



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 18, 2026 – 04:44 AM UTC

PDB ID : 4WZD / pdb_00004wzd
Title : Complex of 70S ribosome with cognate tRNA-Tyr in the P-site
Authors : Rozov, A.; Demeshkina, N.; Yusupov, M.; Yusupova, G.
Deposited on : 2014-11-19
Resolution : 3.10 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

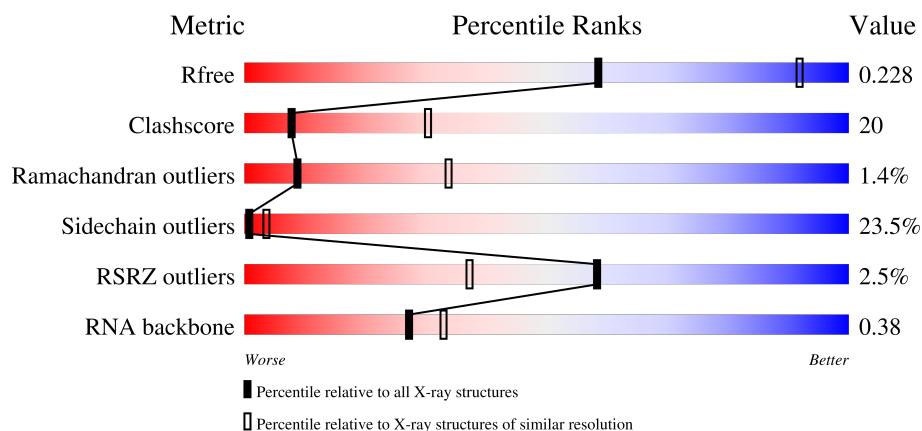
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.10 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1456 (3.10-3.10)
Clashscore	190562	1539 (3.10-3.10)
Ramachandran outliers	187476	1467 (3.10-3.10)
Sidechain outliers	187428	1467 (3.10-3.10)
RSRZ outliers	180081	1456 (3.10-3.10)
RNA backbone	3983	1022 (3.32-2.88)

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

Mol	Chain	Length	Quality of chain
1	13	1522	33% 50% 15% •
1	1G	1522	36% 48% 15% ••
2	12	256	4% 38% 41% 13% 7% •
2	1E	256	2% 34% 42% 16% 7% •

Continued on next page...

Continued from previous page...

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	

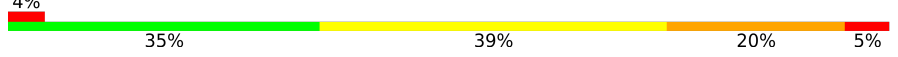
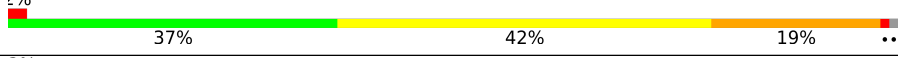
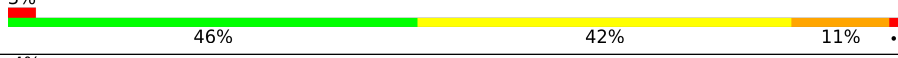
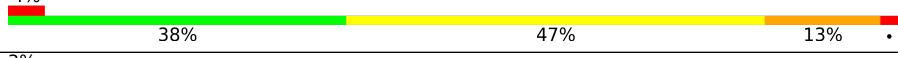
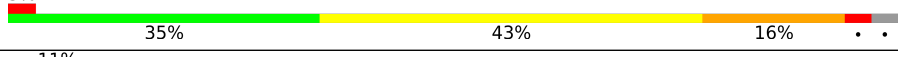
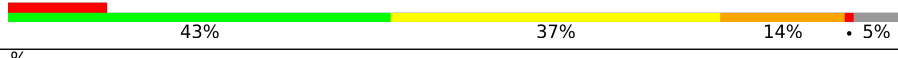
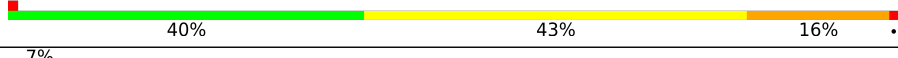
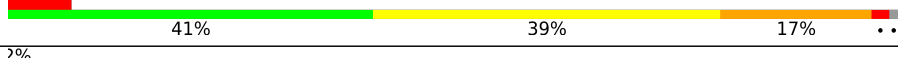
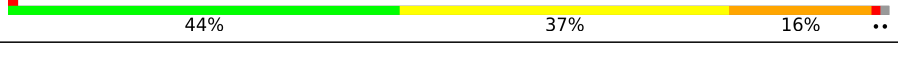
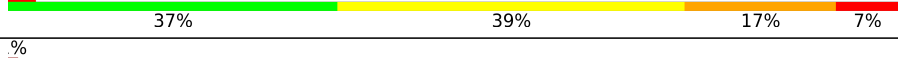
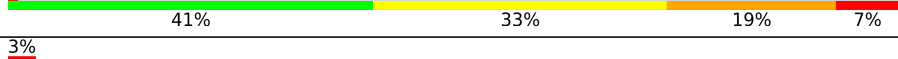
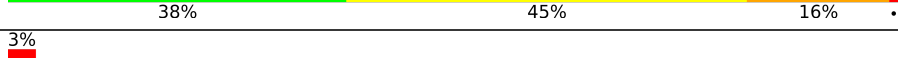
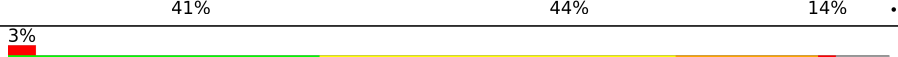
Continued on next page...

Continued from previous page...

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	2K	85	
22	2L	85	
22	3K	85	
22	3L	85	
23	4K	30	
23	4L	30	
24	14	2917	
24	1H	2917	
25	16	122	
25	1J	122	
26	71	229	
26	79	229	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
27	11	276	
27	19	276	
28	21	206	
28	29	206	
29	31	210	
29	39	210	
30	41	182	
30	49	182	
31	51	180	
31	59	180	
32	61	148	
32	69	148	
33	15	140	
33	58	140	
34	25	122	
34	68	122	
35	35	150	
35	78	150	
36	45	141	
36	88	141	
37	55	118	
37	98	118	
38	65	112	
38	A8	112	
39	75	146	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
39	B8	146	
40	85	118	
40	C8	118	
41	95	101	
41	D8	101	
42	A5	113	
42	E8	113	
43	B5	96	
43	F8	96	
44	C5	110	
44	G8	110	
45	D5	206	
45	H8	206	
46	E5	85	
46	I8	85	
47	F5	98	
47	J8	98	
48	G5	72	
48	K8	72	
49	H5	60	
49	L8	60	
50	I5	71	
50	M8	71	
51	J5	60	
51	N8	60	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
52	K5	54	
52	O8	54	
53	L5	49	
53	P8	49	
54	M5	65	
54	Q8	65	

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
55	MG	13	1624	-	-	-	X
55	MG	13	1668	-	-	-	X
55	MG	13	1681	-	-	-	X
55	MG	13	1684	-	-	-	X
55	MG	13	1688	-	-	-	X
55	MG	13	1689	-	-	-	X
55	MG	13	1692	-	-	-	X
55	MG	13	1700	-	-	-	X
55	MG	13	1708	-	-	-	X
55	MG	13	1714	-	-	-	X
55	MG	14	3105	-	-	-	X
55	MG	14	3119	-	-	-	X
55	MG	14	3157	-	-	-	X
55	MG	14	3287	-	-	-	X
55	MG	14	3314	-	-	-	X
55	MG	14	3324	-	-	-	X
55	MG	1G	1610	-	-	-	X
55	MG	1G	1656	-	-	-	X
55	MG	1G	1674	-	-	-	X
55	MG	1G	1691	-	-	-	X
55	MG	1G	1700	-	-	-	X
55	MG	1G	1721	-	-	-	X
55	MG	1G	1727	-	-	-	X
55	MG	1H	3044	-	-	-	X
55	MG	1H	3168	-	-	-	X
55	MG	1H	3203	-	-	-	X
55	MG	1H	3209	-	-	-	X

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
55	MG	1H	3325	-	-	-	X
55	MG	1H	3332	-	-	-	X
55	MG	1H	3357	-	-	-	X
55	MG	1H	3360	-	-	-	X
55	MG	1H	3389	-	-	-	X
55	MG	4A	201	-	-	-	X
55	MG	I8	101	-	-	-	X

2 Entry composition [i](#)

There are 57 unique types of molecules in this entry. The entry contains 299705 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	1499	Total	C	N	O	P	0	5	0
			32337	14392	5999	10442	1504			
1	1G	1503	Total	C	N	O	P	0	0	0
			32309	14381	5990	10436	1502			

- 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	155	Total	C	N	O	S	0	0	0
			1256	781	252	217	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			

Continued on next page...

Continued from previous page...

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	2I	116	Total	C	N	O	S	0	0	0
			864	537	164	160	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	125	Total	C	N	O	S	0	0	0
			975	614	196	164	1			
12	3A	125	Total	C	N	O	S	0	0	0
			975	614	196	164	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	4I	116	Total	C	N	O	S	0	0	0
			928	574	191	161	2			
13	4A	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	60	Total	C	N	O	S	0	0	0
			491	312	104	71	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	100	Total	C	N	O	S	0	0	0
			834	534	155	143	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	83	Total	C	N	O	S	0	0	0
			665	424	124	115	2			
19	AA	79	Total	C	N	O	S	0	0	0
			633	404	117	110	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	25	Total	C	N	O	0	0	0
			217	134	52	31			

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

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
22	2K	82	Total	C	N	O	P	S	0	0	0
			1765	795	315	571	82	2			
22	3K	85	Total	C	N	O	P	S	0	0	0
			1824	822	323	592	85	2			
22	2L	78	Total	C	N	O	P	S	0	0	0
			1678	756	297	545	78	2			
22	3L	85	Total	C	N	O	P	S	0	0	0
			1825	822	323	593	85	2			

- Molecule 23 is a RNA chain called mRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
23	4K	16	Total	C	N	O	P	0	0	0
			348	157	72	103	16			
23	4L	8	Total	C	N	O	P	0	0	0
			170	77	32	53	8			

- Molecule 24 is a RNA chain called 23S ribosomal RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
24	1H	2912	Total	C	N	O	P	0	0	0
			62707	27911	11722	20163	2911			
24	14	2909	Total	C	N	O	P	0	0	0
			62647	27884	11716	20139	2908			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
1H	161	U	-	insertion	GB 48268
1H	493	G	-	insertion	GB 48268
1H	1228	G	-	insertion	GB 48268
14	161	U	-	insertion	GB 48268
14	493	G	-	insertion	GB 48268
14	1228	G	-	insertion	GB 48268

- Molecule 25 is a RNA chain called 5S ribosomal RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
25	16	122	Total	C	N	O	P	0	0	0
			2617	1166	486	844	121			
25	1J	122	Total	C	N	O	P	0	0	0
			2617	1166	486	844	121			

- Molecule 26 is a protein called 50S ribosomal protein L1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
26	71	135	Total	C	N	O	S	0	0	0
			1049	662	197	189	1			
26	79	135	Total	C	N	O	S	0	0	0
			1049	662	197	189	1			

- Molecule 27 is a protein called 50S ribosomal protein L2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
27	11	272	Total	C	N	O	S	0	0	0
			2115	1335	420	357	3			
27	19	273	Total	C	N	O	S	0	0	0
			2120	1338	421	358	3			

- Molecule 28 is a protein called 50S ribosomal protein L3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
28	21	205	Total	C	N	O	S	0	0	0
			1568	991	300	271	6			
28	29	205	Total	C	N	O	S	0	0	0
			1568	991	300	271	6			

- Molecule 29 is a protein called 50S ribosomal protein L4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
29	31	202	Total	C	N	O	S	0	0	0
			1585	1011	297	275	2			
29	39	208	Total	C	N	O	S	0	0	0
			1627	1037	304	283	3			

- Molecule 30 is a protein called 50S ribosomal protein L5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
30	41	181	Total	C	N	O	S	0	0	0
			1473	942	268	259	4			
30	49	181	Total	C	N	O	S	0	0	0
			1473	942	268	259	4			

- Molecule 31 is a protein called 50S ribosomal protein L6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
31	51	174	Total	C	N	O	S	0	0	0
			1336	848	251	236	1			
31	59	171	Total	C	N	O	S	0	0	0
			1312	832	246	233	1			

- Molecule 32 is a protein called 50S ribosomal protein L9.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
32	61	146	Total	C	N	O	S	0	0	0
			1136	726	201	208	1			
32	69	146	Total	C	N	O	S	0	0	0
			1136	726	201	208	1			

- Molecule 33 is a protein called 50S ribosomal protein L13.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
33	58	138	Total	C	N	O	S	0	0	0
			1104	712	206	182	4			
33	15	138	Total	C	N	O	S	0	0	0
			1104	712	206	182	4			

- Molecule 34 is a protein called 50S ribosomal protein L14.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
34	68	122	Total	C	N	O	S	0	0	0
			932	588	171	169	4			
34	25	122	Total	C	N	O	S	0	0	0
			932	588	171	169	4			

- Molecule 35 is a protein called 50S ribosomal protein L15.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
35	78	150	Total	C	N	O	S	0	0	0
			1144	712	232	197	3			

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
35	35	150	Total	C	N	O	S	0	0	0
			1144	712	232	197	3			

- Molecule 36 is a protein called 50S ribosomal protein L16.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
36	88	141	Total	C	N	O	S	0	0	0
			1121	715	212	187	7			
36	45	141	Total	C	N	O	S	0	0	0
			1121	715	212	187	7			

- Molecule 37 is a protein called 50S ribosomal protein L17.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
37	98	118	Total	C	N	O	S	0	0	0
			967	604	203	159	1			
37	55	117	Total	C	N	O		0	0	0
			959	599	202	158				

- Molecule 38 is a protein called 50S ribosomal protein L18.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
38	A8	111	Total	C	N	O	0	0	0
			881	556	176	149			
38	65	111	Total	C	N	O	0	0	0
			881	556	176	149			

- Molecule 39 is a protein called 50S ribosomal protein L19.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
39	B8	137	Total	C	N	O	S	0	0	0
			1141	710	234	196	1			
39	75	137	Total	C	N	O		0	0	0
			1131	704	232	195				

- Molecule 40 is a protein called 50S ribosomal protein L20.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
40	C8	117	Total	C	N	O	S	0	0	0
			963	610	202	150	1			
40	85	117	Total	C	N	O	S	0	0	0
			963	610	202	150	1			

- Molecule 41 is a protein called 50S ribosomal protein L21.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
41	D8	101	Total	C	N	O	S	0	0	0
			778	501	142	134	1			
41	95	101	Total	C	N	O	S	0	0	0
			778	501	142	134	1			

- Molecule 42 is a protein called 50S ribosomal protein L22.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
42	E8	113	Total	C	N	O	S	0	0	0
			899	566	177	154	2			
42	A5	113	Total	C	N	O	S	0	0	0
			899	566	177	154	2			

- Molecule 43 is a protein called 50S ribosomal protein L23.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
43	F8	92	Total	C	N	O	0	0	0
			725	471	131	123			
43	B5	93	Total	C	N	O	0	0	0
			730	474	132	124			

- Molecule 44 is a protein called 50S ribosomal protein L24.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
44	G8	104	Total	C	N	O	S	0	0	0
			791	510	149	127	5			
44	C5	104	Total	C	N	O	S	0	0	0
			794	510	152	127	5			

- Molecule 45 is a protein called 50S ribosomal protein L25.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
45	H8	175	Total	C	N	O	S	0	0	0
			1397	892	251	251	3			
45	D5	179	Total	C	N	O	S	0	0	0
			1428	911	255	259	3			

- Molecule 46 is a protein called 50S ribosomal protein L27.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
46	I8	83	Total	C	N	O	S	0	0	0
			656	407	139	109	1			
46	E5	77	Total	C	N	O	S	0	0	0
			612	379	129	103	1			

- Molecule 47 is a protein called 50S ribosomal protein L28.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
47	J8	97	Total	C	N	O	S	0	0	0
			762	481	150	130	1			
47	F5	97	Total	C	N	O	S	0	0	0
			762	481	150	130	1			

- Molecule 48 is a protein called 50S ribosomal protein L29.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
48	K8	66	Total	C	N	O	S	0	0	0
			558	346	113	98	1			
48	G5	69	Total	C	N	O	S	0	0	0
			580	358	118	103	1			

- Molecule 49 is a protein called 50S ribosomal protein L30.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
49	L8	59	Total	C	N	O	0	0	0
			468	298	90	80			
49	H5	59	Total	C	N	O	0	0	0
			468	298	90	80			

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

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

- Molecule 51 is a protein called 50S ribosomal protein L32.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
51	N8	59	Total	C	N	O	S	0	0	0
			458	288	90	75	5			

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
51	J5	59	Total	C	N	O	S	0	0	0
			458	288	90	75	5			

- Molecule 52 is a protein called 50S ribosomal protein L33.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
52	O8	45	Total	C	N	O	S	0	0	0
			389	241	79	65	4			
52	K5	45	Total	C	N	O	S	0	0	0
			389	241	79	65	4			

- Molecule 53 is a protein called 50S ribosomal protein L34.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
53	P8	47	Total	C	N	O	S	0	0	0
			409	251	102	54	2			
53	L5	49	Total	C	N	O	S	0	0	0
			429	263	108	56	2			

- Molecule 54 is a protein called 50S ribosomal protein L35.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
54	Q8	62	Total	C	N	O	S	0	0	0
			483	308	98	75	2			
54	M5	62	Total	C	N	O	S	0	0	0
			495	317	100	76	2			

- Molecule 55 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
55	13	139	Total	Mg	0	0
			139	139		
55	3E	1	Total	Mg	0	0
			1	1		
55	5E	1	Total	Mg	0	0
			1	1		
55	7E	1	Total	Mg	0	0
			1	1		
55	3I	1	Total	Mg	0	0
			1	1		
55	2K	5	Total	Mg	0	0
			5	5		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
55	4K	1	Total 1	Mg 1	0	0
55	1H	523	Total 523	Mg 523	0	0
55	16	15	Total 15	Mg 15	0	0
55	11	2	Total 2	Mg 2	0	0
55	21	2	Total 2	Mg 2	0	0
55	88	1	Total 1	Mg 1	0	0
55	98	1	Total 1	Mg 1	0	0
55	G8	1	Total 1	Mg 1	0	0
55	I8	3	Total 3	Mg 3	0	0
55	Q8	2	Total 2	Mg 2	0	0
55	1G	148	Total 148	Mg 148	0	0
55	32	1	Total 1	Mg 1	0	0
55	42	1	Total 1	Mg 1	0	0
55	52	1	Total 1	Mg 1	0	0
55	3A	1	Total 1	Mg 1	0	0
55	4A	1	Total 1	Mg 1	0	0
55	2L	4	Total 4	Mg 4	0	0
55	3L	1	Total 1	Mg 1	0	0
55	14	465	Total 465	Mg 465	0	0
55	1J	10	Total 10	Mg 10	0	0
55	19	1	Total 1	Mg 1	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
55	29	4	Total 4	Mg 4	0	0
55	39	1	Total 1	Mg 1	0	0
55	15	1	Total 1	Mg 1	0	0
55	25	1	Total 1	Mg 1	0	0
55	45	1	Total 1	Mg 1	0	0
55	55	1	Total 1	Mg 1	0	0
55	C5	1	Total 1	Mg 1	0	0
55	E5	1	Total 1	Mg 1	0	0
55	F5	1	Total 1	Mg 1	0	0

- Molecule 56 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
56	3E	1	Total 1	Zn 1	0	0
56	5I	1	Total 1	Zn 1	0	0
56	G8	1	Total 1	Zn 1	0	0
56	32	1	Total 1	Zn 1	0	0
56	5A	1	Total 1	Zn 1	0	0
56	C5	1	Total 1	Zn 1	0	0

- Molecule 57 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
57	13	125	Total 125	O 125	0	0
57	5I	1	Total 1	O 1	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
57	AI	3	Total 3	O 3	0	0
57	2K	2	Total 2	O 2	0	0
57	4K	3	Total 3	O 3	0	0
57	1H	652	Total 652	O 652	0	0
57	16	12	Total 12	O 12	0	0
57	11	8	Total 8	O 8	0	0
57	21	2	Total 2	O 2	0	0
57	31	5	Total 5	O 5	0	0
57	78	4	Total 4	O 4	0	0
57	98	1	Total 1	O 1	0	0
57	C8	2	Total 2	O 2	0	0
57	E8	1	Total 1	O 1	0	0
57	F8	2	Total 2	O 2	0	0
57	G8	2	Total 2	O 2	0	0
57	1G	96	Total 96	O 96	0	0
57	32	1	Total 1	O 1	0	0
57	5A	1	Total 1	O 1	0	0
57	7A	2	Total 2	O 2	0	0
57	BA	1	Total 1	O 1	0	0
57	2L	6	Total 6	O 6	0	0
57	14	523	Total 523	O 523	0	0

Continued on next page...

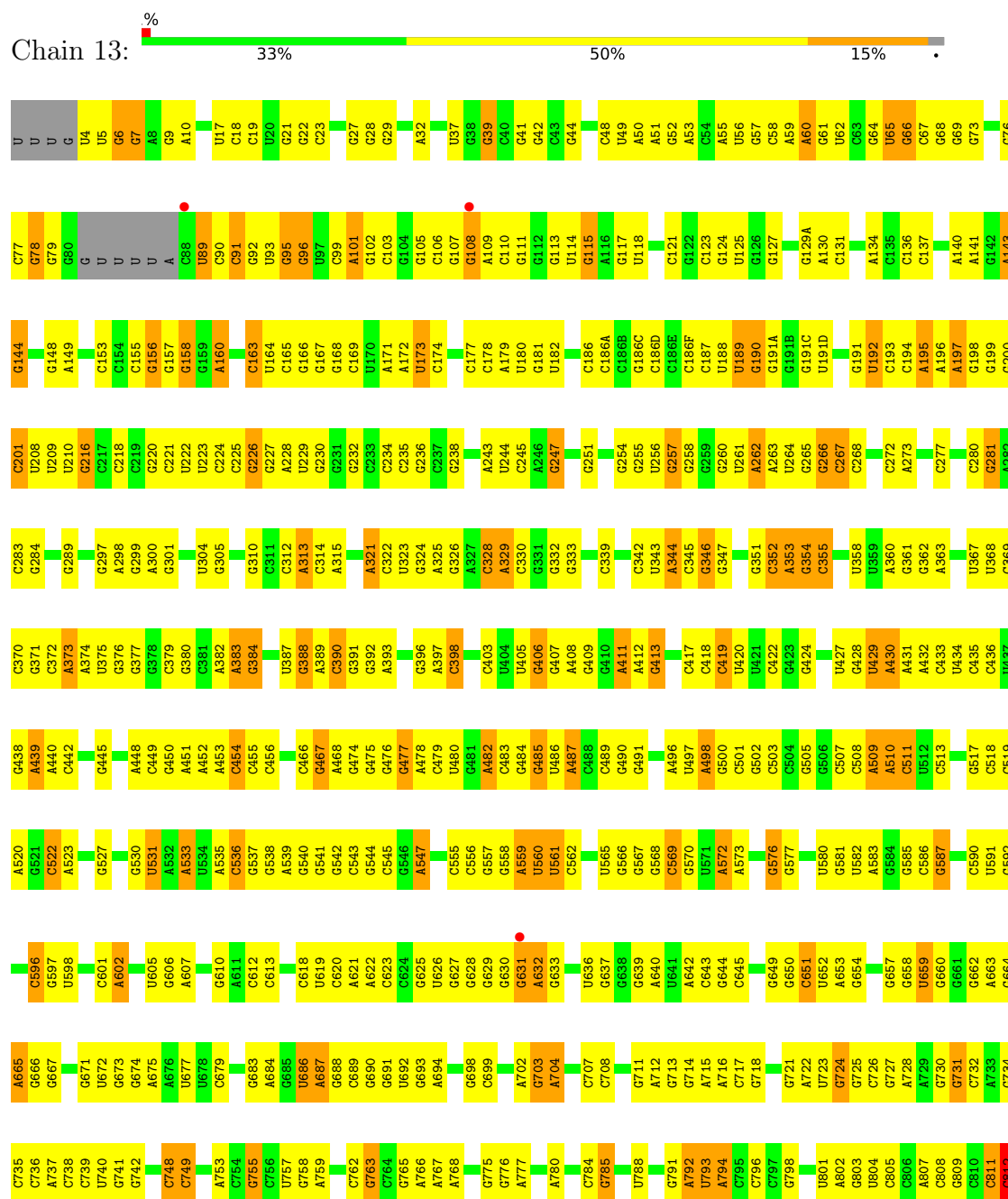
Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
57	1J	22	Total 22	O 22	0	0
57	19	11	Total 11	O 11	0	0
57	39	3	Total 3	O 3	0	0
57	25	6	Total 6	O 6	0	0
57	35	1	Total 1	O 1	0	0
57	75	1	Total 1	O 1	0	0
57	85	4	Total 4	O 4	0	0
57	F5	1	Total 1	O 1	0	0
57	H5	2	Total 2	O 2	0	0

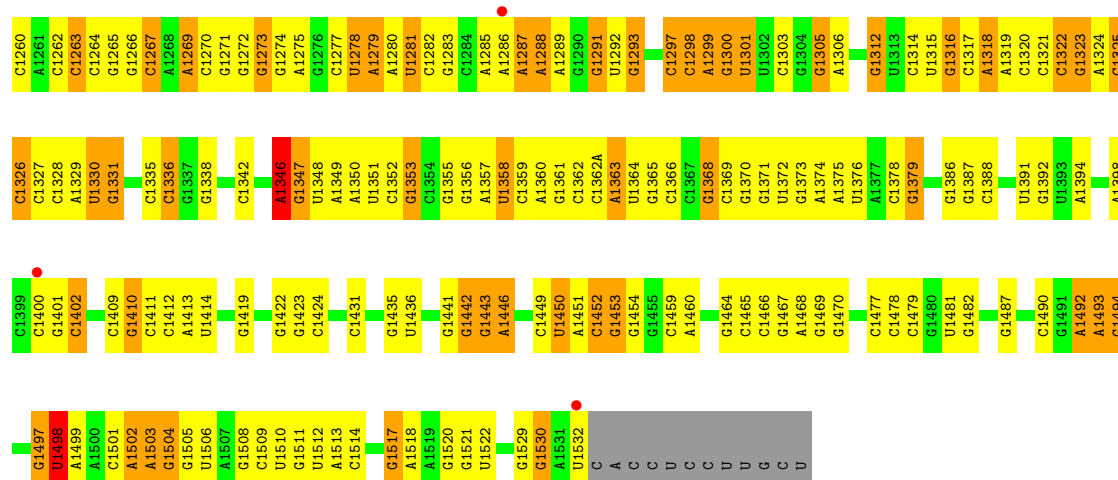
3 Residue-property plots

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

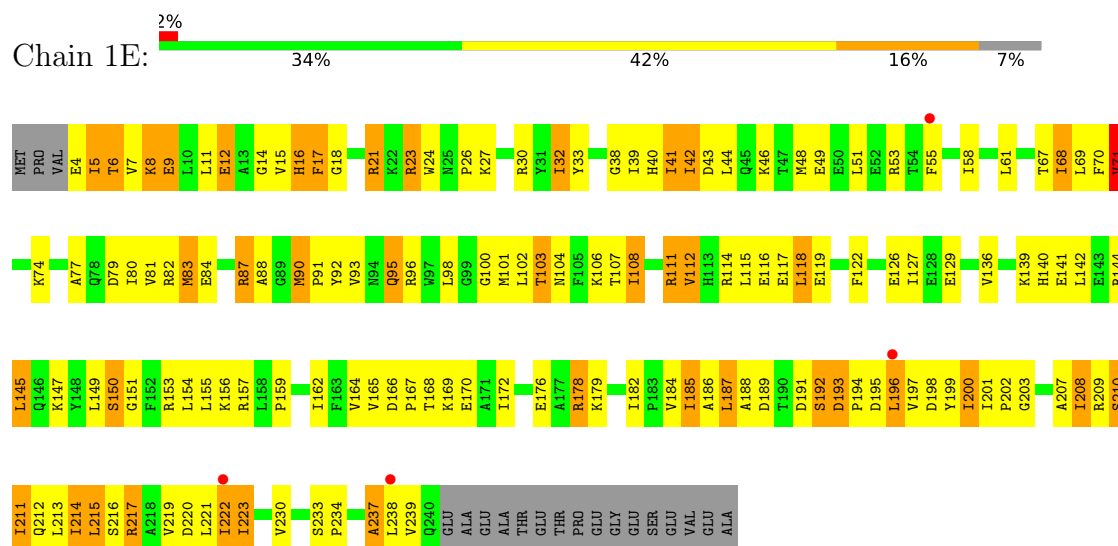
• Molecule 1: 16S ribosomal RNA



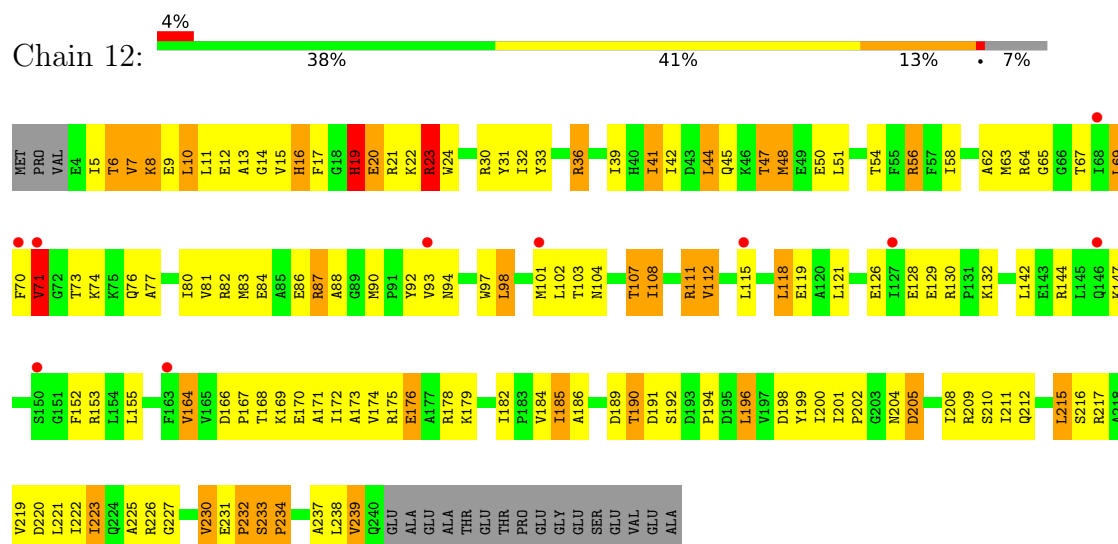
U1196	G1133	G1066	G941	G861	A780	G890	C613	C543	A468	G391	G318	U222	G148
G1197	G1134	A1067	G944	C862	A781	G891	A614	G544	G474	G392	G319	U223	A149
U1198	U1135	G1068	G945	U863	A782	U892	C615	C545	G475	A393	A321	G232	C150
U1199	U1136	A1005	A864	A863	C783	U893	G616	G546	G476	G396	G322	G233	A151
C1200	G1072	U1073	A946	A865	A787	A694	G617	A547	G477	A397	G323	C234	A152
A1201	U1074	C948	C948	C868	A790	A702	C620	G548	G481	C398	G324	C235	C153
G1202	G1009	U950	U950	G869	G791	G709	A621	C549	G481	A327	A327	A243	C154
C1203	G1010	U951	U951	A872	G792	G710	A622	U852	G484	C403	C328	A244	A160
U1204	G1011	C951	C951	A873	U793	G711	C623	A553	G485	U404	A329	U245	C163
G1205	A1014	U952	U952	A874	G794	G712	C624	C554	U486	U405	C330	C245	U164
C1206	A1015	G953	G953	G874	A794	A713	G625	C555	G490	G406	G331	A246	U165
G1207	A1016	U954	U954	C877	C797	G714	U626	C556	G491	G407	G332	G247	G166
A1208	G1017	U955	U955	G878	G798	G715	G627	A559	G492	A408	G333	A250	G167
G1209	C1018	U956	U956	G879	A716	A716	C628	U560	G493	G409	C337	G251	G168
U1210	U1018	U957	U957	C880	G799	A716	G629	U561	U494	G410	A338	U252	C169
U1211	G1021	A958	A958	U884	G800	C719	G631	C562	U495	A411	A339	U253	U170
U1212	G1022	A959	A959	C885	U801	G720	A632	A563	A496	A412	G340	G254	C173
G1215	G1023	U960	U960	U886	G802	C721	G633	C564	U497	A413	C341	G255	C174
C1216	U1024	U961	U961	C887	G803	G722	G634	C565	U498	A414	C342	G256	C175
G1217	U1025	C962	C962	A889	U804	A722	A640	U566	C500	C418	C345	G257	C176
C1218	G1026	U963	U963	C890	C905	G723	A642	G567	C501	C419	G346	G261	C177
U1219	C1027	A964	A964	C891	G806	G724	A643	G568	C502	U421	G347	A262	C178
G1220	C1028	G965	G965	C892	A807	A728	C643	C569	C503	U422	C347	A263	U173
A1221	C1028A	A966	A966	C893	C811	A729	G644	G570	C504	G423	G350	U264	U182
G1222	G1028B	C967	C967	A900	C812	G730	C645	U571	G505	G424	G351	G265	G183
C1223	U1029	A968	A968	A901	C813	G731	U646	A572	A509	G425	C352	G266	C186
G1224	G1030	U969	U969	A902	A814	C947	C647	A573	A510	G426	A353	C267	C186A
A1225	G1031	C970	C970	C894	A815	G734	G650	A574	C511	U427	G354	C268	C186B
C1226	A1032	G903	G903	C895	A816	C735	G651	G575	U512	G428	C269	G269	G186C
U1227	G1032A	C904	C904	C896	C817	G736	U652	G576	U513	U429	A360	A270	C186D
C1228	U1032B	A974	A974	A908	C818	A737	A653	G577	C514	A430	A361	A271	C186E
A1229	G1033	U975	U975	A909	U820	C738	G654	U580	C515	A431	A362	G275	C186F
G1233	A1035	G976	G976	C897	U821	G741	G660	G581	C516	A432	A363	G276	C187
C1234	G1036	A977	A977	A913	G825	C748	G661	U582	C517	C433	U367	G277	U188
U1235	U1037	A978	A978	A914	C826	C749	G662	A583	C518	U434	U368	G278	U189
A1236	C1038	C980	C980	A915	U827	G750	A663	G584	A520	C435	U369	G279	G190
C1237	U1040	U981	U981	A916	U828	G751	A665	G587	C522	G438	C370	G280	U191D
U1238	G1043	G982	G982	A917	A828	C754	G670	G588	A523	A439	G371	G281	G191E
A1239	C1044	C984	C984	A918	U833	G755	G671	C589	C524	A440	C372	G282	U191F
U1240	U1045	U920	U920	A919	C834	C756	G672	C590	C525	C441	A373	A288	G191
G1243	A1046	U921	U921	A923	U835	U757	U673	C591	C526	G444	U374	G289	A195
C1244	U1052	A986	A986	A924	G836	G758	G674	C596	G530	G445	U375	U296	A196
A1245	G1053	C987	C987	A925	G837	A759	A675	C597	C531	G446	G376	G297	A197
C1246	C1054	C988	C988	A926	U841	G761	A676	C598	C532	A448	G378	A298	G198
U1247	A1055	G989	G989	A927	C842	G765	U677	C599	A533	C449	C379	G299	G199
C1248	U1056	U991	U991	A928	U843	A766	U678	C600	U534	G450	G380	G301	G200
A1250	G1057	U992	U992	A929	C844	A767	C679	C601	C535	A451	A382	G309	C201
U1251	U1058	G993	G993	A930	U845	U772	G683	C602	C536	A452	A383	G310	U208
C1252	C1059	C995	C995	A931	G851	G773	G684	U603	G537	C457	G384	G311	U209
G1253	U1060	U996	U996	A932	G852	U774	A685	U604	C538	G458	G385	U210	U210
U1254	G1061	A997	A997	A933	C857	G775	U686	G606	A539	G464	C388	A313	G216
C1255	U1062	G998	G998	A934	C858	A777	U687	A607	C540	A465	A389	C314	G220
A1256	C1063	A1000	A1000	A935	A859	G778	G688	C612	G541	C466	G390	A315	C221
U1257	U1064	G1001	G1001	A936	A860	C779	C689		G542	G467			

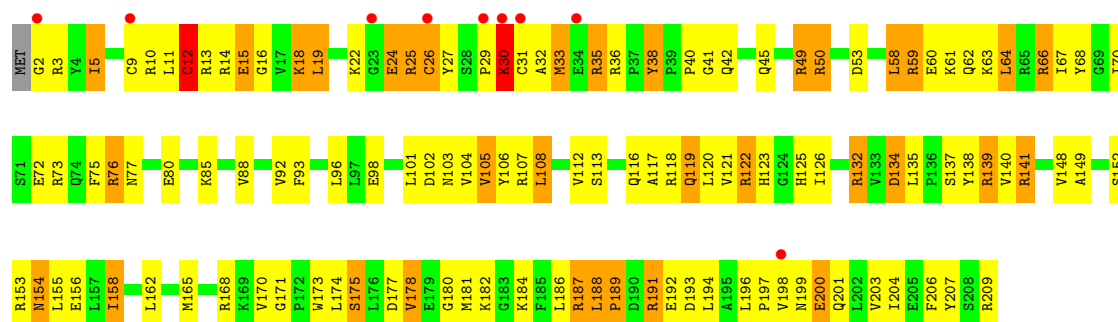


• Molecule 2: 30S ribosomal protein S2

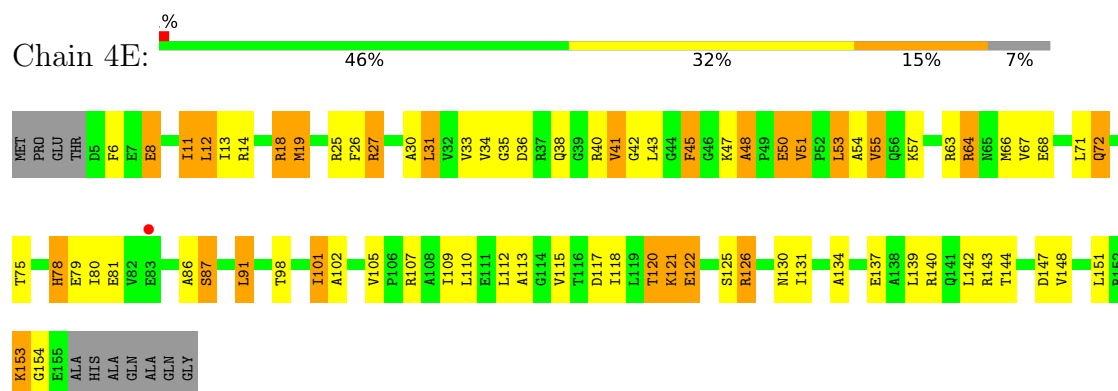


• Molecule 2: 30S ribosomal protein S2

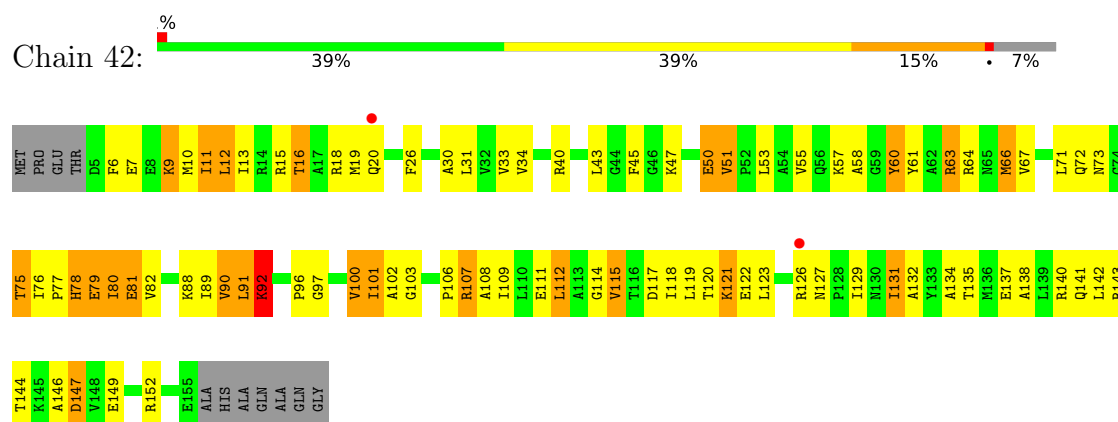




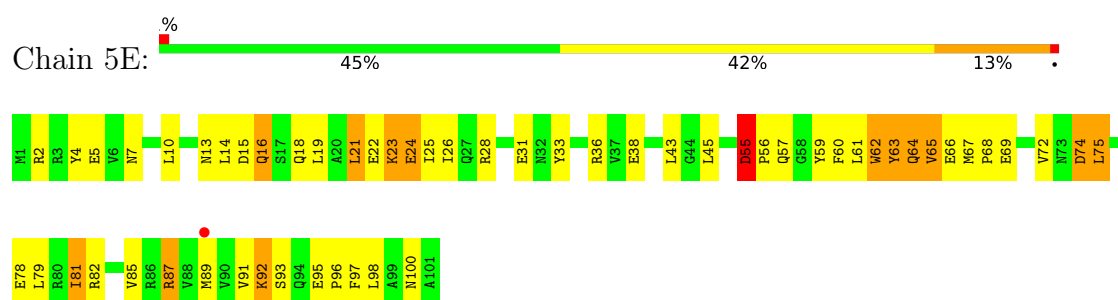
• Molecule 5: 30S ribosomal protein S5



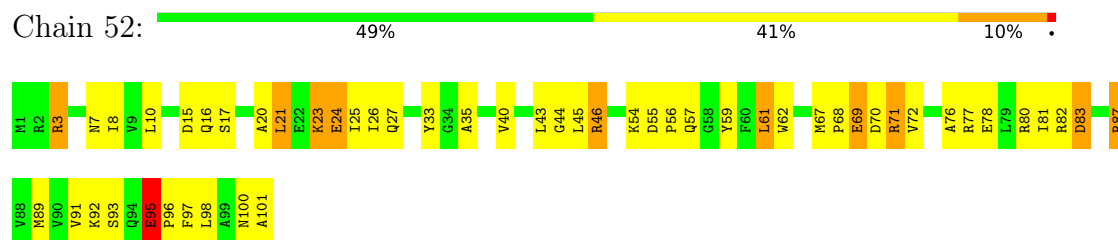
• Molecule 5: 30S ribosomal protein S5



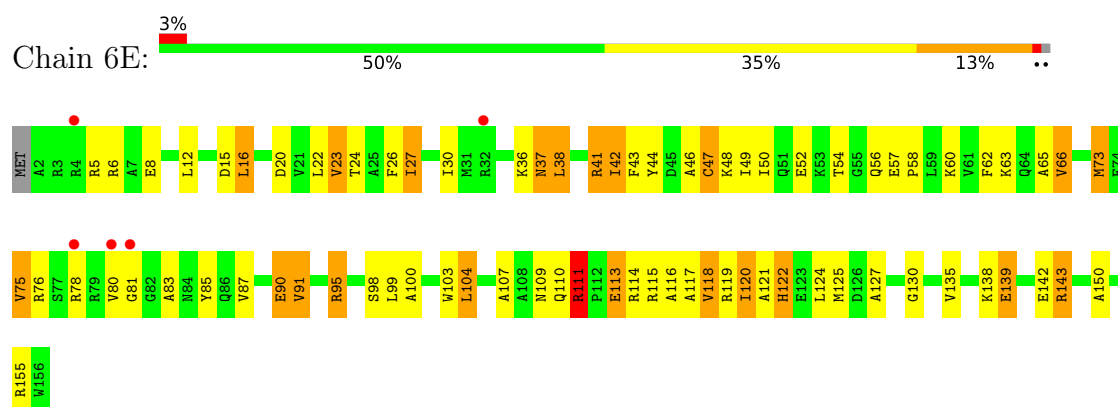
• Molecule 6: 30S ribosomal protein S6



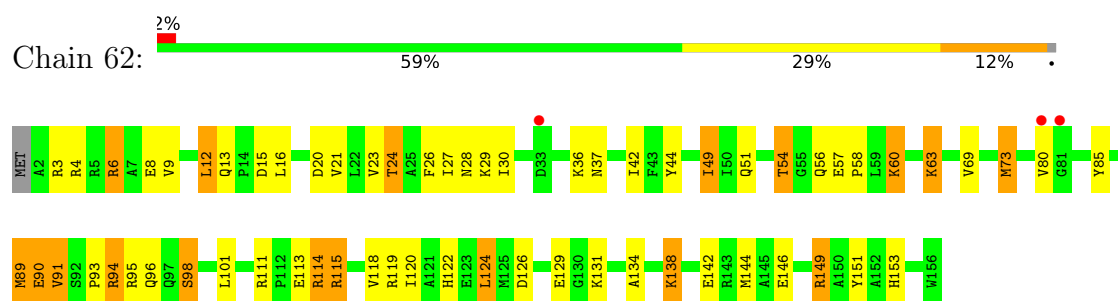
• Molecule 6: 30S ribosomal protein S6



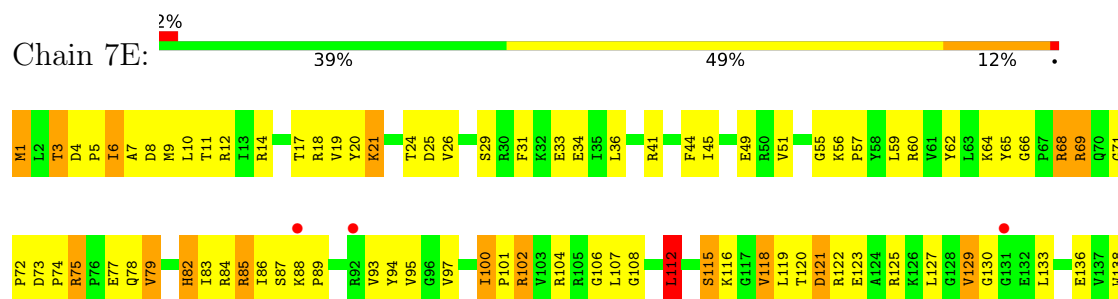
• Molecule 7: 30S ribosomal protein S7



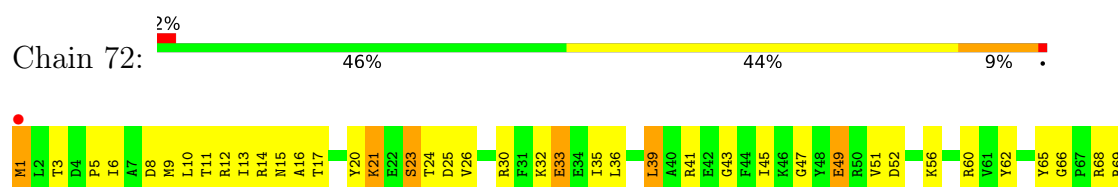
• Molecule 7: 30S ribosomal protein S7

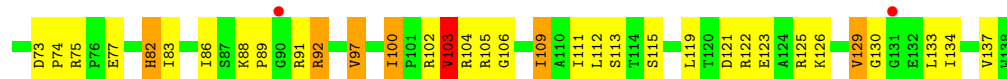


• Molecule 8: 30S ribosomal protein S8

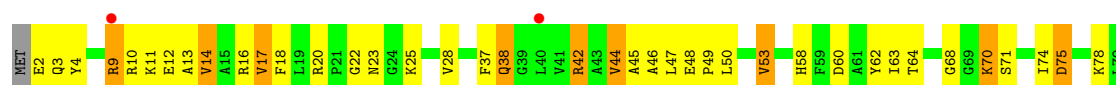


• Molecule 8: 30S ribosomal protein S8

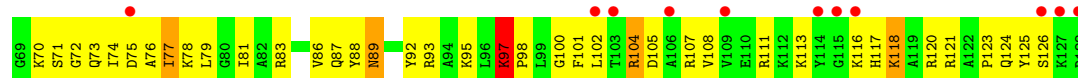
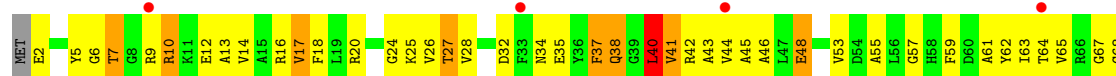




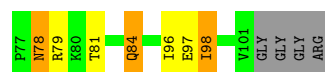
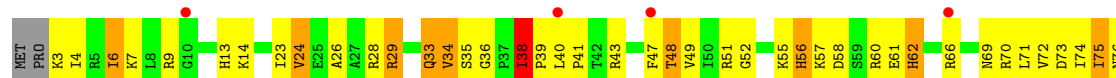
• Molecule 9: 30S ribosomal protein S9



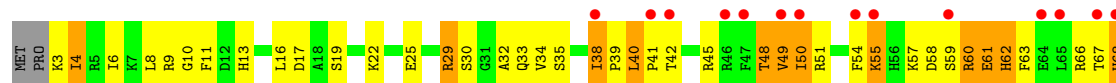
• Molecule 9: 30S ribosomal protein S9



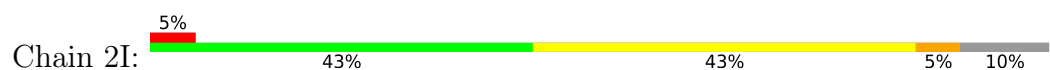
• Molecule 10: 30S ribosomal protein S10

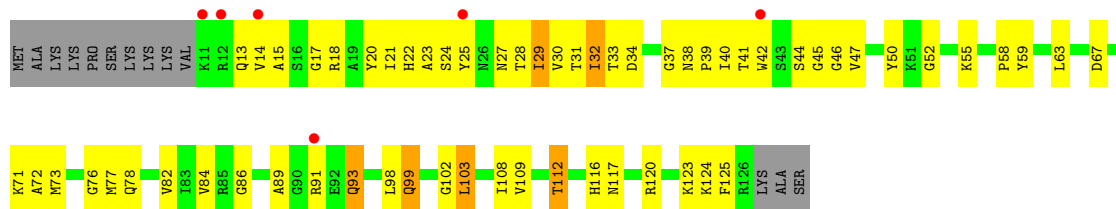


• Molecule 10: 30S ribosomal protein S10

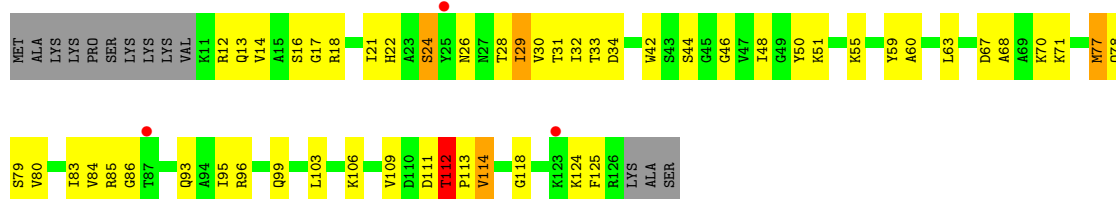


• Molecule 11: 30S ribosomal protein S11

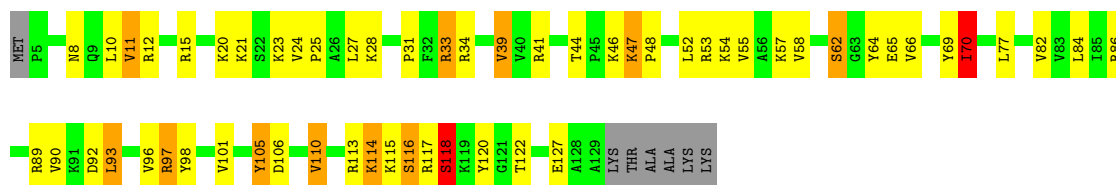




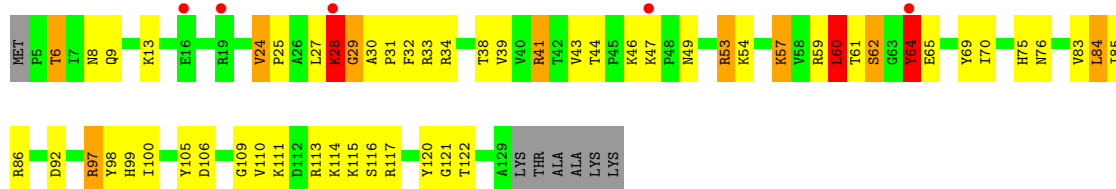
• Molecule 11: 30S ribosomal protein S11



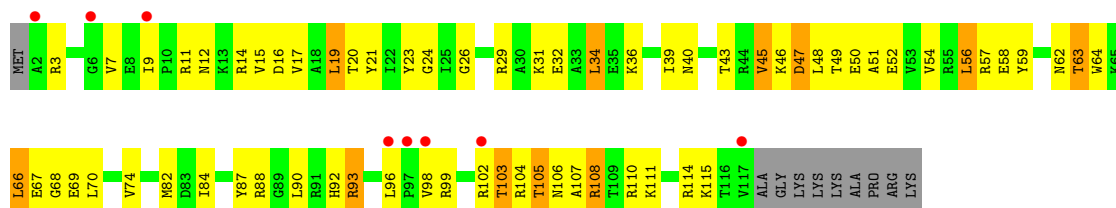
• Molecule 12: 30S ribosomal protein S12



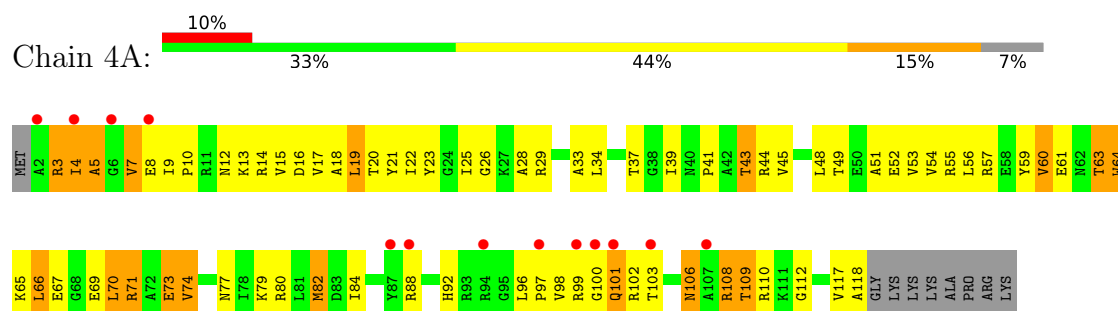
• Molecule 12: 30S ribosomal protein S12



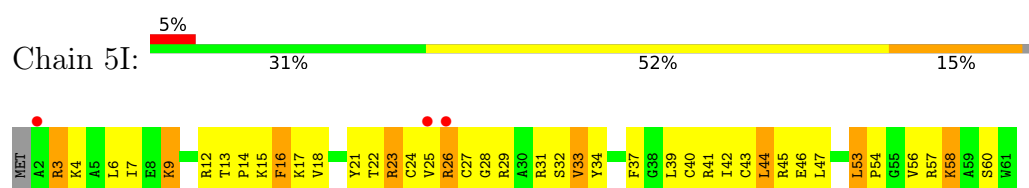
• Molecule 13: 30S ribosomal protein S13



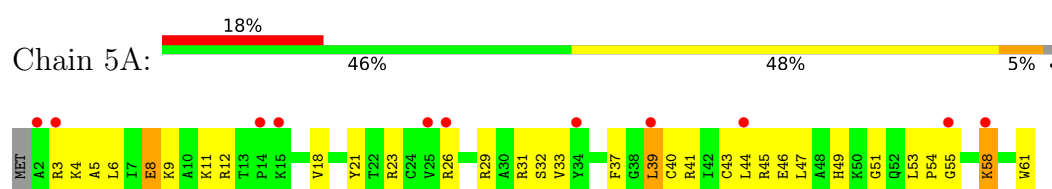
- Molecule 13: 30S ribosomal protein S13



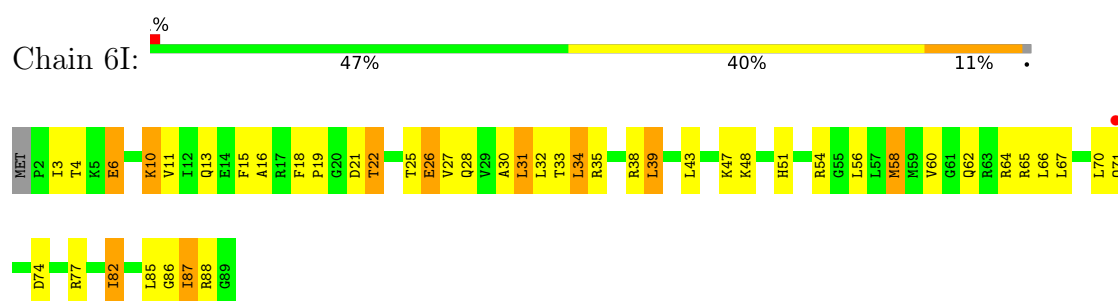
- Molecule 14: 30S ribosomal protein S14 type Z



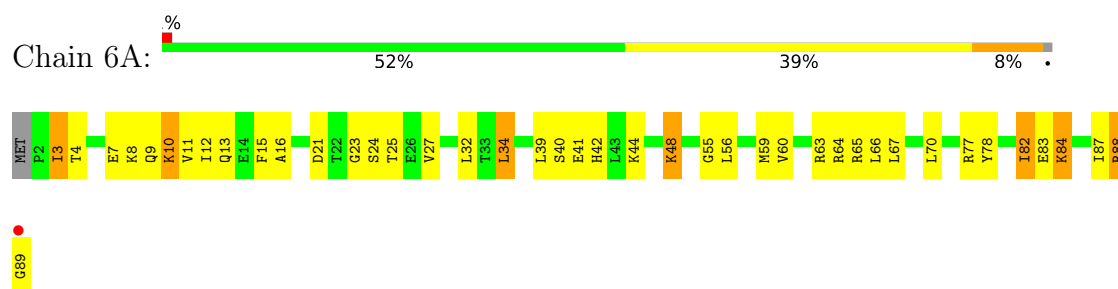
- Molecule 14: 30S ribosomal protein S14 type Z



- Molecule 15: 30S ribosomal protein S15

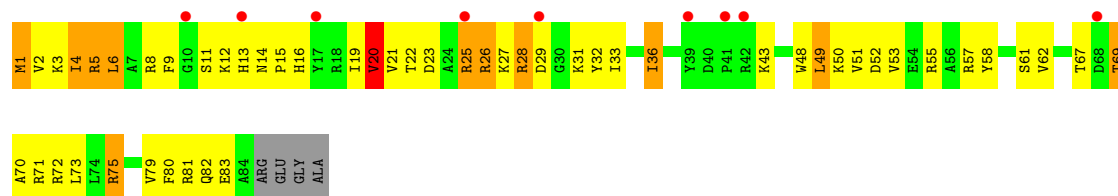


- Molecule 15: 30S ribosomal protein S15



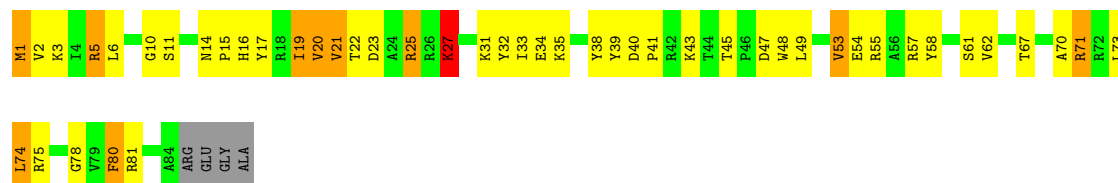
- Molecule 16: 30S ribosomal protein S16





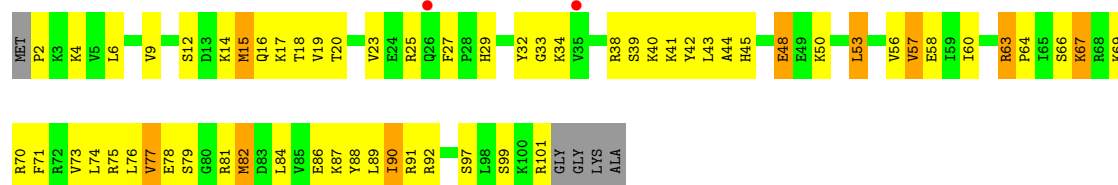
- Molecule 16: 30S ribosomal protein S16

Chain 7A: 41% 42% 11% 5%



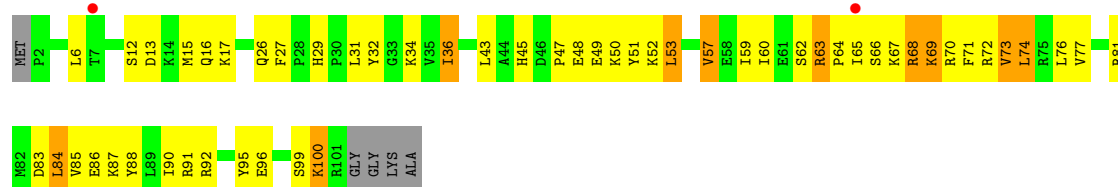
- Molecule 17: 30S ribosomal protein S17

Chain 8I: 2% 37% 50% 9% 5%



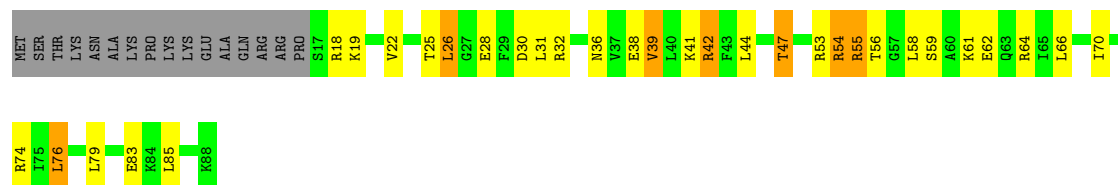
- Molecule 17: 30S ribosomal protein S17

Chain 8A: 2% 44% 42% 10% 5%

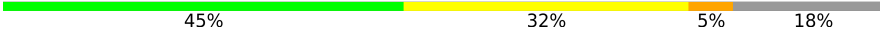


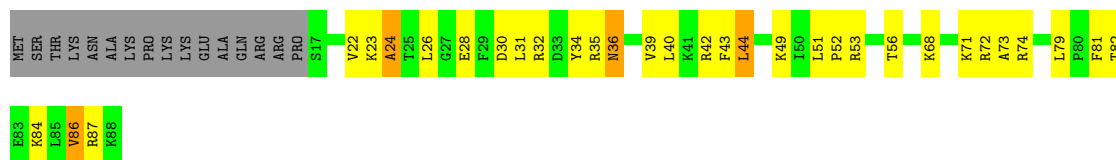
- Molecule 18: 30S ribosomal protein S18

Chain 9I: 45% 28% 8% 18%

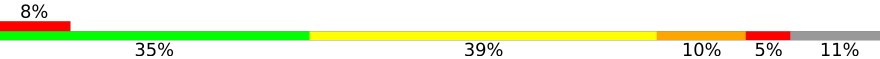


- Molecule 18: 30S ribosomal protein S18

Chain 9A: 

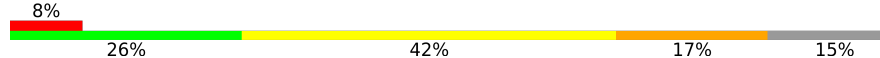


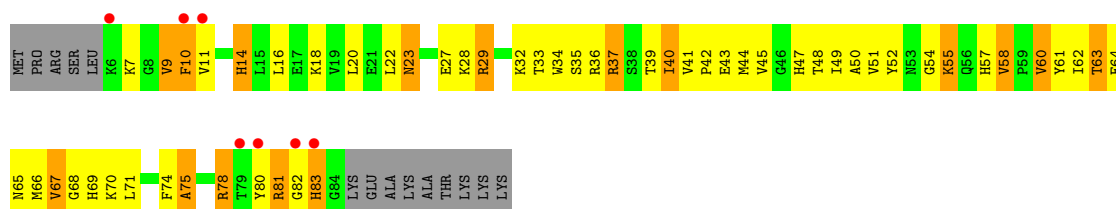
- Molecule 19: 30S ribosomal protein S19

Chain AI: 



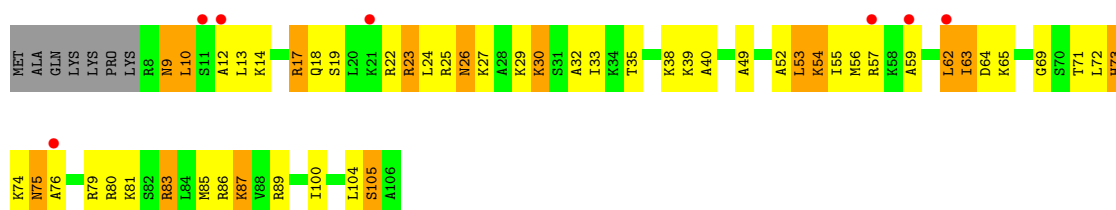
- Molecule 19: 30S ribosomal protein S19

Chain AA: 



- Molecule 20: 30S ribosomal protein S20

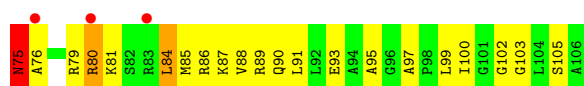
Chain BI: 



- Molecule 20: 30S ribosomal protein S20

Chain BA: 





- Molecule 21: 30S ribosomal protein Thx



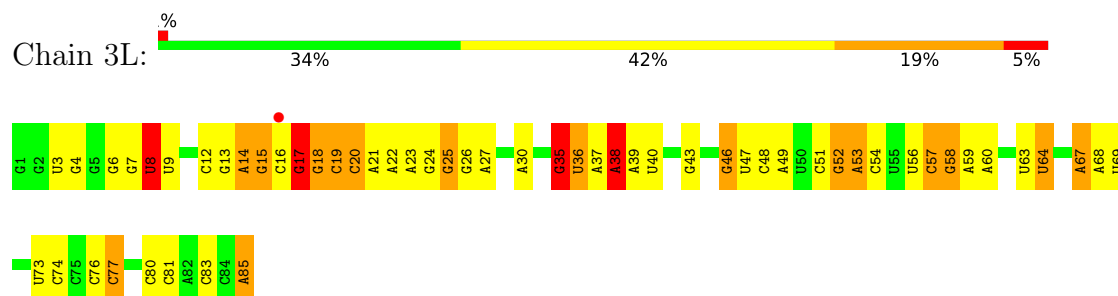
- Molecule 21: 30S ribosomal protein Thx



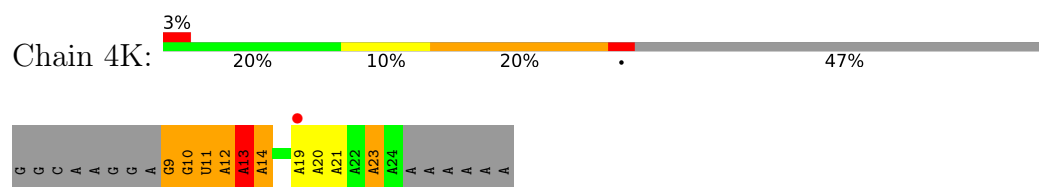
- Molecule 22: tRNA-Tyr



- Molecule 22: tRNA-Tyr



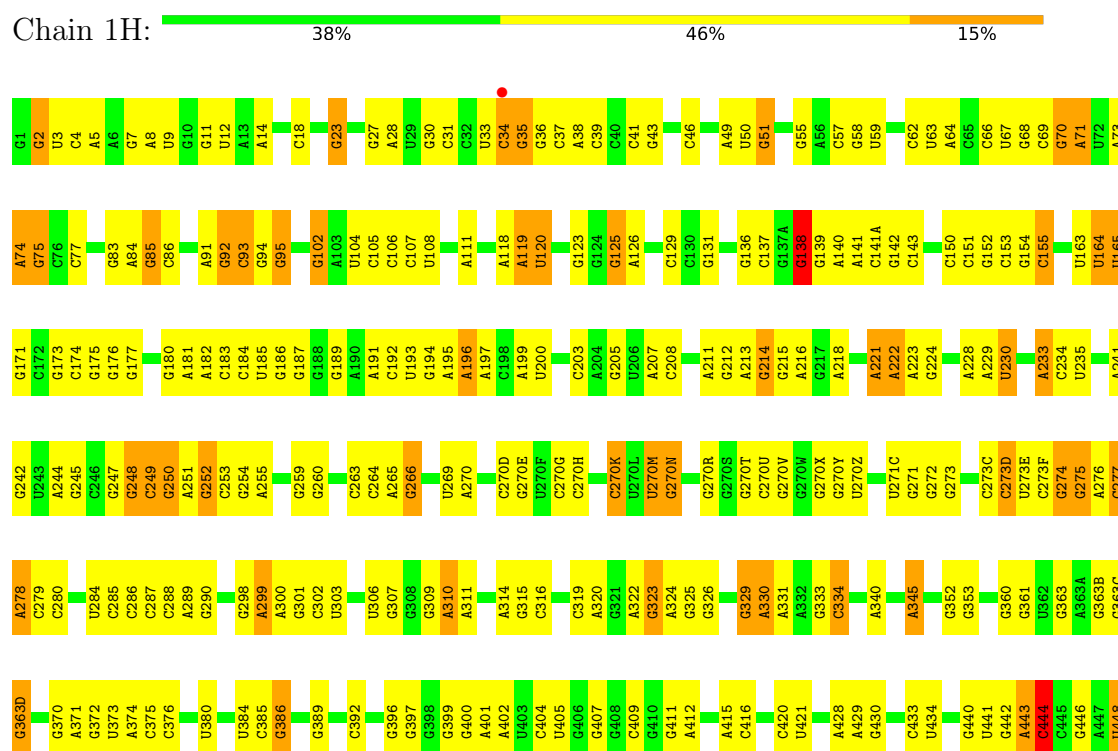
- Molecule 23: mRNA



- Molecule 23: mRNA

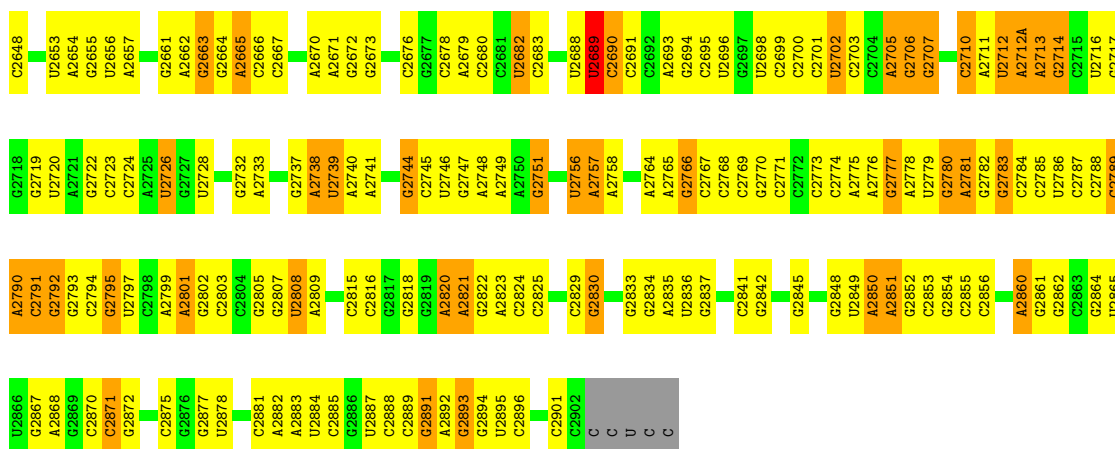


- Molecule 24: 23S ribosomal RNA



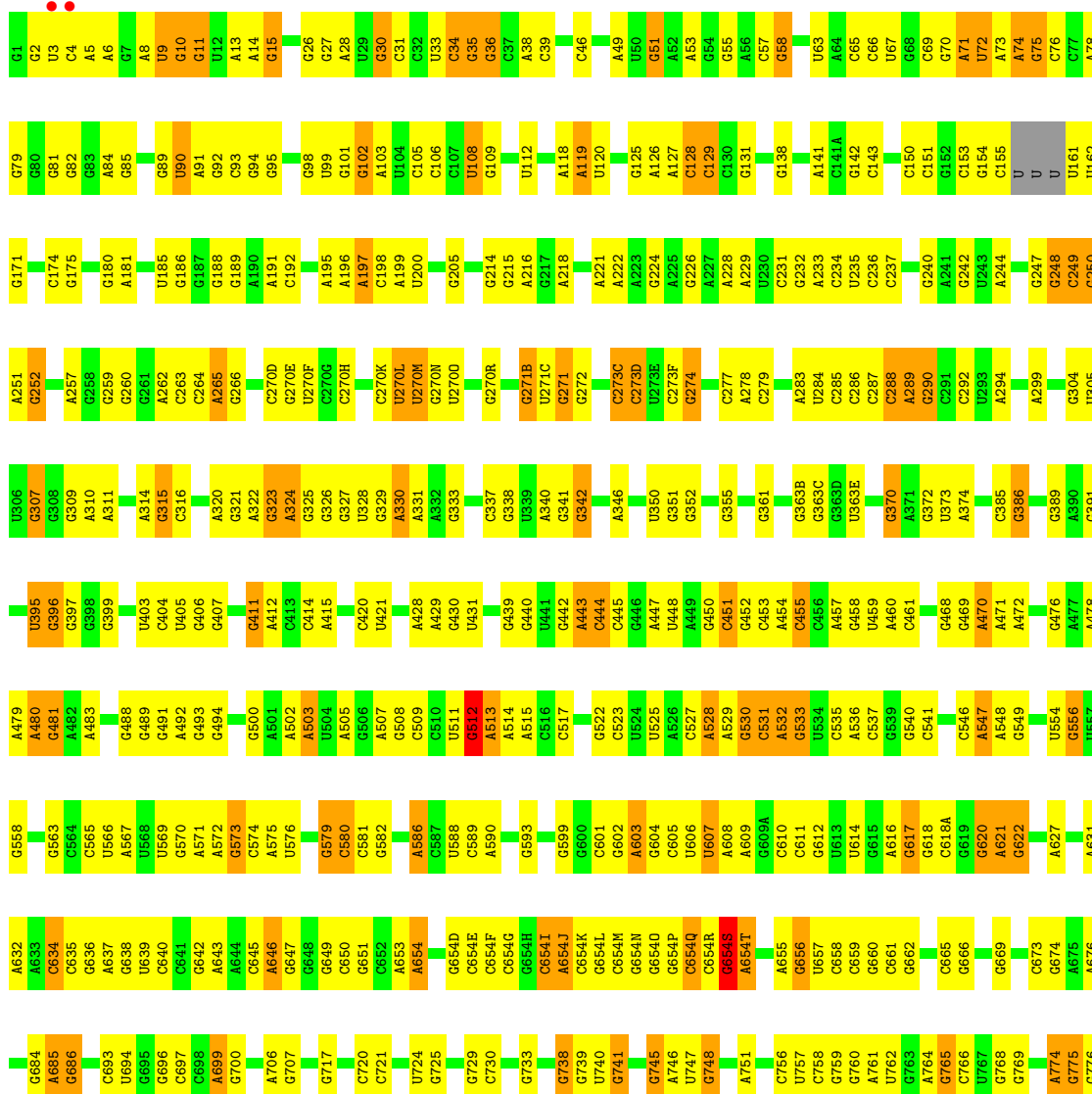


C2573	G2485	G2410	U2344	G2280	C2126	A2054	C1979	C1902	A1809	G1899	A1614	A1536
G2486	G2411	A2411	G2345	C2281	G2127	C2055	G1980	G1903	A1810	A1700	C1615	C1837
G2487	G2415	G2415	A2346	C2282	C2128	C2056	A1981	G1906	G1811	A1709	C1617	G1538
G2489	G2416	G2416	C2347	C2283	C2129	A2057	C1982	G1906	G1812	C1710	G1619	G1539
	G2417	G2417	G2348	C2284	U2130	A2058	G1983	G1906	G1813		G1619	G1540
	G2418	G2418	G2349	C2285	U2131	G2061	G1984	A1912	G1814			U1541
	G2419	G2419	C2350	C2286	U2132	G2062	G1985	A1913	A1815	G1726	G1542	G1541
	G2420	G2420	G2351	U2208	U2133	A2062		A1914	G1816	G1727	A1943	G1542
	G2421	G2421	C2352	C2209	A2134	C2063	G1989	C1915	G1728	U1727	A1544	A1544
	G2422	G2422	G2353	G2210	A2135	C2064	C1990	U1915	A1820	G1729	C1544	C1544
	G2423	G2423	G2354	G2211	C2065	C2065	A1990	U1916	U1820	A1729	A1545	A1545
	G2424	G2424	C2355	A2212	C2136	C2066	G1993	U1917	G1826	U1730	A1546	A1546
	G2425	G2425	C2356	U2213	C2137	G2067	C1994	A1918	G1827	G1731	C1547	C1547
	G2426	G2426	U2215	G2215	C2138	G2068	U1995	A1919	G1828	A1732	C1548	C1548
	G2427	G2427	G2216	G2216	C2139	C2069	C1996	C1920	A1829	G1733	C1549	C1549
	G2428	G2428	G2219	G2219	C2140	G2070	G1997	U1926	C1742		G1643	G1643
	G2429	G2429	G2224	G2224	G2141	A2071	G1998	A1927	G1743		G1643	A1554
	G2430	G2430	A2225	A2225	C2145	U2074	C1999	A1928	A1749	G1647	G1647	C1557
	G2431	G2431	C2226	C2226	C2146		G2002	G1930	G1750	G1648	C1557	C1557
	G2432	G2432	U2233	U2233	C2147	A2077		G1930	G1750	G1649	A1558	A1558
	G2433	G2433	G2234	G2234	C2148	C2078	A2005	U1931	C1838	G1650	G1559	G1559
	G2434	G2434	G2235	G2235	C2149	C2079	C2006	G1932	G1839	G1651	G1560	G1560
	G2435	G2435	G2237	G2237	U2150	C2081	C2006	G1933	C1752	G1652	G1561	G1561
	G2436	G2436	G2238	G2238	G2151	A2082	G2009	C1934	G1756	G1653	A1562	A1562
	G2437	G2437	C2239	C2239	C2152	C2083	G2010	G1935	C1843	A1654		
	G2438	G2438	G2240	G2240	C2153	U2086	A2013	A1936	A1847	A1655	C1565	C1565
	G2439	G2439	U2241	U2241	G2154	G2087	A2014	A1937	G1763	C1656	A1566	A1566
	G2440	G2440	U2242	U2242	C2155		A2015	A1938	G1764	C1657	A1567	A1567
	G2441	G2441	U2243	U2243	G2156	U2096	C2021	G1954	A1871	C1658	G1568	G1568
	G2442	G2442	U2244	U2244	C2157	C2097	G2022	U1955	A1872	U1659	A1569	A1569
	G2443	G2443	U2245	U2245	A2158	U2098	U2022	U1956	G1878	A1664	A1570	A1570
	G2444	G2444	G2251	G2251	C2162	U2102	G2033	A1952	U1884		A1571	A1571
	G2445	G2445	C2252	C2252	C2163	C2103	G2034	A1953	G1889	G1674		
	G2446	G2446	G2253	G2253	C2164	C2104	U2028	G1954	G1883	C1675	C1575	C1575
	G2447	G2447	G2254	G2254	C2165	G2104	U2029	U1955	C1676	A1677	U1576	U1576
	G2448	G2448	G2255	G2255	C2166	C2104	G2035	U1956	G1678	A1784	C1577	C1577
	G2449	G2449	G2256	G2256	U2167	U2099	C2036	G1959	U1875	U1785	U1578	U1578
	G2450	G2450	G2257	G2257	C2168	U2102	G2037	A1960	G1878	A1786	A1586	A1586
	G2451	G2451	G2258	G2258	A2169	C2103	G2038	C1882	U1791	C1792	A1587	A1587
	G2452	G2452	G2259	G2259	C2170	C2104	G2039	G1883	G1792	C1683	C1588	C1588
	G2453	G2453	G2260	G2260	U2172	C2108	A2031	U1963	C1793	C1684	U1589	U1589
	G2454	G2454	G2261	G2261	C2173	U2109	G2032	G1964	A1884	G1685	G1591	G1591
	G2455	G2455	U2262	U2262	C2174	G2110	A2033	C1965	C1885	C1686	C1592	C1592
	G2456	G2456	C2263	C2263	C2175	C2111	G2034	C1966	U1794	G1795	G1593	G1593
	G2457	G2457	G2264	G2264	A2176	G2112	C2035	A1966	C1886	U1796	G1594	G1594
	G2458	G2458	A2267	A2267	C2177	U2113	G2036	C1967	U1887	C1797	G1595	G1595
	G2459	G2459	G2268	G2268	C2178	G2114	G2037	G1968	A1889	U1798	A1603	A1603
	G2460	G2460	A2269	A2269	U2180	G2115	G2038	A1969	A1890	C1799	C1607	C1607
	G2461	G2461	G2270	G2270	U2181	G2116	A2042	U1970	C1891	C1800	A1808	A1808
	G2462	G2462	G2271	G2271	A2117	G2117	C2043	A1971	C1895	C1691	A1609	A1609
	G2463	G2463	A2274	A2274	C2184	U2118	G2043	C1895	U1898	U1693	A1610	A1610
	G2464	G2464	G2275	G2275	C2185	A2119	C2043	G1972	C1895	C1694	C1697	C1697
	G2465	G2465	G2276	G2276	G2186	C2120	G2048	G1973	U1898	A1802	A1698	A1698
	G2466	G2466	G2277	G2277	U2189	G2123	A2051	U1976	G1899	C1804		
	G2467	G2467	A2278	A2278	C2124	G2124	G2052	A1977	C1899	U1805		
	G2468	G2468	G2279	G2279	G2125	G2125	G2053	A1978	A1901			
	G2469	G2469	G2280	G2280	C2191	G2125						
	G2470	G2470	G2281	G2281								
	G2471	G2471	G2282	G2282								
	G2472	G2472	G2283	G2283								
	G2473	G2473	G2284	G2284								
	G2474	G2474	G2285	G2285								
	G2475	G2475	G2286	G2286								
	G2476	G2476	G2287	G2287								
	G2477	G2477	G2288	G2288								
	G2478	G2478	G2289	G2289								
	G2479	G2479	G2290	G2290								
	G2480	G2480	G2291	G2291								
	G2481	G2481	G2292	G2292								
	G2482	G2482	G2293	G2293								
	G2483	G2483	G2294	G2294								
	G2484	G2484	G2295	G2295								
	G2485	G2485	A2360	A2360								
	G2486	G2486	A2361	A2361								
	G2487	G2487	A2362	A2362								
	G2488	G2488	A2363	A2363								
	G2489	G2489	A2364	A2364								
	G2490	G2490	A2365	A2365								
	G2491	G2491	A2366	A2366								
	G2492	G2492	A2367	A2367								
	G2493	G2493	A2368	A2368								
	G2494	G2494	A2369	A2369								
	G2495	G2495	A2370	A2370								
	G2496	G2496	A2371	A2371								
	G2497	G2497	A2372	A2372								
	G2498	G2498	A2373	A2373								
	G2499	G2499	A2374	A2374								
	G2500	G2500	A2375	A2375								
	G2501	G2501	A2376	A2376								
	G2502	G2502	A2377	A2377								
	G2503	G2503	A2378	A2378								
	G2504	G2504	A2379	A2379								
	G2505	G2505	A2380	A2380								
	G2506	G2506	A2381	A2381								
	G2507	G2507	A2382	A2382								
	G2508	G2508	A2383	A2383								
	G2509	G2509	A2384	A2384								
	G2510	G2510	A2385	A2385								
	G2511	G2511	A2386	A2386								
	G2512	G2512	A2387	A2387								
	G2513	G2513	A2388	A2388								
	G2514	G2514	A2389	A2389								
	G2515	G2515	A2390	A2390								
	G2516	G2516	A2391	A2391								
	G2517	G2517	A2392	A2392								
	G2518	G2518	A2393	A2393								
	G2519	G2519	A2394	A2394								
	G2520	G2520	A2395	A2395								
	G2521	G2521	A2396	A2396								
	G2522	G2522	A2397	A2397								
	G2523	G2523	A2398	A2398								
	G2524	G2524	A2399	A2399								
	G2525	G2525	A2400	A2400								
	G2526	G2526	A2401	A2401								
	G2527	G2527	A2402	A2402								
	G2528	G2528	A2403	A2403								
	G2529	G2529	A2404	A2404								
	G2530	G2530	A2405	A2405								
	G2531	G2531	A2406	A2406								
	G2532	G2532	A2407	A2407								
	G2533	G2533	A2408	A2408								
	G2534	G2534	A2409	A2409								
	G2535	G2535	A2410	A2410								
	G2536	G2536	A2411	A2411								
	G2537	G2537	A2412	A2412								
	G2538	G2538	A2413	A2413								
	G2539	G2539	A2414	A2414								
	G2540	G2540	A2415	A2415								
	G2541	G2541	A2416	A2416								
	G2542	G2542	A2417	A2417								
	G2543	G2543	A2418	A2418								
	G2544	G2544	A2419	A2419								

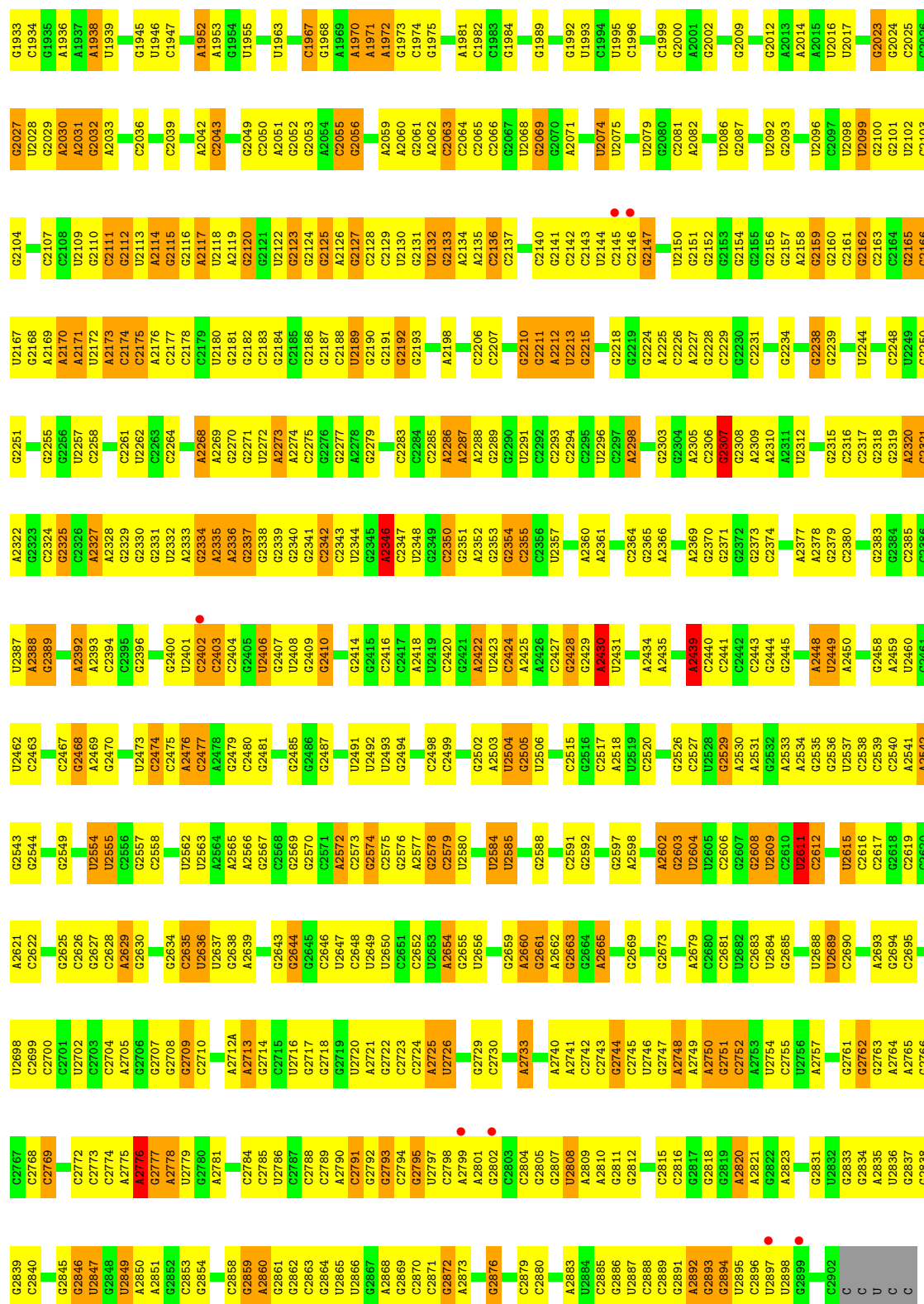


• Molecule 24: 23S ribosomal RNA

Chain 14:

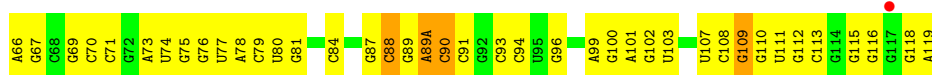




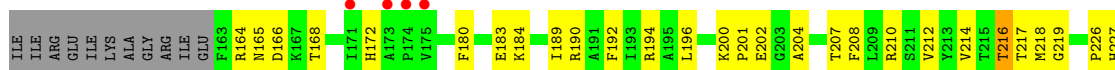
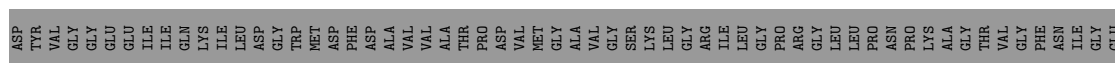




Chain 1J:

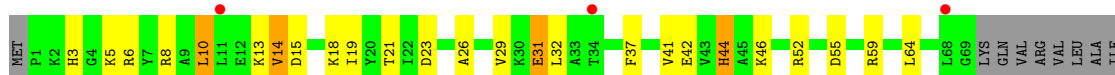


Chain 71: 3% 39% 19% 41%

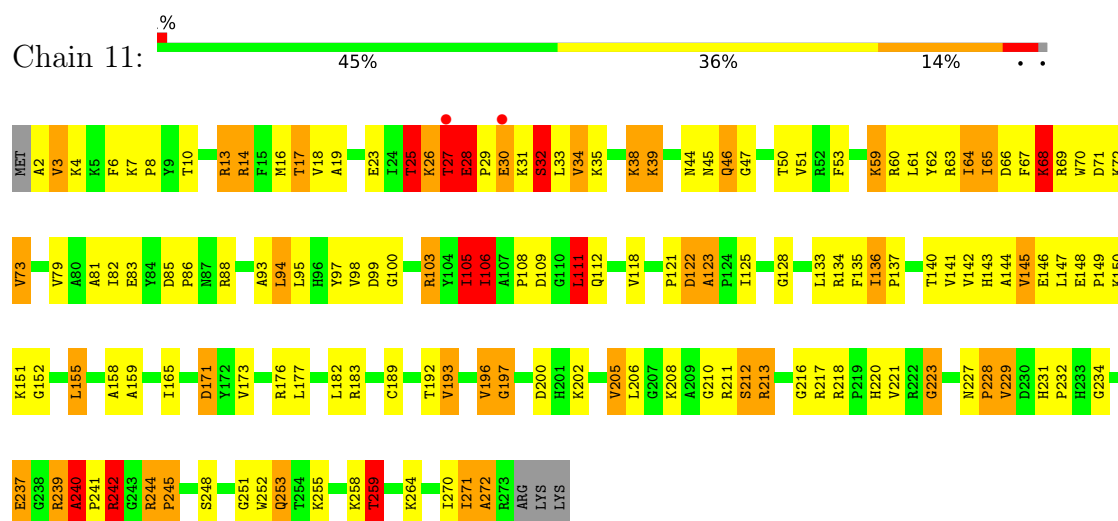


S228

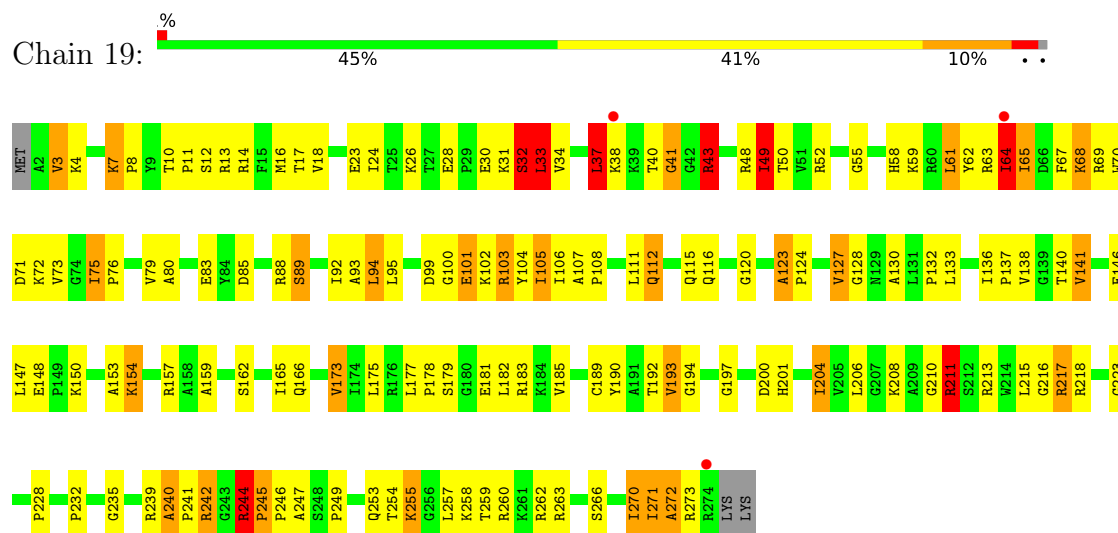
Chain 79: 3% 34% 21% 41%



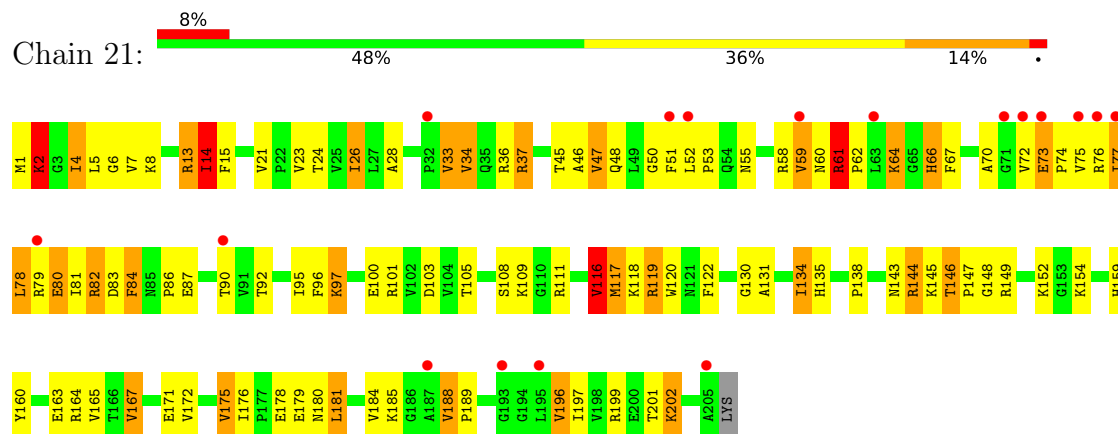
WORLDWIDE
PDB
PROTEIN DATA BANK



• Molecule 27: 50S ribosomal protein L2

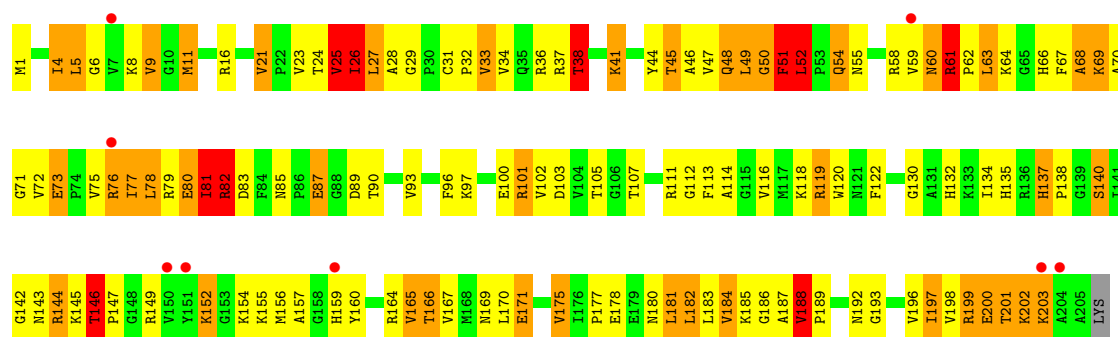


• Molecule 28: 50S ribosomal protein L3



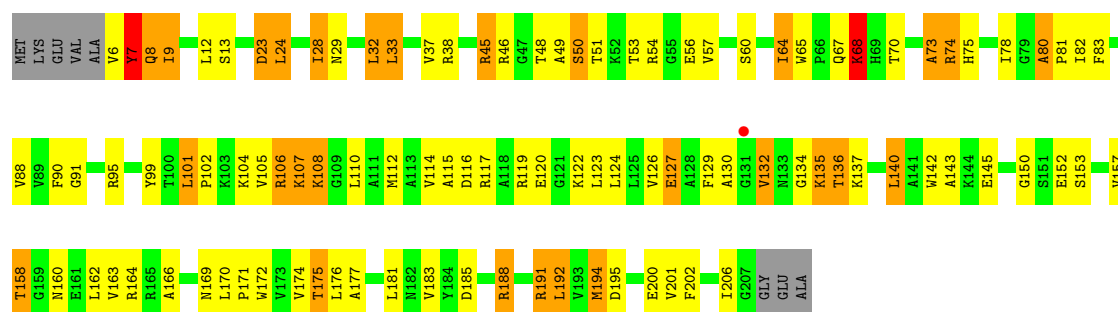
• Molecule 28: 50S ribosomal protein L3





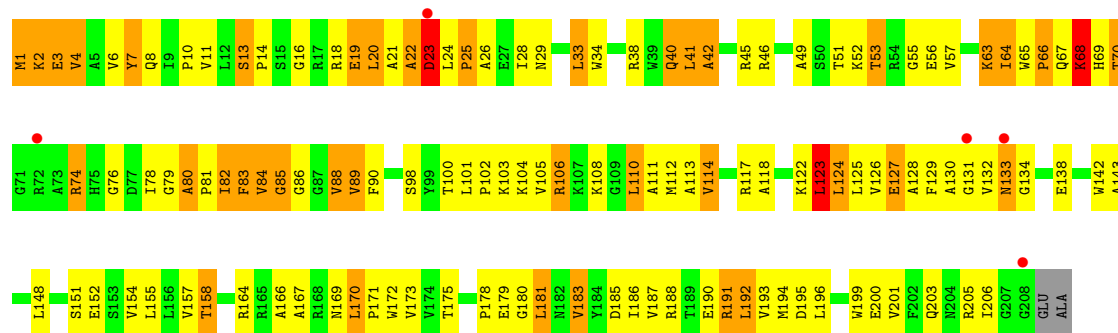
• Molecule 29: 50S ribosomal protein L4

Chain 31: 47% 35% 13% ..



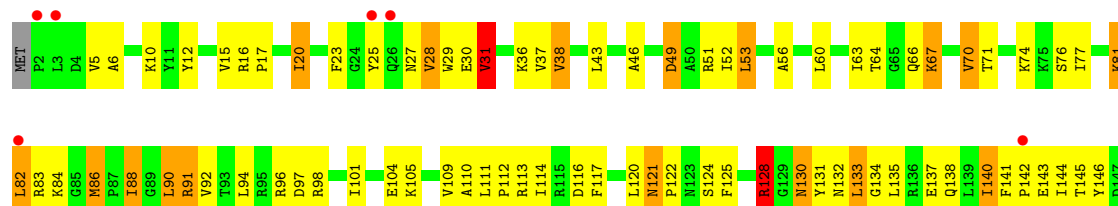
• Molecule 29: 50S ribosomal protein L4

Chain 39: 2% 37% 42% 19% ..



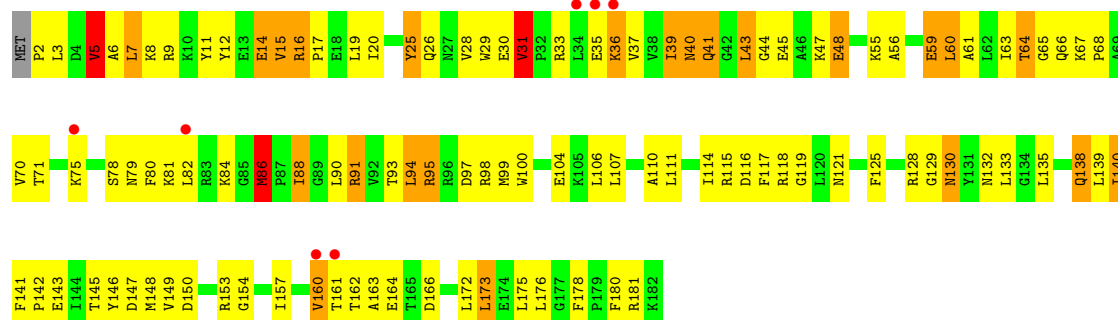
• Molecule 30: 50S ribosomal protein L5

Chain 41: 3% 46% 42% 11% ..

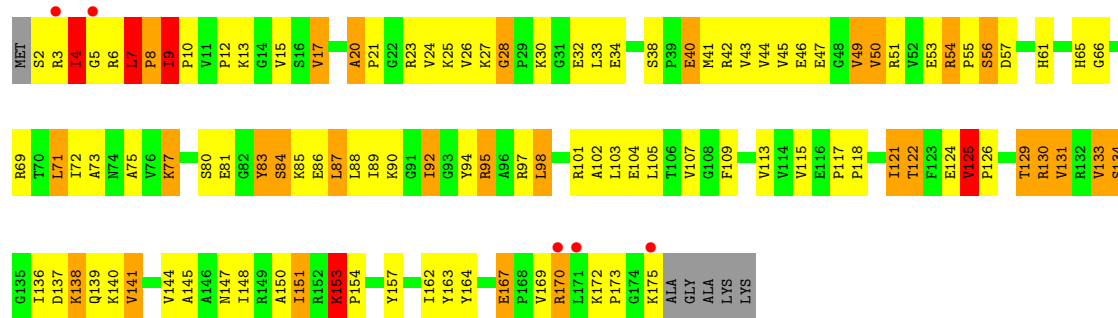




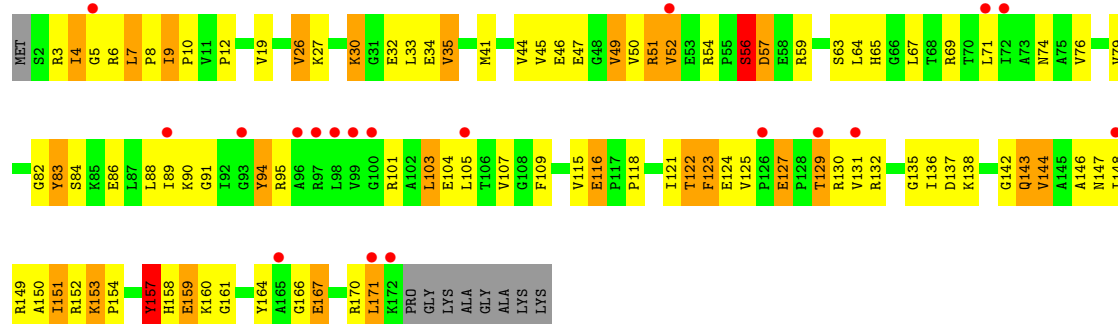
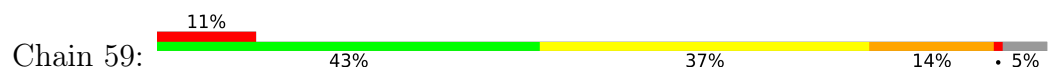
• Molecule 30: 50S ribosomal protein L5



• Molecule 31: 50S ribosomal protein L6

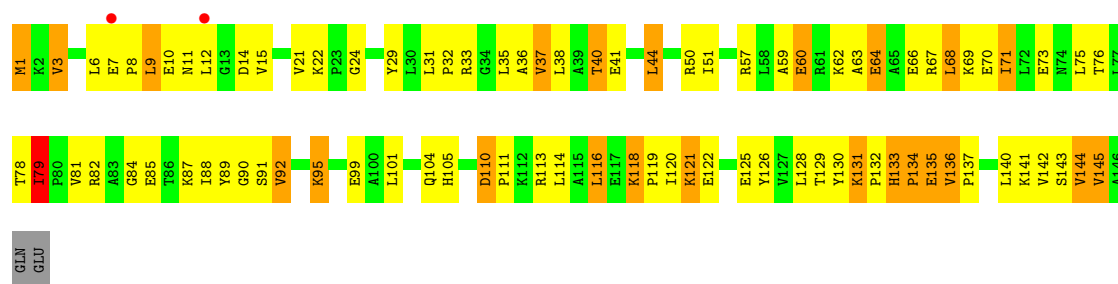


• Molecule 31: 50S ribosomal protein L6

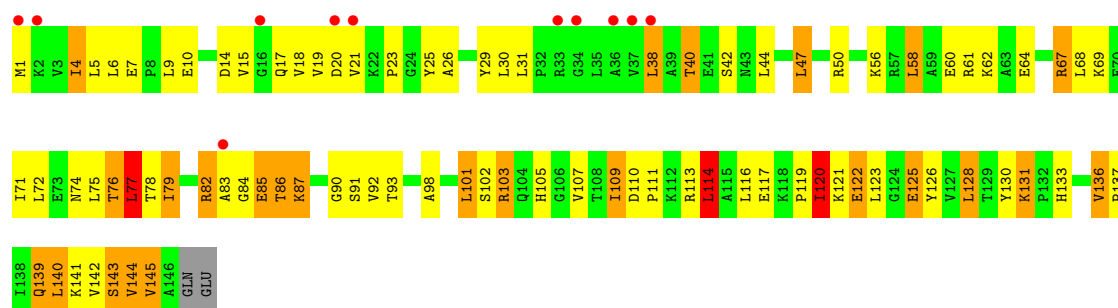
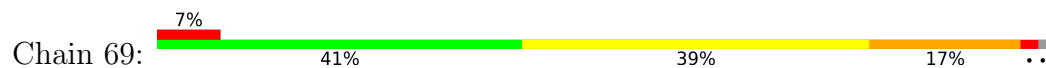


• Molecule 32: 50S ribosomal protein L9

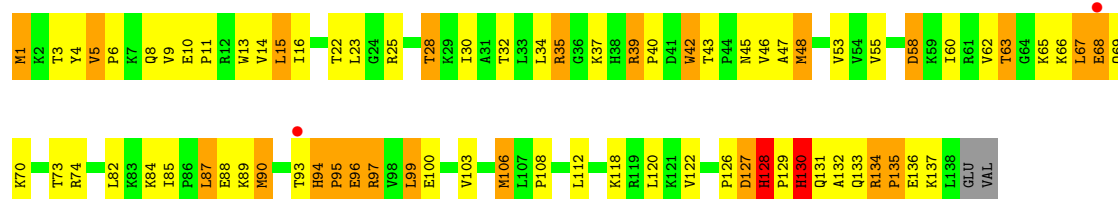




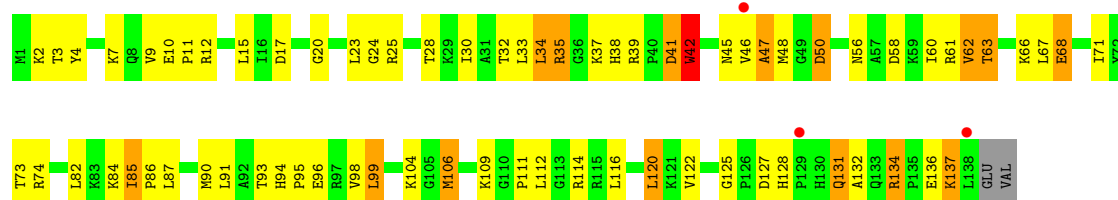
- Molecule 32: 50S ribosomal protein L9



- Molecule 33: 50S ribosomal protein L13

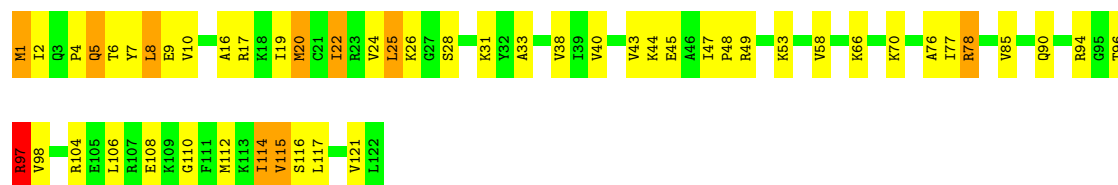


- Molecule 33: 50S ribosomal protein L13



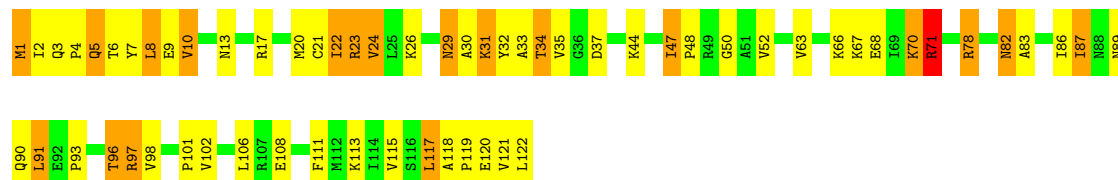
- Molecule 34: 50S ribosomal protein L14





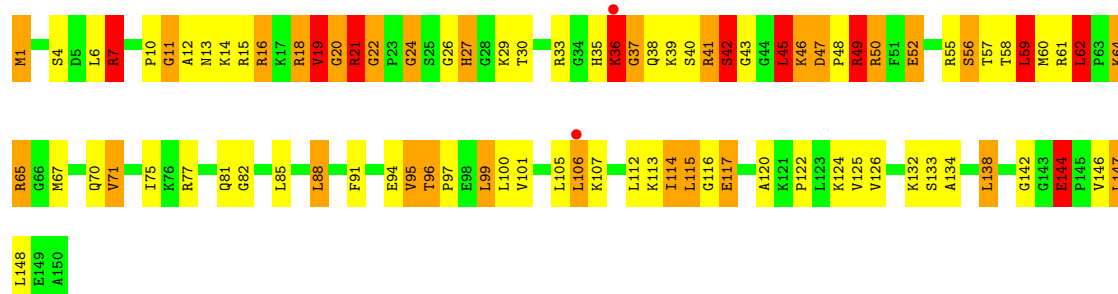
- Molecule 34: 50S ribosomal protein L14

Chain 25: 49% 34% 16% .



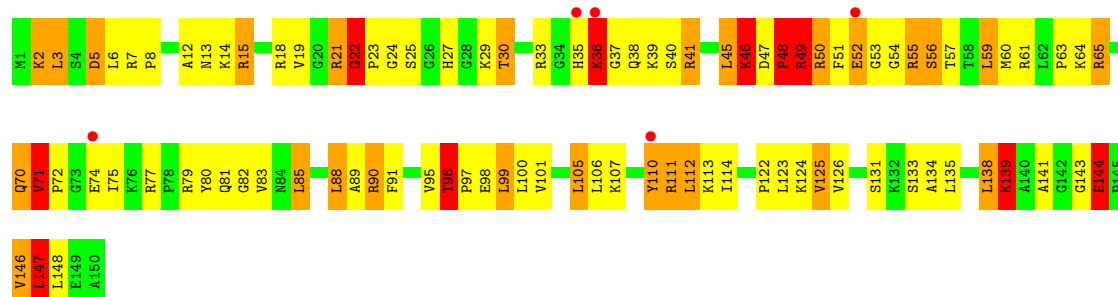
- Molecule 35: 50S ribosomal protein L15

Chain 78: 41% 33% 19% 7%



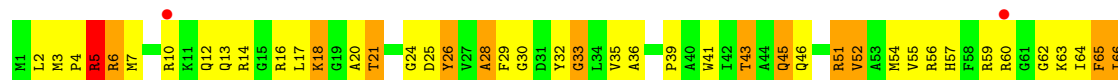
- Molecule 35: 50S ribosomal protein L15

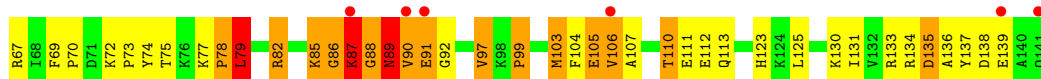
Chain 35: 37% 39% 17% 7%



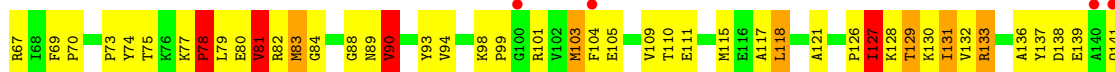
- Molecule 36: 50S ribosomal protein L16

Chain 88: 6% 40% 38% 18%

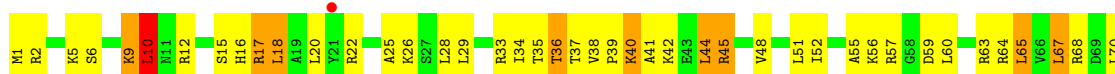




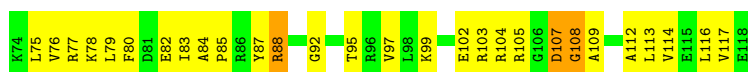
- Molecule 36: 50S ribosomal protein L16



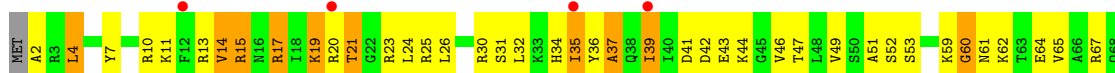
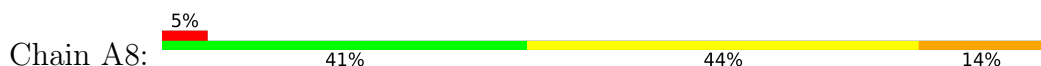
- Molecule 37: 50S ribosomal protein L17



- Molecule 37: 50S ribosomal protein L17

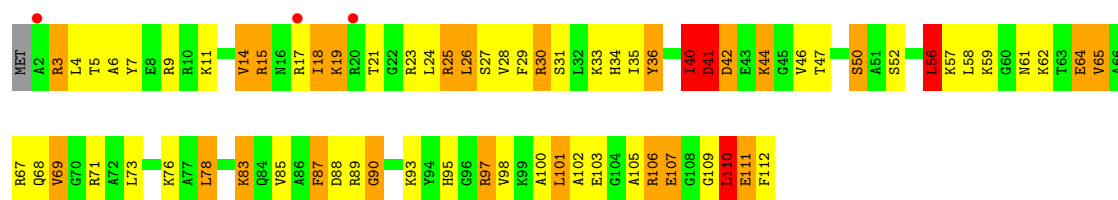


- Molecule 38: 50S ribosomal protein L18

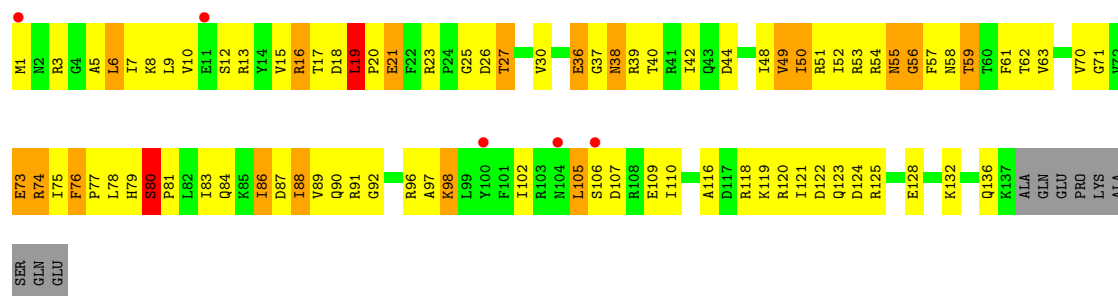


- Molecule 38: 50S ribosomal protein L18

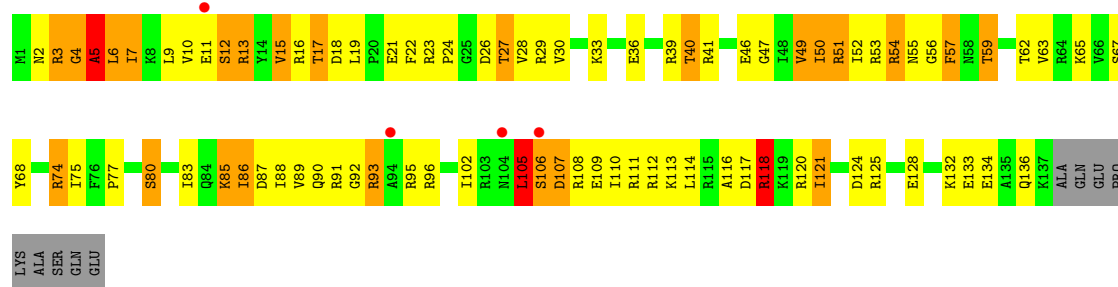




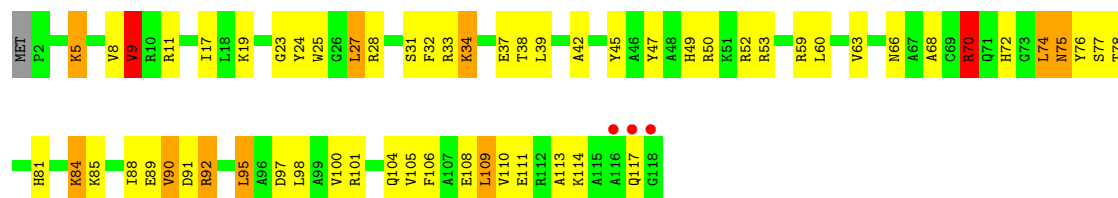
• Molecule 39: 50S ribosomal protein L19



• Molecule 39: 50S ribosomal protein L19



• Molecule 40: 50S ribosomal protein L20

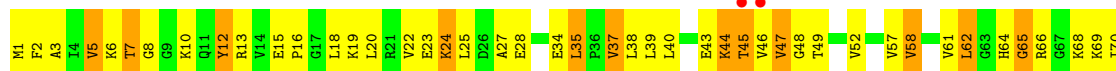
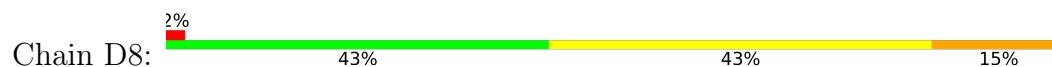


• Molecule 40: 50S ribosomal protein L20

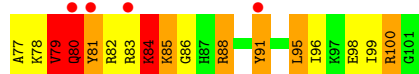




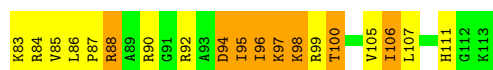
- Molecule 41: 50S ribosomal protein L21



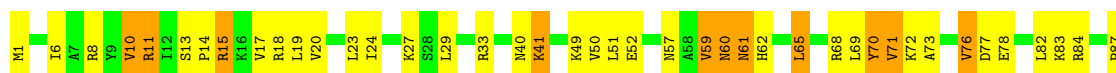
- Molecule 41: 50S ribosomal protein L21



- Molecule 42: 50S ribosomal protein L22

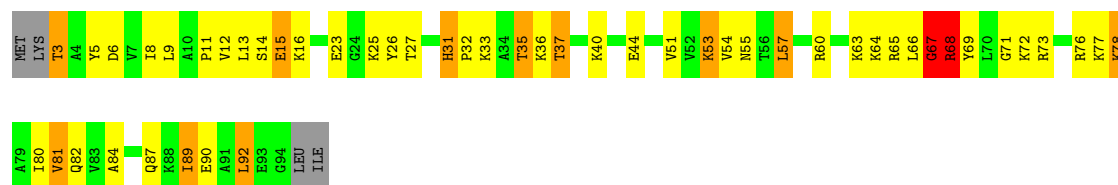


- Molecule 42: 50S ribosomal protein L22

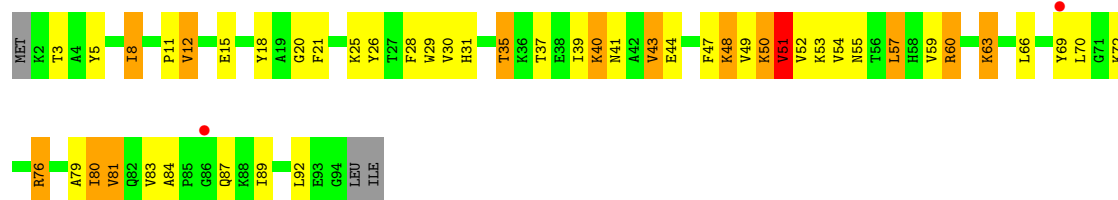


- Molecule 43: 50S ribosomal protein L23

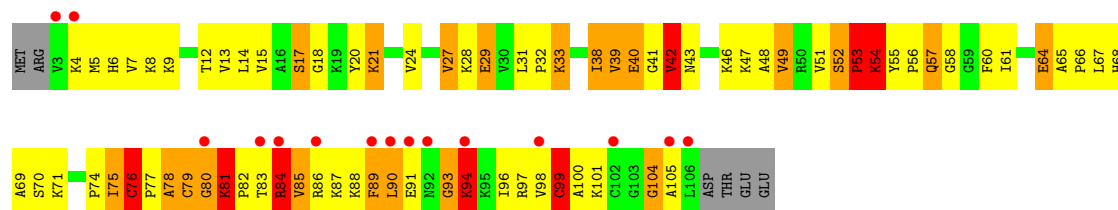




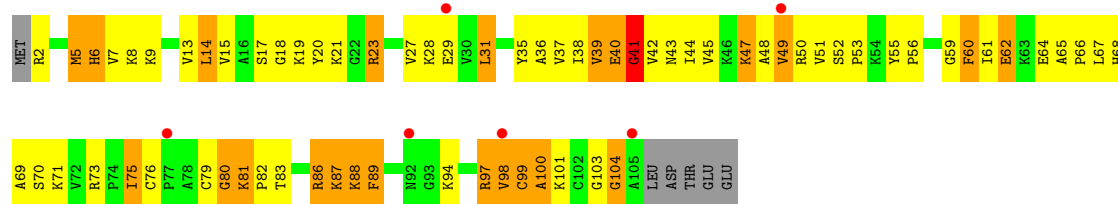
- Molecule 43: 50S ribosomal protein L23



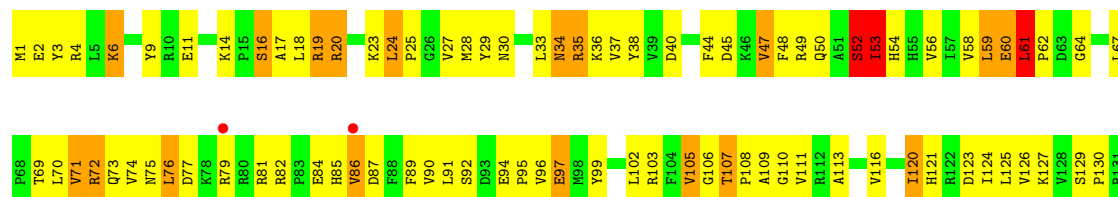
- Molecule 44: 50S ribosomal protein L24

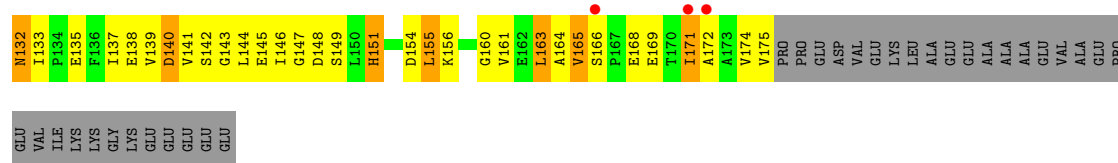


- Molecule 44: 50S ribosomal protein L24

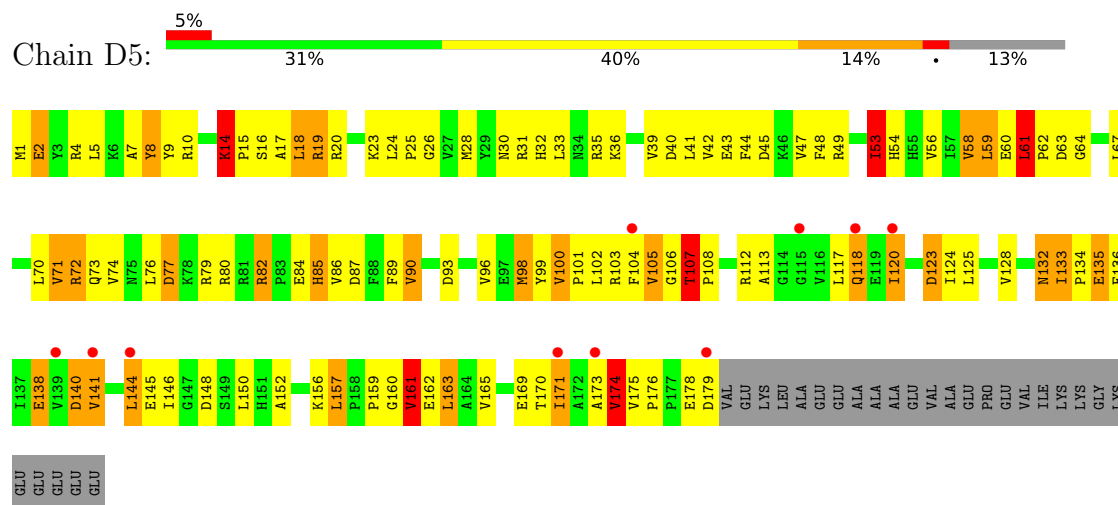


- Molecule 45: 50S ribosomal protein L25

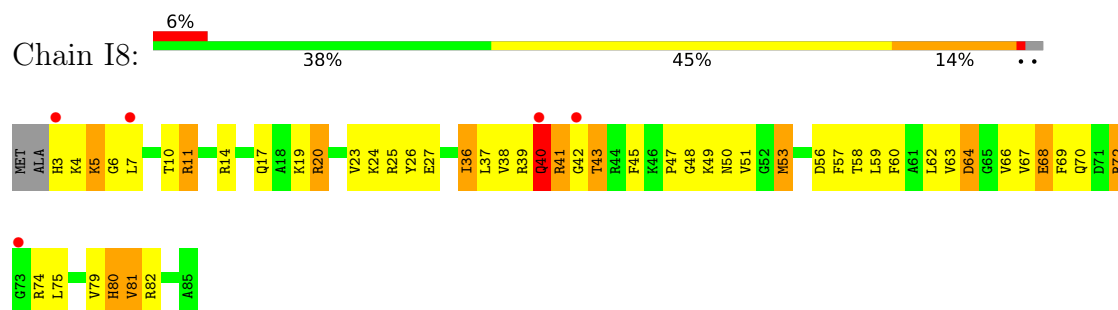




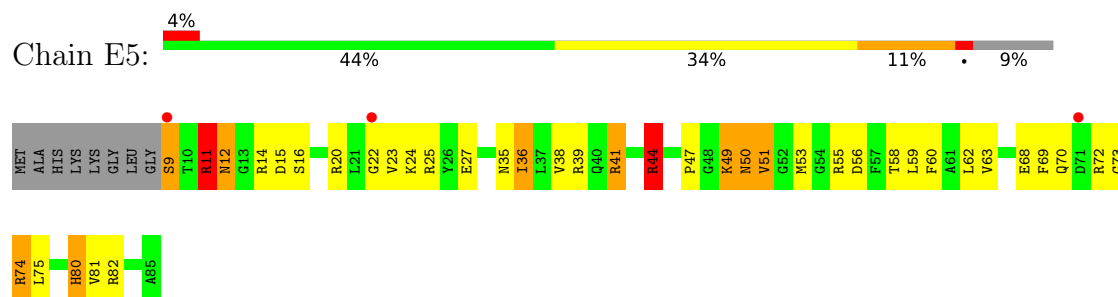
• Molecule 45: 50S ribosomal protein L25



• Molecule 46: 50S ribosomal protein L27

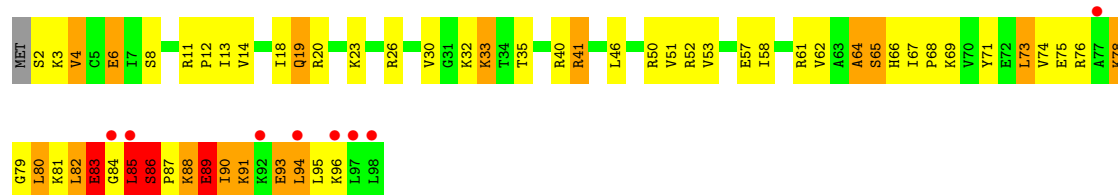


• Molecule 46: 50S ribosomal protein L27

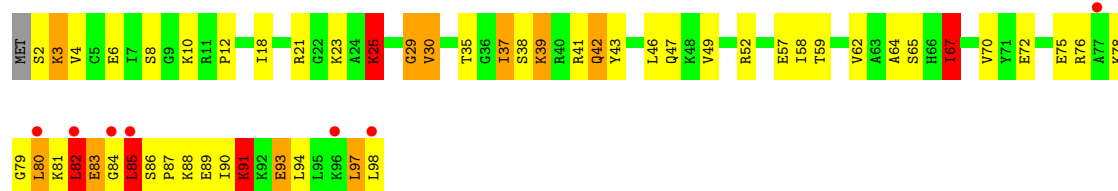


• Molecule 47: 50S ribosomal protein L28

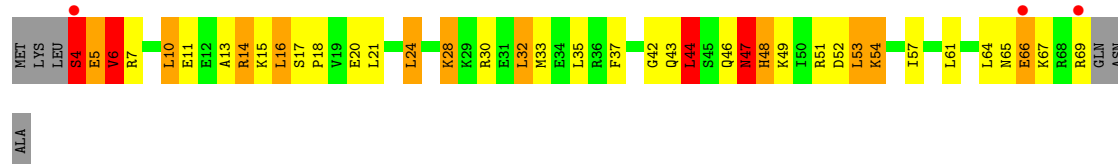




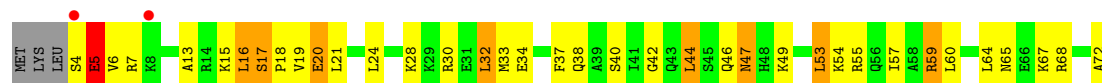
• Molecule 47: 50S ribosomal protein L28



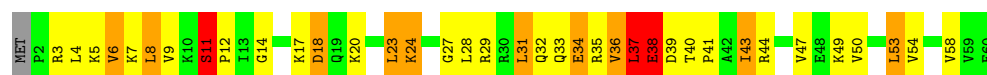
• Molecule 48: 50S ribosomal protein L29



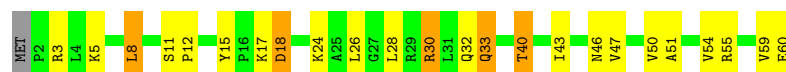
• Molecule 48: 50S ribosomal protein L29



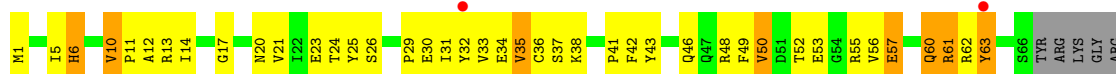
• Molecule 49: 50S ribosomal protein L30



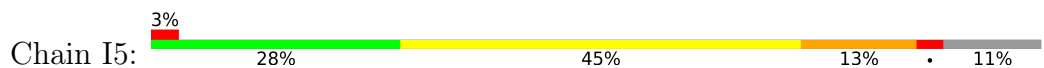
• Molecule 49: 50S ribosomal protein L30



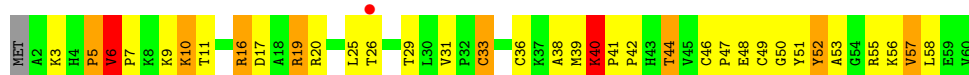
• Molecule 50: 50S ribosomal protein L31



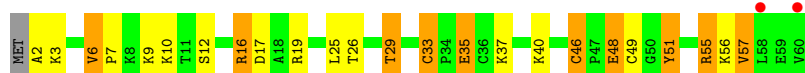
- Molecule 50: 50S ribosomal protein L31



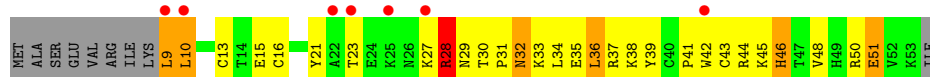
- Molecule 51: 50S ribosomal protein L32



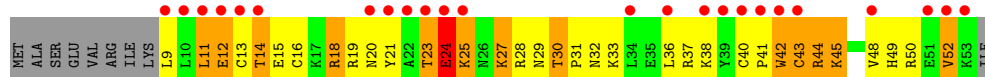
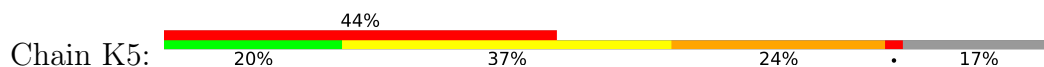
- Molecule 51: 50S ribosomal protein L32



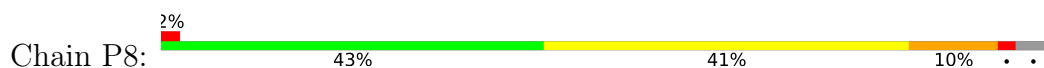
- Molecule 52: 50S ribosomal protein L33

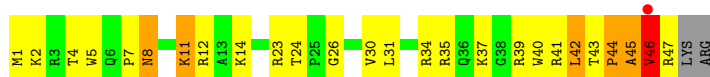


- Molecule 52: 50S ribosomal protein L33



- Molecule 53: 50S ribosomal protein L34





- Molecule 53: 50S ribosomal protein L34



- Molecule 54: 50S ribosomal protein L35



- Molecule 54: 50S ribosomal protein L35



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	210.70Å 448.40Å 616.30Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	153.54 – 3.10 153.54 – 3.10	Depositor EDS
% Data completeness (in resolution range)	99.8 (153.54-3.10) 91.1 (153.54-3.10)	Depositor EDS
R_{merge}	0.22	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.83 (at 3.07Å)	Xtriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.227 , 0.193 0.194 , 0.228	Depositor DCC
R_{free} test set	2000 reflections (0.19%)	wwPDB-VP
Wilson B-factor (Å ²)	84.3	Xtriage
Anisotropy	0.119	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 69.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	299705	wwPDB-VP
Average B, all atoms (Å ²)	114.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.48% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

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	0.45	0/36199	0.70	4/56498 (0.0%)
1	1G	0.45	0/36167	0.71	12/56448 (0.0%)
2	12	0.53	0/1959	1.02	9/2642 (0.3%)
2	1E	0.56	0/1959	0.98	4/2642 (0.2%)
3	22	0.62	0/1636	0.98	2/2205 (0.1%)
3	2E	0.61	0/1629	0.96	1/2195 (0.0%)
4	32	0.69	1/1732 (0.1%)	1.16	12/2318 (0.5%)
4	3E	0.76	1/1732 (0.1%)	1.19	13/2318 (0.6%)
5	42	0.72	0/1171	1.21	9/1576 (0.6%)
5	4E	0.72	0/1171	1.11	7/1576 (0.4%)
6	52	0.73	0/855	1.08	3/1154 (0.3%)
6	5E	0.68	0/855	1.08	2/1154 (0.2%)
7	62	0.61	0/1275	1.03	3/1709 (0.2%)
7	6E	0.59	0/1275	1.01	5/1709 (0.3%)
8	72	0.68	0/1135	1.10	2/1527 (0.1%)
8	7E	0.67	0/1135	1.27	12/1527 (0.8%)
9	82	0.59	0/1028	1.04	5/1379 (0.4%)
9	8E	0.57	0/1028	0.94	0/1379
10	1A	0.57	0/814	0.98	2/1095 (0.2%)
10	1I	0.61	0/814	1.08	8/1095 (0.7%)
11	2A	0.74	0/879	1.17	6/1187 (0.5%)
11	2I	0.73	0/879	1.15	2/1187 (0.2%)
12	3A	0.84	0/991	1.21	9/1327 (0.7%)
12	3I	0.85	0/991	1.31	6/1327 (0.5%)
13	4A	0.54	0/943	0.94	3/1265 (0.2%)
13	4I	0.54	0/938	1.09	4/1258 (0.3%)
14	5A	0.60	0/500	1.09	1/664 (0.2%)
14	5I	0.68	1/500 (0.2%)	1.12	3/664 (0.5%)
15	6A	0.77	0/744	1.02	1/992 (0.1%)
15	6I	0.76	0/744	1.08	0/992
16	7A	0.75	0/721	1.10	3/970 (0.3%)
16	7I	0.67	0/721	1.12	3/970 (0.3%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
17	8A	0.70	0/847	1.13	4/1131 (0.4%)
17	8I	0.65	0/847	1.06	1/1131 (0.1%)
18	9A	0.71	0/595	1.11	1/790 (0.1%)
18	9I	0.69	0/595	1.05	3/790 (0.4%)
19	AA	0.61	0/647	1.12	3/871 (0.3%)
19	AI	0.55	0/680	1.17	6/915 (0.7%)
20	BA	0.73	0/764	1.19	5/1007 (0.5%)
20	BI	0.59	0/764	1.07	1/1007 (0.1%)
21	1B	0.54	0/221	0.97	0/288
21	1F	0.52	0/221	0.96	0/288
22	2K	0.47	1/1784 (0.1%)	0.80	1/2771 (0.0%)
22	2L	0.47	0/1686	0.75	0/2618
22	3K	0.29	0/1850	0.49	0/2875
22	3L	0.31	0/1851	0.51	0/2877
23	4K	0.68	0/392	0.87	1/609 (0.2%)
23	4L	0.56	0/190	0.83	0/293
24	14	0.59	0/70167	0.82	20/109541 (0.0%)
24	1H	0.63	0/70233	0.86	36/109643 (0.0%)
25	16	0.48	0/2928	0.74	0/4568
25	1J	0.48	0/2928	0.78	0/4568
26	71	0.39	0/1072	0.84	2/1447 (0.1%)
26	79	0.40	0/1072	0.90	6/1447 (0.4%)
27	11	1.17	8/2165 (0.4%)	1.63	43/2919 (1.5%)
27	19	1.06	3/2170 (0.1%)	1.45	26/2926 (0.9%)
28	21	0.93	1/1601 (0.1%)	1.43	18/2160 (0.8%)
28	29	0.97	1/1601 (0.1%)	1.49	25/2160 (1.2%)
29	31	1.01	1/1620 (0.1%)	1.38	17/2194 (0.8%)
29	39	0.89	0/1662	1.38	15/2249 (0.7%)
30	41	0.57	0/1498	1.01	6/2016 (0.3%)
30	49	0.55	0/1498	1.02	5/2016 (0.2%)
31	51	0.85	0/1362	1.46	27/1841 (1.5%)
31	59	0.55	0/1337	1.19	17/1809 (0.9%)
32	61	0.73	0/1151	1.15	11/1558 (0.7%)
32	69	0.69	0/1151	1.12	9/1558 (0.6%)
33	15	0.75	0/1131	1.21	8/1525 (0.5%)
33	58	0.83	0/1131	1.20	6/1525 (0.4%)
34	25	1.04	1/942 (0.1%)	1.28	7/1269 (0.6%)
34	68	0.95	0/942	1.25	2/1269 (0.2%)
35	35	0.92	0/1161	1.60	21/1544 (1.4%)
35	78	1.04	2/1161 (0.2%)	1.53	17/1544 (1.1%)
36	45	0.87	1/1142 (0.1%)	1.36	7/1527 (0.5%)
36	88	0.98	1/1142 (0.1%)	1.38	15/1527 (1.0%)
37	55	0.94	0/973	1.26	1/1302 (0.1%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
37	98	0.91	1/981 (0.1%)	1.30	7/1312 (0.5%)
38	65	0.76	0/891	1.22	9/1187 (0.8%)
38	A8	0.77	0/891	1.19	3/1187 (0.3%)
39	75	0.94	0/1145	1.28	8/1531 (0.5%)
39	B8	0.87	0/1155	1.31	13/1542 (0.8%)
40	85	0.85	0/981	1.16	3/1306 (0.2%)
40	C8	0.94	0/981	1.20	2/1306 (0.2%)
41	95	2.58	9/789 (1.1%)	1.66	17/1057 (1.6%)
41	D8	0.88	0/789	1.23	3/1057 (0.3%)
42	A5	0.96	0/910	1.23	6/1220 (0.5%)
42	E8	1.02	0/910	1.28	4/1220 (0.3%)
43	B5	0.99	0/744	1.19	3/1000 (0.3%)
43	F8	1.06	1/739 (0.1%)	1.27	2/993 (0.2%)
44	C5	0.89	1/807 (0.1%)	1.33	12/1076 (1.1%)
44	G8	1.13	2/804 (0.2%)	1.63	19/1073 (1.8%)
45	D5	0.61	0/1460	1.14	15/1982 (0.8%)
45	H8	0.61	0/1427	1.15	10/1935 (0.5%)
46	E5	0.88	0/620	1.30	6/827 (0.7%)
46	I8	1.01	0/665	1.30	2/885 (0.2%)
47	F5	0.89	1/769 (0.1%)	1.29	7/1022 (0.7%)
47	J8	0.91	0/769	1.39	8/1022 (0.8%)
48	G5	0.75	0/582	1.25	2/771 (0.3%)
48	K8	1.02	1/560 (0.2%)	1.39	5/741 (0.7%)
49	H5	0.79	0/473	1.26	2/635 (0.3%)
49	L8	0.88	1/473 (0.2%)	1.44	8/635 (1.3%)
50	I5	0.65	0/527	1.06	3/709 (0.4%)
50	M8	0.51	0/545	0.92	0/733
51	J5	0.87	0/472	1.24	4/639 (0.6%)
51	N8	1.05	1/472 (0.2%)	1.32	7/639 (1.1%)
52	K5	0.78	0/396	1.24	6/529 (1.1%)
52	O8	0.74	0/396	1.22	4/529 (0.8%)
53	L5	1.08	1/437 (0.2%)	1.31	2/575 (0.3%)
53	P8	1.18	0/417	1.34	1/550 (0.2%)
54	M5	1.20	1/502 (0.2%)	1.63	12/661 (1.8%)
54	Q8	1.26	2/488 (0.4%)	1.68	6/641 (0.9%)
All	All	0.65	45/321962 (0.0%)	0.93	770/481589 (0.2%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
2	12	0	2
2	1E	0	1
3	22	0	1
4	3E	0	3
9	82	0	2
12	3A	0	4
14	5I	0	1
19	AA	0	1
19	AI	0	3
20	BA	0	2
27	11	0	4
27	19	0	5
28	29	0	7
29	31	0	1
29	39	0	1
30	49	0	1
31	59	0	1
32	61	0	1
33	15	0	1
34	25	0	1
35	35	0	7
35	78	0	7
36	45	0	1
36	88	0	3
38	65	0	1
38	A8	0	2
39	75	0	3
39	B8	0	1
40	85	0	1
41	95	0	2
43	F8	0	1
44	C5	0	3
44	G8	0	5
45	D5	0	3
47	F5	0	2
47	J8	0	2
48	K8	0	2
49	L8	0	1
51	J5	0	1
52	K5	0	1
53	P8	0	2
54	M5	0	2
54	Q8	0	4

Continued on next page...

Continued from previous page...

Mol	Chain	#Chirality outliers	#Planarity outliers
All	All	0	100

The worst 5 of 45 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
41	95	91	TYR	CD1-CE1	30.02	2.28	1.38
41	95	91	TYR	CD2-CE2	29.01	2.25	1.38
41	95	21	ARG	CD-NE	28.53	1.86	1.46
41	95	91	TYR	CE2-CZ	22.59	1.92	1.38
41	95	91	TYR	CE1-CZ	21.76	1.90	1.38

The worst 5 of 770 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
41	95	21	ARG	CD-NE-CZ	22.47	155.86	124.40
54	Q8	41	ILE	N-CA-C	-17.43	97.85	111.62
27	11	28	GLU	CA-C-N	-15.72	104.47	120.03
27	11	28	GLU	C-N-CA	-15.72	104.47	120.03
31	51	9	ILE	CA-C-N	-13.16	107.00	120.03

There are no chirality outliers.

5 of 100 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	1E	71	VAL	Peptide
4	3E	166	LYS	Peptide
4	3E	193	ASP	Peptide
4	3E	29	PRO	Peptide
14	5I	13	THR	Peptide

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	13	32337	0	16321	895	0
1	1G	32309	0	16307	842	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	12	1924	0	1975	102	0
2	1E	1924	0	1975	123	0
3	22	1612	0	1677	96	0
3	2E	1605	0	1668	72	0
4	32	1702	0	1763	117	1
4	3E	1702	0	1763	83	0
5	42	1155	0	1213	75	0
5	4E	1155	0	1213	58	0
6	52	842	0	857	39	0
6	5E	842	0	857	47	1
7	62	1256	0	1296	42	0
7	6E	1256	0	1296	60	0
8	72	1115	0	1177	52	0
8	7E	1115	0	1177	74	0
9	82	1009	0	1037	77	0
9	8E	1009	0	1037	67	0
10	1A	801	0	849	55	0
10	1I	801	0	849	44	0
11	2A	864	0	881	28	0
11	2I	864	0	881	40	0
12	3A	975	0	1062	39	0
12	3I	975	0	1062	43	0
13	4A	933	0	992	58	0
13	4I	928	0	987	52	0
14	5A	491	0	529	38	0
14	5I	491	0	529	46	0
15	6A	733	0	771	28	0
15	6I	733	0	771	36	0
16	7A	705	0	725	35	0
16	7I	705	0	725	51	0
17	8A	834	0	904	47	0
17	8I	834	0	904	49	0
18	9A	590	0	662	27	0
18	9I	590	0	662	22	0
19	AA	633	0	649	48	0
19	AI	665	0	686	38	0
20	BA	762	0	861	38	0
20	BI	762	0	861	55	0
21	1B	217	0	234	16	0
21	1F	217	0	234	12	0
22	2K	1765	0	916	67	0
22	2L	1678	0	872	65	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
22	3K	1824	0	945	58	0
22	3L	1825	0	946	51	0
23	4K	348	0	175	9	0
23	4L	170	0	87	3	0
24	14	62647	0	31572	1465	0
24	1H	62707	0	31606	1615	0
25	16	2617	0	1328	87	0
25	1J	2617	0	1328	93	0
26	71	1049	0	1071	32	0
26	79	1049	0	1071	42	0
27	11	2115	0	2195	136	0
27	19	2120	0	2197	116	0
28	21	1568	0	1634	98	0
28	29	1568	0	1634	127	0
29	31	1585	0	1632	86	0
29	39	1627	0	1680	107	0
30	41	1473	0	1535	75	0
30	49	1473	0	1535	90	0
31	51	1336	0	1418	92	0
31	59	1312	0	1384	65	0
32	61	1136	0	1223	56	0
32	69	1136	0	1223	68	0
33	15	1104	0	1180	50	0
33	58	1104	0	1180	55	0
34	25	932	0	996	45	0
34	68	932	0	996	34	0
35	35	1144	0	1228	84	0
35	78	1144	0	1228	92	0
36	45	1121	0	1179	75	0
36	88	1121	0	1179	87	0
37	55	959	0	1021	54	0
37	98	967	0	1033	69	0
38	65	881	0	943	77	0
38	A8	881	0	943	49	0
39	75	1131	0	1180	89	0
39	B8	1141	0	1202	58	0
40	85	963	0	1022	58	0
40	C8	963	0	1022	61	0
41	95	778	0	852	87	0
41	D8	778	0	852	33	0
42	A5	899	0	964	36	0
42	E8	899	0	964	41	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
43	B5	730	0	780	41	0
43	F8	725	0	778	47	0
44	C5	794	0	884	58	0
44	G8	791	0	880	68	0
45	D5	1428	0	1454	92	0
45	H8	1397	0	1430	89	0
46	E5	612	0	633	39	0
46	I8	656	0	683	56	0
47	F5	762	0	848	36	0
47	J8	762	0	848	49	0
48	G5	580	0	629	28	0
48	K8	558	0	610	33	0
49	H5	468	0	518	14	0
49	L8	468	0	518	36	0
50	I5	515	0	514	44	0
50	M8	533	0	526	41	0
51	J5	458	0	480	19	0
51	N8	458	0	480	36	0
52	K5	389	0	404	25	0
52	O8	389	0	404	26	0
53	L5	429	0	480	33	0
53	P8	409	0	454	20	0
54	M5	495	0	567	37	0
54	Q8	483	0	555	43	0
55	11	2	0	0	0	0
55	13	139	0	0	0	0
55	14	465	0	0	0	0
55	15	1	0	0	0	0
55	16	15	0	0	0	0
55	19	1	0	0	0	0
55	1G	148	0	0	0	0
55	1H	523	0	0	0	0
55	1J	10	0	0	0	0
55	21	2	0	0	0	0
55	25	1	0	0	0	0
55	29	4	0	0	0	0
55	2K	5	0	0	0	0
55	2L	4	0	0	0	0
55	32	1	0	0	0	0
55	39	1	0	0	0	0
55	3A	1	0	0	0	0
55	3E	1	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
55	3I	1	0	0	0	0
55	3L	1	0	0	0	0
55	42	1	0	0	0	0
55	45	1	0	0	0	0
55	4A	1	0	0	0	0
55	4K	1	0	0	0	0
55	52	1	0	0	0	0
55	55	1	0	0	0	0
55	5E	1	0	0	0	0
55	7E	1	0	0	0	0
55	88	1	0	0	0	0
55	98	1	0	0	0	0
55	C5	1	0	0	0	0
55	E5	1	0	0	0	0
55	F5	1	0	0	0	0
55	G8	1	0	0	0	0
55	I8	3	0	0	0	0
55	Q8	2	0	0	0	0
56	32	1	0	0	0	0
56	3E	1	0	0	0	0
56	5A	1	0	0	0	0
56	5I	1	0	0	0	0
56	C5	1	0	0	0	0
56	G8	1	0	0	0	0
57	11	8	0	0	2	0
57	13	125	0	0	23	0
57	14	523	0	0	116	0
57	16	12	0	0	3	0
57	19	11	0	0	3	0
57	1G	96	0	0	18	0
57	1H	652	0	0	172	0
57	1J	22	0	0	2	0
57	21	2	0	0	2	0
57	25	6	0	0	0	0
57	2K	2	0	0	0	0
57	2L	6	0	0	0	0
57	31	5	0	0	0	0
57	32	1	0	0	0	0
57	35	1	0	0	0	0
57	39	3	0	0	0	0
57	4K	3	0	0	0	0
57	5A	1	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
57	5I	1	0	0	0	0
57	75	1	0	0	0	0
57	78	4	0	0	2	0
57	7A	2	0	0	0	0
57	85	4	0	0	0	0
57	98	1	0	0	2	0
57	AI	3	0	0	0	0
57	BA	1	0	0	0	0
57	C8	2	0	0	0	0
57	E8	1	0	0	0	0
57	F5	1	0	0	0	0
57	F8	2	0	0	0	0
57	G8	2	0	0	1	0
57	H5	2	0	0	0	0
All	All	299705	0	201607	9522	1

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 20.

The worst 5 of 9522 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)
41:95:91:TYR:CG	41:95:91:TYR:CD1	1.79	1.67
41:95:91:TYR:CG	41:95:91:TYR:CD2	1.79	1.65
41:95:91:TYR:CE1	41:95:91:TYR:CZ	1.90	1.56
41:95:91:TYR:CZ	41:95:91:TYR:CE2	1.92	1.55
22:2K:35:QUO:C4	22:2K:35:QUO:N3	1.68	1.55

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

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:5E:15:ASP:OD1	4:32:27:TYR:OH[4_555]	2.04	0.16

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%)	196 (83%)	35 (15%)	4 (2%)	7	30
2	1E	235/256 (92%)	199 (85%)	32 (14%)	4 (2%)	7	30
3	22	204/239 (85%)	175 (86%)	29 (14%)	0	100	100
3	2E	203/239 (85%)	185 (91%)	18 (9%)	0	100	100
4	32	206/209 (99%)	176 (85%)	26 (13%)	4 (2%)	6	27
4	3E	206/209 (99%)	191 (93%)	15 (7%)	0	100	100
5	42	149/162 (92%)	142 (95%)	7 (5%)	0	100	100
5	4E	149/162 (92%)	141 (95%)	7 (5%)	1 (1%)	18	49
6	52	99/101 (98%)	95 (96%)	4 (4%)	0	100	100
6	5E	99/101 (98%)	93 (94%)	6 (6%)	0	100	100
7	62	153/156 (98%)	145 (95%)	8 (5%)	0	100	100
7	6E	153/156 (98%)	142 (93%)	11 (7%)	0	100	100
8	72	136/138 (99%)	127 (93%)	7 (5%)	2 (2%)	8	32
8	7E	136/138 (99%)	125 (92%)	11 (8%)	0	100	100
9	82	125/128 (98%)	112 (90%)	12 (10%)	1 (1%)	16	47
9	8E	125/128 (98%)	114 (91%)	11 (9%)	0	100	100
10	1A	97/105 (92%)	85 (88%)	12 (12%)	0	100	100
10	1I	97/105 (92%)	84 (87%)	13 (13%)	0	100	100
11	2A	114/129 (88%)	102 (90%)	12 (10%)	0	100	100
11	2I	114/129 (88%)	102 (90%)	11 (10%)	1 (1%)	14	44
12	3A	123/132 (93%)	111 (90%)	12 (10%)	0	100	100
12	3I	123/132 (93%)	112 (91%)	11 (9%)	0	100	100
13	4A	115/126 (91%)	98 (85%)	12 (10%)	5 (4%)	2	12
13	4I	114/126 (90%)	98 (86%)	16 (14%)	0	100	100
14	5A	58/61 (95%)	48 (83%)	10 (17%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
14	5I	58/61 (95%)	52 (90%)	5 (9%)	1 (2%)	7	30
15	6A	86/89 (97%)	80 (93%)	6 (7%)	0	100	100
15	6I	86/89 (97%)	77 (90%)	9 (10%)	0	100	100
16	7A	82/88 (93%)	76 (93%)	5 (6%)	1 (1%)	10	37
16	7I	82/88 (93%)	79 (96%)	3 (4%)	0	100	100
17	8A	98/105 (93%)	92 (94%)	6 (6%)	0	100	100
17	8I	98/105 (93%)	90 (92%)	7 (7%)	1 (1%)	12	41
18	9A	70/88 (80%)	65 (93%)	5 (7%)	0	100	100
18	9I	70/88 (80%)	63 (90%)	6 (9%)	1 (1%)	9	34
19	AA	77/93 (83%)	57 (74%)	17 (22%)	3 (4%)	2	14
19	AI	81/93 (87%)	66 (82%)	13 (16%)	2 (2%)	4	21
20	BA	97/106 (92%)	83 (86%)	14 (14%)	0	100	100
20	BI	97/106 (92%)	84 (87%)	13 (13%)	0	100	100
21	1B	23/27 (85%)	22 (96%)	1 (4%)	0	100	100
21	1F	23/27 (85%)	21 (91%)	2 (9%)	0	100	100
26	7I	131/229 (57%)	130 (99%)	1 (1%)	0	100	100
26	79	131/229 (57%)	129 (98%)	2 (2%)	0	100	100
27	11	270/276 (98%)	254 (94%)	12 (4%)	4 (2%)	8	32
27	19	271/276 (98%)	253 (93%)	15 (6%)	3 (1%)	11	39
28	21	203/206 (98%)	174 (86%)	28 (14%)	1 (0%)	24	57
28	29	203/206 (98%)	160 (79%)	34 (17%)	9 (4%)	2	12
29	31	200/210 (95%)	189 (94%)	10 (5%)	1 (0%)	24	57
29	39	206/210 (98%)	176 (85%)	21 (10%)	9 (4%)	2	12
30	41	179/182 (98%)	154 (86%)	24 (13%)	1 (1%)	21	52
30	49	179/182 (98%)	151 (84%)	25 (14%)	3 (2%)	7	30
31	51	172/180 (96%)	146 (85%)	20 (12%)	6 (4%)	3	16
31	59	169/180 (94%)	133 (79%)	35 (21%)	1 (1%)	21	52
32	61	144/148 (97%)	120 (83%)	21 (15%)	3 (2%)	5	25
32	69	144/148 (97%)	122 (85%)	19 (13%)	3 (2%)	5	25
33	15	136/140 (97%)	128 (94%)	7 (5%)	1 (1%)	18	49
33	58	136/140 (97%)	116 (85%)	13 (10%)	7 (5%)	1	10

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
34	25	120/122 (98%)	111 (92%)	9 (8%)	0	100	100
34	68	120/122 (98%)	115 (96%)	4 (3%)	1 (1%)	16	47
35	35	148/150 (99%)	118 (80%)	24 (16%)	6 (4%)	2	13
35	78	148/150 (99%)	117 (79%)	28 (19%)	3 (2%)	6	25
36	45	139/141 (99%)	114 (82%)	20 (14%)	5 (4%)	2	16
36	88	139/141 (99%)	111 (80%)	23 (16%)	5 (4%)	2	16
37	55	115/118 (98%)	103 (90%)	11 (10%)	1 (1%)	14	44
37	98	116/118 (98%)	104 (90%)	10 (9%)	2 (2%)	7	30
38	65	109/112 (97%)	93 (85%)	14 (13%)	2 (2%)	6	28
38	A8	109/112 (97%)	94 (86%)	13 (12%)	2 (2%)	6	28
39	75	135/146 (92%)	113 (84%)	19 (14%)	3 (2%)	5	24
39	B8	135/146 (92%)	117 (87%)	18 (13%)	0	100	100
40	85	115/118 (98%)	106 (92%)	9 (8%)	0	100	100
40	C8	115/118 (98%)	109 (95%)	6 (5%)	0	100	100
41	95	99/101 (98%)	82 (83%)	12 (12%)	5 (5%)	1	10
41	D8	99/101 (98%)	89 (90%)	9 (9%)	1 (1%)	12	41
42	A5	111/113 (98%)	104 (94%)	7 (6%)	0	100	100
42	E8	111/113 (98%)	103 (93%)	8 (7%)	0	100	100
43	B5	91/96 (95%)	86 (94%)	4 (4%)	1 (1%)	11	39
43	F8	90/96 (94%)	84 (93%)	4 (4%)	2 (2%)	5	24
44	C5	102/110 (93%)	72 (71%)	27 (26%)	3 (3%)	3	19
44	G8	102/110 (93%)	84 (82%)	12 (12%)	6 (6%)	1	8
45	D5	177/206 (86%)	145 (82%)	25 (14%)	7 (4%)	2	13
45	H8	173/206 (84%)	134 (78%)	32 (18%)	7 (4%)	2	13
46	E5	75/85 (88%)	73 (97%)	2 (3%)	0	100	100
46	I8	81/85 (95%)	70 (86%)	11 (14%)	0	100	100
47	F5	95/98 (97%)	87 (92%)	7 (7%)	1 (1%)	11	39
47	J8	95/98 (97%)	83 (87%)	10 (10%)	2 (2%)	5	25
48	G5	67/72 (93%)	56 (84%)	11 (16%)	0	100	100
48	K8	64/72 (89%)	61 (95%)	0	3 (5%)	2	11
49	H5	57/60 (95%)	55 (96%)	2 (4%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
49	L8	57/60 (95%)	54 (95%)	3 (5%)	0	100	100
50	I5	61/71 (86%)	33 (54%)	24 (39%)	4 (7%)	1	6
50	M8	64/71 (90%)	45 (70%)	17 (27%)	2 (3%)	3	18
51	J5	57/60 (95%)	48 (84%)	8 (14%)	1 (2%)	6	28
51	N8	57/60 (95%)	49 (86%)	6 (10%)	2 (4%)	3	16
52	K5	43/54 (80%)	28 (65%)	15 (35%)	0	100	100
52	O8	43/54 (80%)	32 (74%)	11 (26%)	0	100	100
53	L5	47/49 (96%)	47 (100%)	0	0	100	100
53	P8	45/49 (92%)	39 (87%)	4 (9%)	2 (4%)	2	12
54	M5	60/65 (92%)	51 (85%)	6 (10%)	3 (5%)	1	11
54	Q8	60/65 (92%)	51 (85%)	7 (12%)	2 (3%)	3	17
All	All	11616/12512 (93%)	10210 (88%)	1239 (11%)	167 (1%)	9	34

5 of 167 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
18	9I	22	VAL
27	11	240	ALA
36	88	87	LYS
43	F8	68	ARG
44	G8	53	PRO

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%)	162 (79%)	43 (21%)	1	5
2	1E	205/220 (93%)	148 (72%)	57 (28%)	0	1
3	22	160/188 (85%)	121 (76%)	39 (24%)	1	3
3	2E	159/188 (85%)	128 (80%)	31 (20%)	1	6
4	32	180/181 (99%)	141 (78%)	39 (22%)	1	5

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	3E	180/181 (99%)	143 (79%)	37 (21%)	1	5
5	42	116/123 (94%)	86 (74%)	30 (26%)	0	2
5	4E	116/123 (94%)	85 (73%)	31 (27%)	0	2
6	52	90/90 (100%)	74 (82%)	16 (18%)	2	9
6	5E	90/90 (100%)	71 (79%)	19 (21%)	1	5
7	62	126/127 (99%)	97 (77%)	29 (23%)	1	4
7	6E	126/127 (99%)	96 (76%)	30 (24%)	1	3
8	72	119/119 (100%)	97 (82%)	22 (18%)	1	8
8	7E	119/119 (100%)	98 (82%)	21 (18%)	2	9
9	82	98/99 (99%)	77 (79%)	21 (21%)	1	5
9	8E	98/99 (99%)	80 (82%)	18 (18%)	1	8
10	1A	89/92 (97%)	64 (72%)	25 (28%)	0	1
10	1I	89/92 (97%)	73 (82%)	16 (18%)	2	8
11	2A	88/99 (89%)	70 (80%)	18 (20%)	1	5
11	2I	88/99 (89%)	73 (83%)	15 (17%)	2	10
12	3A	104/109 (95%)	89 (86%)	15 (14%)	3	14
12	3I	104/109 (95%)	87 (84%)	17 (16%)	2	11
13	4A	94/101 (93%)	73 (78%)	21 (22%)	1	4
13	4I	94/101 (93%)	74 (79%)	20 (21%)	1	5
14	5A	49/50 (98%)	44 (90%)	5 (10%)	7	28
14	5I	49/50 (98%)	37 (76%)	12 (24%)	1	3
15	6A	79/80 (99%)	66 (84%)	13 (16%)	2	11
15	6I	79/80 (99%)	64 (81%)	15 (19%)	1	7
16	7A	72/74 (97%)	56 (78%)	16 (22%)	1	4
16	7I	72/74 (97%)	55 (76%)	17 (24%)	1	3
17	8A	95/97 (98%)	75 (79%)	20 (21%)	1	5
17	8I	95/97 (98%)	77 (81%)	18 (19%)	1	7
18	9A	63/77 (82%)	53 (84%)	10 (16%)	2	12
18	9I	63/77 (82%)	54 (86%)	9 (14%)	3	14
19	AA	68/80 (85%)	50 (74%)	18 (26%)	0	2
19	AI	72/80 (90%)	54 (75%)	18 (25%)	0	2

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
20	BA	76/82 (93%)	62 (82%)	14 (18%)	1	8
20	BI	76/82 (93%)	60 (79%)	16 (21%)	1	5
21	1B	20/22 (91%)	18 (90%)	2 (10%)	7	29
21	1F	20/22 (91%)	19 (95%)	1 (5%)	22	53
26	71	111/181 (61%)	104 (94%)	7 (6%)	16	45
26	79	111/181 (61%)	97 (87%)	14 (13%)	4	19
27	11	214/218 (98%)	170 (79%)	44 (21%)	1	5
27	19	214/218 (98%)	172 (80%)	42 (20%)	1	6
28	21	165/166 (99%)	127 (77%)	38 (23%)	1	4
28	29	165/166 (99%)	122 (74%)	43 (26%)	0	2
29	31	161/166 (97%)	117 (73%)	44 (27%)	0	1
29	39	165/166 (99%)	121 (73%)	44 (27%)	0	2
30	41	155/156 (99%)	125 (81%)	30 (19%)	1	7
30	49	155/156 (99%)	115 (74%)	40 (26%)	0	2
31	51	145/148 (98%)	105 (72%)	40 (28%)	0	1
31	59	142/148 (96%)	106 (75%)	36 (25%)	0	2
32	61	122/124 (98%)	92 (75%)	30 (25%)	1	3
32	69	122/124 (98%)	86 (70%)	36 (30%)	0	1
33	15	117/119 (98%)	88 (75%)	29 (25%)	1	2
33	58	117/119 (98%)	81 (69%)	36 (31%)	0	0
34	25	100/100 (100%)	75 (75%)	25 (25%)	0	2
34	68	100/100 (100%)	78 (78%)	22 (22%)	1	4
35	35	116/116 (100%)	78 (67%)	38 (33%)	0	0
35	78	116/116 (100%)	70 (60%)	46 (40%)	0	0
36	45	111/111 (100%)	86 (78%)	25 (22%)	1	4
36	88	111/111 (100%)	86 (78%)	25 (22%)	1	4
37	55	100/101 (99%)	77 (77%)	23 (23%)	1	4
37	98	101/101 (100%)	79 (78%)	22 (22%)	1	5
38	65	87/88 (99%)	55 (63%)	32 (37%)	0	0
38	A8	87/88 (99%)	67 (77%)	20 (23%)	1	4
39	75	117/127 (92%)	91 (78%)	26 (22%)	1	4

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
39	B8	120/127 (94%)	83 (69%)	37 (31%)	0	0
40	85	93/94 (99%)	76 (82%)	17 (18%)	2	8
40	C8	93/94 (99%)	74 (80%)	19 (20%)	1	5
41	95	82/82 (100%)	62 (76%)	20 (24%)	1	3
41	D8	82/82 (100%)	53 (65%)	29 (35%)	0	0
42	A5	92/92 (100%)	70 (76%)	22 (24%)	1	3
42	E8	92/92 (100%)	64 (70%)	28 (30%)	0	0
43	B5	74/78 (95%)	57 (77%)	17 (23%)	1	4
43	F8	74/78 (95%)	53 (72%)	21 (28%)	0	1
44	C5	85/91 (93%)	62 (73%)	23 (27%)	0	2
44	G8	85/91 (93%)	58 (68%)	27 (32%)	0	0
45	D5	158/179 (88%)	120 (76%)	38 (24%)	1	3
45	H8	154/179 (86%)	116 (75%)	38 (25%)	1	2
46	E5	62/67 (92%)	49 (79%)	13 (21%)	1	5
46	I8	66/67 (98%)	48 (73%)	18 (27%)	0	1
47	F5	82/83 (99%)	56 (68%)	26 (32%)	0	0
47	J8	82/83 (99%)	54 (66%)	28 (34%)	0	0
48	G5	64/67 (96%)	47 (73%)	17 (27%)	0	2
48	K8	62/67 (92%)	45 (73%)	17 (27%)	0	1
49	H5	51/52 (98%)	43 (84%)	8 (16%)	2	12
49	L8	51/52 (98%)	37 (72%)	14 (28%)	0	1
50	I5	57/63 (90%)	43 (75%)	14 (25%)	1	3
50	M8	59/63 (94%)	50 (85%)	9 (15%)	3	12
51	J5	51/52 (98%)	36 (71%)	15 (29%)	0	1
51	N8	51/52 (98%)	37 (72%)	14 (28%)	0	1
52	K5	44/52 (85%)	27 (61%)	17 (39%)	0	0
52	O8	44/52 (85%)	33 (75%)	11 (25%)	0	2
53	L5	42/42 (100%)	32 (76%)	10 (24%)	1	3
53	P8	40/42 (95%)	32 (80%)	8 (20%)	1	6
54	M5	52/55 (94%)	36 (69%)	16 (31%)	0	0
54	Q8	50/55 (91%)	30 (60%)	20 (40%)	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	9806/10360 (95%)	7504 (76%)	2302 (24%)	1 3

5 of 2302 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
33	15	104	LYS
54	M5	36	LYS
35	35	91	PHE
33	15	98	VAL
42	A5	71	VAL

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

Mol	Chain	Res	Type
43	F8	55	ASN
45	D5	118	GLN
4	32	42	GLN
45	D5	32	HIS
30	49	58	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	13	1492/1522 (98%)	354 (23%)	26 (1%)
1	1G	1502/1522 (98%)	372 (24%)	39 (2%)
22	2K	79/85 (92%)	34 (43%)	5 (6%)
22	2L	76/85 (89%)	26 (34%)	8 (10%)
22	3K	83/85 (97%)	25 (30%)	3 (3%)
22	3L	84/85 (98%)	24 (28%)	3 (3%)
23	4K	16/30 (53%)	7 (43%)	3 (18%)
23	4L	7/30 (23%)	4 (57%)	1 (14%)
24	14	2908/2917 (99%)	688 (23%)	48 (1%)
24	1H	2911/2917 (99%)	704 (24%)	56 (1%)
25	16	121/122 (99%)	38 (31%)	0
25	1J	121/122 (99%)	34 (28%)	0
All	All	9400/9522 (98%)	2310 (24%)	192 (2%)

5 of 2310 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	13	5	U
1	13	6	G
1	13	7	G
1	13	9	G
1	13	32	A

5 of 192 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	1G	974	A
23	4L	12	A
1	1G	1094	G
1	1G	1453	G
24	14	310	A

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
22	PSU	3K	40	22	18,21,22	1.16	1 (5%)	21,30,33	1.66	2 (9%)
22	PSU	2K	40	22	18,21,22	1.05	1 (5%)	21,30,33	1.92	4 (19%)
22	MIA	3K	38	22	28,31,32	2.32	3 (10%)	38,44,47	2.94	14 (36%)
22	MIA	2K	38	22	28,31,32	2.29	3 (10%)	38,44,47	3.55	11 (28%)
22	4SU	3L	8	22,55	18,21,22	2.07	5 (27%)	25,30,33	2.04	4 (16%)
22	QUO	3K	35	22	32,35,36	4.91	13 (40%)	36,52,55	5.06	11 (30%)
22	MIA	2L	38	22	28,31,32	2.19	3 (10%)	38,44,47	2.74	12 (31%)
22	MIA	3L	38	22	28,31,32	2.36	4 (14%)	38,44,47	3.11	17 (44%)
22	4SU	2L	8	22	18,21,22	1.79	4 (22%)	25,30,33	2.16	7 (28%)
22	4SU	2K	8	22	18,21,22	2.13	3 (16%)	25,30,33	2.96	7 (28%)
22	PSU	2L	64	22	18,21,22	1.33	2 (11%)	21,30,33	1.68	4 (19%)
22	PSU	2L	40	22	18,21,22	1.37	1 (5%)	21,30,33	1.69	4 (19%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
22	QUO	3L	35	22	32,35,36	4.82	13 (40%)	36,52,55	4.75	13 (36%)
22	4SU	3K	8	22	18,21,22	1.85	3 (16%)	25,30,33	2.69	4 (16%)
22	PSU	3K	64	22	18,21,22	1.26	2 (11%)	21,30,33	1.90	3 (14%)
22	5MU	3L	63	22	19,22,23	3.95	5 (26%)	27,32,35	3.32	9 (33%)
22	PSU	2K	64	22,55	18,21,22	1.35	2 (11%)	21,30,33	2.16	6 (28%)
22	QUO	2L	35	22,23	32,35,36	4.80	12 (37%)	36,52,55	4.83	13 (36%)
22	QUO	2K	35	22,23	32,35,36	4.80	13 (40%)	36,52,55	4.61	11 (30%)
22	PSU	3L	64	22	18,21,22	1.35	1 (5%)	21,30,33	1.66	2 (9%)
22	PSU	3L	40	22	18,21,22	1.27	1 (5%)	21,30,33	1.79	3 (14%)
22	OMG	2L	17	22	23,26,27	4.92	10 (43%)	32,38,41	4.55	18 (56%)
22	OMG	2K	17	22	23,26,27	5.05	11 (47%)	32,38,41	4.59	18 (56%)
22	5MU	2L	63	22	19,22,23	3.90	5 (26%)	27,32,35	3.54	10 (37%)
22	OMG	3K	17	22	23,26,27	5.23	11 (47%)	32,38,41	4.83	16 (50%)
22	OMG	3L	17	22	23,26,27	5.20	11 (47%)	32,38,41	4.74	17 (53%)
22	5MU	3K	63	22	19,22,23	3.89	5 (26%)	27,32,35	3.09	10 (37%)
22	5MU	2K	63	22	19,22,23	4.14	5 (26%)	27,32,35	3.60	10 (37%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	PSU	3K	40	22	-	0/7/25/26	0/2/2/2
22	PSU	2K	40	22	-	0/7/25/26	0/2/2/2
22	MIA	3K	38	22	-	8/15/33/34	0/3/3/3
22	MIA	2K	38	22	-	5/15/33/34	0/3/3/3
22	4SU	3L	8	22,55	-	0/7/25/26	0/2/2/2
22	QUO	3K	35	22	-	3/12/43/44	0/4/4/4
22	MIA	2L	38	22	-	3/15/33/34	0/3/3/3
22	MIA	3L	38	22	-	8/15/33/34	0/3/3/3
22	4SU	2L	8	22	-	0/7/25/26	0/2/2/2
22	4SU	2K	8	22	-	0/7/25/26	0/2/2/2
22	PSU	2L	64	22	-	0/7/25/26	0/2/2/2
22	PSU	2L	40	22	-	0/7/25/26	0/2/2/2
22	QUO	3L	35	22	-	4/12/43/44	0/4/4/4
22	4SU	3K	8	22	-	0/7/25/26	0/2/2/2

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	PSU	3K	64	22	-	0/7/25/26	0/2/2/2
22	5MU	3L	63	22	-	0/7/25/26	0/2/2/2
22	PSU	2K	64	22,55	-	2/7/25/26	0/2/2/2
22	QUO	2L	35	22,23	-	1/12/43/44	0/4/4/4
22	QUO	2K	35	22,23	-	2/12/43/44	0/4/4/4
22	PSU	3L	64	22	-	4/7/25/26	0/2/2/2
22	PSU	3L	40	22	-	0/7/25/26	0/2/2/2
22	OMG	2L	17	22	-	1/9/27/28	0/3/3/3
22	OMG	2K	17	22	-	3/9/27/28	0/3/3/3
22	5MU	2L	63	22	-	3/7/25/26	0/2/2/2
22	OMG	3K	17	22	-	2/9/27/28	0/3/3/3
22	OMG	3L	17	22	-	3/9/27/28	0/3/3/3
22	5MU	3K	63	22	-	0/7/25/26	0/2/2/2
22	5MU	2K	63	22	-	5/7/25/26	0/2/2/2

The worst 5 of 153 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	2L	35	QUO	C4-N3	16.38	1.71	1.34
22	3L	35	QUO	C4-N3	16.33	1.71	1.34
22	3K	35	QUO	C4-N3	16.30	1.71	1.34
22	2K	35	QUO	C4-N3	15.16	1.68	1.34
22	2K	63	5MU	C2-N1	14.02	1.60	1.38

The worst 5 of 260 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	3L	35	QUO	C5-C4-N3	-19.71	104.90	127.53
22	3K	35	QUO	C5-C4-N3	-19.34	105.33	127.53
22	2K	35	QUO	C5-C4-N3	-18.53	106.26	127.53
22	2L	35	QUO	C5-C4-N3	-18.15	106.69	127.53
22	2K	38	MIA	C11-S10-C2	15.14	113.61	102.25

There are no chirality outliers.

5 of 57 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
22	2K	35	QUO	O4'-C4'-C5'-O5'
22	2K	35	QUO	C3'-C4'-C5'-O5'
22	2K	38	MIA	N1-C2-S10-C11

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
22	2K	38	MIA	N3-C2-S10-C11
22	2K	38	MIA	N6-C12-C13-C14

There are no ring outliers.

21 monomers are involved in 47 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
22	3K	38	MIA	5	0
22	2K	38	MIA	2	0
22	3L	8	4SU	1	0
22	3K	35	QUO	2	0
22	2L	38	MIA	2	0
22	3L	38	MIA	1	0
22	2L	8	4SU	3	0
22	2L	64	PSU	2	0
22	3L	35	QUO	3	0
22	3K	8	4SU	2	0
22	3K	64	PSU	1	0
22	2K	64	PSU	4	0
22	2L	35	QUO	5	0
22	2K	35	QUO	2	0
22	3L	64	PSU	1	0
22	2L	17	OMG	2	0
22	2K	17	OMG	6	0
22	2L	63	5MU	5	0
22	3K	17	OMG	1	0
22	3L	17	OMG	2	0
22	3K	63	5MU	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 1351 ligands modelled in this entry, 1351 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](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	13	1499/1522 (98%)	-0.16	10 (0%) 84 68	52, 116, 206, 445	5 (0%)
1	1G	1503/1522 (98%)	-0.23	13 (0%) 81 63	68, 115, 190, 453	0
2	12	237/256 (92%)	0.46	10 (4%) 40 22	127, 170, 220, 245	0
2	1E	237/256 (92%)	0.40	4 (1%) 69 48	120, 163, 212, 246	0
3	22	206/239 (86%)	0.29	5 (2%) 59 38	120, 147, 179, 189	0
3	2E	205/239 (85%)	0.23	3 (1%) 72 52	111, 138, 196, 212	0
4	32	208/209 (99%)	0.48	9 (4%) 40 22	94, 119, 152, 172	0
4	3E	208/209 (99%)	0.31	6 (2%) 53 32	87, 119, 147, 176	0
5	42	151/162 (93%)	0.08	2 (1%) 75 56	94, 113, 140, 210	0
5	4E	151/162 (93%)	0.18	1 (0%) 84 68	87, 114, 139, 206	0
6	52	101/101 (100%)	-0.35	0 100 100	85, 106, 127, 146	0
6	5E	101/101 (100%)	0.13	1 (0%) 79 61	95, 122, 138, 154	0
7	62	155/156 (99%)	0.10	3 (1%) 66 45	111, 129, 145, 152	0
7	6E	155/156 (99%)	0.29	5 (3%) 50 30	106, 137, 161, 172	0
8	72	138/138 (100%)	0.09	3 (2%) 62 41	98, 117, 133, 158	0
8	7E	138/138 (100%)	0.09	3 (2%) 62 41	101, 121, 136, 150	0
9	82	127/128 (99%)	1.00	15 (11%) 9 5	111, 160, 187, 206	0
9	8E	127/128 (99%)	0.65	9 (7%) 22 12	104, 155, 177, 184	0
10	1A	99/105 (94%)	0.96	16 (16%) 4 2	121, 161, 193, 210	0
10	1I	99/105 (94%)	0.65	4 (4%) 42 23	105, 164, 206, 215	0
11	2A	116/129 (89%)	0.00	3 (2%) 57 36	81, 110, 134, 164	0
11	2I	116/129 (89%)	0.18	6 (5%) 33 17	79, 114, 153, 224	0
12	3A	125/132 (94%)	0.27	5 (4%) 42 23	86, 102, 141, 189	0
12	3I	125/132 (94%)	-0.13	0 100 100	79, 92, 125, 247	0

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
13	4A	117/126 (92%)	0.54	13 (11%) 10 5	122, 164, 193, 228	0
13	4I	116/126 (92%)	0.71	8 (6%) 23 12	117, 165, 186, 205	0
14	5A	60/61 (98%)	1.30	11 (18%) 3 1	131, 150, 178, 185	0
14	5I	60/61 (98%)	0.73	3 (5%) 34 18	112, 128, 148, 170	0
15	6A	88/89 (98%)	-0.05	1 (1%) 78 59	84, 115, 134, 141	0
15	6I	88/89 (98%)	0.13	1 (1%) 78 59	92, 112, 133, 151	0
16	7A	84/88 (95%)	0.30	0 100 100	94, 108, 132, 195	0
16	7I	84/88 (95%)	0.79	9 (10%) 11 6	107, 127, 154, 194	0
17	8A	100/105 (95%)	0.03	2 (2%) 65 44	91, 108, 126, 176	0
17	8I	100/105 (95%)	0.26	2 (2%) 65 44	97, 119, 133, 142	0
18	9A	72/88 (81%)	-0.17	0 100 100	91, 112, 166, 208	0
18	9I	72/88 (81%)	-0.04	0 100 100	100, 121, 150, 227	0
19	AA	79/93 (84%)	0.66	7 (8%) 15 8	144, 187, 220, 228	0
19	AI	83/93 (89%)	0.56	7 (8%) 17 9	142, 168, 204, 221	0
20	BA	99/106 (93%)	0.30	7 (7%) 22 12	86, 114, 153, 193	0
20	BI	99/106 (93%)	0.63	7 (7%) 22 12	112, 138, 188, 193	0
21	1B	25/27 (92%)	1.85	11 (44%) 0 0	117, 140, 171, 190	0
21	1F	25/27 (92%)	1.12	5 (20%) 3 1	125, 139, 170, 187	0
22	2K	75/85 (88%)	-0.14	0 100 100	74, 113, 195, 247	0
22	2L	71/85 (83%)	-0.16	1 (1%) 73 53	73, 115, 176, 193	0
22	3K	78/85 (91%)	-0.18	2 (2%) 57 36	85, 189, 296, 344	0
22	3L	78/85 (91%)	-0.13	1 (1%) 75 56	79, 195, 286, 321	0
23	4K	16/30 (53%)	0.55	1 (6%) 26 14	82, 126, 168, 170	0
23	4L	8/30 (26%)	0.99	2 (25%) 2 1	93, 107, 190, 231	0
24	14	2909/2917 (99%)	-0.60	10 (0%) 90 80	53, 84, 260, 407	0
24	1H	2912/2917 (99%)	-0.60	10 (0%) 90 80	48, 80, 247, 440	0
25	16	122/122 (100%)	-0.19	0 100 100	85, 118, 144, 247	0
25	1J	122/122 (100%)	-0.17	2 (1%) 70 49	86, 123, 143, 217	0
26	71	135/229 (58%)	0.52	7 (5%) 33 17	156, 219, 251, 258	0
26	79	135/229 (58%)	0.48	7 (5%) 33 17	152, 228, 253, 265	0
27	11	272/276 (98%)	-0.33	2 (0%) 84 68	48, 69, 90, 122	0

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
27	19	273/276 (98%)	-0.26	3 (1%) 78 59	50, 73, 91, 122	0
28	21	205/206 (99%)	0.37	17 (8%) 17 9	54, 94, 152, 211	0
28	29	205/206 (99%)	0.16	8 (3%) 43 24	57, 88, 164, 238	0
29	31	202/210 (96%)	-0.30	1 (0%) 87 73	47, 81, 123, 148	0
29	39	208/210 (99%)	0.09	5 (2%) 59 38	60, 98, 174, 203	0
30	41	181/182 (99%)	0.45	6 (3%) 49 29	123, 154, 197, 210	0
30	49	181/182 (99%)	0.21	7 (3%) 43 24	120, 146, 190, 208	0
31	51	174/180 (96%)	0.17	5 (2%) 53 32	90, 117, 139, 161	0
31	59	171/180 (95%)	0.78	19 (11%) 10 5	141, 208, 248, 354	0
32	61	146/148 (98%)	0.04	2 (1%) 73 53	84, 128, 153, 169	0
32	69	146/148 (98%)	0.40	11 (7%) 20 11	81, 137, 164, 177	0
33	15	138/140 (98%)	0.03	3 (2%) 62 41	72, 101, 142, 174	0
33	58	138/140 (98%)	0.21	2 (1%) 73 53	73, 98, 154, 181	0
34	25	122/122 (100%)	-0.27	0 100 100	64, 82, 100, 110	0
34	68	122/122 (100%)	-0.37	0 100 100	58, 85, 103, 114	0
35	35	150/150 (100%)	0.14	5 (3%) 49 29	61, 105, 144, 203	0
35	78	150/150 (100%)	0.11	2 (1%) 75 56	55, 91, 117, 251	0
36	45	141/141 (100%)	0.18	4 (2%) 55 34	67, 104, 131, 154	0
36	88	141/141 (100%)	0.23	8 (5%) 29 16	64, 99, 134, 181	0
37	55	117/118 (99%)	-0.11	3 (2%) 57 36	62, 82, 99, 121	0
37	98	118/118 (100%)	-0.11	1 (0%) 82 65	68, 88, 107, 125	0
38	65	111/112 (99%)	0.31	3 (2%) 56 35	93, 118, 148, 171	0
38	A8	111/112 (99%)	0.74	6 (5%) 31 17	97, 119, 163, 218	0
39	75	137/146 (93%)	0.14	4 (2%) 53 32	75, 91, 161, 227	0
39	B8	137/146 (93%)	0.09	5 (3%) 46 26	84, 102, 165, 218	0
40	85	117/118 (99%)	-0.05	0 100 100	65, 95, 135, 167	0
40	C8	117/118 (99%)	0.13	3 (2%) 57 36	57, 83, 130, 183	0
41	95	101/101 (100%)	0.32	9 (8%) 15 8	67, 124, 148, 194	0
41	D8	101/101 (100%)	0.22	2 (1%) 65 44	58, 106, 160, 237	0
42	A5	113/113 (100%)	-0.36	0 100 100	63, 77, 110, 206	0
42	E8	113/113 (100%)	-0.25	0 100 100	61, 77, 109, 231	0

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
43	B5	93/96 (96%)	-0.07	2 (2%) 62 41	73, 86, 119, 127	0
43	F8	92/96 (95%)	-0.40	0 100 100	64, 74, 98, 112	0
44	C5	104/110 (94%)	0.72	6 (5%) 29 16	89, 130, 221, 252	0
44	G8	104/110 (94%)	0.44	15 (14%) 6 3	71, 96, 149, 186	0
45	D5	179/206 (86%)	0.45	10 (5%) 30 16	111, 160, 262, 335	0
45	H8	175/206 (84%)	0.39	5 (2%) 53 32	105, 160, 274, 301	0
46	E5	77/85 (90%)	0.16	3 (3%) 43 24	74, 89, 109, 178	0
46	I8	83/85 (97%)	0.42	5 (6%) 27 15	70, 90, 112, 158	0
47	F5	97/98 (98%)	0.27	7 (7%) 21 11	60, 83, 157, 204	0
47	J8	97/98 (98%)	0.24	8 (8%) 17 10	57, 82, 168, 218	0
48	G5	69/72 (95%)	0.18	2 (2%) 53 32	84, 109, 145, 187	0
48	K8	66/72 (91%)	-0.13	3 (4%) 38 20	63, 82, 115, 177	0
49	H5	59/60 (98%)	-0.05	0 100 100	79, 97, 156, 188	0
49	L8	59/60 (98%)	-0.30	0 100 100	73, 91, 138, 151	0
50	I5	63/71 (88%)	0.38	2 (3%) 50 30	161, 233, 263, 283	0
50	M8	66/71 (92%)	0.48	2 (3%) 52 31	152, 233, 267, 285	0
51	J5	59/60 (98%)	-0.07	2 (3%) 48 28	58, 87, 207, 244	0
51	N8	59/60 (98%)	0.23	1 (1%) 69 48	52, 92, 216, 240	0
52	K5	45/54 (83%)	2.69	24 (53%) 0 0	161, 210, 253, 272	0
52	O8	45/54 (83%)	1.06	7 (15%) 5 2	164, 213, 245, 256	0
53	L5	49/49 (100%)	-0.18	1 (2%) 65 44	56, 61, 106, 147	0
53	P8	47/49 (95%)	-0.40	1 (2%) 63 42	48, 54, 72, 121	0
54	M5	62/65 (95%)	0.32	6 (9%) 13 7	67, 77, 100, 127	0
54	Q8	62/65 (95%)	0.52	3 (4%) 35 19	62, 80, 108, 129	0
All	All	21209/22034 (96%)	-0.07	534 (2%) 58 37	47, 108, 216, 453	5 (0%)

The worst 5 of 534 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
52	K5	23	THR	9.5
9	82	115	GLY	8.9
52	K5	13	CYS	8.8
52	K5	22	ALA	8.6
7	62	81	GLY	7.2

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, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q<0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
22	PSU	2L	64	20/21	0.66	0.10	138,148,163,166	0
22	PSU	3K	64	20/21	0.68	0.12	182,190,202,202	0
22	PSU	3L	64	20/21	0.68	0.12	180,200,211,213	0
22	5MU	3K	63	21/22	0.72	0.09	176,183,187,190	0
22	5MU	3L	63	21/22	0.77	0.11	174,186,190,192	0
22	OMG	2K	17	24/25	0.79	0.10	142,148,151,151	0
22	OMG	2L	17	24/25	0.81	0.10	136,152,154,155	0
22	4SU	3L	8	20/21	0.82	0.11	184,194,207,207	0
22	PSU	2K	64	20/21	0.83	0.10	133,144,150,155	0
22	5MU	2K	63	21/22	0.83	0.10	135,139,149,156	0
22	OMG	3K	17	24/25	0.84	0.12	194,212,234,239	0
22	5MU	2L	63	21/22	0.84	0.10	141,149,156,167	0
22	4SU	3K	8	20/21	0.85	0.07	186,202,212,214	0
22	4SU	2K	8	20/21	0.87	0.09	106,112,119,121	0
22	OMG	3L	17	24/25	0.87	0.14	200,216,227,230	0
22	4SU	2L	8	20/21	0.88	0.10	112,122,128,139	0
22	PSU	3K	40	20/21	0.90	0.07	118,124,129,130	0
22	QUO	3L	35	32/33	0.91	0.12	105,114,128,132	0
22	PSU	3L	40	20/21	0.91	0.10	107,122,124,127	0
22	QUO	2K	35	32/33	0.92	0.15	84,96,115,117	6
22	QUO	3K	35	32/33	0.93	0.13	108,114,124,127	0
22	MIA	3K	38	29/30	0.94	0.10	114,122,132,135	0
22	MIA	3L	38	29/30	0.94	0.10	118,123,131,133	0
22	MIA	2K	38	29/30	0.94	0.10	82,94,106,112	0
22	QUO	2L	35	32/33	0.94	0.16	91,112,118,124	0
22	PSU	2L	40	20/21	0.94	0.13	89,100,105,105	0
22	MIA	2L	38	29/30	0.96	0.10	92,101,113,119	0
22	PSU	2K	40	20/21	0.97	0.07	83,91,99,105	0

6.3 Carbohydrates ⓘ

There are no oligosaccharides 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, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
55	MG	1H	3360	1/1	-0.08	0.43	167,167,167,167	0
55	MG	1G	1691	1/1	-0.03	0.40	132,132,132,132	0
55	MG	13	1703	1/1	0.10	0.39	147,147,147,147	0
55	MG	13	1712	1/1	0.30	0.28	123,123,123,123	0
55	MG	14	3356	1/1	0.31	0.20	195,195,195,195	0
55	MG	14	3331	1/1	0.32	0.25	138,138,138,138	0
55	MG	1G	1708	1/1	0.32	0.30	133,133,133,133	0
55	MG	1G	1704	1/1	0.35	0.29	117,117,117,117	0
55	MG	14	3354	1/1	0.36	0.28	134,134,134,134	0
55	MG	14	3113	1/1	0.39	0.36	97,97,97,97	0
55	MG	13	1656	1/1	0.39	0.34	120,120,120,120	0
55	MG	1G	1692	1/1	0.39	0.39	120,120,120,120	0
55	MG	1G	1721	1/1	0.39	0.44	129,129,129,129	0
55	MG	2K	101	1/1	0.41	0.27	118,118,118,118	0
55	MG	1G	1726	1/1	0.41	0.38	124,124,124,124	0
55	MG	1G	1719	1/1	0.41	0.33	104,104,104,104	0
55	MG	3E	301	1/1	0.43	0.14	156,156,156,156	0
55	MG	1H	3385	1/1	0.45	0.30	97,97,97,97	0
55	MG	13	1702	1/1	0.45	0.36	147,147,147,147	0
55	MG	13	1692	1/1	0.45	0.45	132,132,132,132	0
55	MG	13	1689	1/1	0.46	0.49	116,116,116,116	0
55	MG	14	3299	1/1	0.48	0.37	100,100,100,100	0
55	MG	16	208	1/1	0.48	0.25	113,113,113,113	0
55	MG	13	1617	1/1	0.51	0.33	122,122,122,122	0
55	MG	1H	3396	1/1	0.52	0.32	104,104,104,104	0
55	MG	13	1624	1/1	0.53	0.41	107,107,107,107	0
55	MG	1G	1718	1/1	0.54	0.35	118,118,118,118	0
55	MG	13	1695	1/1	0.54	0.28	90,90,90,90	0
55	MG	1H	3346	1/1	0.54	0.30	113,113,113,113	0
55	MG	1H	3301	1/1	0.55	0.36	79,79,79,79	0
55	MG	1H	3379	1/1	0.55	0.15	245,245,245,245	0
55	MG	13	1714	1/1	0.55	0.59	117,117,117,117	0
55	MG	1H	3221	1/1	0.56	0.32	108,108,108,108	0
55	MG	1G	1694	1/1	0.56	0.28	118,118,118,118	0
55	MG	1H	3384	1/1	0.56	0.35	108,108,108,108	0
55	MG	13	1708	1/1	0.56	0.45	127,127,127,127	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
55	MG	4A	201	1/1	0.56	0.46	115,115,115,115	0
55	MG	1H	3330	1/1	0.57	0.32	90,90,90,90	0
55	MG	14	3186	1/1	0.57	0.31	113,113,113,113	0
55	MG	13	1611	1/1	0.57	0.24	83,83,83,83	0
55	MG	13	1672	1/1	0.58	0.22	119,119,119,119	0
55	MG	13	1644	1/1	0.59	0.37	116,116,116,116	0
55	MG	1H	3343	1/1	0.59	0.19	90,90,90,90	0
55	MG	1H	3121	1/1	0.59	0.36	98,98,98,98	0
55	MG	1G	1685	1/1	0.59	0.36	116,116,116,116	0
55	MG	14	3329	1/1	0.60	0.24	101,101,101,101	0
55	MG	16	211	1/1	0.61	0.23	98,98,98,98	0
55	MG	16	213	1/1	0.61	0.26	113,113,113,113	0
55	MG	1H	3364	1/1	0.61	0.23	103,103,103,103	0
55	MG	1H	3361	1/1	0.61	0.20	155,155,155,155	0
55	MG	1H	3162	1/1	0.62	0.28	94,94,94,94	0
55	MG	1G	1667	1/1	0.62	0.27	103,103,103,103	0
55	MG	1H	3283	1/1	0.63	0.32	104,104,104,104	0
55	MG	13	1674	1/1	0.63	0.23	106,106,106,106	0
55	MG	13	1688	1/1	0.64	0.49	91,91,91,91	0
55	MG	1H	3226	1/1	0.64	0.20	114,114,114,114	0
55	MG	14	3287	1/1	0.65	0.45	98,98,98,98	0
55	MG	1G	1703	1/1	0.65	0.38	99,99,99,99	0
55	MG	1H	3186	1/1	0.65	0.23	70,70,70,70	0
55	MG	2L	102	1/1	0.65	0.38	102,102,102,102	0
55	MG	1H	3240	1/1	0.65	0.28	92,92,92,92	0
55	MG	1G	1724	1/1	0.65	0.23	99,99,99,99	0
55	MG	1H	3194	1/1	0.66	0.35	68,68,68,68	0
55	MG	14	3324	1/1	0.66	0.45	101,101,101,101	0
55	MG	1H	3220	1/1	0.66	0.32	92,92,92,92	0
55	MG	13	1658	1/1	0.66	0.27	108,108,108,108	0
55	MG	1H	3307	1/1	0.66	0.19	83,83,83,83	0
55	MG	13	1681	1/1	0.66	0.43	104,104,104,104	0
55	MG	14	3373	1/1	0.66	0.24	98,98,98,98	0
55	MG	14	3328	1/1	0.67	0.31	115,115,115,115	0
55	MG	13	1678	1/1	0.67	0.35	104,104,104,104	0
55	MG	1H	3203	1/1	0.67	0.44	99,99,99,99	0
55	MG	1H	3205	1/1	0.68	0.36	103,103,103,103	0
55	MG	14	3325	1/1	0.68	0.34	78,78,78,78	0
55	MG	13	1673	1/1	0.68	0.27	109,109,109,109	0
55	MG	32	301	1/1	0.68	0.39	113,113,113,113	0
55	MG	14	3300	1/1	0.69	0.20	83,83,83,83	0
55	MG	1H	3076	1/1	0.69	0.28	77,77,77,77	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
55	MG	1H	3282	1/1	0.69	0.35	90,90,90,90	0
55	MG	1H	3043	1/1	0.69	0.29	92,92,92,92	0
55	MG	1G	1664	1/1	0.69	0.33	104,104,104,104	0
55	MG	14	3132	1/1	0.69	0.29	120,120,120,120	0
55	MG	1H	3398	1/1	0.69	0.20	106,106,106,106	0
55	MG	1G	1674	1/1	0.69	0.41	111,111,111,111	0
55	MG	1G	1727	1/1	0.69	0.65	104,104,104,104	0
55	MG	1J	205	1/1	0.69	0.29	122,122,122,122	0
56	ZN	G8	202	1/1	0.69	0.22	203,203,203,203	0
55	MG	13	1700	1/1	0.70	0.47	97,97,97,97	0
55	MG	1H	3325	1/1	0.70	0.41	97,97,97,97	0
55	MG	14	3224	1/1	0.70	0.25	112,112,112,112	0
55	MG	14	3357	1/1	0.70	0.22	76,76,76,76	0
55	MG	14	3261	1/1	0.70	0.40	105,105,105,105	0
55	MG	1H	3131	1/1	0.70	0.28	75,75,75,75	0
55	MG	14	3296	1/1	0.70	0.27	97,97,97,97	0
55	MG	4K	101	1/1	0.71	0.21	111,111,111,111	0
55	MG	14	3119	1/1	0.71	0.46	70,70,70,70	0
55	MG	14	3302	1/1	0.71	0.23	91,91,91,91	0
55	MG	14	3267	1/1	0.71	0.20	90,90,90,90	0
55	MG	14	3286	1/1	0.71	0.32	100,100,100,100	0
55	MG	1G	1649	1/1	0.71	0.37	93,93,93,93	0
55	MG	13	1613	1/1	0.71	0.30	99,99,99,99	0
55	MG	14	3171	1/1	0.72	0.32	86,86,86,86	0
55	MG	1H	3363	1/1	0.72	0.26	104,104,104,104	0
55	MG	16	204	1/1	0.72	0.28	99,99,99,99	0
55	MG	14	3025	1/1	0.72	0.34	86,86,86,86	0
55	MG	14	3318	1/1	0.72	0.19	80,80,80,80	0
55	MG	1G	1653	1/1	0.72	0.39	103,103,103,103	0
55	MG	1H	3209	1/1	0.72	0.42	99,99,99,99	0
55	MG	1H	3312	1/1	0.72	0.23	81,81,81,81	0
55	MG	13	1659	1/1	0.73	0.29	102,102,102,102	0
55	MG	13	1616	1/1	0.73	0.24	141,141,141,141	0
55	MG	13	1701	1/1	0.73	0.22	100,100,100,100	0
55	MG	13	1621	1/1	0.73	0.30	87,87,87,87	0
55	MG	14	3353	1/1	0.73	0.21	84,84,84,84	0
55	MG	1G	1699	1/1	0.73	0.31	101,101,101,101	0
55	MG	14	3169	1/1	0.73	0.40	100,100,100,100	0
55	MG	1H	3164	1/1	0.73	0.36	90,90,90,90	0
55	MG	1H	3167	1/1	0.73	0.21	66,66,66,66	0
55	MG	14	3218	1/1	0.73	0.26	88,88,88,88	0
55	MG	1G	1678	1/1	0.73	0.36	102,102,102,102	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
55	MG	1H	3138	1/1	0.74	0.34	87,87,87,87	0
55	MG	14	3304	1/1	0.74	0.40	99,99,99,99	0
55	MG	14	3314	1/1	0.74	0.40	105,105,105,105	0
55	MG	1G	1643	1/1	0.74	0.28	106,106,106,106	0
55	MG	14	3323	1/1	0.74	0.20	87,87,87,87	0
55	MG	1G	1693	1/1	0.74	0.30	95,95,95,95	0
55	MG	2K	103	1/1	0.74	0.30	94,94,94,94	0
55	MG	1H	3252	1/1	0.74	0.25	98,98,98,98	0
55	MG	1H	3163	1/1	0.74	0.33	82,82,82,82	0
55	MG	13	1663	1/1	0.74	0.32	105,105,105,105	0
55	MG	14	3273	1/1	0.74	0.35	87,87,87,87	0
55	MG	13	1668	1/1	0.74	0.56	102,102,102,102	0
55	MG	1H	3168	1/1	0.74	0.41	85,85,85,85	0
55	MG	14	3292	1/1	0.74	0.33	90,90,90,90	0
55	MG	1H	3181	1/1	0.74	0.20	62,62,62,62	0
55	MG	1G	1720	1/1	0.74	0.34	95,95,95,95	0
55	MG	14	3161	1/1	0.74	0.32	89,89,89,89	0
55	MG	1G	1607	1/1	0.75	0.36	95,95,95,95	0
55	MG	1G	1609	1/1	0.75	0.34	99,99,99,99	0
55	MG	1G	1621	1/1	0.75	0.24	91,91,91,91	0
55	MG	14	3361	1/1	0.75	0.21	90,90,90,90	0
55	MG	1G	1632	1/1	0.75	0.34	79,79,79,79	0
55	MG	1H	3268	1/1	0.75	0.28	100,100,100,100	0
55	MG	1H	3309	1/1	0.75	0.31	85,85,85,85	0
55	MG	1G	1644	1/1	0.76	0.27	115,115,115,115	0
55	MG	13	1618	1/1	0.76	0.38	96,96,96,96	0
55	MG	1G	1723	1/1	0.76	0.25	98,98,98,98	0
55	MG	1G	1675	1/1	0.76	0.35	99,99,99,99	0
55	MG	14	3174	1/1	0.76	0.32	107,107,107,107	0
55	MG	14	3108	1/1	0.76	0.35	85,85,85,85	0
55	MG	1H	3362	1/1	0.76	0.30	103,103,103,103	0
55	MG	1H	3073	1/1	0.76	0.21	77,77,77,77	0
55	MG	14	3238	1/1	0.76	0.37	81,81,81,81	0
55	MG	1G	1654	1/1	0.77	0.35	91,91,91,91	0
55	MG	1G	1656	1/1	0.77	0.45	94,94,94,94	0
55	MG	1H	3134	1/1	0.77	0.24	65,65,65,65	0
55	MG	1G	1640	1/1	0.77	0.30	107,107,107,107	0
55	MG	1H	3405	1/1	0.77	0.21	74,74,74,74	0
55	MG	1G	1700	1/1	0.77	0.45	94,94,94,94	0
55	MG	16	203	1/1	0.77	0.17	92,92,92,92	0
55	MG	14	3158	1/1	0.77	0.29	97,97,97,97	0
55	MG	14	3372	1/1	0.77	0.31	96,96,96,96	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
55	MG	14	3159	1/1	0.77	0.40	85,85,85,85	0
55	MG	1H	3322	1/1	0.77	0.24	92,92,92,92	0
55	MG	13	1610	1/1	0.77	0.28	115,115,115,115	0
55	MG	1H	3293	1/1	0.78	0.23	95,95,95,95	0
55	MG	1G	1702	1/1	0.78	0.24	95,95,95,95	0
55	MG	1H	3296	1/1	0.78	0.30	84,84,84,84	0
55	MG	1H	3059	1/1	0.78	0.29	83,83,83,83	0
55	MG	14	3157	1/1	0.78	0.41	80,80,80,80	0
55	MG	16	210	1/1	0.78	0.22	96,96,96,96	0
55	MG	1H	3305	1/1	0.78	0.23	104,104,104,104	0
55	MG	1H	3151	1/1	0.78	0.31	76,76,76,76	0
55	MG	1H	3232	1/1	0.78	0.26	103,103,103,103	0
55	MG	13	1684	1/1	0.78	0.46	94,94,94,94	0
55	MG	1G	1682	1/1	0.78	0.24	87,87,87,87	0
55	MG	1G	1684	1/1	0.78	0.35	99,99,99,99	0
55	MG	14	3215	1/1	0.78	0.24	76,76,76,76	0
55	MG	1H	3320	1/1	0.78	0.35	109,109,109,109	0
55	MG	14	3337	1/1	0.78	0.19	105,105,105,105	0
55	MG	13	1698	1/1	0.78	0.32	78,78,78,78	0
55	MG	1H	3389	1/1	0.78	0.68	101,101,101,101	0
55	MG	14	3255	1/1	0.78	0.29	92,92,92,92	0
55	MG	13	1667	1/1	0.78	0.24	94,94,94,94	0
55	MG	13	1707	1/1	0.78	0.29	100,100,100,100	0
55	MG	14	3269	1/1	0.78	0.31	68,68,68,68	0
55	MG	1H	3044	1/1	0.78	0.44	98,98,98,98	0
55	MG	1J	201	1/1	0.78	0.25	100,100,100,100	0
55	MG	14	3070	1/1	0.78	0.29	66,66,66,66	0
55	MG	14	3082	1/1	0.78	0.20	64,64,64,64	0
55	MG	14	3301	1/1	0.79	0.34	82,82,82,82	0
55	MG	1G	1652	1/1	0.79	0.28	82,82,82,82	0
55	MG	13	1625	1/1	0.79	0.26	95,95,95,95	0
55	MG	1G	1725	1/1	0.79	0.22	93,93,93,93	0
55	MG	1H	3304	1/1	0.79	0.28	82,82,82,82	0
55	MG	14	3182	1/1	0.79	0.38	77,77,77,77	0
55	MG	1G	1610	1/1	0.79	0.43	99,99,99,99	0
55	MG	1G	1698	1/1	0.79	0.26	96,96,96,96	0
55	MG	1G	1659	1/1	0.79	0.29	107,107,107,107	0
55	MG	1H	3280	1/1	0.79	0.34	70,70,70,70	0
55	MG	1G	1629	1/1	0.79	0.29	86,86,86,86	0
55	MG	14	3335	1/1	0.79	0.30	90,90,90,90	0
55	MG	13	1694	1/1	0.79	0.20	92,92,92,92	0
55	MG	1G	1637	1/1	0.79	0.29	71,71,71,71	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
55	MG	14	3105	1/1	0.79	0.46	72,72,72,72	0
55	MG	1H	3047	1/1	0.79	0.36	76,76,76,76	0
55	MG	1G	1710	1/1	0.79	0.29	101,101,101,101	0
55	MG	14	3117	1/1	0.79	0.38	93,93,93,93	0
55	MG	1G	1713	1/1	0.79	0.21	107,107,107,107	0
55	MG	1H	3357	1/1	0.79	0.44	92,92,92,92	0
55	MG	1H	3031	1/1	0.79	0.36	82,82,82,82	0
55	MG	1H	3253	1/1	0.79	0.29	71,71,71,71	0
55	MG	1G	1686	1/1	0.79	0.32	95,95,95,95	0
55	MG	1H	3340	1/1	0.80	0.26	77,77,77,77	0
55	MG	1H	3342	1/1	0.80	0.29	89,89,89,89	0
55	MG	14	3143	1/1	0.80	0.35	87,87,87,87	0
55	MG	14	3297	1/1	0.80	0.23	78,78,78,78	0
55	MG	1H	3294	1/1	0.80	0.39	85,85,85,85	0
55	MG	1G	1611	1/1	0.80	0.25	132,132,132,132	0
55	MG	1H	3390	1/1	0.80	0.32	88,88,88,88	0
55	MG	1G	1722	1/1	0.80	0.14	91,91,91,91	0
55	MG	1G	1623	1/1	0.80	0.26	87,87,87,87	0
55	MG	13	1647	1/1	0.80	0.29	110,110,110,110	0
55	MG	14	3317	1/1	0.80	0.36	83,83,83,83	0
55	MG	14	3172	1/1	0.80	0.20	85,85,85,85	0
55	MG	1H	3349	1/1	0.80	0.21	77,77,77,77	0
55	MG	1H	3400	1/1	0.80	0.28	84,84,84,84	0
55	MG	1H	3314	1/1	0.80	0.33	97,97,97,97	0
55	MG	14	3206	1/1	0.80	0.34	76,76,76,76	0
55	MG	1H	3207	1/1	0.80	0.22	67,67,67,67	0
55	MG	1H	3119	1/1	0.80	0.31	77,77,77,77	0
55	MG	1H	3323	1/1	0.80	0.29	80,80,80,80	0
55	MG	1G	1650	1/1	0.80	0.26	90,90,90,90	0
55	MG	14	3349	1/1	0.80	0.20	100,100,100,100	0
55	MG	14	3252	1/1	0.80	0.23	81,81,81,81	0
55	MG	13	1653	1/1	0.80	0.33	104,104,104,104	0
55	MG	14	3260	1/1	0.80	0.29	99,99,99,99	0
55	MG	13	1655	1/1	0.80	0.30	92,92,92,92	0
55	MG	1H	3332	1/1	0.80	0.44	87,87,87,87	0
55	MG	14	3366	1/1	0.80	0.36	99,99,99,99	0
55	MG	I8	101	1/1	0.80	0.45	83,83,83,83	0
55	MG	14	3272	1/1	0.80	0.34	94,94,94,94	0
55	MG	I8	103	1/1	0.80	0.19	92,92,92,92	0
55	MG	1J	204	1/1	0.80	0.26	101,101,101,101	0
55	MG	14	3282	1/1	0.80	0.43	87,87,87,87	0
55	MG	1G	1602	1/1	0.80	0.37	75,75,75,75	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
55	MG	14	3069	1/1	0.81	0.35	96,96,96,96	0
55	MG	1H	3341	1/1	0.81	0.29	76,76,76,76	0
55	MG	1G	1701	1/1	0.81	0.18	93,93,93,93	0
55	MG	1H	3397	1/1	0.81	0.13	94,94,94,94	0
55	MG	1H	3012	1/1	0.81	0.29	57,57,57,57	0
55	MG	1H	3029	1/1	0.81	0.27	71,71,71,71	0
55	MG	Q8	102	1/1	0.81	0.49	81,81,81,81	0
55	MG	14	3276	1/1	0.81	0.22	73,73,73,73	0
55	MG	14	3200	1/1	0.81	0.35	100,100,100,100	0
55	MG	13	1693	1/1	0.81	0.33	100,100,100,100	0
55	MG	14	3211	1/1	0.81	0.30	77,77,77,77	0
55	MG	14	3214	1/1	0.81	0.24	66,66,66,66	0
55	MG	1H	3264	1/1	0.81	0.33	100,100,100,100	0
55	MG	1H	3159	1/1	0.81	0.27	66,66,66,66	0
55	MG	14	3222	1/1	0.81	0.25	79,79,79,79	0
55	MG	14	3362	1/1	0.81	0.24	111,111,111,111	0
55	MG	14	3364	1/1	0.81	0.14	68,68,68,68	0
55	MG	1H	3313	1/1	0.81	0.16	91,91,91,91	0
55	MG	14	3228	1/1	0.81	0.31	84,84,84,84	0
55	MG	14	3020	1/1	0.81	0.26	72,72,72,72	0
55	MG	14	3248	1/1	0.81	0.46	78,78,78,78	0
55	MG	14	3308	1/1	0.81	0.24	80,80,80,80	0
55	MG	14	3249	1/1	0.81	0.20	87,87,87,87	0
55	MG	29	304	1/1	0.81	0.54	89,89,89,89	0
55	MG	13	1648	1/1	0.81	0.28	105,105,105,105	0
55	MG	1H	3315	1/1	0.82	0.29	88,88,88,88	0
55	MG	1G	1745	1/1	0.82	0.19	93,93,93,93	0
55	MG	1G	1748	1/1	0.82	0.26	90,90,90,90	0
55	MG	1H	3350	1/1	0.82	0.37	89,89,89,89	0
55	MG	14	3185	1/1	0.82	0.29	90,90,90,90	0
55	MG	42	201	1/1	0.82	0.33	101,101,101,101	0
55	MG	1G	1608	1/1	0.82	0.20	85,85,85,85	0
55	MG	13	1645	1/1	0.82	0.33	98,98,98,98	0
55	MG	14	3312	1/1	0.82	0.32	81,81,81,81	0
55	MG	13	1711	1/1	0.82	0.40	90,90,90,90	0
55	MG	1G	1658	1/1	0.82	0.13	99,99,99,99	0
55	MG	14	3040	1/1	0.82	0.28	69,69,69,69	0
55	MG	1H	3057	1/1	0.82	0.27	84,84,84,84	0
55	MG	14	3220	1/1	0.82	0.25	89,89,89,89	0
55	MG	1G	1660	1/1	0.82	0.17	87,87,87,87	0
55	MG	1H	3150	1/1	0.82	0.31	78,78,78,78	0
55	MG	14	3093	1/1	0.82	0.27	84,84,84,84	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
55	MG	1H	3188	1/1	0.82	0.36	81,81,81,81	0
55	MG	14	3333	1/1	0.82	0.17	89,89,89,89	0
55	MG	1G	1669	1/1	0.82	0.33	86,86,86,86	0
55	MG	14	3336	1/1	0.82	0.15	73,73,73,73	0
55	MG	14	3111	1/1	0.82	0.16	54,54,54,54	0
55	MG	1G	1670	1/1	0.82	0.36	92,92,92,92	0
55	MG	14	3352	1/1	0.82	0.31	93,93,93,93	0
55	MG	1G	1627	1/1	0.82	0.35	93,93,93,93	0
55	MG	14	3258	1/1	0.82	0.29	70,70,70,70	0
55	MG	13	1636	1/1	0.82	0.28	88,88,88,88	0
55	MG	14	3123	1/1	0.82	0.21	50,50,50,50	0
55	MG	1H	3376	1/1	0.82	0.30	94,94,94,94	0
55	MG	13	1662	1/1	0.82	0.25	86,86,86,86	0
55	MG	14	3271	1/1	0.82	0.28	82,82,82,82	0
55	MG	14	3365	1/1	0.82	0.21	78,78,78,78	0
55	MG	14	3155	1/1	0.82	0.35	77,77,77,77	0
55	MG	14	3369	1/1	0.82	0.27	78,78,78,78	0
55	MG	14	3156	1/1	0.82	0.19	75,75,75,75	0
55	MG	1H	3160	1/1	0.82	0.34	68,68,68,68	0
55	MG	1G	1642	1/1	0.82	0.24	87,87,87,87	0
55	MG	14	3283	1/1	0.82	0.26	87,87,87,87	0
55	MG	13	1615	1/1	0.82	0.28	98,98,98,98	0
55	MG	1H	3032	1/1	0.82	0.23	95,95,95,95	0
55	MG	13	1664	1/1	0.82	0.47	93,93,93,93	0
55	MG	1G	1626	1/1	0.83	0.22	107,107,107,107	0
55	MG	13	1704	1/1	0.83	0.15	87,87,87,87	0
55	MG	13	1671	1/1	0.83	0.14	70,70,70,70	0
55	MG	1H	3178	1/1	0.83	0.19	77,77,77,77	0
55	MG	13	1699	1/1	0.83	0.30	109,109,109,109	0
55	MG	1G	1683	1/1	0.83	0.46	103,103,103,103	0
55	MG	14	3232	1/1	0.83	0.20	98,98,98,98	0
55	MG	13	1665	1/1	0.83	0.16	90,90,90,90	0
55	MG	14	3239	1/1	0.83	0.46	87,87,87,87	0
55	MG	14	3244	1/1	0.83	0.25	86,86,86,86	0
55	MG	14	3127	1/1	0.83	0.30	84,84,84,84	0
55	MG	1H	3027	1/1	0.83	0.26	86,86,86,86	0
55	MG	1H	3190	1/1	0.83	0.29	101,101,101,101	0
55	MG	14	3150	1/1	0.83	0.34	107,107,107,107	0
55	MG	13	1682	1/1	0.83	0.41	85,85,85,85	0
55	MG	1H	3366	1/1	0.83	0.24	84,84,84,84	0
55	MG	1H	3375	1/1	0.83	0.16	85,85,85,85	0
55	MG	14	3342	1/1	0.83	0.48	94,94,94,94	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
55	MG	14	3263	1/1	0.83	0.22	72,72,72,72	0
55	MG	1H	3153	1/1	0.83	0.25	86,86,86,86	0
55	MG	1H	3329	1/1	0.83	0.22	85,85,85,85	0
55	MG	52	201	1/1	0.83	0.13	84,84,84,84	0
55	MG	14	3165	1/1	0.83	0.20	74,74,74,74	0
55	MG	1H	3156	1/1	0.83	0.21	72,72,72,72	0
55	MG	14	3275	1/1	0.83	0.35	90,90,90,90	0
55	MG	13	1638	1/1	0.83	0.20	85,85,85,85	0
55	MG	14	3280	1/1	0.83	0.15	75,75,75,75	0
55	MG	1H	3093	1/1	0.83	0.36	82,82,82,82	0
55	MG	1H	3211	1/1	0.83	0.26	79,79,79,79	0
55	MG	14	3028	1/1	0.83	0.28	77,77,77,77	0
55	MG	14	3036	1/1	0.83	0.26	91,91,91,91	0
55	MG	1H	3104	1/1	0.83	0.20	85,85,85,85	0
55	MG	14	3193	1/1	0.83	0.31	56,56,56,56	0
55	MG	1H	3108	1/1	0.83	0.39	77,77,77,77	0
55	MG	1G	1665	1/1	0.83	0.20	69,69,69,69	0
55	MG	13	1639	1/1	0.83	0.19	66,66,66,66	0
55	MG	1G	1624	1/1	0.83	0.28	78,78,78,78	0
55	MG	21	301	1/1	0.84	0.29	58,58,58,58	0
55	MG	13	1686	1/1	0.84	0.40	85,85,85,85	0
55	MG	1G	1679	1/1	0.84	0.32	97,97,97,97	0
55	MG	1H	3380	1/1	0.84	0.37	88,88,88,88	0
55	MG	14	3087	1/1	0.84	0.27	65,65,65,65	0
55	MG	1H	3127	1/1	0.84	0.25	60,60,60,60	0
55	MG	14	3094	1/1	0.84	0.37	81,81,81,81	0
55	MG	1H	3284	1/1	0.84	0.30	73,73,73,73	0
55	MG	1G	1603	1/1	0.84	0.31	76,76,76,76	0
55	MG	1H	3130	1/1	0.84	0.26	69,69,69,69	0
55	MG	14	3208	1/1	0.84	0.20	88,88,88,88	0
55	MG	1G	1689	1/1	0.84	0.25	90,90,90,90	0
55	MG	1H	3356	1/1	0.84	0.47	91,91,91,91	0
55	MG	13	1660	1/1	0.84	0.25	80,80,80,80	0
55	MG	1H	3094	1/1	0.84	0.23	60,60,60,60	0
55	MG	14	3290	1/1	0.84	0.34	77,77,77,77	0
55	MG	1G	1657	1/1	0.84	0.29	87,87,87,87	0
55	MG	1H	3297	1/1	0.84	0.38	81,81,81,81	0
55	MG	2K	104	1/1	0.84	0.38	101,101,101,101	0
55	MG	14	3144	1/1	0.84	0.41	98,98,98,98	0
55	MG	14	3147	1/1	0.84	0.39	83,83,83,83	0
55	MG	1H	3106	1/1	0.84	0.33	85,85,85,85	0
55	MG	1H	3260	1/1	0.84	0.14	70,70,70,70	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
55	MG	13	1614	1/1	0.84	0.21	95,95,95,95	0
55	MG	3L	101	1/1	0.84	0.14	180,180,180,180	0
55	MG	14	3309	1/1	0.84	0.39	84,84,84,84	0
55	MG	1H	3369	1/1	0.84	0.20	94,94,94,94	0
55	MG	1H	3372	1/1	0.84	0.28	94,94,94,94	0
55	MG	1H	3173	1/1	0.84	0.23	90,90,90,90	0
55	MG	13	1604	1/1	0.84	0.14	86,86,86,86	0
56	ZN	C5	202	1/1	0.84	0.14	219,219,219,219	0
55	MG	1H	3124	1/1	0.85	0.24	59,59,59,59	0
55	MG	1H	3407	1/1	0.85	0.40	89,89,89,89	0
55	MG	1H	3180	1/1	0.85	0.21	86,86,86,86	0
55	MG	1H	3279	1/1	0.85	0.20	96,96,96,96	0
55	MG	16	206	1/1	0.85	0.10	101,101,101,101	0
55	MG	14	3163	1/1	0.85	0.31	80,80,80,80	0
55	MG	13	1685	1/1	0.85	0.12	89,89,89,89	0
55	MG	16	209	1/1	0.85	0.21	80,80,80,80	0
55	MG	13	1676	1/1	0.85	0.25	84,84,84,84	0
55	MG	1H	3006	1/1	0.85	0.29	67,67,67,67	0
55	MG	13	1650	1/1	0.85	0.22	88,88,88,88	0
55	MG	1H	3353	1/1	0.85	0.29	83,83,83,83	0
55	MG	14	3303	1/1	0.85	0.35	99,99,99,99	0
55	MG	1H	3286	1/1	0.85	0.34	82,82,82,82	0
55	MG	1H	3193	1/1	0.85	0.29	77,77,77,77	0
55	MG	14	3187	1/1	0.85	0.27	94,94,94,94	0
55	MG	1H	3358	1/1	0.85	0.46	98,98,98,98	0
55	MG	14	3195	1/1	0.85	0.24	65,65,65,65	0
55	MG	1H	3074	1/1	0.85	0.25	82,82,82,82	0
55	MG	1H	3200	1/1	0.85	0.35	99,99,99,99	0
55	MG	1G	1605	1/1	0.85	0.37	92,92,92,92	0
55	MG	1H	3143	1/1	0.85	0.30	73,73,73,73	0
55	MG	13	1661	1/1	0.85	0.25	95,95,95,95	0
55	MG	1H	3077	1/1	0.85	0.18	59,59,59,59	0
55	MG	14	3054	1/1	0.85	0.40	81,81,81,81	0
55	MG	14	3056	1/1	0.85	0.26	75,75,75,75	0
55	MG	14	3221	1/1	0.85	0.23	76,76,76,76	0
55	MG	1H	3088	1/1	0.85	0.12	52,52,52,52	0
55	MG	1H	3367	1/1	0.85	0.18	67,67,67,67	0
55	MG	1G	1619	1/1	0.85	0.39	73,73,73,73	0
55	MG	13	1691	1/1	0.85	0.41	83,83,83,83	0
55	MG	14	3091	1/1	0.85	0.29	81,81,81,81	0
55	MG	13	1607	1/1	0.85	0.31	86,86,86,86	0
55	MG	14	3241	1/1	0.85	0.29	89,89,89,89	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
55	MG	5E	201	1/1	0.85	0.20	106,106,106,106	0
55	MG	14	3096	1/1	0.85	0.24	94,94,94,94	0
55	MG	14	3100	1/1	0.85	0.21	79,79,79,79	0
55	MG	1H	3223	1/1	0.85	0.37	97,97,97,97	0
55	MG	1H	3035	1/1	0.85	0.22	75,75,75,75	0
55	MG	1H	3037	1/1	0.85	0.28	60,60,60,60	0
55	MG	1G	1631	1/1	0.85	0.22	90,90,90,90	0
55	MG	1H	3234	1/1	0.85	0.31	88,88,88,88	0
55	MG	1H	3238	1/1	0.85	0.34	82,82,82,82	0
55	MG	1H	3112	1/1	0.85	0.29	73,73,73,73	0
55	MG	1G	1705	1/1	0.85	0.30	96,96,96,96	0
55	MG	13	1683	1/1	0.85	0.18	122,122,122,122	0
55	MG	13	1608	1/1	0.85	0.31	101,101,101,101	0
55	MG	1H	3123	1/1	0.85	0.23	78,78,78,78	0
55	MG	1J	206	1/1	0.85	0.23	96,96,96,96	0
55	MG	1H	3263	1/1	0.85	0.40	84,84,84,84	0
55	MG	1H	3399	1/1	0.85	0.18	77,77,77,77	0
55	MG	1H	3334	1/1	0.85	0.24	108,108,108,108	0
55	MG	14	3038	1/1	0.86	0.23	86,86,86,86	0
55	MG	14	3180	1/1	0.86	0.31	82,82,82,82	0
55	MG	1H	3100	1/1	0.86	0.25	61,61,61,61	0
55	MG	14	3291	1/1	0.86	0.33	82,82,82,82	0
55	MG	1H	3377	1/1	0.86	0.33	81,81,81,81	0
55	MG	13	1705	1/1	0.86	0.20	76,76,76,76	0
55	MG	1H	3140	1/1	0.86	0.17	52,52,52,52	0
55	MG	1H	3061	1/1	0.86	0.24	71,71,71,71	0
55	MG	1H	3146	1/1	0.86	0.18	48,48,48,48	0
55	MG	14	3197	1/1	0.86	0.49	81,81,81,81	0
55	MG	1H	3387	1/1	0.86	0.23	75,75,75,75	0
55	MG	1G	1709	1/1	0.86	0.30	96,96,96,96	0
55	MG	1H	3107	1/1	0.86	0.35	81,81,81,81	0
55	MG	14	3209	1/1	0.86	0.20	88,88,88,88	0
55	MG	1H	3025	1/1	0.86	0.40	80,80,80,80	0
55	MG	1G	1717	1/1	0.86	0.20	107,107,107,107	0
55	MG	1H	3391	1/1	0.86	0.42	92,92,92,92	0
55	MG	14	3216	1/1	0.86	0.27	72,72,72,72	0
55	MG	1H	3040	1/1	0.86	0.40	71,71,71,71	0
55	MG	14	3319	1/1	0.86	0.18	89,89,89,89	0
55	MG	1G	1614	1/1	0.86	0.27	92,92,92,92	0
55	MG	1G	1618	1/1	0.86	0.28	79,79,79,79	0
55	MG	14	3112	1/1	0.86	0.31	68,68,68,68	0
55	MG	1H	3118	1/1	0.86	0.39	83,83,83,83	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
55	MG	13	1687	1/1	0.86	0.27	77,77,77,77	0
55	MG	1H	3266	1/1	0.86	0.25	101,101,101,101	0
55	MG	14	3236	1/1	0.86	0.51	94,94,94,94	0
55	MG	1H	3120	1/1	0.86	0.22	69,69,69,69	0
55	MG	14	3126	1/1	0.86	0.34	83,83,83,83	0
55	MG	1H	3271	1/1	0.86	0.18	90,90,90,90	0
55	MG	1H	3276	1/1	0.86	0.25	88,88,88,88	0
55	MG	14	3345	1/1	0.86	0.27	78,78,78,78	0
55	MG	14	3247	1/1	0.86	0.14	79,79,79,79	0
55	MG	13	1734	1/1	0.86	0.07	178,178,178,178	0
55	MG	1H	3084	1/1	0.86	0.35	62,62,62,62	0
55	MG	14	3251	1/1	0.86	0.20	67,67,67,67	0
55	MG	14	3145	1/1	0.86	0.23	78,78,78,78	0
55	MG	1H	3365	1/1	0.86	0.26	86,86,86,86	0
55	MG	13	1633	1/1	0.86	0.25	79,79,79,79	0
55	MG	1G	1688	1/1	0.86	0.30	102,102,102,102	0
55	MG	1G	1638	1/1	0.86	0.34	88,88,88,88	0
55	MG	1H	3049	1/1	0.86	0.26	71,71,71,71	0
55	MG	13	1623	1/1	0.86	0.14	107,107,107,107	0
55	MG	14	3368	1/1	0.86	0.18	76,76,76,76	0
55	MG	14	3014	1/1	0.86	0.26	84,84,84,84	0
55	MG	14	3018	1/1	0.86	0.09	64,64,64,64	0
55	MG	1H	3370	1/1	0.86	0.30	73,73,73,73	0
55	MG	1H	3096	1/1	0.86	0.35	71,71,71,71	0
55	MG	1J	203	1/1	0.86	0.14	92,92,92,92	0
55	MG	14	3166	1/1	0.86	0.14	71,71,71,71	0
55	MG	14	3167	1/1	0.86	0.33	83,83,83,83	0
55	MG	14	3278	1/1	0.86	0.30	84,84,84,84	0
55	MG	1J	210	1/1	0.86	0.09	144,144,144,144	0
55	MG	1G	1646	1/1	0.86	0.23	93,93,93,93	0
55	MG	14	3031	1/1	0.86	0.28	73,73,73,73	0
55	MG	1H	3290	1/1	0.86	0.31	80,80,80,80	0
55	MG	1G	1625	1/1	0.87	0.31	85,85,85,85	0
55	MG	1G	1747	1/1	0.87	0.20	86,86,86,86	0
55	MG	1H	3081	1/1	0.87	0.32	73,73,73,73	0
55	MG	14	3305	1/1	0.87	0.43	89,89,89,89	0
55	MG	1H	3239	1/1	0.87	0.31	74,74,74,74	0
55	MG	1H	3197	1/1	0.87	0.37	85,85,85,85	0
55	MG	1H	3243	1/1	0.87	0.36	52,52,52,52	0
55	MG	1H	3244	1/1	0.87	0.27	55,55,55,55	0
55	MG	1H	3303	1/1	0.87	0.26	63,63,63,63	0
55	MG	1H	3247	1/1	0.87	0.28	51,51,51,51	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
55	MG	16	207	1/1	0.87	0.28	85,85,85,85	0
55	MG	1H	3105	1/1	0.87	0.29	90,90,90,90	0
55	MG	1H	3060	1/1	0.87	0.23	80,80,80,80	0
55	MG	1G	1696	1/1	0.87	0.39	92,92,92,92	0
55	MG	14	3326	1/1	0.87	0.30	90,90,90,90	0
55	MG	14	3327	1/1	0.87	0.36	110,110,110,110	0
55	MG	1H	3256	1/1	0.87	0.24	78,78,78,78	0
55	MG	1H	3257	1/1	0.87	0.34	83,83,83,83	0
55	MG	1G	1648	1/1	0.87	0.29	89,89,89,89	0
55	MG	14	3254	1/1	0.87	0.39	85,85,85,85	0
55	MG	1H	3204	1/1	0.87	0.38	83,83,83,83	0
55	MG	1H	3171	1/1	0.87	0.33	82,82,82,82	0
55	MG	14	3051	1/1	0.87	0.30	62,62,62,62	0
55	MG	14	3338	1/1	0.87	0.19	78,78,78,78	0
55	MG	14	3340	1/1	0.87	0.17	79,79,79,79	0
55	MG	1G	1651	1/1	0.87	0.56	96,96,96,96	0
55	MG	14	3262	1/1	0.87	0.31	86,86,86,86	0
55	MG	13	1713	1/1	0.87	0.33	100,100,100,100	0
55	MG	14	3351	1/1	0.87	0.30	87,87,87,87	0
55	MG	14	3264	1/1	0.87	0.32	84,84,84,84	0
55	MG	14	3067	1/1	0.87	0.30	71,71,71,71	0
55	MG	1H	3125	1/1	0.87	0.29	73,73,73,73	0
55	MG	1H	3267	1/1	0.87	0.20	57,57,57,57	0
55	MG	1H	3126	1/1	0.87	0.34	61,61,61,61	0
55	MG	1H	3269	1/1	0.87	0.31	82,82,82,82	0
55	MG	1G	1711	1/1	0.87	0.26	73,73,73,73	0
55	MG	14	3191	1/1	0.87	0.34	92,92,92,92	0
55	MG	1H	3215	1/1	0.87	0.32	91,91,91,91	0
55	MG	1H	3218	1/1	0.87	0.33	82,82,82,82	0
55	MG	1H	3277	1/1	0.87	0.36	74,74,74,74	0
55	MG	1H	3219	1/1	0.87	0.39	72,72,72,72	0
55	MG	14	3202	1/1	0.87	0.32	74,74,74,74	0
55	MG	1H	3339	1/1	0.87	0.29	91,91,91,91	0
55	MG	13	1677	1/1	0.87	0.12	83,83,83,83	0
55	MG	1H	3038	1/1	0.87	0.26	59,59,59,59	0
55	MG	1H	3116	1/1	0.87	0.45	74,74,74,74	0
55	MG	14	3293	1/1	0.87	0.16	75,75,75,75	0
55	MG	1H	3023	1/1	0.87	0.25	55,55,55,55	0
55	MG	1H	3192	1/1	0.87	0.21	87,87,87,87	0
55	MG	29	303	1/1	0.87	0.14	74,74,74,74	0
55	MG	1H	3348	1/1	0.87	0.26	88,88,88,88	0
55	MG	E5	101	1/1	0.87	0.40	88,88,88,88	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
55	MG	13	1706	1/1	0.87	0.50	93,93,93,93	0
55	MG	14	3219	1/1	0.87	0.19	67,67,67,67	0
55	MG	1H	3317	1/1	0.88	0.32	63,63,63,63	0
55	MG	14	3129	1/1	0.88	0.34	70,70,70,70	0
55	MG	14	3130	1/1	0.88	0.12	72,72,72,72	0
55	MG	14	3223	1/1	0.88	0.14	64,64,64,64	0
55	MG	1H	3285	1/1	0.88	0.15	89,89,89,89	0
55	MG	14	3225	1/1	0.88	0.27	75,75,75,75	0
55	MG	14	3134	1/1	0.88	0.26	80,80,80,80	0
55	MG	14	3137	1/1	0.88	0.24	69,69,69,69	0
55	MG	14	3234	1/1	0.88	0.17	51,51,51,51	0
55	MG	1G	1695	1/1	0.88	0.15	86,86,86,86	0
55	MG	14	3321	1/1	0.88	0.34	89,89,89,89	0
55	MG	1H	3258	1/1	0.88	0.34	91,91,91,91	0
55	MG	1G	1697	1/1	0.88	0.36	85,85,85,85	0
55	MG	14	3017	1/1	0.88	0.25	83,83,83,83	0
55	MG	14	3242	1/1	0.88	0.45	86,86,86,86	0
55	MG	13	1666	1/1	0.88	0.47	104,104,104,104	0
55	MG	14	3154	1/1	0.88	0.32	87,87,87,87	0
55	MG	1H	3102	1/1	0.88	0.17	49,49,49,49	0
55	MG	13	1690	1/1	0.88	0.08	118,118,118,118	0
55	MG	1H	3295	1/1	0.88	0.39	87,87,87,87	0
55	MG	1H	3403	1/1	0.88	0.15	111,111,111,111	0
55	MG	1H	3404	1/1	0.88	0.19	80,80,80,80	0
55	MG	1H	3236	1/1	0.88	0.31	89,89,89,89	0
55	MG	1H	3333	1/1	0.88	0.25	81,81,81,81	0
55	MG	14	3046	1/1	0.88	0.28	75,75,75,75	0
55	MG	13	1637	1/1	0.88	0.49	90,90,90,90	0
55	MG	1H	3299	1/1	0.88	0.18	57,57,57,57	0
55	MG	14	3346	1/1	0.88	0.31	84,84,84,84	0
55	MG	14	3348	1/1	0.88	0.20	65,65,65,65	0
55	MG	1G	1668	1/1	0.88	0.22	82,82,82,82	0
55	MG	14	3060	1/1	0.88	0.22	64,64,64,64	0
55	MG	13	1697	1/1	0.88	0.45	84,84,84,84	0
55	MG	1H	3184	1/1	0.88	0.33	85,85,85,85	0
55	MG	1G	1714	1/1	0.88	0.31	98,98,98,98	0
55	MG	1G	1673	1/1	0.88	0.19	88,88,88,88	0
55	MG	1H	3374	1/1	0.88	0.16	67,67,67,67	0
55	MG	14	3090	1/1	0.88	0.28	70,70,70,70	0
55	MG	1H	3083	1/1	0.88	0.25	58,58,58,58	0
55	MG	13	1733	1/1	0.88	0.07	141,141,141,141	0
55	MG	13	1640	1/1	0.88	0.22	89,89,89,89	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
55	MG	1G	1681	1/1	0.88	0.47	88,88,88,88	0
55	MG	14	3367	1/1	0.88	0.13	72,72,72,72	0
55	MG	1H	3041	1/1	0.88	0.26	63,63,63,63	0
55	MG	14	3284	1/1	0.88	0.20	95,95,95,95	0
55	MG	14	3101	1/1	0.88	0.24	65,65,65,65	0
55	MG	1H	3064	1/1	0.88	0.31	70,70,70,70	0
55	MG	14	3465	1/1	0.88	0.30	64,64,64,64	0
55	MG	1H	3381	1/1	0.88	0.37	62,62,62,62	0
55	MG	1J	202	1/1	0.88	0.40	90,90,90,90	0
55	MG	14	3207	1/1	0.88	0.24	77,77,77,77	0
55	MG	1H	3254	1/1	0.88	0.22	69,69,69,69	0
55	MG	1H	3030	1/1	0.88	0.27	91,91,91,91	0
55	MG	14	3295	1/1	0.88	0.28	72,72,72,72	0
55	MG	1G	1601	1/1	0.88	0.21	76,76,76,76	0
55	MG	14	3115	1/1	0.88	0.14	58,58,58,58	0
55	MG	1G	1647	1/1	0.88	0.23	80,80,80,80	0
55	MG	55	201	1/1	0.88	0.27	68,68,68,68	0
55	MG	1G	1690	1/1	0.88	0.27	98,98,98,98	0
55	MG	1H	3355	1/1	0.88	0.51	107,107,107,107	0
55	MG	1H	3099	1/1	0.88	0.32	52,52,52,52	0
55	MG	14	3160	1/1	0.89	0.18	74,74,74,74	0
55	MG	1G	1630	1/1	0.89	0.33	81,81,81,81	0
55	MG	14	3061	1/1	0.89	0.25	70,70,70,70	0
55	MG	1H	3292	1/1	0.89	0.41	82,82,82,82	0
55	MG	1H	3373	1/1	0.89	0.32	79,79,79,79	0
55	MG	1G	1680	1/1	0.89	0.35	88,88,88,88	0
55	MG	1G	1633	1/1	0.89	0.36	80,80,80,80	0
55	MG	1H	3072	1/1	0.89	0.31	75,75,75,75	0
55	MG	13	1632	1/1	0.89	0.39	74,74,74,74	0
55	MG	16	212	1/1	0.89	0.15	85,85,85,85	0
55	MG	14	3259	1/1	0.89	0.22	82,82,82,82	0
55	MG	1H	3147	1/1	0.89	0.36	60,60,60,60	0
55	MG	1H	3033	1/1	0.89	0.18	83,83,83,83	0
55	MG	88	201	1/1	0.89	0.18	98,98,98,98	0
55	MG	14	3098	1/1	0.89	0.26	46,46,46,46	0
55	MG	13	1606	1/1	0.89	0.20	92,92,92,92	0
55	MG	14	3265	1/1	0.89	0.31	76,76,76,76	0
55	MG	14	3266	1/1	0.89	0.49	88,88,88,88	0
55	MG	14	3189	1/1	0.89	0.26	63,63,63,63	0
55	MG	1H	3298	1/1	0.89	0.43	87,87,87,87	0
55	MG	1H	3265	1/1	0.89	0.23	83,83,83,83	0
55	MG	1H	3187	1/1	0.89	0.17	83,83,83,83	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
55	MG	1H	3056	1/1	0.89	0.37	68,68,68,68	0
55	MG	1H	3154	1/1	0.89	0.28	79,79,79,79	0
55	MG	1H	3155	1/1	0.89	0.28	38,38,38,38	0
55	MG	13	1635	1/1	0.89	0.23	95,95,95,95	0
55	MG	1H	3273	1/1	0.89	0.26	103,103,103,103	0
55	MG	14	3281	1/1	0.89	0.39	82,82,82,82	0
55	MG	14	3358	1/1	0.89	0.12	85,85,85,85	0
55	MG	14	3001	1/1	0.89	0.24	70,70,70,70	0
55	MG	14	3002	1/1	0.89	0.16	67,67,67,67	0
55	MG	14	3007	1/1	0.89	0.24	58,58,58,58	0
55	MG	14	3213	1/1	0.89	0.26	68,68,68,68	0
55	MG	14	3009	1/1	0.89	0.22	58,58,58,58	0
55	MG	1G	1655	1/1	0.89	0.45	74,74,74,74	0
55	MG	1H	3275	1/1	0.89	0.18	69,69,69,69	0
55	MG	13	1675	1/1	0.89	0.27	85,85,85,85	0
55	MG	13	1710	1/1	0.89	0.20	103,103,103,103	0
55	MG	1H	3004	1/1	0.89	0.33	49,49,49,49	0
55	MG	14	3026	1/1	0.89	0.24	78,78,78,78	0
55	MG	1H	3109	1/1	0.89	0.23	76,76,76,76	0
55	MG	1H	3111	1/1	0.89	0.20	71,71,71,71	0
55	MG	14	3034	1/1	0.89	0.30	73,73,73,73	0
55	MG	13	1629	1/1	0.89	0.25	60,60,60,60	0
55	MG	14	3152	1/1	0.89	0.30	72,72,72,72	0
55	MG	14	3231	1/1	0.89	0.21	76,76,76,76	0
55	MG	1H	3065	1/1	0.89	0.24	64,64,64,64	0
55	MG	1H	3117	1/1	0.89	0.31	75,75,75,75	0
55	MG	14	3235	1/1	0.89	0.10	63,63,63,63	0
55	MG	1H	3326	1/1	0.89	0.10	78,78,78,78	0
55	MG	1H	3327	1/1	0.89	0.21	63,63,63,63	0
55	MG	1H	3142	1/1	0.89	0.20	74,74,74,74	0
55	MG	1H	3213	1/1	0.89	0.47	84,84,84,84	0
55	MG	1H	3354	1/1	0.90	0.32	88,88,88,88	0
55	MG	13	1622	1/1	0.90	0.35	74,74,74,74	0
55	MG	14	3212	1/1	0.90	0.21	66,66,66,66	0
55	MG	1G	1620	1/1	0.90	0.46	96,96,96,96	0
55	MG	1H	3007	1/1	0.90	0.28	62,62,62,62	0
55	MG	1H	3189	1/1	0.90	0.09	83,83,83,83	0
55	MG	13	1715	1/1	0.90	0.13	70,70,70,70	0
55	MG	1H	3316	1/1	0.90	0.10	61,61,61,61	0
55	MG	14	3118	1/1	0.90	0.16	84,84,84,84	0
55	MG	1H	3016	1/1	0.90	0.21	56,56,56,56	0
55	MG	1H	3087	1/1	0.90	0.22	49,49,49,49	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
55	MG	14	3124	1/1	0.90	0.16	56,56,56,56	0
55	MG	14	3313	1/1	0.90	0.16	86,86,86,86	0
55	MG	14	3125	1/1	0.90	0.30	88,88,88,88	0
55	MG	14	3316	1/1	0.90	0.22	70,70,70,70	0
55	MG	1G	1628	1/1	0.90	0.18	90,90,90,90	0
55	MG	1H	3514	1/1	0.90	0.20	109,109,109,109	0
55	MG	1H	3522	1/1	0.90	0.13	68,68,68,68	0
55	MG	14	3229	1/1	0.90	0.26	64,64,64,64	0
55	MG	14	3230	1/1	0.90	0.29	75,75,75,75	0
55	MG	16	201	1/1	0.90	0.10	110,110,110,110	0
55	MG	14	3131	1/1	0.90	0.14	66,66,66,66	0
55	MG	13	1669	1/1	0.90	0.28	77,77,77,77	0
55	MG	1H	3157	1/1	0.90	0.31	79,79,79,79	0
55	MG	14	3135	1/1	0.90	0.18	64,64,64,64	0
55	MG	16	205	1/1	0.90	0.10	109,109,109,109	0
55	MG	14	3330	1/1	0.90	0.24	81,81,81,81	0
55	MG	14	3140	1/1	0.90	0.41	77,77,77,77	0
55	MG	14	3332	1/1	0.90	0.21	83,83,83,83	0
55	MG	14	3240	1/1	0.90	0.20	95,95,95,95	0
55	MG	1H	3052	1/1	0.90	0.20	73,73,73,73	0
55	MG	13	1643	1/1	0.90	0.38	86,86,86,86	0
55	MG	13	1738	1/1	0.90	0.10	138,138,138,138	0
55	MG	14	3246	1/1	0.90	0.30	83,83,83,83	0
55	MG	14	3339	1/1	0.90	0.26	74,74,74,74	0
55	MG	13	1679	1/1	0.90	0.25	80,80,80,80	0
55	MG	13	1680	1/1	0.90	0.27	77,77,77,77	0
55	MG	3I	201	1/1	0.90	0.14	80,80,80,80	0
55	MG	14	3153	1/1	0.90	0.50	82,82,82,82	0
55	MG	1H	3063	1/1	0.90	0.20	63,63,63,63	0
55	MG	14	3029	1/1	0.90	0.32	51,51,51,51	0
55	MG	1H	3212	1/1	0.90	0.26	78,78,78,78	0
55	MG	11	301	1/1	0.90	0.19	54,54,54,54	0
55	MG	14	3035	1/1	0.90	0.25	57,57,57,57	0
55	MG	1H	3336	1/1	0.90	0.30	83,83,83,83	0
55	MG	14	3037	1/1	0.90	0.34	71,71,71,71	0
55	MG	13	1709	1/1	0.90	0.27	78,78,78,78	0
55	MG	13	1620	1/1	0.90	0.27	66,66,66,66	0
55	MG	14	3359	1/1	0.90	0.11	89,89,89,89	0
55	MG	14	3360	1/1	0.90	0.21	74,74,74,74	0
55	MG	1H	3217	1/1	0.90	0.32	92,92,92,92	0
55	MG	1H	3300	1/1	0.90	0.23	77,77,77,77	0
55	MG	14	3052	1/1	0.90	0.38	65,65,65,65	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
55	MG	1G	1707	1/1	0.90	0.33	90,90,90,90	0
55	MG	14	3170	1/1	0.90	0.20	79,79,79,79	0
55	MG	14	3055	1/1	0.90	0.25	61,61,61,61	0
55	MG	1H	3068	1/1	0.90	0.18	61,61,61,61	0
55	MG	1H	3344	1/1	0.90	0.43	84,84,84,84	0
55	MG	13	1651	1/1	0.90	0.28	73,73,73,73	0
55	MG	1H	3386	1/1	0.90	0.20	66,66,66,66	0
55	MG	1G	1712	1/1	0.90	0.14	109,109,109,109	0
55	MG	14	3279	1/1	0.90	0.41	84,84,84,84	0
55	MG	13	1603	1/1	0.90	0.17	96,96,96,96	0
55	MG	14	3078	1/1	0.90	0.28	60,60,60,60	0
55	MG	1H	3388	1/1	0.90	0.21	74,74,74,74	0
55	MG	1G	1715	1/1	0.90	0.15	106,106,106,106	0
55	MG	1G	1663	1/1	0.90	0.31	81,81,81,81	0
55	MG	1H	3002	1/1	0.90	0.20	53,53,53,53	0
55	MG	1H	3185	1/1	0.90	0.33	91,91,91,91	0
55	MG	1G	1666	1/1	0.90	0.31	72,72,72,72	0
55	MG	1H	3352	1/1	0.90	0.40	97,97,97,97	0
55	MG	13	1654	1/1	0.90	0.26	72,72,72,72	0
55	MG	1G	1615	1/1	0.90	0.19	78,78,78,78	0
55	MG	1G	1617	1/1	0.90	0.38	71,71,71,71	0
55	MG	14	3039	1/1	0.91	0.10	67,67,67,67	0
55	MG	13	1612	1/1	0.91	0.27	102,102,102,102	0
55	MG	14	3041	1/1	0.91	0.29	58,58,58,58	0
55	MG	14	3307	1/1	0.91	0.39	89,89,89,89	0
55	MG	1H	3225	1/1	0.91	0.33	77,77,77,77	0
55	MG	21	302	1/1	0.91	0.20	68,68,68,68	0
55	MG	1H	3289	1/1	0.91	0.25	78,78,78,78	0
55	MG	1H	3128	1/1	0.91	0.32	63,63,63,63	0
55	MG	1H	3291	1/1	0.91	0.20	68,68,68,68	0
55	MG	1H	3324	1/1	0.91	0.33	66,66,66,66	0
55	MG	14	3148	1/1	0.91	0.47	86,86,86,86	0
55	MG	14	3057	1/1	0.91	0.31	54,54,54,54	0
55	MG	14	3059	1/1	0.91	0.21	60,60,60,60	0
55	MG	1H	3259	1/1	0.91	0.25	93,93,93,93	0
55	MG	1G	1687	1/1	0.91	0.31	79,79,79,79	0
55	MG	14	3062	1/1	0.91	0.32	72,72,72,72	0
55	MG	14	3065	1/1	0.91	0.32	50,50,50,50	0
55	MG	14	3066	1/1	0.91	0.18	63,63,63,63	0
55	MG	1H	3228	1/1	0.91	0.27	63,63,63,63	0
55	MG	14	3243	1/1	0.91	0.18	78,78,78,78	0
55	MG	14	3068	1/1	0.91	0.29	66,66,66,66	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
55	MG	1G	1741	1/1	0.91	0.14	112,112,112,112	0
55	MG	1H	3229	1/1	0.91	0.13	54,54,54,54	0
55	MG	14	3076	1/1	0.91	0.40	47,47,47,47	0
55	MG	1G	1604	1/1	0.91	0.11	78,78,78,78	0
55	MG	1H	3208	1/1	0.91	0.41	69,69,69,69	0
55	MG	1H	3402	1/1	0.91	0.13	77,77,77,77	0
55	MG	14	3253	1/1	0.91	0.21	105,105,105,105	0
55	MG	1H	3233	1/1	0.91	0.24	72,72,72,72	0
55	MG	1H	3014	1/1	0.91	0.20	51,51,51,51	0
55	MG	14	3092	1/1	0.91	0.39	70,70,70,70	0
55	MG	13	1619	1/1	0.91	0.24	74,74,74,74	0
55	MG	14	3173	1/1	0.91	0.29	70,70,70,70	0
55	MG	1H	3003	1/1	0.91	0.22	54,54,54,54	0
55	MG	14	3175	1/1	0.91	0.34	85,85,85,85	0
55	MG	14	3178	1/1	0.91	0.37	81,81,81,81	0
55	MG	1G	1612	1/1	0.91	0.10	84,84,84,84	0
55	MG	1G	1613	1/1	0.91	0.06	92,92,92,92	0
55	MG	1H	3469	1/1	0.91	0.09	115,115,115,115	0
55	MG	1H	3502	1/1	0.91	0.09	148,148,148,148	0
55	MG	14	3104	1/1	0.91	0.29	59,59,59,59	0
55	MG	14	3270	1/1	0.91	0.39	76,76,76,76	0
55	MG	14	3188	1/1	0.91	0.31	76,76,76,76	0
55	MG	13	1646	1/1	0.91	0.38	90,90,90,90	0
55	MG	14	3190	1/1	0.91	0.36	95,95,95,95	0
55	MG	14	3107	1/1	0.91	0.34	80,80,80,80	0
55	MG	14	3192	1/1	0.91	0.14	56,56,56,56	0
55	MG	14	3363	1/1	0.91	0.11	61,61,61,61	0
55	MG	14	3277	1/1	0.91	0.31	78,78,78,78	0
55	MG	1H	3177	1/1	0.91	0.15	69,69,69,69	0
55	MG	14	3109	1/1	0.91	0.25	85,85,85,85	0
55	MG	1H	3241	1/1	0.91	0.18	69,69,69,69	0
55	MG	14	3198	1/1	0.91	0.28	70,70,70,70	0
55	MG	14	3199	1/1	0.91	0.12	60,60,60,60	0
55	MG	1H	3216	1/1	0.91	0.39	90,90,90,90	0
55	MG	13	1696	1/1	0.91	0.16	86,86,86,86	0
55	MG	14	3285	1/1	0.91	0.29	93,93,93,93	0
55	MG	1H	3306	1/1	0.91	0.15	83,83,83,83	0
55	MG	14	3116	1/1	0.91	0.23	49,49,49,49	0
55	MG	1H	3245	1/1	0.91	0.31	86,86,86,86	0
55	MG	2K	105	1/1	0.91	0.18	76,76,76,76	0
55	MG	1H	3347	1/1	0.91	0.27	72,72,72,72	0
55	MG	1H	3250	1/1	0.91	0.09	73,73,73,73	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
55	MG	14	3032	1/1	0.91	0.29	64,64,64,64	0
55	MG	14	3033	1/1	0.91	0.35	71,71,71,71	0
55	MG	1G	1671	1/1	0.91	0.20	92,92,92,92	0
55	MG	15	201	1/1	0.91	0.35	99,99,99,99	0
55	MG	1H	3039	1/1	0.91	0.27	68,68,68,68	0
55	MG	1H	3145	1/1	0.91	0.20	46,46,46,46	0
55	MG	F5	101	1/1	0.91	0.29	77,77,77,77	0
55	MG	1H	3351	1/1	0.91	0.15	90,90,90,90	0
55	MG	1H	3103	1/1	0.91	0.36	71,71,71,71	0
55	MG	14	3294	1/1	0.92	0.17	81,81,81,81	0
55	MG	14	3201	1/1	0.92	0.27	61,61,61,61	0
55	MG	1H	3132	1/1	0.92	0.32	76,76,76,76	0
55	MG	14	3204	1/1	0.92	0.35	70,70,70,70	0
55	MG	14	3010	1/1	0.92	0.19	47,47,47,47	0
55	MG	1H	3278	1/1	0.92	0.36	76,76,76,76	0
55	MG	1H	3010	1/1	0.92	0.29	66,66,66,66	0
55	MG	1H	3136	1/1	0.92	0.35	85,85,85,85	0
55	MG	14	3019	1/1	0.92	0.33	68,68,68,68	0
55	MG	1H	3196	1/1	0.92	0.35	80,80,80,80	0
55	MG	14	3022	1/1	0.92	0.24	60,60,60,60	0
55	MG	14	3306	1/1	0.92	0.16	74,74,74,74	0
55	MG	14	3023	1/1	0.92	0.20	72,72,72,72	0
55	MG	1H	3137	1/1	0.92	0.20	60,60,60,60	0
55	MG	1H	3199	1/1	0.92	0.10	72,72,72,72	0
55	MG	14	3122	1/1	0.92	0.18	61,61,61,61	0
55	MG	1H	3328	1/1	0.92	0.33	85,85,85,85	0
55	MG	1H	3042	1/1	0.92	0.15	95,95,95,95	0
55	MG	14	3030	1/1	0.92	0.24	60,60,60,60	0
55	MG	1G	1645	1/1	0.92	0.15	79,79,79,79	0
55	MG	1H	3202	1/1	0.92	0.14	94,94,94,94	0
55	MG	14	3128	1/1	0.92	0.32	76,76,76,76	0
55	MG	1H	3331	1/1	0.92	0.15	84,84,84,84	0
55	MG	1H	3165	1/1	0.92	0.34	74,74,74,74	0
55	MG	1H	3166	1/1	0.92	0.18	67,67,67,67	0
55	MG	1H	3139	1/1	0.92	0.47	69,69,69,69	0
55	MG	98	201	1/1	0.92	0.54	89,89,89,89	0
55	MG	1H	3248	1/1	0.92	0.16	61,61,61,61	0
55	MG	1G	1706	1/1	0.92	0.32	86,86,86,86	0
55	MG	1H	3382	1/1	0.92	0.12	79,79,79,79	0
55	MG	14	3141	1/1	0.92	0.41	85,85,85,85	0
55	MG	Q8	101	1/1	0.92	0.16	99,99,99,99	0
55	MG	14	3042	1/1	0.92	0.35	67,67,67,67	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
55	MG	14	3043	1/1	0.92	0.28	62,62,62,62	0
55	MG	1H	3337	1/1	0.92	0.19	94,94,94,94	0
55	MG	14	3048	1/1	0.92	0.29	55,55,55,55	0
55	MG	14	3149	1/1	0.92	0.09	66,66,66,66	0
55	MG	1H	3079	1/1	0.92	0.28	66,66,66,66	0
55	MG	14	3245	1/1	0.92	0.32	64,64,64,64	0
55	MG	1H	3169	1/1	0.92	0.35	83,83,83,83	0
55	MG	14	3341	1/1	0.92	0.09	95,95,95,95	0
55	MG	14	3053	1/1	0.92	0.19	59,59,59,59	0
55	MG	13	1652	1/1	0.92	0.17	88,88,88,88	0
55	MG	1H	3172	1/1	0.92	0.19	69,69,69,69	0
55	MG	1H	3255	1/1	0.92	0.10	92,92,92,92	0
55	MG	1G	1662	1/1	0.92	0.33	84,84,84,84	0
55	MG	1G	1606	1/1	0.92	0.17	80,80,80,80	0
55	MG	1H	3026	1/1	0.92	0.16	66,66,66,66	0
55	MG	1H	3174	1/1	0.92	0.23	89,89,89,89	0
55	MG	14	3257	1/1	0.92	0.21	75,75,75,75	0
55	MG	1H	3392	1/1	0.92	0.27	73,73,73,73	0
55	MG	1H	3395	1/1	0.92	0.43	76,76,76,76	0
55	MG	1H	3176	1/1	0.92	0.27	73,73,73,73	0
55	MG	1H	3144	1/1	0.92	0.34	69,69,69,69	0
55	MG	1H	3122	1/1	0.92	0.19	82,82,82,82	0
55	MG	1H	3179	1/1	0.92	0.07	60,60,60,60	0
55	MG	1H	3045	1/1	0.92	0.20	88,88,88,88	0
55	MG	14	3075	1/1	0.92	0.21	52,52,52,52	0
55	MG	1H	3036	1/1	0.92	0.14	70,70,70,70	0
55	MG	1G	1739	1/1	0.92	0.12	154,154,154,154	0
55	MG	14	3079	1/1	0.92	0.26	82,82,82,82	0
55	MG	14	3081	1/1	0.92	0.29	70,70,70,70	0
55	MG	13	1627	1/1	0.92	0.44	65,65,65,65	0
55	MG	14	3179	1/1	0.92	0.60	88,88,88,88	0
55	MG	14	3083	1/1	0.92	0.27	68,68,68,68	0
55	MG	14	3181	1/1	0.92	0.32	70,70,70,70	0
55	MG	14	3380	1/1	0.92	0.11	79,79,79,79	0
55	MG	14	3436	1/1	0.92	0.09	107,107,107,107	0
55	MG	14	3450	1/1	0.92	0.15	105,105,105,105	0
55	MG	14	3085	1/1	0.92	0.33	72,72,72,72	0
55	MG	14	3086	1/1	0.92	0.22	51,51,51,51	0
55	MG	1G	1676	1/1	0.92	0.34	98,98,98,98	0
55	MG	1H	3090	1/1	0.92	0.16	47,47,47,47	0
55	MG	1H	3311	1/1	0.92	0.41	83,83,83,83	0
55	MG	1H	3092	1/1	0.92	0.30	62,62,62,62	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
55	MG	1H	3465	1/1	0.92	0.15	87,87,87,87	0
55	MG	1H	3015	1/1	0.92	0.29	46,46,46,46	0
55	MG	1H	3227	1/1	0.92	0.35	76,76,76,76	0
55	MG	1H	3129	1/1	0.92	0.20	63,63,63,63	0
55	MG	14	3194	1/1	0.92	0.17	46,46,46,46	0
55	MG	1H	3518	1/1	0.92	0.07	135,135,135,135	0
55	MG	13	1642	1/1	0.92	0.41	66,66,66,66	0
55	MG	14	3103	1/1	0.92	0.28	58,58,58,58	0
55	MG	1H	3021	1/1	0.92	0.17	51,51,51,51	0
55	MG	1H	3318	1/1	0.92	0.22	75,75,75,75	0
55	MG	1H	3095	1/1	0.93	0.28	46,46,46,46	0
55	MG	14	3050	1/1	0.93	0.10	65,65,65,65	0
55	MG	14	3274	1/1	0.93	0.14	69,69,69,69	0
55	MG	14	3334	1/1	0.93	0.35	84,84,84,84	0
55	MG	2L	101	1/1	0.93	0.12	77,77,77,77	0
55	MG	1H	3335	1/1	0.93	0.29	70,70,70,70	0
55	MG	14	3168	1/1	0.93	0.34	76,76,76,76	0
55	MG	13	1605	1/1	0.93	0.12	84,84,84,84	0
55	MG	1H	3075	1/1	0.93	0.35	87,87,87,87	0
55	MG	13	1634	1/1	0.93	0.27	73,73,73,73	0
55	MG	14	3004	1/1	0.93	0.25	57,57,57,57	0
55	MG	14	3005	1/1	0.93	0.22	52,52,52,52	0
55	MG	14	3058	1/1	0.93	0.13	63,63,63,63	0
55	MG	13	1736	1/1	0.93	0.06	132,132,132,132	0
55	MG	13	1657	1/1	0.93	0.38	74,74,74,74	0
55	MG	1H	3191	1/1	0.93	0.40	64,64,64,64	0
55	MG	14	3350	1/1	0.93	0.23	77,77,77,77	0
55	MG	14	3011	1/1	0.93	0.25	47,47,47,47	0
55	MG	14	3289	1/1	0.93	0.15	175,175,175,175	0
55	MG	14	3064	1/1	0.93	0.23	52,52,52,52	0
55	MG	14	3237	1/1	0.93	0.28	74,74,74,74	0
55	MG	14	3355	1/1	0.93	0.25	73,73,73,73	0
55	MG	14	3012	1/1	0.93	0.26	53,53,53,53	0
55	MG	1G	1639	1/1	0.93	0.48	97,97,97,97	0
55	MG	14	3015	1/1	0.93	0.10	64,64,64,64	0
55	MG	1H	3467	1/1	0.93	0.13	72,72,72,72	0
55	MG	1G	1677	1/1	0.93	0.48	89,89,89,89	0
55	MG	1H	3281	1/1	0.93	0.30	80,80,80,80	0
55	MG	14	3298	1/1	0.93	0.27	69,69,69,69	0
55	MG	1H	3497	1/1	0.93	0.09	105,105,105,105	0
55	MG	1H	3501	1/1	0.93	0.10	99,99,99,99	0
55	MG	1H	3080	1/1	0.93	0.18	62,62,62,62	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
55	MG	13	1601	1/1	0.93	0.17	103,103,103,103	0
55	MG	1H	3170	1/1	0.93	0.25	89,89,89,89	0
55	MG	1H	3082	1/1	0.93	0.36	72,72,72,72	0
55	MG	1H	3224	1/1	0.93	0.26	83,83,83,83	0
55	MG	1H	3287	1/1	0.93	0.36	78,78,78,78	0
55	MG	1H	3034	1/1	0.93	0.11	54,54,54,54	0
55	MG	1H	3009	1/1	0.93	0.20	44,44,44,44	0
55	MG	14	3413	1/1	0.93	0.09	70,70,70,70	0
55	MG	14	3088	1/1	0.93	0.29	70,70,70,70	0
55	MG	14	3449	1/1	0.93	0.08	108,108,108,108	0
55	MG	14	3311	1/1	0.93	0.32	87,87,87,87	0
55	MG	14	3455	1/1	0.93	0.10	108,108,108,108	0
55	MG	14	3256	1/1	0.93	0.36	67,67,67,67	0
55	MG	1H	3152	1/1	0.93	0.30	80,80,80,80	0
55	MG	13	1626	1/1	0.93	0.32	65,65,65,65	0
55	MG	14	3205	1/1	0.93	0.30	70,70,70,70	0
55	MG	1H	3067	1/1	0.93	0.16	47,47,47,47	0
55	MG	1H	3231	1/1	0.93	0.52	88,88,88,88	0
55	MG	1H	3001	1/1	0.93	0.27	50,50,50,50	0
55	MG	1J	209	1/1	0.93	0.07	128,128,128,128	0
55	MG	1H	3071	1/1	0.93	0.26	51,51,51,51	0
55	MG	1G	1622	1/1	0.93	0.39	86,86,86,86	0
55	MG	1H	3206	1/1	0.93	0.35	72,72,72,72	0
55	MG	1H	3235	1/1	0.93	0.39	88,88,88,88	0
55	MG	1H	3135	1/1	0.93	0.19	72,72,72,72	0
55	MG	C5	201	1/1	0.93	0.24	86,86,86,86	0
55	MG	14	3268	1/1	0.93	0.40	85,85,85,85	0
55	MG	1H	3028	1/1	0.93	0.20	53,53,53,53	0
55	MG	1H	3055	1/1	0.93	0.47	77,77,77,77	0
55	MG	14	3217	1/1	0.93	0.24	55,55,55,55	0
55	MG	1H	3022	1/1	0.94	0.09	60,60,60,60	0
55	MG	13	1609	1/1	0.94	0.16	83,83,83,83	0
55	MG	14	3347	1/1	0.94	0.17	83,83,83,83	0
55	MG	13	1641	1/1	0.94	0.20	67,67,67,67	0
55	MG	1H	3013	1/1	0.94	0.26	47,47,47,47	0
55	MG	13	1670	1/1	0.94	0.09	106,106,106,106	0
55	MG	1G	1738	1/1	0.94	0.12	140,140,140,140	0
55	MG	1H	3148	1/1	0.94	0.14	86,86,86,86	0
55	MG	1H	3242	1/1	0.94	0.17	45,45,45,45	0
55	MG	1G	1743	1/1	0.94	0.16	105,105,105,105	0
55	MG	14	3196	1/1	0.94	0.08	60,60,60,60	0
55	MG	1H	3274	1/1	0.94	0.40	71,71,71,71	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
55	MG	1H	3393	1/1	0.94	0.10	62,62,62,62	0
55	MG	14	3089	1/1	0.94	0.30	71,71,71,71	0
55	MG	1H	3113	1/1	0.94	0.16	40,40,40,40	0
55	MG	1H	3115	1/1	0.94	0.17	51,51,51,51	0
55	MG	13	1602	1/1	0.94	0.13	78,78,78,78	0
55	MG	14	3203	1/1	0.94	0.20	55,55,55,55	0
55	MG	1H	3195	1/1	0.94	0.14	79,79,79,79	0
55	MG	11	302	1/1	0.94	0.18	85,85,85,85	0
55	MG	14	3095	1/1	0.94	0.15	65,65,65,65	0
55	MG	1H	3078	1/1	0.94	0.24	71,71,71,71	0
55	MG	1H	3222	1/1	0.94	0.30	65,65,65,65	0
55	MG	14	3047	1/1	0.94	0.23	57,57,57,57	0
55	MG	14	3210	1/1	0.94	0.21	68,68,68,68	0
55	MG	14	3371	1/1	0.94	0.22	84,84,84,84	0
55	MG	1H	3368	1/1	0.94	0.27	72,72,72,72	0
55	MG	14	3102	1/1	0.94	0.18	61,61,61,61	0
55	MG	14	3376	1/1	0.94	0.09	66,66,66,66	0
55	MG	1H	3048	1/1	0.94	0.18	58,58,58,58	0
55	MG	14	3385	1/1	0.94	0.08	73,73,73,73	0
55	MG	1H	3198	1/1	0.94	0.25	77,77,77,77	0
55	MG	1H	3008	1/1	0.94	0.19	44,44,44,44	0
55	MG	14	3438	1/1	0.94	0.09	83,83,83,83	0
55	MG	14	3322	1/1	0.94	0.13	70,70,70,70	0
55	MG	1H	3066	1/1	0.94	0.30	70,70,70,70	0
55	MG	14	3006	1/1	0.94	0.20	56,56,56,56	0
55	MG	1G	1635	1/1	0.94	0.44	70,70,70,70	0
55	MG	14	3110	1/1	0.94	0.37	63,63,63,63	0
55	MG	1G	1636	1/1	0.94	0.35	80,80,80,80	0
55	MG	1H	3425	1/1	0.94	0.12	61,61,61,61	0
55	MG	1H	3017	1/1	0.94	0.24	47,47,47,47	0
55	MG	1H	3345	1/1	0.94	0.24	67,67,67,67	0
55	MG	1H	3054	1/1	0.94	0.19	51,51,51,51	0
55	MG	1H	3070	1/1	0.94	0.15	60,60,60,60	0
55	MG	1H	3161	1/1	0.94	0.21	69,69,69,69	0
55	MG	19	301	1/1	0.94	0.28	67,67,67,67	0
55	MG	1H	3182	1/1	0.94	0.08	70,70,70,70	0
55	MG	14	3177	1/1	0.94	0.35	76,76,76,76	0
55	MG	39	301	1/1	0.94	0.13	83,83,83,83	0
55	MG	1H	3508	1/1	0.94	0.06	119,119,119,119	0
55	MG	1H	3262	1/1	0.94	0.10	71,71,71,71	0
55	MG	14	3021	1/1	0.94	0.06	63,63,63,63	0
55	MG	1H	3141	1/1	0.94	0.29	65,65,65,65	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
55	MG	1H	3520	1/1	0.94	0.10	103,103,103,103	0
55	MG	13	1739	1/1	0.94	0.14	90,90,90,90	0
55	MG	14	3071	1/1	0.94	0.15	62,62,62,62	0
55	MG	1H	3158	1/1	0.95	0.25	71,71,71,71	0
55	MG	1H	3513	1/1	0.95	0.06	116,116,116,116	0
55	MG	1H	3058	1/1	0.95	0.31	60,60,60,60	0
55	MG	14	3045	1/1	0.95	0.12	41,41,41,41	0
55	MG	14	3146	1/1	0.95	0.29	64,64,64,64	0
55	MG	1G	1672	1/1	0.95	0.33	79,79,79,79	0
55	MG	1H	3011	1/1	0.95	0.34	54,54,54,54	0
55	MG	1H	3089	1/1	0.95	0.24	38,38,38,38	0
55	MG	1H	3046	1/1	0.95	0.21	71,71,71,71	0
55	MG	14	3097	1/1	0.95	0.25	54,54,54,54	0
55	MG	1G	1641	1/1	0.95	0.31	83,83,83,83	0
55	MG	14	3099	1/1	0.95	0.14	67,67,67,67	0
55	MG	14	3008	1/1	0.95	0.19	53,53,53,53	0
55	MG	1H	3523	1/1	0.95	0.07	78,78,78,78	0
55	MG	1H	3394	1/1	0.95	0.08	69,69,69,69	0
55	MG	16	202	1/1	0.95	0.17	84,84,84,84	0
55	MG	1H	3018	1/1	0.95	0.16	50,50,50,50	0
55	MG	14	3315	1/1	0.95	0.34	85,85,85,85	0
55	MG	1H	3321	1/1	0.95	0.34	79,79,79,79	0
55	MG	1H	3020	1/1	0.95	0.21	52,52,52,52	0
55	MG	13	1630	1/1	0.95	0.13	61,61,61,61	0
55	MG	1H	3114	1/1	0.95	0.06	56,56,56,56	0
55	MG	1G	1616	1/1	0.95	0.10	62,62,62,62	0
55	MG	1H	3051	1/1	0.95	0.17	47,47,47,47	0
55	MG	1H	3401	1/1	0.95	0.14	67,67,67,67	0
55	MG	1H	3230	1/1	0.95	0.30	71,71,71,71	0
55	MG	14	3432	1/1	0.95	0.14	100,100,100,100	0
55	MG	1H	3149	1/1	0.95	0.32	82,82,82,82	0
55	MG	14	3024	1/1	0.95	0.20	49,49,49,49	0
55	MG	1H	3302	1/1	0.95	0.09	74,74,74,74	0
55	MG	13	1649	1/1	0.95	0.39	84,84,84,84	0
55	MG	14	3454	1/1	0.95	0.10	106,106,106,106	0
55	MG	1H	3133	1/1	0.95	0.11	49,49,49,49	0
55	MG	14	3462	1/1	0.95	0.05	130,130,130,130	0
55	MG	14	3463	1/1	0.95	0.09	130,130,130,130	0
55	MG	13	1720	1/1	0.95	0.09	129,129,129,129	0
55	MG	14	3227	1/1	0.95	0.33	80,80,80,80	0
55	MG	14	3176	1/1	0.95	0.25	63,63,63,63	0
55	MG	14	3073	1/1	0.95	0.15	58,58,58,58	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
55	MG	14	3074	1/1	0.95	0.14	47,47,47,47	0
55	MG	1G	1740	1/1	0.95	0.08	140,140,140,140	0
55	MG	1H	3449	1/1	0.95	0.19	94,94,94,94	0
55	MG	14	3077	1/1	0.95	0.20	61,61,61,61	0
55	MG	1H	3457	1/1	0.95	0.12	102,102,102,102	0
55	MG	1G	1661	1/1	0.95	0.37	76,76,76,76	0
55	MG	1H	3024	1/1	0.95	0.19	61,61,61,61	0
55	MG	1H	3069	1/1	0.95	0.17	51,51,51,51	0
55	MG	1H	3237	1/1	0.95	0.23	67,67,67,67	0
55	MG	14	3343	1/1	0.95	0.33	86,86,86,86	0
55	MG	2K	102	1/1	0.95	0.24	93,93,93,93	0
55	MG	1H	3499	1/1	0.95	0.06	111,111,111,111	0
55	MG	1H	3005	1/1	0.95	0.15	44,44,44,44	0
55	MG	14	3138	1/1	0.95	0.15	58,58,58,58	0
55	MG	14	3139	1/1	0.95	0.36	69,69,69,69	0
55	MG	1H	3086	1/1	0.95	0.17	59,59,59,59	0
55	MG	14	3310	1/1	0.96	0.36	75,75,75,75	0
55	MG	14	3080	1/1	0.96	0.39	81,81,81,81	0
55	MG	1H	3439	1/1	0.96	0.11	92,92,92,92	0
55	MG	14	3003	1/1	0.96	0.13	47,47,47,47	0
55	MG	1H	3251	1/1	0.96	0.18	56,56,56,56	0
55	MG	1H	3452	1/1	0.96	0.07	58,58,58,58	0
55	MG	1H	3310	1/1	0.96	0.23	72,72,72,72	0
55	MG	1H	3019	1/1	0.96	0.15	61,61,61,61	0
55	MG	1H	3359	1/1	0.96	0.21	77,77,77,77	0
55	MG	13	1731	1/1	0.96	0.12	153,153,153,153	0
55	MG	14	3320	1/1	0.96	0.09	88,88,88,88	0
55	MG	14	3049	1/1	0.96	0.12	55,55,55,55	0
55	MG	14	3370	1/1	0.96	0.24	75,75,75,75	0
55	MG	1H	3482	1/1	0.96	0.11	70,70,70,70	0
55	MG	14	3183	1/1	0.96	0.25	56,56,56,56	0
55	MG	1H	3488	1/1	0.96	0.11	66,66,66,66	0
55	MG	1H	3495	1/1	0.96	0.06	79,79,79,79	0
55	MG	14	3013	1/1	0.96	0.13	56,56,56,56	0
55	MG	14	3233	1/1	0.96	0.37	67,67,67,67	0
55	MG	14	3407	1/1	0.96	0.07	83,83,83,83	0
55	MG	1H	3097	1/1	0.96	0.25	70,70,70,70	0
55	MG	14	3424	1/1	0.96	0.09	81,81,81,81	0
55	MG	14	3429	1/1	0.96	0.14	77,77,77,77	0
55	MG	14	3431	1/1	0.96	0.05	102,102,102,102	0
55	MG	13	1631	1/1	0.96	0.07	60,60,60,60	0
55	MG	1H	3091	1/1	0.96	0.26	59,59,59,59	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
55	MG	1H	3270	1/1	0.96	0.06	84,84,84,84	0
55	MG	14	3443	1/1	0.96	0.07	103,103,103,103	0
55	MG	14	3446	1/1	0.96	0.07	87,87,87,87	0
55	MG	1H	3383	1/1	0.96	0.15	60,60,60,60	0
55	MG	1H	3510	1/1	0.96	0.07	111,111,111,111	0
55	MG	1H	3511	1/1	0.96	0.06	119,119,119,119	0
55	MG	1H	3214	1/1	0.96	0.21	64,64,64,64	0
55	MG	14	3458	1/1	0.96	0.06	108,108,108,108	0
55	MG	1H	3101	1/1	0.96	0.14	50,50,50,50	0
55	MG	14	3063	1/1	0.96	0.20	51,51,51,51	0
55	MG	1G	1634	1/1	0.96	0.43	80,80,80,80	0
55	MG	14	3106	1/1	0.96	0.39	75,75,75,75	0
55	MG	1H	3517	1/1	0.96	0.05	113,113,113,113	0
55	MG	1G	1744	1/1	0.96	0.09	128,128,128,128	0
55	MG	1H	3246	1/1	0.96	0.10	48,48,48,48	0
55	MG	1G	1746	1/1	0.96	0.09	134,134,134,134	0
55	MG	14	3344	1/1	0.96	0.08	95,95,95,95	0
55	MG	1H	3519	1/1	0.96	0.07	103,103,103,103	0
55	MG	1H	3085	1/1	0.96	0.12	63,63,63,63	0
55	MG	1H	3261	1/1	0.96	0.26	72,72,72,72	0
55	MG	29	301	1/1	0.96	0.22	72,72,72,72	0
55	MG	29	302	1/1	0.96	0.22	51,51,51,51	0
55	MG	14	3114	1/1	0.96	0.15	56,56,56,56	0
55	MG	7E	201	1/1	0.96	0.21	83,83,83,83	0
55	MG	14	3164	1/1	0.96	0.25	60,60,60,60	0
55	MG	1H	3408	1/1	0.96	0.09	54,54,54,54	0
55	MG	45	201	1/1	0.96	0.29	76,76,76,76	0
55	MG	1H	3410	1/1	0.96	0.12	52,52,52,52	0
55	MG	1H	3423	1/1	0.96	0.10	61,61,61,61	0
55	MG	13	1628	1/1	0.96	0.23	71,71,71,71	0
55	MG	14	3121	1/1	0.96	0.11	54,54,54,54	0
55	MG	1H	3436	1/1	0.96	0.05	94,94,94,94	0
55	MG	1H	3438	1/1	0.96	0.12	60,60,60,60	0
55	MG	1H	3494	1/1	0.97	0.06	81,81,81,81	0
55	MG	14	3374	1/1	0.97	0.07	52,52,52,52	0
55	MG	1H	3371	1/1	0.97	0.05	62,62,62,62	0
55	MG	1H	3272	1/1	0.97	0.19	76,76,76,76	0
55	MG	14	3288	1/1	0.97	0.08	171,171,171,171	0
55	MG	14	3391	1/1	0.97	0.07	62,62,62,62	0
55	MG	1H	3110	1/1	0.97	0.27	47,47,47,47	0
55	MG	1H	3210	1/1	0.97	0.34	79,79,79,79	0
55	MG	14	3414	1/1	0.97	0.07	56,56,56,56	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
55	MG	14	3420	1/1	0.97	0.06	89,89,89,89	0
55	MG	1H	3050	1/1	0.97	0.24	47,47,47,47	0
55	MG	14	3425	1/1	0.97	0.06	96,96,96,96	0
55	MG	1H	3504	1/1	0.97	0.08	80,80,80,80	0
55	MG	1H	3288	1/1	0.97	0.23	72,72,72,72	0
55	MG	14	3250	1/1	0.97	0.22	70,70,70,70	0
55	MG	1H	3509	1/1	0.97	0.09	85,85,85,85	0
55	MG	14	3437	1/1	0.97	0.07	85,85,85,85	0
55	MG	1G	1732	1/1	0.97	0.04	113,113,113,113	0
55	MG	14	3439	1/1	0.97	0.05	101,101,101,101	0
55	MG	14	3442	1/1	0.97	0.06	107,107,107,107	0
55	MG	1G	1733	1/1	0.97	0.05	93,93,93,93	0
55	MG	1G	1735	1/1	0.97	0.06	96,96,96,96	0
55	MG	1G	1737	1/1	0.97	0.04	114,114,114,114	0
55	MG	1H	3429	1/1	0.97	0.07	71,71,71,71	0
55	MG	14	3452	1/1	0.97	0.12	100,100,100,100	0
55	MG	14	3016	1/1	0.97	0.12	63,63,63,63	0
55	MG	1H	3183	1/1	0.97	0.40	63,63,63,63	0
55	MG	14	3457	1/1	0.97	0.04	125,125,125,125	0
55	MG	1H	3378	1/1	0.97	0.06	91,91,91,91	0
55	MG	14	3460	1/1	0.97	0.06	112,112,112,112	0
55	MG	1H	3175	1/1	0.97	0.40	74,74,74,74	0
55	MG	14	3133	1/1	0.97	0.28	71,71,71,71	0
55	MG	14	3464	1/1	0.97	0.10	101,101,101,101	0
55	MG	1G	1742	1/1	0.97	0.06	112,112,112,112	0
55	MG	1H	3515	1/1	0.97	0.05	106,106,106,106	0
55	MG	14	3136	1/1	0.97	0.28	75,75,75,75	0
55	MG	I8	102	1/1	0.97	0.26	65,65,65,65	0
55	MG	1H	3443	1/1	0.97	0.05	75,75,75,75	0
55	MG	1H	3062	1/1	0.97	0.12	48,48,48,48	0
55	MG	13	1735	1/1	0.97	0.09	106,106,106,106	0
55	MG	1J	208	1/1	0.97	0.06	97,97,97,97	0
55	MG	13	1722	1/1	0.97	0.07	101,101,101,101	0
55	MG	14	3184	1/1	0.97	0.20	71,71,71,71	0
55	MG	14	3142	1/1	0.97	0.27	72,72,72,72	0
55	MG	14	3027	1/1	0.97	0.15	71,71,71,71	0
55	MG	13	1737	1/1	0.97	0.06	111,111,111,111	0
55	MG	1H	3308	1/1	0.97	0.07	106,106,106,106	0
55	MG	1H	3338	1/1	0.97	0.06	78,78,78,78	0
55	MG	3A	201	1/1	0.97	0.14	81,81,81,81	0
55	MG	1H	3481	1/1	0.97	0.05	64,64,64,64	0
55	MG	25	201	1/1	0.97	0.05	111,111,111,111	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
55	MG	13	1718	1/1	0.97	0.05	85,85,85,85	0
55	MG	1H	3484	1/1	0.97	0.05	118,118,118,118	0
55	MG	14	3151	1/1	0.97	0.39	78,78,78,78	0
55	MG	14	3072	1/1	0.97	0.24	54,54,54,54	0
55	MG	2L	103	1/1	0.97	0.05	130,130,130,130	0
56	ZN	3E	302	1/1	0.97	0.22	102,102,102,102	0
55	MG	1H	3249	1/1	0.97	0.41	66,66,66,66	0
56	ZN	5A	101	1/1	0.97	0.06	133,133,133,133	0
55	MG	1H	3490	1/1	0.97	0.07	89,89,89,89	0
55	MG	14	3400	1/1	0.98	0.06	65,65,65,65	0
55	MG	14	3401	1/1	0.98	0.08	82,82,82,82	0
55	MG	14	3402	1/1	0.98	0.07	82,82,82,82	0
55	MG	14	3406	1/1	0.98	0.04	61,61,61,61	0
55	MG	1H	3500	1/1	0.98	0.11	65,65,65,65	0
55	MG	14	3409	1/1	0.98	0.07	64,64,64,64	0
55	MG	13	1732	1/1	0.98	0.06	128,128,128,128	0
55	MG	13	1717	1/1	0.98	0.06	66,66,66,66	0
55	MG	14	3416	1/1	0.98	0.06	52,52,52,52	0
55	MG	1H	3430	1/1	0.98	0.05	76,76,76,76	0
55	MG	1H	3506	1/1	0.98	0.05	110,110,110,110	0
55	MG	1H	3434	1/1	0.98	0.07	60,60,60,60	0
55	MG	13	1721	1/1	0.98	0.04	88,88,88,88	0
55	MG	1H	3437	1/1	0.98	0.04	66,66,66,66	0
55	MG	13	1716	1/1	0.98	0.05	74,74,74,74	0
55	MG	14	3434	1/1	0.98	0.04	98,98,98,98	0
55	MG	1H	3512	1/1	0.98	0.04	115,115,115,115	0
55	MG	1G	1736	1/1	0.98	0.06	94,94,94,94	0
55	MG	13	1724	1/1	0.98	0.07	107,107,107,107	0
55	MG	13	1726	1/1	0.98	0.04	89,89,89,89	0
55	MG	14	3441	1/1	0.98	0.05	86,86,86,86	0
55	MG	1H	3447	1/1	0.98	0.05	62,62,62,62	0
55	MG	1H	3516	1/1	0.98	0.06	88,88,88,88	0
55	MG	14	3444	1/1	0.98	0.10	90,90,90,90	0
55	MG	1H	3448	1/1	0.98	0.05	63,63,63,63	0
55	MG	14	3447	1/1	0.98	0.05	102,102,102,102	0
55	MG	1H	3201	1/1	0.98	0.31	66,66,66,66	0
55	MG	14	3162	1/1	0.98	0.28	71,71,71,71	0
55	MG	1H	3319	1/1	0.98	0.06	60,60,60,60	0
55	MG	13	1727	1/1	0.98	0.06	108,108,108,108	0
55	MG	1H	3461	1/1	0.98	0.06	54,54,54,54	0
55	MG	14	3456	1/1	0.98	0.06	102,102,102,102	0
55	MG	14	3120	1/1	0.98	0.36	54,54,54,54	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
55	MG	13	1729	1/1	0.98	0.04	112,112,112,112	0
55	MG	14	3459	1/1	0.98	0.03	130,130,130,130	0
55	MG	1H	3466	1/1	0.98	0.05	59,59,59,59	0
55	MG	14	3461	1/1	0.98	0.09	82,82,82,82	0
55	MG	13	1730	1/1	0.98	0.05	115,115,115,115	0
55	MG	13	1719	1/1	0.98	0.04	94,94,94,94	0
55	MG	1H	3470	1/1	0.98	0.10	74,74,74,74	0
55	MG	1H	3476	1/1	0.98	0.05	59,59,59,59	0
55	MG	1H	3477	1/1	0.98	0.04	74,74,74,74	0
55	MG	1H	3409	1/1	0.98	0.05	62,62,62,62	0
55	MG	1H	3053	1/1	0.98	0.09	61,61,61,61	0
55	MG	1H	3483	1/1	0.98	0.07	84,84,84,84	0
55	MG	1H	3412	1/1	0.98	0.05	69,69,69,69	0
55	MG	2L	104	1/1	0.98	0.05	93,93,93,93	0
55	MG	1H	3486	1/1	0.98	0.09	79,79,79,79	0
55	MG	14	3226	1/1	0.98	0.08	55,55,55,55	0
55	MG	14	3044	1/1	0.98	0.12	43,43,43,43	0
55	MG	1H	3487	1/1	0.98	0.11	81,81,81,81	0
55	MG	1H	3414	1/1	0.98	0.05	59,59,59,59	0
55	MG	16	215	1/1	0.98	0.04	93,93,93,93	0
55	MG	1H	3416	1/1	0.98	0.07	71,71,71,71	0
55	MG	1H	3491	1/1	0.98	0.03	52,52,52,52	0
55	MG	1H	3493	1/1	0.98	0.05	103,103,103,103	0
55	MG	1H	3418	1/1	0.98	0.10	63,63,63,63	0
55	MG	14	3378	1/1	0.98	0.05	78,78,78,78	0
55	MG	1H	3421	1/1	0.98	0.06	52,52,52,52	0
55	MG	14	3381	1/1	0.98	0.06	52,52,52,52	0
55	MG	14	3382	1/1	0.98	0.05	55,55,55,55	0
55	MG	14	3383	1/1	0.98	0.05	81,81,81,81	0
55	MG	1H	3098	1/1	0.98	0.15	42,42,42,42	0
55	MG	1H	3424	1/1	0.98	0.07	58,58,58,58	0
56	ZN	5I	101	1/1	0.98	0.03	116,116,116,116	0
55	MG	14	3394	1/1	0.98	0.07	89,89,89,89	0
55	MG	14	3395	1/1	0.98	0.05	65,65,65,65	0
55	MG	14	3396	1/1	0.98	0.05	67,67,67,67	0
55	MG	14	3411	1/1	0.99	0.03	63,63,63,63	0
55	MG	1H	3462	1/1	0.99	0.03	49,49,49,49	0
55	MG	1H	3505	1/1	0.99	0.07	69,69,69,69	0
55	MG	14	3415	1/1	0.99	0.07	62,62,62,62	0
55	MG	1H	3463	1/1	0.99	0.04	52,52,52,52	0
55	MG	14	3417	1/1	0.99	0.03	51,51,51,51	0
55	MG	14	3419	1/1	0.99	0.03	94,94,94,94	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
55	MG	1H	3507	1/1	0.99	0.07	62,62,62,62	0
55	MG	14	3421	1/1	0.99	0.07	82,82,82,82	0
55	MG	1H	3433	1/1	0.99	0.05	54,54,54,54	0
55	MG	1H	3419	1/1	0.99	0.04	48,48,48,48	0
55	MG	14	3426	1/1	0.99	0.04	91,91,91,91	0
55	MG	14	3427	1/1	0.99	0.05	75,75,75,75	0
55	MG	14	3428	1/1	0.99	0.03	69,69,69,69	0
55	MG	1H	3435	1/1	0.99	0.04	76,76,76,76	0
55	MG	14	3430	1/1	0.99	0.04	67,67,67,67	0
55	MG	1H	3468	1/1	0.99	0.04	59,59,59,59	0
55	MG	1G	1728	1/1	0.99	0.04	73,73,73,73	0
55	MG	1G	1729	1/1	0.99	0.06	93,93,93,93	0
55	MG	1G	1730	1/1	0.99	0.08	82,82,82,82	0
55	MG	1G	1731	1/1	0.99	0.10	110,110,110,110	0
55	MG	1H	3420	1/1	0.99	0.03	52,52,52,52	0
55	MG	1H	3411	1/1	0.99	0.04	67,67,67,67	0
55	MG	14	3440	1/1	0.99	0.03	101,101,101,101	0
55	MG	1G	1734	1/1	0.99	0.03	81,81,81,81	0
55	MG	1H	3471	1/1	0.99	0.03	71,71,71,71	0
55	MG	1H	3472	1/1	0.99	0.03	82,82,82,82	0
55	MG	1H	3473	1/1	0.99	0.06	64,64,64,64	0
55	MG	1H	3475	1/1	0.99	0.04	70,70,70,70	0
55	MG	13	1723	1/1	0.99	0.04	86,86,86,86	0
55	MG	14	3448	1/1	0.99	0.06	87,87,87,87	0
55	MG	1H	3413	1/1	0.99	0.04	44,44,44,44	0
55	MG	1H	3478	1/1	0.99	0.07	82,82,82,82	0
55	MG	14	3451	1/1	0.99	0.05	74,74,74,74	0
55	MG	1H	3479	1/1	0.99	0.04	58,58,58,58	0
55	MG	14	3453	1/1	0.99	0.05	76,76,76,76	0
55	MG	1H	3441	1/1	0.99	0.13	63,63,63,63	0
55	MG	1H	3442	1/1	0.99	0.03	43,43,43,43	0
55	MG	13	1725	1/1	0.99	0.03	99,99,99,99	0
55	MG	1H	3444	1/1	0.99	0.03	59,59,59,59	0
55	MG	1H	3485	1/1	0.99	0.05	75,75,75,75	0
55	MG	14	3084	1/1	0.99	0.12	73,73,73,73	0
55	MG	1H	3446	1/1	0.99	0.05	52,52,52,52	0
55	MG	1H	3427	1/1	0.99	0.03	107,107,107,107	0
55	MG	14	3375	1/1	0.99	0.04	51,51,51,51	0
55	MG	1H	3428	1/1	0.99	0.03	74,74,74,74	0
55	MG	14	3377	1/1	0.99	0.04	57,57,57,57	0
55	MG	13	1728	1/1	0.99	0.04	76,76,76,76	0
55	MG	14	3379	1/1	0.99	0.05	53,53,53,53	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
55	MG	1H	3450	1/1	0.99	0.10	53,53,53,53	0
55	MG	1H	3492	1/1	0.99	0.02	83,83,83,83	0
55	MG	1H	3406	1/1	0.99	0.53	91,91,91,91	0
55	MG	1H	3453	1/1	0.99	0.03	42,42,42,42	0
55	MG	14	3384	1/1	0.99	0.05	54,54,54,54	0
55	MG	1J	207	1/1	0.99	0.03	88,88,88,88	0
55	MG	1H	3454	1/1	0.99	0.04	49,49,49,49	0
55	MG	14	3388	1/1	0.99	0.04	61,61,61,61	0
55	MG	14	3390	1/1	0.99	0.03	52,52,52,52	0
55	MG	16	214	1/1	0.99	0.05	86,86,86,86	0
55	MG	14	3392	1/1	0.99	0.04	54,54,54,54	0
55	MG	14	3393	1/1	0.99	0.03	53,53,53,53	0
55	MG	1H	3496	1/1	0.99	0.03	78,78,78,78	0
55	MG	1H	3456	1/1	0.99	0.02	51,51,51,51	0
55	MG	1H	3498	1/1	0.99	0.05	77,77,77,77	0
55	MG	14	3397	1/1	0.99	0.05	70,70,70,70	0
55	MG	14	3398	1/1	0.99	0.06	83,83,83,83	0
55	MG	14	3399	1/1	0.99	0.04	82,82,82,82	0
55	MG	1H	3431	1/1	0.99	0.05	70,70,70,70	0
55	MG	1H	3459	1/1	0.99	0.06	75,75,75,75	0
55	MG	1G	1716	1/1	0.99	0.04	110,110,110,110	0
55	MG	14	3404	1/1	0.99	0.10	79,79,79,79	0
55	MG	14	3405	1/1	0.99	0.05	64,64,64,64	0
55	MG	1H	3460	1/1	0.99	0.04	87,87,87,87	0
55	MG	1H	3432	1/1	0.99	0.05	68,68,68,68	0
56	ZN	32	302	1/1	0.99	0.19	111,111,111,111	0
55	MG	G8	201	1/1	0.99	0.05	77,77,77,77	0
55	MG	14	3410	1/1	0.99	0.05	58,58,58,58	0
55	MG	1H	3464	1/1	1.00	0.01	52,52,52,52	0
55	MG	1H	3455	1/1	1.00	0.02	47,47,47,47	0
55	MG	1H	3489	1/1	1.00	0.02	67,67,67,67	0
55	MG	14	3418	1/1	1.00	0.04	72,72,72,72	0
55	MG	14	3445	1/1	1.00	0.02	58,58,58,58	0
55	MG	1H	3503	1/1	1.00	0.02	57,57,57,57	0
55	MG	1H	3422	1/1	1.00	0.03	56,56,56,56	0
55	MG	1H	3426	1/1	1.00	0.02	67,67,67,67	0
55	MG	14	3422	1/1	1.00	0.06	53,53,53,53	0
55	MG	14	3423	1/1	1.00	0.02	84,84,84,84	0
55	MG	1H	3458	1/1	1.00	0.04	70,70,70,70	0
55	MG	1H	3521	1/1	1.00	0.04	47,47,47,47	0
55	MG	1H	3480	1/1	1.00	0.03	47,47,47,47	0
55	MG	14	3403	1/1	1.00	0.02	69,69,69,69	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
55	MG	1H	3415	1/1	1.00	0.01	50,50,50,50	0
55	MG	14	3386	1/1	1.00	0.02	56,56,56,56	0
55	MG	14	3387	1/1	1.00	0.02	58,58,58,58	0
55	MG	1H	3451	1/1	1.00	0.01	54,54,54,54	0
55	MG	14	3408	1/1	1.00	0.04	56,56,56,56	0
55	MG	14	3433	1/1	1.00	0.03	87,87,87,87	0
55	MG	14	3389	1/1	1.00	0.03	53,53,53,53	0
55	MG	14	3435	1/1	1.00	0.02	95,95,95,95	0
55	MG	1H	3445	1/1	1.00	0.03	59,59,59,59	0
55	MG	1H	3440	1/1	1.00	0.03	91,91,91,91	0
55	MG	14	3412	1/1	1.00	0.03	49,49,49,49	0
55	MG	1H	3417	1/1	1.00	0.03	40,40,40,40	0
55	MG	1H	3474	1/1	1.00	0.02	79,79,79,79	0

6.5 Other polymers [i](#)

There are no such residues in this entry.