



# wwPDB X-ray Structure Validation Summary Report ⓘ

May 15, 2020 – 08:11 pm BST

PDB ID : 4WZO  
Title : Complex of 70S ribosome with tRNA-fMet and mRNA  
Authors : Rozov, A.; Demeshkina, N.; Yusupov, M.; Yusupova, G.  
Deposited on : 2014-11-20  
Resolution : 3.30 Å(reported)

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

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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

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



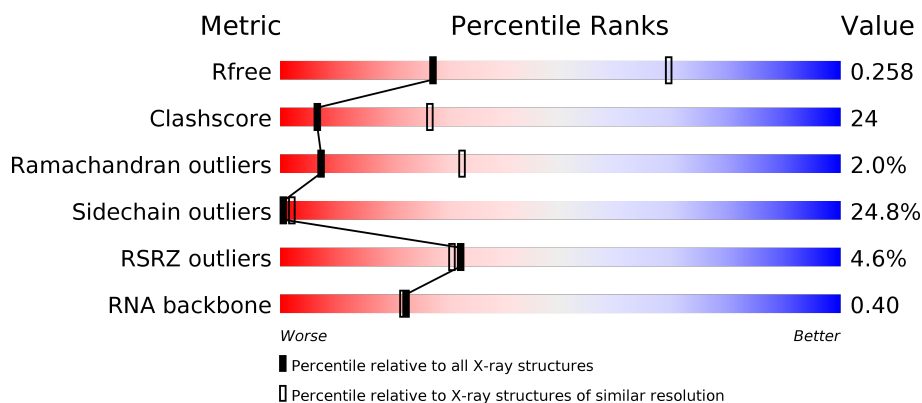
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.30 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	130704	1149 (3.34-3.26)
Clashscore	141614	1205 (3.34-3.26)
Ramachandran outliers	138981	1183 (3.34-3.26)
Sidechain outliers	138945	1182 (3.34-3.26)
RSRZ outliers	127900	1115 (3.34-3.26)
RNA backbone	3102	1117 (3.70-2.90)

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

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

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

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Mol	Chain	Length	Quality of chain
15	6I	89	
16	7A	88	
16	7I	88	
17	8A	105	
17	8I	105	
18	9A	88	
18	9I	88	
19	AA	93	
19	AI	93	
20	BA	106	
20	BI	106	
21	1B	27	
21	1F	27	
22	1K	77	
23	2K	77	
24	3K	76	
24	3L	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	% 49% 35% 14% ..
30	21	206	11% 41% 43% 15% .
30	29	206	3% 35% 47% 16% .
31	31	210	% 39% 44% 13% .
31	39	210	5% 31% 51% 13% ..
32	41	182	5% 31% 51% 18% ..
32	49	182	21% 31% 52% 16% .
33	51	180	2% 41% 41% 14% ..
33	59	180	24% 31% 46% 18% 6%
34	61	148	10% 39% 43% 15% ..
34	69	148	11% 39% 46% 14% ..
35	15	140	3% 46% 42% 11% .
35	58	140	3% 39% 41% 19% .
36	25	122	3% 43% 39% 17%
36	68	122	3% 51% 37% 12%
37	35	150	12% 31% 39% 23% 5% .
37	78	150	2% 36% 44% 17% .
38	45	141	21% 40% 44% 14% .
38	88	141	5% 45% 34% 16% ..
39	55	118	4% 31% 54% 14% .
39	98	118	3% 33% 53% 13% .
40	65	112	7% 33% 54% 11% ..
40	A8	112	13% 32% 44% 21% ..
41	75	146	3% 33% 44% 17% 6%
41	B8	146	% 41% 36% 16% . 6%

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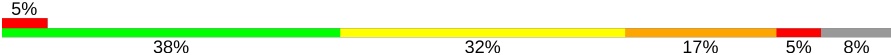

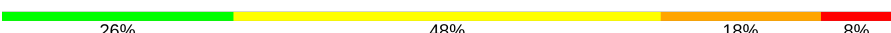
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Mol	Chain	Length	Quality of chain
42	85	118	
42	C8	118	
43	95	101	
43	D8	101	
44	A5	113	
44	E8	113	
45	B5	96	
45	F8	96	
46	C5	110	
46	G8	110	
47	D5	206	
47	H8	206	
48	E5	85	
48	I8	85	
49	F5	98	
49	J8	98	
50	G5	72	
50	K8	72	
51	H5	60	
51	L8	60	
52	I5	71	
52	M8	71	
53	J5	60	
53	N8	60	
54	L5	49	

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Mol	Chain	Length	Quality of chain
54	P8	49	
55	M5	65	
55	Q8	65	
56	2L	77	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
57	MG	13	1626	-	-	-	X
57	MG	13	1642	-	-	-	X
57	MG	13	1659	-	-	-	X
57	MG	13	1661	-	-	-	X
57	MG	13	1662	-	-	-	X
57	MG	13	1664	-	-	-	X
57	MG	13	1671	-	-	-	X
57	MG	14	3069	-	-	-	X
57	MG	14	3086	-	-	-	X
57	MG	14	3094	-	-	-	X
57	MG	14	3102	-	-	-	X
57	MG	14	3124	-	-	-	X
57	MG	14	3156	-	-	-	X
57	MG	14	3164	-	-	-	X
57	MG	14	3166	-	-	-	X
57	MG	14	3170	-	-	-	X
57	MG	14	3174	-	-	-	X
57	MG	14	3176	-	-	-	X
57	MG	14	3179	-	-	-	X
57	MG	14	3201	-	-	-	X
57	MG	14	3211	-	-	-	X
57	MG	14	3212	-	-	-	X
57	MG	14	3213	-	-	-	X
57	MG	14	3216	-	-	-	X
57	MG	14	3218	-	-	-	X
57	MG	1G	1621	-	-	-	X
57	MG	1G	1635	-	-	-	X
57	MG	1G	1651	-	-	-	X
57	MG	1H	3053	-	-	-	X
57	MG	1H	3162	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
57	MG	1H	3169	-	-	-	X
57	MG	1H	3170	-	-	-	X
57	MG	1H	3188	-	-	-	X
57	MG	1H	3198	-	-	-	X
57	MG	1H	3204	-	-	-	X
57	MG	1H	3224	-	-	-	X
57	MG	1H	3225	-	-	-	X
57	MG	1H	3230	-	-	-	X
57	MG	1H	3242	-	-	-	X
57	MG	1H	3244	-	-	-	X
57	MG	1H	3252	-	-	-	X
57	MG	1H	3261	-	-	-	X
57	MG	1H	3262	-	-	-	X
57	MG	1H	3271	-	-	-	X
57	MG	1H	3277	-	-	-	X



## 2 Entry composition

There are 59 unique types of molecules in this entry. The entry contains 295920 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	1497	Total	C	N	O	P	0	0	0
			32185	14324	5968	10396	1497			
1	1G	1497	Total	C	N	O	P	0	0	0
			32182	14324	5968	10394	1496			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	1E	237	Total	C	N	O	S	0	0	0
			1924	1228	344	347	5			
2	12	237	Total	C	N	O	S	0	0	0
			1924	1228	344	347	5			

- 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	206	Total	C	N	O	S	0	0	0
			1612	1016	314	281	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	151	Total	C	N	O	S	0	0	0
			1155	729	218	204	4			
5	42	151	Total	C	N	O	S	0	0	0
			1155	729	218	204	4			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	5E	101	Total	C	N	O	S	0	0	0
			842	531	155	153	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	155	Total	C	N	O	S	0	0	0
			1256	781	252	217	6			
7	62	147	Total	C	N	O	S	0	0	0
			1194	744	237	207	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
			1009	639	197	173				
9	82	127	Total	C	N	O		0	0	0
			1009	639	197	173				

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	1I	99	Total	C	N	O	S	0	0	0
			801	504	157	139	1			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	1A	66	Total	C	N	O	S	0	0	0
			522	327	99	95	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	2I	119	Total	C	N	O	S	0	0	0
			884	549	168	164	3			
11	2A	116	Total	C	N	O	S	0	0	0
			864	537	164	160	3			

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
14	5I	60	Total	C	N	O	S	0	0	0
			491	312	104	71	4			
14	5A	52	Total	C	N	O	S	0	0	0
			418	262	90	62	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	88	Total	C	N	O	S	0	0	0
			733	459	147	125	2			



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

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

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

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

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
18	9I	72	Total	C	N	O	0	0	0
			590	376	117	97			
18	9A	72	Total	C	N	O	0	0	0
			590	376	117	97			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
19	AI	81	Total	C	N	O	S	0	0	0
			647	413	119	113	2			
19	AA	78	Total	C	N	O	S	0	0	0
			624	398	115	109	2			

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

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

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



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
21	1F	25	Total	C	N	O	0	0	0
			217	134	52	31			
21	1B	22	Total	C	N	O	0	0	0
			188	116	44	28			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
22	1K	70	Total	C	N	O	P	0	0	0
			1497	669	274	485	69			

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

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

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

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
24	3K	76	Total	C	N	O	P	S	0	0	0
			1627	730	290	530	75	2			
24	3L	76	Total	C	N	O	P	S	0	0	0
			1627	730	290	530	75	2			

- Molecule 25 is a RNA chain called mRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
25	4K	13	Total	C	N	O	P	0	0	0
			285	129	62	81	13			
25	4L	9	Total	C	N	O	P	0	0	0
			197	89	42	57	9			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
26	1H	2902	Total	C	N	O	P	0	0	0
			62497	27816	11684	20095	2902			
26	14	2877	Total	C	N	O	P	0	0	0
			61968	27579	11594	19918	2877			

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



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

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
28	71	93	Total	C	N	O	0	0	0
			737	465	139	133			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
29	11	272	Total	C	N	O	S	0	0	0
			2115	1335	420	357	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	205	Total	C	N	O	S	0	0	0
			1568	991	300	271	6			
30	29	205	Total	C	N	O	S	0	0	0
			1568	991	300	271	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	206	Total	C	N	O	S	0	0	0
			1610	1026	301	281	2			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
32	41	181	Total	C	N	O	S	0	0	0
			1473	942	268	259	4			
32	49	181	Total	C	N	O	S	0	0	0
			1473	942	268	259	4			



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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
33	51	174	Total	C	N	O	S	0	0	0
			1336	848	251	236	1			
33	59	170	Total	C	N	O	S	0	0	0
			1307	829	245	232	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
34	61	146	Total	C	N	O	S	0	0	0
			1136	726	201	208	1			
34	69	146	Total	C	N	O	S	0	0	0
			1136	726	201	208	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	138	Total	C	N	O	S	0	0	0
			1104	712	206	182	4			

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
37	78	150	Total	C	N	O	S	0	0	0
			1144	712	232	197	3			
37	35	147	Total	C	N	O	S	0	0	0
			1122	698	229	192	3			

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



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
38	88	137	Total	C	N	O	S	0	0	0
			1077	688	206	177	6			
38	45	141	Total	C	N	O	S	0	0	0
			1121	715	212	187	7			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
39	98	118	Total	C	N	O	S	0	0	0
			967	604	203	159	1			
39	55	117	Total	C	N	O		0	0	0
			959	599	202	158				

- 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	111	Total	C	N	O	0	0	0
			881	556	176	149			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
41	B8	137	Total	C	N	O	S	0	0	0
			1141	710	234	196	1			
41	75	137	Total	C	N	O	S	0	0	0
			1141	710	234	196	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
42	C8	117	Total	C	N	O	S	0	0	0
			963	610	202	150	1			
42	85	117	Total	C	N	O	S	0	0	0
			963	610	202	150	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
43	D8	101	Total	C	N	O	S	0	0	0
			778	501	142	134	1			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
43	95	101	Total	C	N	O	S	0	0	0
			778	501	142	134	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
44	E8	113	Total	C	N	O	S	0	0	0
			899	566	177	154	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	94	Total	C	N	O	S	0	0	0
			742	482	134	125	1			
45	B5	92	Total	C	N	O		0	0	0
			725	471	131	123				

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
46	G8	104	Total	C	N	O	S	0	0	0
			791	510	149	127	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	135	Total	C	N	O	S	0	0	0
			1110	714	202	192	2			
47	D5	137	Total	C	N	O	S	0	0	0
			1126	725	202	197	2			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
48	I8	80	Total	C	N	O	S	0	0	0
			626	388	132	105	1			
48	E5	77	Total	C	N	O	S	0	0	0
			612	379	129	103	1			



There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
I8	6	ALA	GLY	conflict	UNP P60493
I8	8	ALA	GLY	conflict	UNP P60493
E5	6	ALA	GLY	conflict	UNP P60493
E5	8	ALA	GLY	conflict	UNP P60493

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
49	J8	97	Total	C	N	O	S	0	0	0
			762	481	150	130	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	67	Total	C	N	O	S	0	0	0
			563	349	114	99	1			
50	G5	66	Total	C	N	O	S	0	0	0
			558	346	113	98	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
51	L8	57	Total	C	N	O	S	0	0	0
			452	288	88	76				
51	H5	59	Total	C	N	O	S	0	0	0
			468	298	90	80				

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
52	M8	66	Total	C	N	O	S	0	0	0
			533	335	96	97	5			
52	I5	63	Total	C	N	O	S	0	0	0
			515	326	93	91	5			

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



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
53	N8	54	Total	C	N	O	S	0	0	0
			422	264	85	68	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
			409	251	102	54	2			
54	L5	46	Total	C	N	O	S	0	0	0
			398	245	98	53	2			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
55	Q8	60	Total	C	N	O	S	0	0	0
			480	306	98	74	2			
55	M5	60	Total	C	N	O	S	0	0	0
			477	303	98	74	2			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
56	2L	77	Total	C	N	O	P	S	0	0
			1645	734	298	535	77	1		

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
57	98	1	Total	Mg	0	0
			1	1		
57	45	1	Total	Mg	0	0
			1	1		
57	P8	1	Total	Mg	0	0
			1	1		
57	13	99	Total	Mg	0	0
			99	99		
57	1J	3	Total	Mg	0	0
			3	3		
57	35	1	Total	Mg	0	0
			1	1		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
57	16	11	Total 11	Mg 11	0	0
57	25	1	Total 1	Mg 1	0	0
57	M5	1	Total 1	Mg 1	0	0
57	2K	2	Total 2	Mg 2	0	0
57	L8	1	Total 1	Mg 1	0	0
57	4I	1	Total 1	Mg 1	0	0
57	I8	2	Total 2	Mg 2	0	0
57	68	2	Total 2	Mg 2	0	0
57	29	2	Total 2	Mg 2	0	0
57	78	2	Total 2	Mg 2	0	0
57	J8	2	Total 2	Mg 2	0	0
57	1G	72	Total 72	Mg 72	0	0
57	4E	1	Total 1	Mg 1	0	0
57	11	3	Total 3	Mg 3	0	0
57	1H	444	Total 444	Mg 444	0	0
57	88	1	Total 1	Mg 1	0	0
57	14	327	Total 327	Mg 327	0	0
57	3E	1	Total 1	Mg 1	0	0
57	55	1	Total 1	Mg 1	0	0
57	3L	2	Total 2	Mg 2	0	0
57	41	2	Total 2	Mg 2	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
57	2L	2	Total	Mg	0	0
			2	2		

- Molecule 58 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
58	32	1	Total	Zn	0	0
			1	1		
58	3E	1	Total	Zn	0	0
			1	1		
58	5I	1	Total	Zn	0	0
			1	1		
58	5A	1	Total	Zn	0	0
			1	1		
58	G8	1	Total	Zn	0	0
			1	1		
58	C5	1	Total	Zn	0	0
			1	1		

- Molecule 59 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
59	13	144	Total	O	0	0
			144	144		
59	3E	2	Total	O	0	0
			2	2		
59	1I	1	Total	O	0	0
			1	1		
59	3I	2	Total	O	0	0
			2	2		
59	5I	2	Total	O	0	0
			2	2		
59	2K	6	Total	O	0	0
			6	6		
59	4K	2	Total	O	0	0
			2	2		
59	1H	933	Total	O	0	0
			933	933		
59	16	22	Total	O	0	0
			22	22		
59	11	11	Total	O	0	0
			11	11		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
59	21	3	Total 3	O 3	0	0
59	31	9	Total 9	O 9	0	0
59	78	6	Total 6	O 6	0	0
59	D8	1	Total 1	O 1	0	0
59	F8	2	Total 2	O 2	0	0
59	G8	2	Total 2	O 2	0	0
59	I8	5	Total 5	O 5	0	0
59	J8	1	Total 1	O 1	0	0
59	L8	1	Total 1	O 1	0	0
59	P8	2	Total 2	O 2	0	0
59	Q8	1	Total 1	O 1	0	0
59	1G	48	Total 48	O 48	0	0
59	14	592	Total 592	O 592	0	0
59	19	8	Total 8	O 8	0	0
59	29	5	Total 5	O 5	0	0
59	39	4	Total 4	O 4	0	0
59	25	6	Total 6	O 6	0	0
59	35	2	Total 2	O 2	0	0
59	55	3	Total 3	O 3	0	0
59	75	1	Total 1	O 1	0	0
59	A5	1	Total 1	O 1	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
59	H5	2	Total	O	0	0
			2	2		
59	L5	1	Total	O	0	0
			1	1		
59	M5	1	Total	O	0	0
			1	1		





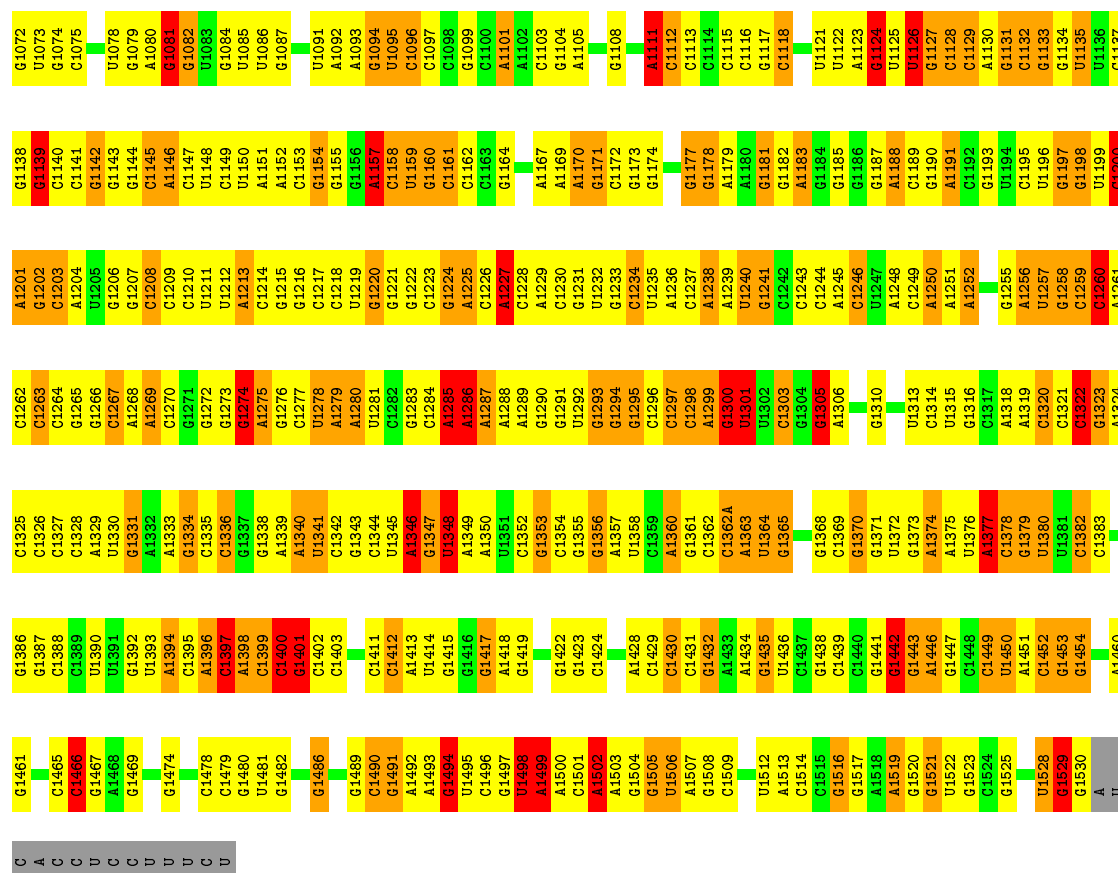




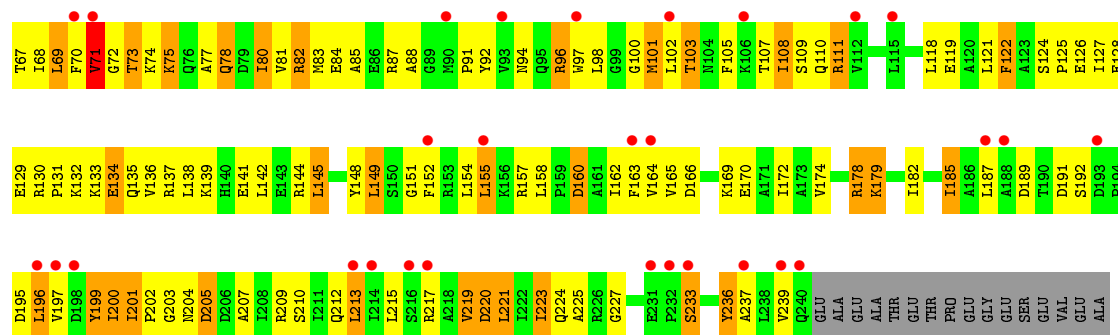


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A1015	G954	U891	A814	U743	A676	G543	A480	G406	G332	U265	G191E	C137	G66
A1016	U955	U890	A815	C744	U677	C545	G481	G407	G333	G266	G191F	G138	C67
G1017	U956	A892	A816	C745	U678	C546	A482	A408	G334	C267	G191G	G139	
C1018	U957	C893	C817	C746	U679	A547	C483	G409	C335		U192	A140	G73
G1019	A958	G894	G818	C747	G682	G548	G484	G410	C336	C271	C193	A141	G74
U1020	A959	G895	A819	C748	G683	C549	G485	A411	C337	C272	C194	G142	C75
G1023	U960	C896	U820	C749	A684	G550	U486	A412	A338	A273	A195	A143	G76
G1024	U961	C897	G821	G750	G685	U551	A487	G413	C339	G274	A196	G144	G77
G1025	C962	G898	C822	U751	U686	U552	C488	A414	U340	G275	A197	G145	G78
U1026	G963	C899	G823	G752	A687	A553	C489	A415	G341	G276	G198	G146	G79
C1027	A964	A900	C824	A753	G688	C554	G490	G416	C342	C277	G199	G147	G80
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C1028B	C967	C904	U827	C756	A621	G557			G346	A279	U208	C150	U
G1029	A968	U905	A828	G757	C623	G558	A496	U421		A282	U209	A151	U
G1030	G969	G906	G829	U758	G693	C624	A497	G423	A349	C283	U210	G154	A
C1031	C970	A907	G830		A694	G625	U497	G424	G350	G284	C217	C155	C
G1032	G971	A908	U831	G763	A695	U626	A498	G425	G351	G285	C218	G156	
G1032A	C972	A909	G832	C764	U696	G627	A499	G426	C352	G286	C219	G157	U89
G1032B	G973	C910	U833	G765	U697	G628	C501	G427	A353	U287	G220	G158	C90
G1033	A974	U911	G838	A766	G698	G629	G502	U427	G354	A288	C221	G159	C91
G1033A	C975	C912	U841	A767	C699	G630	C503	G428	G357	G289	U222	A160	G95
G1034	G976	A813	C842	A768	G700	G631	C504	U429	U359	G290	U223	A161	G96
A1035	A977	A914	U843	G769	C701	A632	G505	A430	U358	U294	C224	A162	U97
G1036	A978	A915	U844	C770	A704	G633	G506		A360		C225	C163	
C1037	C979	C916	C849	G771		G634	C507	C433	A361		C226	U164	G102
C1038	G980	G917	U851	U772	G707	G635	C508	U434	G361	A298	G227	G165	C103
G1039	U981	A918	G855	G773	C707	U636	A509	C435	G362	G299	G228	G166	G104
U1040	A982	A919	C856	G774	G708	G637	A510	C436	A363	A300	A228	G167	
A1041	U983	U920	C857	G775	G709	G638	C511	U437	G364	G301	U229	G168	G105
G1042	C984	U921	G858	G776	G710	A642	U512	G438	U365	G302	G230	G169	C106
C1043	A985	G922	U860	G777	A712	C643	C513	A439	C366	A303	G231	U170	G107
G1044	G986	C924	G861	C778	G713	G644	G515	A440	U367	U304	C232	A171	C108
C1045	G987	G925	C862	A780		C645	U516		G371	G305	C233	A172	C109
A1046	U991	G926	U863		G718	C646	G517	C444	C372	G306	C234	U173	G111
G1047	U992	G927	A864	C783	C719	U646	G518	G445	A372	C307	G235	C174	
U1048	G993		A865	C784	C720	C647	C519	G447	A373	C308	G236	C175	U114
G1050	A994		C866	G785	G721	A648	A520	G448	U375	C309	C237	C176	G115
C1051	C995	C932	G867	G786	A722	G650	G521	C449	G376	G310	C242	C177	A116
U1052	A996	G933	C868	G787	G723	C651	G522	G450	G377	G311	U244	C178	G117
G1053	U997	A935	G869	U788	G724	U652	A523	A451	A382	G312	C245	A179	U118
C1054	G998	C936	U870	U789	G725	A653		A452	A383	G314	G246	U180	C121
A1055	C998A	A937	U871	A790	C726	G658	C526	A453	A384	A315	A246	G181	G122
U1056	U999	A938	A872	G791	G727	G659	G527	C454	G384	G316	G247	U182	G123
G1057	A1000	G939	A873	A792	A728	U659	C528	C455	C385	G317	C250	G186	G124
C1058	G1001	C940	G874	U793	A729	G660	U591	C456	C386	G318	G251		U125
U1059	G1002	G941	C875	A794	G730	G661	G592	C457	U387	G319	G252	G187	G125
	G1003	G942	C876		G731	G664	G593	C458	G388	C320	G253	U188	A130
	U1004	U943	G877	C797	C732	A665	A532	G464	A389	A321	G254	U189	C131
C1063	A1005	G944	G878		A733	A666	A533	A465	C390	G322	G255	G190	G126
G1064	C1006	G945	C879	U801	G734	G667	U534	C466	C391	U323	G256	G191A	G127
U1065	C1007	A946	C880	A802	C735	G667	A535	G467	G392	G324	U257	G191B	G128
C1066	G1008	G947	G881	G803	C736	G668	A536	A468	A393	A325	G258		U129
A1067	G1009	C948	C882	U804	A737	U669	C800	G474	G396	G326	G259		A130
G1068	G1010	U949	U884	C805	C738	G670	A601	G475	G397	A327	G260		C132
	U1011	U950	U885		C739	G671	A602	G476	C398	C328	U261		U133
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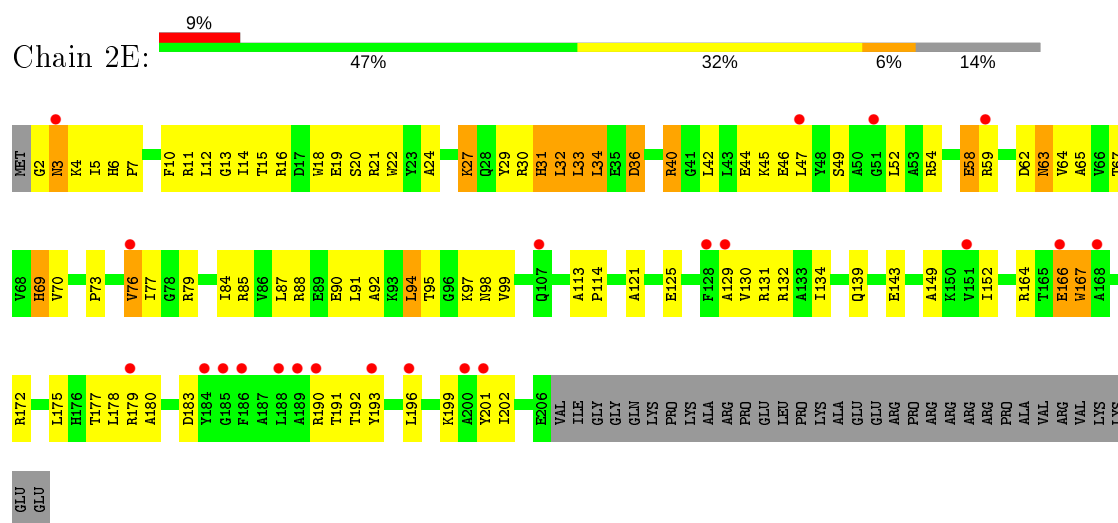




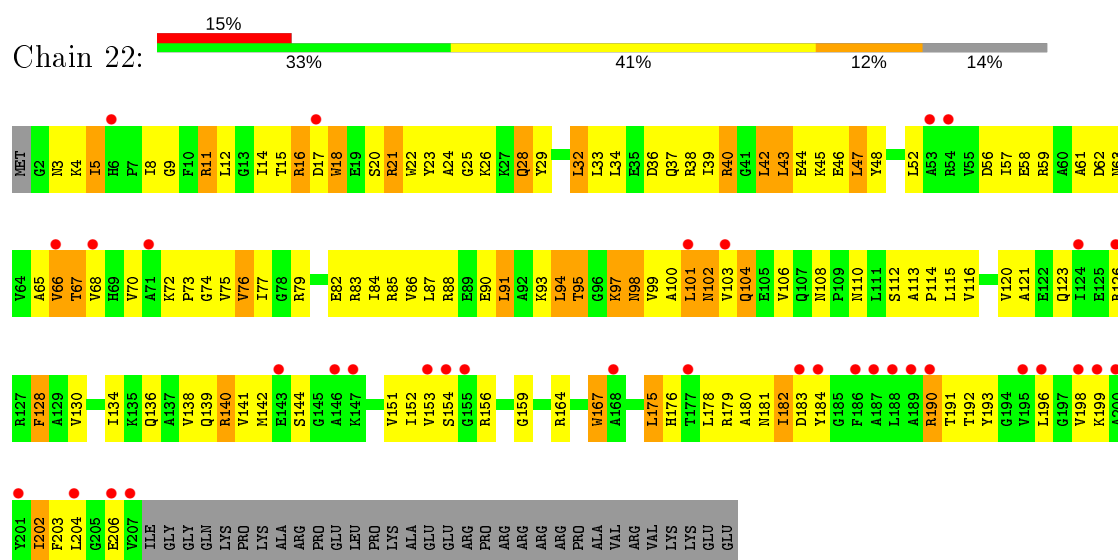




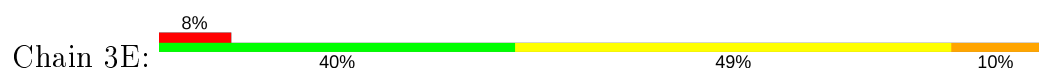
• Molecule 3: 30S ribosomal protein S3



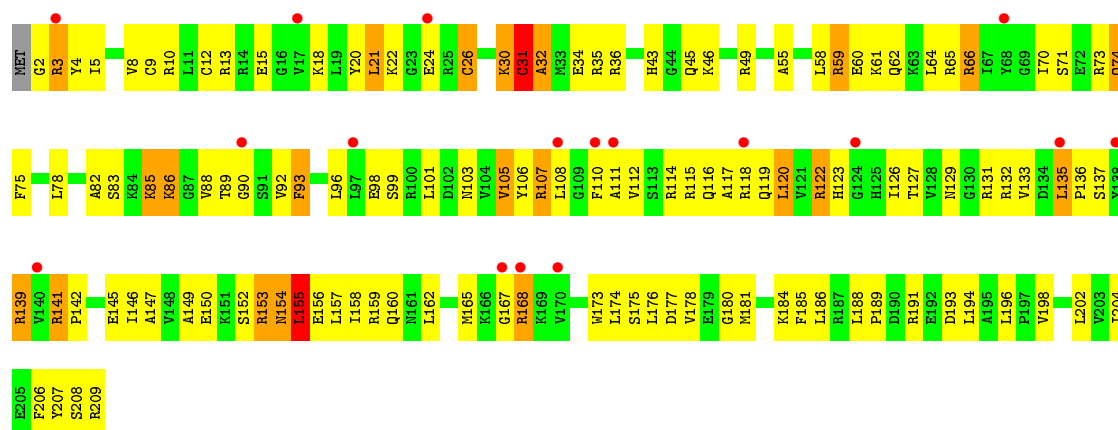
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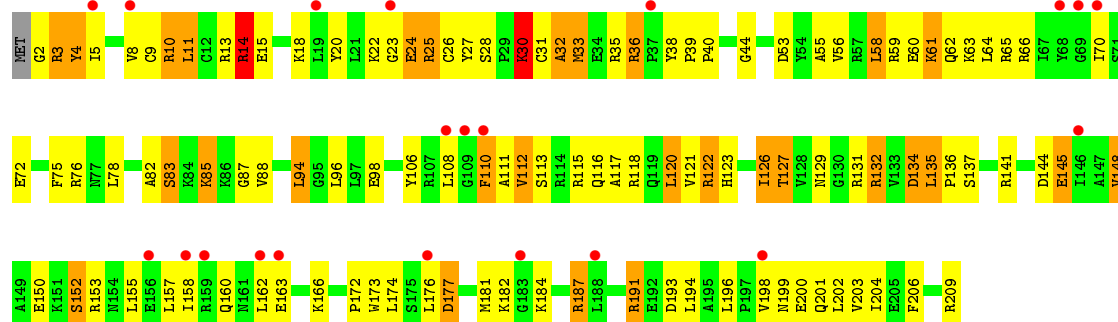
• Molecule 4: 30S ribosomal protein S4



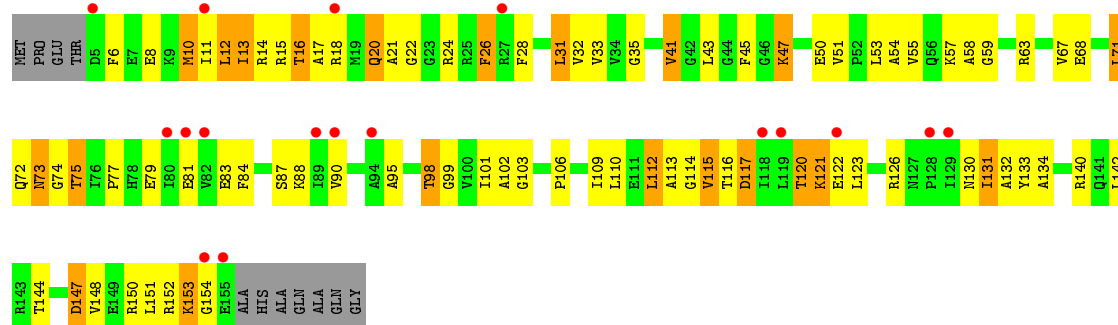




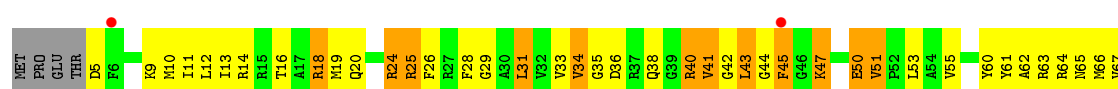
• Molecule 4: 30S ribosomal protein S4



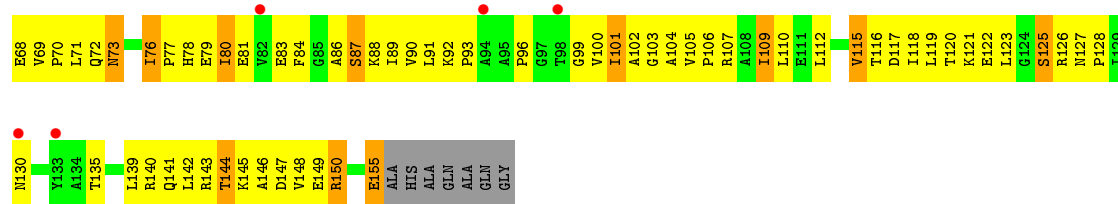
• Molecule 5: 30S ribosomal protein S5



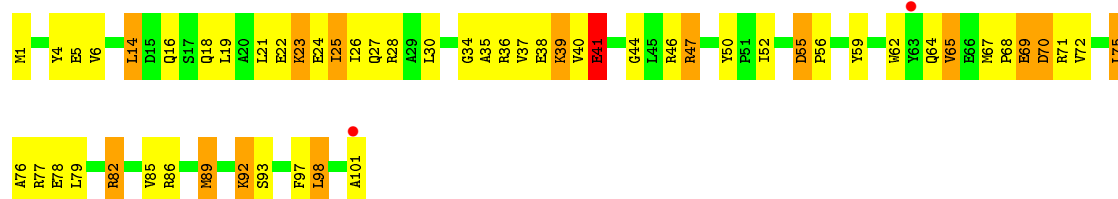
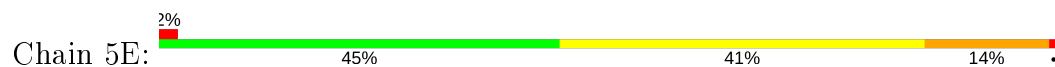
• Molecule 5: 30S ribosomal protein S5



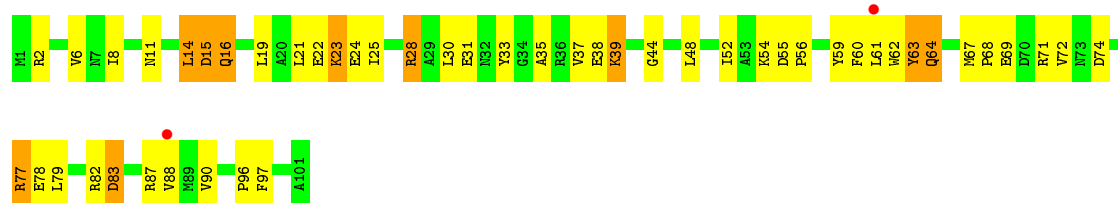




• Molecule 6: 30S ribosomal protein S6



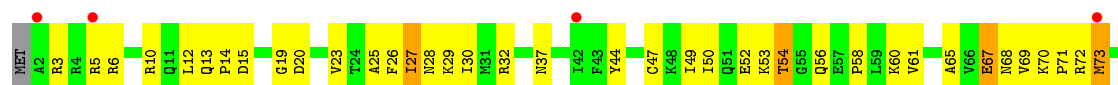
• Molecule 6: 30S ribosomal protein S6



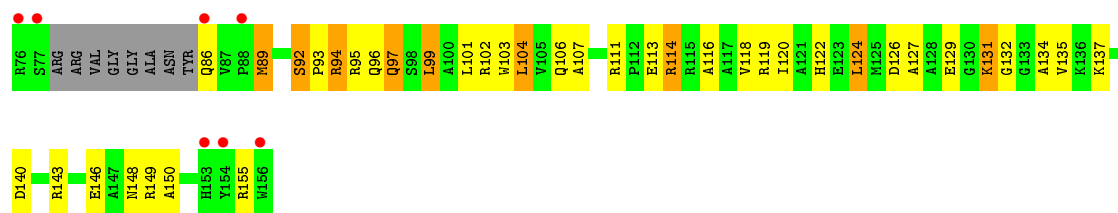
• Molecule 7: 30S ribosomal protein S7



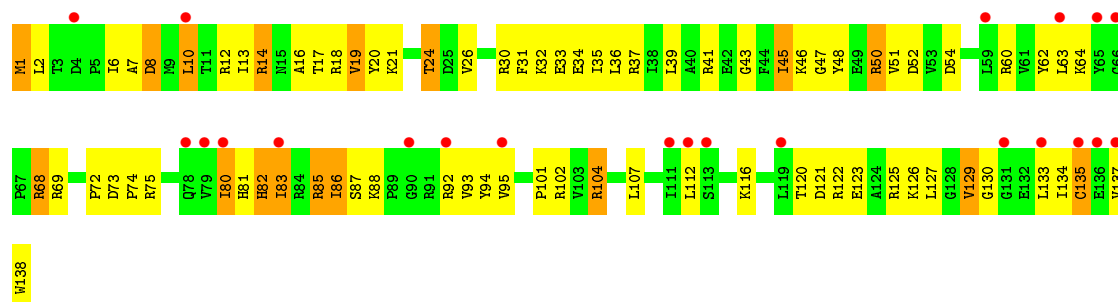
• Molecule 7: 30S ribosomal protein S7



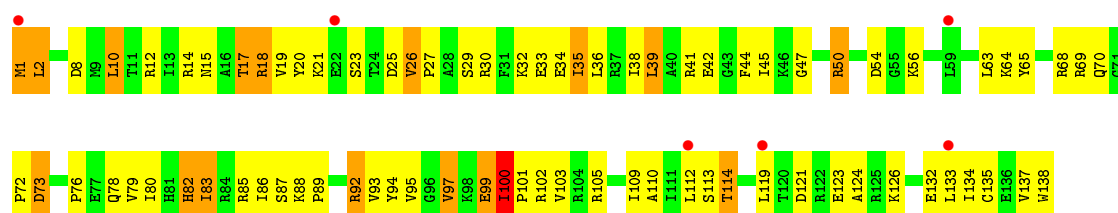




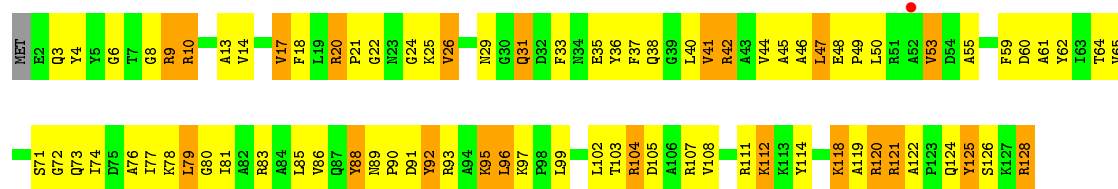
• Molecule 8: 30S ribosomal protein S8



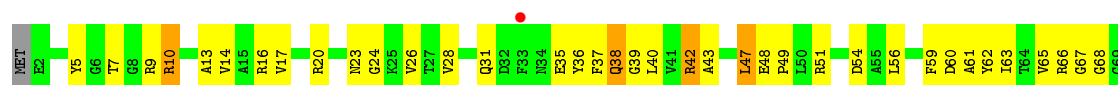
• Molecule 8: 30S ribosomal protein S8



• Molecule 9: 30S ribosomal protein S9



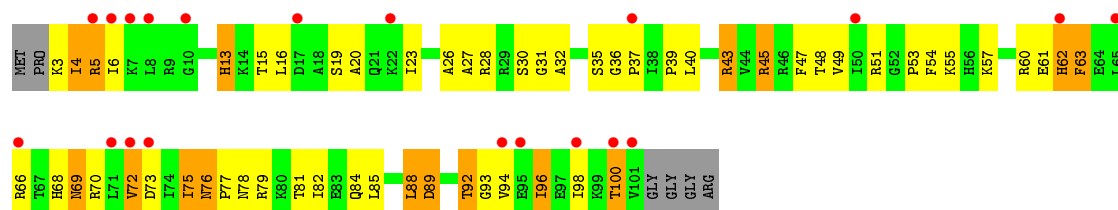
• Molecule 9: 30S ribosomal protein S9



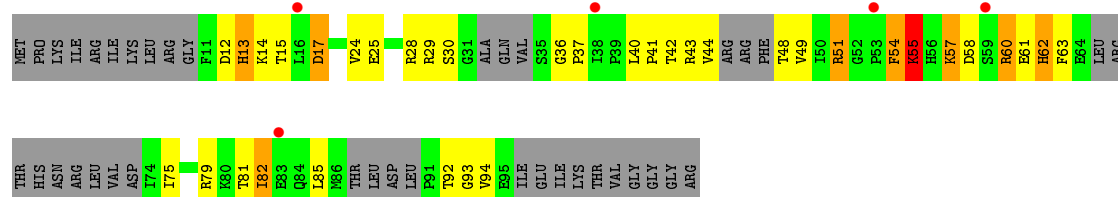
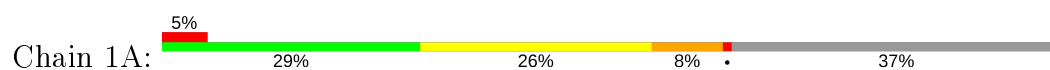




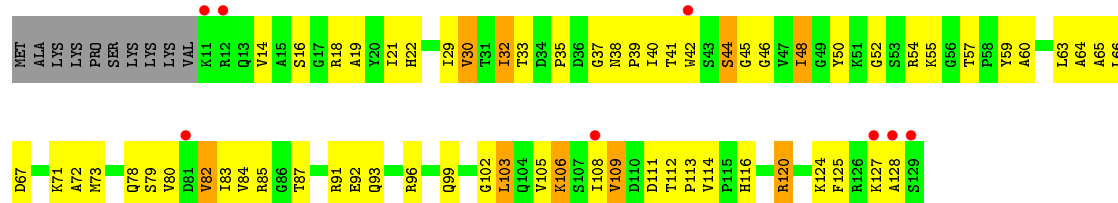
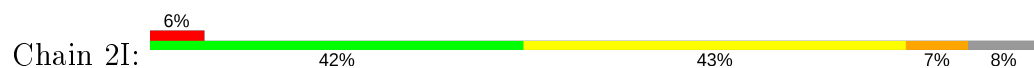
• Molecule 10: 30S ribosomal protein S10



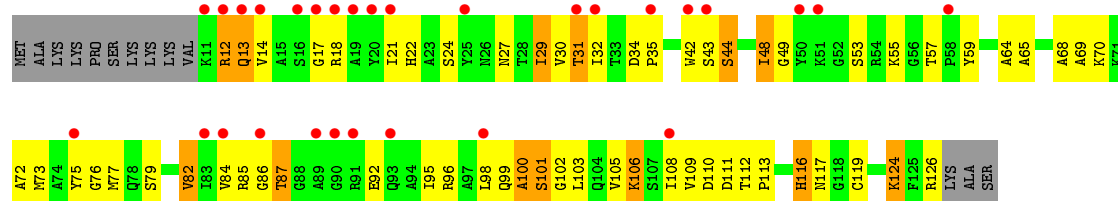
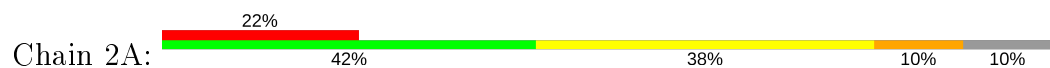
• Molecule 10: 30S ribosomal protein S10



• Molecule 11: 30S ribosomal protein S11



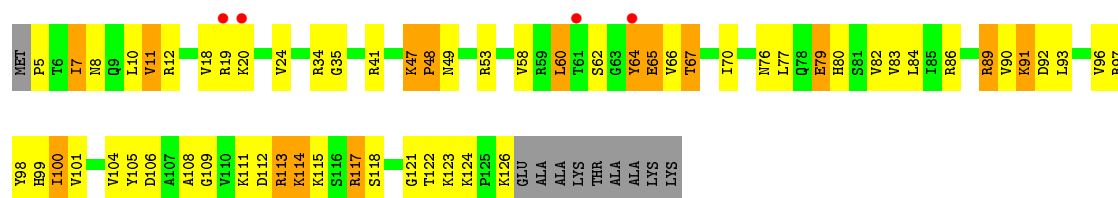
• Molecule 11: 30S ribosomal protein S11



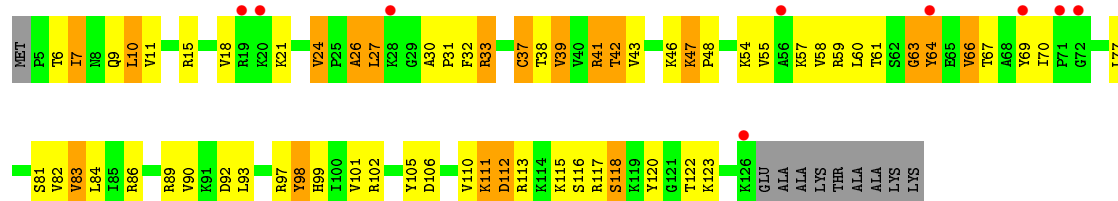
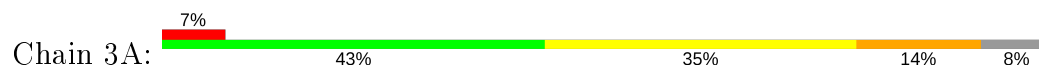
• Molecule 12: 30S ribosomal protein S12



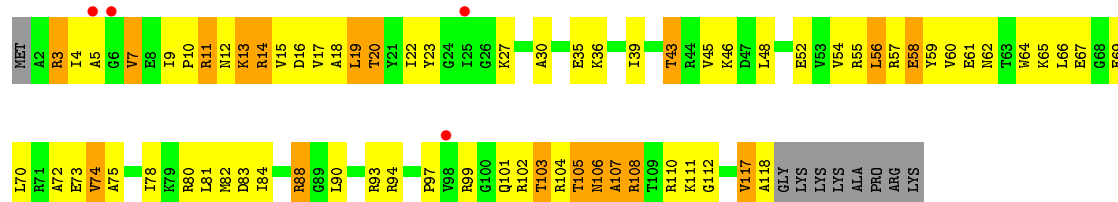




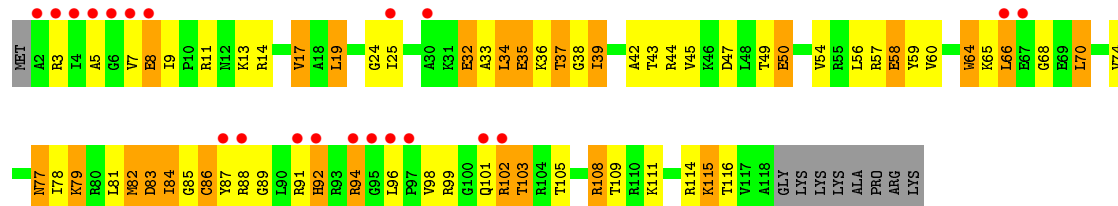
- Molecule 12: 30S ribosomal protein S12



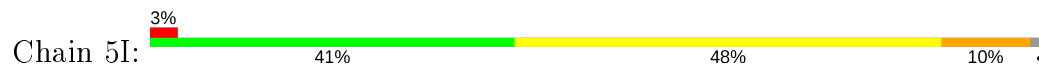
- Molecule 13: 30S ribosomal protein S13



- Molecule 13: 30S ribosomal protein S13



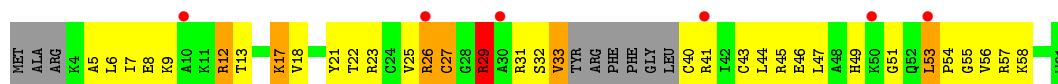
- Molecule 14: 30S ribosomal protein S14 type Z



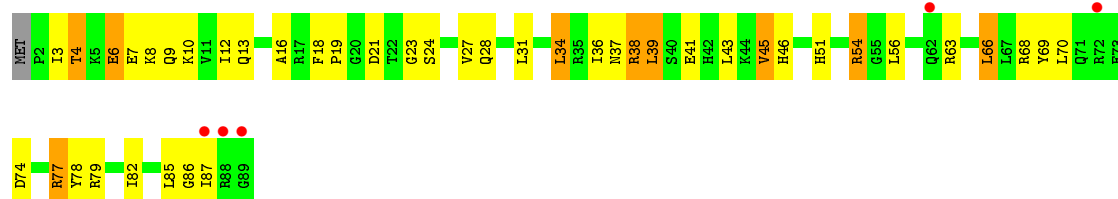
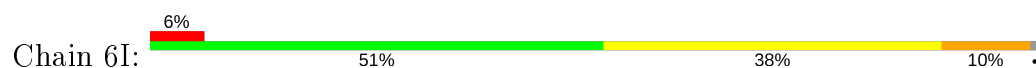
- Molecule 14: 30S ribosomal protein S14 type Z



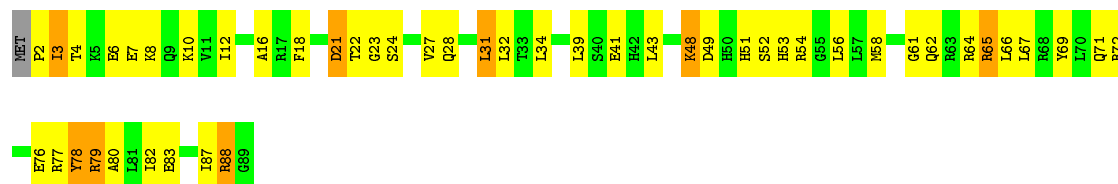




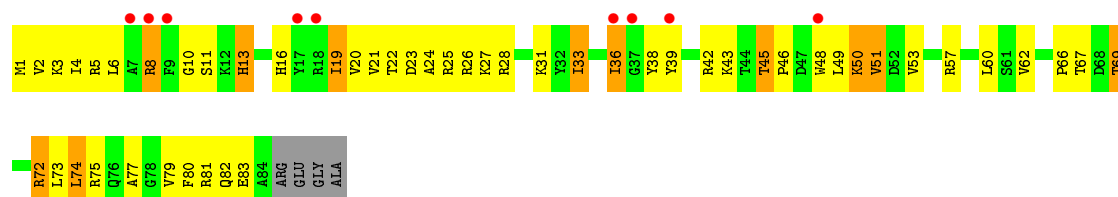
- Molecule 15: 30S ribosomal protein S15



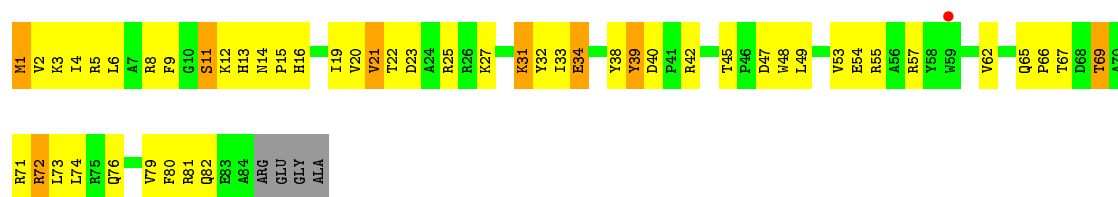
- Molecule 15: 30S ribosomal protein S15



- Molecule 16: 30S ribosomal protein S16



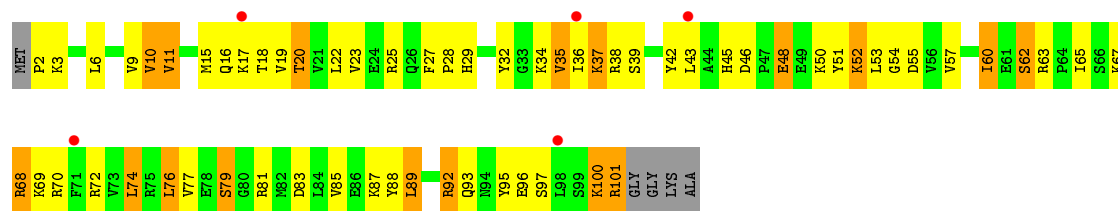
- Molecule 16: 30S ribosomal protein S16



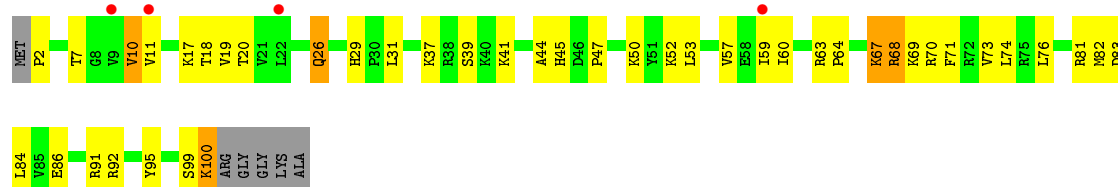
- Molecule 17: 30S ribosomal protein S17



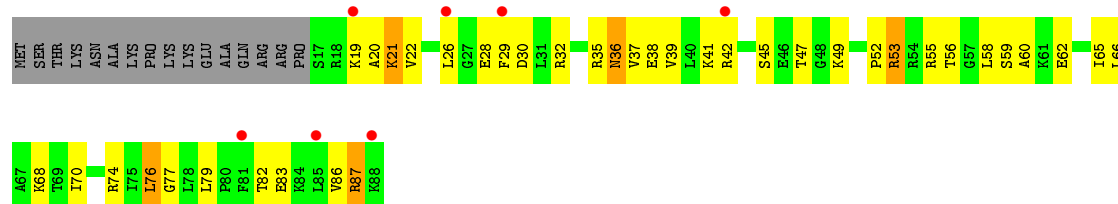




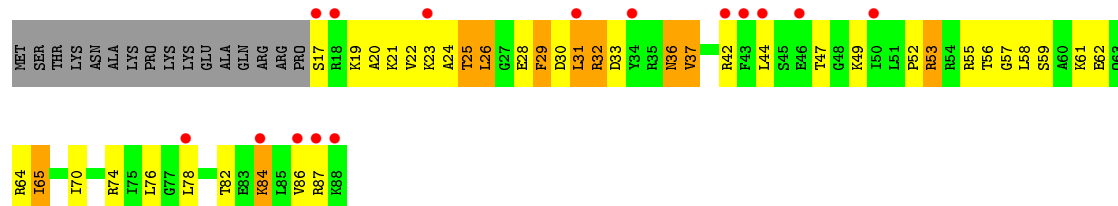
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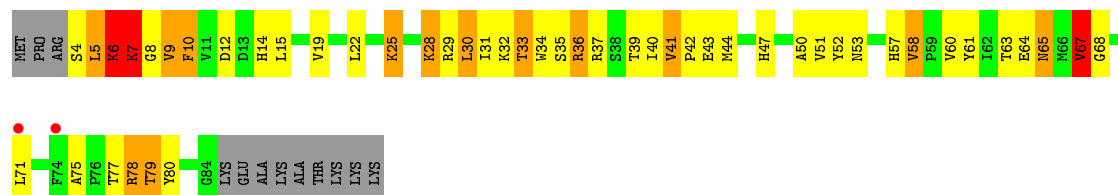
• Molecule 18: 30S ribosomal protein S18



• Molecule 18: 30S ribosomal protein S18

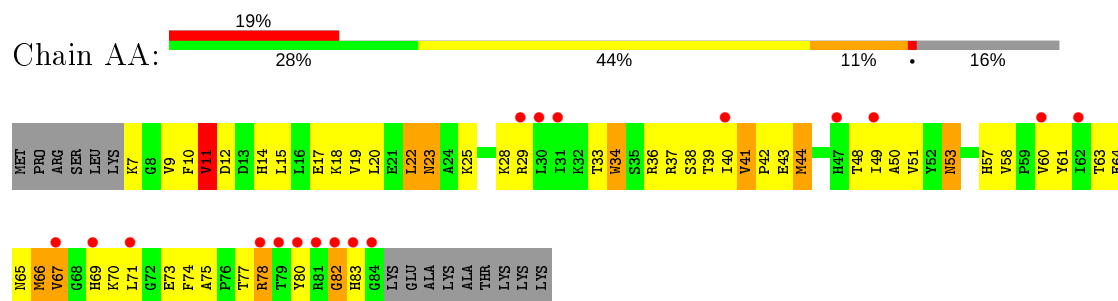


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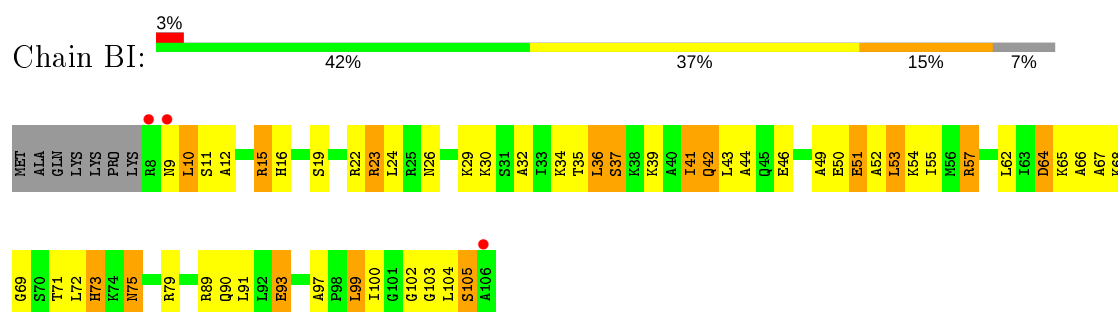




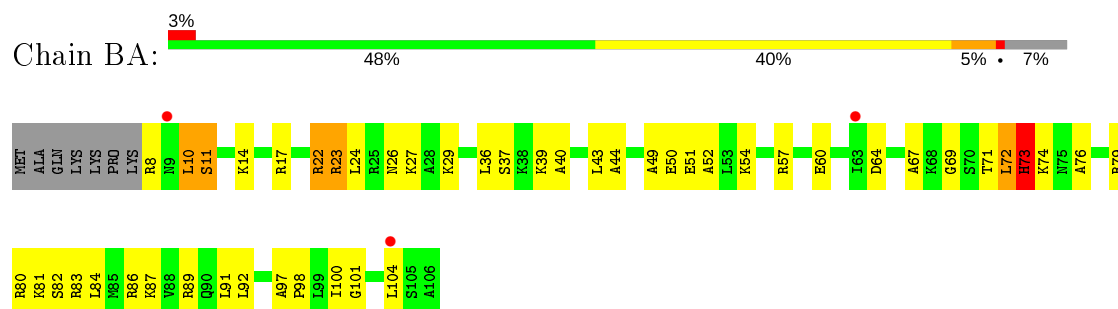
- Molecule 19: 30S ribosomal protein S19



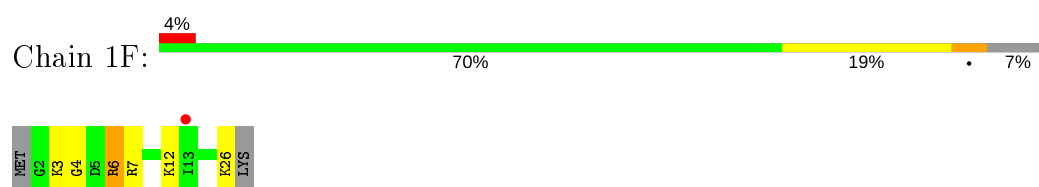
- Molecule 20: 30S ribosomal protein S20



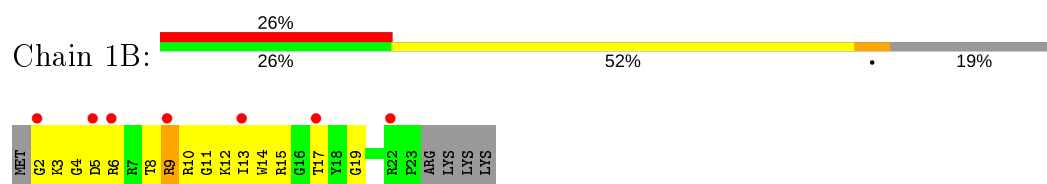
- Molecule 20: 30S ribosomal protein S20



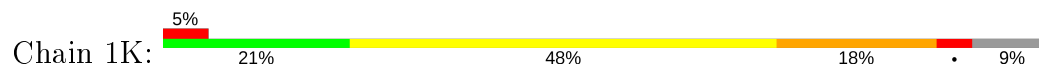
- Molecule 21: 30S ribosomal protein Thx



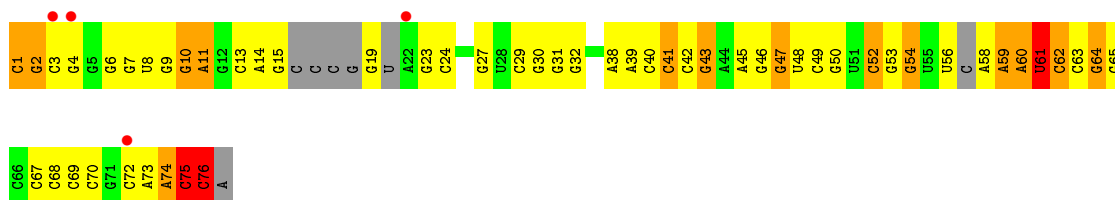
- Molecule 21: 30S ribosomal protein Thx



- Molecule 22: tRNA-fMet

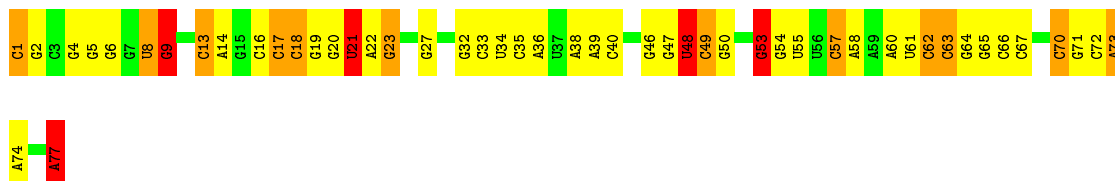






- Molecule 23: tRNA-fMet

Chain 2K:



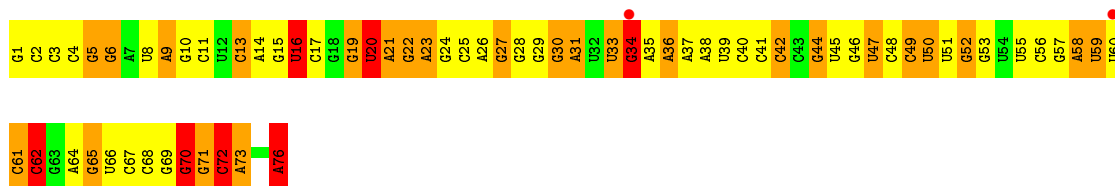
- Molecule 24: tRNA-Phe

Chain 3K:



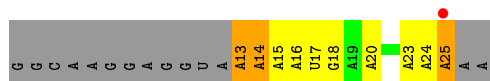
- Molecule 24: tRNA-Phe

Chain 3L:



- Molecule 25: mRNA

Chain 4K:



- Molecule 25: mRNA

Chain 4L:





Chain 1H: 



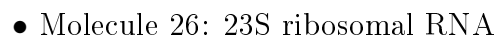


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G1453	A																						













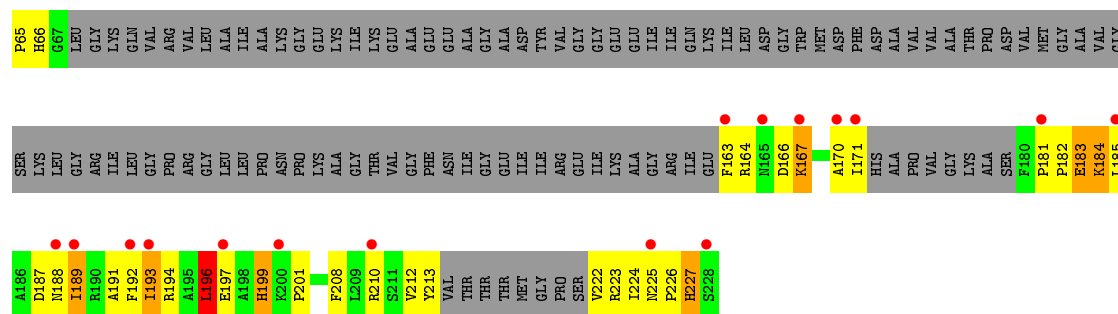


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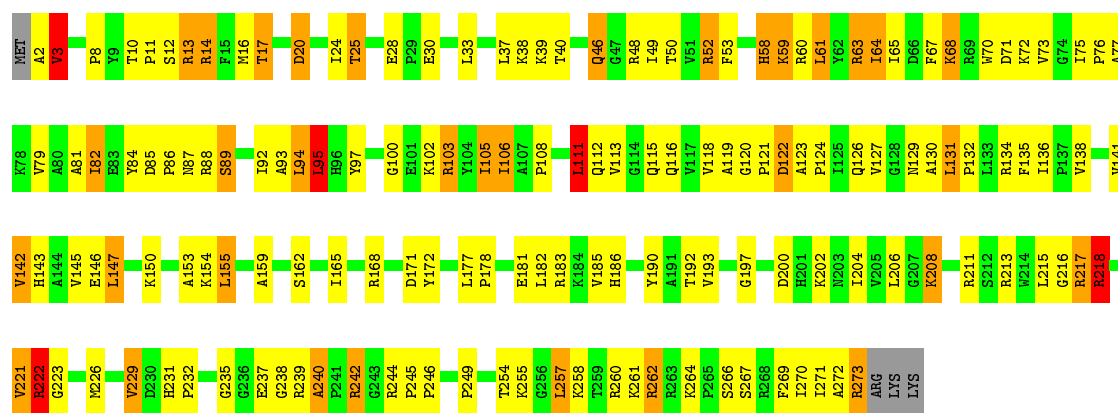






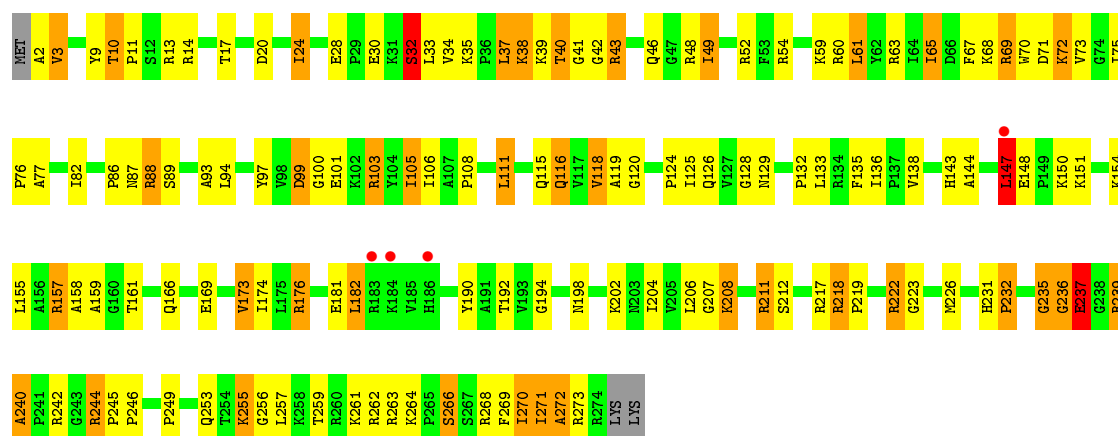
• Molecule 29: 50S ribosomal protein L2

Chain 11: 43% 42% 12% ..



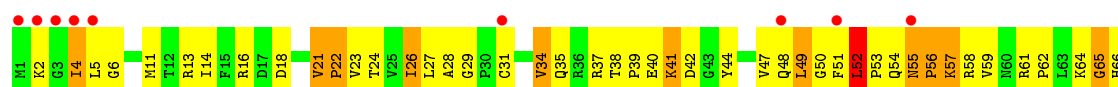
• Molecule 29: 50S ribosomal protein L2

Chain 19: 49% 35% 14% ..

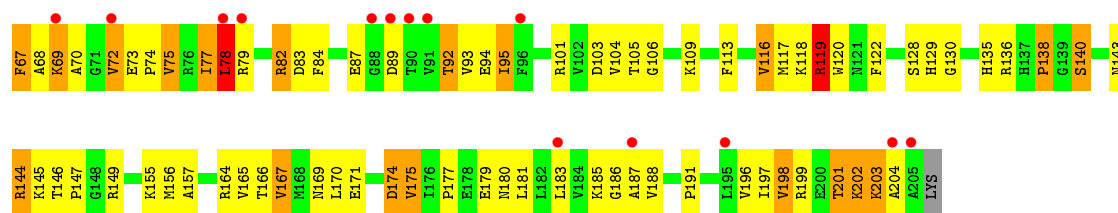


• Molecule 30: 50S ribosomal protein L3

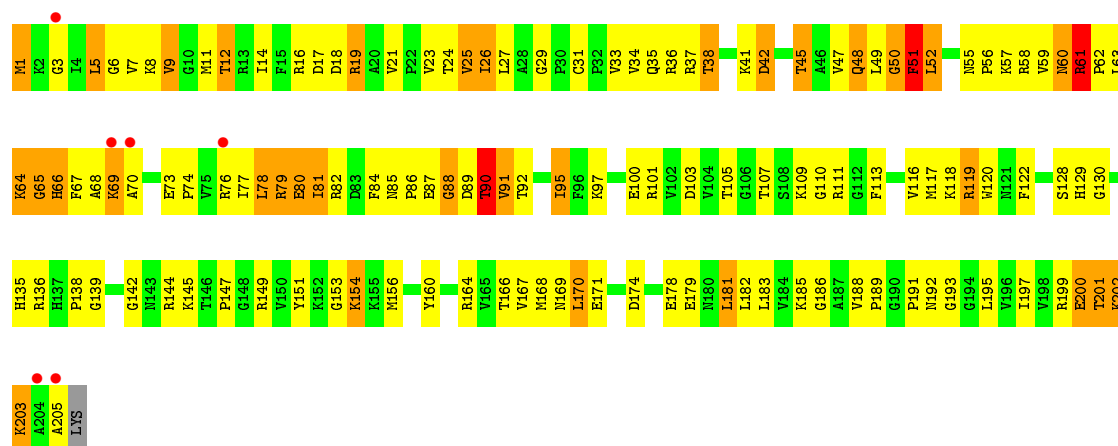
Chain 21: 11% 41% 43% 15% .



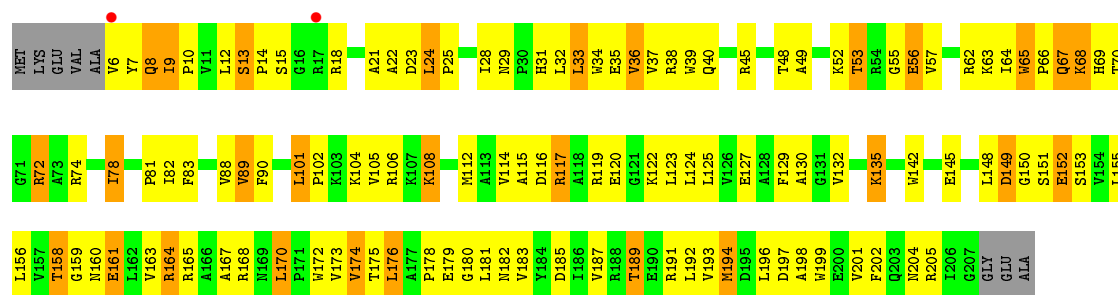




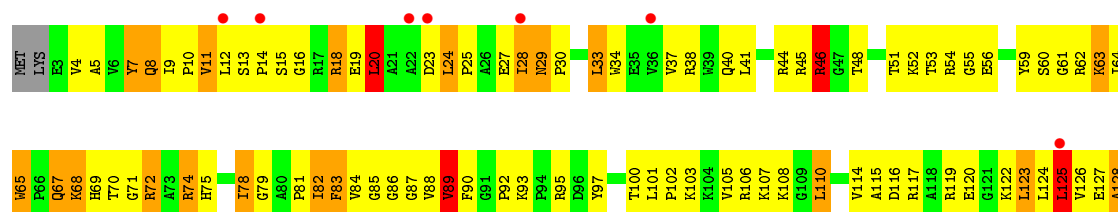
• Molecule 30: 50S ribosomal protein L3



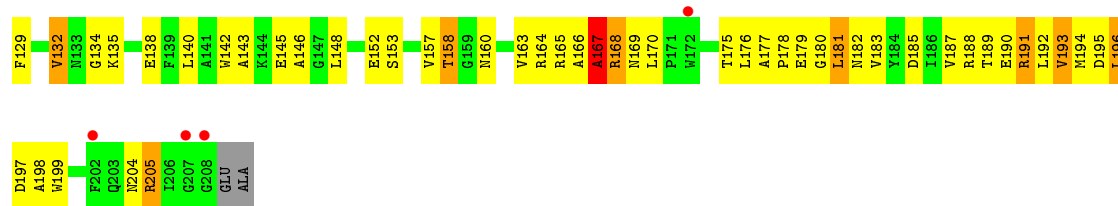
• Molecule 31: 50S ribosomal protein L4



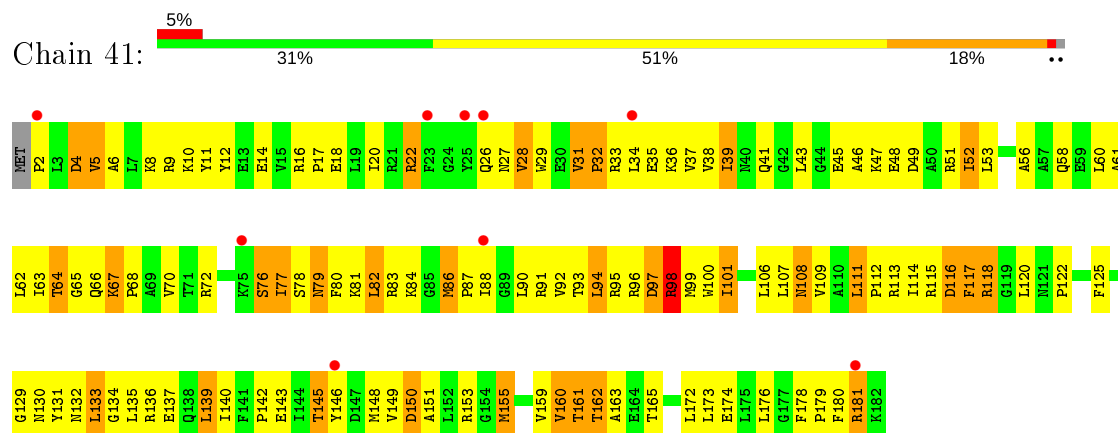
• Molecule 31: 50S ribosomal protein L4



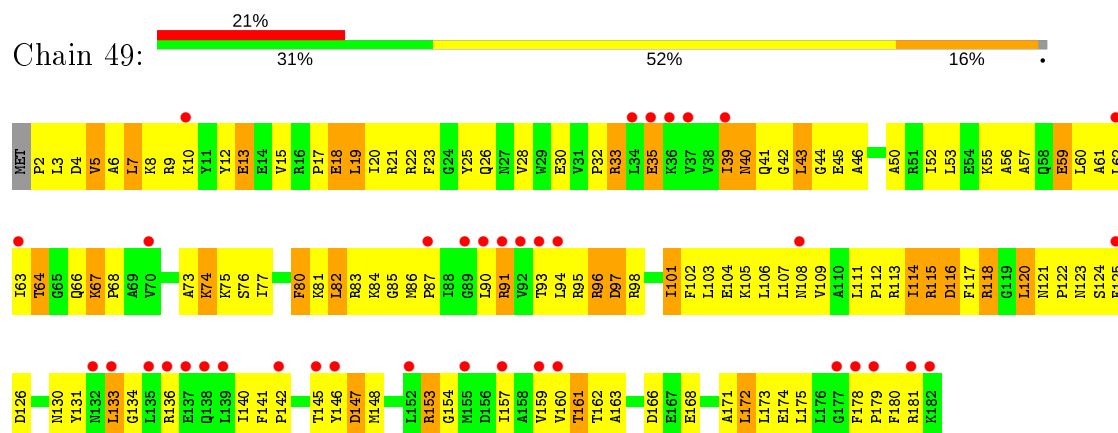




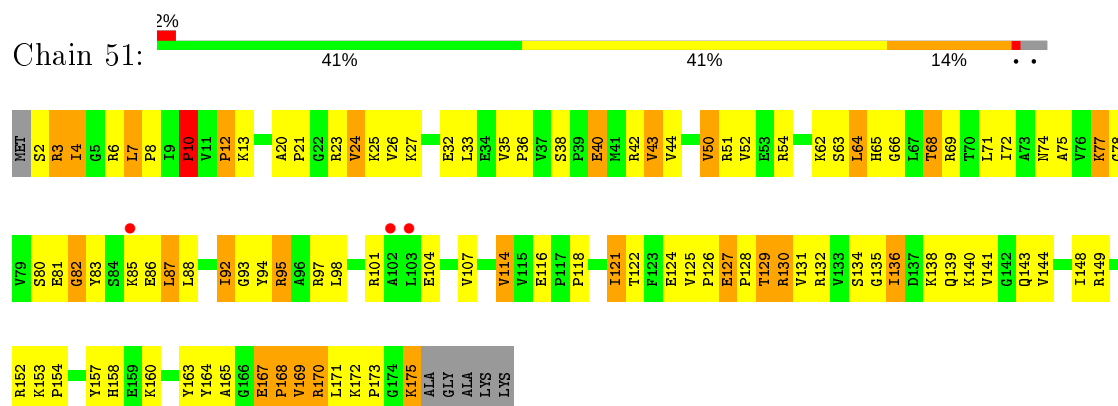
• Molecule 32: 50S ribosomal protein L5



• Molecule 32: 50S ribosomal protein L5

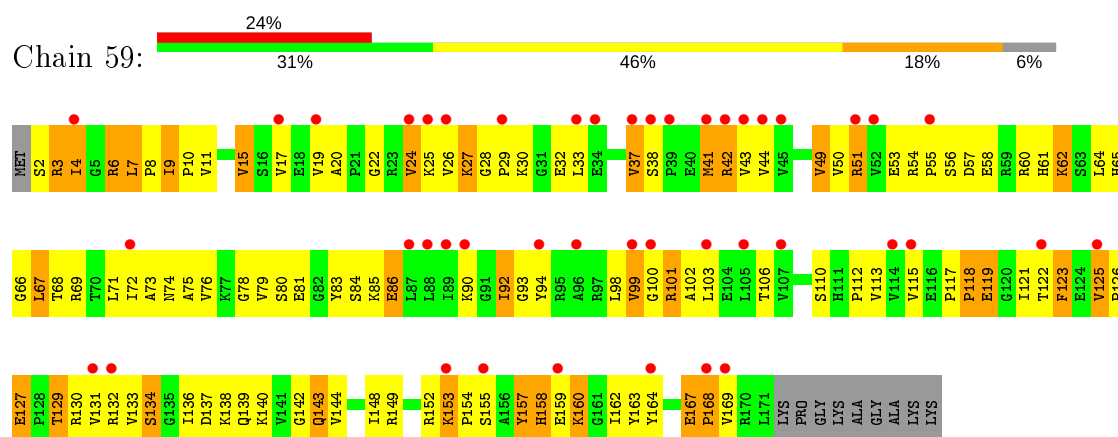


• Molecule 33: 50S ribosomal protein L6

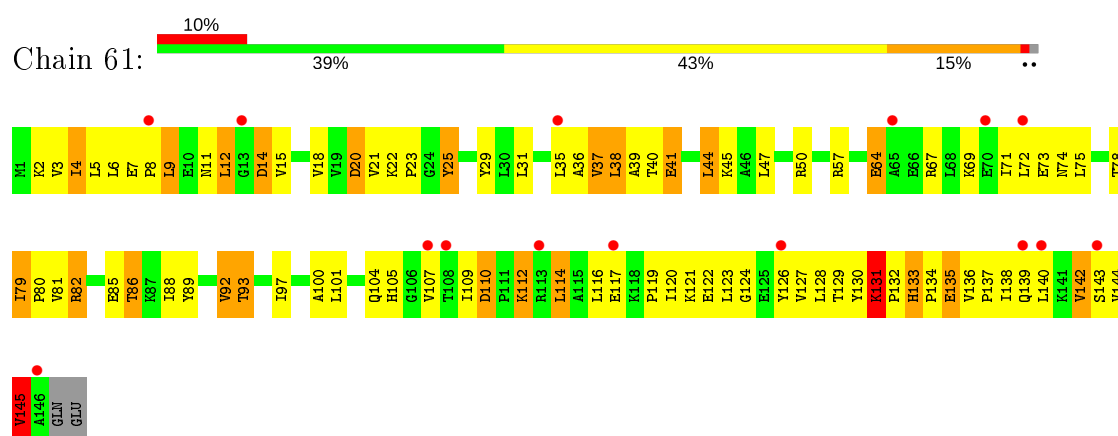


• Molecule 33: 50S ribosomal protein L6

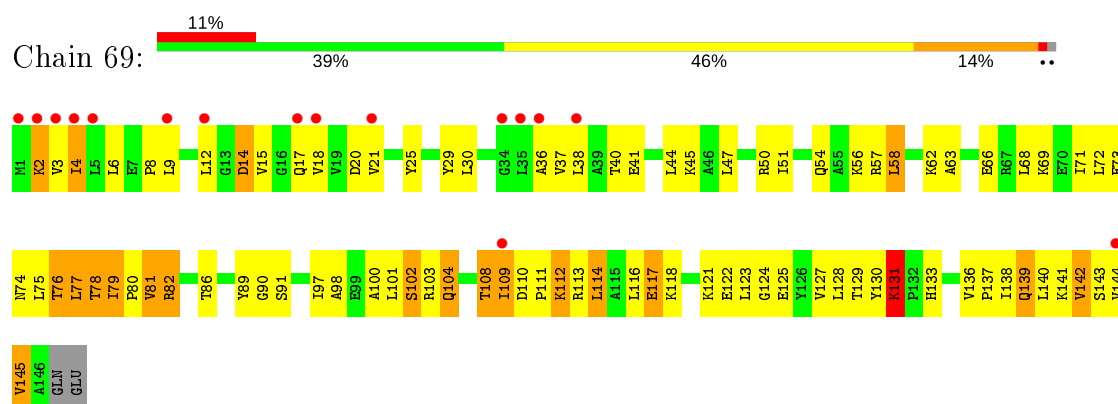




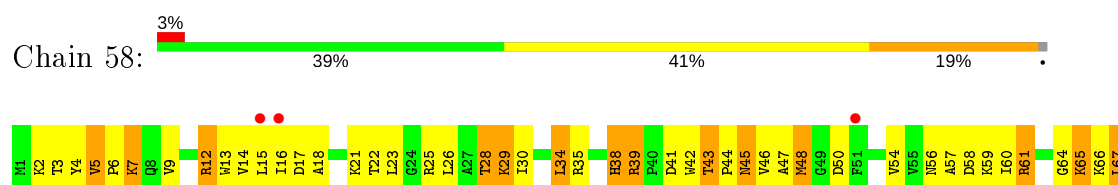
• Molecule 34: 50S ribosomal protein L9



• Molecule 34: 50S ribosomal protein L9



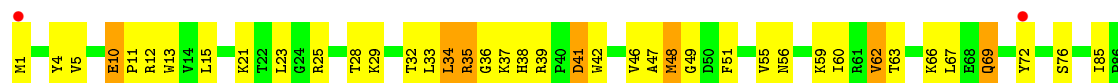
• Molecule 35: 50S ribosomal protein L13



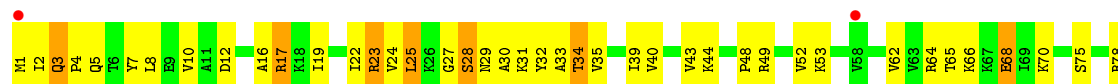




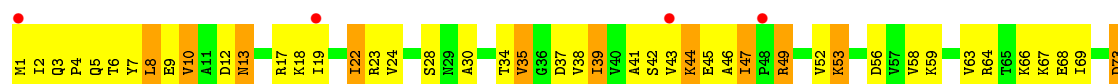
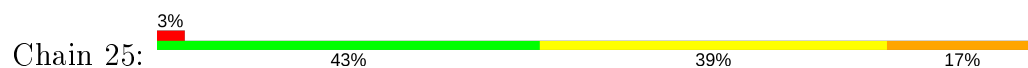
- Molecule 35: 50S ribosomal protein L13



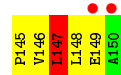
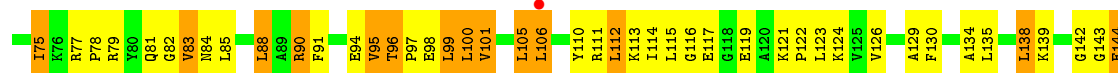
- Molecule 36: 50S ribosomal protein L14



- Molecule 36: 50S ribosomal protein L14

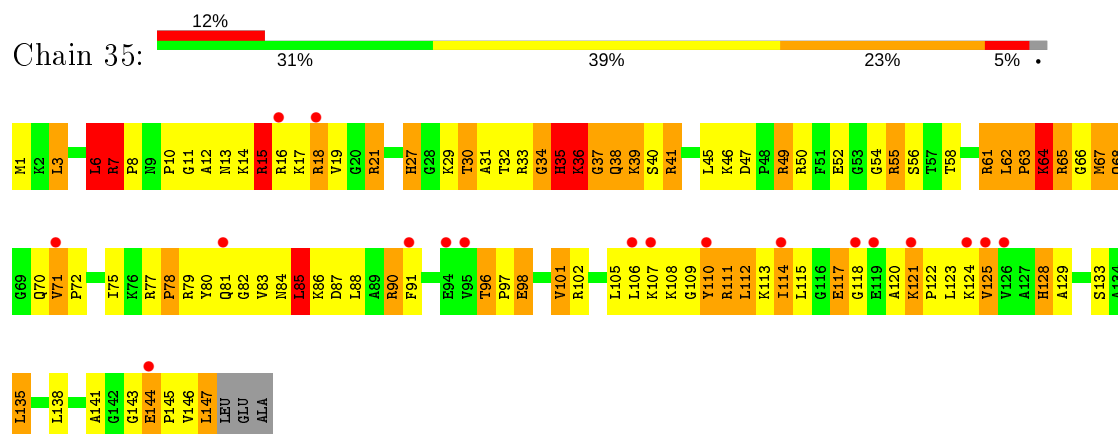


- Molecule 37: 50S ribosomal protein L15

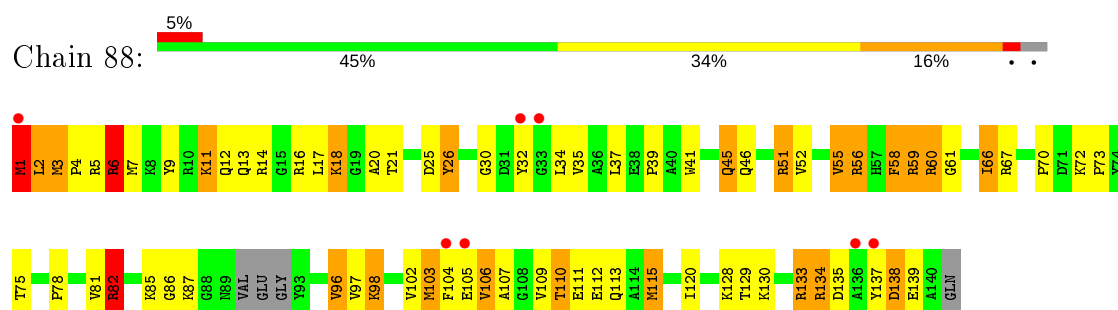




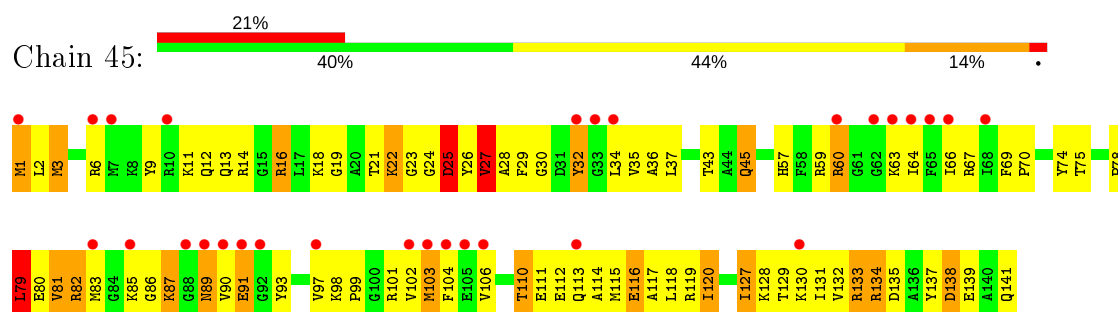
- Molecule 37: 50S ribosomal protein L15



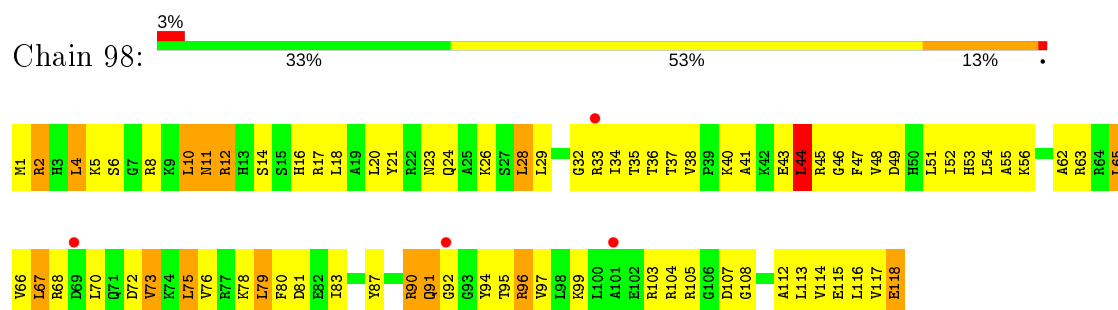
- Molecule 38: 50S ribosomal protein L16



- Molecule 38: 50S ribosomal protein L16



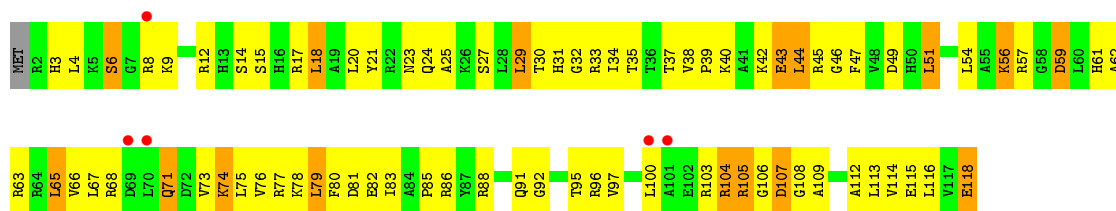
- Molecule 39: 50S ribosomal protein L17



- Molecule 39: 50S ribosomal protein L17

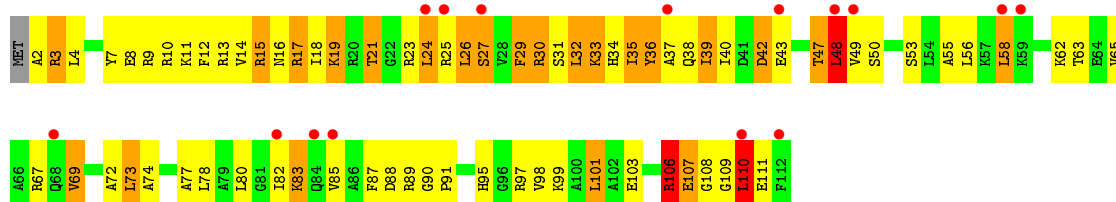






• Molecule 40: 50S ribosomal protein L18

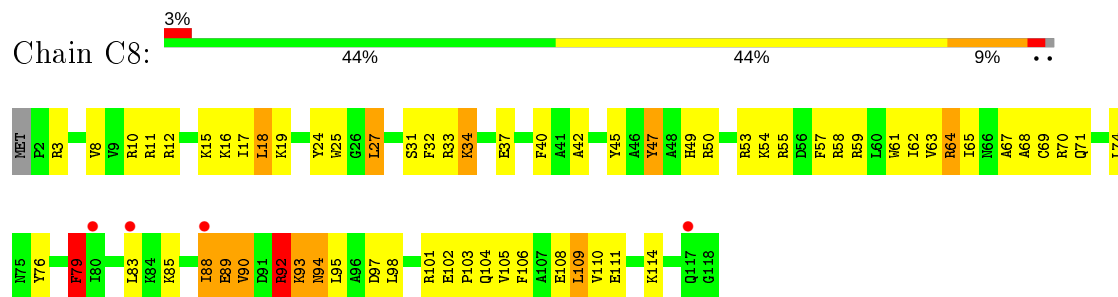
Chain A8: ..



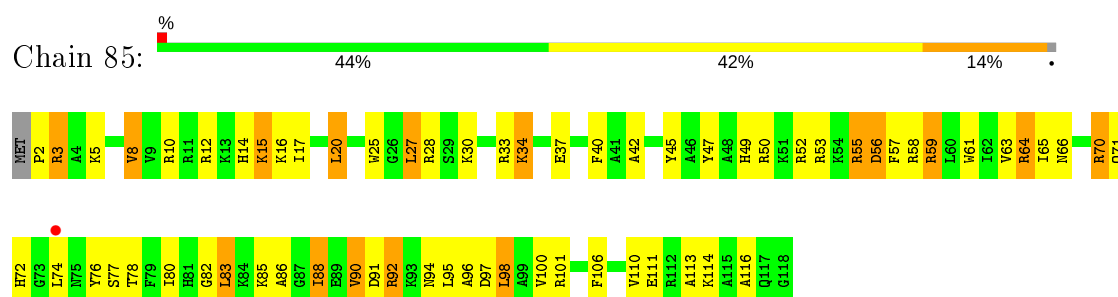


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PRO  
LYS  
ALA  
SER  
GLN  
GLU

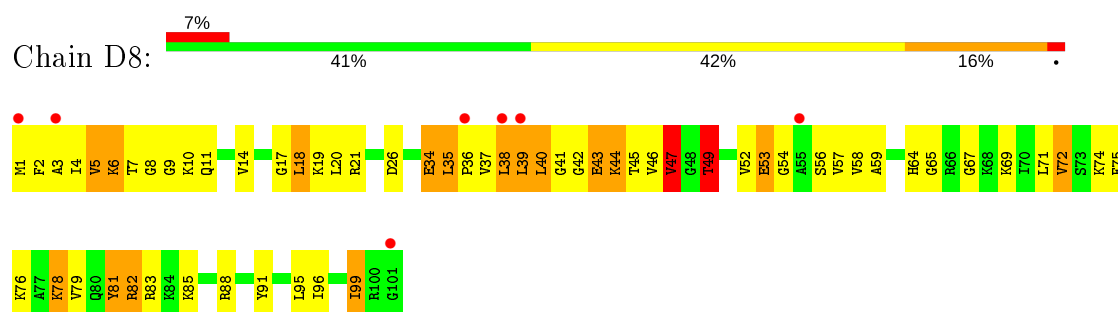
• Molecule 42: 50S ribosomal protein L20



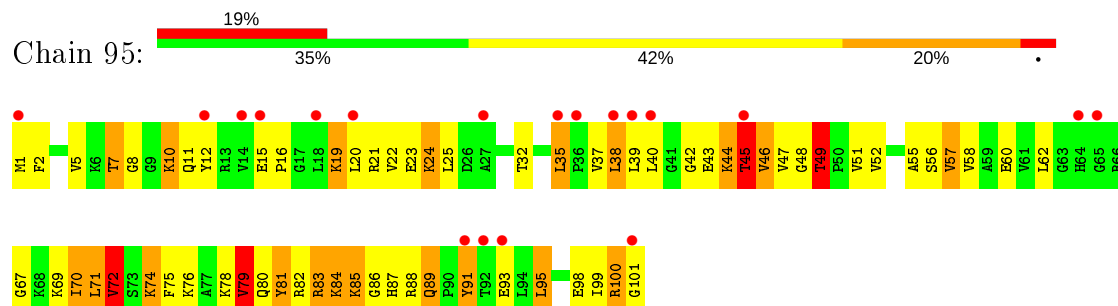
• Molecule 42: 50S ribosomal protein L20



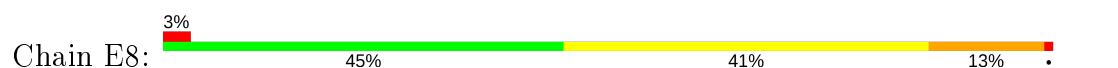
• Molecule 43: 50S ribosomal protein L21



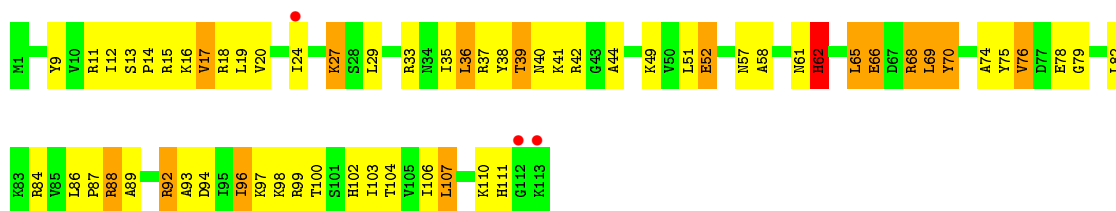
• Molecule 43: 50S ribosomal protein L21



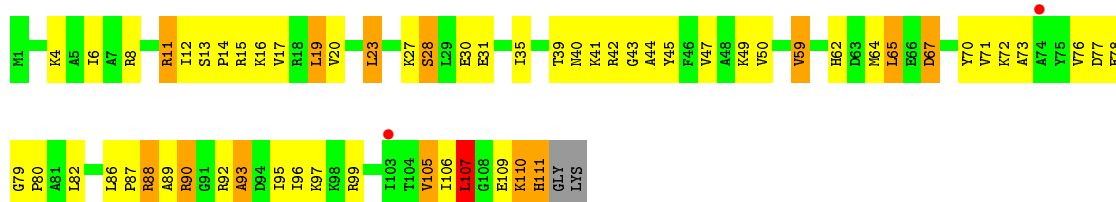
• Molecule 44: 50S ribosomal protein L22







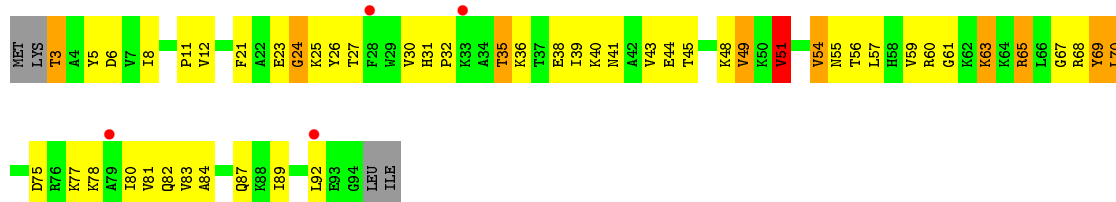
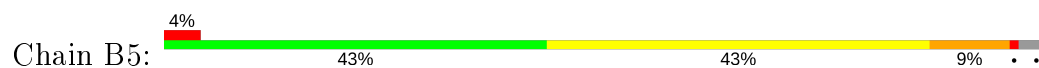
- Molecule 44: 50S ribosomal protein L22



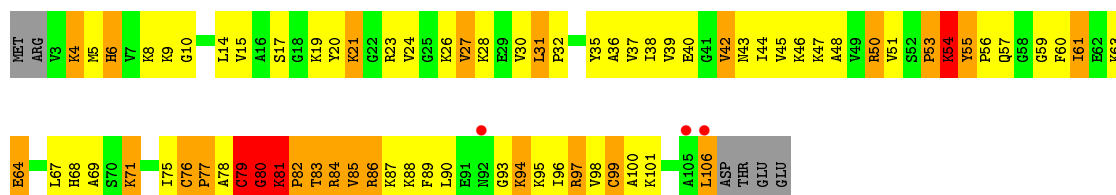
- Molecule 45: 50S ribosomal protein L23



- Molecule 45: 50S ribosomal protein L23

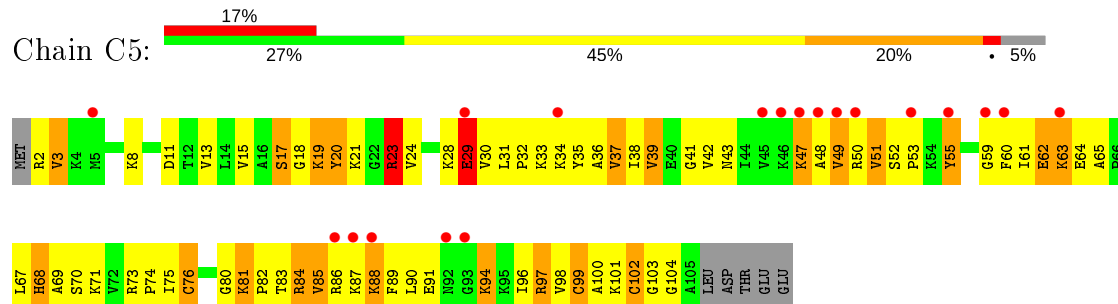


- Molecule 46: 50S ribosomal protein L24

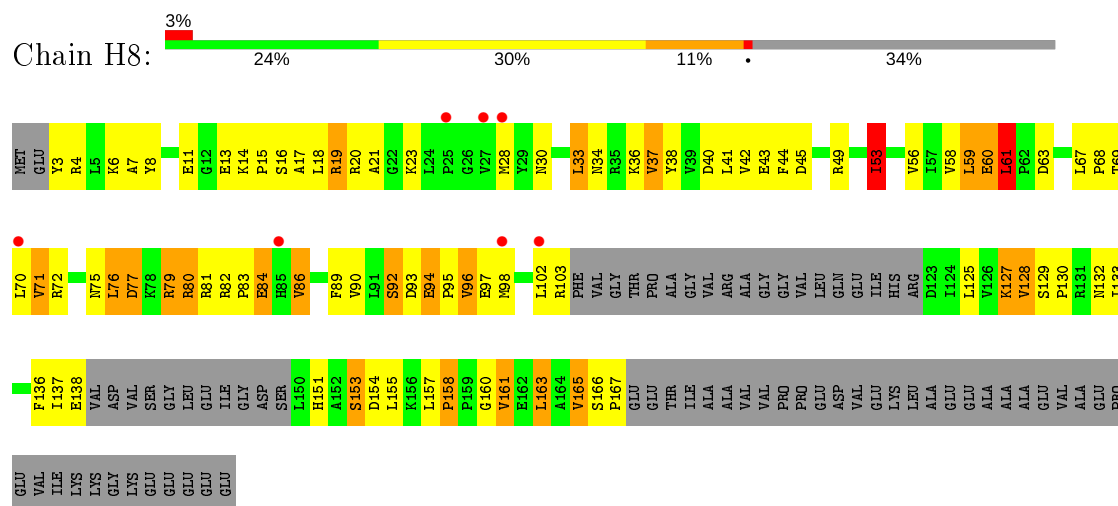




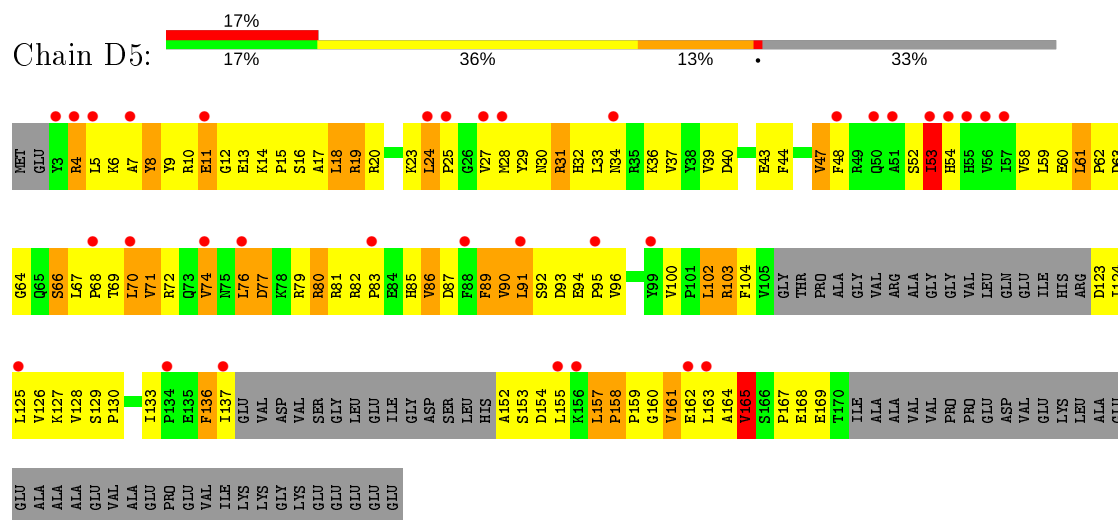
- Molecule 46: 50S ribosomal protein L24



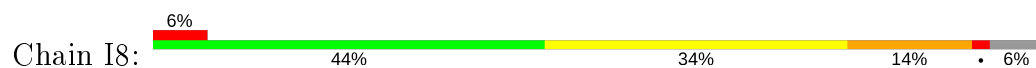
- Molecule 47: 50S ribosomal protein L25



- Molecule 47: 50S ribosomal protein L25

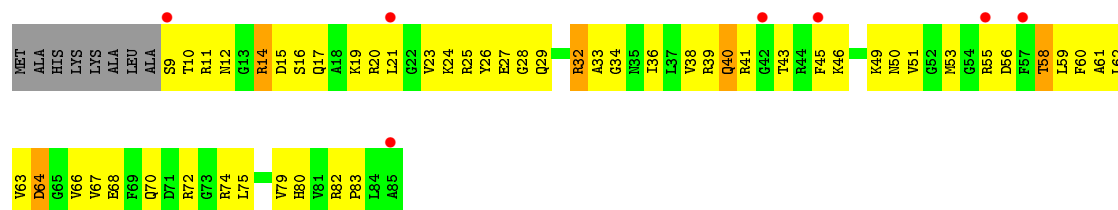


- Molecule 48: 50S ribosomal protein L27

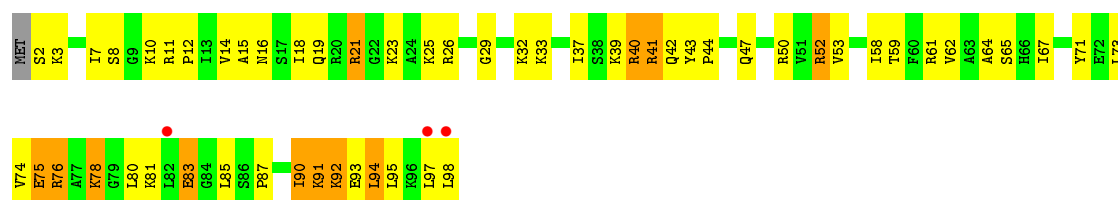
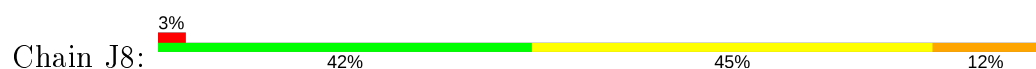




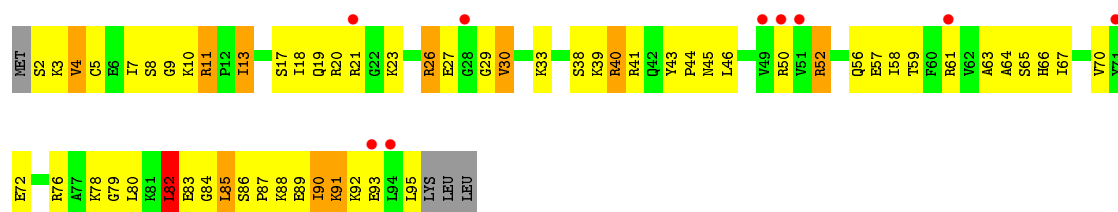
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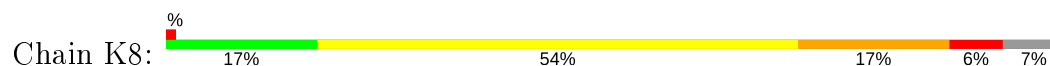
- Molecule 49: 50S ribosomal protein L28



- Molecule 49: 50S ribosomal protein L28



- Molecule 50: 50S ribosomal protein L29

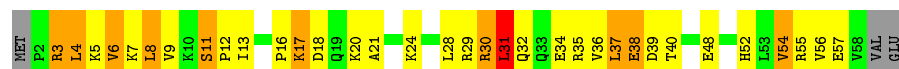


- Molecule 50: 50S ribosomal protein L29

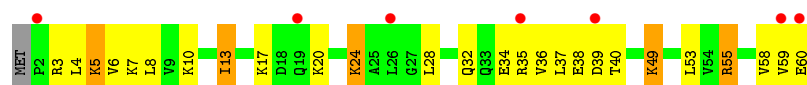




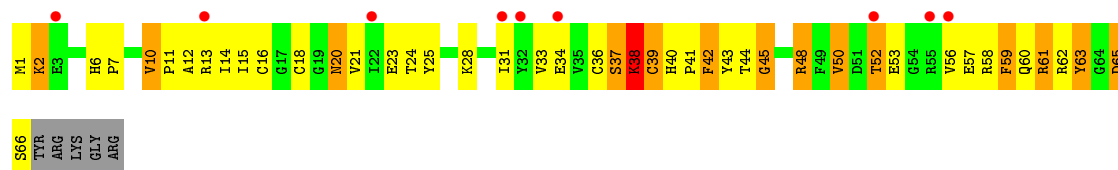
- Molecule 51: 50S ribosomal protein L30



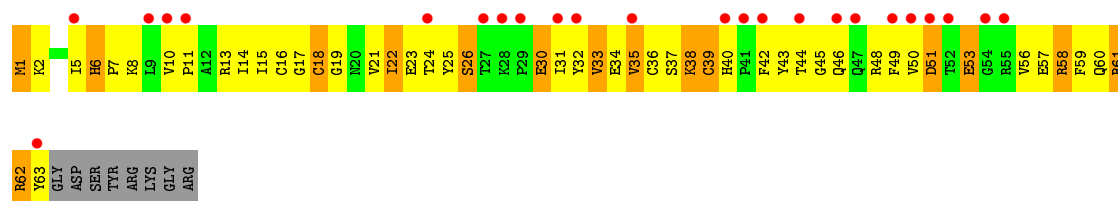
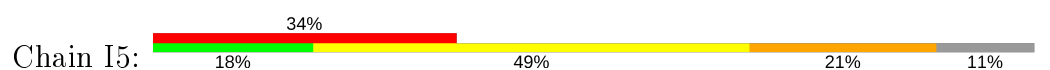
- Molecule 51: 50S ribosomal protein L30



- Molecule 52: 50S ribosomal protein L31



- Molecule 52: 50S ribosomal protein L31

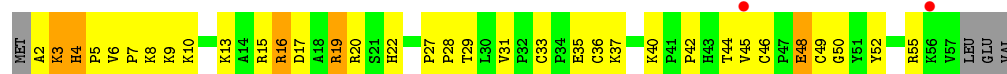


- Molecule 53: 50S ribosomal protein L32



- Molecule 53: 50S ribosomal protein L32

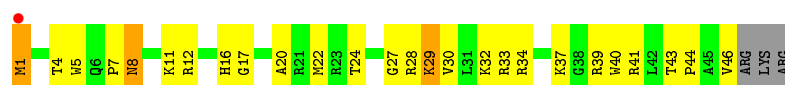
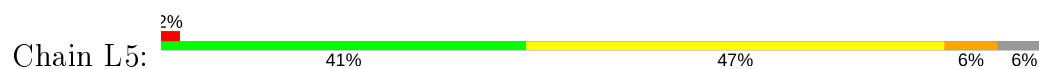




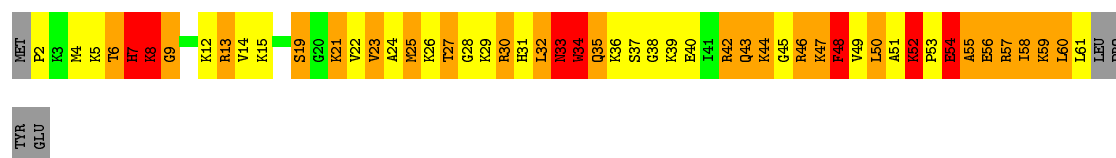
- Molecule 54: 50S ribosomal protein L34



- Molecule 54: 50S ribosomal protein L34



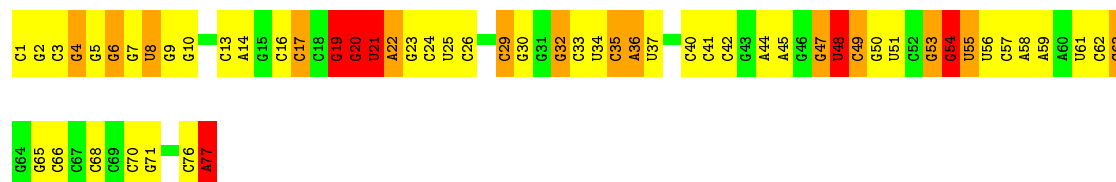
- Molecule 55: 50S ribosomal protein L35



- Molecule 55: 50S ribosomal protein L35



- Molecule 56: tRNA-fMet





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	210.20 Å 448.80 Å 621.00 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	153.41 – 3.30 153.41 – 3.30	Depositor EDS
% Data completeness (in resolution range)	99.9 (153.41-3.30) 92.6 (153.41-3.30)	Depositor EDS
$R_{merge}$	0.46	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	0.96 (at 3.33 Å)	Xtriage
Refinement program	PHENIX	Depositor
R, $R_{free}$	0.191 , 0.258 0.191 , 0.258	Depositor DCC
$R_{free}$ test set	2000 reflections (0.23%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	96.5	Xtriage
Anisotropy	0.268	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.27 , 88.8	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.43$ , $\langle L^2 \rangle = 0.26$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	295920	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	115.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.44% of the height of the origin peak. No significant pseudotranslation is detected.*

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

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



## 5 Model quality ⓘ

### 5.1 Standard geometry ⓘ

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z  > 5$	RMSZ	$\# Z  > 5$
1	13	0.84	15/36028 (0.0%)	1.50	521/56231 (0.9%)
1	1G	0.74	0/36025	1.40	370/56227 (0.7%)
2	12	0.43	0/1959	0.71	3/2642 (0.1%)
2	1E	0.46	0/1959	0.74	1/2642 (0.0%)
3	22	0.43	0/1636	0.67	1/2205 (0.0%)
3	2E	0.54	0/1629	0.72	0/2195
4	32	0.50	0/1732	0.76	0/2318
4	3E	0.58	0/1732	0.77	2/2318 (0.1%)
5	42	0.54	0/1171	0.75	0/1576
5	4E	0.57	0/1171	0.74	0/1576
6	52	0.55	0/855	0.70	0/1154
6	5E	0.59	0/855	0.72	0/1154
7	62	0.47	0/1211	0.64	0/1622
7	6E	0.53	0/1275	0.64	0/1709
8	72	0.48	0/1135	0.69	0/1527
8	7E	0.56	0/1135	0.79	0/1527
9	82	0.44	0/1028	0.69	0/1379
9	8E	0.49	0/1028	0.72	0/1379
10	1A	0.48	0/529	0.70	0/706
10	1I	0.46	0/814	0.71	0/1095
11	2A	0.49	0/879	0.72	0/1187
11	2I	0.61	0/899	0.83	1/1213 (0.1%)
12	3A	0.60	0/972	0.81	0/1301
12	3I	0.67	0/972	0.87	0/1301
13	4A	0.41	0/943	0.66	0/1265
13	4I	0.55	0/943	0.76	0/1265
14	5A	0.52	0/423	0.75	0/560
14	5I	0.75	1/500 (0.2%)	0.74	0/664
15	6A	0.53	0/744	0.70	0/992
15	6I	0.63	0/744	0.81	0/992
16	7A	0.49	0/721	0.73	0/970
16	7I	0.48	0/721	0.74	1/970 (0.1%)



Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
17	8A	0.54	0/836	0.70	0/1117
17	8I	0.62	0/847	0.76	0/1131
18	9A	0.51	0/595	0.71	0/790
18	9I	0.57	0/595	0.79	0/790
19	AA	0.42	0/638	0.70	1/860 (0.1%)
19	AI	0.55	0/661	0.88	1/890 (0.1%)
20	BA	0.47	0/764	0.77	0/1007
20	BI	0.44	0/764	0.70	0/1007
21	1B	0.55	0/192	0.71	0/252
21	1F	0.51	0/221	0.76	0/288
22	1K	0.73	1/1623 (0.1%)	1.34	22/2521 (0.9%)
23	2K	1.17	6/1721 (0.3%)	1.62	36/2682 (1.3%)
24	3K	0.98	11/1669 (0.7%)	1.28	13/2599 (0.5%)
24	3L	1.00	11/1669 (0.7%)	1.37	33/2599 (1.3%)
25	4K	0.96	0/322	1.53	8/500 (1.6%)
25	4L	0.85	0/222	1.36	2/344 (0.6%)
26	14	1.00	78/69405 (0.1%)	1.72	1985/108348 (1.8%)
26	1H	1.21	256/69998 (0.4%)	1.93	3118/109276 (2.9%)
27	16	0.93	2/2928 (0.1%)	1.75	90/4568 (2.0%)
27	1J	0.75	0/2928	1.52	41/4568 (0.9%)
28	71	0.82	0/749	0.80	0/1004
29	11	0.89	3/2165 (0.1%)	1.04	7/2919 (0.2%)
29	19	0.76	0/2170	0.95	3/2926 (0.1%)
30	21	0.73	0/1601	0.98	5/2160 (0.2%)
30	29	0.70	0/1601	0.99	5/2160 (0.2%)
31	31	0.81	1/1620 (0.1%)	0.93	3/2194 (0.1%)
31	39	0.67	1/1645 (0.1%)	0.94	2/2228 (0.1%)
32	41	0.62	0/1498	0.82	2/2016 (0.1%)
32	49	0.45	0/1498	0.73	0/2016
33	51	0.66	0/1362	0.89	3/1841 (0.2%)
33	59	0.48	0/1332	0.84	1/1802 (0.1%)
34	61	0.59	0/1151	0.86	0/1558
34	69	0.53	0/1151	0.77	2/1558 (0.1%)
35	15	0.56	0/1131	0.80	0/1525
35	58	0.69	0/1131	0.94	0/1525
36	25	0.68	0/942	0.82	0/1269
36	68	0.76	0/942	0.82	0/1269
37	35	0.66	0/1139	1.01	6/1514 (0.4%)
37	78	0.75	0/1161	1.05	1/1544 (0.1%)
38	45	0.69	0/1142	0.94	3/1527 (0.2%)
38	88	0.86	0/1097	1.10	3/1466 (0.2%)
39	55	0.69	0/973	0.93	1/1302 (0.1%)
39	98	0.65	0/981	0.96	2/1312 (0.2%)



Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
40	65	0.57	0/891	0.96	2/1187 (0.2%)
40	A8	0.78	0/891	1.02	4/1187 (0.3%)
41	75	0.65	0/1155	0.82	1/1542 (0.1%)
41	B8	0.73	0/1155	0.94	1/1542 (0.1%)
42	85	0.60	0/981	0.79	1/1306 (0.1%)
42	C8	0.80	0/981	0.98	3/1306 (0.2%)
43	95	0.65	0/789	0.90	1/1057 (0.1%)
43	D8	0.73	0/789	0.94	2/1057 (0.2%)
44	A5	0.74	0/897	0.88	1/1204 (0.1%)
44	E8	0.77	0/910	0.92	1/1220 (0.1%)
45	B5	0.78	0/739	0.86	0/993
45	F8	0.92	2/756 (0.3%)	1.00	1/1014 (0.1%)
46	C5	0.73	0/807	1.03	3/1076 (0.3%)
46	G8	0.79	0/804	1.09	5/1073 (0.5%)
47	D5	0.46	0/1151	0.74	0/1557
47	H8	0.60	0/1135	0.88	0/1535
48	E5	0.67	0/620	0.87	0/827
48	I8	0.80	0/634	1.00	0/847
49	F5	0.63	0/744	0.92	1/989 (0.1%)
49	J8	0.83	0/769	1.00	0/1022
50	G5	0.61	0/560	0.82	0/741
50	K8	0.82	0/565	1.01	1/748 (0.1%)
51	H5	0.59	0/473	0.74	0/635
51	L8	0.74	0/457	1.04	1/613 (0.2%)
52	I5	0.52	0/527	0.92	0/709
52	M8	0.58	0/545	0.96	1/733 (0.1%)
53	J5	0.73	0/448	0.93	0/606
53	N8	0.65	0/436	0.87	0/589
54	L5	0.75	0/406	0.95	0/536
54	P8	0.88	0/417	0.99	0/550
55	M5	0.96	1/483 (0.2%)	1.14	3/634 (0.5%)
55	Q8	1.27	3/486 (0.6%)	1.65	9/638 (1.4%)
56	2L	1.26	13/1742 (0.7%)	1.51	30/2712 (1.1%)
All	All	0.92	405/318291 (0.1%)	1.52	6371/476619 (1.3%)

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	2
4	32	0	3
4	3E	0	1
6	5E	0	1
9	82	0	1
10	1A	0	1
11	2A	0	1
12	3A	0	1
13	4A	0	1
13	4I	0	1
14	5A	0	1
19	AI	0	2
20	BA	0	3
29	11	0	2
29	19	0	5
30	21	0	4
30	29	0	5
31	31	0	1
31	39	0	4
32	41	0	1
32	49	0	1
33	59	0	1
34	61	0	4
34	69	0	1
35	15	0	1
36	25	0	1
37	35	0	3
37	78	0	2
38	45	0	5
38	88	0	3
39	98	0	1
40	65	0	1
40	A8	0	2
41	75	0	2
41	B8	0	2
42	85	0	3
42	C8	0	2
43	95	0	1
44	A5	0	2
45	B5	0	2
46	C5	0	3
46	G8	0	3

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Mol	Chain	#Chirality outliers	#Planarity outliers
47	D5	0	2
47	H8	0	3
48	E5	0	1
48	I8	0	2
49	J8	0	1
50	G5	0	2
50	K8	0	3
52	I5	0	2
52	M8	0	1
53	N8	0	1
55	M5	0	2
55	Q8	0	7
All	All	0	116

The worst 5 of 405 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
56	2L	55	U	N1-C2	22.39	1.58	1.38
23	2K	21	U	C5-C6	18.80	1.51	1.34
56	2L	21	U	C5-C6	18.33	1.50	1.34
24	3L	20	U	C5-C6	17.50	1.49	1.34
24	3K	16	U	C5-C6	17.45	1.49	1.34

The worst 5 of 6371 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	1H	1899	G	N3-C4-N9	-22.03	112.78	126.00
26	1H	2430	A	C2-N3-C4	-19.32	100.94	110.60
26	1H	783	A	C5-N7-C8	-17.81	94.99	103.90
26	1H	774	A	C2-N3-C4	-17.32	101.94	110.60
26	1H	2430	A	N1-C6-N6	16.97	128.78	118.60

There are no chirality outliers.

5 of 116 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	1E	15	VAL	Peptide
2	1E	237	ALA	Peptide
4	3E	31	CYS	Peptide
13	4I	107	ALA	Peptide
6	5E	41	GLU	Peptide



## 5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	13	32185	0	16244	1069	0
1	1G	32182	0	16244	1090	0
2	12	1924	0	1975	113	0
2	1E	1924	0	1975	127	0
3	22	1612	0	1677	111	0
3	2E	1605	0	1668	60	0
4	32	1702	0	1763	110	0
4	3E	1702	0	1762	110	0
5	42	1155	0	1213	83	0
5	4E	1155	0	1213	68	0
6	52	842	0	857	35	0
6	5E	842	0	857	47	0
7	62	1194	0	1234	58	0
7	6E	1256	0	1296	61	0
8	72	1115	0	1177	59	0
8	7E	1115	0	1177	68	0
9	82	1009	0	1037	81	0
9	8E	1009	0	1037	78	0
10	1A	522	0	530	31	0
10	1I	801	0	849	54	0
11	2A	864	0	881	52	0
11	2I	884	0	904	44	0
12	3A	956	0	1046	56	0
12	3I	956	0	1046	48	0
13	4A	933	0	992	62	0
13	4I	933	0	992	60	0
14	5A	418	0	456	36	0
14	5I	491	0	529	38	0
15	6A	733	0	771	40	0
15	6I	733	0	771	43	0
16	7A	705	0	725	36	0
16	7I	705	0	725	57	0
17	8A	823	0	891	27	0
17	8I	834	0	904	63	0
18	9A	590	0	662	27	0
18	9I	590	0	662	31	0
19	AA	624	0	636	51	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
19	AI	647	0	665	46	0
20	BA	762	0	861	41	0
20	BI	762	0	861	51	0
21	1B	188	0	195	16	0
21	1F	217	0	234	7	0
22	1K	1497	0	770	36	0
23	2K	1646	0	845	38	0
24	3K	1627	0	838	64	0
24	3L	1627	0	838	78	0
25	4K	285	0	143	16	0
25	4L	197	0	99	6	0
26	14	61968	0	31239	1915	0
26	1H	62497	0	31504	1930	2
27	16	2617	0	1328	93	0
27	1J	2617	0	1328	122	0
28	71	737	0	743	64	0
29	11	2115	0	2195	124	0
29	19	2120	0	2197	121	0
30	21	1568	0	1634	105	0
30	29	1568	0	1634	131	0
31	31	1585	0	1632	108	0
31	39	1610	0	1655	144	0
32	41	1473	0	1535	107	0
32	49	1473	0	1535	101	0
33	51	1336	0	1418	96	0
33	59	1307	0	1382	93	0
34	61	1136	0	1223	70	0
34	69	1136	0	1223	59	0
35	15	1104	0	1180	54	0
35	58	1104	0	1180	74	0
36	25	932	0	996	59	0
36	68	932	0	996	45	0
37	35	1122	0	1206	121	0
37	78	1144	0	1228	111	0
38	45	1121	0	1179	91	0
38	88	1077	0	1121	77	0
39	55	959	0	1021	70	0
39	98	967	0	1033	76	0
40	65	881	0	943	73	0
40	A8	881	0	943	70	0
41	75	1141	0	1202	71	0
41	B8	1141	0	1202	77	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
42	85	963	0	1022	69	0
42	C8	963	0	1022	63	0
43	95	778	0	852	81	0
43	D8	778	0	852	56	0
44	A5	886	0	948	40	0
44	E8	899	0	964	50	0
45	B5	725	0	778	33	0
45	F8	742	0	803	47	0
46	C5	794	0	884	67	0
46	G8	791	0	881	66	0
47	D5	1126	0	1154	92	0
47	H8	1110	0	1141	75	0
48	E5	612	0	633	42	0
48	I8	626	0	642	41	0
49	F5	737	0	813	35	0
49	J8	762	0	848	41	0
50	G5	558	0	610	26	1
50	K8	563	0	612	52	0
51	H5	468	0	518	15	1
51	L8	452	0	503	29	0
52	I5	515	0	514	60	0
52	M8	533	0	526	54	0
53	J5	434	0	454	33	0
53	N8	422	0	440	27	0
54	L5	398	0	441	25	0
54	P8	409	0	454	14	0
55	M5	477	0	540	47	0
55	Q8	480	0	549	104	0
56	2L	1645	0	843	40	0
57	11	3	0	0	0	0
57	13	99	0	0	0	0
57	14	327	0	0	0	0
57	16	11	0	0	0	0
57	1G	72	0	0	0	0
57	1H	444	0	0	0	0
57	1J	3	0	0	0	0
57	25	1	0	0	0	0
57	29	2	0	0	0	0
57	2K	2	0	0	0	0
57	2L	2	0	0	0	0
57	35	1	0	0	0	0
57	3E	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
57	3L	2	0	0	0	0
57	4I	2	0	0	0	0
57	45	1	0	0	0	0
57	4E	1	0	0	0	0
57	4I	1	0	0	0	0
57	55	1	0	0	0	0
57	68	2	0	0	0	0
57	78	2	0	0	0	0
57	88	1	0	0	0	0
57	98	1	0	0	0	0
57	I8	2	0	0	0	0
57	J8	2	0	0	0	0
57	L8	1	0	0	0	0
57	M5	1	0	0	0	0
57	P8	1	0	0	0	0
58	32	1	0	0	0	0
58	3E	1	0	0	0	0
58	5A	1	0	0	0	0
58	5I	1	0	0	0	0
58	C5	1	0	0	0	0
58	G8	1	0	0	0	0
59	11	11	0	0	1	0
59	13	144	0	0	30	0
59	14	592	0	0	151	0
59	16	22	0	0	0	0
59	19	8	0	0	1	0
59	1G	48	0	0	9	0
59	1H	933	0	0	316	0
59	1I	1	0	0	0	0
59	21	3	0	0	1	0
59	25	6	0	0	1	0
59	29	5	0	0	2	0
59	2K	6	0	0	0	0
59	31	9	0	0	0	0
59	35	2	0	0	0	0
59	39	4	0	0	0	0
59	3E	2	0	0	1	0
59	3I	2	0	0	0	0
59	4K	2	0	0	0	0
59	55	3	0	0	2	0
59	5I	2	0	0	0	0
59	75	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
59	78	6	0	0	2	0
59	A5	1	0	0	0	0
59	D8	1	0	0	0	0
59	F8	2	0	0	0	0
59	G8	2	0	0	0	0
59	H5	2	0	0	1	0
59	I8	5	0	0	2	0
59	J8	1	0	0	0	0
59	L5	1	0	0	0	0
59	L8	1	0	0	1	0
59	M5	1	0	0	0	0
59	P8	2	0	0	0	0
59	Q8	1	0	0	0	0
All	All	295920	0	197803	11212	2

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 24.

The worst 5 of 11212 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)
26:1H:270(L):U:H3	34:61:50:ARG:HG2	1.19	1.06
26:1H:2714:G:OP2	59:1H:3574:HOH:O	1.71	1.06
26:1H:2781:A:H5'	26:1H:2782:G:H5'	1.35	1.06
26:1H:741:G:OP1	59:1H:3910:HOH:O	1.74	1.05
26:1H:1614:A:OP1	59:1H:3862:HOH:O	1.75	1.04

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

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:1H:654(H):G:O2'	51:H5:55:ARG:NH2[2_464]	2.11	0.09
26:1H:277:C:O2'	50:G5:49:LYS:NZ[2_564]	2.16	0.04



## 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	235/256 (92%)	192 (82%)	37 (16%)	6 (3%)	5	27
2	1E	235/256 (92%)	193 (82%)	39 (17%)	3 (1%)	12	40
3	22	204/239 (85%)	182 (89%)	22 (11%)	0	100	100
3	2E	203/239 (85%)	185 (91%)	18 (9%)	0	100	100
4	32	206/209 (99%)	180 (87%)	22 (11%)	4 (2%)	8	34
4	3E	206/209 (99%)	190 (92%)	13 (6%)	3 (2%)	10	38
5	42	149/162 (92%)	135 (91%)	13 (9%)	1 (1%)	22	54
5	4E	149/162 (92%)	139 (93%)	9 (6%)	1 (1%)	22	54
6	52	99/101 (98%)	97 (98%)	2 (2%)	0	100	100
6	5E	99/101 (98%)	93 (94%)	6 (6%)	0	100	100
7	62	143/156 (92%)	135 (94%)	7 (5%)	1 (1%)	22	54
7	6E	153/156 (98%)	143 (94%)	10 (6%)	0	100	100
8	72	136/138 (99%)	124 (91%)	10 (7%)	2 (2%)	10	38
8	7E	136/138 (99%)	124 (91%)	11 (8%)	1 (1%)	22	54
9	82	125/128 (98%)	112 (90%)	12 (10%)	1 (1%)	19	51
9	8E	125/128 (98%)	106 (85%)	18 (14%)	1 (1%)	19	51
10	1A	56/105 (53%)	48 (86%)	8 (14%)	0	100	100
10	1I	97/105 (92%)	88 (91%)	8 (8%)	1 (1%)	15	46
11	2A	114/129 (88%)	101 (89%)	10 (9%)	3 (3%)	5	27
11	2I	117/129 (91%)	100 (86%)	16 (14%)	1 (1%)	17	48
12	3A	120/132 (91%)	101 (84%)	14 (12%)	5 (4%)	3	17
12	3I	120/132 (91%)	103 (86%)	17 (14%)	0	100	100
13	4A	115/126 (91%)	97 (84%)	16 (14%)	2 (2%)	9	35
13	4I	115/126 (91%)	95 (83%)	19 (16%)	1 (1%)	17	48
14	5A	48/61 (79%)	38 (79%)	9 (19%)	1 (2%)	7	31

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
14	5I	58/61 (95%)	45 (78%)	11 (19%)	2 (3%)	3	22
15	6A	86/89 (97%)	74 (86%)	12 (14%)	0	100	100
15	6I	86/89 (97%)	75 (87%)	11 (13%)	0	100	100
16	7A	82/88 (93%)	76 (93%)	6 (7%)	0	100	100
16	7I	82/88 (93%)	76 (93%)	5 (6%)	1 (1%)	13	42
17	8A	97/105 (92%)	92 (95%)	5 (5%)	0	100	100
17	8I	98/105 (93%)	93 (95%)	5 (5%)	0	100	100
18	9A	70/88 (80%)	61 (87%)	9 (13%)	0	100	100
18	9I	70/88 (80%)	62 (89%)	7 (10%)	1 (1%)	11	38
19	AA	76/93 (82%)	59 (78%)	14 (18%)	3 (4%)	3	18
19	AI	79/93 (85%)	65 (82%)	10 (13%)	4 (5%)	2	13
20	BA	97/106 (92%)	85 (88%)	11 (11%)	1 (1%)	15	46
20	BI	97/106 (92%)	83 (86%)	14 (14%)	0	100	100
21	1B	20/27 (74%)	19 (95%)	1 (5%)	0	100	100
21	1F	23/27 (85%)	21 (91%)	2 (9%)	0	100	100
28	7I	83/229 (36%)	79 (95%)	2 (2%)	2 (2%)	6	28
29	11	270/276 (98%)	253 (94%)	13 (5%)	4 (2%)	10	38
29	19	271/276 (98%)	248 (92%)	18 (7%)	5 (2%)	8	35
30	21	203/206 (98%)	160 (79%)	33 (16%)	10 (5%)	2	14
30	29	203/206 (98%)	149 (73%)	45 (22%)	9 (4%)	2	16
31	31	200/210 (95%)	180 (90%)	19 (10%)	1 (0%)	29	61
31	39	204/210 (97%)	163 (80%)	34 (17%)	7 (3%)	3	22
32	41	179/182 (98%)	155 (87%)	20 (11%)	4 (2%)	6	30
32	49	179/182 (98%)	150 (84%)	28 (16%)	1 (1%)	25	57
33	51	172/180 (96%)	146 (85%)	19 (11%)	7 (4%)	3	17
33	59	168/180 (93%)	125 (74%)	35 (21%)	8 (5%)	2	14
34	61	144/148 (97%)	119 (83%)	21 (15%)	4 (3%)	5	25
34	69	144/148 (97%)	115 (80%)	26 (18%)	3 (2%)	7	31
35	15	136/140 (97%)	119 (88%)	15 (11%)	2 (2%)	10	38
35	58	136/140 (97%)	114 (84%)	18 (13%)	4 (3%)	4	24
36	25	120/122 (98%)	111 (92%)	8 (7%)	1 (1%)	19	51

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
36	68	120/122 (98%)	114 (95%)	5 (4%)	1 (1%)	19	51
37	35	145/150 (97%)	110 (76%)	26 (18%)	9 (6%)	1	10
37	78	148/150 (99%)	117 (79%)	26 (18%)	5 (3%)	3	22
38	45	139/141 (99%)	109 (78%)	27 (19%)	3 (2%)	6	30
38	88	133/141 (94%)	110 (83%)	19 (14%)	4 (3%)	4	24
39	55	115/118 (98%)	107 (93%)	7 (6%)	1 (1%)	17	48
39	98	116/118 (98%)	99 (85%)	16 (14%)	1 (1%)	17	48
40	65	109/112 (97%)	85 (78%)	20 (18%)	4 (4%)	3	20
40	A8	109/112 (97%)	87 (80%)	20 (18%)	2 (2%)	8	35
41	75	135/146 (92%)	117 (87%)	17 (13%)	1 (1%)	22	54
41	B8	135/146 (92%)	114 (84%)	20 (15%)	1 (1%)	22	54
42	85	115/118 (98%)	99 (86%)	16 (14%)	0	100	100
42	C8	115/118 (98%)	102 (89%)	11 (10%)	2 (2%)	9	35
43	95	99/101 (98%)	79 (80%)	16 (16%)	4 (4%)	3	18
43	D8	99/101 (98%)	91 (92%)	6 (6%)	2 (2%)	7	32
44	A5	109/113 (96%)	97 (89%)	9 (8%)	3 (3%)	5	25
44	E8	111/113 (98%)	98 (88%)	13 (12%)	0	100	100
45	B5	90/96 (94%)	80 (89%)	8 (9%)	2 (2%)	6	30
45	F8	92/96 (96%)	83 (90%)	8 (9%)	1 (1%)	14	45
46	C5	102/110 (93%)	75 (74%)	20 (20%)	7 (7%)	1	8
46	G8	102/110 (93%)	80 (78%)	15 (15%)	7 (7%)	1	8
47	D5	131/206 (64%)	101 (77%)	24 (18%)	6 (5%)	2	15
47	H8	129/206 (63%)	104 (81%)	19 (15%)	6 (5%)	2	14
48	E5	75/85 (88%)	65 (87%)	9 (12%)	1 (1%)	12	40
48	I8	78/85 (92%)	67 (86%)	9 (12%)	2 (3%)	5	27
49	F5	92/98 (94%)	84 (91%)	7 (8%)	1 (1%)	14	45
49	J8	95/98 (97%)	85 (90%)	8 (8%)	2 (2%)	7	31
50	G5	64/72 (89%)	58 (91%)	4 (6%)	2 (3%)	4	23
50	K8	65/72 (90%)	56 (86%)	5 (8%)	4 (6%)	1	10
51	H5	57/60 (95%)	50 (88%)	7 (12%)	0	100	100
51	L8	55/60 (92%)	50 (91%)	4 (7%)	1 (2%)	8	35

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
52	I5	61/71 (86%)	33 (54%)	25 (41%)	3 (5%)	2	14
52	M8	64/71 (90%)	39 (61%)	22 (34%)	3 (5%)	2	14
53	J5	54/60 (90%)	49 (91%)	5 (9%)	0	100	100
53	N8	52/60 (87%)	43 (83%)	7 (14%)	2 (4%)	3	19
54	L5	44/49 (90%)	43 (98%)	1 (2%)	0	100	100
54	P8	45/49 (92%)	43 (96%)	2 (4%)	0	100	100
55	M5	58/65 (89%)	46 (79%)	9 (16%)	3 (5%)	2	13
55	Q8	58/65 (89%)	36 (62%)	15 (26%)	7 (12%)	0	2
All	All	11153/12175 (92%)	9578 (86%)	1350 (12%)	225 (2%)	7	32

5 of 225 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
18	9I	22	VAL
30	21	78	LEU
30	21	83	ASP
33	51	169	VAL
37	78	57	THR

### 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	205/220 (93%)	148 (72%)	57 (28%)	0	1
2	1E	205/220 (93%)	158 (77%)	47 (23%)	1	3
3	22	160/188 (85%)	121 (76%)	39 (24%)	0	2
3	2E	159/188 (85%)	128 (80%)	31 (20%)	1	5
4	32	180/181 (99%)	140 (78%)	40 (22%)	1	3
4	3E	180/181 (99%)	146 (81%)	34 (19%)	1	6
5	42	116/123 (94%)	80 (69%)	36 (31%)	0	1
5	4E	116/123 (94%)	86 (74%)	30 (26%)	0	2

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
6	52	90/90 (100%)	73 (81%)	17 (19%)	1	6
6	5E	90/90 (100%)	70 (78%)	20 (22%)	1	3
7	62	121/127 (95%)	97 (80%)	24 (20%)	1	5
7	6E	126/127 (99%)	98 (78%)	28 (22%)	1	3
8	72	119/119 (100%)	91 (76%)	28 (24%)	1	3
8	7E	119/119 (100%)	93 (78%)	26 (22%)	1	4
9	82	98/99 (99%)	77 (79%)	21 (21%)	1	4
9	8E	98/99 (99%)	71 (72%)	27 (28%)	0	1
10	1A	58/92 (63%)	43 (74%)	15 (26%)	0	2
10	1I	89/92 (97%)	68 (76%)	21 (24%)	1	3
11	2A	88/99 (89%)	72 (82%)	16 (18%)	1	7
11	2I	90/99 (91%)	73 (81%)	17 (19%)	1	6
12	3A	103/109 (94%)	81 (79%)	22 (21%)	1	4
12	3I	103/109 (94%)	80 (78%)	23 (22%)	1	3
13	4A	94/101 (93%)	60 (64%)	34 (36%)	0	0
13	4I	94/101 (93%)	71 (76%)	23 (24%)	0	2
14	5A	43/50 (86%)	33 (77%)	10 (23%)	1	3
14	5I	49/50 (98%)	42 (86%)	7 (14%)	3	15
15	6A	79/80 (99%)	64 (81%)	15 (19%)	1	6
15	6I	79/80 (99%)	68 (86%)	11 (14%)	3	16
16	7A	72/74 (97%)	53 (74%)	19 (26%)	0	1
16	7I	72/74 (97%)	56 (78%)	16 (22%)	1	3
17	8A	94/97 (97%)	80 (85%)	14 (15%)	3	13
17	8I	95/97 (98%)	73 (77%)	22 (23%)	1	3
18	9A	63/77 (82%)	44 (70%)	19 (30%)	0	1
18	9I	63/77 (82%)	53 (84%)	10 (16%)	2	11
19	AA	67/80 (84%)	54 (81%)	13 (19%)	1	5
19	AI	70/80 (88%)	45 (64%)	25 (36%)	0	0
20	BA	76/82 (93%)	66 (87%)	10 (13%)	4	17
20	BI	76/82 (93%)	55 (72%)	21 (28%)	0	1
21	1B	17/22 (77%)	16 (94%)	1 (6%)	19	49

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
21	1F	20/22 (91%)	19 (95%)	1 (5%)	24	55
28	71	77/181 (42%)	58 (75%)	19 (25%)	0	2
29	11	214/218 (98%)	162 (76%)	52 (24%)	0	2
29	19	214/218 (98%)	162 (76%)	52 (24%)	0	2
30	21	165/166 (99%)	130 (79%)	35 (21%)	1	4
30	29	165/166 (99%)	128 (78%)	37 (22%)	1	3
31	31	161/166 (97%)	123 (76%)	38 (24%)	1	3
31	39	163/166 (98%)	125 (77%)	38 (23%)	1	3
32	41	155/156 (99%)	109 (70%)	46 (30%)	0	1
32	49	155/156 (99%)	112 (72%)	43 (28%)	0	1
33	51	145/148 (98%)	112 (77%)	33 (23%)	1	3
33	59	142/148 (96%)	108 (76%)	34 (24%)	0	2
34	61	122/124 (98%)	89 (73%)	33 (27%)	0	1
34	69	122/124 (98%)	87 (71%)	35 (29%)	0	1
35	15	117/119 (98%)	93 (80%)	24 (20%)	1	4
35	58	117/119 (98%)	85 (73%)	32 (27%)	0	1
36	25	100/100 (100%)	72 (72%)	28 (28%)	0	1
36	68	100/100 (100%)	78 (78%)	22 (22%)	1	3
37	35	114/116 (98%)	70 (61%)	44 (39%)	0	0
37	78	116/116 (100%)	79 (68%)	37 (32%)	0	1
38	45	111/111 (100%)	85 (77%)	26 (23%)	1	3
38	88	103/111 (93%)	73 (71%)	30 (29%)	0	1
39	55	100/101 (99%)	78 (78%)	22 (22%)	1	3
39	98	101/101 (100%)	80 (79%)	21 (21%)	1	4
40	65	87/88 (99%)	68 (78%)	19 (22%)	1	4
40	A8	87/88 (99%)	58 (67%)	29 (33%)	0	1
41	75	120/127 (94%)	83 (69%)	37 (31%)	0	1
41	B8	120/127 (94%)	85 (71%)	35 (29%)	0	1
42	85	93/94 (99%)	71 (76%)	22 (24%)	1	2
42	C8	93/94 (99%)	73 (78%)	20 (22%)	1	4
43	95	82/82 (100%)	53 (65%)	29 (35%)	0	0

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
43	D8	82/82 (100%)	56 (68%)	26 (32%)	0	1
44	A5	91/92 (99%)	65 (71%)	26 (29%)	0	1
44	E8	92/92 (100%)	68 (74%)	24 (26%)	0	2
45	B5	74/78 (95%)	57 (77%)	17 (23%)	1	3
45	F8	76/78 (97%)	56 (74%)	20 (26%)	0	2
46	C5	85/91 (93%)	60 (71%)	25 (29%)	0	1
46	G8	85/91 (93%)	57 (67%)	28 (33%)	0	1
47	D5	126/179 (70%)	95 (75%)	31 (25%)	0	2
47	H8	124/179 (69%)	96 (77%)	28 (23%)	1	3
48	E5	62/67 (92%)	48 (77%)	14 (23%)	1	3
48	I8	61/67 (91%)	44 (72%)	17 (28%)	0	1
49	F5	79/83 (95%)	56 (71%)	23 (29%)	0	1
49	J8	82/83 (99%)	61 (74%)	21 (26%)	0	2
50	G5	62/67 (92%)	41 (66%)	21 (34%)	0	1
50	K8	62/67 (92%)	44 (71%)	18 (29%)	0	1
51	H5	51/52 (98%)	38 (74%)	13 (26%)	0	2
51	L8	49/52 (94%)	33 (67%)	16 (33%)	0	1
52	I5	57/63 (90%)	40 (70%)	17 (30%)	0	1
52	M8	59/63 (94%)	43 (73%)	16 (27%)	0	1
53	J5	48/52 (92%)	34 (71%)	14 (29%)	0	1
53	N8	47/52 (90%)	35 (74%)	12 (26%)	0	2
54	L5	39/42 (93%)	31 (80%)	8 (20%)	1	4
54	P8	40/42 (95%)	31 (78%)	9 (22%)	1	3
55	M5	49/55 (89%)	36 (74%)	13 (26%)	0	1
55	Q8	50/55 (91%)	33 (66%)	17 (34%)	0	1
All	All	9429/10075 (94%)	7093 (75%)	2336 (25%)	0	2

5 of 2336 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
48	I8	44	ARG
4	32	191	ARG
46	C5	19	LYS

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Mol	Chain	Res	Type
50	K8	9	GLN
2	12	56	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 31 such sidechains are listed below:

Mol	Chain	Res	Type
48	I8	29	GLN
5	42	127	ASN
40	65	34	HIS
2	12	19	HIS
5	42	130	ASN

### 5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	13	1495/1522 (98%)	395 (26%)	38 (2%)
1	1G	1495/1522 (98%)	396 (26%)	36 (2%)
22	1K	65/77 (84%)	28 (43%)	3 (4%)
23	2K	76/77 (98%)	16 (21%)	1 (1%)
24	3K	75/76 (98%)	35 (46%)	6 (8%)
24	3L	74/76 (97%)	38 (51%)	2 (2%)
25	4K	12/27 (44%)	2 (16%)	0
25	4L	9/27 (33%)	4 (44%)	1 (11%)
26	14	2874/2917 (98%)	803 (27%)	48 (1%)
26	1H	2901/2917 (99%)	734 (25%)	52 (1%)
27	16	121/122 (99%)	25 (20%)	0
27	1J	121/122 (99%)	39 (32%)	1 (0%)
56	2L	75/77 (97%)	22 (29%)	3 (4%)
All	All	9393/9559 (98%)	2537 (27%)	191 (2%)

5 of 2537 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	13	5	U
1	13	6	G
1	13	7	G
1	13	8	A
1	13	9	G

5 of 191 RNA pucker outliers are listed below:



Mol	Chain	Res	Type
26	1H	2062	A
1	1G	274	A
26	14	2157	G
26	1H	2167	U
26	1H	2611	U

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

23 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$
24	PSU	3K	55	24	17,21,22	1.16	3 (17%)	20,30,33	3.03	7 (35%)
24	4SU	3K	8	24	14,21,22	3.38	2 (14%)	15,30,33	1.25	2 (13%)
24	MIA	3L	37	24	24,31,32	2.66	4 (16%)	26,44,47	3.09	10 (38%)
23	7MG	2K	47	23	22,26,27	3.32	7 (31%)	28,39,42	2.61	10 (35%)
23	PSU	2K	56	23	17,21,22	1.12	2 (11%)	20,30,33	2.72	4 (20%)
22	OMC	1K	33	22	15,22,23	2.19	4 (26%)	17,31,34	1.55	3 (17%)
22	5MU	1K	55	22	15,22,23	2.14	3 (20%)	16,32,35	1.69	2 (12%)
24	4SU	3L	8	24	14,21,22	3.38	2 (14%)	15,30,33	1.59	2 (13%)
24	PSU	3L	55	24	17,21,22	1.02	1 (5%)	20,30,33	3.20	6 (30%)
23	5MU	2K	55	23	15,22,23	2.23	3 (20%)	16,32,35	1.80	2 (12%)
24	7MG	3K	46	24	22,26,27	3.39	6 (27%)	28,39,42	2.56	11 (39%)
24	7MG	3L	46	24	22,26,27	3.55	6 (27%)	28,39,42	2.41	11 (39%)
56	OMC	2L	33	56	15,22,23	2.17	4 (26%)	17,31,34	1.63	3 (17%)
56	PSU	2L	56	56	17,21,22	1.18	1 (5%)	20,30,33	3.30	6 (30%)
24	PSU	3L	32	24	17,21,22	1.17	1 (5%)	20,30,33	3.50	6 (30%)
24	PSU	3K	39	24	17,21,22	1.07	1 (5%)	20,30,33	3.24	6 (30%)
24	PSU	3K	32	24	17,21,22	1.05	1 (5%)	20,30,33	3.30	5 (25%)
23	OMC	2K	33	23	15,22,23	2.26	4 (26%)	17,31,34	1.40	2 (11%)
56	4SU	2L	8	56	14,21,22	3.47	2 (14%)	15,30,33	0.96	1 (6%)



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
56	7MG	2L	47	56	22,26,27	3.37	6 (27%)	28,39,42	2.54	10 (35%)
24	MIA	3K	37	24	24,31,32	2.39	4 (16%)	26,44,47	3.43	10 (38%)
23	4SU	2K	8	23	14,21,22	3.08	2 (14%)	15,30,33	0.66	0
24	PSU	3L	39	24	17,21,22	1.06	1 (5%)	20,30,33	3.17	6 (30%)

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
24	PSU	3K	55	24	-	2/7/25/26	0/2/2/2
24	4SU	3K	8	24	-	1/5/25/26	0/2/2/2
24	MIA	3L	37	24	-	7/11/33/34	0/3/3/3
23	7MG	2K	47	23	-	4/7/37/38	0/3/3/3
23	PSU	2K	56	23	-	0/7/25/26	0/2/2/2
22	OMC	1K	33	22	-	0/7/27/28	0/2/2/2
22	5MU	1K	55	22	-	0/5/25/26	0/2/2/2
24	4SU	3L	8	24	-	2/5/25/26	0/2/2/2
24	PSU	3L	55	24	-	0/7/25/26	0/2/2/2
23	5MU	2K	55	23	-	0/5/25/26	0/2/2/2
24	7MG	3K	46	24	-	2/7/37/38	0/3/3/3
24	7MG	3L	46	24	-	2/7/37/38	0/3/3/3
56	OMC	2L	33	56	-	0/7/27/28	0/2/2/2
56	PSU	2L	56	56	-	0/7/25/26	0/2/2/2
24	PSU	3L	32	24	-	0/7/25/26	0/2/2/2
24	PSU	3K	39	24	-	0/7/25/26	0/2/2/2
24	PSU	3K	32	24	-	0/7/25/26	0/2/2/2
23	OMC	2K	33	23	-	1/7/27/28	0/2/2/2
56	4SU	2L	8	56	-	2/5/25/26	0/2/2/2
56	7MG	2L	47	56	-	3/7/37/38	0/3/3/3
24	MIA	3K	37	24	-	6/11/33/34	0/3/3/3
23	4SU	2K	8	23	-	0/5/25/26	0/2/2/2
24	PSU	3L	39	24	-	2/7/25/26	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)
24	3L	46	7MG	C4-N3	11.15	1.48	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	3K	46	7MG	C4-N3	10.93	1.48	1.34
56	2L	47	7MG	C4-N3	10.90	1.48	1.34
23	2K	47	7MG	C4-N3	10.76	1.47	1.34
24	3L	8	4SU	C5-C4	9.98	1.49	1.38

The worst 5 of 125 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	3L	32	PSU	N1-C2-N3	-12.18	118.75	128.43
24	3K	32	PSU	N1-C2-N3	-11.41	119.36	128.43
24	3K	37	MIA	C11-S10-C2	11.38	110.77	102.27
24	3L	55	PSU	N1-C2-N3	-11.31	119.44	128.43
24	3L	39	PSU	N1-C2-N3	-10.88	119.78	128.43

There are no chirality outliers.

5 of 34 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
24	3L	37	MIA	O4'-C4'-C5'-O5'
24	3L	37	MIA	C3'-C4'-C5'-O5'
24	3L	37	MIA	C5-C6-N6-C12
24	3L	37	MIA	N1-C2-S10-C11
24	3L	37	MIA	N3-C2-S10-C11

There are no ring outliers.

16 monomers are involved in 29 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
24	3K	55	PSU	2	0
24	3K	8	4SU	1	0
24	3L	37	MIA	2	0
23	2K	47	7MG	3	0
24	3L	8	4SU	5	0
24	3L	55	PSU	1	0
23	2K	55	5MU	1	0
24	3K	46	7MG	2	0
56	2L	33	OMC	1	0
56	2L	56	PSU	2	0
24	3K	39	PSU	2	0
23	2K	33	OMC	2	0
56	2L	8	4SU	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
56	2L	47	7MG	2	0
24	3K	37	MIA	1	0
23	2K	8	4SU	1	0

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 995 ligands modelled in this entry, 995 are monoatomic - leaving 0 for Mogul analysis.

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](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
56	2L	1
22	1K	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	1K	69:C	O3'	70:C	P	5.53
1	2L	54:G	O3'	55:U	P	2.94



## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	13	1497/1522 (98%)	-0.58	0 100 100	70, 114, 187, 287	0
1	1G	1497/1522 (98%)	-0.66	0 100 100	79, 129, 197, 297	0
2	12	237/256 (92%)	0.88	43 (18%) 1 1	143, 175, 203, 210	0
2	1E	237/256 (92%)	0.26	14 (5%) 22 22	124, 155, 178, 191	0
3	22	206/239 (86%)	1.02	35 (16%) 1 1	132, 155, 182, 195	0
3	2E	205/239 (85%)	0.72	22 (10%) 6 5	101, 124, 154, 164	0
4	32	208/209 (99%)	0.73	21 (10%) 7 6	118, 137, 157, 163	0
4	3E	208/209 (99%)	0.60	17 (8%) 11 11	100, 127, 145, 153	0
5	42	151/162 (93%)	0.37	7 (4%) 32 30	115, 132, 153, 171	0
5	4E	151/162 (93%)	0.75	17 (11%) 5 5	93, 117, 136, 166	0
6	52	101/101 (100%)	0.49	2 (1%) 65 64	102, 116, 134, 144	0
6	5E	101/101 (100%)	0.33	2 (1%) 65 64	89, 112, 132, 144	0
7	62	147/156 (94%)	0.28	11 (7%) 14 13	122, 138, 151, 165	0
7	6E	155/156 (99%)	0.35	14 (9%) 9 9	108, 123, 152, 169	0
8	72	138/138 (100%)	0.36	6 (4%) 35 34	111, 137, 150, 157	0
8	7E	138/138 (100%)	0.72	22 (15%) 1 2	107, 122, 136, 144	0
9	82	127/128 (99%)	0.42	4 (3%) 49 48	125, 161, 179, 186	0
9	8E	127/128 (99%)	0.30	1 (0%) 86 86	98, 142, 161, 174	0
10	1A	66/105 (62%)	0.47	5 (7%) 13 13	130, 158, 176, 188	0
10	1I	99/105 (94%)	0.91	20 (20%) 1 1	98, 147, 178, 183	0
11	2A	116/129 (89%)	1.32	29 (25%) 0 0	103, 124, 142, 169	0
11	2I	119/129 (92%)	0.67	8 (6%) 17 17	85, 112, 156, 180	0
12	3A	122/132 (92%)	0.50	9 (7%) 14 14	97, 113, 129, 145	0
12	3I	122/132 (92%)	0.24	4 (3%) 46 44	83, 93, 119, 143	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
13	4A	117/126 (92%)	0.67	21 (17%) 1 1	125, 155, 178, 192	0
13	4I	117/126 (92%)	0.15	4 (3%) 45 43	95, 131, 145, 162	0
14	5A	52/61 (85%)	0.83	6 (11%) 4 4	138, 151, 163, 167	0
14	5I	60/61 (98%)	0.45	2 (3%) 46 44	101, 113, 127, 134	0
15	6A	88/89 (98%)	-0.04	0 100 100	99, 120, 141, 148	0
15	6I	88/89 (98%)	0.17	5 (5%) 23 23	87, 110, 128, 134	0
16	7A	84/88 (95%)	0.23	1 (1%) 79 78	108, 123, 139, 168	0
16	7I	84/88 (95%)	0.67	9 (10%) 6 5	113, 127, 155, 174	0
17	8A	99/105 (94%)	0.35	4 (4%) 38 36	101, 116, 131, 136	0
17	8I	100/105 (95%)	0.34	5 (5%) 28 27	100, 117, 127, 131	0
18	9A	72/88 (81%)	1.34	15 (20%) 1 1	109, 130, 167, 194	0
18	9I	72/88 (81%)	0.81	7 (9%) 7 8	96, 115, 152, 185	0
19	AA	78/93 (83%)	1.07	18 (23%) 0 1	137, 178, 195, 198	0
19	AI	81/93 (87%)	0.21	2 (2%) 57 54	107, 129, 146, 157	0
20	BA	99/106 (93%)	0.38	3 (3%) 50 49	104, 122, 141, 156	0
20	BI	99/106 (93%)	0.29	3 (3%) 50 49	120, 135, 156, 164	0
21	1B	22/27 (81%)	1.42	7 (31%) 0 0	122, 142, 149, 152	0
21	1F	25/27 (92%)	0.42	1 (4%) 38 36	106, 118, 135, 147	0
22	1K	68/77 (88%)	0.51	4 (5%) 22 22	117, 196, 214, 216	0
23	2K	72/77 (93%)	-0.41	0 100 100	80, 108, 138, 146	0
24	3K	70/76 (92%)	-0.25	1 (1%) 75 75	83, 231, 262, 266	0
24	3L	70/76 (92%)	-0.09	2 (2%) 51 50	96, 239, 268, 279	0
25	4K	13/27 (48%)	0.30	1 (7%) 13 12	83, 115, 170, 170	0
25	4L	9/27 (33%)	-0.03	0 100 100	100, 136, 151, 157	0
26	14	2877/2917 (98%)	-0.38	16 (0%) 89 90	62, 96, 237, 329	0
26	1H	2902/2917 (99%)	-0.36	13 (0%) 92 93	50, 81, 226, 314	0
27	16	122/122 (100%)	-0.64	1 (0%) 86 86	76, 99, 116, 199	0
27	1J	122/122 (100%)	-0.75	0 100 100	98, 136, 162, 199	0
28	7I	93/229 (40%)	1.10	21 (22%) 0 1	109, 115, 131, 143	0
29	11	272/276 (98%)	0.12	0 100 100	52, 71, 87, 95	0
29	19	273/276 (98%)	0.28	4 (1%) 73 72	60, 83, 100, 111	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
30	21	205/206 (99%)	0.60	23 (11%) 5 5	59, 95, 137, 152	0
30	29	205/206 (99%)	0.23	6 (2%) 51 50	70, 104, 144, 178	0
31	31	202/210 (96%)	0.10	2 (0%) 82 82	55, 84, 120, 142	0
31	39	206/210 (98%)	0.55	11 (5%) 26 24	70, 110, 163, 190	0
32	41	181/182 (99%)	0.42	9 (4%) 28 27	85, 110, 141, 149	0
32	49	181/182 (99%)	0.98	38 (20%) 1 1	133, 152, 174, 187	0
33	51	174/180 (96%)	0.20	3 (1%) 70 68	88, 108, 123, 136	0
33	59	170/180 (94%)	1.27	44 (25%) 0 0	131, 193, 221, 241	0
34	61	146/148 (98%)	0.58	15 (10%) 6 6	81, 135, 151, 154	0
34	69	146/148 (98%)	0.46	16 (10%) 5 5	97, 138, 155, 163	0
35	15	138/140 (98%)	0.45	4 (2%) 51 50	87, 114, 146, 168	0
35	58	138/140 (98%)	0.34	4 (2%) 51 50	73, 95, 129, 147	0
36	25	122/122 (100%)	0.38	4 (3%) 46 44	75, 96, 112, 124	0
36	68	122/122 (100%)	0.52	4 (3%) 46 44	65, 85, 103, 115	0
37	35	147/150 (98%)	0.82	18 (12%) 4 3	70, 114, 145, 159	0
37	78	150/150 (100%)	0.01	3 (2%) 65 64	57, 85, 111, 159	0
38	45	141/141 (100%)	1.18	29 (20%) 1 1	80, 111, 139, 153	0
38	88	137/141 (97%)	0.39	7 (5%) 28 26	63, 84, 103, 146	0
39	55	117/118 (99%)	0.32	5 (4%) 35 34	69, 88, 105, 121	0
39	98	118/118 (100%)	0.53	4 (3%) 45 43	70, 91, 111, 121	0
40	65	111/112 (99%)	0.51	8 (7%) 15 15	104, 128, 140, 146	0
40	A8	111/112 (99%)	0.80	15 (13%) 3 3	81, 95, 120, 129	0
41	75	137/146 (93%)	0.13	4 (2%) 51 50	86, 104, 164, 200	0
41	B8	137/146 (93%)	0.11	1 (0%) 87 88	80, 99, 151, 186	0
42	85	117/118 (99%)	0.24	1 (0%) 84 84	76, 103, 142, 163	0
42	C8	117/118 (99%)	0.22	4 (3%) 45 43	63, 83, 117, 136	0
43	95	101/101 (100%)	0.98	19 (18%) 1 1	72, 129, 143, 161	0
43	D8	101/101 (100%)	0.45	7 (6%) 16 16	63, 108, 131, 145	0
44	A5	111/113 (98%)	0.30	2 (1%) 68 67	69, 83, 117, 151	0
44	E8	113/113 (100%)	0.26	3 (2%) 54 52	66, 80, 116, 158	0
45	B5	92/96 (95%)	0.60	4 (4%) 35 34	78, 94, 113, 133	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
45	F8	94/96 (97%)	0.60	5 (5%) 26 24	65, 77, 101, 118	0
46	C5	104/110 (94%)	0.84	19 (18%) 1 1	98, 120, 152, 163	0
46	G8	104/110 (94%)	0.17	3 (2%) 51 50	76, 98, 132, 143	0
47	D5	137/206 (66%)	1.18	34 (24%) 0 0	118, 147, 190, 205	0
47	H8	135/206 (65%)	0.51	7 (5%) 27 25	89, 115, 161, 183	0
48	E5	77/85 (90%)	0.84	7 (9%) 9 9	81, 97, 115, 148	0
48	I8	80/85 (94%)	0.42	5 (6%) 20 20	66, 78, 106, 122	0
49	F5	94/98 (95%)	0.66	9 (9%) 8 8	72, 94, 135, 145	0
49	J8	97/98 (98%)	0.28	3 (3%) 49 48	60, 79, 122, 155	0
50	G5	66/72 (91%)	0.61	4 (6%) 21 20	95, 113, 128, 155	0
50	K8	67/72 (93%)	0.36	1 (1%) 73 72	70, 89, 107, 139	0
51	H5	59/60 (98%)	0.76	7 (11%) 4 4	87, 104, 146, 161	0
51	L8	57/60 (95%)	0.09	0 100 100	70, 86, 105, 121	0
52	I5	63/71 (88%)	1.50	24 (38%) 0 0	163, 192, 207, 213	0
52	M8	66/71 (92%)	0.77	9 (13%) 3 2	120, 156, 195, 205	0
53	J5	56/60 (93%)	0.13	2 (3%) 42 40	69, 94, 139, 149	0
53	N8	54/60 (90%)	0.20	2 (3%) 41 38	62, 100, 155, 165	0
54	L5	46/49 (93%)	0.09	1 (2%) 62 60	61, 71, 82, 95	0
54	P8	47/49 (95%)	-0.18	0 100 100	53, 60, 76, 85	0
55	M5	60/65 (92%)	0.57	3 (5%) 28 27	78, 90, 114, 129	0
55	Q8	60/65 (92%)	0.13	0 100 100	64, 77, 102, 113	0
56	2L	73/77 (94%)	-0.33	0 100 100	91, 123, 156, 173	0
All	All	20765/21734 (95%)	0.08	951 (4%) 32 30	50, 110, 186, 329	0

The worst 5 of 951 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
13	4A	6	GLY	10.5
31	39	208	GLY	9.4
30	21	204	ALA	8.0
18	9A	88	LYS	8.0
38	45	65	PHE	7.8



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

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
24	4SU	3K	8	20/21	0.44	0.22	240,248,252,254	0
24	7MG	3K	46	24/25	0.68	0.19	234,242,250,254	0
24	4SU	3L	8	20/21	0.70	0.12	239,245,250,250	0
24	PSU	3L	55	20/21	0.71	0.18	244,253,256,256	0
24	7MG	3L	46	24/25	0.75	0.16	242,245,250,252	0
24	PSU	3K	55	20/21	0.78	0.16	233,248,253,253	0
24	MIA	3L	37	29/30	0.78	0.28	158,185,200,208	0
24	PSU	3L	32	20/21	0.80	0.18	165,176,183,185	0
22	5MU	1K	55	21/22	0.87	0.19	147,158,168,170	0
24	PSU	3K	32	20/21	0.88	0.19	149,154,157,159	0
24	PSU	3L	39	20/21	0.89	0.15	156,173,181,188	0
24	MIA	3K	37	29/30	0.90	0.19	139,155,160,161	0
56	4SU	2L	8	20/21	0.91	0.17	127,132,138,139	0
56	PSU	2L	56	20/21	0.92	0.10	116,124,129,135	0
23	4SU	2K	8	20/21	0.92	0.15	101,110,114,119	0
23	PSU	2K	56	20/21	0.92	0.12	95,103,113,113	0
22	OMC	1K	33	21/22	0.93	0.18	114,132,138,141	0
23	7MG	2K	47	24/25	0.94	0.13	113,121,127,130	0
24	PSU	3K	39	20/21	0.94	0.12	126,143,151,159	0
56	7MG	2L	47	24/25	0.94	0.13	137,143,153,157	0
23	OMC	2K	33	21/22	0.95	0.16	84,91,99,106	0
23	5MU	2K	55	21/22	0.95	0.13	96,109,114,116	0
56	OMC	2L	33	21/22	0.96	0.15	105,114,117,119	0

## 6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 6.4 Ligands ⓘ

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



Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
57	MG	1H	3252	1/1	0.17	0.65	92,92,92,92	0
57	MG	13	1667	1/1	0.19	0.38	119,119,119,119	0
57	MG	1G	1631	1/1	0.37	0.24	97,97,97,97	0
57	MG	1H	3199	1/1	0.44	0.29	98,98,98,98	0
57	MG	1H	3259	1/1	0.45	0.27	73,73,73,73	0
57	MG	13	1626	1/1	0.45	0.46	73,73,73,73	0
57	MG	1H	3225	1/1	0.45	0.78	95,95,95,95	0
57	MG	14	3176	1/1	0.49	0.58	85,85,85,85	0
57	MG	13	1662	1/1	0.49	0.56	88,88,88,88	0
57	MG	13	1659	1/1	0.50	0.41	100,100,100,100	0
57	MG	1H	3232	1/1	0.50	0.31	102,102,102,102	0
57	MG	14	3108	1/1	0.51	0.35	77,77,77,77	0
57	MG	14	3164	1/1	0.52	0.76	94,94,94,94	0
57	MG	1H	3096	1/1	0.52	0.27	65,65,65,65	0
57	MG	16	207	1/1	0.53	0.27	88,88,88,88	0
57	MG	14	3213	1/1	0.53	0.41	102,102,102,102	0
57	MG	1H	3174	1/1	0.55	0.29	88,88,88,88	0
57	MG	14	3069	1/1	0.56	0.46	97,97,97,97	0
57	MG	1G	1655	1/1	0.57	0.37	82,82,82,82	0
57	MG	14	3200	1/1	0.57	0.38	90,90,90,90	0
57	MG	14	3179	1/1	0.57	0.56	100,100,100,100	0
57	MG	16	205	1/1	0.58	0.40	90,90,90,90	0
57	MG	1G	1635	1/1	0.59	0.58	79,79,79,79	0
57	MG	13	1671	1/1	0.59	0.46	97,97,97,97	0
57	MG	1H	3148	1/1	0.60	0.16	64,64,64,64	0
57	MG	14	3102	1/1	0.60	0.62	81,81,81,81	0
57	MG	1H	3167	1/1	0.60	0.37	79,79,79,79	0
57	MG	1H	3262	1/1	0.60	0.50	75,75,75,75	0
57	MG	14	3218	1/1	0.61	0.43	74,74,74,74	0
57	MG	1H	3190	1/1	0.61	0.29	94,94,94,94	0
57	MG	14	3094	1/1	0.64	0.56	94,94,94,94	0
57	MG	1G	1672	1/1	0.64	0.09	117,117,117,117	0
57	MG	14	3086	1/1	0.64	0.43	82,82,82,82	0
57	MG	1H	3240	1/1	0.64	0.30	73,73,73,73	0
57	MG	1H	3053	1/1	0.66	0.66	76,76,76,76	0
57	MG	14	3103	1/1	0.66	0.38	74,74,74,74	0
57	MG	14	3166	1/1	0.66	0.48	82,82,82,82	0
57	MG	13	1664	1/1	0.66	0.58	95,95,95,95	0
57	MG	2L	102	1/1	0.66	0.28	96,96,96,96	0
57	MG	14	3124	1/1	0.67	0.49	97,97,97,97	0
57	MG	1H	3100	1/1	0.67	0.40	84,84,84,84	0
57	MG	14	3211	1/1	0.68	0.47	101,101,101,101	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
57	MG	M5	101	1/1	0.68	0.36	85,85,85,85	0
57	MG	1H	3270	1/1	0.68	0.35	102,102,102,102	0
57	MG	14	3107	1/1	0.69	0.32	76,76,76,76	0
57	MG	45	201	1/1	0.69	0.16	98,98,98,98	0
57	MG	1H	3162	1/1	0.70	0.44	83,83,83,83	0
57	MG	1J	201	1/1	0.70	0.32	88,88,88,88	0
57	MG	1H	3169	1/1	0.70	0.70	72,72,72,72	0
57	MG	1G	1648	1/1	0.70	0.26	99,99,99,99	0
57	MG	14	3212	1/1	0.70	1.00	86,86,86,86	0
57	MG	14	3142	1/1	0.70	0.21	86,86,86,86	0
57	MG	14	3170	1/1	0.70	0.80	83,83,83,83	0
57	MG	1G	1663	1/1	0.70	0.25	89,89,89,89	0
57	MG	14	3216	1/1	0.70	0.67	84,84,84,84	0
57	MG	1H	3074	1/1	0.71	0.21	63,63,63,63	0
57	MG	1G	1656	1/1	0.71	0.40	97,97,97,97	0
57	MG	14	3099	1/1	0.71	0.18	108,108,108,108	0
57	MG	14	3167	1/1	0.71	0.31	91,91,91,91	0
57	MG	1H	3102	1/1	0.71	0.28	82,82,82,82	0
57	MG	13	1693	1/1	0.71	0.08	118,118,118,118	0
57	MG	14	3151	1/1	0.71	0.35	71,71,71,71	0
57	MG	1G	1651	1/1	0.71	0.59	94,94,94,94	0
57	MG	1H	3428	1/1	0.71	0.07	103,103,103,103	0
57	MG	1H	3255	1/1	0.71	0.33	81,81,81,81	0
57	MG	1H	3314	1/1	0.71	0.09	86,86,86,86	0
57	MG	1H	3188	1/1	0.72	0.51	82,82,82,82	0
57	MG	14	3291	1/1	0.72	0.11	126,126,126,126	0
57	MG	13	1661	1/1	0.72	0.40	89,89,89,89	0
57	MG	1H	3404	1/1	0.72	0.06	110,110,110,110	0
57	MG	14	3139	1/1	0.72	0.14	93,93,93,93	0
57	MG	1H	3242	1/1	0.72	0.54	79,79,79,79	0
57	MG	1H	3219	1/1	0.72	0.30	77,77,77,77	0
57	MG	1H	3129	1/1	0.72	0.29	93,93,93,93	0
57	MG	1H	3181	1/1	0.73	0.25	75,75,75,75	0
57	MG	16	208	1/1	0.73	0.09	102,102,102,102	0
57	MG	1H	3228	1/1	0.74	0.40	83,83,83,83	0
57	MG	14	3180	1/1	0.74	0.39	112,112,112,112	0
57	MG	1H	3186	1/1	0.75	0.35	72,72,72,72	0
57	MG	13	1645	1/1	0.75	0.23	89,89,89,89	0
57	MG	14	3156	1/1	0.76	0.43	107,107,107,107	0
57	MG	1H	3224	1/1	0.76	0.52	66,66,66,66	0
57	MG	1H	3152	1/1	0.76	0.38	92,92,92,92	0
57	MG	14	3304	1/1	0.76	0.12	103,103,103,103	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
57	MG	1H	3098	1/1	0.76	0.27	83,83,83,83	0
57	MG	1H	3247	1/1	0.76	0.18	97,97,97,97	0
57	MG	1H	3140	1/1	0.76	0.33	74,74,74,74	0
57	MG	1H	3170	1/1	0.76	0.49	88,88,88,88	0
57	MG	29	302	1/1	0.77	0.17	68,68,68,68	0
57	MG	14	3098	1/1	0.77	0.36	78,78,78,78	0
57	MG	13	1612	1/1	0.77	0.24	84,84,84,84	0
57	MG	1H	3248	1/1	0.77	0.34	76,76,76,76	0
57	MG	1H	3277	1/1	0.77	0.46	89,89,89,89	0
57	MG	14	3307	1/1	0.77	0.15	91,91,91,91	0
57	MG	13	1634	1/1	0.77	0.19	110,110,110,110	0
57	MG	1H	3018	1/1	0.78	0.12	80,80,80,80	0
57	MG	1H	3230	1/1	0.78	0.73	97,97,97,97	0
57	MG	1H	3177	1/1	0.78	0.24	57,57,57,57	0
57	MG	1H	3024	1/1	0.78	0.23	72,72,72,72	0
57	MG	1H	3163	1/1	0.78	0.28	65,65,65,65	0
57	MG	1H	3198	1/1	0.78	0.62	77,77,77,77	0
57	MG	1G	1621	1/1	0.78	0.76	92,92,92,92	0
57	MG	1H	3204	1/1	0.78	0.94	77,77,77,77	0
57	MG	14	3194	1/1	0.78	0.28	79,79,79,79	0
57	MG	1H	3073	1/1	0.78	0.36	55,55,55,55	0
57	MG	68	201	1/1	0.79	0.37	80,80,80,80	0
57	MG	1H	3078	1/1	0.79	0.15	73,73,73,73	0
57	MG	1H	3064	1/1	0.79	0.26	52,52,52,52	0
57	MG	1H	3244	1/1	0.79	0.53	88,88,88,88	0
57	MG	1H	3423	1/1	0.79	0.09	65,65,65,65	0
57	MG	1H	3271	1/1	0.79	0.59	90,90,90,90	0
57	MG	1G	1661	1/1	0.79	0.16	109,109,109,109	0
57	MG	14	3189	1/1	0.79	0.28	69,69,69,69	0
57	MG	2K	102	1/1	0.79	0.11	111,111,111,111	0
57	MG	1H	3261	1/1	0.79	0.68	80,80,80,80	0
57	MG	14	3310	1/1	0.79	0.10	102,102,102,102	0
57	MG	1H	3164	1/1	0.79	0.31	66,66,66,66	0
57	MG	14	3160	1/1	0.79	0.22	83,83,83,83	0
57	MG	14	3122	1/1	0.80	0.18	76,76,76,76	0
57	MG	14	3135	1/1	0.80	0.37	74,74,74,74	0
57	MG	1H	3172	1/1	0.80	0.39	73,73,73,73	0
57	MG	13	1642	1/1	0.80	0.47	80,80,80,80	0
57	MG	14	3022	1/1	0.80	0.08	89,89,89,89	0
57	MG	14	3111	1/1	0.80	0.34	89,89,89,89	0
57	MG	14	3201	1/1	0.80	0.61	78,78,78,78	0
57	MG	14	3302	1/1	0.80	0.10	106,106,106,106	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
57	MG	14	3174	1/1	0.80	0.86	87,87,87,87	0
57	MG	1H	3236	1/1	0.81	0.37	80,80,80,80	0
57	MG	1H	3191	1/1	0.81	0.62	102,102,102,102	0
57	MG	13	1663	1/1	0.81	0.76	77,77,77,77	0
57	MG	1H	3443	1/1	0.81	0.08	100,100,100,100	0
57	MG	14	3060	1/1	0.81	0.55	83,83,83,83	0
57	MG	1H	3257	1/1	0.81	0.59	90,90,90,90	0
57	MG	14	3112	1/1	0.81	0.38	78,78,78,78	0
57	MG	68	202	1/1	0.81	0.45	91,91,91,91	0
57	MG	1H	3111	1/1	0.81	0.39	71,71,71,71	0
57	MG	14	3271	1/1	0.81	0.13	92,92,92,92	0
57	MG	1H	3059	1/1	0.81	0.28	75,75,75,75	0
57	MG	1H	3269	1/1	0.81	0.69	74,74,74,74	0
57	MG	1H	3274	1/1	0.81	0.88	86,86,86,86	0
57	MG	1H	3427	1/1	0.81	0.07	122,122,122,122	0
57	MG	1H	3251	1/1	0.81	0.58	84,84,84,84	0
57	MG	1H	3136	1/1	0.81	0.22	55,55,55,55	0
57	MG	14	3195	1/1	0.81	0.52	88,88,88,88	0
58	ZN	G8	201	1/1	0.81	0.26	176,176,176,176	0
57	MG	14	3083	1/1	0.81	0.41	57,57,57,57	0
57	MG	14	3020	1/1	0.81	0.60	76,76,76,76	0
57	MG	1H	3110	1/1	0.82	0.52	84,84,84,84	0
57	MG	13	1632	1/1	0.82	0.50	74,74,74,74	0
57	MG	1H	3070	1/1	0.82	0.31	64,64,64,64	0
57	MG	14	3327	1/1	0.82	0.08	108,108,108,108	0
57	MG	1G	1658	1/1	0.82	0.13	132,132,132,132	0
57	MG	14	3178	1/1	0.82	0.29	76,76,76,76	0
57	MG	1H	3377	1/1	0.82	0.07	103,103,103,103	0
57	MG	1H	3130	1/1	0.82	0.41	81,81,81,81	0
57	MG	1G	1652	1/1	0.82	0.31	82,82,82,82	0
57	MG	1H	3095	1/1	0.82	0.36	74,74,74,74	0
57	MG	1H	3109	1/1	0.82	0.27	76,76,76,76	0
57	MG	1J	202	1/1	0.82	0.36	74,74,74,74	0
57	MG	1H	3143	1/1	0.82	0.37	64,64,64,64	0
57	MG	14	3143	1/1	0.82	0.16	92,92,92,92	0
57	MG	13	1655	1/1	0.83	0.40	81,81,81,81	0
57	MG	1H	3182	1/1	0.83	0.25	78,78,78,78	0
57	MG	1G	1659	1/1	0.83	0.30	101,101,101,101	0
57	MG	14	3027	1/1	0.83	0.14	94,94,94,94	0
57	MG	1H	3119	1/1	0.83	0.67	62,62,62,62	0
57	MG	1G	1644	1/1	0.83	0.37	90,90,90,90	0
57	MG	13	1652	1/1	0.83	0.16	104,104,104,104	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
57	MG	1H	3178	1/1	0.83	0.19	91,91,91,91	0
57	MG	1G	1620	1/1	0.83	0.50	71,71,71,71	0
57	MG	1H	3087	1/1	0.83	0.31	80,80,80,80	0
57	MG	14	3116	1/1	0.83	0.35	60,60,60,60	0
57	MG	1H	3278	1/1	0.83	0.66	68,68,68,68	0
57	MG	1G	1614	1/1	0.83	0.49	72,72,72,72	0
57	MG	1H	3201	1/1	0.83	0.55	68,68,68,68	0
57	MG	1H	3218	1/1	0.84	0.56	91,91,91,91	0
57	MG	1H	3107	1/1	0.84	0.29	81,81,81,81	0
57	MG	1G	1670	1/1	0.84	0.11	129,129,129,129	0
57	MG	14	3318	1/1	0.84	0.14	84,84,84,84	0
57	MG	1H	3229	1/1	0.84	0.12	72,72,72,72	0
57	MG	14	3125	1/1	0.84	0.58	68,68,68,68	0
57	MG	1H	3099	1/1	0.84	0.09	88,88,88,88	0
57	MG	1G	1657	1/1	0.84	0.76	91,91,91,91	0
57	MG	1H	3138	1/1	0.84	0.11	67,67,67,67	0
57	MG	13	1627	1/1	0.84	0.52	84,84,84,84	0
57	MG	13	1650	1/1	0.84	0.34	88,88,88,88	0
57	MG	1G	1624	1/1	0.84	0.37	71,71,71,71	0
57	MG	1G	1612	1/1	0.84	0.14	99,99,99,99	0
57	MG	1H	3392	1/1	0.84	0.16	96,96,96,96	0
57	MG	14	3089	1/1	0.85	0.20	56,56,56,56	0
57	MG	1H	3444	1/1	0.85	0.08	96,96,96,96	0
57	MG	1H	3253	1/1	0.85	0.41	67,67,67,67	0
58	ZN	C5	201	1/1	0.85	0.22	187,187,187,187	0
57	MG	11	303	1/1	0.85	0.64	48,48,48,48	0
57	MG	13	1665	1/1	0.85	0.40	86,86,86,86	0
57	MG	1G	1636	1/1	0.85	0.24	96,96,96,96	0
57	MG	1H	3221	1/1	0.85	0.42	79,79,79,79	0
57	MG	1H	3243	1/1	0.85	0.52	65,65,65,65	0
57	MG	1G	1668	1/1	0.85	0.07	120,120,120,120	0
57	MG	1H	3168	1/1	0.85	0.43	100,100,100,100	0
57	MG	14	3084	1/1	0.85	0.18	82,82,82,82	0
57	MG	14	3214	1/1	0.85	0.25	84,84,84,84	0
57	MG	1H	3126	1/1	0.85	0.30	67,67,67,67	0
57	MG	1G	1641	1/1	0.85	0.22	113,113,113,113	0
57	MG	14	3093	1/1	0.85	0.20	62,62,62,62	0
57	MG	14	3157	1/1	0.85	0.76	79,79,79,79	0
57	MG	14	3172	1/1	0.86	0.38	68,68,68,68	0
57	MG	1H	3197	1/1	0.86	0.36	53,53,53,53	0
57	MG	14	3100	1/1	0.86	0.32	82,82,82,82	0
57	MG	1H	3215	1/1	0.86	0.34	79,79,79,79	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
57	MG	11	301	1/1	0.86	0.31	62,62,62,62	0
57	MG	13	1670	1/1	0.86	0.12	101,101,101,101	0
57	MG	1H	3216	1/1	0.86	0.38	75,75,75,75	0
57	MG	1H	3042	1/1	0.86	0.27	77,77,77,77	0
57	MG	14	3185	1/1	0.86	0.70	71,71,71,71	0
57	MG	1H	3154	1/1	0.86	0.37	101,101,101,101	0
57	MG	13	1614	1/1	0.86	0.61	70,70,70,70	0
57	MG	1H	3092	1/1	0.86	0.30	67,67,67,67	0
57	MG	14	3206	1/1	0.86	0.29	78,78,78,78	0
57	MG	1H	3202	1/1	0.86	0.36	84,84,84,84	0
57	MG	1H	3141	1/1	0.86	0.33	81,81,81,81	0
57	MG	14	3169	1/1	0.86	0.32	59,59,59,59	0
57	MG	1H	3116	1/1	0.86	0.18	80,80,80,80	0
57	MG	1H	3196	1/1	0.86	0.29	84,84,84,84	0
57	MG	1H	3075	1/1	0.86	0.46	59,59,59,59	0
57	MG	1G	1611	1/1	0.86	0.11	98,98,98,98	0
57	MG	13	1630	1/1	0.86	0.27	83,83,83,83	0
57	MG	1H	3142	1/1	0.87	0.36	55,55,55,55	0
57	MG	14	3171	1/1	0.87	0.56	71,71,71,71	0
57	MG	1H	3088	1/1	0.87	0.25	65,65,65,65	0
57	MG	1H	3414	1/1	0.87	0.09	87,87,87,87	0
57	MG	14	3109	1/1	0.87	0.31	84,84,84,84	0
57	MG	14	3288	1/1	0.87	0.09	108,108,108,108	0
57	MG	14	3299	1/1	0.87	0.05	114,114,114,114	0
57	MG	14	3199	1/1	0.87	0.54	95,95,95,95	0
57	MG	1H	3150	1/1	0.87	0.28	65,65,65,65	0
57	MG	1H	3091	1/1	0.87	0.21	71,71,71,71	0
57	MG	1H	3106	1/1	0.87	0.40	69,69,69,69	0
57	MG	13	1618	1/1	0.87	0.39	63,63,63,63	0
57	MG	13	1696	1/1	0.87	0.05	101,101,101,101	0
57	MG	1H	3151	1/1	0.87	0.39	75,75,75,75	0
57	MG	1H	3400	1/1	0.87	0.08	85,85,85,85	0
57	MG	1H	3227	1/1	0.87	0.67	66,66,66,66	0
57	MG	14	3161	1/1	0.87	0.47	88,88,88,88	0
57	MG	1H	3115	1/1	0.87	0.20	63,63,63,63	0
57	MG	14	3031	1/1	0.87	0.42	73,73,73,73	0
57	MG	1H	3157	1/1	0.87	0.13	89,89,89,89	0
57	MG	14	3294	1/1	0.87	0.09	107,107,107,107	0
57	MG	1H	3121	1/1	0.87	0.55	73,73,73,73	0
57	MG	14	3210	1/1	0.88	0.20	78,78,78,78	0
57	MG	14	3153	1/1	0.88	0.49	87,87,87,87	0
57	MG	13	1646	1/1	0.88	0.18	102,102,102,102	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
57	MG	1H	3390	1/1	0.88	0.08	99,99,99,99	0
57	MG	14	3095	1/1	0.88	0.42	83,83,83,83	0
57	MG	1G	1664	1/1	0.88	0.65	87,87,87,87	0
57	MG	1H	3263	1/1	0.88	0.70	75,75,75,75	0
57	MG	14	3191	1/1	0.88	0.22	72,72,72,72	0
57	MG	14	3217	1/1	0.88	0.11	83,83,83,83	0
57	MG	14	3264	1/1	0.88	0.19	57,57,57,57	0
57	MG	1G	1634	1/1	0.88	0.21	93,93,93,93	0
57	MG	1G	1615	1/1	0.88	0.49	90,90,90,90	0
57	MG	1H	3418	1/1	0.88	0.06	82,82,82,82	0
57	MG	L8	101	1/1	0.88	0.35	70,70,70,70	0
57	MG	14	3203	1/1	0.88	0.42	83,83,83,83	0
57	MG	1H	3082	1/1	0.88	0.29	60,60,60,60	0
57	MG	1G	1623	1/1	0.88	0.53	66,66,66,66	0
57	MG	1H	3160	1/1	0.88	0.39	67,67,67,67	0
57	MG	1H	3114	1/1	0.88	0.40	77,77,77,77	0
57	MG	1H	3060	1/1	0.88	0.29	63,63,63,63	0
57	MG	1H	3233	1/1	0.88	0.80	86,86,86,86	0
57	MG	1H	3180	1/1	0.88	0.16	80,80,80,80	0
57	MG	1H	3175	1/1	0.88	0.48	64,64,64,64	0
57	MG	1H	3331	1/1	0.88	0.08	74,74,74,74	0
57	MG	13	1677	1/1	0.89	0.14	98,98,98,98	0
57	MG	14	3260	1/1	0.89	0.09	86,86,86,86	0
57	MG	13	1672	1/1	0.89	0.88	84,84,84,84	0
57	MG	14	3283	1/1	0.89	0.14	74,74,74,74	0
57	MG	14	3219	1/1	0.89	0.56	81,81,81,81	0
57	MG	14	3092	1/1	0.89	0.77	79,79,79,79	0
57	MG	14	3090	1/1	0.89	0.20	77,77,77,77	0
57	MG	1H	3025	1/1	0.89	0.18	66,66,66,66	0
57	MG	1H	3354	1/1	0.89	0.20	66,66,66,66	0
57	MG	1H	3179	1/1	0.89	0.41	81,81,81,81	0
57	MG	13	1628	1/1	0.89	0.19	90,90,90,90	0
57	MG	1G	1642	1/1	0.89	0.26	93,93,93,93	0
57	MG	14	3074	1/1	0.89	0.27	82,82,82,82	0
57	MG	1H	3226	1/1	0.89	0.42	70,70,70,70	0
57	MG	14	3182	1/1	0.89	0.24	84,84,84,84	0
57	MG	14	3096	1/1	0.89	0.35	70,70,70,70	0
57	MG	14	3041	1/1	0.89	0.24	60,60,60,60	0
57	MG	14	3229	1/1	0.89	0.09	82,82,82,82	0
57	MG	16	203	1/1	0.89	0.10	98,98,98,98	0
57	MG	1H	3068	1/1	0.89	0.10	63,63,63,63	0
57	MG	3E	301	1/1	0.89	0.13	127,127,127,127	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
57	MG	14	3244	1/1	0.89	0.10	93,93,93,93	0
57	MG	1H	3062	1/1	0.89	0.61	78,78,78,78	0
57	MG	16	204	1/1	0.89	0.10	78,78,78,78	0
57	MG	14	3292	1/1	0.89	0.08	91,91,91,91	0
57	MG	14	3325	1/1	0.89	0.10	104,104,104,104	0
57	MG	1H	3076	1/1	0.89	0.28	77,77,77,77	0
57	MG	16	211	1/1	0.89	0.07	99,99,99,99	0
57	MG	13	1687	1/1	0.89	0.08	103,103,103,103	0
57	MG	13	1633	1/1	0.89	0.39	90,90,90,90	0
57	MG	1H	3184	1/1	0.89	0.34	86,86,86,86	0
57	MG	1H	3090	1/1	0.89	0.33	47,47,47,47	0
57	MG	1H	3012	1/1	0.89	0.39	69,69,69,69	0
57	MG	1H	3069	1/1	0.89	0.15	69,69,69,69	0
57	MG	14	3196	1/1	0.89	0.37	86,86,86,86	0
57	MG	1H	3146	1/1	0.89	0.51	80,80,80,80	0
57	MG	14	3228	1/1	0.89	0.08	69,69,69,69	0
57	MG	14	3198	1/1	0.89	0.66	86,86,86,86	0
57	MG	1H	3256	1/1	0.89	0.52	72,72,72,72	0
57	MG	13	1615	1/1	0.89	0.34	85,85,85,85	0
57	MG	1H	3382	1/1	0.89	0.07	74,74,74,74	0
57	MG	14	3296	1/1	0.90	0.12	110,110,110,110	0
57	MG	1H	3173	1/1	0.90	0.57	99,99,99,99	0
57	MG	14	3234	1/1	0.90	0.12	86,86,86,86	0
57	MG	1H	3396	1/1	0.90	0.07	80,80,80,80	0
57	MG	1G	1654	1/1	0.90	0.38	92,92,92,92	0
57	MG	1H	3166	1/1	0.90	0.41	75,75,75,75	0
57	MG	13	1619	1/1	0.90	0.28	72,72,72,72	0
57	MG	14	3132	1/1	0.90	0.29	81,81,81,81	0
57	MG	1G	1622	1/1	0.90	0.41	80,80,80,80	0
57	MG	14	3036	1/1	0.90	0.38	64,64,64,64	0
57	MG	1H	3267	1/1	0.90	0.34	106,106,106,106	0
57	MG	1G	1653	1/1	0.90	0.26	91,91,91,91	0
57	MG	1H	3320	1/1	0.90	0.14	76,76,76,76	0
57	MG	14	3263	1/1	0.90	0.06	99,99,99,99	0
57	MG	14	3257	1/1	0.90	0.12	89,89,89,89	0
57	MG	14	3207	1/1	0.90	0.33	70,70,70,70	0
57	MG	1H	3254	1/1	0.90	0.44	94,94,94,94	0
57	MG	13	1640	1/1	0.90	0.08	141,141,141,141	0
57	MG	13	1657	1/1	0.90	0.24	129,129,129,129	0
57	MG	14	3047	1/1	0.90	0.43	56,56,56,56	0
57	MG	13	1673	1/1	0.90	0.32	87,87,87,87	0
57	MG	13	1616	1/1	0.90	0.38	93,93,93,93	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
57	MG	14	3117	1/1	0.90	0.37	80,80,80,80	0
57	MG	1G	1626	1/1	0.90	0.28	81,81,81,81	0
57	MG	14	3148	1/1	0.90	0.31	93,93,93,93	0
57	MG	1H	3183	1/1	0.90	0.60	87,87,87,87	0
57	MG	13	1699	1/1	0.90	0.07	119,119,119,119	0
57	MG	1H	3316	1/1	0.90	0.08	75,75,75,75	0
57	MG	1H	3135	1/1	0.90	0.28	74,74,74,74	0
57	MG	1H	3123	1/1	0.90	0.28	58,58,58,58	0
57	MG	14	3197	1/1	0.90	0.32	78,78,78,78	0
57	MG	1H	3371	1/1	0.90	0.13	66,66,66,66	0
57	MG	13	1638	1/1	0.90	0.56	84,84,84,84	0
57	MG	14	3278	1/1	0.90	0.04	109,109,109,109	0
57	MG	11	302	1/1	0.90	0.35	48,48,48,48	0
57	MG	13	1643	1/1	0.90	0.23	91,91,91,91	0
57	MG	1H	3239	1/1	0.91	0.52	71,71,71,71	0
57	MG	13	1698	1/1	0.91	0.11	105,105,105,105	0
57	MG	13	1647	1/1	0.91	0.31	81,81,81,81	0
57	MG	1H	3037	1/1	0.91	0.37	55,55,55,55	0
57	MG	14	3137	1/1	0.91	0.12	76,76,76,76	0
57	MG	14	3141	1/1	0.91	0.29	67,67,67,67	0
57	MG	14	3175	1/1	0.91	0.31	75,75,75,75	0
57	MG	1H	3348	1/1	0.91	0.12	90,90,90,90	0
57	MG	13	1656	1/1	0.91	0.18	96,96,96,96	0
57	MG	1H	3385	1/1	0.91	0.08	112,112,112,112	0
57	MG	13	1649	1/1	0.91	0.07	97,97,97,97	0
57	MG	14	3150	1/1	0.91	0.23	79,79,79,79	0
57	MG	1H	3275	1/1	0.91	0.21	63,63,63,63	0
57	MG	1G	1665	1/1	0.91	0.07	117,117,117,117	0
57	MG	1H	3386	1/1	0.91	0.06	96,96,96,96	0
57	MG	1H	3250	1/1	0.91	0.29	71,71,71,71	0
57	MG	1H	3279	1/1	0.91	0.27	78,78,78,78	0
57	MG	1H	3223	1/1	0.91	0.31	63,63,63,63	0
57	MG	1H	3203	1/1	0.91	0.28	62,62,62,62	0
57	MG	14	3312	1/1	0.91	0.09	115,115,115,115	0
57	MG	1H	3346	1/1	0.91	0.09	58,58,58,58	0
57	MG	13	1689	1/1	0.91	0.10	115,115,115,115	0
57	MG	14	3119	1/1	0.91	0.24	67,67,67,67	0
57	MG	1H	3147	1/1	0.91	0.16	74,74,74,74	0
57	MG	1H	3235	1/1	0.91	0.52	69,69,69,69	0
57	MG	1H	3101	1/1	0.91	0.41	70,70,70,70	0
57	MG	1H	3089	1/1	0.91	0.29	74,74,74,74	0
57	MG	14	3277	1/1	0.91	0.07	98,98,98,98	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
57	MG	14	3044	1/1	0.91	0.29	82,82,82,82	0
57	MG	1H	3085	1/1	0.91	0.15	58,58,58,58	0
57	MG	1H	3205	1/1	0.92	0.64	73,73,73,73	0
57	MG	14	3043	1/1	0.92	0.29	71,71,71,71	0
57	MG	1H	3402	1/1	0.92	0.10	88,88,88,88	0
57	MG	13	1623	1/1	0.92	0.21	77,77,77,77	0
57	MG	1H	3124	1/1	0.92	0.12	61,61,61,61	0
57	MG	1H	3276	1/1	0.92	0.37	67,67,67,67	0
57	MG	13	1674	1/1	0.92	0.13	83,83,83,83	0
57	MG	1H	3023	1/1	0.92	0.18	68,68,68,68	0
57	MG	13	1639	1/1	0.92	0.61	83,83,83,83	0
57	MG	16	206	1/1	0.92	0.32	83,83,83,83	0
57	MG	1H	3379	1/1	0.92	0.12	83,83,83,83	0
57	MG	1H	3034	1/1	0.92	0.18	62,62,62,62	0
57	MG	1H	3220	1/1	0.92	0.40	62,62,62,62	0
57	MG	14	3186	1/1	0.92	0.35	75,75,75,75	0
57	MG	1H	3388	1/1	0.92	0.09	75,75,75,75	0
57	MG	13	1660	1/1	0.92	0.28	61,61,61,61	0
57	MG	1H	3077	1/1	0.92	0.51	65,65,65,65	0
57	MG	1H	3391	1/1	0.92	0.07	91,91,91,91	0
57	MG	1G	1608	1/1	0.92	0.31	88,88,88,88	0
57	MG	1G	1646	1/1	0.92	0.16	117,117,117,117	0
57	MG	1H	3194	1/1	0.92	0.13	83,83,83,83	0
57	MG	1H	3300	1/1	0.92	0.08	68,68,68,68	0
57	MG	1H	3158	1/1	0.92	0.35	59,59,59,59	0
57	MG	1H	3195	1/1	0.92	0.89	70,70,70,70	0
57	MG	1H	3043	1/1	0.92	0.14	75,75,75,75	0
57	MG	16	201	1/1	0.92	0.17	90,90,90,90	0
57	MG	35	201	1/1	0.92	0.14	77,77,77,77	0
57	MG	14	3097	1/1	0.92	0.10	62,62,62,62	0
57	MG	1H	3287	1/1	0.92	0.10	71,71,71,71	0
57	MG	14	3025	1/1	0.92	0.23	95,95,95,95	0
57	MG	14	3184	1/1	0.92	0.65	75,75,75,75	0
57	MG	13	1624	1/1	0.92	0.17	84,84,84,84	0
57	MG	I8	101	1/1	0.92	0.08	91,91,91,91	0
57	MG	1H	3171	1/1	0.92	0.47	84,84,84,84	0
57	MG	41	201	1/1	0.92	0.09	82,82,82,82	0
57	MG	1H	3083	1/1	0.92	0.31	61,61,61,61	0
57	MG	14	3105	1/1	0.92	0.23	89,89,89,89	0
57	MG	14	3315	1/1	0.92	0.10	80,80,80,80	0
57	MG	14	3048	1/1	0.92	0.27	59,59,59,59	0
57	MG	14	3243	1/1	0.92	0.11	74,74,74,74	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
57	MG	1H	3017	1/1	0.92	0.20	81,81,81,81	0
57	MG	1G	1645	1/1	0.92	0.20	107,107,107,107	0
57	MG	1H	3315	1/1	0.92	0.21	81,81,81,81	0
57	MG	1H	3021	1/1	0.92	0.36	62,62,62,62	0
57	MG	1H	3416	1/1	0.92	0.09	81,81,81,81	0
57	MG	1H	3308	1/1	0.92	0.05	91,91,91,91	0
57	MG	1H	3398	1/1	0.92	0.07	98,98,98,98	0
57	MG	1H	3268	1/1	0.92	0.17	96,96,96,96	0
57	MG	13	1683	1/1	0.92	0.11	96,96,96,96	0
57	MG	1G	1660	1/1	0.92	0.23	124,124,124,124	0
57	MG	1G	1605	1/1	0.92	0.10	104,104,104,104	0
57	MG	1H	3210	1/1	0.93	0.15	70,70,70,70	0
57	MG	1H	3397	1/1	0.93	0.15	76,76,76,76	0
57	MG	14	3220	1/1	0.93	0.26	84,84,84,84	0
57	MG	1H	3222	1/1	0.93	0.63	81,81,81,81	0
57	MG	14	3183	1/1	0.93	0.40	77,77,77,77	0
57	MG	14	3306	1/1	0.93	0.07	82,82,82,82	0
57	MG	14	3223	1/1	0.93	0.13	79,79,79,79	0
57	MG	1H	3217	1/1	0.93	0.36	97,97,97,97	0
57	MG	1G	1633	1/1	0.93	0.09	141,141,141,141	0
57	MG	1H	3122	1/1	0.93	0.39	81,81,81,81	0
57	MG	13	1666	1/1	0.93	0.23	116,116,116,116	0
57	MG	78	201	1/1	0.93	0.26	60,60,60,60	0
57	MG	4E	201	1/1	0.93	0.46	88,88,88,88	0
57	MG	14	3032	1/1	0.93	0.38	98,98,98,98	0
57	MG	14	3127	1/1	0.93	0.22	77,77,77,77	0
57	MG	14	3308	1/1	0.93	0.07	106,106,106,106	0
57	MG	1H	3237	1/1	0.93	0.51	64,64,64,64	0
57	MG	1H	3249	1/1	0.93	0.24	79,79,79,79	0
57	MG	1H	3326	1/1	0.93	0.11	105,105,105,105	0
57	MG	14	3246	1/1	0.93	0.09	96,96,96,96	0
57	MG	1H	3265	1/1	0.93	0.20	83,83,83,83	0
57	MG	14	3293	1/1	0.93	0.08	84,84,84,84	0
57	MG	14	3326	1/1	0.93	0.09	104,104,104,104	0
57	MG	14	3140	1/1	0.93	0.20	54,54,54,54	0
57	MG	1H	3071	1/1	0.93	0.27	66,66,66,66	0
57	MG	1H	3156	1/1	0.93	0.31	81,81,81,81	0
57	MG	1G	1606	1/1	0.93	0.22	92,92,92,92	0
57	MG	1H	3439	1/1	0.93	0.15	65,65,65,65	0
57	MG	14	3323	1/1	0.93	0.11	73,73,73,73	0
57	MG	1H	3131	1/1	0.93	0.31	67,67,67,67	0
57	MG	13	1635	1/1	0.93	0.20	92,92,92,92	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
57	MG	14	3114	1/1	0.93	0.46	88,88,88,88	0
57	MG	14	3046	1/1	0.93	0.44	61,61,61,61	0
57	MG	1G	1613	1/1	0.93	0.17	89,89,89,89	0
57	MG	1H	3022	1/1	0.93	0.23	64,64,64,64	0
57	MG	14	3215	1/1	0.93	0.28	97,97,97,97	0
57	MG	1H	3231	1/1	0.93	0.44	79,79,79,79	0
57	MG	1G	1610	1/1	0.93	0.20	111,111,111,111	0
57	MG	14	3162	1/1	0.93	0.19	102,102,102,102	0
57	MG	1H	3241	1/1	0.93	0.37	73,73,73,73	0
57	MG	14	3254	1/1	0.93	0.17	69,69,69,69	0
57	MG	14	3013	1/1	0.93	0.37	55,55,55,55	0
57	MG	1G	1616	1/1	0.93	0.20	105,105,105,105	0
57	MG	1H	3441	1/1	0.93	0.13	70,70,70,70	0
57	MG	14	3250	1/1	0.93	0.12	56,56,56,56	0
57	MG	1H	3097	1/1	0.93	0.41	93,93,93,93	0
57	MG	1H	3434	1/1	0.93	0.14	68,68,68,68	0
57	MG	1H	3145	1/1	0.93	0.66	66,66,66,66	0
57	MG	1G	1639	1/1	0.93	0.15	90,90,90,90	0
57	MG	14	3190	1/1	0.93	0.46	72,72,72,72	0
57	MG	13	1611	1/1	0.93	0.18	107,107,107,107	0
57	MG	13	1621	1/1	0.93	0.22	88,88,88,88	0
57	MG	1J	203	1/1	0.93	0.36	90,90,90,90	0
57	MG	1H	3011	1/1	0.93	0.55	63,63,63,63	0
57	MG	1H	3324	1/1	0.93	0.05	76,76,76,76	0
57	MG	1H	3245	1/1	0.93	0.49	96,96,96,96	0
57	MG	1H	3318	1/1	0.93	0.12	55,55,55,55	0
57	MG	1H	3207	1/1	0.93	0.37	80,80,80,80	0
57	MG	13	1610	1/1	0.93	0.24	72,72,72,72	0
57	MG	14	3039	1/1	0.93	0.59	75,75,75,75	0
57	MG	14	3061	1/1	0.93	0.56	67,67,67,67	0
57	MG	1H	3258	1/1	0.93	0.41	86,86,86,86	0
57	MG	14	3181	1/1	0.93	0.44	85,85,85,85	0
57	MG	1H	3289	1/1	0.93	0.10	48,48,48,48	0
57	MG	14	3063	1/1	0.93	0.25	80,80,80,80	0
57	MG	14	3075	1/1	0.94	0.26	103,103,103,103	0
57	MG	1H	3117	1/1	0.94	0.23	74,74,74,74	0
57	MG	98	201	1/1	0.94	0.44	70,70,70,70	0
57	MG	14	3238	1/1	0.94	0.13	76,76,76,76	0
57	MG	1H	3125	1/1	0.94	0.46	77,77,77,77	0
57	MG	1H	3411	1/1	0.94	0.09	133,133,133,133	0
57	MG	14	3227	1/1	0.94	0.13	64,64,64,64	0
57	MG	13	1608	1/1	0.94	0.15	88,88,88,88	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
57	MG	14	3205	1/1	0.94	0.62	80,80,80,80	0
57	MG	1H	3084	1/1	0.94	0.15	53,53,53,53	0
57	MG	13	1617	1/1	0.94	0.62	70,70,70,70	0
57	MG	1H	3234	1/1	0.94	0.56	86,86,86,86	0
57	MG	1G	1650	1/1	0.94	0.31	86,86,86,86	0
57	MG	14	3088	1/1	0.94	0.30	76,76,76,76	0
57	MG	1H	3419	1/1	0.94	0.10	83,83,83,83	0
57	MG	1H	3104	1/1	0.94	0.30	69,69,69,69	0
57	MG	1H	3328	1/1	0.94	0.05	91,91,91,91	0
57	MG	1H	3406	1/1	0.94	0.12	106,106,106,106	0
57	MG	14	3134	1/1	0.94	0.14	72,72,72,72	0
57	MG	16	210	1/1	0.94	0.05	88,88,88,88	0
57	MG	1H	3189	1/1	0.94	0.26	70,70,70,70	0
57	MG	14	3021	1/1	0.94	0.40	65,65,65,65	0
57	MG	14	3239	1/1	0.94	0.09	92,92,92,92	0
57	MG	1H	3035	1/1	0.94	0.18	64,64,64,64	0
57	MG	13	1676	1/1	0.94	0.11	110,110,110,110	0
57	MG	14	3281	1/1	0.94	0.09	95,95,95,95	0
57	MG	1H	3417	1/1	0.94	0.07	73,73,73,73	0
57	MG	14	3128	1/1	0.94	0.16	98,98,98,98	0
57	MG	1H	3408	1/1	0.94	0.07	67,67,67,67	0
57	MG	1H	3415	1/1	0.94	0.09	105,105,105,105	0
57	MG	14	3290	1/1	0.94	0.03	114,114,114,114	0
57	MG	14	3268	1/1	0.94	0.11	84,84,84,84	0
57	MG	1G	1625	1/1	0.94	0.42	81,81,81,81	0
57	MG	14	3058	1/1	0.94	0.32	77,77,77,77	0
57	MG	14	3026	1/1	0.94	0.07	83,83,83,83	0
57	MG	1H	3159	1/1	0.94	0.46	67,67,67,67	0
57	MG	1H	3403	1/1	0.94	0.11	76,76,76,76	0
57	MG	14	3245	1/1	0.94	0.04	99,99,99,99	0
57	MG	14	3023	1/1	0.94	0.33	50,50,50,50	0
57	MG	1H	3357	1/1	0.94	0.05	77,77,77,77	0
57	MG	1H	3103	1/1	0.94	0.23	80,80,80,80	0
57	MG	1H	3272	1/1	0.94	0.35	71,71,71,71	0
57	MG	14	3104	1/1	0.94	0.48	68,68,68,68	0
57	MG	1H	3094	1/1	0.94	0.36	60,60,60,60	0
57	MG	14	3113	1/1	0.94	0.22	76,76,76,76	0
57	MG	29	301	1/1	0.94	0.34	67,67,67,67	0
57	MG	1G	1607	1/1	0.94	0.12	98,98,98,98	0
57	MG	13	1637	1/1	0.94	0.17	105,105,105,105	0
57	MG	1H	3384	1/1	0.94	0.08	68,68,68,68	0
57	MG	1G	1628	1/1	0.94	0.17	108,108,108,108	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
57	MG	1G	1647	1/1	0.94	0.56	101,101,101,101	0
57	MG	13	1685	1/1	0.94	0.13	93,93,93,93	0
57	MG	1H	3282	1/1	0.94	0.09	65,65,65,65	0
57	MG	1H	3336	1/1	0.94	0.10	67,67,67,67	0
57	MG	13	1669	1/1	0.94	0.40	79,79,79,79	0
57	MG	J8	102	1/1	0.94	0.19	68,68,68,68	0
57	MG	1H	3280	1/1	0.94	0.44	72,72,72,72	0
57	MG	1H	3273	1/1	0.94	0.61	85,85,85,85	0
57	MG	1H	3108	1/1	0.94	0.99	73,73,73,73	0
57	MG	14	3230	1/1	0.94	0.10	65,65,65,65	0
57	MG	14	3311	1/1	0.94	0.11	78,78,78,78	0
57	MG	1H	3086	1/1	0.94	0.46	48,48,48,48	0
57	MG	13	1668	1/1	0.94	0.17	119,119,119,119	0
57	MG	1H	3120	1/1	0.94	0.42	56,56,56,56	0
57	MG	1H	3337	1/1	0.94	0.10	65,65,65,65	0
57	MG	1H	3317	1/1	0.94	0.12	76,76,76,76	0
57	MG	14	3303	1/1	0.94	0.06	85,85,85,85	0
57	MG	41	202	1/1	0.94	0.18	93,93,93,93	0
57	MG	1G	1637	1/1	0.94	0.47	85,85,85,85	0
57	MG	P8	101	1/1	0.94	0.41	65,65,65,65	0
57	MG	1H	3050	1/1	0.94	0.19	68,68,68,68	0
57	MG	14	3313	1/1	0.94	0.06	101,101,101,101	0
57	MG	1H	3016	1/1	0.94	0.24	71,71,71,71	0
57	MG	1H	3356	1/1	0.95	0.07	81,81,81,81	0
57	MG	1H	3296	1/1	0.95	0.13	51,51,51,51	0
57	MG	14	3115	1/1	0.95	0.39	71,71,71,71	0
57	MG	14	3080	1/1	0.95	0.41	89,89,89,89	0
57	MG	14	3163	1/1	0.95	0.49	72,72,72,72	0
57	MG	1H	3284	1/1	0.95	0.12	51,51,51,51	0
57	MG	14	3053	1/1	0.95	0.39	64,64,64,64	0
57	MG	1H	3380	1/1	0.95	0.07	57,57,57,57	0
57	MG	1H	3187	1/1	0.95	0.88	81,81,81,81	0
57	MG	1H	3310	1/1	0.95	0.09	91,91,91,91	0
57	MG	1H	3342	1/1	0.95	0.17	63,63,63,63	0
57	MG	1H	3067	1/1	0.95	0.33	70,70,70,70	0
57	MG	1H	3344	1/1	0.95	0.12	57,57,57,57	0
57	MG	1H	3367	1/1	0.95	0.12	90,90,90,90	0
57	MG	1H	3374	1/1	0.95	0.07	83,83,83,83	0
57	MG	1H	3311	1/1	0.95	0.08	70,70,70,70	0
57	MG	1H	3322	1/1	0.95	0.12	74,74,74,74	0
57	MG	13	1692	1/1	0.95	0.06	100,100,100,100	0
57	MG	13	1607	1/1	0.95	0.22	88,88,88,88	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
57	MG	1H	3080	1/1	0.95	0.25	81,81,81,81	0
57	MG	14	3154	1/1	0.95	0.43	59,59,59,59	0
57	MG	14	3101	1/1	0.95	0.42	84,84,84,84	0
57	MG	1H	3139	1/1	0.95	0.55	62,62,62,62	0
57	MG	1H	3214	1/1	0.95	0.45	55,55,55,55	0
57	MG	1H	3407	1/1	0.95	0.09	77,77,77,77	0
57	MG	1H	3368	1/1	0.95	0.08	65,65,65,65	0
57	MG	1H	3105	1/1	0.95	0.13	81,81,81,81	0
57	MG	1G	1630	1/1	0.95	0.17	102,102,102,102	0
57	MG	1H	3019	1/1	0.95	0.30	72,72,72,72	0
57	MG	1H	3294	1/1	0.95	0.07	65,65,65,65	0
57	MG	1H	3193	1/1	0.95	0.35	65,65,65,65	0
57	MG	14	3145	1/1	0.95	0.59	64,64,64,64	0
57	MG	1G	1603	1/1	0.95	0.34	77,77,77,77	0
57	MG	14	3279	1/1	0.95	0.10	69,69,69,69	0
57	MG	14	3209	1/1	0.95	0.26	84,84,84,84	0
57	MG	78	202	1/1	0.95	0.33	84,84,84,84	0
57	MG	1H	3372	1/1	0.95	0.10	62,62,62,62	0
57	MG	13	1680	1/1	0.95	0.09	91,91,91,91	0
57	MG	1H	3307	1/1	0.95	0.05	114,114,114,114	0
57	MG	14	3082	1/1	0.95	0.23	63,63,63,63	0
57	MG	14	3273	1/1	0.95	0.10	69,69,69,69	0
57	MG	1H	3394	1/1	0.95	0.07	83,83,83,83	0
57	MG	14	3193	1/1	0.95	0.85	78,78,78,78	0
57	MG	1H	3313	1/1	0.95	0.06	84,84,84,84	0
57	MG	1H	3281	1/1	0.95	0.11	55,55,55,55	0
57	MG	1H	3185	1/1	0.95	0.08	121,121,121,121	0
57	MG	1H	3093	1/1	0.95	0.25	69,69,69,69	0
57	MG	14	3091	1/1	0.95	0.54	69,69,69,69	0
57	MG	14	3158	1/1	0.95	0.10	94,94,94,94	0
57	MG	1H	3054	1/1	0.95	0.50	41,41,41,41	0
57	MG	14	3282	1/1	0.95	0.05	92,92,92,92	0
57	MG	14	3192	1/1	0.95	0.37	74,74,74,74	0
57	MG	55	201	1/1	0.95	0.18	57,57,57,57	0
57	MG	14	3076	1/1	0.95	0.20	80,80,80,80	0
57	MG	13	1609	1/1	0.95	0.17	82,82,82,82	0
57	MG	14	3035	1/1	0.95	0.38	59,59,59,59	0
57	MG	14	3187	1/1	0.95	0.35	81,81,81,81	0
57	MG	13	1613	1/1	0.95	0.48	74,74,74,74	0
57	MG	1H	3440	1/1	0.95	0.15	64,64,64,64	0
57	MG	1H	3343	1/1	0.95	0.09	57,57,57,57	0
57	MG	14	3065	1/1	0.95	0.33	58,58,58,58	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
57	MG	1H	3335	1/1	0.95	0.17	74,74,74,74	0
57	MG	14	3085	1/1	0.95	0.23	64,64,64,64	0
57	MG	1H	3134	1/1	0.95	0.47	62,62,62,62	0
57	MG	1H	3206	1/1	0.95	0.65	73,73,73,73	0
57	MG	1H	3420	1/1	0.95	0.12	60,60,60,60	0
57	MG	14	3126	1/1	0.95	0.37	66,66,66,66	0
57	MG	14	3144	1/1	0.95	0.42	72,72,72,72	0
57	MG	14	3258	1/1	0.95	0.15	80,80,80,80	0
57	MG	14	3033	1/1	0.95	0.20	74,74,74,74	0
57	MG	14	3017	1/1	0.95	0.15	75,75,75,75	0
57	MG	13	1678	1/1	0.95	0.05	106,106,106,106	0
57	MG	14	3231	1/1	0.95	0.18	66,66,66,66	0
57	MG	1H	3361	1/1	0.95	0.05	95,95,95,95	0
57	MG	14	3287	1/1	0.95	0.14	101,101,101,101	0
57	MG	14	3235	1/1	0.95	0.18	66,66,66,66	0
57	MG	13	1686	1/1	0.95	0.13	89,89,89,89	0
57	MG	14	3237	1/1	0.95	0.10	69,69,69,69	0
57	MG	1H	3015	1/1	0.95	0.23	52,52,52,52	0
57	MG	14	3034	1/1	0.95	0.18	82,82,82,82	0
57	MG	14	3012	1/1	0.95	0.59	60,60,60,60	0
57	MG	1H	3133	1/1	0.95	0.20	54,54,54,54	0
57	MG	14	3045	1/1	0.95	0.30	66,66,66,66	0
57	MG	1H	3036	1/1	0.96	0.27	57,57,57,57	0
57	MG	1H	3426	1/1	0.96	0.07	97,97,97,97	0
57	MG	14	3010	1/1	0.96	0.33	58,58,58,58	0
57	MG	1H	3437	1/1	0.96	0.13	64,64,64,64	0
57	MG	1H	3046	1/1	0.96	0.46	75,75,75,75	0
57	MG	1H	3431	1/1	0.96	0.13	66,66,66,66	0
57	MG	1G	1640	1/1	0.96	0.04	107,107,107,107	0
57	MG	1G	1669	1/1	0.96	0.10	129,129,129,129	0
57	MG	1H	3327	1/1	0.96	0.11	81,81,81,81	0
57	MG	13	1651	1/1	0.96	0.09	110,110,110,110	0
57	MG	14	3062	1/1	0.96	0.29	70,70,70,70	0
57	MG	14	3070	1/1	0.96	0.30	74,74,74,74	0
57	MG	13	1636	1/1	0.96	0.08	103,103,103,103	0
57	MG	13	1644	1/1	0.96	0.40	78,78,78,78	0
57	MG	1H	3200	1/1	0.96	0.22	73,73,73,73	0
57	MG	1G	1629	1/1	0.96	0.18	96,96,96,96	0
57	MG	14	3297	1/1	0.96	0.07	92,92,92,92	0
57	MG	13	1648	1/1	0.96	0.32	84,84,84,84	0
57	MG	14	3241	1/1	0.96	0.12	69,69,69,69	0
57	MG	14	3138	1/1	0.96	0.45	74,74,74,74	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
57	MG	14	3133	1/1	0.96	0.21	77,77,77,77	0
57	MG	14	3317	1/1	0.96	0.07	76,76,76,76	0
57	MG	14	3266	1/1	0.96	0.11	73,73,73,73	0
57	MG	14	3056	1/1	0.96	0.22	65,65,65,65	0
57	MG	13	1625	1/1	0.96	0.37	80,80,80,80	0
57	MG	13	1601	1/1	0.96	0.25	82,82,82,82	0
57	MG	1H	3137	1/1	0.96	0.32	62,62,62,62	0
57	MG	1H	3304	1/1	0.96	0.07	76,76,76,76	0
57	MG	1H	3389	1/1	0.96	0.09	87,87,87,87	0
57	MG	14	3028	1/1	0.96	0.39	67,67,67,67	0
57	MG	14	3262	1/1	0.96	0.21	55,55,55,55	0
57	MG	14	3232	1/1	0.96	0.09	67,67,67,67	0
57	MG	1H	3364	1/1	0.96	0.10	93,93,93,93	0
57	MG	13	1682	1/1	0.96	0.16	84,84,84,84	0
57	MG	1H	3048	1/1	0.96	0.30	69,69,69,69	0
57	MG	1H	3264	1/1	0.96	0.32	65,65,65,65	0
57	MG	14	3014	1/1	0.96	0.31	72,72,72,72	0
57	MG	1H	3153	1/1	0.96	0.63	83,83,83,83	0
57	MG	1H	3329	1/1	0.96	0.08	80,80,80,80	0
57	MG	1H	3112	1/1	0.96	0.42	76,76,76,76	0
57	MG	1H	3393	1/1	0.96	0.10	58,58,58,58	0
57	MG	1G	1671	1/1	0.96	0.12	117,117,117,117	0
57	MG	1H	3209	1/1	0.96	0.27	76,76,76,76	0
57	MG	1H	3432	1/1	0.96	0.11	56,56,56,56	0
57	MG	1H	3425	1/1	0.96	0.09	110,110,110,110	0
57	MG	1H	3211	1/1	0.96	0.32	78,78,78,78	0
57	MG	1H	3001	1/1	0.96	0.62	83,83,83,83	0
57	MG	14	3081	1/1	0.96	0.20	94,94,94,94	0
57	MG	14	3149	1/1	0.96	0.31	96,96,96,96	0
57	MG	1H	3113	1/1	0.96	0.28	81,81,81,81	0
57	MG	1H	3401	1/1	0.96	0.05	80,80,80,80	0
57	MG	1H	3351	1/1	0.96	0.06	79,79,79,79	0
57	MG	1H	3044	1/1	0.96	0.24	60,60,60,60	0
57	MG	13	1606	1/1	0.96	0.17	83,83,83,83	0
57	MG	1H	3363	1/1	0.96	0.10	69,69,69,69	0
57	MG	14	3130	1/1	0.96	0.19	84,84,84,84	0
57	MG	13	1620	1/1	0.96	0.20	61,61,61,61	0
57	MG	14	3255	1/1	0.96	0.11	72,72,72,72	0
57	MG	14	3309	1/1	0.96	0.11	86,86,86,86	0
57	MG	1G	1618	1/1	0.96	0.27	100,100,100,100	0
57	MG	14	3118	1/1	0.96	0.16	58,58,58,58	0
57	MG	14	3316	1/1	0.96	0.07	88,88,88,88	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
57	MG	1H	3291	1/1	0.96	0.14	56,56,56,56	0
57	MG	1H	3295	1/1	0.96	0.09	76,76,76,76	0
57	MG	14	3204	1/1	0.96	0.30	71,71,71,71	0
57	MG	1H	3056	1/1	0.96	0.18	46,46,46,46	0
57	MG	4I	201	1/1	0.96	0.06	97,97,97,97	0
57	MG	14	3222	1/1	0.96	0.16	62,62,62,62	0
57	MG	13	1605	1/1	0.96	0.19	75,75,75,75	0
57	MG	1H	3299	1/1	0.96	0.13	49,49,49,49	0
57	MG	1H	3260	1/1	0.96	0.48	71,71,71,71	0
57	MG	14	3110	1/1	0.96	0.24	82,82,82,82	0
58	ZN	3E	302	1/1	0.96	0.32	95,95,95,95	0
57	MG	1H	3340	1/1	0.96	0.14	64,64,64,64	0
57	MG	1H	3058	1/1	0.96	0.11	71,71,71,71	0
57	MG	14	3106	1/1	0.96	0.64	86,86,86,86	0
57	MG	13	1675	1/1	0.96	0.14	70,70,70,70	0
57	MG	14	3120	1/1	0.96	0.34	49,49,49,49	0
57	MG	1G	1649	1/1	0.96	0.42	70,70,70,70	0
57	MG	14	3270	1/1	0.96	0.08	97,97,97,97	0
57	MG	1H	3298	1/1	0.96	0.14	65,65,65,65	0
57	MG	1H	3031	1/1	0.96	0.29	87,87,87,87	0
57	MG	13	1690	1/1	0.96	0.10	83,83,83,83	0
57	MG	1H	3435	1/1	0.96	0.20	90,90,90,90	0
57	MG	14	3233	1/1	0.96	0.15	82,82,82,82	0
57	MG	1H	3369	1/1	0.96	0.16	60,60,60,60	0
57	MG	13	1641	1/1	0.96	0.37	74,74,74,74	0
57	MG	14	3322	1/1	0.96	0.14	79,79,79,79	0
57	MG	1H	3049	1/1	0.96	0.16	58,58,58,58	0
57	MG	14	3040	1/1	0.96	0.42	62,62,62,62	0
57	MG	14	3087	1/1	0.96	0.38	76,76,76,76	0
57	MG	1G	1627	1/1	0.96	0.30	103,103,103,103	0
57	MG	1H	3161	1/1	0.96	0.27	71,71,71,71	0
57	MG	1H	3266	1/1	0.96	0.35	85,85,85,85	0
57	MG	14	3324	1/1	0.96	0.11	77,77,77,77	0
57	MG	14	3298	1/1	0.96	0.08	78,78,78,78	0
57	MG	1H	3238	1/1	0.96	0.39	101,101,101,101	0
57	MG	14	3236	1/1	0.96	0.12	63,63,63,63	0
57	MG	1H	3213	1/1	0.96	0.58	77,77,77,77	0
58	ZN	5A	101	1/1	0.96	0.10	139,139,139,139	0
57	MG	14	3280	1/1	0.97	0.14	75,75,75,75	0
57	MG	1H	3144	1/1	0.97	0.21	95,95,95,95	0
57	MG	1H	3323	1/1	0.97	0.05	83,83,83,83	0
57	MG	1H	3376	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
57	MG	1G	1667	1/1	0.97	0.10	98,98,98,98	0
57	MG	14	3286	1/1	0.97	0.06	91,91,91,91	0
57	MG	14	3242	1/1	0.97	0.13	65,65,65,65	0
57	MG	14	3284	1/1	0.97	0.05	84,84,84,84	0
57	MG	3L	101	1/1	0.97	0.43	156,156,156,156	0
57	MG	1H	3128	1/1	0.97	0.18	52,52,52,52	0
57	MG	14	3015	1/1	0.97	0.32	69,69,69,69	0
57	MG	1H	3421	1/1	0.97	0.08	104,104,104,104	0
57	MG	14	3177	1/1	0.97	0.29	65,65,65,65	0
57	MG	1H	3395	1/1	0.97	0.09	73,73,73,73	0
57	MG	3L	102	1/1	0.97	0.28	165,165,165,165	0
57	MG	1H	3063	1/1	0.97	0.29	56,56,56,56	0
57	MG	1H	3045	1/1	0.97	0.31	70,70,70,70	0
57	MG	14	3289	1/1	0.97	0.06	106,106,106,106	0
57	MG	1H	3118	1/1	0.97	0.21	76,76,76,76	0
57	MG	14	3295	1/1	0.97	0.09	78,78,78,78	0
57	MG	13	1684	1/1	0.97	0.11	95,95,95,95	0
57	MG	14	3248	1/1	0.97	0.09	103,103,103,103	0
57	MG	13	1688	1/1	0.97	0.10	74,74,74,74	0
57	MG	1G	1609	1/1	0.97	0.11	106,106,106,106	0
57	MG	14	3314	1/1	0.97	0.06	91,91,91,91	0
57	MG	1H	3009	1/1	0.97	0.20	47,47,47,47	0
57	MG	14	3129	1/1	0.97	0.33	90,90,90,90	0
57	MG	1H	3149	1/1	0.97	0.23	61,61,61,61	0
57	MG	16	202	1/1	0.97	0.28	62,62,62,62	0
57	MG	1H	3430	1/1	0.97	0.16	50,50,50,50	0
57	MG	1H	3349	1/1	0.97	0.11	68,68,68,68	0
57	MG	1H	3429	1/1	0.97	0.08	60,60,60,60	0
57	MG	1H	3032	1/1	0.97	0.30	75,75,75,75	0
57	MG	1H	3405	1/1	0.97	0.10	72,72,72,72	0
57	MG	1H	3303	1/1	0.97	0.10	61,61,61,61	0
57	MG	13	1622	1/1	0.97	0.33	65,65,65,65	0
57	MG	1H	3010	1/1	0.97	0.33	51,51,51,51	0
57	MG	J8	101	1/1	0.97	0.37	62,62,62,62	0
57	MG	14	3016	1/1	0.97	0.18	86,86,86,86	0
57	MG	14	3226	1/1	0.97	0.13	67,67,67,67	0
57	MG	1H	3334	1/1	0.97	0.08	54,54,54,54	0
57	MG	1H	3030	1/1	0.97	0.28	79,79,79,79	0
57	MG	14	3168	1/1	0.97	0.48	51,51,51,51	0
57	MG	1H	3409	1/1	0.97	0.04	99,99,99,99	0
57	MG	1H	3373	1/1	0.97	0.05	55,55,55,55	0
57	MG	14	3067	1/1	0.97	0.46	71,71,71,71	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
57	MG	1H	3006	1/1	0.97	0.43	58,58,58,58	0
57	MG	14	3024	1/1	0.97	0.22	78,78,78,78	0
57	MG	14	3019	1/1	0.97	0.41	77,77,77,77	0
57	MG	1H	3321	1/1	0.97	0.12	74,74,74,74	0
57	MG	1H	3359	1/1	0.97	0.07	79,79,79,79	0
57	MG	14	3064	1/1	0.97	0.19	84,84,84,84	0
57	MG	1H	3352	1/1	0.97	0.05	68,68,68,68	0
57	MG	1H	3366	1/1	0.97	0.13	75,75,75,75	0
57	MG	14	3224	1/1	0.97	0.13	55,55,55,55	0
57	MG	1H	3033	1/1	0.97	0.18	54,54,54,54	0
57	MG	1H	3360	1/1	0.97	0.10	67,67,67,67	0
57	MG	1H	3433	1/1	0.97	0.12	56,56,56,56	0
57	MG	14	3265	1/1	0.97	0.08	72,72,72,72	0
57	MG	1H	3362	1/1	0.97	0.15	60,60,60,60	0
57	MG	1H	3312	1/1	0.97	0.17	93,93,93,93	0
57	MG	13	1697	1/1	0.97	0.10	76,76,76,76	0
57	MG	14	3256	1/1	0.97	0.15	57,57,57,57	0
57	MG	1H	3292	1/1	0.97	0.18	58,58,58,58	0
57	MG	1G	1604	1/1	0.97	0.21	91,91,91,91	0
57	MG	1H	3055	1/1	0.97	0.53	64,64,64,64	0
57	MG	1H	3081	1/1	0.97	0.21	47,47,47,47	0
57	MG	14	3321	1/1	0.97	0.10	78,78,78,78	0
57	MG	1H	3309	1/1	0.97	0.11	66,66,66,66	0
57	MG	1H	3212	1/1	0.97	0.24	62,62,62,62	0
57	MG	1H	3410	1/1	0.97	0.11	102,102,102,102	0
57	MG	13	1603	1/1	0.97	0.22	78,78,78,78	0
57	MG	16	209	1/1	0.97	0.07	76,76,76,76	0
57	MG	1H	3004	1/1	0.97	0.21	56,56,56,56	0
57	MG	14	3051	1/1	0.97	0.39	74,74,74,74	0
57	MG	1H	3325	1/1	0.97	0.10	75,75,75,75	0
57	MG	14	3068	1/1	0.97	0.34	81,81,81,81	0
57	MG	1H	3003	1/1	0.97	0.24	53,53,53,53	0
57	MG	1H	3127	1/1	0.97	0.36	63,63,63,63	0
57	MG	1H	3039	1/1	0.97	0.29	69,69,69,69	0
57	MG	1H	3387	1/1	0.97	0.11	82,82,82,82	0
57	MG	1G	1602	1/1	0.97	0.41	79,79,79,79	0
57	MG	1H	3057	1/1	0.97	0.18	60,60,60,60	0
57	MG	1H	3041	1/1	0.97	0.30	68,68,68,68	0
57	MG	14	3221	1/1	0.97	0.18	67,67,67,67	0
57	MG	I8	102	1/1	0.97	0.06	69,69,69,69	0
57	MG	14	3253	1/1	0.98	0.13	66,66,66,66	0
57	MG	1H	3208	1/1	0.98	0.37	48,48,48,48	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
57	MG	14	3042	1/1	0.98	0.40	75,75,75,75	0
57	MG	14	3259	1/1	0.98	0.10	71,71,71,71	0
57	MG	14	3225	1/1	0.98	0.11	55,55,55,55	0
57	MG	14	3159	1/1	0.98	0.33	73,73,73,73	0
57	MG	1H	3350	1/1	0.98	0.10	74,74,74,74	0
57	MG	1G	1662	1/1	0.98	0.38	91,91,91,91	0
57	MG	1H	3345	1/1	0.98	0.15	53,53,53,53	0
57	MG	14	3001	1/1	0.98	0.39	58,58,58,58	0
57	MG	14	3305	1/1	0.98	0.11	74,74,74,74	0
57	MG	1H	3319	1/1	0.98	0.11	60,60,60,60	0
57	MG	14	3005	1/1	0.98	0.31	61,61,61,61	0
57	MG	13	1604	1/1	0.98	0.19	79,79,79,79	0
57	MG	13	1694	1/1	0.98	0.09	111,111,111,111	0
57	MG	13	1691	1/1	0.98	0.12	78,78,78,78	0
57	MG	14	3052	1/1	0.98	0.28	63,63,63,63	0
57	MG	1H	3020	1/1	0.98	0.25	70,70,70,70	0
57	MG	14	3029	1/1	0.98	0.21	78,78,78,78	0
57	MG	14	3006	1/1	0.98	0.41	53,53,53,53	0
57	MG	14	3123	1/1	0.98	0.31	73,73,73,73	0
57	MG	1H	3246	1/1	0.98	0.43	78,78,78,78	0
57	MG	14	3285	1/1	0.98	0.11	87,87,87,87	0
57	MG	14	3208	1/1	0.98	0.33	77,77,77,77	0
57	MG	14	3276	1/1	0.98	0.10	83,83,83,83	0
57	MG	14	3272	1/1	0.98	0.22	58,58,58,58	0
57	MG	14	3251	1/1	0.98	0.07	77,77,77,77	0
57	MG	13	1679	1/1	0.98	0.07	100,100,100,100	0
57	MG	1H	3038	1/1	0.98	0.26	55,55,55,55	0
57	MG	1H	3290	1/1	0.98	0.11	49,49,49,49	0
57	MG	14	3300	1/1	0.98	0.08	87,87,87,87	0
57	MG	14	3066	1/1	0.98	0.50	63,63,63,63	0
57	MG	14	3059	1/1	0.98	0.32	45,45,45,45	0
57	MG	1H	3014	1/1	0.98	0.37	67,67,67,67	0
57	MG	1H	3375	1/1	0.98	0.16	60,60,60,60	0
57	MG	1H	3301	1/1	0.98	0.12	61,61,61,61	0
57	MG	1H	3165	1/1	0.98	0.22	96,96,96,96	0
57	MG	14	3188	1/1	0.98	0.42	87,87,87,87	0
57	MG	1H	3027	1/1	0.98	0.34	35,35,35,35	0
57	MG	1H	3285	1/1	0.98	0.12	53,53,53,53	0
57	MG	1H	3007	1/1	0.98	0.38	47,47,47,47	0
57	MG	2L	101	1/1	0.98	0.31	80,80,80,80	0
57	MG	1G	1638	1/1	0.98	0.20	83,83,83,83	0
57	MG	1H	3338	1/1	0.98	0.12	60,60,60,60	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
57	MG	1H	3302	1/1	0.98	0.15	60,60,60,60	0
57	MG	1H	3286	1/1	0.98	0.10	62,62,62,62	0
57	MG	1H	3370	1/1	0.98	0.17	60,60,60,60	0
57	MG	1H	3442	1/1	0.98	0.06	73,73,73,73	0
57	MG	14	3319	1/1	0.98	0.10	63,63,63,63	0
57	MG	1H	3155	1/1	0.98	0.34	68,68,68,68	0
57	MG	1H	3365	1/1	0.98	0.12	68,68,68,68	0
57	MG	14	3073	1/1	0.98	0.31	81,81,81,81	0
57	MG	14	3249	1/1	0.98	0.12	62,62,62,62	0
57	MG	1H	3072	1/1	0.98	0.36	66,66,66,66	0
57	MG	1H	3066	1/1	0.98	0.39	59,59,59,59	0
57	MG	1H	3399	1/1	0.98	0.04	111,111,111,111	0
57	MG	1G	1632	1/1	0.98	0.13	131,131,131,131	0
57	MG	14	3146	1/1	0.98	0.39	71,71,71,71	0
57	MG	1H	3347	1/1	0.98	0.07	64,64,64,64	0
57	MG	14	3054	1/1	0.98	0.64	53,53,53,53	0
58	ZN	5I	101	1/1	0.98	0.13	100,100,100,100	0
57	MG	13	1654	1/1	0.98	0.12	133,133,133,133	0
57	MG	1H	3028	1/1	0.98	0.33	71,71,71,71	0
57	MG	14	3011	1/1	0.98	0.42	60,60,60,60	0
57	MG	14	3072	1/1	0.98	0.23	62,62,62,62	0
57	MG	1H	3013	1/1	0.98	0.21	63,63,63,63	0
57	MG	14	3055	1/1	0.98	0.26	62,62,62,62	0
57	MG	14	3152	1/1	0.98	0.38	93,93,93,93	0
57	MG	14	3165	1/1	0.98	0.46	86,86,86,86	0
57	MG	1H	3293	1/1	0.98	0.17	62,62,62,62	0
57	MG	14	3136	1/1	0.98	0.20	66,66,66,66	0
57	MG	14	3071	1/1	0.98	0.23	68,68,68,68	0
57	MG	1H	3005	1/1	0.98	0.40	51,51,51,51	0
57	MG	14	3147	1/1	0.98	0.42	79,79,79,79	0
57	MG	1H	3422	1/1	0.98	0.08	86,86,86,86	0
57	MG	1G	1617	1/1	0.98	0.25	88,88,88,88	0
57	MG	1H	3383	1/1	0.98	0.07	82,82,82,82	0
58	ZN	32	301	1/1	0.98	0.30	117,117,117,117	0
57	MG	1H	3378	1/1	0.98	0.13	59,59,59,59	0
57	MG	13	1653	1/1	0.98	0.12	92,92,92,92	0
57	MG	1G	1601	1/1	0.98	0.27	90,90,90,90	0
57	MG	1H	3339	1/1	0.98	0.13	50,50,50,50	0
57	MG	1G	1666	1/1	0.98	0.14	89,89,89,89	0
57	MG	1H	3047	1/1	0.98	0.30	61,61,61,61	0
57	MG	1H	3065	1/1	0.98	0.18	58,58,58,58	0
57	MG	1H	3341	1/1	0.98	0.08	47,47,47,47	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
57	MG	14	3049	1/1	0.98	0.38	63,63,63,63	0
57	MG	14	3121	1/1	0.98	0.15	65,65,65,65	0
57	MG	1H	3330	1/1	0.98	0.16	49,49,49,49	0
57	MG	1H	3061	1/1	0.98	0.32	52,52,52,52	0
57	MG	2K	101	1/1	0.98	0.37	77,77,77,77	0
57	MG	13	1695	1/1	0.98	0.09	87,87,87,87	0
57	MG	1H	3008	1/1	0.98	0.34	53,53,53,53	0
57	MG	1H	3358	1/1	0.98	0.08	73,73,73,73	0
57	MG	14	3173	1/1	0.98	0.28	44,44,44,44	0
57	MG	1H	3436	1/1	0.98	0.16	50,50,50,50	0
57	MG	14	3008	1/1	0.98	0.32	59,59,59,59	0
57	MG	14	3037	1/1	0.98	0.26	61,61,61,61	0
57	MG	1H	3192	1/1	0.98	0.32	66,66,66,66	0
57	MG	88	201	1/1	0.98	0.39	76,76,76,76	0
57	MG	1H	3288	1/1	0.98	0.07	55,55,55,55	0
57	MG	14	3002	1/1	0.98	0.33	64,64,64,64	0
57	MG	14	3320	1/1	0.98	0.15	73,73,73,73	0
57	MG	1G	1619	1/1	0.98	0.29	103,103,103,103	0
57	MG	14	3030	1/1	0.98	0.24	64,64,64,64	0
57	MG	14	3267	1/1	0.98	0.15	48,48,48,48	0
57	MG	25	201	1/1	0.98	0.05	111,111,111,111	0
57	MG	1H	3413	1/1	0.98	0.08	57,57,57,57	0
57	MG	14	3274	1/1	0.98	0.10	74,74,74,74	0
57	MG	1H	3424	1/1	0.98	0.08	94,94,94,94	0
57	MG	1H	3381	1/1	0.98	0.11	58,58,58,58	0
57	MG	1H	3332	1/1	0.98	0.08	49,49,49,49	0
57	MG	14	3050	1/1	0.98	0.35	63,63,63,63	0
57	MG	14	3007	1/1	0.98	0.27	76,76,76,76	0
57	MG	1G	1643	1/1	0.98	0.10	97,97,97,97	0
57	MG	1H	3002	1/1	0.98	0.38	47,47,47,47	0
57	MG	14	3301	1/1	0.98	0.06	92,92,92,92	0
57	MG	14	3018	1/1	0.99	0.39	66,66,66,66	0
57	MG	14	3261	1/1	0.99	0.23	56,56,56,56	0
57	MG	1H	3306	1/1	0.99	0.09	70,70,70,70	0
57	MG	14	3004	1/1	0.99	0.30	60,60,60,60	0
57	MG	1H	3051	1/1	0.99	0.32	50,50,50,50	0
57	MG	1H	3079	1/1	0.99	0.23	66,66,66,66	0
57	MG	1H	3353	1/1	0.99	0.09	62,62,62,62	0
57	MG	14	3155	1/1	0.99	0.31	70,70,70,70	0
57	MG	14	3079	1/1	0.99	0.31	56,56,56,56	0
57	MG	1H	3412	1/1	0.99	0.05	94,94,94,94	0
57	MG	1H	3040	1/1	0.99	0.25	67,67,67,67	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
57	MG	14	3202	1/1	0.99	0.21	88,88,88,88	0
57	MG	13	1631	1/1	0.99	0.26	83,83,83,83	0
57	MG	14	3247	1/1	0.99	0.12	65,65,65,65	0
57	MG	14	3275	1/1	0.99	0.10	90,90,90,90	0
57	MG	14	3077	1/1	0.99	0.12	61,61,61,61	0
57	MG	1H	3132	1/1	0.99	0.14	49,49,49,49	0
57	MG	1H	3026	1/1	0.99	0.21	62,62,62,62	0
57	MG	1H	3176	1/1	0.99	0.23	42,42,42,42	0
57	MG	13	1681	1/1	0.99	0.09	71,71,71,71	0
57	MG	1H	3438	1/1	0.99	0.10	55,55,55,55	0
57	MG	14	3038	1/1	0.99	0.39	55,55,55,55	0
57	MG	1H	3355	1/1	0.99	0.17	56,56,56,56	0
57	MG	1H	3333	1/1	0.99	0.10	54,54,54,54	0
57	MG	13	1629	1/1	0.99	0.42	74,74,74,74	0
57	MG	13	1658	1/1	0.99	0.25	91,91,91,91	0
57	MG	1H	3283	1/1	0.99	0.15	65,65,65,65	0
57	MG	14	3009	1/1	0.99	0.36	59,59,59,59	0
57	MG	1H	3297	1/1	0.99	0.12	47,47,47,47	0
57	MG	1H	3029	1/1	0.99	0.25	55,55,55,55	0
57	MG	14	3269	1/1	0.99	0.08	108,108,108,108	0
57	MG	1H	3305	1/1	0.99	0.13	49,49,49,49	0
57	MG	14	3003	1/1	0.99	0.27	54,54,54,54	0
57	MG	14	3057	1/1	0.99	0.47	78,78,78,78	0
57	MG	14	3131	1/1	0.99	0.17	76,76,76,76	0
57	MG	14	3252	1/1	0.99	0.08	71,71,71,71	0
57	MG	14	3078	1/1	0.99	0.10	70,70,70,70	0
57	MG	1H	3052	1/1	0.99	0.36	42,42,42,42	0
57	MG	13	1602	1/1	0.99	0.27	80,80,80,80	0
57	MG	14	3240	1/1	0.99	0.08	71,71,71,71	0

## 6.5 Other polymers ⓘ

There are no such residues in this entry.