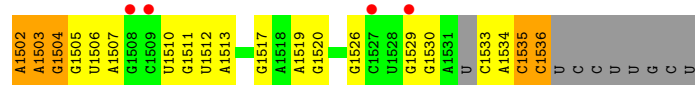
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
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61	7A	1	Total 1	O 1	0	0
61	BA	1	Total 1	O 1	0	0
61	14	717	Total 717	O 717	0	0
61	1J	6	Total 6	O 6	0	0
61	19	10	Total 10	O 10	0	0
61	29	3	Total 3	O 3	0	0
61	39	3	Total 3	O 3	0	0
61	15	1	Total 1	O 1	0	0
61	35	3	Total 3	O 3	0	0
61	75	2	Total 2	O 2	0	0
61	85	3	Total 3	O 3	0	0
61	M5	3	Total 3	O 3	0	0

3 Residue-property plots

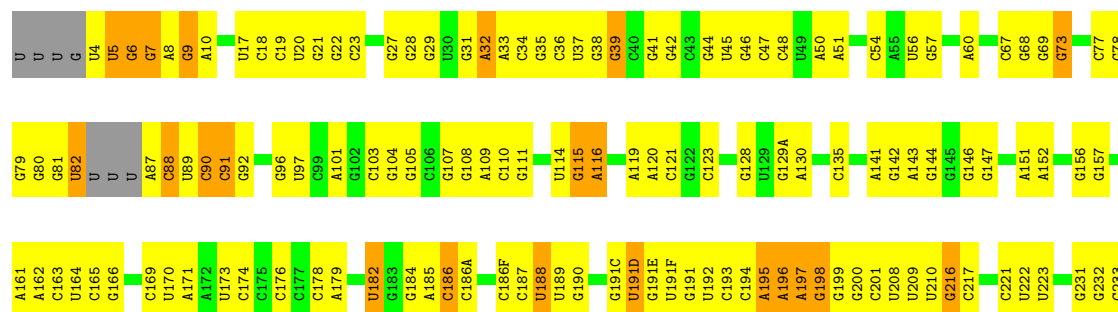
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

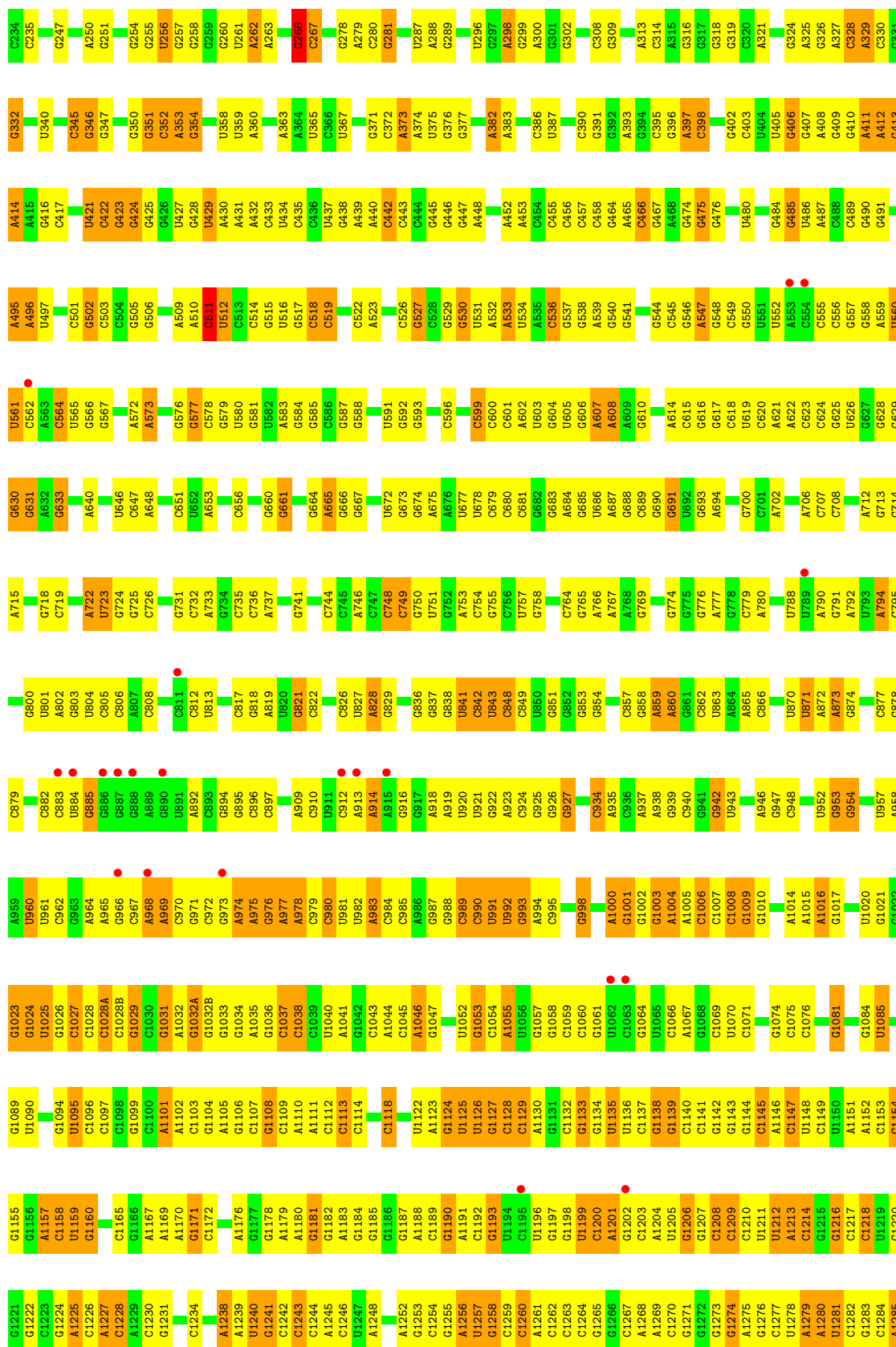
• Molecule 1: 16S ribosomal RNA

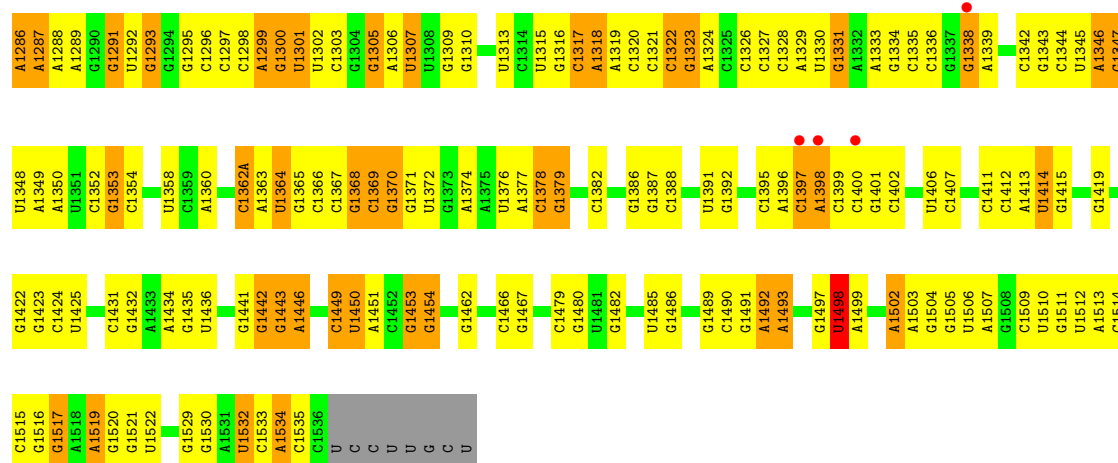




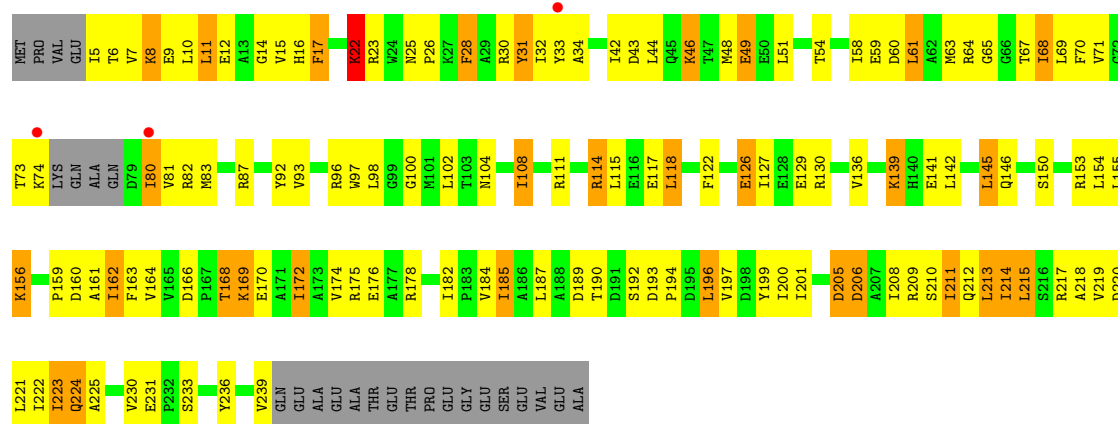
Chain 1G:



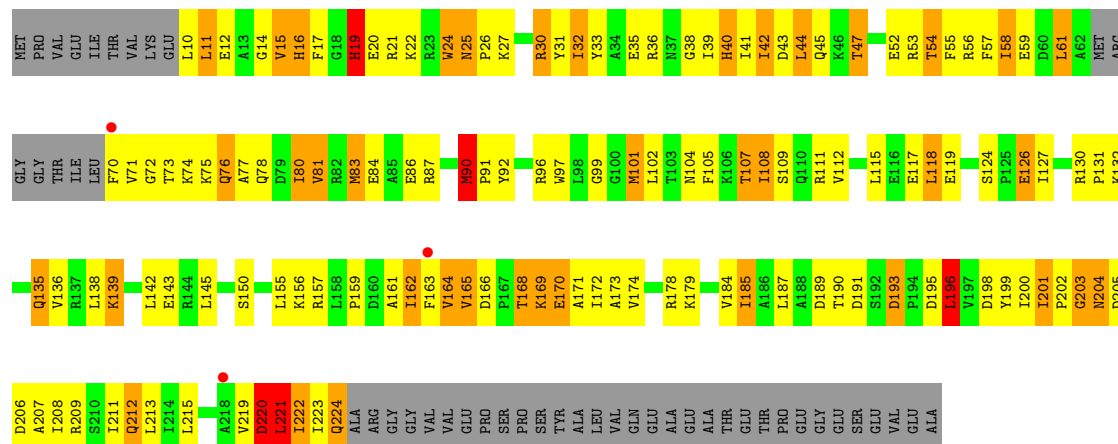
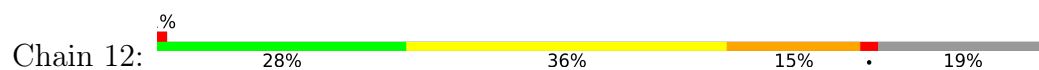




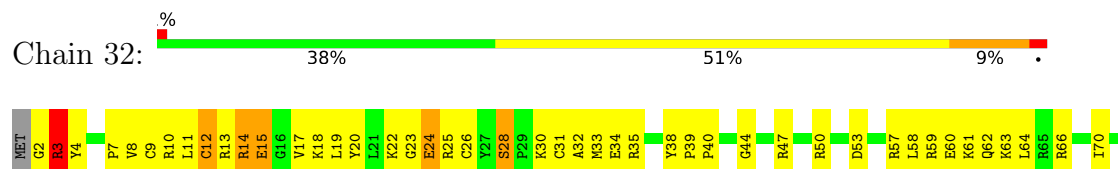
• Molecule 2: 30S ribosomal protein S2

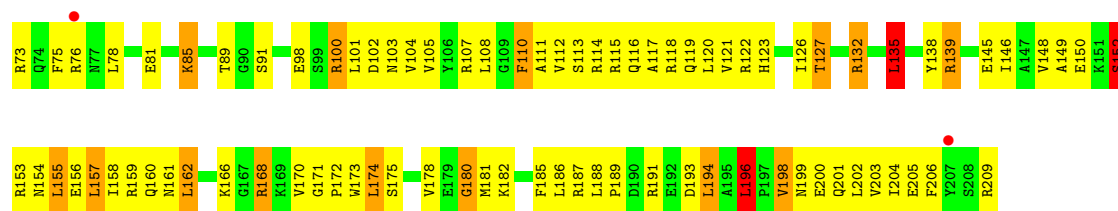


• Molecule 2: 30S ribosomal protein S2

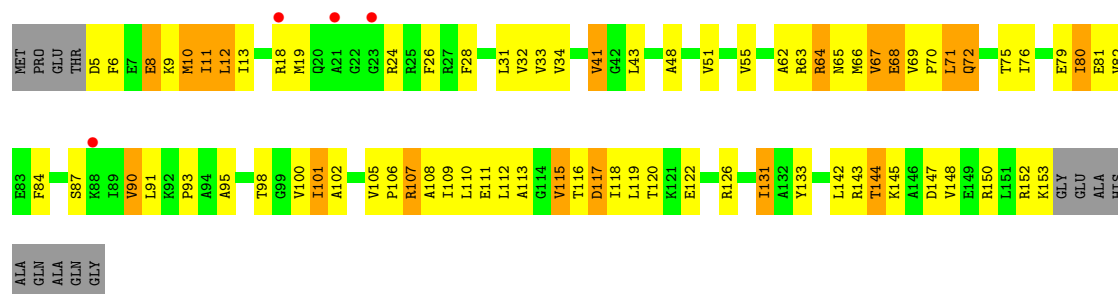


• Molecule 3: 30S ribosomal protein S3

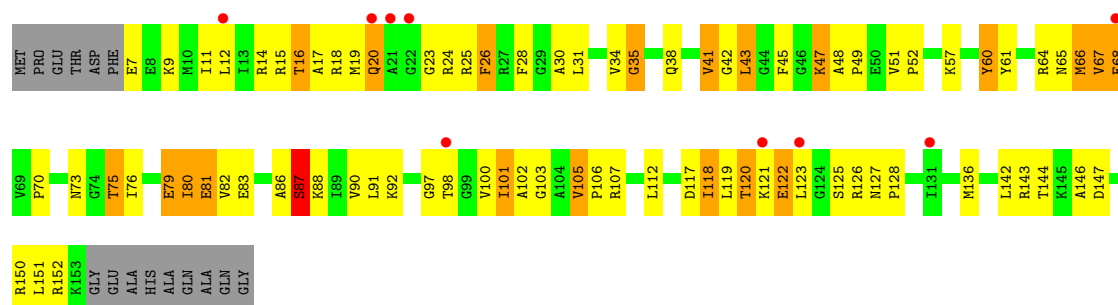
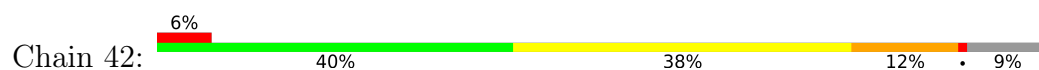




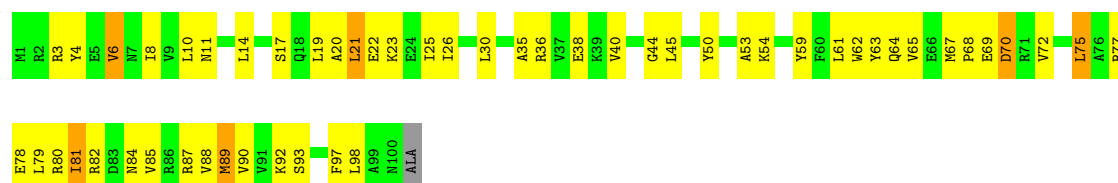
• Molecule 5: 30S ribosomal protein S5



• Molecule 5: 30S ribosomal protein S5

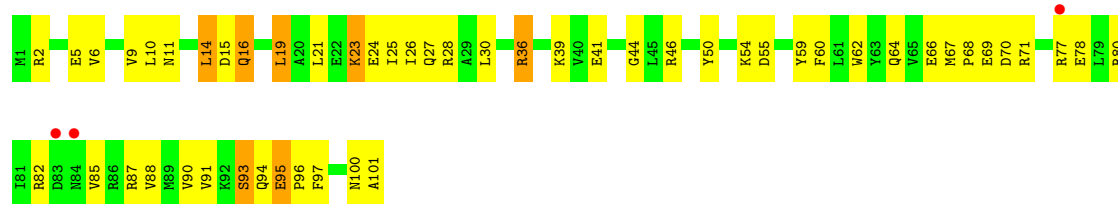


• Molecule 6: 30S ribosomal protein S6

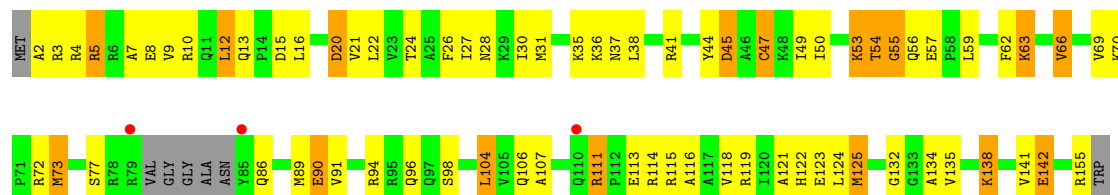


• Molecule 6: 30S ribosomal protein S6

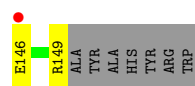
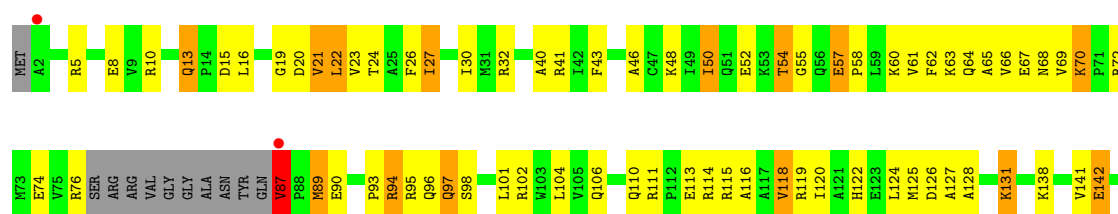




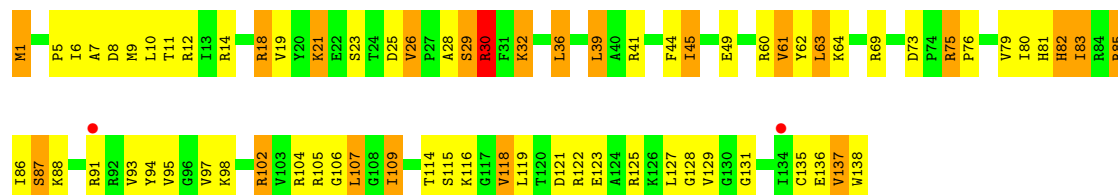
• Molecule 7: 30S ribosomal protein S7



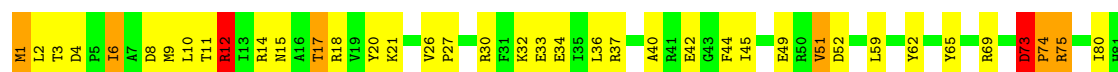
• Molecule 7: 30S ribosomal protein S7

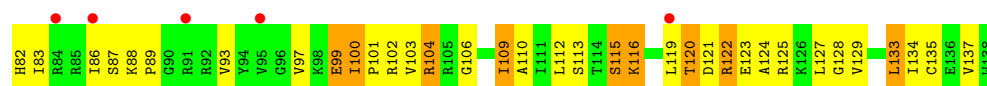


• Molecule 8: 30S ribosomal protein S8

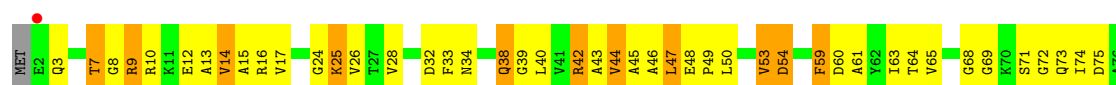


• Molecule 8: 30S ribosomal protein S8

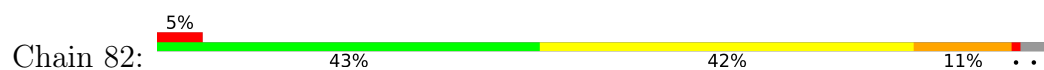




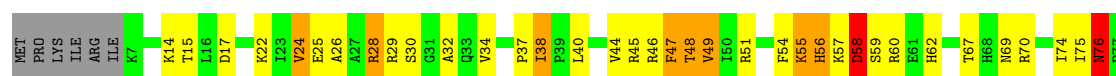
• Molecule 9: 30S ribosomal protein S9



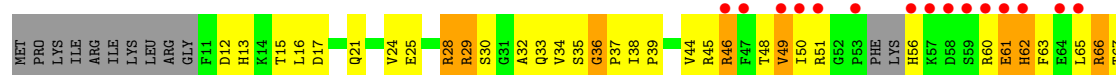
• Molecule 9: 30S ribosomal protein S9



• Molecule 10: 30S ribosomal protein S10

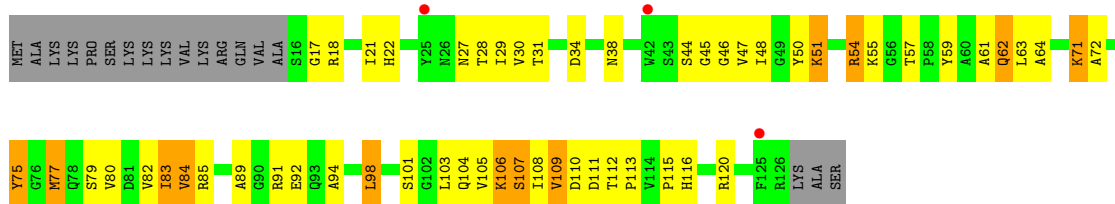


• Molecule 10: 30S ribosomal protein S10

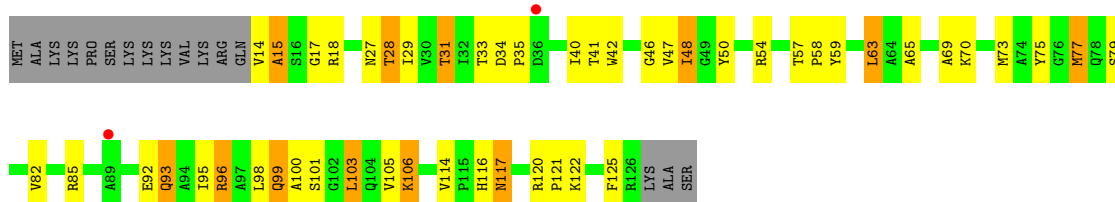


• Molecule 11: 30S ribosomal protein S11

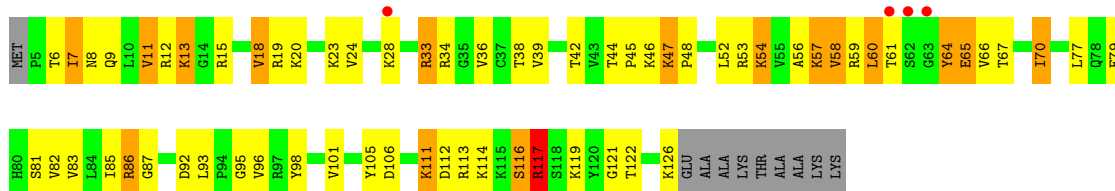
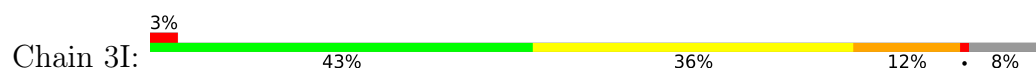




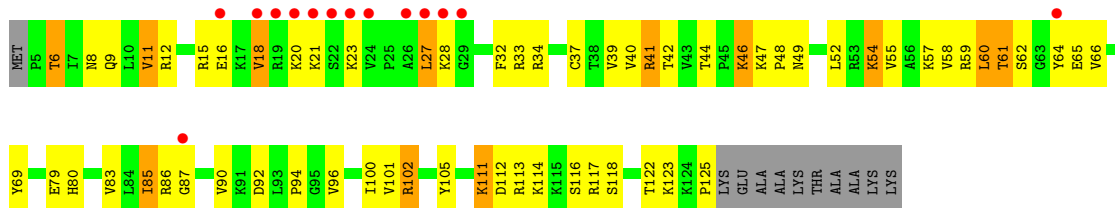
• Molecule 11: 30S ribosomal protein S11



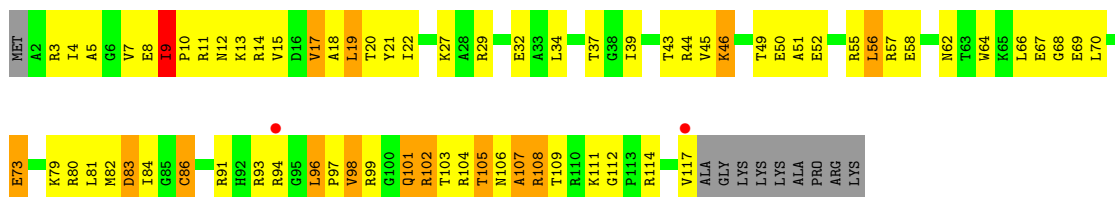
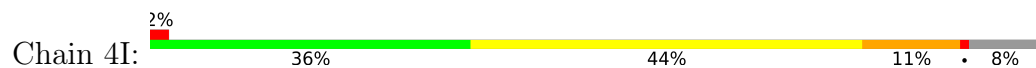
• Molecule 12: 30S ribosomal protein S12



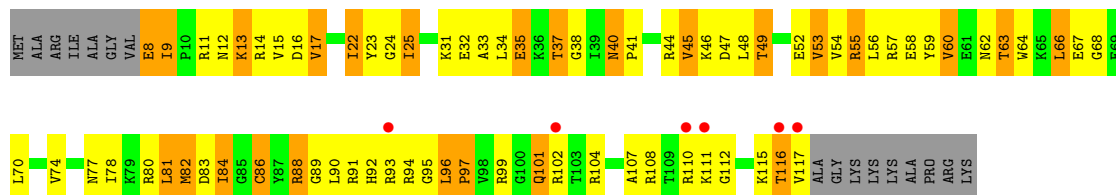
• Molecule 12: 30S ribosomal protein S12



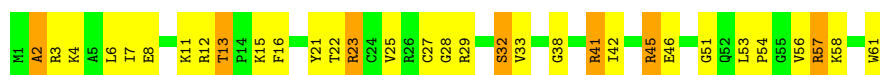
• Molecule 13: 30S ribosomal protein S13



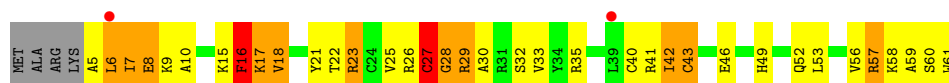
- Molecule 13: 30S ribosomal protein S13



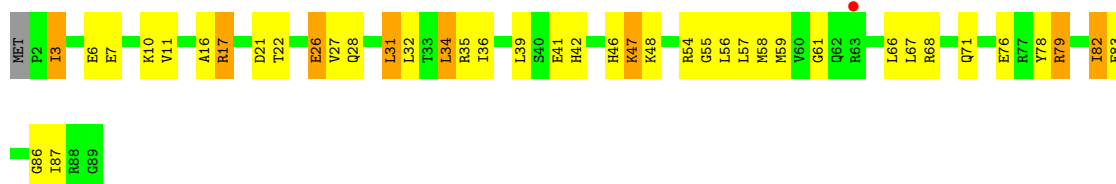
- Molecule 14: 30S ribosomal protein S14 type Z



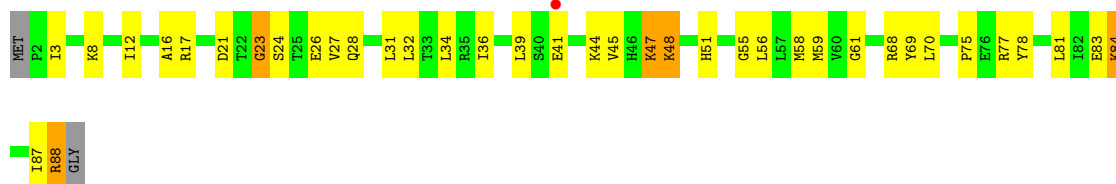
- Molecule 14: 30S ribosomal protein S14 type Z



- Molecule 15: 30S ribosomal protein S15



- Molecule 15: 30S ribosomal protein S15

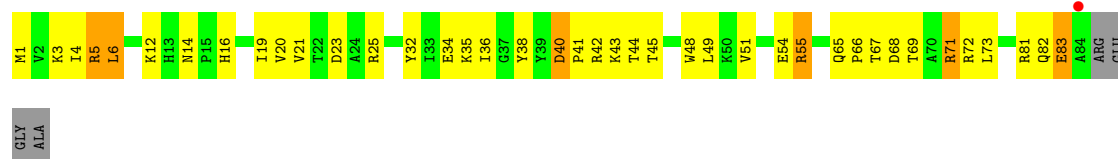


- Molecule 16: 30S ribosomal protein S16

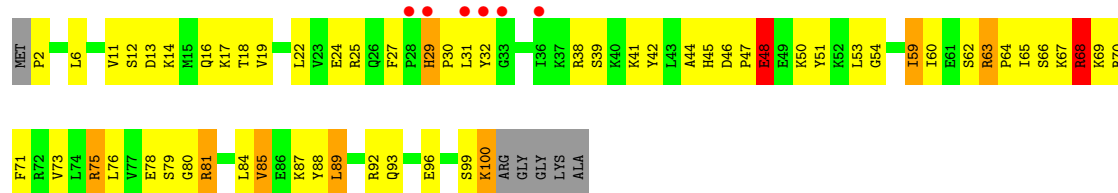




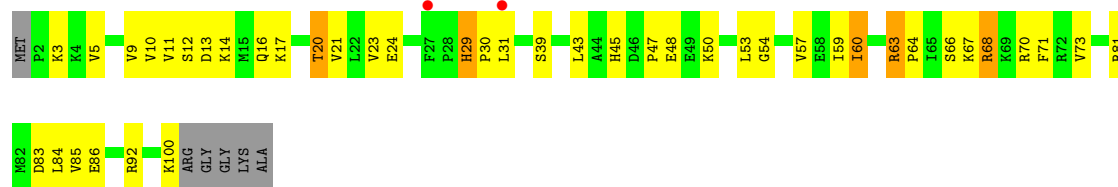
• Molecule 16: 30S ribosomal protein S16



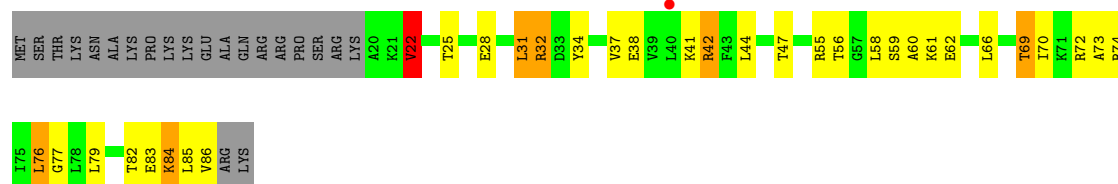
• Molecule 17: 30S ribosomal protein S17



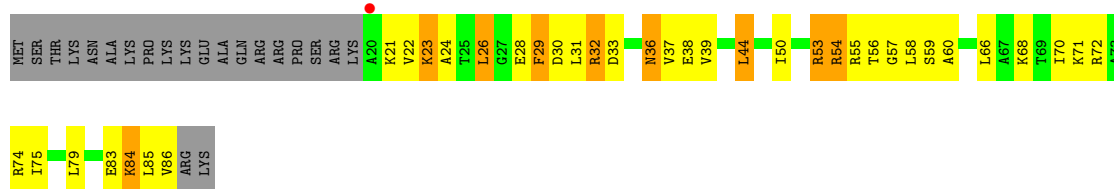
• Molecule 17: 30S ribosomal protein S17



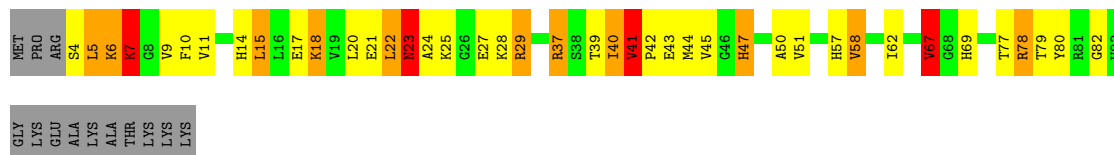
• Molecule 18: 30S ribosomal protein S18



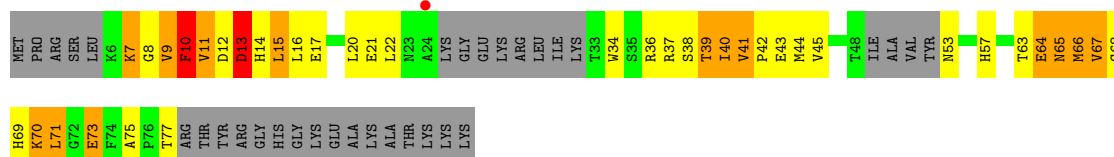
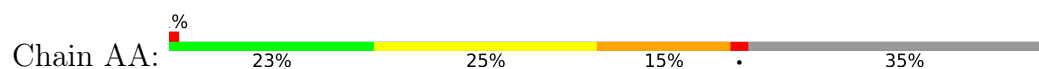
• Molecule 18: 30S ribosomal protein S18



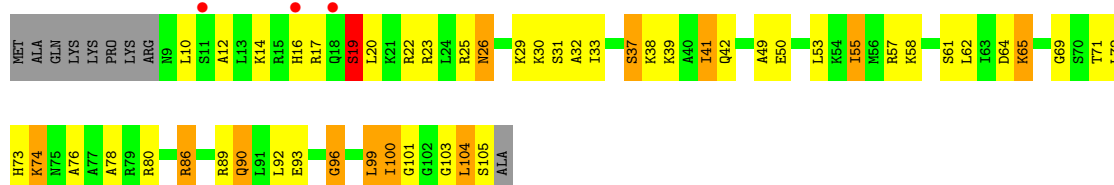
- Molecule 19: 30S ribosomal protein S19



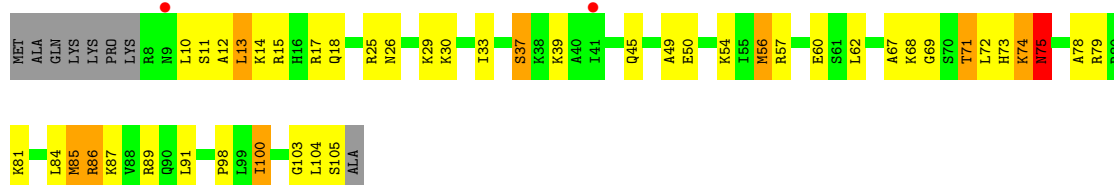
- Molecule 19: 30S ribosomal protein S19



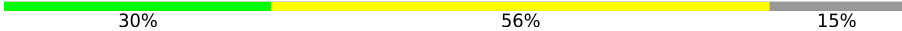
- Molecule 20: 30S ribosomal protein S20

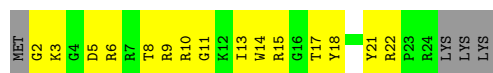


- Molecule 20: 30S ribosomal protein S20

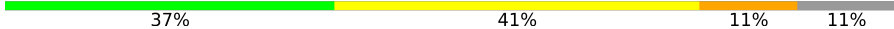


- Molecule 21: 30S ribosomal protein Thx

Chain 1F: 

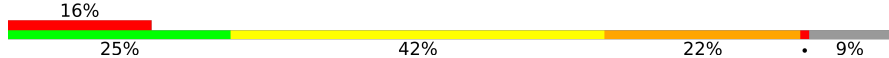


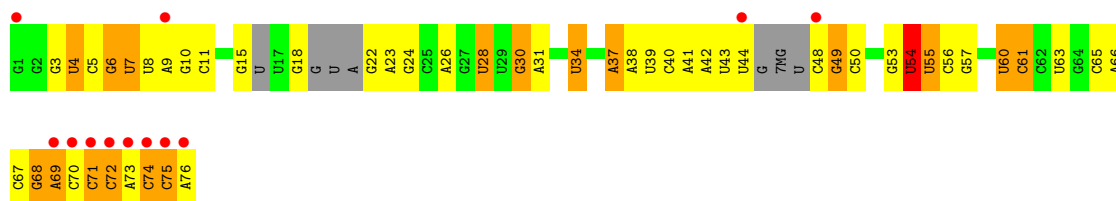
- Molecule 21: 30S ribosomal protein Thx

Chain 1B: 



- Molecule 22: tRNA-Lys

Chain 1K: 



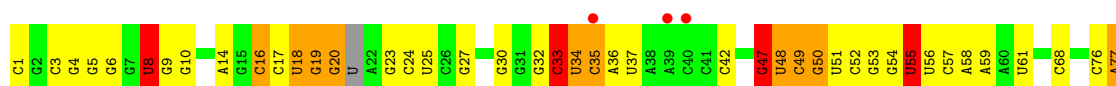
- Molecule 23: tRNA-fMet

Chain 2K: 

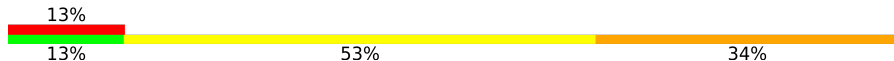


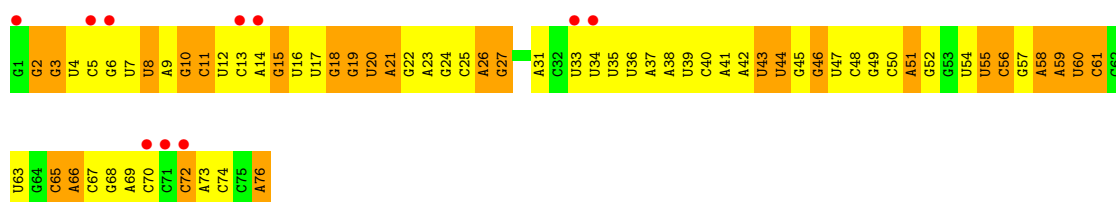
- Molecule 23: tRNA-fMet

Chain 2L: 



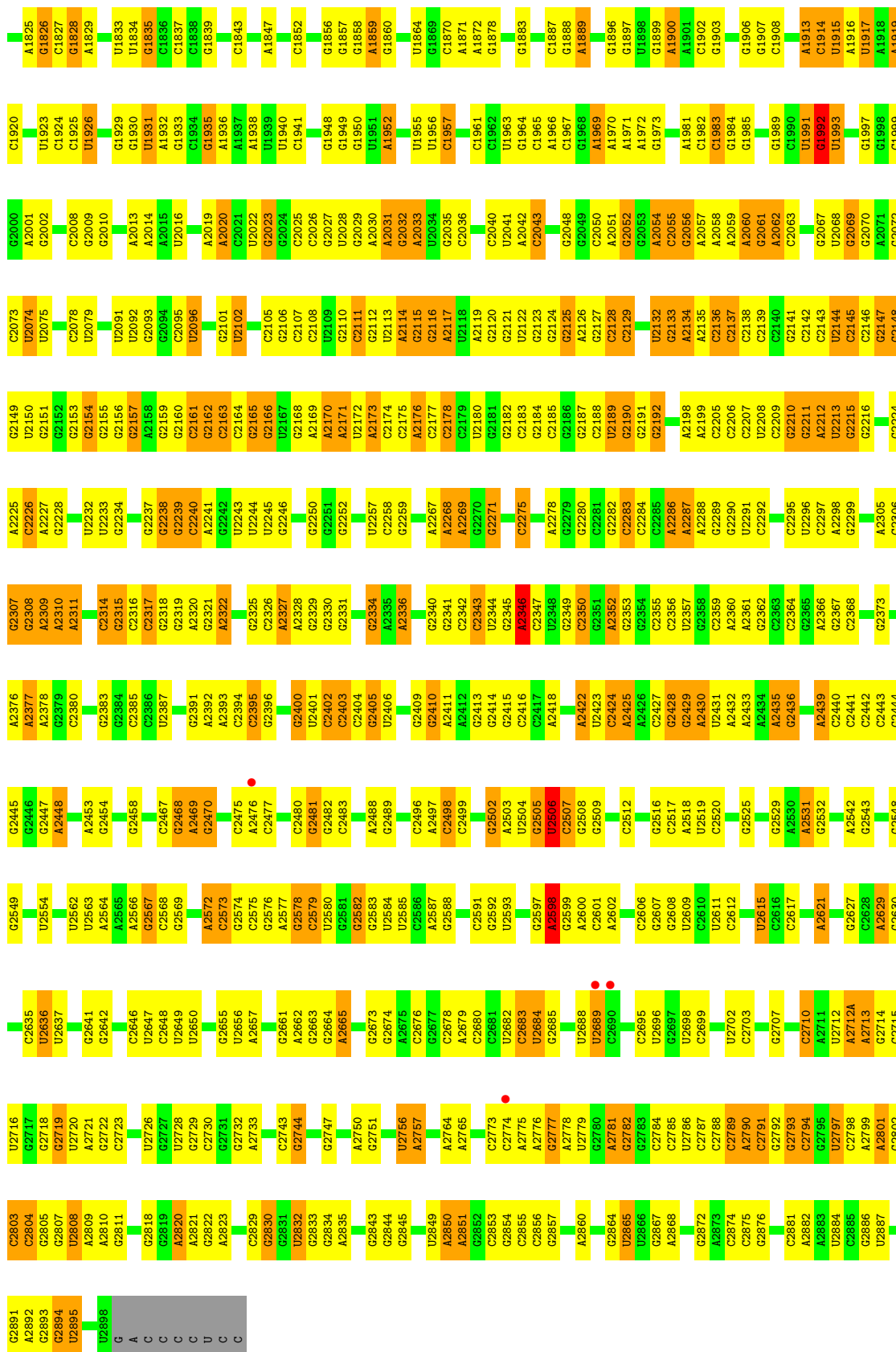
- Molecule 24: tRNA-Lys

Chain 3K: 

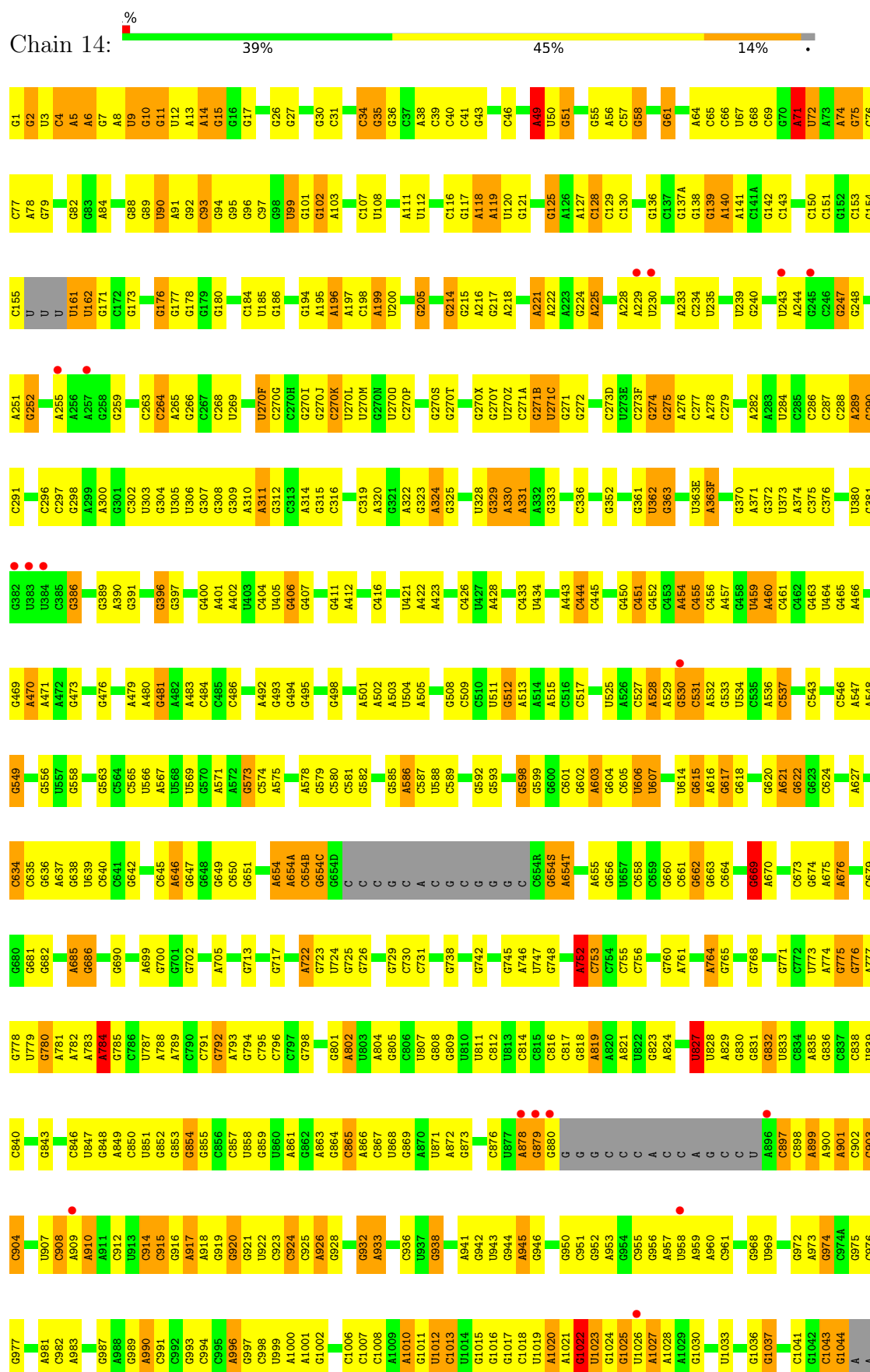


- Molecule 25: mRNA

A1732	G1647	A1566	G1426	G1348	A1272	C1201	C1121	U	G968	C893	U822	G748
G1748	C1648	A1567	A1427	A1349	U1273	C1202	G1122	G	U969	C894	G823	C749
A1749	G1651	G1568	C1428	U1352	A1274	G1203	C1123	U	C971	A	A824	A750
G1753	A1652	A1569	C1430	A1353	A1275	A1205	A1126	G	G972	C895	U827	A752
A1756	A1653	A1570	C1431	A1354	G1276	A1206	A1127	C	A973	C898	U828	C753
G1757	A1654	A1571	C1432	G1355	A1278	G1207	A1128	C	G974	A899	A829	C754
U1757	A1655	A1572	C1433	G1356	G1279	C1208	A1129	U	C974A	A900	G830	C755
G1758	A1656	G1573	A1434	U1357	G1280	G1209	U1130	U	A980	A901	G831	C756
A1762	C1577	C1577	C1437	G1358	G1283	G1210	G1131	A	A983	C902	G832	U757
G1763	U1578	U1578	U1438	A1359	A1284	U1211	A1132	G	A983	C903	U833	C758
G1764	A1580	A1579	A1439	G1360	G1285	G1212	U1133	A	A983	C904	C834	G759
C1765	G1581	G1581	G1440	G1364	A1286	A1213	C1135	A	A990	G905	A835	G760
A1766	A1582	A1582	G1441	A1365	A1287	A1214	G1136	G	C991	G906	G836	A761
C1767	A1583	A1583	G1442	A1366	U1288	G1137	G1137	C	C992	U907	C837	U762
U1768	A1585	A1585	G1443	G1371	U1289	G1219	G1139	A	G993	C908	C838	G763
A1668	A1586	A1586	G1444	G1372	C1290	G1219	C1140	G	C994	A909	U839	A764
A1669	A1587	A1587	A1444A	U1372	C1291	A1220	U1141	C	C995	A910	C840	G765
C1771	C1588	C1588	C1445	A1373	U1292	C1221	U1142	C	A996	A911		
G1772	U1589	U1589	C1446	G1374	C1293	C1222	A1142A	A	A997	C912	C844	G768
A1773	G1525	G1525	G1447	C1375	G1296	G1228	A1155	U	C998	U913	G845	G769
G1776	G1526	G1526	G1448	G1376	C1297	G1229	A1156	C	C998	C914	G846	G770
U1777	G1527	G1527	A1449	G1377	C1298	G1229A	G1157	U	C1005	C915	U847	G775
U1778	A1528	A1528	G1449A	A1378	C1299			U	C1006	A916	G848	G776
C1782	A1529	A1529	U1454	A1379	U1300	G1236	G1160	A	C1007	A917	G849	
A1783	G1530	G1530	G1455	G1380	A1301	A1237		A	C1008	A918	G850	
A1784	C1533	C1533	G1456	G1385		G1237	G1163	A	A1009	G919	U851	U779
A1785	U1535	U1535	G1459	G1386	C1304	G1238	G1164	A	A1010	U930	G855	G780
A1786	A1536	A1536	A1460	G1387	C1305	G1239	G1165	G	G1011	C931		A781
A1787	G1537	G1537	A1461	G1388	C1306	U1240	U1166	A	U1012	G932	U858	A782
U1788	C1538	C1538	C1462	G1389		U1241	C1166	G	C1013	A933	U859	A783
A1789	G1539	G1539	C1467	A1392	G1311	G1243	G1169	U	A1021	G934	U860	A784
A1791	G1540	G1540	C1467	A1393	U1312	G1244	G1170	G	G1022	C935	A861	G785
G1792	U1541	U1541	G1470	U1394	U1313	A1247	G1171	C	U1023	U937	G862	U787
C1793	A1543	A1543	A1471	A1395		G1247	G1173	U	G1024	G938	A866	A788
G1794	C1544	C1544	A1472	U1396	A1317	G1248	A1174	A	G1025	G939	C867	G792
C1795	A1545	A1545	G1475	U1397	C1318	U1249	U1175	A	U1026	G940	U868	A793
U1796	A1545A	A1545A	G1476	C1403	G1324	G1250	G1176	U	A1027	A941	U869	G794
C1797	C1546	C1546	G1478	U1405		C1251	A1177	A	U1028	G942		C795
U1798	G1547	G1547	G1479	U1406	G1328	A1252	C1178	G	C1033	U943	G873	C796
G1699	C1548	C1548	G1479	C1407	C1329	A1254	C1179	C	U1033	G944	G874	C797
G1705	C1549	C1549	G1483	C1408	C1330	U1255	C1180	U	C1038	G945	G875	C798
U1706	C1550	C1550	G1484	G1412	A1331	G1256	C1181	C	G1039	A946	C876	G799
A1802	C1551	C1551	G1485	G1413	C1332	C1257	A1182	A	C1040	G950	U877	A800
C1804	A1553	A1553	A1486	A1414	G1333	G1258	G1183	U	A1045	C951	G879	A802
U1805	A1554	A1554	G1487	G1416	G1334	G1260	C1184	G	A1046	G952	G881	G805
A1814	C1557	C1557	G1487	G1417	G1338	U1263	G1187	G	G1047	A953	G882	C806
A1815	A1558	A1558	A1490	G1418	G1339	G1264	G1188	U	A1048	G956	G	U807
G1816	C1640	C1640	G1491	U1340	U1341	A1265	A1189	C	G1051	A957	C	U811
G1817	G1492	G1492	U1420	A1419	U1341	G1266	G1190	C	C1052	U958	C	C812
U1818	C1493	C1493	G1421	G1422	A1342	U1267	G1191	A	C1053	A959	C	U813
A1819	G1422	G1422	G1422	G1422	G1344	A1268	A1194	C	A	C961	C	
U1820	G1423	G1423	G1423	G1423	G1345	A1269	G1195	C	G	G962	C	G818
A1821	C1564	C1564	U1496	U1496	C1345	C1270	C1196	A	A	U963	A	
	G1731	G1731	C1498	G1425	G1347	G1271	G1197	G	A		G	A821



- Molecule 26: 23S ribosomal RNA



C2039	A1885	A1789	G1696	A1608	A1529	A1453	G1385	A1174	C1109	G1047
A2042	C1886	C1790	G1686	A1609	G1530	U1454	C1386	U1175	G1110	A1048
C2043	G1887	A1791	A1700	C1611	C1532	G1455	C1387	G1244	G1111	C1049
	A1889	C1792	A1701	A1614	C1533	G1458	C1389	A1247	U1113	A1050
G2049	C1893	C1795	G1703	C1615	U1535	A1460	U1390	U1249	G1114	A1054
C2050	C1894	C1796	G1703	A1616	U1536	G1461	A1393	C1251	G1115	G1055
A2051	G1897	C1797	C1711	G1619	C1537	G1462	U1394	C1181	G1116	G1056
G2052	U1898	C1798	U1716	G1712	U1538	C1463	A1395	A1182	G1117	A1057
A2054	U1899	C1799	U1716	G1717	G1539	C1464	A1396	G1183	C1118	U1058
C2055	A1900	C1800	G1717	G1717	U1540	U1467	U1397	G1184	C1119	G1059
G2056	A1901	G1801	G1718	G1718	U1541		C1398	G1185	G1120	U1060
A2057	C1902	A1802	G1725	C1625	G1542		C1399	G1187		U1061
	G1903	C1806	U1726	U1629	A1543	A1471	G1400	U1188	C1124	G1062
A2060	G1904	C1806	U1728	U1629	G1552	A1472	G1403	A1189	G1125	G1063
G2061	C1905	A1810	G1728	A1631	G1552	C1473	C1403	A1126	A1126	C
C2063	G1906	C1811	U1730	A1632	C1556	C1474	U1405	G1190	A1127	U
G2064	C1909	A1812	G1731	G1633	C1557	A1477	U1406	G1191	A1128	U
C2065	U1910		C1735	A1634	C1558	G1478	C1407	G1192	A1129	A
G2066	U1911	G1816	G1735	G1635	G1559	G1479	C1408	G1193	U1130	G
G2067	U1912	G1817	C1741	C1636	G1560	G1480	G1338	U1198	G1131	A1069
U2068	A1913	U1818	G1742	A1637		U1482	G1339	U1199	U1132	A1070
G2069	C1914	A1819	G1743	U1639	A1566	G1483	U1340	G1200	G1135	C1072
A2071	U1917	U1820	G1750	C1644	A1567	A1486	U1341	C1201	G1136	A1073
U2074	A1918	G1823	C1751	C1644	G1568	G1487	A1342	G1202	G1137	G1074
U2075	U1919	C1826	C1752	G1648	A1569	G1488	G1343	C1203	G1138	C1075
U2076	C1920	G1827	G1753	G1649	A1570	G1489	U1345	A1204	G1139	A
A2077	G1921	G1828	C1754	G1651	A1572	A1490	G1346	U1205	C1140	A
G2078	U1922	A1829	U1755	G1650	G1573	G1491	G1347		U1141	U
U2079	U1926		U1757	G1651	U1576	G1492	G1348	A1213	U1142	C
A2082	A1927	C1832	G1758	G1652	U1577	G1493	A1349	G1212	A1142A	A
G2086	U1928	U1833	A1759	A1654	U1578	A1496	G1425	A1213	A1143	U
G2087	G1930	C1838	A1762	A1655	A1580	G1500	U1352	G1218	A1148	A1086
U2088		G1839	G1763	C1656	G1581	U1503	G1358	C1219	G1149	G1087
U2089	A1936	G1840	G1764	C1658	C1582	C1504	A1360	A1220	C1150	A1088
G2093	U1937	A1847	G1769	A1665	C1585	A1507	A1286	C1221	C1151	G1089
G2094	A1938	A1848	G1770	G1666	A1586	A1508	A1287	C1222	C1152	U1090
C2095	U1939		C1771	G1667	C1587	C1509	U1288	C1223	C1153	G1091
U2096	C1941	G1856	G1772	G1670	C1588	A1510	C1289	G1224	G1154	C1092
U2099	C1942	G1857	A1773	C1671	C1592	A1511	C1290	C1225	A1155	G1093
G2100	U1943	G1858	G1776	G1674	G1593	U1512	U1291	G1226	A	U
G2101	G1944	G1859	U1777	C1675	G1594	U1513	G1369	U1159	U1159	A
U2102	G1945	G1860	U1778	A1676	A1596	U1514	C1370	G1229	C1160	U
C2103	U1946		U1779	A1677	U1597	C1515	G1371	G1229A	C1161	A1098
G2104	G1949	U1864	C1781	A1677	A1598	U1516	U1372	C1230	G1162	G1099
C2105	U1950	A1871	C1781	U1678	C1599	U1517	C1375	G1232	U1165	C1100
	A1951	A1872	U1679	U1679	C1599	C1518	A1301	C1233	C1166	C1101
C2108	U1952	G1878	U1681	U1680	G1600	G1519	A1447	U1234	U1167	C1102
	A1953	C1879	A1784	G1681	G1601	U1520	A1378	G1235	C1168	A1103
	G1954		A1785	U1682	U1602	G1521	A1379	G1236	G1169	C1104
C2111	U1955	G1883	A1786	U1688	A1603	G1522	G1380		G1170	U1105
G	U1956	A1884	A1787	U1688	C1607	A1528	U1312	G1239	G1171	G1106
U2113			C1788	U1693			U1313	U1240	G1173	U1108



Response	Percentage
Yes	41%
No	45%
Don't know	13%



Chain 1J:

Amino Acid	Chain 1J Count	Chain 1K Count
A66	1	1
A0	1	1
U1	1	1
C2	1	1
C3	1	1
C4	1	1
C5	1	1
C6	1	1
U7	1	1
G8	1	1
G9	1	1
C12	1	1
A13	1	1
U14	1	1
C15	1	1
G16	1	1
C17	1	1
G18	1	1
G19	1	1
C20	1	1
G21	1	1
U22	1	1
G23	1	1
G24	1	1
A25	1	1
A26	1	1
C27	1	1
C28	1	1
A29	1	1
C30	1	1
G33	1	1
U34	1	1
U40	1	1
U41	1	1
C42	1	1
C43	1	1
G44	1	1
A45	1	1
A46	1	1
C47	1	1
A48	1	1
C49	1	1
G50	1	1
G51	1	1
A52	1	1
U55	1	1
G56	1	1
A57	1	1
A58	1	1
A59	1	1
C60	1	1
G61	1	1
C62	1	1
G63	1	1
C64	1	1
C65	1	1
A66	1	1
G67	1	1
C68	1	1
G69	1	1
C70	1	1
C71	1	1
G72	1	1
A73	1	1
U74	1	1
G75	1	1
A78	1	1
C79	1	1
U80	1	1
G81	1	1
G82	1	1
G83	1	1
C88	1	1
G89	1	1
A89A	1	1
C90	1	1
C93	1	1
C94	1	1
U95	1	1
G96	1	1
A99	1	1
G100	1	1
A101	1	1
G102	1	1
U103	1	1
A104	1	1
G105	1	1
C108	1	1
G109	1	1
G110	1	1
G115	1	1
G116	1	1
G117	1	1
G118	1	1
A119	1	1

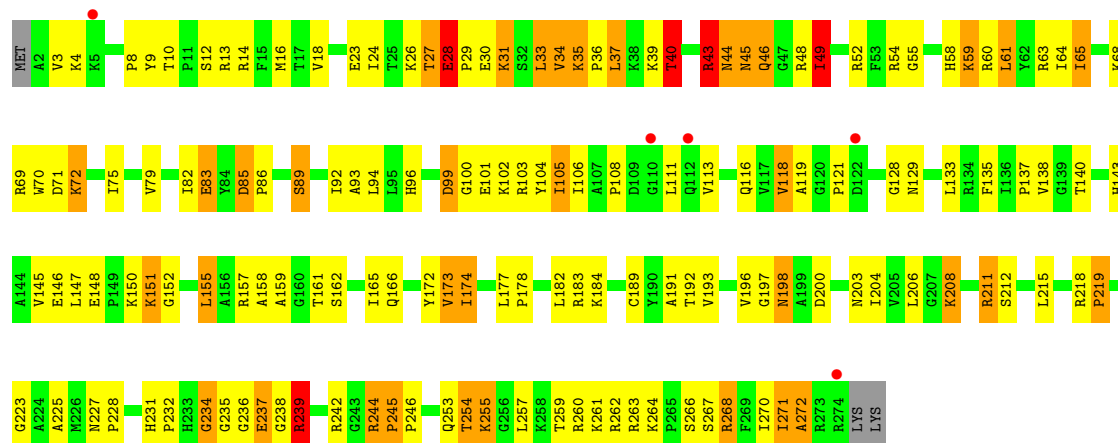
[illegible]

Chain 11:

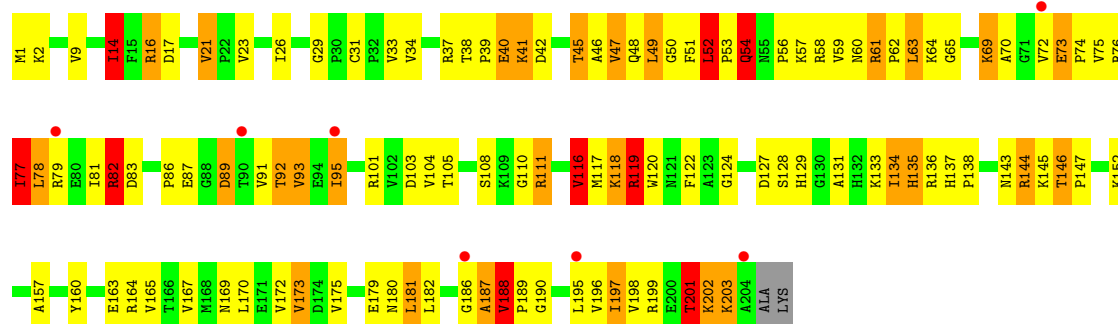
47% 36% 14% 2%

Met, A2, V3, F6, K7, P8, T10, P11, S12, R13, R14, F15, M16, T17, D20, K26, T27, E28, P29, E30, K31, S32, L33, V34, K35, P36, L37, K38, K39, T40, G41, G42, R43, T50, V51, R52, F53, L61, Y62, R63, I64, I65, D66, K68, R69, W70, D71, K72, V73, G74, I75, V76

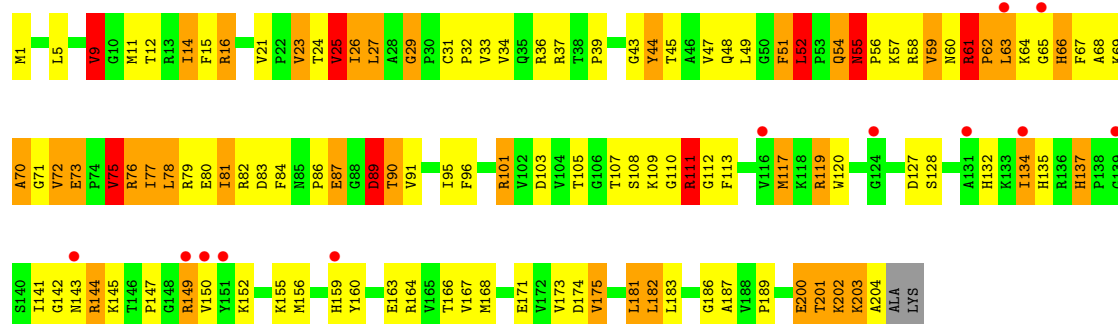
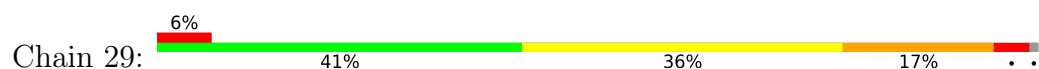
Chain 19: 2% 44% 40% 13% ..



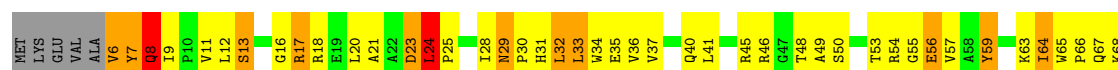
• Molecule 30: 50S ribosomal protein L3

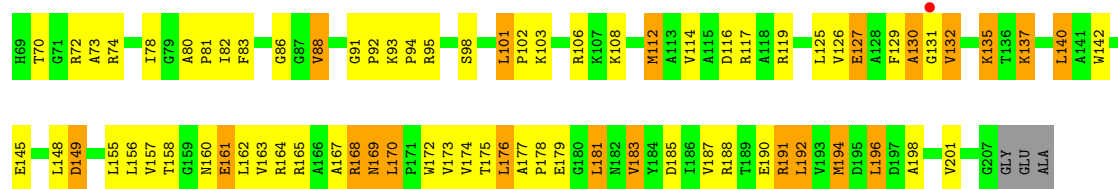


• Molecule 30: 50S ribosomal protein L3



• Molecule 31: 50S ribosomal protein L4





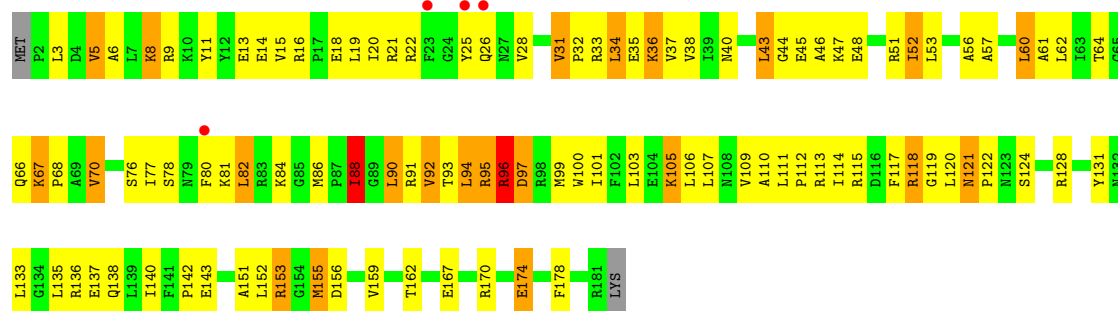
• Molecule 31: 50S ribosomal protein L4

Chain 39: 36% 47% 11% . .



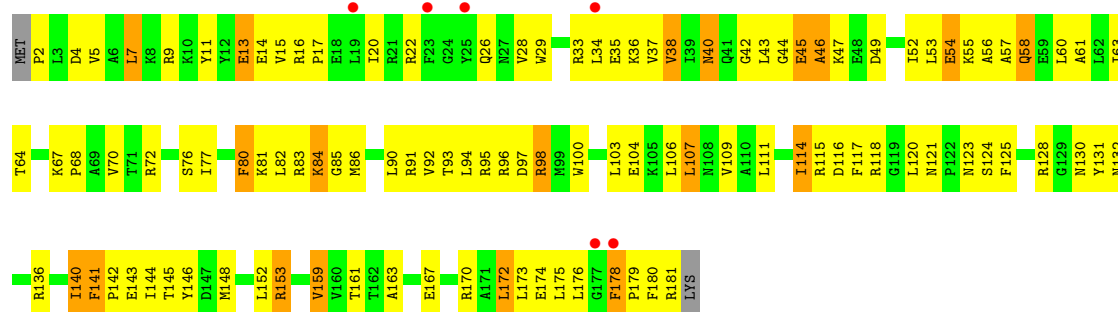
• Molecule 32: 50S ribosomal protein L5

Chain 41: 2% 41% 45% 12% ..

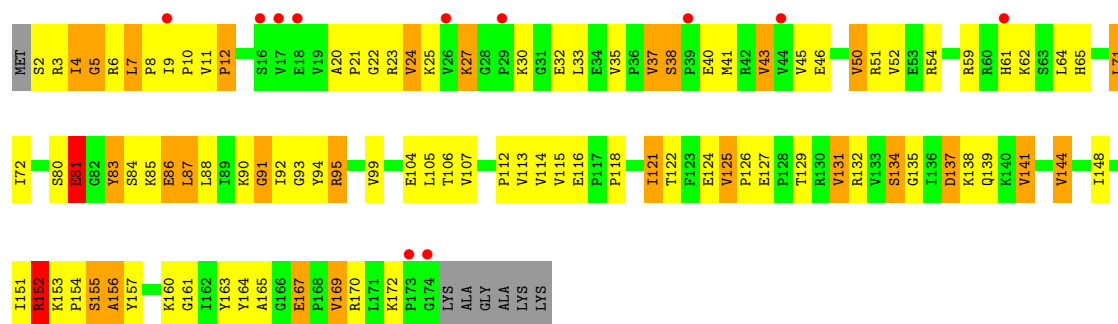


• Molecule 32: 50S ribosomal protein L5

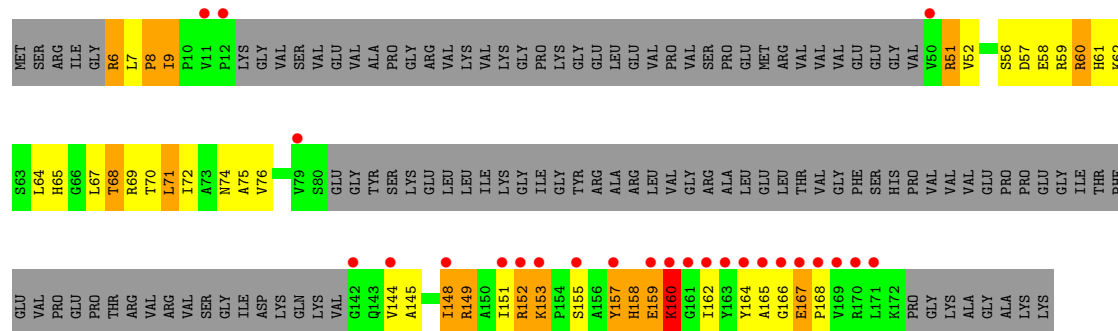
Chain 49: 3% 39% 49% 10% .



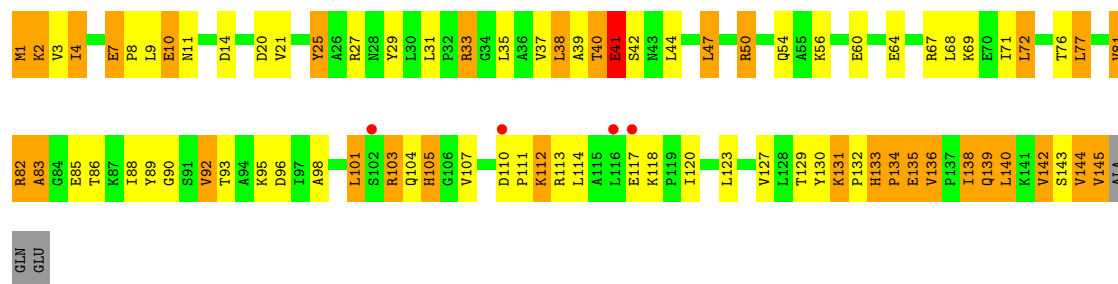
Chain 51:



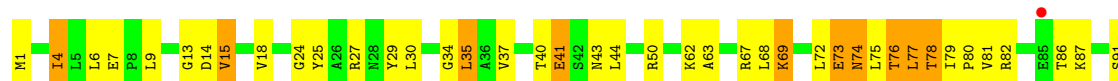
Chain 59: 14% 15% 14% 8% 62%



Chain 61: 3% 43% 32% 22%

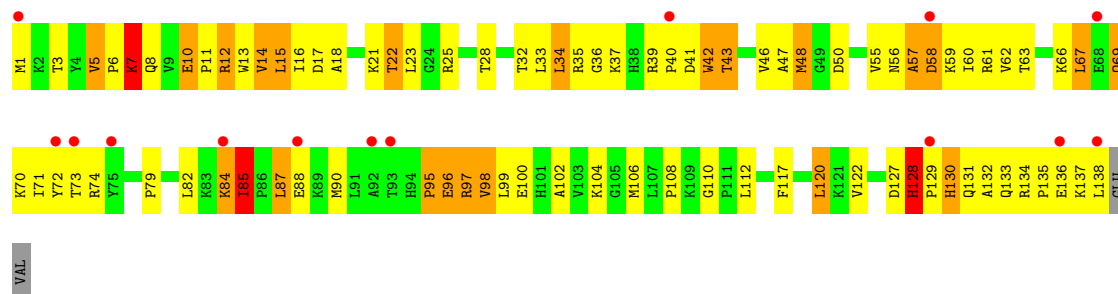


Chain 69: %

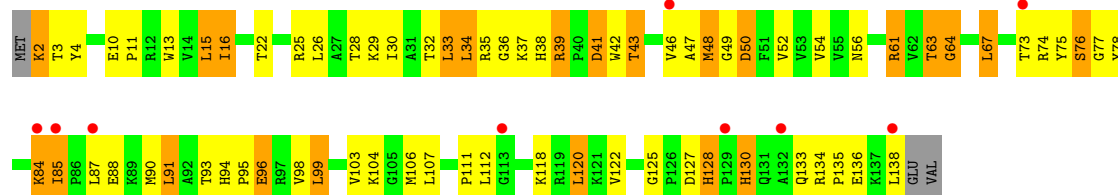




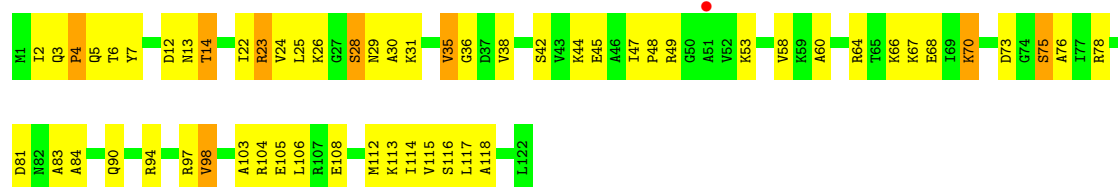
- Molecule 35: 50S ribosomal protein L13



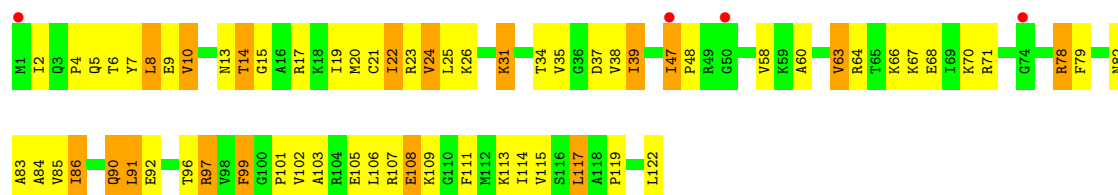
- Molecule 35: 50S ribosomal protein L13



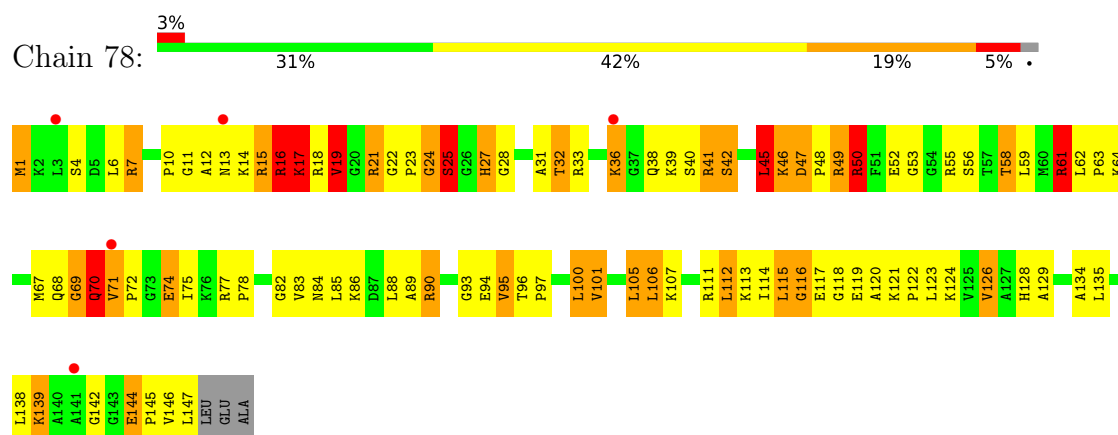
- Molecule 36: 50S ribosomal protein L14



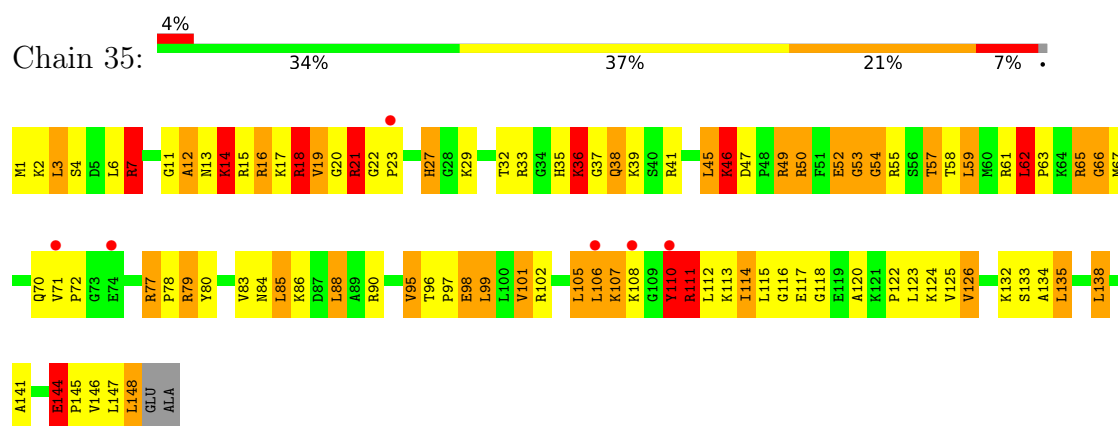
- Molecule 36: 50S ribosomal protein L14



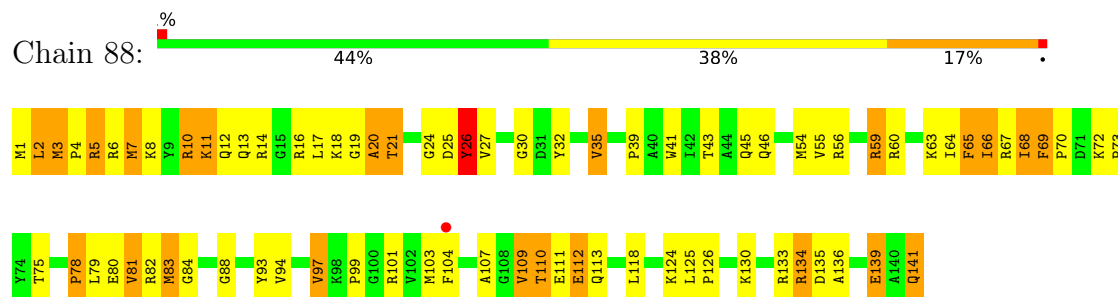
- Molecule 37: 50S ribosomal protein L15



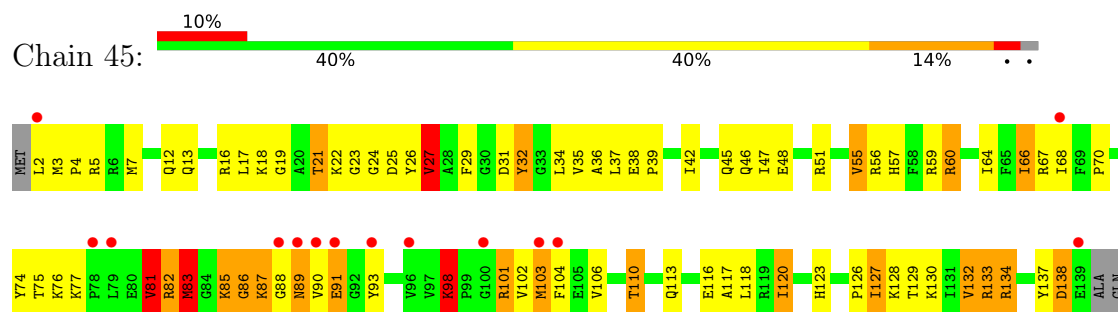
- Molecule 37: 50S ribosomal protein L15



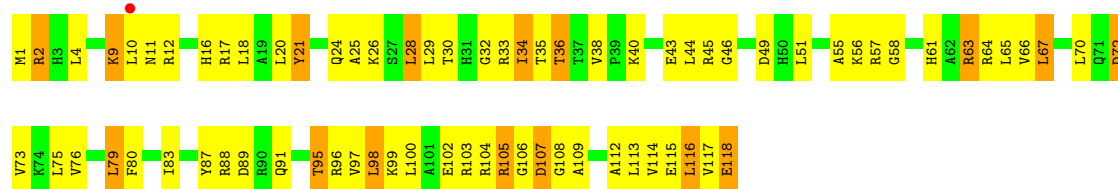
- Molecule 38: 50S ribosomal protein L16



- Molecule 38: 50S ribosomal protein L16



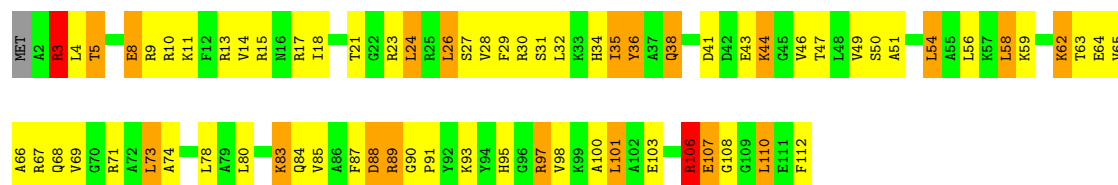
- Molecule 39: 50S ribosomal protein L17



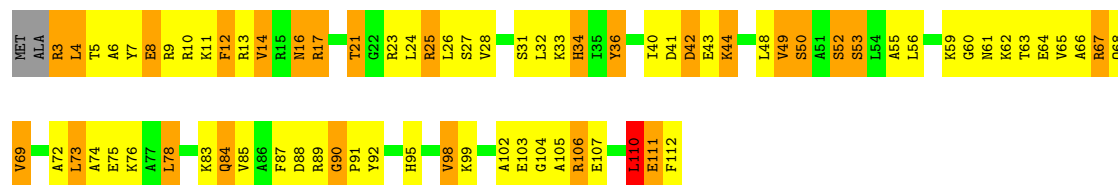
• Molecule 39: 50S ribosomal protein L17



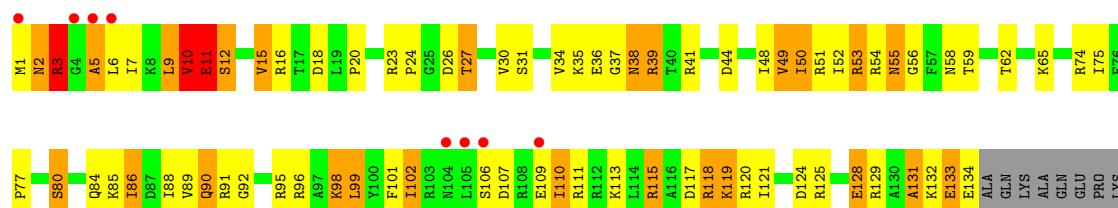
• Molecule 40: 50S ribosomal protein L18



• Molecule 40: 50S ribosomal protein L18

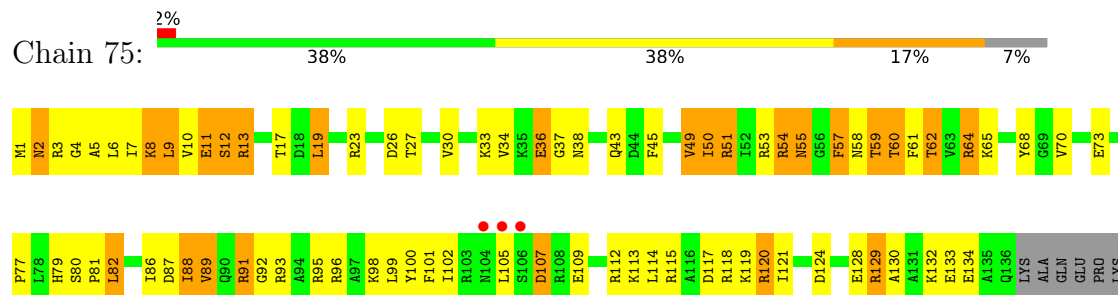


• Molecule 41: 50S ribosomal protein L19



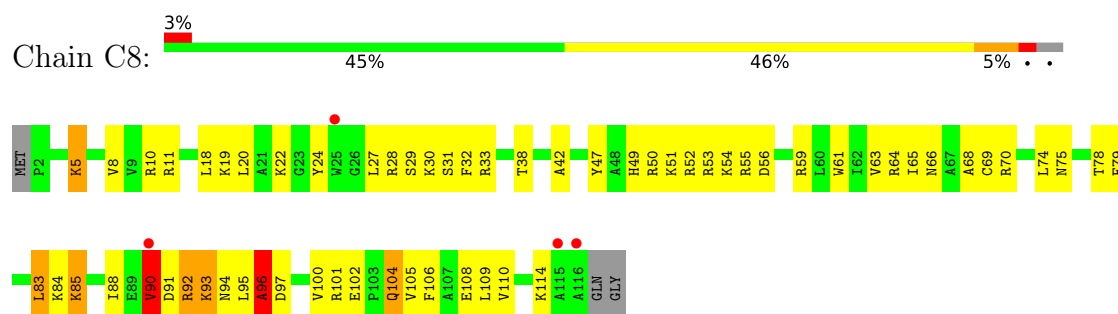
ALA
SER
GLN
GLU

• Molecule 41: 50S ribosomal protein L19

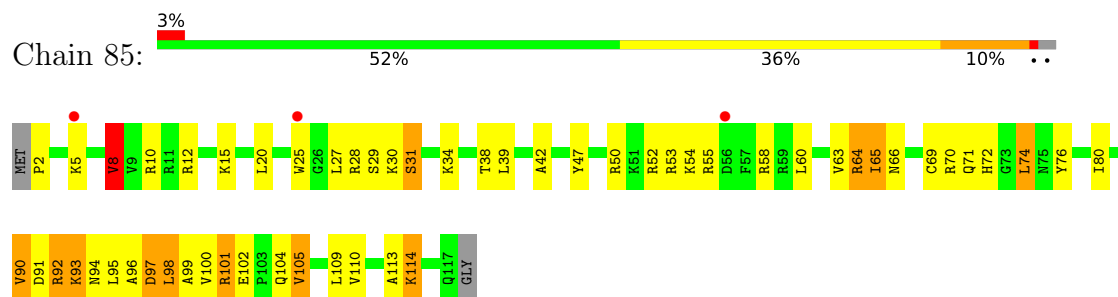


ALA
SER
GLN
GLU

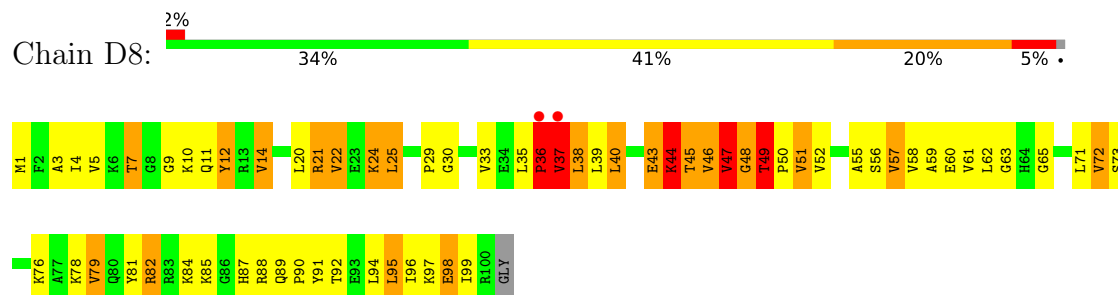
• Molecule 42: 50S ribosomal protein L20



• Molecule 42: 50S ribosomal protein L20

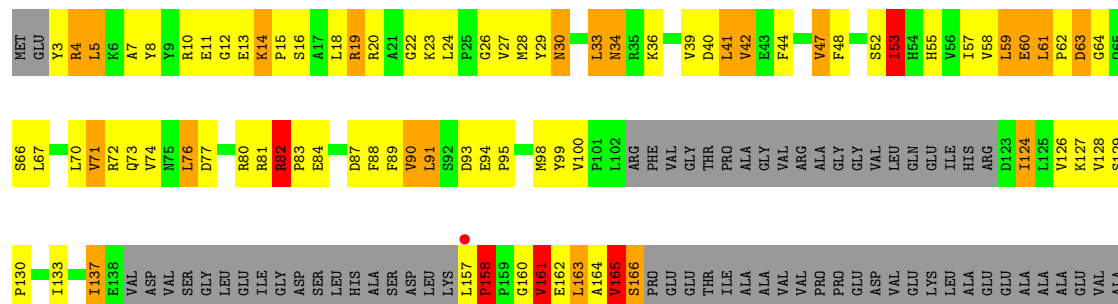
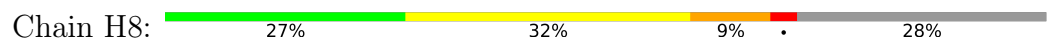


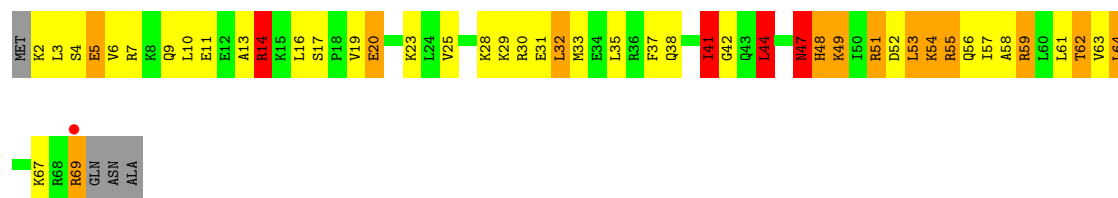
• Molecule 43: 50S ribosomal protein L21



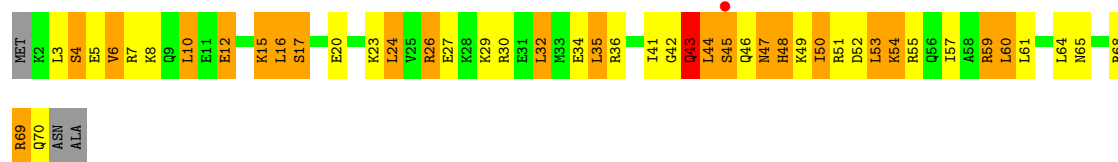
• Molecule 43: 50S ribosomal protein L21

Chain G8:

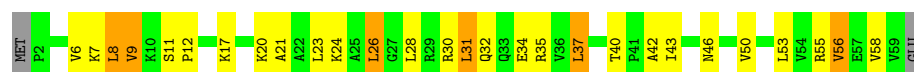




- Molecule 50: 50S ribosomal protein L29



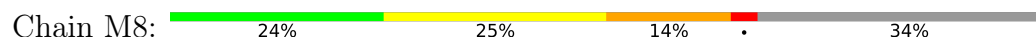
- Molecule 51: 50S ribosomal protein L30



- Molecule 51: 50S ribosomal protein L30



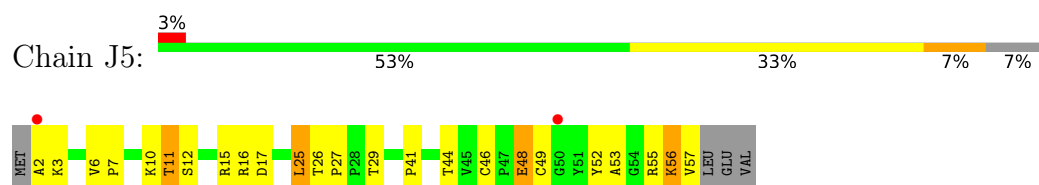
- Molecule 52: 50S ribosomal protein L31



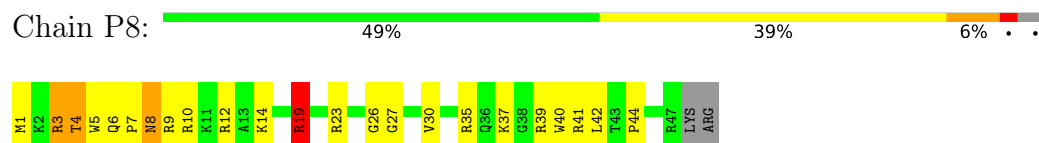
- Molecule 53: 50S ribosomal protein L32



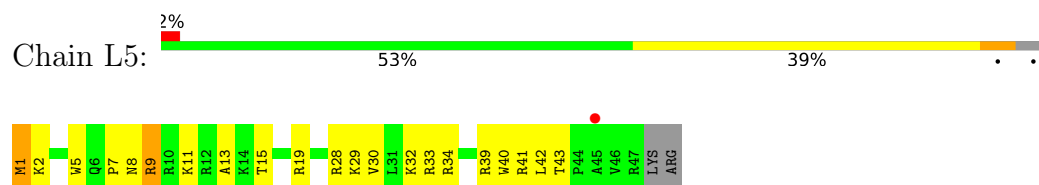
- Molecule 53: 50S ribosomal protein L32



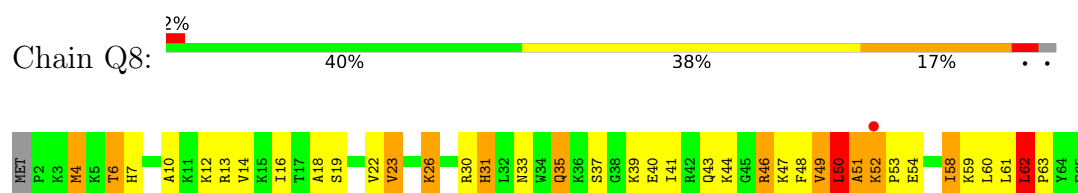
- Molecule 54: 50S ribosomal protein L34



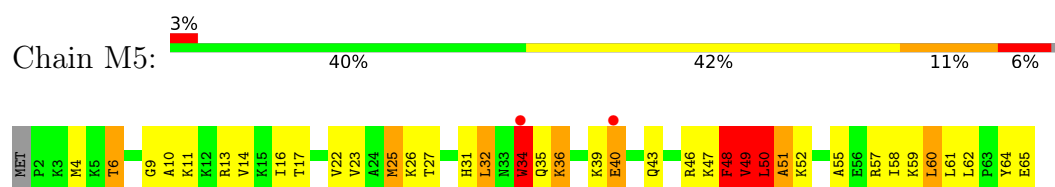
- Molecule 54: 50S ribosomal protein L34



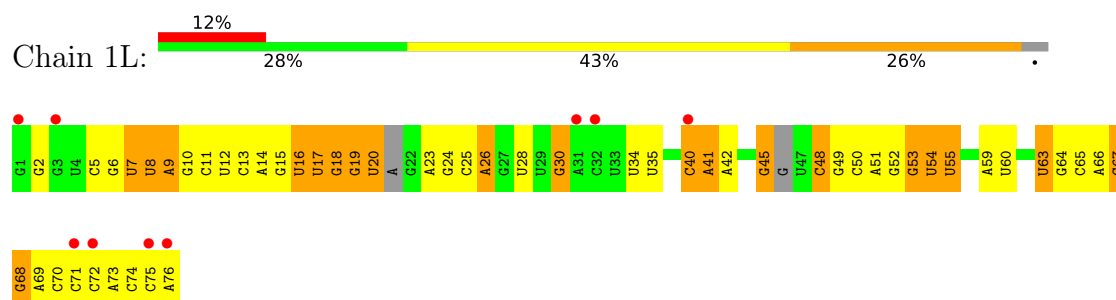
- Molecule 55: 50S ribosomal protein L35



- Molecule 55: 50S ribosomal protein L35

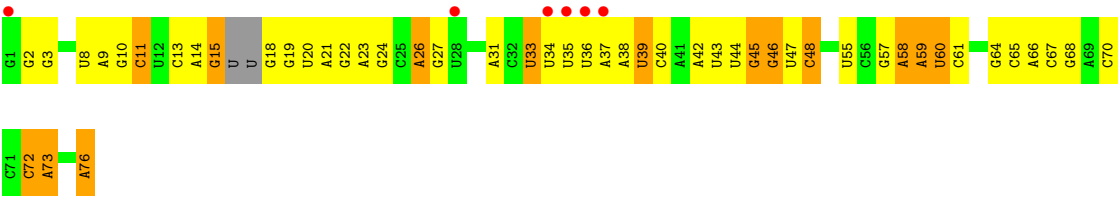


- Molecule 56: tRNA-Lys



- Molecule 57: tRNA-Lys





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	208.90Å 447.80Å 617.50Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	151.53 – 3.15 151.53 – 3.15	Depositor EDS
% Data completeness (in resolution range)	100.0 (151.53-3.15) 93.3 (151.53-3.15)	Depositor EDS
R_{merge}	0.31	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.79 (at 3.13Å)	Xtriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.193 , 0.251 0.195 , 0.253	Depositor DCC
R_{free} test set	2000 reflections (0.20%)	wwPDB-VP
Wilson B-factor (Å ²)	85.9	Xtriage
Anisotropy	0.296	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.27 , 54.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.44$, $\langle L^2 \rangle = 0.26$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	294304	wwPDB-VP
Average B, all atoms (Å ²)	106.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.46% 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: T6A, 5MU, MG, ZN, PSU, OMC, U8U, SF4, 4SU, 7MG

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	0.44	0/35994	0.69	11/56171 (0.0%)
1	1G	0.37	0/36258	0.60	4/56589 (0.0%)
2	12	0.67	1/1742 (0.1%)	1.22	21/2346 (0.9%)
2	1E	0.59	0/1908	1.06	8/2573 (0.3%)
3	22	0.59	0/1552	1.08	11/2093 (0.5%)
3	2E	0.68	0/1629	1.03	2/2195 (0.1%)
4	32	0.59	0/1732	1.12	13/2318 (0.6%)
4	3E	0.72	0/1732	1.17	10/2318 (0.4%)
5	42	0.63	0/1138	1.15	9/1532 (0.6%)
5	4E	0.73	0/1158	1.12	7/1559 (0.4%)
6	52	0.64	0/855	1.03	5/1154 (0.4%)
6	5E	0.64	0/850	1.01	1/1147 (0.1%)
7	62	0.59	0/1122	1.15	12/1500 (0.8%)
7	6E	0.59	0/1230	1.04	9/1645 (0.5%)
8	72	0.53	0/1135	0.96	3/1527 (0.2%)
8	7E	0.63	0/1135	1.10	5/1527 (0.3%)
9	82	0.57	0/1002	1.00	5/1346 (0.4%)
9	8E	0.62	0/1024	1.04	2/1374 (0.1%)
10	1A	0.64	0/636	1.05	4/855 (0.5%)
10	1I	0.67	0/747	1.11	5/1006 (0.5%)
11	2A	0.66	0/850	1.10	3/1150 (0.3%)
11	2I	0.73	0/838	1.21	10/1133 (0.9%)
12	3A	0.72	0/963	1.07	2/1290 (0.2%)
12	3I	0.96	1/972 (0.1%)	1.36	8/1301 (0.6%)
13	4A	0.65	0/898	1.09	9/1204 (0.7%)
13	4I	0.69	0/938	1.11	5/1258 (0.4%)
14	5A	0.60	0/475	1.14	2/632 (0.3%)
14	5I	0.72	2/505 (0.4%)	1.09	2/671 (0.3%)
15	6A	0.56	0/740	0.95	1/987 (0.1%)
15	6I	0.66	0/744	1.04	1/992 (0.1%)
16	7A	0.60	0/721	1.09	5/970 (0.5%)
16	7I	0.63	0/687	1.15	6/925 (0.6%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
17	8A	0.58	0/836	0.97	3/1117 (0.3%)
17	8I	0.75	0/836	1.13	7/1117 (0.6%)
18	9A	0.62	0/549	1.00	0/732
18	9I	0.67	0/549	1.07	1/732 (0.1%)
19	AA	0.57	0/480	1.13	2/648 (0.3%)
19	AI	0.73	1/657 (0.2%)	1.23	5/885 (0.6%)
20	BA	0.62	0/759	1.02	2/1000 (0.2%)
20	BI	0.60	0/748	1.03	4/986 (0.4%)
21	1B	0.53	0/212	0.87	0/277
21	1F	0.51	0/203	0.94	0/266
22	1K	0.38	0/1516	0.56	0/2350
23	2K	0.47	0/1721	0.69	0/2682
23	2L	0.39	0/1698	0.62	0/2644
24	3K	0.37	0/1799	0.57	0/2801
25	4K	0.47	0/495	0.66	0/771
25	4L	0.38	0/420	0.53	0/654
26	14	0.51	0/69023	0.76	21/107740 (0.0%)
26	1H	0.58	0/68351	0.83	25/106700 (0.0%)
27	16	0.47	0/2928	0.76	1/4568 (0.0%)
27	1J	0.41	0/2928	0.68	0/4568
28	71	0.79	1/1055 (0.1%)	1.17	8/1425 (0.6%)
29	11	1.05	4/2175 (0.2%)	1.49	37/2933 (1.3%)
29	19	1.04	6/2170 (0.3%)	1.48	31/2926 (1.1%)
30	21	0.88	2/1596 (0.1%)	1.48	27/2153 (1.3%)
30	29	0.86	1/1596 (0.1%)	1.41	23/2153 (1.1%)
31	31	0.95	1/1620 (0.1%)	1.33	17/2194 (0.8%)
31	39	0.79	1/1641 (0.1%)	1.27	15/2223 (0.7%)
32	41	0.68	0/1489	1.08	6/2005 (0.3%)
32	49	0.54	0/1489	1.17	11/2005 (0.5%)
33	51	0.79	0/1353	1.34	19/1830 (1.0%)
33	59	0.75	0/548	1.35	7/738 (0.9%)
34	61	0.68	0/1146	1.10	12/1551 (0.8%)
34	69	0.65	0/1146	1.12	9/1551 (0.6%)
35	15	0.65	1/1123 (0.1%)	1.12	5/1515 (0.3%)
35	58	0.81	0/1131	1.27	14/1525 (0.9%)
36	25	0.78	0/942	1.19	6/1269 (0.5%)
36	68	0.85	0/942	1.18	3/1269 (0.2%)
37	35	0.88	1/1147 (0.1%)	1.54	26/1525 (1.7%)
37	78	0.96	1/1139 (0.1%)	1.48	19/1514 (1.3%)
38	45	0.85	2/1120 (0.2%)	1.27	10/1498 (0.7%)
38	88	0.97	1/1134 (0.1%)	1.34	13/1519 (0.9%)
39	55	0.83	0/981	1.08	0/1312
39	98	0.82	1/981 (0.1%)	1.15	4/1312 (0.3%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
40	65	0.69	0/886	1.19	7/1180 (0.6%)
40	A8	0.83	0/891	1.21	3/1187 (0.3%)
41	75	0.78	0/1146	1.21	3/1531 (0.2%)
41	B8	0.88	0/1132	1.33	10/1512 (0.7%)
42	85	0.74	0/977	1.08	2/1301 (0.2%)
42	C8	0.89	1/968 (0.1%)	1.14	3/1289 (0.2%)
43	95	0.96	3/774 (0.4%)	1.35	6/1038 (0.6%)
43	D8	0.87	0/785	1.26	8/1052 (0.8%)
44	A5	0.82	0/897	1.11	2/1204 (0.2%)
44	E8	0.92	0/901	1.18	2/1209 (0.2%)
45	B5	0.92	0/752	1.24	4/1010 (0.4%)
45	F8	0.99	0/765	1.27	5/1029 (0.5%)
46	C5	0.87	0/807	1.24	5/1076 (0.5%)
46	G8	1.04	3/796 (0.4%)	1.58	19/1062 (1.8%)
47	D5	0.64	0/1057	1.24	7/1430 (0.5%)
47	H8	0.68	1/1248 (0.1%)	1.14	8/1687 (0.5%)
48	E5	0.79	0/624	1.34	9/832 (1.1%)
48	I8	0.98	1/624 (0.2%)	1.23	1/832 (0.1%)
49	F5	0.86	0/744	1.21	4/989 (0.4%)
49	J8	0.88	1/744 (0.1%)	1.30	5/989 (0.5%)
50	G5	0.71	0/575	1.22	3/762 (0.4%)
50	K8	0.90	0/573	1.19	5/759 (0.7%)
51	H5	0.64	0/464	1.13	2/623 (0.3%)
51	L8	0.77	0/464	1.26	2/623 (0.3%)
52	M8	0.70	0/375	1.29	7/507 (1.4%)
53	J5	0.81	1/448 (0.2%)	1.32	4/606 (0.7%)
53	N8	0.93	0/394	1.40	5/534 (0.9%)
54	L5	0.91	0/409	1.30	1/540 (0.2%)
54	P8	1.08	0/409	1.34	2/540 (0.4%)
55	M5	1.00	0/524	1.26	3/691 (0.4%)
55	Q8	1.02	0/524	1.53	7/691 (1.0%)
56	1L	0.36	0/1705	0.53	0/2649
57	3L	0.33	0/1732	0.50	0/2695
All	All	0.59	39/316396 (0.0%)	0.88	748/474130 (0.2%)

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	2

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Mol	Chain	#Chirality outliers	#Planarity outliers
2	1E	0	1
4	32	0	2
4	3E	0	4
7	62	0	1
7	6E	0	1
10	1A	0	1
12	3A	0	2
12	3I	0	2
13	4I	0	2
14	5A	0	1
19	AA	0	1
19	AI	0	3
28	71	0	1
29	11	0	4
29	19	0	2
30	21	0	2
30	29	0	6
31	31	0	2
31	39	0	6
32	41	0	1
32	49	0	2
33	51	0	3
33	59	0	1
34	61	0	3
34	69	0	1
35	58	0	1
37	35	0	10
37	78	0	7
38	45	0	4
38	88	0	1
40	65	0	1
40	A8	0	1
41	75	0	3
41	B8	0	4
42	85	0	2
42	C8	0	3
43	D8	0	3
45	B5	0	3
45	F8	0	1
46	C5	0	4
46	G8	0	2
47	D5	0	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
47	H8	0	2
50	G5	0	3
52	M8	0	2
55	M5	0	2
55	Q8	0	2
All	All	0	119

The worst 5 of 39 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
28	71	189	ILE	CA-CB	10.59	1.68	1.54
29	19	40	THR	CA-C	8.37	1.62	1.52
43	95	80	GLN	CA-C	8.07	1.63	1.52
29	19	34	VAL	CA-CB	7.58	1.63	1.53
29	19	272	ALA	CA-CB	-7.49	1.48	1.54

The worst 5 of 748 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	19	272	ALA	N-CA-C	14.46	125.12	108.49
29	19	235	GLY	N-CA-C	14.44	126.77	112.04
30	21	73	GLU	CA-C-N	13.99	134.16	119.89
30	21	73	GLU	C-N-CA	13.99	134.16	119.89
47	D5	157	LEU	CA-C-N	13.81	134.60	120.38

There are no chirality outliers.

5 of 119 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	1E	169	LYS	Peptide
4	3E	77	ASN	Peptide
4	3E	82	ALA	Peptide
4	3E	87	GLY	Peptide
4	3E	88	VAL	Peptide

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	13	32157	0	16233	799	0
1	1G	32391	0	16352	818	1
2	12	1711	0	1751	92	0
2	1E	1874	0	1926	87	0
3	22	1529	0	1592	72	0
3	2E	1605	0	1668	50	0
4	32	1702	0	1766	101	0
4	3E	1702	0	1762	108	0
5	42	1123	0	1191	58	0
5	4E	1142	0	1204	48	0
6	52	842	0	857	33	0
6	5E	837	0	852	48	0
7	62	1110	0	1163	53	0
7	6E	1214	0	1259	41	0
8	72	1115	0	1177	46	0
8	7E	1115	0	1177	56	0
9	82	983	0	1006	58	0
9	8E	1005	0	1033	76	0
10	1A	626	0	639	34	0
10	1I	734	0	761	50	0
11	2A	835	0	847	40	0
11	2I	823	0	833	33	0
12	3A	947	0	1033	51	0
12	3I	956	0	1046	43	0
13	4A	888	0	941	67	0
13	4I	928	0	987	53	0
14	5A	466	0	499	39	0
14	5I	496	0	535	25	0
15	6A	729	0	768	29	0
15	6I	733	0	771	25	0
16	7A	705	0	725	31	0
16	7I	671	0	693	41	0
17	8A	823	0	891	33	0
17	8I	823	0	891	48	0
18	9A	544	0	605	30	0
18	9I	544	0	605	30	0
19	AA	471	0	464	35	0
19	AI	643	0	662	37	0
20	BA	757	0	856	37	0
20	BI	746	0	843	43	0
21	1B	208	0	221	27	0
21	1F	199	0	208	7	0
22	1K	1477	0	758	31	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
23	2K	1646	0	844	29	0
23	2L	1626	0	835	30	0
24	3K	1611	0	817	57	0
25	4K	439	0	218	14	0
25	4L	373	0	185	9	0
26	14	61630	0	31070	1405	1
26	1H	61028	0	30763	1412	0
27	16	2617	0	1328	71	0
27	1J	2617	0	1328	87	0
28	71	1033	0	1048	55	0
29	11	2125	0	2199	124	0
29	19	2120	0	2197	119	0
30	21	1563	0	1629	98	0
30	29	1563	0	1629	114	0
31	31	1585	0	1632	105	0
31	39	1606	0	1652	99	0
32	41	1464	0	1522	78	0
32	49	1464	0	1522	73	0
33	51	1327	0	1405	62	0
33	59	539	0	563	35	0
34	61	1131	0	1218	51	0
34	69	1131	0	1218	55	0
35	15	1096	0	1168	64	0
35	58	1104	0	1180	68	0
36	25	932	0	996	47	0
36	68	932	0	996	42	0
37	35	1130	0	1217	98	0
37	78	1122	0	1206	93	0
38	45	1099	0	1154	68	0
38	88	1113	0	1157	56	0
39	55	967	0	1033	47	0
39	98	967	0	1033	48	0
40	65	876	0	938	81	0
40	A8	881	0	943	61	0
41	75	1132	0	1189	75	0
41	B8	1118	0	1176	64	0
42	85	959	0	1019	67	0
42	C8	950	0	1011	56	0
43	95	763	0	836	72	0
43	D8	774	0	849	53	0
44	A5	886	0	948	25	0
44	E8	890	0	951	32	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
45	B5	738	0	792	37	0
45	F8	751	0	807	41	0
46	C5	794	0	886	55	0
46	G8	783	0	873	67	0
47	D5	1034	0	1061	72	0
47	H8	1222	0	1247	79	0
48	E5	616	0	633	37	0
48	I8	616	0	633	27	0
49	F5	737	0	813	45	0
49	J8	737	0	813	40	0
50	G5	573	0	616	34	0
50	K8	571	0	623	36	0
51	H5	459	0	512	17	0
51	L8	459	0	512	17	0
52	M8	366	0	370	31	0
53	J5	434	0	454	18	0
53	N8	381	0	397	29	0
54	L5	401	0	436	18	0
54	P8	401	0	436	21	0
55	M5	516	0	582	34	0
55	Q8	516	0	582	34	0
56	1L	1570	0	798	34	0
57	3L	1571	0	798	35	0
58	11	1	0	0	0	0
58	13	142	0	0	0	0
58	14	421	0	0	0	0
58	16	11	0	0	0	0
58	19	1	0	0	0	0
58	1G	95	0	0	0	0
58	1H	495	0	0	0	0
58	1I	1	0	0	0	0
58	1J	6	0	0	0	0
58	1K	1	0	0	0	0
58	21	2	0	0	0	0
58	25	1	0	0	0	0
58	29	3	0	0	0	0
58	2I	1	0	0	0	0
58	2K	2	0	0	0	0
58	2L	2	0	0	0	0
58	39	2	0	0	0	0
58	3I	1	0	0	0	0
58	3L	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
58	4I	1	0	0	0	0
58	45	3	0	0	0	0
58	4I	1	0	0	0	0
58	4K	1	0	0	0	0
58	5I	1	0	0	0	0
58	78	1	0	0	0	0
58	7I	1	0	0	0	0
58	88	3	0	0	0	0
58	E5	1	0	0	0	0
58	I8	1	0	0	0	0
58	J8	1	0	0	0	0
58	N8	1	0	0	0	0
58	P8	1	0	0	0	0
58	Q8	1	0	0	0	0
59	32	8	0	0	0	0
59	3E	8	0	0	0	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	9	0	0	2	0
61	13	207	0	0	36	0
61	14	717	0	0	118	0
61	15	1	0	0	0	0
61	16	22	0	0	3	0
61	19	10	0	0	4	0
61	1G	117	0	0	23	0
61	1H	819	0	0	164	0
61	1I	1	0	0	0	0
61	1J	6	0	0	0	0
61	21	6	0	0	3	0
61	29	3	0	0	0	0
61	2A	1	0	0	0	0
61	31	4	0	0	1	0
61	32	2	0	0	0	0
61	35	3	0	0	0	0
61	39	3	0	0	0	0
61	3E	2	0	0	0	0
61	3I	2	0	0	0	0
61	4E	2	0	0	0	0
61	4K	4	0	0	0	0
61	5I	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
61	6A	2	0	0	1	0
61	6I	1	0	0	0	0
61	75	2	0	0	0	0
61	78	1	0	0	0	0
61	7A	1	0	0	0	0
61	85	3	0	0	1	0
61	8E	1	0	0	0	0
61	B8	1	0	0	0	0
61	BA	1	0	0	0	0
61	C8	3	0	0	1	0
61	F8	1	0	0	0	0
61	I8	5	0	0	0	0
61	J8	2	0	0	0	0
61	L8	3	0	0	0	0
61	M5	3	0	0	0	0
All	All	294304	0	195547	8678	1

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

The worst 5 of 8678 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)
1:13:788:U:H2'	1:13:789:U:H5'	1.29	1.06
30:21:135:HIS:NE2	61:21:401:HOH:O	1.87	1.06
26:1H:511:U:OP2	61:1H:3501:HOH:O	1.72	1.05
47:H8:5:LEU:HD11	47:H8:44:PHE:HA	1.40	1.02
26:14:1899:G:H21	26:14:1902:C:N4	1.56	1.02

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1G:82:U:O2'	26:14:271(C):U:O4[3_545]	2.15	0.05

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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	204/256 (80%)	170 (83%)	32 (16%)	2 (1%)	12	41
2	1E	227/256 (89%)	191 (84%)	34 (15%)	2 (1%)	14	43
3	22	190/239 (80%)	173 (91%)	15 (8%)	2 (1%)	11	39
3	2E	203/239 (85%)	187 (92%)	16 (8%)	0	100	100
4	32	206/209 (99%)	183 (89%)	22 (11%)	1 (0%)	24	55
4	3E	206/209 (99%)	188 (91%)	13 (6%)	5 (2%)	4	23
5	42	145/162 (90%)	136 (94%)	8 (6%)	1 (1%)	18	49
5	4E	147/162 (91%)	139 (95%)	7 (5%)	1 (1%)	18	49
6	52	99/101 (98%)	93 (94%)	6 (6%)	0	100	100
6	5E	98/101 (97%)	95 (97%)	3 (3%)	0	100	100
7	62	134/156 (86%)	126 (94%)	8 (6%)	0	100	100
7	6E	145/156 (93%)	136 (94%)	9 (6%)	0	100	100
8	72	136/138 (99%)	126 (93%)	8 (6%)	2 (2%)	8	33
8	7E	136/138 (99%)	129 (95%)	7 (5%)	0	100	100
9	82	122/128 (95%)	111 (91%)	11 (9%)	0	100	100
9	8E	125/128 (98%)	111 (89%)	13 (10%)	1 (1%)	16	46
10	1A	72/105 (69%)	64 (89%)	8 (11%)	0	100	100
10	1I	89/105 (85%)	81 (91%)	7 (8%)	1 (1%)	11	39
11	2A	111/129 (86%)	99 (89%)	11 (10%)	1 (1%)	14	43
11	2I	109/129 (84%)	99 (91%)	8 (7%)	2 (2%)	6	29
12	3A	119/132 (90%)	99 (83%)	19 (16%)	1 (1%)	16	46
12	3I	120/132 (91%)	104 (87%)	15 (12%)	1 (1%)	16	46
13	4A	108/126 (86%)	87 (81%)	20 (18%)	1 (1%)	14	43
13	4I	114/126 (90%)	93 (82%)	19 (17%)	2 (2%)	6	29
14	5A	55/61 (90%)	46 (84%)	8 (14%)	1 (2%)	6	29

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
14	5I	59/61 (97%)	51 (86%)	8 (14%)	0	100	100
15	6A	85/89 (96%)	79 (93%)	6 (7%)	0	100	100
15	6I	86/89 (97%)	75 (87%)	10 (12%)	1 (1%)	10	37
16	7A	82/88 (93%)	77 (94%)	5 (6%)	0	100	100
16	7I	78/88 (89%)	76 (97%)	2 (3%)	0	100	100
17	8A	97/105 (92%)	90 (93%)	7 (7%)	0	100	100
17	8I	97/105 (92%)	92 (95%)	5 (5%)	0	100	100
18	9A	65/88 (74%)	61 (94%)	4 (6%)	0	100	100
18	9I	65/88 (74%)	63 (97%)	1 (2%)	1 (2%)	8	33
19	AA	54/93 (58%)	45 (83%)	5 (9%)	4 (7%)	1	4
19	AI	78/93 (84%)	68 (87%)	6 (8%)	4 (5%)	1	10
20	BA	96/106 (91%)	88 (92%)	8 (8%)	0	100	100
20	BI	95/106 (90%)	82 (86%)	13 (14%)	0	100	100
21	1B	22/27 (82%)	21 (96%)	1 (4%)	0	100	100
21	1F	21/27 (78%)	19 (90%)	2 (10%)	0	100	100
28	7I	129/229 (56%)	120 (93%)	9 (7%)	0	100	100
29	11	272/276 (99%)	247 (91%)	16 (6%)	9 (3%)	3	17
29	19	271/276 (98%)	249 (92%)	17 (6%)	5 (2%)	6	29
30	21	202/206 (98%)	173 (86%)	25 (12%)	4 (2%)	6	27
30	29	202/206 (98%)	153 (76%)	36 (18%)	13 (6%)	1	6
31	31	200/210 (95%)	179 (90%)	19 (10%)	2 (1%)	12	41
31	39	203/210 (97%)	174 (86%)	24 (12%)	5 (2%)	4	22
32	41	178/182 (98%)	152 (85%)	23 (13%)	3 (2%)	7	30
32	49	178/182 (98%)	158 (89%)	18 (10%)	2 (1%)	11	39
33	51	171/180 (95%)	132 (77%)	35 (20%)	4 (2%)	5	24
33	59	63/180 (35%)	45 (71%)	17 (27%)	1 (2%)	7	32
34	61	143/148 (97%)	116 (81%)	25 (18%)	2 (1%)	9	34
34	69	143/148 (97%)	116 (81%)	27 (19%)	0	100	100
35	15	135/140 (96%)	123 (91%)	11 (8%)	1 (1%)	18	49
35	58	136/140 (97%)	116 (85%)	17 (12%)	3 (2%)	5	25
36	25	120/122 (98%)	112 (93%)	8 (7%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
36	68	120/122 (98%)	114 (95%)	6 (5%)	0	100	100
37	35	146/150 (97%)	112 (77%)	27 (18%)	7 (5%)	2	11
37	78	145/150 (97%)	118 (81%)	20 (14%)	7 (5%)	2	11
38	45	136/141 (96%)	111 (82%)	22 (16%)	3 (2%)	5	25
38	88	139/141 (99%)	114 (82%)	19 (14%)	6 (4%)	2	13
39	55	116/118 (98%)	110 (95%)	6 (5%)	0	100	100
39	98	116/118 (98%)	102 (88%)	14 (12%)	0	100	100
40	65	108/112 (96%)	92 (85%)	14 (13%)	2 (2%)	6	28
40	A8	109/112 (97%)	94 (86%)	13 (12%)	2 (2%)	6	29
41	75	134/146 (92%)	115 (86%)	18 (13%)	1 (1%)	18	49
41	B8	132/146 (90%)	118 (89%)	14 (11%)	0	100	100
42	85	114/118 (97%)	103 (90%)	10 (9%)	1 (1%)	14	43
42	C8	113/118 (96%)	105 (93%)	6 (5%)	2 (2%)	6	29
43	95	97/101 (96%)	78 (80%)	15 (16%)	4 (4%)	2	14
43	D8	98/101 (97%)	87 (89%)	8 (8%)	3 (3%)	3	18
44	A5	109/113 (96%)	99 (91%)	10 (9%)	0	100	100
44	E8	110/113 (97%)	103 (94%)	7 (6%)	0	100	100
45	B5	92/96 (96%)	85 (92%)	6 (6%)	1 (1%)	11	39
45	F8	94/96 (98%)	83 (88%)	8 (8%)	3 (3%)	3	17
46	C5	102/110 (93%)	69 (68%)	26 (26%)	7 (7%)	1	5
46	G8	101/110 (92%)	90 (89%)	9 (9%)	2 (2%)	6	27
47	D5	120/206 (58%)	92 (77%)	24 (20%)	4 (3%)	3	17
47	H8	142/206 (69%)	120 (84%)	15 (11%)	7 (5%)	1	11
48	E5	76/85 (89%)	73 (96%)	3 (4%)	0	100	100
48	I8	76/85 (89%)	67 (88%)	8 (10%)	1 (1%)	9	36
49	F5	92/98 (94%)	83 (90%)	7 (8%)	2 (2%)	5	25
49	J8	92/98 (94%)	88 (96%)	3 (3%)	1 (1%)	11	39
50	G5	67/72 (93%)	60 (90%)	5 (8%)	2 (3%)	3	19
50	K8	66/72 (92%)	62 (94%)	3 (4%)	1 (2%)	8	33
51	H5	56/60 (93%)	53 (95%)	3 (5%)	0	100	100
51	L8	56/60 (93%)	54 (96%)	2 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
52	M8	45/71 (63%)	26 (58%)	18 (40%)	1 (2%)	5	25
53	J5	54/60 (90%)	47 (87%)	7 (13%)	0	100	100
53	N8	47/60 (78%)	43 (92%)	4 (8%)	0	100	100
54	L5	45/49 (92%)	44 (98%)	1 (2%)	0	100	100
54	P8	45/49 (92%)	42 (93%)	3 (7%)	0	100	100
55	M5	62/65 (95%)	50 (81%)	9 (14%)	3 (5%)	2	11
55	Q8	62/65 (95%)	54 (87%)	4 (6%)	4 (6%)	1	6
All	All	10880/12104 (90%)	9578 (88%)	1134 (10%)	168 (2%)	8	33

5 of 168 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	3E	88	VAL
18	9I	22	VAL
29	11	40	THR
29	11	237	GLU
37	78	16	ARG

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	12	182/220 (83%)	129 (71%)	53 (29%)	0	1
2	1E	200/220 (91%)	147 (74%)	53 (26%)	0	2
3	22	153/188 (81%)	124 (81%)	29 (19%)	1	7
3	2E	159/188 (85%)	127 (80%)	32 (20%)	1	6
4	32	180/181 (99%)	142 (79%)	38 (21%)	1	6
4	3E	180/181 (99%)	149 (83%)	31 (17%)	2	9
5	42	113/123 (92%)	86 (76%)	27 (24%)	1	3
5	4E	115/123 (94%)	85 (74%)	30 (26%)	0	2
6	52	90/90 (100%)	79 (88%)	11 (12%)	5	19

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
6	5E	90/90 (100%)	78 (87%)	12 (13%)	4	17
7	62	114/127 (90%)	90 (79%)	24 (21%)	1	6
7	6E	123/127 (97%)	88 (72%)	35 (28%)	0	1
8	72	119/119 (100%)	94 (79%)	25 (21%)	1	6
8	7E	119/119 (100%)	92 (77%)	27 (23%)	1	4
9	82	95/99 (96%)	73 (77%)	22 (23%)	1	4
9	8E	97/99 (98%)	71 (73%)	26 (27%)	0	2
10	1A	69/92 (75%)	53 (77%)	16 (23%)	1	4
10	1I	81/92 (88%)	61 (75%)	20 (25%)	1	3
11	2A	85/99 (86%)	69 (81%)	16 (19%)	1	8
11	2I	84/99 (85%)	64 (76%)	20 (24%)	1	4
12	3A	102/109 (94%)	82 (80%)	20 (20%)	1	7
12	3I	103/109 (94%)	79 (77%)	24 (23%)	1	4
13	4A	91/101 (90%)	64 (70%)	27 (30%)	0	1
13	4I	94/101 (93%)	69 (73%)	25 (27%)	0	2
14	5A	47/50 (94%)	31 (66%)	16 (34%)	0	0
14	5I	49/50 (98%)	40 (82%)	9 (18%)	1	8
15	6A	79/80 (99%)	68 (86%)	11 (14%)	3	15
15	6I	79/80 (99%)	64 (81%)	15 (19%)	1	7
16	7A	72/74 (97%)	61 (85%)	11 (15%)	3	12
16	7I	69/74 (93%)	51 (74%)	18 (26%)	0	2
17	8A	94/97 (97%)	84 (89%)	10 (11%)	6	24
17	8I	94/97 (97%)	74 (79%)	20 (21%)	1	5
18	9A	58/77 (75%)	44 (76%)	14 (24%)	1	3
18	9I	58/77 (75%)	47 (81%)	11 (19%)	1	7
19	AA	52/80 (65%)	33 (64%)	19 (36%)	0	0
19	AI	70/80 (88%)	51 (73%)	19 (27%)	0	2
20	BA	76/82 (93%)	62 (82%)	14 (18%)	1	8
20	BI	75/82 (92%)	64 (85%)	11 (15%)	3	14
21	1B	19/22 (86%)	16 (84%)	3 (16%)	2	11
21	1F	18/22 (82%)	14 (78%)	4 (22%)	1	5

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
28	71	109/181 (60%)	75 (69%)	34 (31%)	0	1
29	11	214/218 (98%)	161 (75%)	53 (25%)	1	3
29	19	214/218 (98%)	157 (73%)	57 (27%)	0	2
30	21	165/166 (99%)	124 (75%)	41 (25%)	1	3
30	29	165/166 (99%)	129 (78%)	36 (22%)	1	5
31	31	161/166 (97%)	121 (75%)	40 (25%)	1	3
31	39	163/166 (98%)	122 (75%)	41 (25%)	0	3
32	41	154/156 (99%)	111 (72%)	43 (28%)	0	2
32	49	154/156 (99%)	126 (82%)	28 (18%)	2	8
33	51	144/148 (97%)	107 (74%)	37 (26%)	0	3
33	59	56/148 (38%)	40 (71%)	16 (29%)	0	1
34	61	122/124 (98%)	88 (72%)	34 (28%)	0	2
34	69	122/124 (98%)	87 (71%)	35 (29%)	0	1
35	15	116/119 (98%)	87 (75%)	29 (25%)	0	3
35	58	117/119 (98%)	83 (71%)	34 (29%)	0	1
36	25	100/100 (100%)	76 (76%)	24 (24%)	1	3
36	68	100/100 (100%)	79 (79%)	21 (21%)	1	6
37	35	115/116 (99%)	73 (64%)	42 (36%)	0	0
37	78	114/116 (98%)	79 (69%)	35 (31%)	0	1
38	45	109/111 (98%)	79 (72%)	30 (28%)	0	2
38	88	109/111 (98%)	84 (77%)	25 (23%)	1	4
39	55	101/101 (100%)	76 (75%)	25 (25%)	1	3
39	98	101/101 (100%)	73 (72%)	28 (28%)	0	2
40	65	87/88 (99%)	61 (70%)	26 (30%)	0	1
40	A8	87/88 (99%)	58 (67%)	29 (33%)	0	1
41	75	119/127 (94%)	88 (74%)	31 (26%)	0	2
41	B8	118/127 (93%)	85 (72%)	33 (28%)	0	2
42	85	93/94 (99%)	76 (82%)	17 (18%)	2	8
42	C8	92/94 (98%)	78 (85%)	14 (15%)	3	12
43	95	81/82 (99%)	55 (68%)	26 (32%)	0	1
43	D8	82/82 (100%)	51 (62%)	31 (38%)	0	0

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
44	A5	91/92 (99%)	72 (79%)	19 (21%)	1	6
44	E8	91/92 (99%)	66 (72%)	25 (28%)	0	2
45	B5	75/78 (96%)	54 (72%)	21 (28%)	0	2
45	F8	76/78 (97%)	58 (76%)	18 (24%)	1	4
46	C5	85/91 (93%)	59 (69%)	26 (31%)	0	1
46	G8	84/91 (92%)	56 (67%)	28 (33%)	0	1
47	D5	115/179 (64%)	83 (72%)	32 (28%)	0	2
47	H8	137/179 (76%)	104 (76%)	33 (24%)	1	3
48	E5	62/67 (92%)	50 (81%)	12 (19%)	1	7
48	I8	62/67 (92%)	49 (79%)	13 (21%)	1	6
49	F5	79/83 (95%)	53 (67%)	26 (33%)	0	1
49	J8	79/83 (95%)	60 (76%)	19 (24%)	1	3
50	G5	62/67 (92%)	35 (56%)	27 (44%)	0	0
50	K8	63/67 (94%)	40 (64%)	23 (36%)	0	0
51	H5	50/52 (96%)	41 (82%)	9 (18%)	2	8
51	L8	50/52 (96%)	39 (78%)	11 (22%)	1	5
52	M8	42/63 (67%)	31 (74%)	11 (26%)	0	2
53	J5	48/52 (92%)	41 (85%)	7 (15%)	3	14
53	N8	44/52 (85%)	33 (75%)	11 (25%)	0	3
54	L5	38/42 (90%)	31 (82%)	7 (18%)	1	8
54	P8	38/42 (90%)	32 (84%)	6 (16%)	2	11
55	M5	54/55 (98%)	37 (68%)	17 (32%)	0	1
55	Q8	54/55 (98%)	42 (78%)	12 (22%)	1	5
All	All	9210/10012 (92%)	6954 (76%)	2256 (24%)	1	3

5 of 2256 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
36	25	97	ARG
38	45	55	VAL
36	25	92	GLU
45	B5	54	VAL
36	68	108	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 70 such sidechains are listed below:

Mol	Chain	Res	Type
39	55	31	HIS
43	95	87	HIS
48	E5	29	GLN
36	68	3	GLN
32	41	40	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	13	1493/1522 (98%)	374 (25%)	34 (2%)
1	1G	1505/1522 (98%)	379 (25%)	30 (1%)
22	1K	65/76 (85%)	32 (49%)	3 (4%)
23	2K	76/77 (98%)	23 (30%)	3 (3%)
23	2L	74/77 (96%)	20 (27%)	3 (4%)
24	3K	75/76 (98%)	43 (57%)	2 (2%)
25	4K	19/27 (70%)	10 (52%)	2 (10%)
25	4L	16/27 (59%)	7 (43%)	0
26	14	2852/2917 (97%)	734 (25%)	47 (1%)
26	1H	2828/2917 (96%)	710 (25%)	52 (1%)
27	16	121/122 (99%)	25 (20%)	2 (1%)
27	1J	121/122 (99%)	41 (33%)	2 (1%)
56	1L	71/76 (93%)	31 (43%)	4 (5%)
57	3L	72/76 (94%)	21 (29%)	2 (2%)
All	All	9388/9634 (97%)	2450 (26%)	186 (1%)

5 of 2450 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	13	2	U
1	13	5	U
1	13	6	G
1	13	11	G
1	13	31	G

5 of 186 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	1G	913	A
26	14	278	A
1	1G	1145	C

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Mol	Chain	Res	Type
56	1L	67	C
26	14	784	A

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
23	PSU	2L	56	23	18,21,22	1.33	1 (5%)	21,30,33	1.75	3 (14%)
23	4SU	2K	8	23	18,21,22	1.84	3 (16%)	25,30,33	2.44	5 (20%)
23	4SU	2L	8	23	18,21,22	2.01	5 (27%)	25,30,33	2.40	6 (24%)
22	PSU	1K	55	22	18,21,22	1.36	1 (5%)	21,30,33	1.82	5 (23%)
22	U8U	1K	34	25,22	20,24,25	2.35	6 (30%)	22,34,37	1.20	3 (13%)
56	5MU	1L	54	56	19,22,23	3.93	5 (26%)	27,32,35	3.11	11 (40%)
23	5MU	2L	55	23	19,22,23	4.03	5 (26%)	27,32,35	3.20	9 (33%)
57	PSU	3L	39	57	18,21,22	1.22	1 (5%)	21,30,33	1.56	2 (9%)
23	7MG	2K	47	23	23,26,27	3.28	7 (30%)	27,39,42	2.51	10 (37%)
22	T6A	1K	37	22	31,34,35	2.10	9 (29%)	43,49,52	2.21	14 (32%)
23	7MG	2L	47	23	23,26,27	3.04	7 (30%)	27,39,42	2.94	10 (37%)
23	PSU	2K	56	23	18,21,22	1.30	1 (5%)	21,30,33	2.05	4 (19%)
23	OMC	2K	33	23	19,22,23	1.72	3 (15%)	25,31,34	0.95	1 (4%)
22	PSU	1K	39	22	18,21,22	1.19	1 (5%)	21,30,33	1.67	4 (19%)
23	5MU	2K	55	23	19,22,23	3.94	5 (26%)	27,32,35	3.37	10 (37%)
22	5MU	1K	54	22	19,22,23	3.87	5 (26%)	27,32,35	3.24	6 (22%)
56	PSU	1L	55	56	18,21,22	1.19	1 (5%)	21,30,33	1.76	4 (19%)
23	OMC	2L	33	23	19,22,23	1.83	4 (21%)	25,31,34	1.11	1 (4%)

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	PSU	2L	56	23	-	0/7/25/26	0/2/2/2
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
22	PSU	1K	55	22	-	0/7/25/26	0/2/2/2
22	U8U	1K	34	25,22	-	3/10/28/29	0/2/2/2
56	5MU	1L	54	56	-	3/7/25/26	0/2/2/2
23	5MU	2L	55	23	-	2/7/25/26	0/2/2/2
57	PSU	3L	39	57	-	0/7/25/26	0/2/2/2
23	7MG	2K	47	23	-	1/7/37/38	0/3/3/3
22	T6A	1K	37	22	-	4/23/41/42	0/3/3/3
23	7MG	2L	47	23	-	3/7/37/38	0/3/3/3
23	PSU	2K	56	23	-	0/7/25/26	0/2/2/2
23	OMC	2K	33	23	-	0/9/27/28	0/2/2/2
22	PSU	1K	39	22	-	1/7/25/26	0/2/2/2
23	5MU	2K	55	23	-	0/7/25/26	0/2/2/2
22	5MU	1K	54	22	-	2/7/25/26	0/2/2/2
56	PSU	1L	55	56	-	3/7/25/26	0/2/2/2
23	OMC	2L	33	23	-	3/9/27/28	0/2/2/2

The worst 5 of 70 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	2L	55	5MU	C2-N1	13.02	1.58	1.38
23	2K	55	5MU	C2-N1	12.73	1.58	1.38
22	1K	54	5MU	C2-N1	12.62	1.58	1.38
56	1L	54	5MU	C2-N1	12.41	1.57	1.38
23	2K	47	7MG	C5-N7	9.19	1.47	1.35

The worst 5 of 108 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	1K	54	5MU	C5-C4-N3	10.75	124.67	115.32
23	2L	55	5MU	C5-C4-N3	10.10	124.10	115.32
23	2K	55	5MU	C5-C4-N3	10.00	124.02	115.32
56	1L	54	5MU	C5-C4-N3	9.74	123.78	115.32
23	2L	47	7MG	C4-C5-N7	8.20	115.06	105.38

There are no chirality outliers.

5 of 25 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
22	1K	34	U8U	C5-C-N-CA
22	1K	34	U8U	O4'-C4'-C5'-O5'
22	1K	37	T6A	N11-C12-C14-O14
22	1K	37	T6A	N11-C12-C14-C15
22	1K	37	T6A	C13-C12-C14-O14

There are no ring outliers.

12 monomers are involved in 15 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
23	2K	8	4SU	1	0
23	2L	8	4SU	2	0
22	1K	55	PSU	1	0
23	2L	55	5MU	1	0
57	3L	39	PSU	1	0
23	2K	47	7MG	1	0
22	1K	37	T6A	1	0
23	2L	47	7MG	1	0
23	2K	33	OMC	1	0
23	2K	55	5MU	2	0
22	1K	54	5MU	2	0
23	2L	33	OMC	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 1213 ligands modelled in this entry, 1211 are monoatomic - leaving 2 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	$\# Z > 2$
59	SF4	3E	301	4	0,12,12	-	-	-		
59	SF4	32	301	-	0,12,12	-	-	-		

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
59	SF4	3E	301	4	-	-	0/6/5/5
59	SF4	32	301	-	-	-	0/6/5/5

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

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%)	-0.58	11 (0%) 84 69	61, 106, 170, 196	0
1	1G	1507/1522 (99%)	-0.42	25 (1%) 69 48	74, 126, 175, 200	0
2	12	208/256 (81%)	0.01	3 (1%) 73 53	134, 156, 168, 176	0
2	1E	231/256 (90%)	0.04	3 (1%) 75 55	116, 144, 162, 166	0
3	22	194/239 (81%)	0.39	11 (5%) 29 17	129, 148, 164, 167	0
3	2E	205/239 (85%)	0.10	6 (2%) 53 34	89, 111, 139, 148	0
4	32	208/209 (99%)	0.12	2 (0%) 79 62	105, 125, 146, 151	0
4	3E	208/209 (99%)	0.02	5 (2%) 59 39	85, 106, 126, 135	0
5	42	147/162 (90%)	0.41	9 (6%) 27 15	112, 126, 138, 145	0
5	4E	149/162 (91%)	0.01	4 (2%) 56 35	81, 103, 122, 131	0
6	52	101/101 (100%)	0.09	3 (2%) 52 32	92, 111, 128, 134	0
6	5E	100/101 (99%)	-0.04	0 100 100	90, 109, 127, 132	0
7	62	138/156 (88%)	0.13	3 (2%) 62 41	122, 133, 142, 148	0
7	6E	149/156 (95%)	0.09	3 (2%) 65 44	107, 124, 143, 149	0
8	72	138/138 (100%)	-0.03	5 (3%) 46 27	112, 131, 141, 149	0
8	7E	138/138 (100%)	-0.09	2 (1%) 73 53	92, 115, 130, 139	0
9	82	124/128 (96%)	0.15	7 (5%) 30 17	121, 153, 162, 166	0
9	8E	127/128 (99%)	0.38	12 (9%) 14 8	91, 137, 154, 159	0
10	1A	78/105 (74%)	1.03	19 (24%) 2 1	119, 148, 159, 161	0
10	1I	91/105 (86%)	0.02	0 100 100	87, 128, 157, 163	0
11	2A	113/129 (87%)	0.46	2 (1%) 67 47	89, 115, 135, 141	0
11	2I	111/129 (86%)	0.34	3 (2%) 56 35	82, 110, 127, 140	0
12	3A	121/132 (91%)	0.66	14 (11%) 9 6	93, 113, 129, 148	0
12	3I	122/132 (92%)	-0.13	4 (3%) 49 29	72, 80, 103, 132	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
13	4A	110/126 (87%)	0.24	6 (5%) 30 17	135, 149, 160, 164	0
13	4I	116/126 (92%)	0.02	2 (1%) 69 48	94, 127, 141, 150	0
14	5A	57/61 (93%)	0.10	2 (3%) 47 28	134, 146, 155, 158	0
14	5I	61/61 (100%)	-0.28	0 100 100	86, 100, 118, 123	0
15	6A	87/89 (97%)	-0.23	1 (1%) 78 60	93, 119, 139, 144	0
15	6I	88/89 (98%)	-0.25	1 (1%) 78 60	81, 104, 125, 134	0
16	7A	84/88 (95%)	0.06	1 (1%) 76 57	95, 114, 137, 148	0
16	7I	80/88 (90%)	0.08	0 100 100	101, 115, 133, 142	0
17	8A	99/105 (94%)	-0.24	2 (2%) 65 44	102, 119, 130, 135	0
17	8I	99/105 (94%)	0.11	6 (6%) 27 15	93, 109, 125, 130	0
18	9A	67/88 (76%)	-0.05	1 (1%) 72 52	101, 118, 136, 139	0
18	9I	67/88 (76%)	0.08	1 (1%) 72 52	94, 112, 132, 136	0
19	AA	60/93 (64%)	0.21	1 (1%) 69 48	133, 161, 167, 171	0
19	AI	80/93 (86%)	-0.03	0 100 100	105, 121, 143, 150	0
20	BA	98/106 (92%)	-0.17	2 (2%) 65 44	87, 115, 141, 154	0
20	BI	97/106 (91%)	0.15	3 (3%) 51 31	114, 126, 152, 156	0
21	1B	24/27 (88%)	0.07	0 100 100	128, 144, 156, 160	0
21	1F	23/27 (85%)	-0.40	0 100 100	106, 114, 122, 128	0
22	1K	64/76 (84%)	0.89	12 (18%) 3 2	96, 170, 182, 184	0
23	2K	72/77 (93%)	-0.03	1 (1%) 73 53	74, 103, 134, 154	0
23	2L	71/77 (92%)	0.40	3 (4%) 40 23	84, 121, 153, 157	0
24	3K	76/76 (100%)	0.81	10 (13%) 7 5	79, 183, 195, 202	0
25	4K	20/27 (74%)	0.62	2 (10%) 12 7	78, 145, 186, 186	0
25	4L	17/27 (62%)	0.95	2 (11%) 9 5	104, 160, 189, 189	0
26	14	2861/2917 (98%)	-0.63	20 (0%) 84 69	54, 88, 183, 207	0
26	1H	2833/2917 (97%)	-0.74	18 (0%) 85 72	45, 77, 169, 200	0
27	16	122/122 (100%)	-0.96	0 100 100	70, 97, 122, 187	0
27	1J	122/122 (100%)	-0.52	1 (0%) 82 66	94, 131, 151, 186	0
28	7I	133/229 (58%)	0.21	4 (3%) 52 32	126, 158, 171, 177	0
29	11	274/276 (99%)	-0.16	6 (2%) 62 41	47, 69, 89, 99	0
29	19	273/276 (98%)	0.13	5 (1%) 67 47	51, 76, 92, 113	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
30	21	204/206 (99%)	0.23	7 (3%) 48 28	52, 92, 133, 150	0
30	29	204/206 (99%)	0.29	12 (5%) 28 16	59, 96, 131, 135	0
31	31	202/210 (96%)	-0.23	1 (0%) 87 75	51, 81, 113, 135	0
31	39	205/210 (97%)	-0.19	1 (0%) 87 75	61, 104, 144, 171	0
32	41	180/182 (98%)	-0.25	4 (2%) 62 41	90, 110, 144, 155	0
32	49	180/182 (98%)	0.16	6 (3%) 49 29	124, 143, 162, 169	0
33	51	173/180 (96%)	0.31	11 (6%) 25 14	87, 109, 124, 137	0
33	59	69/180 (38%)	1.91	25 (36%) 1 1	136, 158, 168, 170	0
34	61	145/148 (97%)	0.09	4 (2%) 55 34	84, 133, 147, 158	0
34	69	145/148 (97%)	-0.01	1 (0%) 84 69	87, 127, 146, 152	0
35	15	137/140 (97%)	0.44	9 (6%) 24 14	78, 109, 138, 155	0
35	58	138/140 (98%)	0.43	14 (10%) 12 7	69, 92, 132, 145	0
36	25	122/122 (100%)	0.10	4 (3%) 49 29	70, 92, 109, 116	0
36	68	122/122 (100%)	0.13	1 (0%) 82 66	60, 81, 99, 113	0
37	35	148/150 (98%)	0.17	6 (4%) 41 24	59, 105, 140, 156	0
37	78	147/150 (98%)	-0.08	5 (3%) 48 28	52, 84, 108, 119	0
38	45	138/141 (97%)	0.34	14 (10%) 12 7	75, 110, 134, 149	0
38	88	141/141 (100%)	-0.22	1 (0%) 84 69	58, 85, 105, 122	0
39	55	118/118 (100%)	-0.42	0 100 100	64, 84, 102, 119	0
39	98	118/118 (100%)	-0.11	1 (0%) 82 66	66, 87, 108, 130	0
40	65	110/112 (98%)	-0.21	0 100 100	92, 120, 137, 142	0
40	A8	111/112 (99%)	-0.44	0 100 100	75, 93, 115, 135	0
41	75	136/146 (93%)	-0.01	3 (2%) 62 41	80, 100, 138, 155	0
41	B8	134/146 (91%)	0.44	8 (5%) 27 16	74, 95, 137, 155	0
42	85	116/118 (98%)	0.06	3 (2%) 57 36	68, 97, 129, 138	0
42	C8	115/118 (97%)	0.17	4 (3%) 47 28	57, 83, 110, 117	0
43	95	99/101 (98%)	0.39	5 (5%) 33 19	65, 123, 136, 145	0
43	D8	100/101 (99%)	0.46	2 (2%) 65 44	59, 102, 124, 139	0
44	A5	111/113 (98%)	-0.10	0 100 100	65, 77, 107, 135	0
44	E8	112/113 (99%)	-0.02	1 (0%) 81 64	61, 75, 105, 140	0
45	B5	94/96 (97%)	-0.11	2 (2%) 63 42	69, 90, 111, 123	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
45	F8	96/96 (100%)	-0.17	2 (2%) 63 42	53, 74, 112, 125	0
46	C5	104/110 (94%)	1.02	18 (17%) 4 2	91, 119, 148, 157	0
46	G8	103/110 (93%)	0.34	5 (4%) 35 20	74, 93, 127, 130	0
47	D5	126/206 (61%)	-0.04	1 (0%) 82 66	117, 137, 159, 164	0
47	H8	148/206 (71%)	-0.30	0 100 100	86, 121, 154, 160	0
48	E5	78/85 (91%)	0.13	3 (3%) 44 26	73, 93, 110, 138	0
48	I8	78/85 (91%)	-0.36	4 (5%) 33 19	62, 77, 98, 110	0
49	F5	94/98 (95%)	0.36	7 (7%) 20 12	65, 86, 123, 133	0
49	J8	94/98 (95%)	-0.06	2 (2%) 63 42	57, 79, 115, 126	0
50	G5	69/72 (95%)	-0.15	1 (1%) 73 53	89, 109, 131, 150	0
50	K8	68/72 (94%)	-0.08	1 (1%) 72 52	64, 81, 98, 126	0
51	H5	58/60 (96%)	-0.16	1 (1%) 69 48	77, 103, 128, 137	0
51	L8	58/60 (96%)	-0.39	0 100 100	66, 81, 110, 129	0
52	M8	47/71 (66%)	0.07	0 100 100	114, 147, 163, 171	0
53	J5	56/60 (93%)	0.12	2 (3%) 46 27	61, 87, 134, 143	0
53	N8	49/60 (81%)	-0.04	1 (2%) 65 44	55, 82, 140, 150	0
54	L5	47/49 (95%)	-0.33	1 (2%) 63 42	57, 62, 79, 91	0
54	P8	47/49 (95%)	-0.46	0 100 100	49, 55, 78, 89	0
55	M5	64/65 (98%)	0.16	2 (3%) 51 31	72, 82, 97, 124	0
55	Q8	64/65 (98%)	-0.14	1 (1%) 70 50	56, 73, 86, 101	0
56	1L	72/76 (94%)	0.72	9 (12%) 8 5	127, 184, 195, 204	0
57	3L	73/76 (96%)	0.42	6 (8%) 17 10	84, 172, 185, 193	0
All	All	20506/21738 (94%)	-0.22	491 (2%) 59 39	45, 104, 163, 207	0

The worst 5 of 491 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
12	3A	19	ARG	10.3
41	B8	104	ASN	9.0
10	1A	58	ASP	9.0
9	82	115	GLY	8.3
33	59	169	VAL	7.5

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

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
56	5MU	1L	54	21/22	0.75	0.10	143,156,161,162	0
22	PSU	1K	55	20/21	0.76	0.10	121,129,137,142	0
56	PSU	1L	55	20/21	0.81	0.08	137,155,161,162	0
23	PSU	2L	56	20/21	0.83	0.08	133,136,141,142	0
23	5MU	2L	55	21/22	0.85	0.08	131,139,146,151	0
57	PSU	3L	39	20/21	0.86	0.11	147,156,160,160	0
23	PSU	2K	56	20/21	0.86	0.08	103,115,124,125	0
23	OMC	2L	33	21/22	0.86	0.12	106,117,118,119	0
23	5MU	2K	55	21/22	0.88	0.08	117,123,131,135	0
23	4SU	2L	8	20/21	0.88	0.12	110,128,130,136	0
22	5MU	1K	54	21/22	0.89	0.08	118,129,141,147	0
23	4SU	2K	8	20/21	0.90	0.12	90,100,108,111	0
23	7MG	2L	47	24/25	0.90	0.10	133,141,147,149	0
23	7MG	2K	47	24/25	0.92	0.09	103,111,119,127	0
22	PSU	1K	39	20/21	0.92	0.11	104,124,130,132	0
22	T6A	1K	37	32/33	0.93	0.11	89,102,123,128	0
23	OMC	2K	33	21/22	0.94	0.15	80,86,90,95	0
22	U8U	1K	34	23/24	0.94	0.09	88,99,103,104	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
58	MG	13	1680	1/1	-0.12	0.29	149,149,149,149	0
58	MG	1H	3294	1/1	0.34	0.28	141,141,141,141	0
58	MG	1K	101	1/1	0.38	0.36	147,147,147,147	0
58	MG	14	3138	1/1	0.43	0.33	91,91,91,91	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
58	MG	1G	1668	1/1	0.44	0.29	141,141,141,141	0
58	MG	1H	3205	1/1	0.44	0.26	101,101,101,101	0
58	MG	1G	1666	1/1	0.47	0.29	125,125,125,125	0
58	MG	1H	3333	1/1	0.49	0.37	88,88,88,88	0
58	MG	3L	101	1/1	0.50	0.20	160,160,160,160	0
58	MG	1J	203	1/1	0.51	0.29	88,88,88,88	0
58	MG	14	3042	1/1	0.52	0.27	95,95,95,95	0
58	MG	14	3241	1/1	0.53	0.27	115,115,115,115	0
58	MG	14	3219	1/1	0.53	0.20	107,107,107,107	0
58	MG	1H	3327	1/1	0.54	0.27	134,134,134,134	0
58	MG	13	1608	1/1	0.54	0.30	86,86,86,86	0
58	MG	1H	3263	1/1	0.58	0.27	106,106,106,106	0
58	MG	1G	1664	1/1	0.59	0.28	122,122,122,122	0
58	MG	1H	3286	1/1	0.59	0.29	100,100,100,100	0
58	MG	14	3289	1/1	0.59	0.20	99,99,99,99	0
58	MG	13	1679	1/1	0.59	0.20	117,117,117,117	0
58	MG	1G	1654	1/1	0.60	0.23	132,132,132,132	0
58	MG	2L	102	1/1	0.61	0.20	94,94,94,94	0
58	MG	1G	1603	1/1	0.61	0.27	100,100,100,100	0
58	MG	1H	3334	1/1	0.62	0.24	96,96,96,96	0
58	MG	1G	1611	1/1	0.62	0.28	105,105,105,105	0
58	MG	1H	3326	1/1	0.63	0.30	119,119,119,119	0
58	MG	14	3245	1/1	0.64	0.22	90,90,90,90	0
58	MG	14	3257	1/1	0.64	0.30	92,92,92,92	0
58	MG	1H	3272	1/1	0.64	0.24	80,80,80,80	0
58	MG	1G	1616	1/1	0.64	0.15	116,116,116,116	0
58	MG	1H	3284	1/1	0.65	0.34	92,92,92,92	0
58	MG	14	3243	1/1	0.65	0.20	118,118,118,118	0
58	MG	1H	3174	1/1	0.65	0.31	93,93,93,93	0
58	MG	1G	1670	1/1	0.65	0.34	110,110,110,110	0
58	MG	14	3263	1/1	0.65	0.29	86,86,86,86	0
58	MG	14	3199	1/1	0.65	0.29	91,91,91,91	0
58	MG	13	1647	1/1	0.65	0.21	107,107,107,107	0
58	MG	1G	1650	1/1	0.66	0.33	102,102,102,102	0
58	MG	1H	3318	1/1	0.66	0.47	71,71,71,71	0
58	MG	14	3190	1/1	0.66	0.19	106,106,106,106	0
58	MG	1G	1659	1/1	0.66	0.25	107,107,107,107	0
58	MG	14	3201	1/1	0.67	0.27	91,91,91,91	0
58	MG	1H	3201	1/1	0.67	0.18	67,67,67,67	0
58	MG	1H	3293	1/1	0.67	0.36	92,92,92,92	0
58	MG	1H	3313	1/1	0.68	0.27	96,96,96,96	0
58	MG	14	3231	1/1	0.68	0.27	90,90,90,90	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
58	MG	14	3102	1/1	0.68	0.45	76,76,76,76	0
58	MG	14	3115	1/1	0.68	0.23	104,104,104,104	0
58	MG	1G	1655	1/1	0.68	0.33	85,85,85,85	0
58	MG	1G	1648	1/1	0.68	0.33	90,90,90,90	0
58	MG	1G	1660	1/1	0.68	0.26	107,107,107,107	0
58	MG	13	1675	1/1	0.68	0.21	97,97,97,97	0
58	MG	14	3207	1/1	0.68	0.15	66,66,66,66	0
58	MG	14	3226	1/1	0.69	0.41	99,99,99,99	0
58	MG	14	3249	1/1	0.69	0.27	93,93,93,93	0
58	MG	14	3037	1/1	0.69	0.20	55,55,55,55	0
58	MG	13	1690	1/1	0.70	0.30	105,105,105,105	0
58	MG	14	3184	1/1	0.70	0.28	85,85,85,85	0
58	MG	1G	1638	1/1	0.70	0.21	131,131,131,131	0
58	MG	14	3194	1/1	0.70	0.28	74,74,74,74	0
58	MG	13	1701	1/1	0.70	0.20	92,92,92,92	0
58	MG	1G	1656	1/1	0.70	0.20	126,126,126,126	0
58	MG	14	3208	1/1	0.71	0.39	76,76,76,76	0
58	MG	13	1667	1/1	0.71	0.17	90,90,90,90	0
58	MG	13	1668	1/1	0.71	0.21	105,105,105,105	0
58	MG	1H	3160	1/1	0.71	0.24	93,93,93,93	0
58	MG	1H	3162	1/1	0.71	0.25	74,74,74,74	0
58	MG	1G	1671	1/1	0.71	0.27	102,102,102,102	0
58	MG	1G	1674	1/1	0.71	0.21	110,110,110,110	0
58	MG	1G	1633	1/1	0.71	0.18	102,102,102,102	0
58	MG	14	3197	1/1	0.71	0.24	146,146,146,146	0
58	MG	1H	3267	1/1	0.71	0.27	97,97,97,97	0
58	MG	14	3003	1/1	0.71	0.26	74,74,74,74	0
58	MG	1G	1641	1/1	0.71	0.19	102,102,102,102	0
58	MG	14	3160	1/1	0.72	0.31	76,76,76,76	0
58	MG	13	1694	1/1	0.72	0.28	88,88,88,88	0
58	MG	13	1696	1/1	0.72	0.28	105,105,105,105	0
58	MG	13	1686	1/1	0.72	0.15	94,94,94,94	0
58	MG	13	1687	1/1	0.72	0.19	96,96,96,96	0
58	MG	1H	3234	1/1	0.72	0.24	78,78,78,78	0
58	MG	1H	3252	1/1	0.72	0.30	77,77,77,77	0
58	MG	14	3258	1/1	0.72	0.20	100,100,100,100	0
58	MG	13	1670	1/1	0.72	0.32	103,103,103,103	0
58	MG	1G	1612	1/1	0.72	0.25	100,100,100,100	0
58	MG	1G	1673	1/1	0.72	0.13	93,93,93,93	0
58	MG	1H	3302	1/1	0.73	0.27	94,94,94,94	0
58	MG	14	3242	1/1	0.73	0.34	90,90,90,90	0
58	MG	13	1702	1/1	0.73	0.16	157,157,157,157	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
58	MG	14	3104	1/1	0.73	0.34	85,85,85,85	0
58	MG	1G	1647	1/1	0.73	0.29	105,105,105,105	0
58	MG	13	1692	1/1	0.73	0.33	101,101,101,101	0
58	MG	14	3144	1/1	0.73	0.29	82,82,82,82	0
58	MG	1H	3072	1/1	0.73	0.16	80,80,80,80	0
58	MG	13	1666	1/1	0.73	0.24	97,97,97,97	0
58	MG	1H	3271	1/1	0.73	0.32	72,72,72,72	0
58	MG	1H	3042	1/1	0.74	0.32	67,67,67,67	0
58	MG	13	1641	1/1	0.74	0.27	86,86,86,86	0
58	MG	1G	1628	1/1	0.74	0.32	102,102,102,102	0
58	MG	14	3232	1/1	0.74	0.27	84,84,84,84	0
58	MG	14	3206	1/1	0.74	0.33	71,71,71,71	0
58	MG	1H	3300	1/1	0.74	0.27	85,85,85,85	0
58	MG	1H	3034	1/1	0.74	0.23	91,91,91,91	0
58	MG	2I	201	1/1	0.75	0.20	98,98,98,98	0
58	MG	1H	3037	1/1	0.75	0.24	99,99,99,99	0
58	MG	14	3246	1/1	0.75	0.20	90,90,90,90	0
58	MG	1H	3202	1/1	0.75	0.18	84,84,84,84	0
58	MG	13	1698	1/1	0.75	0.20	104,104,104,104	0
58	MG	1H	3295	1/1	0.75	0.30	88,88,88,88	0
58	MG	1H	3219	1/1	0.75	0.21	96,96,96,96	0
58	MG	16	208	1/1	0.75	0.23	82,82,82,82	0
58	MG	1H	3230	1/1	0.75	0.23	85,85,85,85	0
58	MG	14	3077	1/1	0.76	0.28	84,84,84,84	0
58	MG	14	3192	1/1	0.76	0.32	69,69,69,69	0
58	MG	1H	3149	1/1	0.76	0.30	79,79,79,79	0
58	MG	13	1672	1/1	0.76	0.19	112,112,112,112	0
58	MG	14	3107	1/1	0.76	0.28	92,92,92,92	0
58	MG	1H	3068	1/1	0.76	0.24	92,92,92,92	0
58	MG	14	3121	1/1	0.76	0.27	83,83,83,83	0
58	MG	14	3250	1/1	0.76	0.32	87,87,87,87	0
58	MG	13	1699	1/1	0.76	0.22	88,88,88,88	0
58	MG	1H	3226	1/1	0.76	0.30	74,74,74,74	0
58	MG	14	3158	1/1	0.76	0.17	69,69,69,69	0
58	MG	1G	1627	1/1	0.76	0.26	103,103,103,103	0
58	MG	14	3068	1/1	0.76	0.43	86,86,86,86	0
58	MG	1J	205	1/1	0.76	0.26	89,89,89,89	0
58	MG	14	3013	1/1	0.77	0.31	83,83,83,83	0
58	MG	14	3036	1/1	0.77	0.23	115,115,115,115	0
58	MG	1H	3304	1/1	0.77	0.37	94,94,94,94	0
58	MG	14	3227	1/1	0.77	0.32	91,91,91,91	0
58	MG	1H	3288	1/1	0.77	0.26	77,77,77,77	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
58	MG	1H	3317	1/1	0.77	0.48	81,81,81,81	0
58	MG	14	3239	1/1	0.77	0.30	102,102,102,102	0
58	MG	14	3266	1/1	0.77	0.23	72,72,72,72	0
58	MG	14	3276	1/1	0.77	0.28	87,87,87,87	0
58	MG	14	3277	1/1	0.77	0.43	98,98,98,98	0
58	MG	14	3286	1/1	0.77	0.21	103,103,103,103	0
58	MG	1H	3298	1/1	0.77	0.27	84,84,84,84	0
58	MG	1H	3346	1/1	0.77	0.34	80,80,80,80	0
58	MG	1G	1643	1/1	0.77	0.29	83,83,83,83	0
58	MG	1H	3244	1/1	0.78	0.22	100,100,100,100	0
58	MG	13	1605	1/1	0.78	0.33	79,79,79,79	0
58	MG	1H	3024	1/1	0.78	0.22	74,74,74,74	0
58	MG	1H	3075	1/1	0.78	0.27	70,70,70,70	0
58	MG	14	3254	1/1	0.78	0.30	90,90,90,90	0
58	MG	14	3008	1/1	0.78	0.30	85,85,85,85	0
58	MG	1G	1661	1/1	0.78	0.16	96,96,96,96	0
58	MG	14	3152	1/1	0.78	0.33	91,91,91,91	0
58	MG	1H	3092	1/1	0.78	0.26	69,69,69,69	0
58	MG	1H	3131	1/1	0.78	0.33	59,59,59,59	0
58	MG	1H	3281	1/1	0.78	0.32	85,85,85,85	0
58	MG	13	1673	1/1	0.78	0.36	99,99,99,99	0
58	MG	13	1651	1/1	0.78	0.24	105,105,105,105	0
58	MG	13	1671	1/1	0.78	0.15	121,121,121,121	0
58	MG	14	3103	1/1	0.78	0.27	75,75,75,75	0
58	MG	14	3149	1/1	0.79	0.23	83,83,83,83	0
58	MG	14	3021	1/1	0.79	0.16	77,77,77,77	0
58	MG	14	3217	1/1	0.79	0.25	91,91,91,91	0
58	MG	14	3252	1/1	0.79	0.39	82,82,82,82	0
58	MG	1G	1672	1/1	0.79	0.18	110,110,110,110	0
58	MG	1H	3264	1/1	0.79	0.29	87,87,87,87	0
58	MG	14	3105	1/1	0.79	0.25	91,91,91,91	0
58	MG	14	3230	1/1	0.79	0.23	87,87,87,87	0
58	MG	1H	3207	1/1	0.79	0.34	84,84,84,84	0
58	MG	14	3051	1/1	0.79	0.18	88,88,88,88	0
58	MG	1H	3322	1/1	0.79	0.26	78,78,78,78	0
58	MG	14	3136	1/1	0.79	0.21	79,79,79,79	0
58	MG	14	3287	1/1	0.79	0.38	83,83,83,83	0
58	MG	14	3014	1/1	0.79	0.36	78,78,78,78	0
58	MG	14	3140	1/1	0.79	0.17	90,90,90,90	0
58	MG	14	3095	1/1	0.79	0.21	83,83,83,83	0
58	MG	1H	3156	1/1	0.80	0.24	76,76,76,76	0
58	MG	1H	3158	1/1	0.80	0.25	78,78,78,78	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
58	MG	1H	3119	1/1	0.80	0.27	72,72,72,72	0
58	MG	1H	3031	1/1	0.80	0.21	70,70,70,70	0
58	MG	14	3267	1/1	0.80	0.25	94,94,94,94	0
58	MG	14	3113	1/1	0.80	0.24	84,84,84,84	0
58	MG	14	3176	1/1	0.80	0.25	92,92,92,92	0
58	MG	13	1697	1/1	0.80	0.32	95,95,95,95	0
58	MG	1H	3188	1/1	0.80	0.26	90,90,90,90	0
58	MG	1G	1651	1/1	0.80	0.20	100,100,100,100	0
58	MG	14	3290	1/1	0.80	0.23	89,89,89,89	0
58	MG	1H	3265	1/1	0.80	0.22	115,115,115,115	0
58	MG	1H	3289	1/1	0.80	0.16	91,91,91,91	0
58	MG	45	202	1/1	0.80	0.15	102,102,102,102	0
58	MG	1G	1665	1/1	0.81	0.26	85,85,85,85	0
58	MG	13	1683	1/1	0.81	0.15	97,97,97,97	0
58	MG	1H	3155	1/1	0.81	0.19	71,71,71,71	0
58	MG	14	3253	1/1	0.81	0.28	84,84,84,84	0
58	MG	14	3143	1/1	0.81	0.19	60,60,60,60	0
58	MG	13	1642	1/1	0.81	0.19	92,92,92,92	0
58	MG	14	3147	1/1	0.81	0.29	91,91,91,91	0
58	MG	1H	3077	1/1	0.81	0.37	62,62,62,62	0
58	MG	13	1662	1/1	0.81	0.20	81,81,81,81	0
58	MG	1H	3276	1/1	0.81	0.22	67,67,67,67	0
58	MG	1H	3161	1/1	0.81	0.24	71,71,71,71	0
58	MG	1H	3062	1/1	0.81	0.17	88,88,88,88	0
58	MG	14	3233	1/1	0.81	0.22	79,79,79,79	0
58	MG	1G	1618	1/1	0.81	0.12	85,85,85,85	0
58	MG	1G	1658	1/1	0.81	0.20	99,99,99,99	0
58	MG	1H	3122	1/1	0.81	0.17	65,65,65,65	0
58	MG	1H	3249	1/1	0.81	0.18	77,77,77,77	0
58	MG	13	1638	1/1	0.81	0.23	80,80,80,80	0
58	MG	1H	3134	1/1	0.81	0.18	58,58,58,58	0
58	MG	14	3078	1/1	0.82	0.21	76,76,76,76	0
58	MG	1H	3341	1/1	0.82	0.18	81,81,81,81	0
58	MG	1H	3197	1/1	0.82	0.19	91,91,91,91	0
58	MG	1H	3019	1/1	0.82	0.27	64,64,64,64	0
58	MG	13	1607	1/1	0.82	0.32	84,84,84,84	0
58	MG	1H	3303	1/1	0.82	0.26	99,99,99,99	0
58	MG	14	3106	1/1	0.82	0.22	66,66,66,66	0
58	MG	14	3198	1/1	0.82	0.29	69,69,69,69	0
58	MG	1H	3204	1/1	0.82	0.33	81,81,81,81	0
58	MG	1H	3005	1/1	0.82	0.18	52,52,52,52	0
58	MG	1H	3206	1/1	0.82	0.25	69,69,69,69	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
58	MG	1H	3255	1/1	0.82	0.12	68,68,68,68	0
58	MG	14	3134	1/1	0.82	0.23	83,83,83,83	0
58	MG	14	3213	1/1	0.82	0.13	72,72,72,72	0
58	MG	14	3020	1/1	0.82	0.29	78,78,78,78	0
58	MG	14	3270	1/1	0.82	0.20	90,90,90,90	0
58	MG	1H	3259	1/1	0.82	0.40	82,82,82,82	0
58	MG	14	3223	1/1	0.82	0.41	92,92,92,92	0
58	MG	1G	1631	1/1	0.82	0.28	104,104,104,104	0
58	MG	1H	3324	1/1	0.82	0.15	65,65,65,65	0
58	MG	1H	3260	1/1	0.82	0.19	60,60,60,60	0
58	MG	14	3044	1/1	0.82	0.13	85,85,85,85	0
58	MG	1H	3176	1/1	0.82	0.14	76,76,76,76	0
58	MG	1H	3209	1/1	0.82	0.30	87,87,87,87	0
58	MG	1H	3074	1/1	0.82	0.25	44,44,44,44	0
58	MG	1H	3147	1/1	0.83	0.27	90,90,90,90	0
58	MG	1H	3070	1/1	0.83	0.29	68,68,68,68	0
58	MG	14	3122	1/1	0.83	0.27	71,71,71,71	0
58	MG	14	3123	1/1	0.83	0.23	79,79,79,79	0
58	MG	14	3124	1/1	0.83	0.24	86,86,86,86	0
58	MG	1G	1652	1/1	0.83	0.24	81,81,81,81	0
58	MG	14	3048	1/1	0.83	0.22	79,79,79,79	0
58	MG	1H	3211	1/1	0.83	0.35	83,83,83,83	0
58	MG	1H	3182	1/1	0.83	0.18	76,76,76,76	0
58	MG	1H	3114	1/1	0.83	0.35	64,64,64,64	0
58	MG	1H	3014	1/1	0.83	0.24	80,80,80,80	0
58	MG	14	3092	1/1	0.83	0.22	74,74,74,74	0
58	MG	1H	3043	1/1	0.83	0.22	86,86,86,86	0
58	MG	1H	3125	1/1	0.83	0.18	79,79,79,79	0
58	MG	2K	101	1/1	0.83	0.36	72,72,72,72	0
58	MG	1H	3343	1/1	0.83	0.34	77,77,77,77	0
58	MG	14	3015	1/1	0.83	0.30	67,67,67,67	0
58	MG	14	3177	1/1	0.83	0.31	75,75,75,75	0
58	MG	14	3182	1/1	0.83	0.23	89,89,89,89	0
58	MG	13	1652	1/1	0.83	0.24	93,93,93,93	0
58	MG	1H	3168	1/1	0.83	0.20	70,70,70,70	0
58	MG	1H	3285	1/1	0.83	0.12	61,61,61,61	0
58	MG	1H	3301	1/1	0.84	0.31	80,80,80,80	0
58	MG	1H	3099	1/1	0.84	0.26	57,57,57,57	0
58	MG	1H	3268	1/1	0.84	0.16	72,72,72,72	0
58	MG	2L	101	1/1	0.84	0.34	81,81,81,81	0
58	MG	1H	3013	1/1	0.84	0.32	67,67,67,67	0
58	MG	1H	3309	1/1	0.84	0.17	77,77,77,77	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
58	MG	1G	1635	1/1	0.84	0.18	82,82,82,82	0
58	MG	14	3229	1/1	0.84	0.09	85,85,85,85	0
58	MG	13	1649	1/1	0.84	0.24	92,92,92,92	0
58	MG	14	3132	1/1	0.84	0.51	81,81,81,81	0
58	MG	14	3009	1/1	0.84	0.53	73,73,73,73	0
58	MG	14	3010	1/1	0.84	0.29	76,76,76,76	0
58	MG	14	3011	1/1	0.84	0.24	66,66,66,66	0
58	MG	1H	3274	1/1	0.84	0.33	75,75,75,75	0
58	MG	1H	3275	1/1	0.84	0.33	69,69,69,69	0
58	MG	1I	201	1/1	0.84	0.23	79,79,79,79	0
58	MG	13	1669	1/1	0.84	0.34	81,81,81,81	0
58	MG	1H	3325	1/1	0.84	0.22	82,82,82,82	0
58	MG	1H	3030	1/1	0.84	0.12	82,82,82,82	0
58	MG	14	3157	1/1	0.84	0.36	67,67,67,67	0
58	MG	13	1622	1/1	0.84	0.14	109,109,109,109	0
58	MG	1H	3195	1/1	0.84	0.19	85,85,85,85	0
58	MG	14	3165	1/1	0.84	0.19	47,47,47,47	0
58	MG	1H	3287	1/1	0.84	0.20	77,77,77,77	0
58	MG	13	1700	1/1	0.84	0.19	93,93,93,93	0
58	MG	1H	3035	1/1	0.84	0.35	87,87,87,87	0
58	MG	14	3057	1/1	0.84	0.34	64,64,64,64	0
58	MG	14	3185	1/1	0.84	0.20	87,87,87,87	0
58	MG	1H	3290	1/1	0.84	0.22	83,83,83,83	0
58	MG	1H	3447	1/1	0.84	0.10	87,87,87,87	0
58	MG	14	3193	1/1	0.84	0.24	69,69,69,69	0
58	MG	1H	3154	1/1	0.84	0.31	42,42,42,42	0
58	MG	1G	1602	1/1	0.84	0.28	79,79,79,79	0
58	MG	1H	3036	1/1	0.84	0.24	126,126,126,126	0
58	MG	1H	3081	1/1	0.84	0.18	83,83,83,83	0
58	MG	1H	3082	1/1	0.84	0.22	80,80,80,80	0
58	MG	13	1636	1/1	0.84	0.20	76,76,76,76	0
58	MG	1G	1617	1/1	0.84	0.22	101,101,101,101	0
58	MG	14	3166	1/1	0.85	0.23	60,60,60,60	0
58	MG	13	1682	1/1	0.85	0.26	151,151,151,151	0
58	MG	1H	3310	1/1	0.85	0.14	126,126,126,126	0
58	MG	14	3240	1/1	0.85	0.24	82,82,82,82	0
58	MG	13	1693	1/1	0.85	0.20	77,77,77,77	0
58	MG	13	1674	1/1	0.85	0.11	102,102,102,102	0
58	MG	13	1684	1/1	0.85	0.12	101,101,101,101	0
58	MG	1G	1625	1/1	0.85	0.30	87,87,87,87	0
58	MG	1H	3159	1/1	0.85	0.18	70,70,70,70	0
58	MG	14	3033	1/1	0.85	0.21	68,68,68,68	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
58	MG	1H	3126	1/1	0.85	0.34	77,77,77,77	0
58	MG	1H	3128	1/1	0.85	0.25	83,83,83,83	0
58	MG	1G	1632	1/1	0.85	0.20	106,106,106,106	0
58	MG	13	1663	1/1	0.85	0.33	77,77,77,77	0
58	MG	14	3255	1/1	0.85	0.32	79,79,79,79	0
58	MG	1H	3167	1/1	0.85	0.22	78,78,78,78	0
58	MG	14	3139	1/1	0.85	0.30	55,55,55,55	0
58	MG	13	1644	1/1	0.85	0.20	85,85,85,85	0
58	MG	1H	3296	1/1	0.85	0.19	66,66,66,66	0
58	MG	1H	3135	1/1	0.85	0.17	55,55,55,55	0
58	MG	1H	3299	1/1	0.85	0.14	98,98,98,98	0
58	MG	14	3272	1/1	0.85	0.17	71,71,71,71	0
58	MG	14	3218	1/1	0.85	0.19	84,84,84,84	0
58	MG	1H	3136	1/1	0.85	0.29	63,63,63,63	0
58	MG	14	3220	1/1	0.85	0.19	64,64,64,64	0
58	MG	14	3151	1/1	0.85	0.33	65,65,65,65	0
58	MG	13	1604	1/1	0.85	0.26	86,86,86,86	0
58	MG	14	3002	1/1	0.85	0.23	53,53,53,53	0
58	MG	1H	3184	1/1	0.85	0.22	81,81,81,81	0
58	MG	1J	204	1/1	0.85	0.14	99,99,99,99	0
58	MG	1H	3241	1/1	0.85	0.26	71,71,71,71	0
58	MG	1H	3001	1/1	0.85	0.29	52,52,52,52	0
58	MG	1H	3051	1/1	0.86	0.32	45,45,45,45	0
58	MG	1H	3130	1/1	0.86	0.20	67,67,67,67	0
58	MG	1H	3231	1/1	0.86	0.32	75,75,75,75	0
58	MG	1G	1644	1/1	0.86	0.21	93,93,93,93	0
58	MG	14	3168	1/1	0.86	0.18	64,64,64,64	0
58	MG	1H	3055	1/1	0.86	0.24	50,50,50,50	0
58	MG	1H	3104	1/1	0.86	0.24	66,66,66,66	0
58	MG	14	3180	1/1	0.86	0.16	83,83,83,83	0
58	MG	1H	3348	1/1	0.86	0.24	63,63,63,63	0
58	MG	13	1643	1/1	0.86	0.17	90,90,90,90	0
58	MG	1H	3280	1/1	0.86	0.21	90,90,90,90	0
58	MG	1H	3246	1/1	0.86	0.15	75,75,75,75	0
58	MG	14	3114	1/1	0.86	0.17	85,85,85,85	0
58	MG	1H	3308	1/1	0.86	0.26	76,76,76,76	0
58	MG	1H	3116	1/1	0.86	0.23	71,71,71,71	0
58	MG	1H	3138	1/1	0.86	0.34	83,83,83,83	0
58	MG	14	3256	1/1	0.86	0.29	77,77,77,77	0
58	MG	14	3018	1/1	0.86	0.31	63,63,63,63	0
58	MG	1H	3067	1/1	0.86	0.19	88,88,88,88	0
58	MG	14	3131	1/1	0.86	0.23	70,70,70,70	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
58	MG	14	3205	1/1	0.86	0.26	63,63,63,63	0
58	MG	1H	3080	1/1	0.86	0.13	65,65,65,65	0
58	MG	14	3032	1/1	0.86	0.20	62,62,62,62	0
58	MG	13	1637	1/1	0.86	0.32	82,82,82,82	0
58	MG	1H	3321	1/1	0.86	0.12	78,78,78,78	0
58	MG	1H	3178	1/1	0.86	0.23	76,76,76,76	0
58	MG	14	3041	1/1	0.86	0.24	81,81,81,81	0
58	MG	1H	3180	1/1	0.86	0.16	71,71,71,71	0
58	MG	1G	1629	1/1	0.86	0.18	98,98,98,98	0
58	MG	1G	1669	1/1	0.86	0.29	93,93,93,93	0
58	MG	13	1606	1/1	0.86	0.19	124,124,124,124	0
58	MG	1H	3266	1/1	0.86	0.15	82,82,82,82	0
58	MG	1H	3225	1/1	0.86	0.33	56,56,56,56	0
58	MG	39	302	1/1	0.86	0.18	96,96,96,96	0
58	MG	1H	3329	1/1	0.86	0.30	91,91,91,91	0
58	MG	14	3043	1/1	0.87	0.17	85,85,85,85	0
58	MG	1H	3132	1/1	0.87	0.13	74,74,74,74	0
58	MG	1H	3248	1/1	0.87	0.17	77,77,77,77	0
58	MG	1H	3312	1/1	0.87	0.17	80,80,80,80	0
58	MG	1H	3194	1/1	0.87	0.26	79,79,79,79	0
58	MG	14	3066	1/1	0.87	0.24	47,47,47,47	0
58	MG	1H	3095	1/1	0.87	0.32	66,66,66,66	0
58	MG	16	204	1/1	0.87	0.14	80,80,80,80	0
58	MG	14	3195	1/1	0.87	0.21	75,75,75,75	0
58	MG	1H	3253	1/1	0.87	0.18	62,62,62,62	0
58	MG	14	3084	1/1	0.87	0.23	71,71,71,71	0
58	MG	14	3088	1/1	0.87	0.13	70,70,70,70	0
58	MG	Q8	101	1/1	0.87	0.23	72,72,72,72	0
58	MG	13	1611	1/1	0.87	0.14	85,85,85,85	0
58	MG	14	3100	1/1	0.87	0.18	67,67,67,67	0
58	MG	1H	3277	1/1	0.87	0.28	96,96,96,96	0
58	MG	14	3265	1/1	0.87	0.34	83,83,83,83	0
58	MG	1H	3175	1/1	0.87	0.22	84,84,84,84	0
58	MG	1H	3059	1/1	0.87	0.20	66,66,66,66	0
58	MG	14	3153	1/1	0.87	0.25	77,77,77,77	0
58	MG	1G	1649	1/1	0.87	0.18	97,97,97,97	0
58	MG	1H	3061	1/1	0.87	0.25	75,75,75,75	0
58	MG	1H	3142	1/1	0.87	0.35	62,62,62,62	0
58	MG	14	3282	1/1	0.87	0.20	82,82,82,82	0
58	MG	14	3164	1/1	0.87	0.32	70,70,70,70	0
58	MG	14	3108	1/1	0.87	0.16	77,77,77,77	0
58	MG	14	3112	1/1	0.87	0.28	83,83,83,83	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
58	MG	14	3167	1/1	0.87	0.15	50,50,50,50	0
58	MG	1H	3020	1/1	0.87	0.31	52,52,52,52	0
58	MG	14	3170	1/1	0.87	0.20	82,82,82,82	0
58	MG	1H	3242	1/1	0.87	0.17	66,66,66,66	0
58	MG	13	1676	1/1	0.87	0.14	94,94,94,94	0
58	MG	25	201	1/1	0.87	0.27	85,85,85,85	0
58	MG	14	3178	1/1	0.87	0.34	65,65,65,65	0
58	MG	14	3127	1/1	0.88	0.24	69,69,69,69	0
58	MG	1H	3191	1/1	0.88	0.30	67,67,67,67	0
58	MG	1H	3193	1/1	0.88	0.24	89,89,89,89	0
58	MG	14	3222	1/1	0.88	0.19	73,73,73,73	0
58	MG	1H	3336	1/1	0.88	0.10	76,76,76,76	0
58	MG	14	3022	1/1	0.88	0.21	63,63,63,63	0
58	MG	1H	3153	1/1	0.88	0.34	80,80,80,80	0
58	MG	1H	3105	1/1	0.88	0.30	63,63,63,63	0
58	MG	1H	3345	1/1	0.88	0.32	68,68,68,68	0
58	MG	13	1688	1/1	0.88	0.24	85,85,85,85	0
58	MG	14	3038	1/1	0.88	0.26	59,59,59,59	0
58	MG	13	1659	1/1	0.88	0.20	87,87,87,87	0
58	MG	14	3236	1/1	0.88	0.13	74,74,74,74	0
58	MG	13	1618	1/1	0.88	0.17	107,107,107,107	0
58	MG	1H	3012	1/1	0.88	0.29	57,57,57,57	0
58	MG	13	1646	1/1	0.88	0.13	93,93,93,93	0
58	MG	88	203	1/1	0.88	0.17	75,75,75,75	0
58	MG	13	1635	1/1	0.88	0.14	97,97,97,97	0
58	MG	1H	3018	1/1	0.88	0.29	51,51,51,51	0
58	MG	13	1695	1/1	0.88	0.23	80,80,80,80	0
58	MG	14	3248	1/1	0.88	0.39	85,85,85,85	0
58	MG	1G	1608	1/1	0.88	0.19	97,97,97,97	0
58	MG	14	3069	1/1	0.88	0.14	64,64,64,64	0
58	MG	14	3073	1/1	0.88	0.28	57,57,57,57	0
58	MG	14	3074	1/1	0.88	0.24	48,48,48,48	0
58	MG	14	3076	1/1	0.88	0.15	88,88,88,88	0
58	MG	1G	1609	1/1	0.88	0.12	98,98,98,98	0
58	MG	13	1678	1/1	0.88	0.22	89,89,89,89	0
58	MG	1H	3215	1/1	0.88	0.19	67,67,67,67	0
58	MG	1H	3058	1/1	0.88	0.26	54,54,54,54	0
58	MG	1H	3222	1/1	0.88	0.18	74,74,74,74	0
58	MG	1H	3273	1/1	0.88	0.12	80,80,80,80	0
58	MG	1H	3083	1/1	0.88	0.14	99,99,99,99	0
58	MG	1H	3088	1/1	0.88	0.18	58,58,58,58	0
58	MG	1H	3227	1/1	0.88	0.13	77,77,77,77	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
58	MG	1H	3089	1/1	0.88	0.27	50,50,50,50	0
58	MG	1H	3023	1/1	0.88	0.25	78,78,78,78	0
58	MG	1H	3232	1/1	0.88	0.22	75,75,75,75	0
58	MG	14	3280	1/1	0.88	0.24	49,49,49,49	0
58	MG	1H	3282	1/1	0.88	0.09	67,67,67,67	0
58	MG	14	3284	1/1	0.88	0.50	81,81,81,81	0
58	MG	14	3007	1/1	0.88	0.24	52,52,52,52	0
58	MG	7I	101	1/1	0.88	0.12	95,95,95,95	0
58	MG	1G	1636	1/1	0.88	0.23	90,90,90,90	0
58	MG	1G	1637	1/1	0.88	0.16	87,87,87,87	0
58	MG	1H	3183	1/1	0.88	0.34	67,67,67,67	0
58	MG	14	3118	1/1	0.88	0.14	53,53,53,53	0
58	MG	14	3012	1/1	0.88	0.12	58,58,58,58	0
58	MG	29	302	1/1	0.88	0.21	74,74,74,74	0
58	MG	13	1657	1/1	0.88	0.19	72,72,72,72	0
58	MG	1G	1642	1/1	0.88	0.18	78,78,78,78	0
58	MG	1H	3064	1/1	0.88	0.22	57,57,57,57	0
58	MG	13	1623	1/1	0.89	0.15	81,81,81,81	0
58	MG	14	3017	1/1	0.89	0.27	87,87,87,87	0
58	MG	1H	3078	1/1	0.89	0.36	56,56,56,56	0
58	MG	13	1627	1/1	0.89	0.14	97,97,97,97	0
58	MG	1G	1605	1/1	0.89	0.21	102,102,102,102	0
58	MG	1H	3107	1/1	0.89	0.31	69,69,69,69	0
58	MG	13	1602	1/1	0.89	0.17	74,74,74,74	0
58	MG	13	1665	1/1	0.89	0.23	85,85,85,85	0
58	MG	13	1654	1/1	0.89	0.17	76,76,76,76	0
58	MG	1G	1614	1/1	0.89	0.19	120,120,120,120	0
58	MG	14	3187	1/1	0.89	0.24	72,72,72,72	0
58	MG	1H	3170	1/1	0.89	0.20	70,70,70,70	0
58	MG	1H	3270	1/1	0.89	0.27	43,43,43,43	0
58	MG	1H	3237	1/1	0.89	0.26	72,72,72,72	0
58	MG	1G	1621	1/1	0.89	0.29	79,79,79,79	0
58	MG	1H	3297	1/1	0.89	0.30	78,78,78,78	0
58	MG	1H	3240	1/1	0.89	0.22	49,49,49,49	0
58	MG	1H	3143	1/1	0.89	0.17	75,75,75,75	0
58	MG	14	3262	1/1	0.89	0.14	78,78,78,78	0
58	MG	14	3133	1/1	0.89	0.28	66,66,66,66	0
58	MG	13	1648	1/1	0.89	0.14	76,76,76,76	0
58	MG	14	3060	1/1	0.89	0.23	67,67,67,67	0
58	MG	1H	3342	1/1	0.89	0.20	82,82,82,82	0
58	MG	14	3067	1/1	0.89	0.22	60,60,60,60	0
58	MG	1H	3124	1/1	0.89	0.25	56,56,56,56	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
58	MG	14	3273	1/1	0.89	0.58	87,87,87,87	0
58	MG	14	3274	1/1	0.89	0.10	91,91,91,91	0
58	MG	14	3141	1/1	0.89	0.20	80,80,80,80	0
58	MG	1H	3151	1/1	0.89	0.17	76,76,76,76	0
58	MG	13	1681	1/1	0.89	0.21	66,66,66,66	0
58	MG	1H	3347	1/1	0.89	0.17	66,66,66,66	0
58	MG	1H	3210	1/1	0.89	0.26	67,67,67,67	0
58	MG	1H	3349	1/1	0.89	0.28	89,89,89,89	0
58	MG	1H	3032	1/1	0.89	0.33	78,78,78,78	0
58	MG	14	3224	1/1	0.89	0.23	59,59,59,59	0
58	MG	16	202	1/1	0.89	0.13	90,90,90,90	0
58	MG	16	203	1/1	0.89	0.15	84,84,84,84	0
58	MG	14	3228	1/1	0.89	0.25	76,76,76,76	0
58	MG	1H	3015	1/1	0.89	0.19	70,70,70,70	0
58	MG	16	206	1/1	0.89	0.17	77,77,77,77	0
58	MG	39	301	1/1	0.89	0.42	66,66,66,66	0
58	MG	1H	3283	1/1	0.89	0.23	84,84,84,84	0
58	MG	21	301	1/1	0.89	0.18	48,48,48,48	0
58	MG	1H	3096	1/1	0.89	0.18	51,51,51,51	0
58	MG	14	3058	1/1	0.90	0.16	55,55,55,55	0
58	MG	14	3225	1/1	0.90	0.28	84,84,84,84	0
58	MG	1H	3328	1/1	0.90	0.28	65,65,65,65	0
58	MG	1H	3007	1/1	0.90	0.22	83,83,83,83	0
58	MG	14	3146	1/1	0.90	0.24	71,71,71,71	0
58	MG	1H	3010	1/1	0.90	0.24	57,57,57,57	0
58	MG	1H	3169	1/1	0.90	0.10	84,84,84,84	0
58	MG	13	1741	1/1	0.90	0.06	103,103,103,103	0
58	MG	1H	3171	1/1	0.90	0.10	62,62,62,62	0
58	MG	1H	3257	1/1	0.90	0.19	75,75,75,75	0
58	MG	14	3154	1/1	0.90	0.18	66,66,66,66	0
58	MG	14	3156	1/1	0.90	0.19	66,66,66,66	0
58	MG	14	3075	1/1	0.90	0.25	60,60,60,60	0
58	MG	13	1631	1/1	0.90	0.14	55,55,55,55	0
58	MG	14	3159	1/1	0.90	0.18	75,75,75,75	0
58	MG	13	1689	1/1	0.90	0.40	80,80,80,80	0
58	MG	14	3161	1/1	0.90	0.11	99,99,99,99	0
58	MG	1H	3262	1/1	0.90	0.39	78,78,78,78	0
58	MG	1H	3212	1/1	0.90	0.23	42,42,42,42	0
58	MG	1H	3103	1/1	0.90	0.30	75,75,75,75	0
58	MG	14	3090	1/1	0.90	0.25	64,64,64,64	0
58	MG	3I	201	1/1	0.90	0.16	62,62,62,62	0
58	MG	1G	1640	1/1	0.90	0.19	75,75,75,75	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
58	MG	1H	3220	1/1	0.90	0.15	84,84,84,84	0
58	MG	14	3101	1/1	0.90	0.23	61,61,61,61	0
58	MG	1H	3179	1/1	0.90	0.17	76,76,76,76	0
58	MG	1H	3071	1/1	0.90	0.20	80,80,80,80	0
58	MG	1H	3040	1/1	0.90	0.11	89,89,89,89	0
58	MG	14	3259	1/1	0.90	0.39	81,81,81,81	0
58	MG	16	205	1/1	0.90	0.11	88,88,88,88	0
58	MG	1H	3041	1/1	0.90	0.39	86,86,86,86	0
58	MG	1H	3228	1/1	0.90	0.42	68,68,68,68	0
58	MG	5I	101	1/1	0.90	0.16	77,77,77,77	0
58	MG	14	3110	1/1	0.90	0.14	66,66,66,66	0
58	MG	1H	3186	1/1	0.90	0.20	58,58,58,58	0
58	MG	14	3271	1/1	0.90	0.29	77,77,77,77	0
58	MG	P8	101	1/1	0.90	0.17	68,68,68,68	0
58	MG	13	1655	1/1	0.90	0.13	72,72,72,72	0
58	MG	14	3031	1/1	0.90	0.15	75,75,75,75	0
58	MG	13	1664	1/1	0.90	0.19	82,82,82,82	0
58	MG	1H	3235	1/1	0.90	0.33	64,64,64,64	0
58	MG	1H	3278	1/1	0.90	0.19	61,61,61,61	0
58	MG	14	3204	1/1	0.90	0.25	60,60,60,60	0
58	MG	14	3283	1/1	0.90	0.21	78,78,78,78	0
58	MG	1H	3320	1/1	0.90	0.11	84,84,84,84	0
58	MG	13	1640	1/1	0.90	0.15	63,63,63,63	0
58	MG	1H	3056	1/1	0.90	0.28	50,50,50,50	0
58	MG	1G	1662	1/1	0.90	0.18	84,84,84,84	0
58	MG	14	3212	1/1	0.90	0.20	63,63,63,63	0
58	MG	14	3346	1/1	0.90	0.09	144,144,144,144	0
58	MG	1H	3057	1/1	0.90	0.21	51,51,51,51	0
58	MG	14	3215	1/1	0.90	0.12	73,73,73,73	0
58	MG	13	1658	1/1	0.90	0.15	74,74,74,74	0
58	MG	1H	3084	1/1	0.90	0.12	49,49,49,49	0
58	MG	1G	1667	1/1	0.90	0.12	81,81,81,81	0
58	MG	14	3053	1/1	0.90	0.16	74,74,74,74	0
58	MG	14	3055	1/1	0.90	0.28	71,71,71,71	0
58	MG	13	1624	1/1	0.90	0.14	75,75,75,75	0
58	MG	45	203	1/1	0.90	0.19	70,70,70,70	0
60	ZN	G8	201	1/1	0.90	0.22	147,147,147,147	0
58	MG	1H	3102	1/1	0.91	0.26	64,64,64,64	0
58	MG	1H	3203	1/1	0.91	0.07	76,76,76,76	0
58	MG	14	3169	1/1	0.91	0.13	63,63,63,63	0
58	MG	1H	3050	1/1	0.91	0.27	53,53,53,53	0
58	MG	1H	3236	1/1	0.91	0.27	76,76,76,76	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
58	MG	13	1613	1/1	0.91	0.17	76,76,76,76	0
58	MG	1H	3239	1/1	0.91	0.11	58,58,58,58	0
58	MG	1H	3004	1/1	0.91	0.18	54,54,54,54	0
58	MG	1G	1623	1/1	0.91	0.16	80,80,80,80	0
58	MG	1H	3026	1/1	0.91	0.19	60,60,60,60	0
58	MG	1H	3157	1/1	0.91	0.16	67,67,67,67	0
58	MG	14	3046	1/1	0.91	0.12	74,74,74,74	0
58	MG	1H	3108	1/1	0.91	0.23	51,51,51,51	0
58	MG	14	3191	1/1	0.91	0.33	81,81,81,81	0
58	MG	14	3050	1/1	0.91	0.26	71,71,71,71	0
58	MG	1H	3245	1/1	0.91	0.18	72,72,72,72	0
58	MG	1H	3430	1/1	0.91	0.13	112,112,112,112	0
58	MG	14	3129	1/1	0.91	0.24	53,53,53,53	0
58	MG	14	3261	1/1	0.91	0.20	74,74,74,74	0
58	MG	14	3196	1/1	0.91	0.15	87,87,87,87	0
58	MG	14	3130	1/1	0.91	0.22	78,78,78,78	0
58	MG	14	3264	1/1	0.91	0.18	86,86,86,86	0
58	MG	14	3054	1/1	0.91	0.19	54,54,54,54	0
58	MG	1H	3443	1/1	0.91	0.08	86,86,86,86	0
58	MG	1H	3113	1/1	0.91	0.22	52,52,52,52	0
58	MG	1H	3485	1/1	0.91	0.07	116,116,116,116	0
58	MG	1H	3486	1/1	0.91	0.17	98,98,98,98	0
58	MG	14	3063	1/1	0.91	0.17	73,73,73,73	0
58	MG	13	1634	1/1	0.91	0.17	81,81,81,81	0
58	MG	13	1620	1/1	0.91	0.10	87,87,87,87	0
58	MG	14	3210	1/1	0.91	0.10	58,58,58,58	0
58	MG	1H	3141	1/1	0.91	0.14	47,47,47,47	0
58	MG	1H	3163	1/1	0.91	0.15	76,76,76,76	0
58	MG	1H	3319	1/1	0.91	0.13	80,80,80,80	0
58	MG	1H	3192	1/1	0.91	0.08	86,86,86,86	0
58	MG	1H	3224	1/1	0.91	0.21	50,50,50,50	0
58	MG	14	3285	1/1	0.91	0.09	70,70,70,70	0
58	MG	1G	1646	1/1	0.91	0.24	70,70,70,70	0
58	MG	13	1630	1/1	0.91	0.07	62,62,62,62	0
58	MG	N8	101	1/1	0.91	0.19	67,67,67,67	0
58	MG	14	3079	1/1	0.91	0.15	63,63,63,63	0
58	MG	4K	101	1/1	0.91	0.21	85,85,85,85	0
58	MG	14	3419	1/1	0.91	0.25	62,62,62,62	0
58	MG	1J	201	1/1	0.91	0.22	76,76,76,76	0
58	MG	1H	3146	1/1	0.91	0.26	72,72,72,72	0
58	MG	1H	3196	1/1	0.91	0.17	72,72,72,72	0
58	MG	1H	3229	1/1	0.91	0.29	59,59,59,59	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
58	MG	1H	3046	1/1	0.91	0.20	55,55,55,55	0
58	MG	14	3019	1/1	0.91	0.21	83,83,83,83	0
58	MG	1H	3047	1/1	0.91	0.24	43,43,43,43	0
58	MG	14	3162	1/1	0.91	0.27	75,75,75,75	0
58	MG	1H	3330	1/1	0.91	0.19	87,87,87,87	0
58	MG	1G	1657	1/1	0.91	0.27	84,84,84,84	0
58	MG	14	3028	1/1	0.91	0.16	53,53,53,53	0
58	MG	14	3238	1/1	0.92	0.29	82,82,82,82	0
58	MG	1H	3238	1/1	0.92	0.10	63,63,63,63	0
58	MG	1H	3291	1/1	0.92	0.10	64,64,64,64	0
58	MG	1H	3006	1/1	0.92	0.15	56,56,56,56	0
58	MG	1H	3217	1/1	0.92	0.05	67,67,67,67	0
58	MG	1H	3021	1/1	0.92	0.23	64,64,64,64	0
58	MG	14	3173	1/1	0.92	0.12	92,92,92,92	0
58	MG	1H	3172	1/1	0.92	0.11	76,76,76,76	0
58	MG	14	3247	1/1	0.92	0.23	75,75,75,75	0
58	MG	14	3109	1/1	0.92	0.12	66,66,66,66	0
58	MG	1H	3053	1/1	0.92	0.20	54,54,54,54	0
58	MG	14	3047	1/1	0.92	0.20	56,56,56,56	0
58	MG	1G	1639	1/1	0.92	0.31	68,68,68,68	0
58	MG	1H	3065	1/1	0.92	0.24	64,64,64,64	0
58	MG	1H	3332	1/1	0.92	0.12	72,72,72,72	0
58	MG	14	3052	1/1	0.92	0.34	75,75,75,75	0
58	MG	14	3189	1/1	0.92	0.20	90,90,90,90	0
58	MG	14	3119	1/1	0.92	0.20	80,80,80,80	0
58	MG	13	1656	1/1	0.92	0.06	83,83,83,83	0
58	MG	1H	3247	1/1	0.92	0.33	76,76,76,76	0
58	MG	1H	3335	1/1	0.92	0.14	79,79,79,79	0
58	MG	14	3004	1/1	0.92	0.21	57,57,57,57	0
58	MG	14	3126	1/1	0.92	0.30	78,78,78,78	0
58	MG	1H	3177	1/1	0.92	0.16	86,86,86,86	0
58	MG	1H	3339	1/1	0.92	0.26	84,84,84,84	0
58	MG	1H	3340	1/1	0.92	0.26	72,72,72,72	0
58	MG	1H	3121	1/1	0.92	0.11	60,60,60,60	0
58	MG	14	3268	1/1	0.92	0.17	79,79,79,79	0
58	MG	1H	3250	1/1	0.92	0.09	69,69,69,69	0
58	MG	14	3202	1/1	0.92	0.19	77,77,77,77	0
58	MG	1H	3008	1/1	0.92	0.14	90,90,90,90	0
58	MG	13	1625	1/1	0.92	0.23	69,69,69,69	0
58	MG	14	3070	1/1	0.92	0.20	72,72,72,72	0
58	MG	1H	3254	1/1	0.92	0.09	58,58,58,58	0
58	MG	13	1614	1/1	0.92	0.09	81,81,81,81	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
58	MG	1H	3256	1/1	0.92	0.27	70,70,70,70	0
58	MG	1H	3049	1/1	0.92	0.15	57,57,57,57	0
58	MG	14	3142	1/1	0.92	0.16	89,89,89,89	0
58	MG	1G	1622	1/1	0.92	0.16	84,84,84,84	0
58	MG	14	3216	1/1	0.92	0.29	58,58,58,58	0
58	MG	1H	3164	1/1	0.92	0.26	70,70,70,70	0
58	MG	1H	3085	1/1	0.92	0.21	59,59,59,59	0
58	MG	14	3081	1/1	0.92	0.16	56,56,56,56	0
58	MG	1G	1626	1/1	0.92	0.15	93,93,93,93	0
58	MG	14	3086	1/1	0.92	0.25	74,74,74,74	0
58	MG	14	3381	1/1	0.92	0.16	95,95,95,95	0
58	MG	14	3026	1/1	0.92	0.21	51,51,51,51	0
58	MG	1H	3106	1/1	0.92	0.14	46,46,46,46	0
58	MG	1J	202	1/1	0.92	0.26	84,84,84,84	0
58	MG	14	3030	1/1	0.92	0.14	65,65,65,65	0
58	MG	14	3094	1/1	0.92	0.26	67,67,67,67	0
58	MG	1G	1663	1/1	0.92	0.14	99,99,99,99	0
58	MG	1J	206	1/1	0.92	0.06	115,115,115,115	0
58	MG	29	301	1/1	0.92	0.20	58,58,58,58	0
58	MG	14	3096	1/1	0.92	0.19	65,65,65,65	0
58	MG	14	3097	1/1	0.92	0.23	49,49,49,49	0
58	MG	14	3098	1/1	0.92	0.26	57,57,57,57	0
58	MG	14	3099	1/1	0.92	0.24	69,69,69,69	0
58	MG	1H	3190	1/1	0.92	0.23	66,66,66,66	0
58	MG	1H	3087	1/1	0.92	0.19	46,46,46,46	0
58	MG	1G	1630	1/1	0.92	0.21	79,79,79,79	0
58	MG	1G	1653	1/1	0.93	0.14	86,86,86,86	0
58	MG	1H	3214	1/1	0.93	0.20	50,50,50,50	0
58	MG	14	3186	1/1	0.93	0.22	63,63,63,63	0
58	MG	1H	3039	1/1	0.93	0.23	64,64,64,64	0
58	MG	1H	3315	1/1	0.93	0.30	58,58,58,58	0
58	MG	1H	3139	1/1	0.93	0.08	58,58,58,58	0
58	MG	1H	3022	1/1	0.93	0.18	60,60,60,60	0
58	MG	1G	1620	1/1	0.93	0.22	74,74,74,74	0
58	MG	14	3135	1/1	0.93	0.38	71,71,71,71	0
58	MG	1H	3027	1/1	0.93	0.30	83,83,83,83	0
58	MG	14	3137	1/1	0.93	0.20	55,55,55,55	0
58	MG	1H	3052	1/1	0.93	0.11	57,57,57,57	0
58	MG	14	3085	1/1	0.93	0.14	54,54,54,54	0
58	MG	1H	3269	1/1	0.93	0.27	71,71,71,71	0
58	MG	14	3260	1/1	0.93	0.08	65,65,65,65	0
58	MG	1H	3460	1/1	0.93	0.13	87,87,87,87	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
58	MG	14	3200	1/1	0.93	0.07	84,84,84,84	0
58	MG	1H	3476	1/1	0.93	0.10	72,72,72,72	0
58	MG	14	3034	1/1	0.93	0.31	53,53,53,53	0
58	MG	1H	3479	1/1	0.93	0.12	102,102,102,102	0
58	MG	14	3145	1/1	0.93	0.13	87,87,87,87	0
58	MG	1H	3145	1/1	0.93	0.10	53,53,53,53	0
58	MG	1H	3199	1/1	0.93	0.24	68,68,68,68	0
58	MG	14	3269	1/1	0.93	0.18	86,86,86,86	0
58	MG	14	3148	1/1	0.93	0.24	84,84,84,84	0
58	MG	14	3209	1/1	0.93	0.17	70,70,70,70	0
58	MG	1H	3127	1/1	0.93	0.26	64,64,64,64	0
58	MG	14	3211	1/1	0.93	0.13	85,85,85,85	0
58	MG	1H	3181	1/1	0.93	0.28	74,74,74,74	0
58	MG	1H	3028	1/1	0.93	0.24	63,63,63,63	0
58	MG	1H	3066	1/1	0.93	0.13	60,60,60,60	0
58	MG	14	3278	1/1	0.93	0.08	63,63,63,63	0
58	MG	1G	1634	1/1	0.93	0.13	85,85,85,85	0
58	MG	14	3281	1/1	0.93	0.19	93,93,93,93	0
58	MG	13	1639	1/1	0.93	0.20	80,80,80,80	0
58	MG	16	207	1/1	0.93	0.10	84,84,84,84	0
58	MG	1H	3185	1/1	0.93	0.27	63,63,63,63	0
58	MG	1H	3331	1/1	0.93	0.20	84,84,84,84	0
58	MG	88	202	1/1	0.93	0.14	81,81,81,81	0
58	MG	1H	3045	1/1	0.93	0.27	52,52,52,52	0
58	MG	1H	3279	1/1	0.93	0.21	71,71,71,71	0
58	MG	1H	3187	1/1	0.93	0.10	69,69,69,69	0
58	MG	1H	3118	1/1	0.93	0.17	54,54,54,54	0
58	MG	1G	1601	1/1	0.93	0.14	85,85,85,85	0
58	MG	14	3059	1/1	0.93	0.21	63,63,63,63	0
58	MG	1H	3305	1/1	0.93	0.26	90,90,90,90	0
58	MG	14	3062	1/1	0.93	0.23	72,72,72,72	0
58	MG	1H	3307	1/1	0.93	0.22	68,68,68,68	0
58	MG	14	3171	1/1	0.93	0.08	65,65,65,65	0
58	MG	14	3065	1/1	0.93	0.29	67,67,67,67	0
58	MG	14	3235	1/1	0.93	0.23	76,76,76,76	0
58	MG	19	301	1/1	0.93	0.23	70,70,70,70	0
58	MG	14	3175	1/1	0.93	0.13	88,88,88,88	0
58	MG	14	3237	1/1	0.93	0.34	77,77,77,77	0
58	MG	29	303	1/1	0.93	0.14	74,74,74,74	0
58	MG	1G	1604	1/1	0.93	0.11	91,91,91,91	0
58	MG	13	1621	1/1	0.93	0.16	101,101,101,101	0
58	MG	1H	3038	1/1	0.93	0.23	72,72,72,72	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
58	MG	45	201	1/1	0.93	0.13	69,69,69,69	0
58	MG	1H	3213	1/1	0.93	0.20	49,49,49,49	0
58	MG	14	3181	1/1	0.93	0.14	57,57,57,57	0
58	MG	1H	3311	1/1	0.93	0.13	127,127,127,127	0
58	MG	14	3064	1/1	0.94	0.25	62,62,62,62	0
58	MG	14	3188	1/1	0.94	0.14	73,73,73,73	0
58	MG	13	1691	1/1	0.94	0.14	89,89,89,89	0
58	MG	1H	3086	1/1	0.94	0.20	59,59,59,59	0
58	MG	1H	3009	1/1	0.94	0.15	69,69,69,69	0
58	MG	1H	3223	1/1	0.94	0.06	81,81,81,81	0
58	MG	13	1742	1/1	0.94	0.15	85,85,85,85	0
58	MG	1H	3123	1/1	0.94	0.18	63,63,63,63	0
58	MG	14	3071	1/1	0.94	0.10	75,75,75,75	0
58	MG	14	3016	1/1	0.94	0.08	61,61,61,61	0
58	MG	1H	3261	1/1	0.94	0.08	85,85,85,85	0
58	MG	1H	3069	1/1	0.94	0.20	62,62,62,62	0
58	MG	1H	3091	1/1	0.94	0.17	70,70,70,70	0
58	MG	1H	3337	1/1	0.94	0.21	53,53,53,53	0
58	MG	1G	1606	1/1	0.94	0.10	88,88,88,88	0
58	MG	1H	3025	1/1	0.94	0.18	41,41,41,41	0
58	MG	1H	3094	1/1	0.94	0.18	62,62,62,62	0
58	MG	14	3082	1/1	0.94	0.14	85,85,85,85	0
58	MG	14	3027	1/1	0.94	0.13	49,49,49,49	0
58	MG	1H	3054	1/1	0.94	0.26	45,45,45,45	0
58	MG	14	3029	1/1	0.94	0.25	49,49,49,49	0
58	MG	1H	3129	1/1	0.94	0.14	68,68,68,68	0
58	MG	14	3089	1/1	0.94	0.12	80,80,80,80	0
58	MG	13	1650	1/1	0.94	0.11	100,100,100,100	0
58	MG	1H	3233	1/1	0.94	0.20	77,77,77,77	0
58	MG	14	3093	1/1	0.94	0.25	52,52,52,52	0
58	MG	1H	3098	1/1	0.94	0.23	65,65,65,65	0
58	MG	1H	3073	1/1	0.94	0.11	67,67,67,67	0
58	MG	14	3155	1/1	0.94	0.30	69,69,69,69	0
58	MG	1H	3101	1/1	0.94	0.14	47,47,47,47	0
58	MG	13	1633	1/1	0.94	0.26	91,91,91,91	0
58	MG	1H	3002	1/1	0.94	0.17	48,48,48,48	0
58	MG	14	3039	1/1	0.94	0.07	72,72,72,72	0
58	MG	14	3040	1/1	0.94	0.16	49,49,49,49	0
58	MG	1H	3076	1/1	0.94	0.15	56,56,56,56	0
58	MG	1G	1624	1/1	0.94	0.12	100,100,100,100	0
58	MG	1H	3173	1/1	0.94	0.23	66,66,66,66	0
58	MG	1H	3003	1/1	0.94	0.19	38,38,38,38	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
58	MG	14	3339	1/1	0.94	0.06	109,109,109,109	0
58	MG	14	3342	1/1	0.94	0.05	129,129,129,129	0
58	MG	14	3345	1/1	0.94	0.08	90,90,90,90	0
58	MG	1H	3044	1/1	0.94	0.22	41,41,41,41	0
58	MG	14	3372	1/1	0.94	0.06	119,119,119,119	0
58	MG	13	1601	1/1	0.94	0.13	72,72,72,72	0
58	MG	14	3385	1/1	0.94	0.06	86,86,86,86	0
58	MG	14	3409	1/1	0.94	0.06	106,106,106,106	0
58	MG	14	3416	1/1	0.94	0.16	83,83,83,83	0
58	MG	4I	201	1/1	0.94	0.13	84,84,84,84	0
58	MG	14	3049	1/1	0.94	0.19	63,63,63,63	0
58	MG	1H	3112	1/1	0.94	0.25	52,52,52,52	0
58	MG	1H	3063	1/1	0.94	0.07	58,58,58,58	0
58	MG	14	3234	1/1	0.94	0.22	81,81,81,81	0
58	MG	14	3172	1/1	0.94	0.15	75,75,75,75	0
58	MG	13	1715	1/1	0.94	0.08	106,106,106,106	0
58	MG	1H	3115	1/1	0.94	0.14	62,62,62,62	0
58	MG	1H	3323	1/1	0.94	0.09	77,77,77,77	0
58	MG	1H	3150	1/1	0.94	0.27	62,62,62,62	0
58	MG	14	3117	1/1	0.94	0.15	62,62,62,62	0
58	MG	14	3179	1/1	0.94	0.16	91,91,91,91	0
58	MG	1H	3251	1/1	0.94	0.47	78,78,78,78	0
58	MG	13	1738	1/1	0.94	0.11	105,105,105,105	0
58	MG	11	301	1/1	0.94	0.21	50,50,50,50	0
58	MG	1H	3218	1/1	0.94	0.14	48,48,48,48	0
58	MG	21	302	1/1	0.94	0.06	69,69,69,69	0
58	MG	78	201	1/1	0.94	0.27	76,76,76,76	0
58	MG	1H	3338	1/1	0.95	0.21	66,66,66,66	0
58	MG	1G	1680	1/1	0.95	0.07	127,127,127,127	0
58	MG	14	3045	1/1	0.95	0.07	83,83,83,83	0
58	MG	1G	1682	1/1	0.95	0.07	113,113,113,113	0
58	MG	1G	1691	1/1	0.95	0.06	123,123,123,123	0
58	MG	1G	1692	1/1	0.95	0.05	130,130,130,130	0
58	MG	2K	102	1/1	0.95	0.30	79,79,79,79	0
58	MG	13	1724	1/1	0.95	0.08	85,85,85,85	0
58	MG	13	1735	1/1	0.95	0.05	124,124,124,124	0
58	MG	13	1737	1/1	0.95	0.08	111,111,111,111	0
58	MG	13	1629	1/1	0.95	0.18	58,58,58,58	0
58	MG	1H	3344	1/1	0.95	0.06	57,57,57,57	0
58	MG	1H	3109	1/1	0.95	0.26	47,47,47,47	0
58	MG	14	3275	1/1	0.95	0.28	71,71,71,71	0
58	MG	14	3163	1/1	0.95	0.36	65,65,65,65	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
58	MG	1H	3316	1/1	0.95	0.28	79,79,79,79	0
58	MG	13	1685	1/1	0.95	0.09	101,101,101,101	0
58	MG	14	3279	1/1	0.95	0.18	77,77,77,77	0
58	MG	14	3111	1/1	0.95	0.18	48,48,48,48	0
58	MG	1G	1645	1/1	0.95	0.09	96,96,96,96	0
58	MG	13	1619	1/1	0.95	0.14	72,72,72,72	0
58	MG	14	3061	1/1	0.95	0.15	56,56,56,56	0
58	MG	1H	3090	1/1	0.95	0.12	48,48,48,48	0
58	MG	1H	3352	1/1	0.95	0.08	70,70,70,70	0
58	MG	1H	3363	1/1	0.95	0.10	53,53,53,53	0
58	MG	1G	1610	1/1	0.95	0.16	92,92,92,92	0
58	MG	14	3120	1/1	0.95	0.26	70,70,70,70	0
58	MG	13	1677	1/1	0.95	0.16	71,71,71,71	0
58	MG	13	1615	1/1	0.95	0.11	85,85,85,85	0
58	MG	1G	1613	1/1	0.95	0.09	89,89,89,89	0
58	MG	1H	3140	1/1	0.95	0.15	61,61,61,61	0
58	MG	13	1645	1/1	0.95	0.23	75,75,75,75	0
58	MG	1H	3463	1/1	0.95	0.10	99,99,99,99	0
58	MG	14	3379	1/1	0.95	0.09	93,93,93,93	0
58	MG	14	3128	1/1	0.95	0.17	65,65,65,65	0
58	MG	1H	3467	1/1	0.95	0.08	101,101,101,101	0
58	MG	14	3403	1/1	0.95	0.07	119,119,119,119	0
58	MG	14	3408	1/1	0.95	0.06	108,108,108,108	0
58	MG	14	3024	1/1	0.95	0.20	58,58,58,58	0
58	MG	14	3412	1/1	0.95	0.08	113,113,113,113	0
58	MG	14	3415	1/1	0.95	0.12	97,97,97,97	0
58	MG	1G	1619	1/1	0.95	0.07	78,78,78,78	0
58	MG	1H	3060	1/1	0.95	0.20	47,47,47,47	0
58	MG	13	1653	1/1	0.95	0.08	86,86,86,86	0
58	MG	1H	3243	1/1	0.95	0.14	65,65,65,65	0
58	MG	1H	3144	1/1	0.95	0.06	48,48,48,48	0
58	MG	1H	3487	1/1	0.95	0.12	117,117,117,117	0
58	MG	13	1617	1/1	0.95	0.17	74,74,74,74	0
58	MG	14	3083	1/1	0.95	0.15	67,67,67,67	0
58	MG	1H	3079	1/1	0.95	0.25	51,51,51,51	0
58	MG	1H	3221	1/1	0.95	0.12	63,63,63,63	0
58	MG	14	3035	1/1	0.95	0.09	72,72,72,72	0
58	MG	13	1609	1/1	0.95	0.15	79,79,79,79	0
58	MG	1H	3148	1/1	0.95	0.26	77,77,77,77	0
58	MG	13	1628	1/1	0.95	0.29	82,82,82,82	0
58	MG	1H	3198	1/1	0.95	0.34	72,72,72,72	0
58	MG	1H	3306	1/1	0.95	0.13	63,63,63,63	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
58	MG	13	1717	1/1	0.95	0.09	97,97,97,97	0
58	MG	14	3203	1/1	0.95	0.14	71,71,71,71	0
58	MG	1H	3200	1/1	0.95	0.40	72,72,72,72	0
60	ZN	C5	201	1/1	0.95	0.06	153,153,153,153	0
58	MG	1H	3478	1/1	0.96	0.15	64,64,64,64	0
58	MG	13	1603	1/1	0.96	0.24	76,76,76,76	0
58	MG	1H	3120	1/1	0.96	0.09	47,47,47,47	0
58	MG	1H	3093	1/1	0.96	0.32	45,45,45,45	0
58	MG	1H	3048	1/1	0.96	0.20	43,43,43,43	0
58	MG	14	3221	1/1	0.96	0.36	86,86,86,86	0
58	MG	1H	3189	1/1	0.96	0.42	71,71,71,71	0
58	MG	1H	3208	1/1	0.96	0.30	71,71,71,71	0
58	MG	13	1616	1/1	0.96	0.24	62,62,62,62	0
58	MG	14	3025	1/1	0.96	0.16	52,52,52,52	0
58	MG	13	1626	1/1	0.96	0.17	62,62,62,62	0
58	MG	14	3174	1/1	0.96	0.11	53,53,53,53	0
58	MG	1H	3097	1/1	0.96	0.10	56,56,56,56	0
58	MG	1H	3016	1/1	0.96	0.21	52,52,52,52	0
58	MG	1H	3350	1/1	0.96	0.07	49,49,49,49	0
58	MG	1H	3017	1/1	0.96	0.24	54,54,54,54	0
58	MG	1H	3100	1/1	0.96	0.25	38,38,38,38	0
58	MG	1H	3373	1/1	0.96	0.08	76,76,76,76	0
58	MG	14	3288	1/1	0.96	0.12	56,56,56,56	0
58	MG	14	3080	1/1	0.96	0.09	62,62,62,62	0
58	MG	41	201	1/1	0.96	0.10	86,86,86,86	0
58	MG	14	3299	1/1	0.96	0.05	99,99,99,99	0
58	MG	14	3307	1/1	0.96	0.08	67,67,67,67	0
58	MG	14	3183	1/1	0.96	0.10	59,59,59,59	0
58	MG	1H	3376	1/1	0.96	0.06	71,71,71,71	0
58	MG	14	3343	1/1	0.96	0.08	72,72,72,72	0
58	MG	14	3344	1/1	0.96	0.06	96,96,96,96	0
58	MG	88	201	1/1	0.96	0.16	75,75,75,75	0
58	MG	1H	3379	1/1	0.96	0.10	92,92,92,92	0
58	MG	14	3350	1/1	0.96	0.06	89,89,89,89	0
58	MG	14	3354	1/1	0.96	0.05	92,92,92,92	0
58	MG	1G	1679	1/1	0.96	0.04	103,103,103,103	0
58	MG	14	3373	1/1	0.96	0.09	96,96,96,96	0
58	MG	1H	3394	1/1	0.96	0.09	104,104,104,104	0
58	MG	1H	3421	1/1	0.96	0.04	118,118,118,118	0
58	MG	1G	1686	1/1	0.96	0.05	126,126,126,126	0
58	MG	14	3387	1/1	0.96	0.18	89,89,89,89	0
58	MG	14	3393	1/1	0.96	0.06	140,140,140,140	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
58	MG	14	3396	1/1	0.96	0.14	67,67,67,67	0
58	MG	1G	1687	1/1	0.96	0.07	116,116,116,116	0
58	MG	14	3091	1/1	0.96	0.21	66,66,66,66	0
58	MG	1H	3426	1/1	0.96	0.06	103,103,103,103	0
58	MG	13	1726	1/1	0.96	0.05	122,122,122,122	0
58	MG	14	3414	1/1	0.96	0.05	104,104,104,104	0
58	MG	1G	1695	1/1	0.96	0.04	136,136,136,136	0
58	MG	1H	3439	1/1	0.96	0.07	80,80,80,80	0
58	MG	14	3251	1/1	0.96	0.10	66,66,66,66	0
58	MG	1H	3440	1/1	0.96	0.11	102,102,102,102	0
58	MG	13	1612	1/1	0.96	0.12	75,75,75,75	0
58	MG	1H	3117	1/1	0.96	0.20	68,68,68,68	0
58	MG	1H	3452	1/1	0.96	0.05	85,85,85,85	0
58	MG	14	3150	1/1	0.96	0.21	78,78,78,78	0
58	MG	1H	3454	1/1	0.96	0.13	102,102,102,102	0
58	MG	14	3005	1/1	0.96	0.13	51,51,51,51	0
58	MG	14	3006	1/1	0.96	0.33	47,47,47,47	0
58	MG	1H	3458	1/1	0.96	0.06	99,99,99,99	0
58	MG	13	1714	1/1	0.96	0.04	106,106,106,106	0
58	MG	1H	3462	1/1	0.96	0.08	91,91,91,91	0
58	MG	14	3056	1/1	0.96	0.20	50,50,50,50	0
58	MG	1H	3165	1/1	0.96	0.12	76,76,76,76	0
58	MG	1H	3465	1/1	0.96	0.07	97,97,97,97	0
58	MG	1H	3166	1/1	0.96	0.22	77,77,77,77	0
58	MG	1H	3469	1/1	0.96	0.14	81,81,81,81	0
58	MG	1H	3474	1/1	0.96	0.05	97,97,97,97	0
58	MG	1H	3133	1/1	0.96	0.11	60,60,60,60	0
58	MG	1H	3110	1/1	0.97	0.19	60,60,60,60	0
58	MG	14	3308	1/1	0.97	0.05	75,75,75,75	0
58	MG	14	3315	1/1	0.97	0.05	81,81,81,81	0
58	MG	14	3321	1/1	0.97	0.12	87,87,87,87	0
58	MG	14	3324	1/1	0.97	0.07	93,93,93,93	0
58	MG	14	3327	1/1	0.97	0.06	102,102,102,102	0
58	MG	14	3332	1/1	0.97	0.08	103,103,103,103	0
58	MG	14	3334	1/1	0.97	0.06	89,89,89,89	0
58	MG	14	3335	1/1	0.97	0.06	120,120,120,120	0
58	MG	1H	3448	1/1	0.97	0.06	67,67,67,67	0
58	MG	1H	3449	1/1	0.97	0.05	76,76,76,76	0
58	MG	1H	3033	1/1	0.97	0.19	66,66,66,66	0
58	MG	1H	3314	1/1	0.97	0.10	76,76,76,76	0
58	MG	1H	3137	1/1	0.97	0.11	56,56,56,56	0
58	MG	I8	101	1/1	0.97	0.11	90,90,90,90	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
58	MG	J8	101	1/1	0.97	0.10	77,77,77,77	0
58	MG	14	3351	1/1	0.97	0.05	79,79,79,79	0
58	MG	13	1707	1/1	0.97	0.06	87,87,87,87	0
58	MG	14	3362	1/1	0.97	0.05	81,81,81,81	0
58	MG	14	3366	1/1	0.97	0.06	68,68,68,68	0
58	MG	14	3370	1/1	0.97	0.06	80,80,80,80	0
58	MG	1H	3152	1/1	0.97	0.07	64,64,64,64	0
58	MG	1H	3360	1/1	0.97	0.05	70,70,70,70	0
58	MG	14	3376	1/1	0.97	0.04	117,117,117,117	0
58	MG	14	3377	1/1	0.97	0.08	105,105,105,105	0
58	MG	1H	3464	1/1	0.97	0.06	97,97,97,97	0
58	MG	13	1730	1/1	0.97	0.04	95,95,95,95	0
58	MG	14	3382	1/1	0.97	0.08	75,75,75,75	0
58	MG	1H	3367	1/1	0.97	0.09	59,59,59,59	0
58	MG	1H	3369	1/1	0.97	0.07	49,49,49,49	0
58	MG	14	3390	1/1	0.97	0.06	118,118,118,118	0
58	MG	13	1732	1/1	0.97	0.03	120,120,120,120	0
58	MG	14	3394	1/1	0.97	0.07	101,101,101,101	0
58	MG	1G	1677	1/1	0.97	0.05	130,130,130,130	0
58	MG	14	3399	1/1	0.97	0.10	80,80,80,80	0
58	MG	1G	1678	1/1	0.97	0.09	120,120,120,120	0
58	MG	14	3406	1/1	0.97	0.05	100,100,100,100	0
58	MG	13	1734	1/1	0.97	0.03	130,130,130,130	0
58	MG	13	1711	1/1	0.97	0.06	102,102,102,102	0
58	MG	1H	3385	1/1	0.97	0.05	60,60,60,60	0
58	MG	1G	1685	1/1	0.97	0.04	109,109,109,109	0
58	MG	1H	3484	1/1	0.97	0.05	104,104,104,104	0
58	MG	1H	3388	1/1	0.97	0.13	78,78,78,78	0
58	MG	14	3417	1/1	0.97	0.04	113,113,113,113	0
58	MG	1G	1688	1/1	0.97	0.04	122,122,122,122	0
58	MG	13	1736	1/1	0.97	0.06	116,116,116,116	0
58	MG	1H	3397	1/1	0.97	0.07	79,79,79,79	0
58	MG	16	201	1/1	0.97	0.04	99,99,99,99	0
58	MG	1G	1615	1/1	0.97	0.08	132,132,132,132	0
58	MG	1H	3029	1/1	0.97	0.44	67,67,67,67	0
58	MG	1H	3425	1/1	0.97	0.04	110,110,110,110	0
58	MG	1H	3011	1/1	0.97	0.28	62,62,62,62	0
58	MG	1H	3292	1/1	0.97	0.07	68,68,68,68	0
58	MG	1H	3432	1/1	0.97	0.08	78,78,78,78	0
58	MG	14	3244	1/1	0.97	0.19	78,78,78,78	0
58	MG	1H	3437	1/1	0.97	0.06	82,82,82,82	0
58	MG	1H	3216	1/1	0.97	0.07	57,57,57,57	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
58	MG	14	3125	1/1	0.97	0.08	60,60,60,60	0
58	MG	13	1720	1/1	0.97	0.06	111,111,111,111	0
58	MG	13	1660	1/1	0.97	0.33	63,63,63,63	0
58	MG	14	3292	1/1	0.97	0.06	68,68,68,68	0
58	MG	E5	101	1/1	0.97	0.16	53,53,53,53	0
58	MG	14	3087	1/1	0.97	0.15	56,56,56,56	0
60	ZN	5A	101	1/1	0.97	0.05	128,128,128,128	0
58	MG	14	3302	1/1	0.97	0.06	67,67,67,67	0
58	MG	14	3295	1/1	0.98	0.03	61,61,61,61	0
58	MG	14	3298	1/1	0.98	0.04	69,69,69,69	0
58	MG	13	1705	1/1	0.98	0.04	99,99,99,99	0
58	MG	1H	3466	1/1	0.98	0.04	77,77,77,77	0
58	MG	14	3303	1/1	0.98	0.05	72,72,72,72	0
58	MG	1H	3386	1/1	0.98	0.04	59,59,59,59	0
58	MG	1H	3468	1/1	0.98	0.10	108,108,108,108	0
58	MG	14	3310	1/1	0.98	0.04	59,59,59,59	0
58	MG	14	3311	1/1	0.98	0.05	62,62,62,62	0
58	MG	14	3312	1/1	0.98	0.06	56,56,56,56	0
58	MG	13	1721	1/1	0.98	0.04	63,63,63,63	0
58	MG	1H	3470	1/1	0.98	0.04	96,96,96,96	0
58	MG	1H	3473	1/1	0.98	0.04	89,89,89,89	0
58	MG	14	3326	1/1	0.98	0.07	77,77,77,77	0
58	MG	13	1739	1/1	0.98	0.03	110,110,110,110	0
58	MG	14	3331	1/1	0.98	0.04	102,102,102,102	0
58	MG	1G	1675	1/1	0.98	0.04	78,78,78,78	0
58	MG	13	1740	1/1	0.98	0.13	93,93,93,93	0
58	MG	1H	3477	1/1	0.98	0.05	96,96,96,96	0
58	MG	14	3336	1/1	0.98	0.04	107,107,107,107	0
58	MG	14	3337	1/1	0.98	0.07	78,78,78,78	0
58	MG	1H	3398	1/1	0.98	0.04	48,48,48,48	0
58	MG	14	3340	1/1	0.98	0.12	72,72,72,72	0
58	MG	14	3341	1/1	0.98	0.04	92,92,92,92	0
58	MG	1H	3400	1/1	0.98	0.04	71,71,71,71	0
58	MG	1G	1681	1/1	0.98	0.05	88,88,88,88	0
58	MG	1H	3480	1/1	0.98	0.05	98,98,98,98	0
58	MG	1G	1683	1/1	0.98	0.05	106,106,106,106	0
58	MG	1H	3401	1/1	0.98	0.04	71,71,71,71	0
58	MG	14	3347	1/1	0.98	0.04	83,83,83,83	0
58	MG	1H	3406	1/1	0.98	0.05	91,91,91,91	0
58	MG	14	3116	1/1	0.98	0.32	48,48,48,48	0
58	MG	14	3352	1/1	0.98	0.06	69,69,69,69	0
58	MG	1H	3407	1/1	0.98	0.09	59,59,59,59	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
58	MG	14	3361	1/1	0.98	0.05	70,70,70,70	0
58	MG	1H	3409	1/1	0.98	0.04	58,58,58,58	0
58	MG	14	3363	1/1	0.98	0.05	63,63,63,63	0
58	MG	1G	1690	1/1	0.98	0.09	105,105,105,105	0
58	MG	14	3367	1/1	0.98	0.08	67,67,67,67	0
58	MG	1H	3488	1/1	0.98	0.04	92,92,92,92	0
58	MG	1H	3489	1/1	0.98	0.07	83,83,83,83	0
58	MG	1G	1693	1/1	0.98	0.05	123,123,123,123	0
58	MG	1H	3492	1/1	0.98	0.07	95,95,95,95	0
58	MG	1H	3493	1/1	0.98	0.04	96,96,96,96	0
58	MG	1H	3413	1/1	0.98	0.05	72,72,72,72	0
58	MG	1H	3416	1/1	0.98	0.08	108,108,108,108	0
58	MG	14	3001	1/1	0.98	0.06	46,46,46,46	0
58	MG	14	3383	1/1	0.98	0.06	93,93,93,93	0
58	MG	1H	3420	1/1	0.98	0.04	80,80,80,80	0
58	MG	13	1661	1/1	0.98	0.04	86,86,86,86	0
58	MG	1H	3422	1/1	0.98	0.07	83,83,83,83	0
58	MG	14	3391	1/1	0.98	0.05	85,85,85,85	0
58	MG	13	1708	1/1	0.98	0.04	76,76,76,76	0
58	MG	13	1727	1/1	0.98	0.15	79,79,79,79	0
58	MG	1H	3427	1/1	0.98	0.04	84,84,84,84	0
58	MG	16	210	1/1	0.98	0.03	80,80,80,80	0
58	MG	14	3402	1/1	0.98	0.08	110,110,110,110	0
58	MG	16	211	1/1	0.98	0.04	88,88,88,88	0
58	MG	14	3405	1/1	0.98	0.07	107,107,107,107	0
58	MG	14	3072	1/1	0.98	0.11	43,43,43,43	0
58	MG	14	3407	1/1	0.98	0.05	98,98,98,98	0
58	MG	13	1728	1/1	0.98	0.05	76,76,76,76	0
58	MG	13	1610	1/1	0.98	0.06	66,66,66,66	0
58	MG	14	3410	1/1	0.98	0.04	75,75,75,75	0
58	MG	14	3411	1/1	0.98	0.05	113,113,113,113	0
58	MG	1H	3433	1/1	0.98	0.09	45,45,45,45	0
58	MG	1H	3353	1/1	0.98	0.06	54,54,54,54	0
58	MG	1H	3438	1/1	0.98	0.04	79,79,79,79	0
58	MG	1H	3354	1/1	0.98	0.04	49,49,49,49	0
58	MG	1H	3356	1/1	0.98	0.05	56,56,56,56	0
58	MG	13	1632	1/1	0.98	0.06	57,57,57,57	0
58	MG	14	3420	1/1	0.98	0.05	72,72,72,72	0
58	MG	1H	3444	1/1	0.98	0.05	50,50,50,50	0
58	MG	1H	3361	1/1	0.98	0.07	47,47,47,47	0
58	MG	13	1733	1/1	0.98	0.12	83,83,83,83	0
58	MG	1H	3364	1/1	0.98	0.05	48,48,48,48	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
58	MG	1H	3451	1/1	0.98	0.04	68,68,68,68	0
58	MG	14	3214	1/1	0.98	0.06	82,82,82,82	0
58	MG	14	3023	1/1	0.98	0.12	42,42,42,42	0
58	MG	1H	3258	1/1	0.98	0.33	66,66,66,66	0
58	MG	1H	3453	1/1	0.98	0.03	98,98,98,98	0
58	MG	13	1703	1/1	0.98	0.04	64,64,64,64	0
58	MG	1H	3456	1/1	0.98	0.04	93,93,93,93	0
58	MG	13	1704	1/1	0.98	0.06	72,72,72,72	0
58	MG	1H	3459	1/1	0.98	0.09	85,85,85,85	0
58	MG	1G	1607	1/1	0.98	0.10	92,92,92,92	0
58	MG	13	1718	1/1	0.98	0.04	100,100,100,100	0
58	MG	1H	3111	1/1	0.98	0.14	39,39,39,39	0
58	MG	1H	3381	1/1	0.98	0.06	47,47,47,47	0
59	SF4	32	301	8/8	0.98	0.03	119,123,130,133	0
58	MG	1H	3382	1/1	0.98	0.06	58,58,58,58	0
58	MG	14	3293	1/1	0.98	0.09	67,67,67,67	0
58	MG	14	3294	1/1	0.98	0.06	65,65,65,65	0
58	MG	14	3319	1/1	0.99	0.08	50,50,50,50	0
58	MG	14	3320	1/1	0.99	0.06	78,78,78,78	0
58	MG	13	1709	1/1	0.99	0.04	96,96,96,96	0
58	MG	14	3323	1/1	0.99	0.04	61,61,61,61	0
58	MG	1H	3445	1/1	0.99	0.04	49,49,49,49	0
58	MG	14	3325	1/1	0.99	0.07	75,75,75,75	0
58	MG	1H	3446	1/1	0.99	0.07	77,77,77,77	0
58	MG	1H	3355	1/1	0.99	0.03	60,60,60,60	0
58	MG	14	3328	1/1	0.99	0.07	105,105,105,105	0
58	MG	14	3330	1/1	0.99	0.03	73,73,73,73	0
58	MG	1H	3387	1/1	0.99	0.03	51,51,51,51	0
58	MG	13	1722	1/1	0.99	0.09	70,70,70,70	0
58	MG	14	3333	1/1	0.99	0.04	98,98,98,98	0
58	MG	1H	3450	1/1	0.99	0.08	77,77,77,77	0
58	MG	1H	3391	1/1	0.99	0.04	61,61,61,61	0
58	MG	1H	3358	1/1	0.99	0.06	54,54,54,54	0
58	MG	1H	3395	1/1	0.99	0.06	72,72,72,72	0
58	MG	14	3338	1/1	0.99	0.06	64,64,64,64	0
58	MG	1H	3396	1/1	0.99	0.05	75,75,75,75	0
58	MG	1H	3455	1/1	0.99	0.04	65,65,65,65	0
58	MG	1H	3359	1/1	0.99	0.02	43,43,43,43	0
58	MG	13	1723	1/1	0.99	0.02	80,80,80,80	0
58	MG	13	1710	1/1	0.99	0.03	74,74,74,74	0
58	MG	13	1725	1/1	0.99	0.05	83,83,83,83	0
58	MG	1H	3461	1/1	0.99	0.04	80,80,80,80	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
58	MG	1H	3402	1/1	0.99	0.03	60,60,60,60	0
58	MG	1G	1676	1/1	0.99	0.08	91,91,91,91	0
58	MG	14	3348	1/1	0.99	0.03	86,86,86,86	0
58	MG	14	3349	1/1	0.99	0.03	47,47,47,47	0
58	MG	1H	3404	1/1	0.99	0.07	78,78,78,78	0
58	MG	1H	3405	1/1	0.99	0.03	70,70,70,70	0
58	MG	13	1716	1/1	0.99	0.07	75,75,75,75	0
58	MG	14	3353	1/1	0.99	0.04	80,80,80,80	0
58	MG	1H	3365	1/1	0.99	0.06	60,60,60,60	0
58	MG	14	3355	1/1	0.99	0.03	91,91,91,91	0
58	MG	14	3356	1/1	0.99	0.04	61,61,61,61	0
58	MG	14	3357	1/1	0.99	0.07	83,83,83,83	0
58	MG	14	3358	1/1	0.99	0.06	83,83,83,83	0
58	MG	14	3359	1/1	0.99	0.04	70,70,70,70	0
58	MG	14	3360	1/1	0.99	0.04	48,48,48,48	0
58	MG	1H	3408	1/1	0.99	0.03	61,61,61,61	0
58	MG	1H	3366	1/1	0.99	0.06	53,53,53,53	0
58	MG	1H	3410	1/1	0.99	0.04	76,76,76,76	0
58	MG	14	3364	1/1	0.99	0.04	98,98,98,98	0
58	MG	14	3365	1/1	0.99	0.04	55,55,55,55	0
58	MG	1G	1684	1/1	0.99	0.07	82,82,82,82	0
58	MG	1H	3412	1/1	0.99	0.04	55,55,55,55	0
58	MG	14	3368	1/1	0.99	0.06	79,79,79,79	0
58	MG	14	3369	1/1	0.99	0.03	49,49,49,49	0
58	MG	1H	3471	1/1	0.99	0.08	92,92,92,92	0
58	MG	14	3371	1/1	0.99	0.06	89,89,89,89	0
58	MG	1H	3472	1/1	0.99	0.03	60,60,60,60	0
58	MG	13	1706	1/1	0.99	0.03	80,80,80,80	0
58	MG	14	3374	1/1	0.99	0.08	95,95,95,95	0
58	MG	14	3375	1/1	0.99	0.04	49,49,49,49	0
58	MG	1G	1689	1/1	0.99	0.03	98,98,98,98	0
58	MG	1H	3414	1/1	0.99	0.03	59,59,59,59	0
58	MG	1H	3475	1/1	0.99	0.09	80,80,80,80	0
58	MG	14	3380	1/1	0.99	0.02	85,85,85,85	0
58	MG	1H	3415	1/1	0.99	0.03	69,69,69,69	0
58	MG	1H	3368	1/1	0.99	0.03	53,53,53,53	0
58	MG	1G	1694	1/1	0.99	0.05	129,129,129,129	0
58	MG	14	3384	1/1	0.99	0.03	93,93,93,93	0
58	MG	1H	3417	1/1	0.99	0.04	83,83,83,83	0
58	MG	14	3386	1/1	0.99	0.03	82,82,82,82	0
58	MG	1H	3418	1/1	0.99	0.04	74,74,74,74	0
58	MG	14	3388	1/1	0.99	0.03	83,83,83,83	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
58	MG	14	3389	1/1	0.99	0.04	94,94,94,94	0
58	MG	1H	3419	1/1	0.99	0.03	51,51,51,51	0
58	MG	1H	3481	1/1	0.99	0.07	100,100,100,100	0
58	MG	14	3392	1/1	0.99	0.05	88,88,88,88	0
58	MG	1H	3482	1/1	0.99	0.08	95,95,95,95	0
58	MG	1H	3483	1/1	0.99	0.03	99,99,99,99	0
58	MG	14	3395	1/1	0.99	0.08	69,69,69,69	0
58	MG	13	1712	1/1	0.99	0.03	66,66,66,66	0
58	MG	14	3397	1/1	0.99	0.03	89,89,89,89	0
58	MG	1H	3371	1/1	0.99	0.05	66,66,66,66	0
58	MG	14	3400	1/1	0.99	0.09	82,82,82,82	0
58	MG	14	3401	1/1	0.99	0.04	83,83,83,83	0
58	MG	1H	3372	1/1	0.99	0.03	73,73,73,73	0
58	MG	1H	3423	1/1	0.99	0.08	71,71,71,71	0
58	MG	14	3404	1/1	0.99	0.02	85,85,85,85	0
58	MG	1H	3424	1/1	0.99	0.02	66,66,66,66	0
58	MG	13	1729	1/1	0.99	0.06	80,80,80,80	0
58	MG	1H	3490	1/1	0.99	0.03	95,95,95,95	0
58	MG	1H	3374	1/1	0.99	0.05	63,63,63,63	0
58	MG	1H	3375	1/1	0.99	0.04	50,50,50,50	0
58	MG	1H	3494	1/1	0.99	0.04	44,44,44,44	0
58	MG	1H	3495	1/1	0.99	0.06	70,70,70,70	0
58	MG	1H	3428	1/1	0.99	0.03	64,64,64,64	0
58	MG	14	3413	1/1	0.99	0.03	102,102,102,102	0
58	MG	14	3291	1/1	0.99	0.10	55,55,55,55	0
58	MG	1H	3429	1/1	0.99	0.05	105,105,105,105	0
58	MG	13	1719	1/1	0.99	0.04	95,95,95,95	0
58	MG	1H	3431	1/1	0.99	0.03	74,74,74,74	0
58	MG	14	3418	1/1	0.99	0.06	52,52,52,52	0
58	MG	1H	3377	1/1	0.99	0.08	68,68,68,68	0
58	MG	14	3296	1/1	0.99	0.03	67,67,67,67	0
58	MG	14	3421	1/1	0.99	0.04	79,79,79,79	0
58	MG	14	3297	1/1	0.99	0.03	55,55,55,55	0
58	MG	1H	3378	1/1	0.99	0.04	85,85,85,85	0
58	MG	1H	3435	1/1	0.99	0.04	70,70,70,70	0
58	MG	14	3301	1/1	0.99	0.03	49,49,49,49	0
58	MG	1H	3436	1/1	0.99	0.03	73,73,73,73	0
58	MG	1H	3351	1/1	0.99	0.05	49,49,49,49	0
58	MG	14	3304	1/1	0.99	0.04	62,62,62,62	0
58	MG	14	3305	1/1	0.99	0.05	51,51,51,51	0
58	MG	14	3306	1/1	0.99	0.04	64,64,64,64	0
58	MG	1H	3380	1/1	0.99	0.13	56,56,56,56	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
58	MG	13	1731	1/1	0.99	0.04	78,78,78,78	0
58	MG	14	3309	1/1	0.99	0.06	51,51,51,51	0
58	MG	13	1713	1/1	0.99	0.03	84,84,84,84	0
58	MG	1H	3441	1/1	0.99	0.08	78,78,78,78	0
58	MG	1H	3442	1/1	0.99	0.05	64,64,64,64	0
58	MG	14	3313	1/1	0.99	0.03	84,84,84,84	0
58	MG	14	3314	1/1	0.99	0.04	63,63,63,63	0
59	SF4	3E	301	8/8	0.99	0.05	78,90,95,100	0
58	MG	1H	3383	1/1	0.99	0.04	49,49,49,49	0
60	ZN	5I	102	1/1	0.99	0.02	92,92,92,92	0
58	MG	14	3316	1/1	0.99	0.03	59,59,59,59	0
58	MG	14	3317	1/1	0.99	0.04	52,52,52,52	0
58	MG	14	3318	1/1	0.99	0.03	65,65,65,65	0
58	MG	1H	3389	1/1	1.00	0.02	50,50,50,50	0
58	MG	1H	3390	1/1	1.00	0.03	58,58,58,58	0
58	MG	1H	3399	1/1	1.00	0.02	40,40,40,40	0
58	MG	1H	3357	1/1	1.00	0.03	56,56,56,56	0
58	MG	14	3300	1/1	1.00	0.03	57,57,57,57	0
58	MG	1H	3457	1/1	1.00	0.03	75,75,75,75	0
58	MG	1H	3411	1/1	1.00	0.02	63,63,63,63	0
58	MG	1H	3434	1/1	1.00	0.02	45,45,45,45	0
58	MG	1H	3392	1/1	1.00	0.02	50,50,50,50	0
58	MG	1H	3393	1/1	1.00	0.01	51,51,51,51	0
58	MG	14	3322	1/1	1.00	0.02	69,69,69,69	0
58	MG	1H	3403	1/1	1.00	0.04	45,45,45,45	0
58	MG	14	3378	1/1	1.00	0.02	90,90,90,90	0
58	MG	14	3398	1/1	1.00	0.06	67,67,67,67	0
58	MG	1H	3370	1/1	1.00	0.06	72,72,72,72	0
58	MG	16	209	1/1	1.00	0.02	64,64,64,64	0
58	MG	1H	3362	1/1	1.00	0.01	42,42,42,42	0
58	MG	1H	3491	1/1	1.00	0.03	91,91,91,91	0
58	MG	1H	3384	1/1	1.00	0.02	45,45,45,45	0
58	MG	14	3329	1/1	1.00	0.07	75,75,75,75	0

6.5 Other polymers ⓘ

There are no such residues in this entry.