



wwPDB X-ray Structure Validation Summary Report ⓘ

Jun 3, 2020 – 06:07 am BST

PDB ID : 4WZD
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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

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

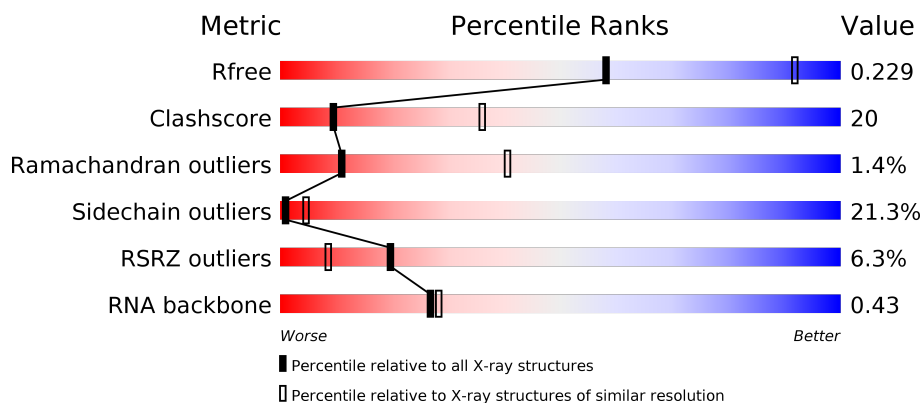
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

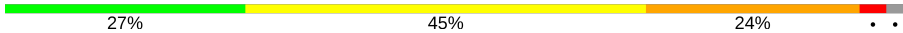
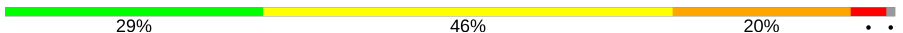


The reported resolution of this entry is 3.10 Å.

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}	130704	1094 (3.10-3.10)
Clashscore	141614	1184 (3.10-3.10)
Ramachandran outliers	138981	1141 (3.10-3.10)
Sidechain outliers	138945	1141 (3.10-3.10)
RSRZ outliers	127900	1067 (3.10-3.10)
RNA backbone	3102	1116 (3.40-2.80)

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

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



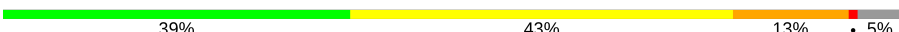
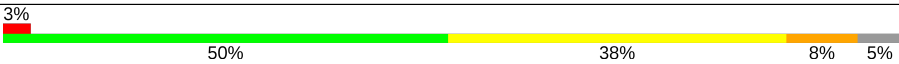
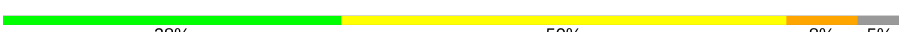
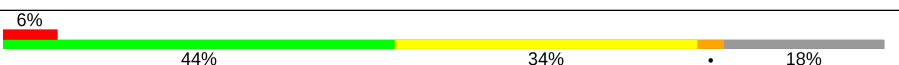
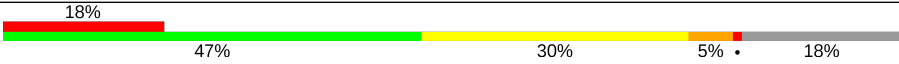
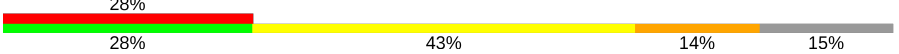
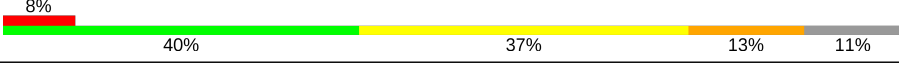




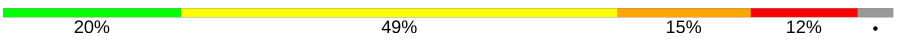

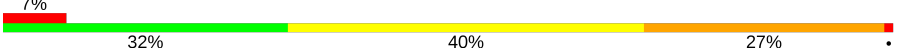



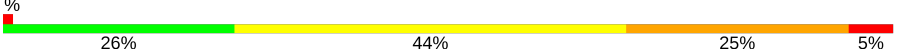


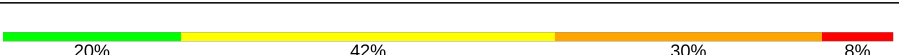
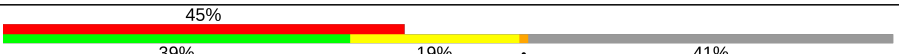
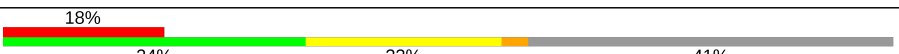
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Mol	Chain	Length	Quality of chain
3	22	239	
3	2E	239	
4	32	209	
4	3E	209	
5	42	162	
5	4E	162	
6	52	101	
6	5E	101	
7	62	156	
7	6E	156	
8	72	138	
8	7E	138	
9	82	128	
9	8E	128	
10	1A	105	
10	1I	105	
11	2A	129	
11	2I	129	
12	3A	132	
12	3I	132	
13	4A	126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








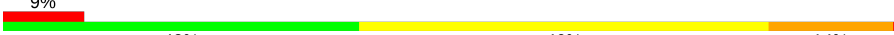



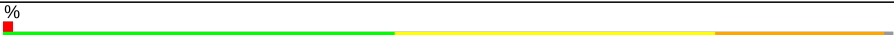


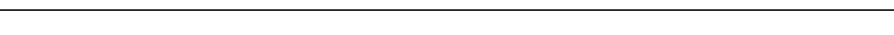
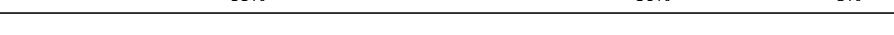

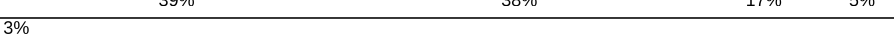







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Mol	Chain	Length	Quality of chain
15	6I	89	
16	7A	88	
16	7I	88	
17	8A	105	
17	8I	105	
18	9A	88	
18	9I	88	
19	AA	93	
19	AI	93	
20	BA	106	
20	BI	106	
21	1B	27	
21	1F	27	
22	2K	85	
22	2L	85	
22	3K	85	
22	3L	85	
23	4K	30	
23	4L	30	
24	14	2917	
24	1H	2917	
25	16	122	
25	1J	122	
26	71	229	
26	79	229	

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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	

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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	

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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	1643	-	-	-	X
55	MG	13	1644	-	-	-	X
55	MG	13	1645	-	-	-	X
55	MG	13	1649	-	-	-	X
55	MG	13	1666	-	-	-	X
55	MG	13	1668	-	-	-	X
55	MG	13	1688	-	-	-	X
55	MG	13	1689	-	-	-	X
55	MG	13	1699	-	-	-	X
55	MG	13	1706	-	-	-	X
55	MG	13	1708	-	-	-	X
55	MG	13	1711	-	-	-	X
55	MG	14	3128	-	-	-	X
55	MG	14	3261	-	-	-	X
55	MG	1G	1620	-	-	-	X
55	MG	1G	1638	-	-	-	X
55	MG	1G	1639	-	-	-	X
55	MG	1G	1699	-	-	-	X
55	MG	1G	1721	-	-	-	X
55	MG	1G	1726	-	-	-	X
55	MG	1H	3058	-	-	-	X
55	MG	1H	3096	-	-	-	X
55	MG	1H	3106	-	-	-	X
55	MG	1H	3116	-	-	-	X
55	MG	1H	3149	-	-	-	X
55	MG	1H	3152	-	-	-	X
55	MG	1H	3185	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
55	MG	1H	3190	-	-	-	X
55	MG	1H	3196	-	-	-	X
55	MG	1H	3203	-	-	-	X
55	MG	1H	3209	-	-	-	X
55	MG	1H	3215	-	-	-	X
55	MG	1H	3216	-	-	-	X
55	MG	1H	3218	-	-	-	X
55	MG	1H	3231	-	-	-	X
55	MG	1H	3282	-	-	-	X
55	MG	1H	3283	-	-	-	X
55	MG	1H	3292	-	-	-	X
55	MG	1H	3294	-	-	-	X
55	MG	1H	3311	-	-	-	X
55	MG	1H	3330	-	-	-	X
55	MG	1H	3336	-	-	-	X
55	MG	1H	3339	-	-	-	X
55	MG	1H	3342	-	-	-	X
55	MG	1H	3350	-	-	-	X
55	MG	1H	3355	-	-	-	X
55	MG	1H	3356	-	-	-	X
55	MG	1H	3406	-	-	-	X
55	MG	29	304	-	-	-	X
55	MG	2K	104	-	-	-	X
55	MG	32	301	-	-	-	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			

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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			

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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			

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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 (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
55	98	1	Total	Mg	0	0
			1	1		
55	45	1	Total	Mg	0	0
			1	1		
55	55	1	Total	Mg	0	0
			1	1		
55	32	1	Total	Mg	0	0
			1	1		
55	C5	1	Total	Mg	0	0
			1	1		
55	13	139	Total	Mg	0	0
			139	139		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
55	1J	10	Total 10	Mg 10	0	0
55	16	15	Total 15	Mg 15	0	0
55	42	1	Total 1	Mg 1	0	0
55	25	1	Total 1	Mg 1	0	0
55	21	2	Total 2	Mg 2	0	0
55	4A	1	Total 1	Mg 1	0	0
55	Q8	2	Total 2	Mg 2	0	0
55	3I	1	Total 1	Mg 1	0	0
55	I8	3	Total 3	Mg 3	0	0
55	52	1	Total 1	Mg 1	0	0
55	5E	1	Total 1	Mg 1	0	0
55	29	4	Total 4	Mg 4	0	0
55	2K	5	Total 5	Mg 5	0	0
55	15	1	Total 1	Mg 1	0	0
55	7E	1	Total 1	Mg 1	0	0
55	39	1	Total 1	Mg 1	0	0
55	1G	148	Total 148	Mg 148	0	0
55	11	2	Total 2	Mg 2	0	0
55	1H	523	Total 523	Mg 523	0	0
55	F5	1	Total 1	Mg 1	0	0
55	E5	1	Total 1	Mg 1	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
55	88	1	Total Mg 1 1	0	0
55	14	465	Total Mg 465 465	0	0
55	3E	1	Total Mg 1 1	0	0
55	19	1	Total Mg 1 1	0	0
55	3L	1	Total Mg 1 1	0	0
55	4K	1	Total Mg 1 1	0	0
55	3A	1	Total Mg 1 1	0	0
55	G8	1	Total Mg 1 1	0	0
55	2L	4	Total Mg 4 4	0	0

- Molecule 56 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

- Molecule 57 is water.

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

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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

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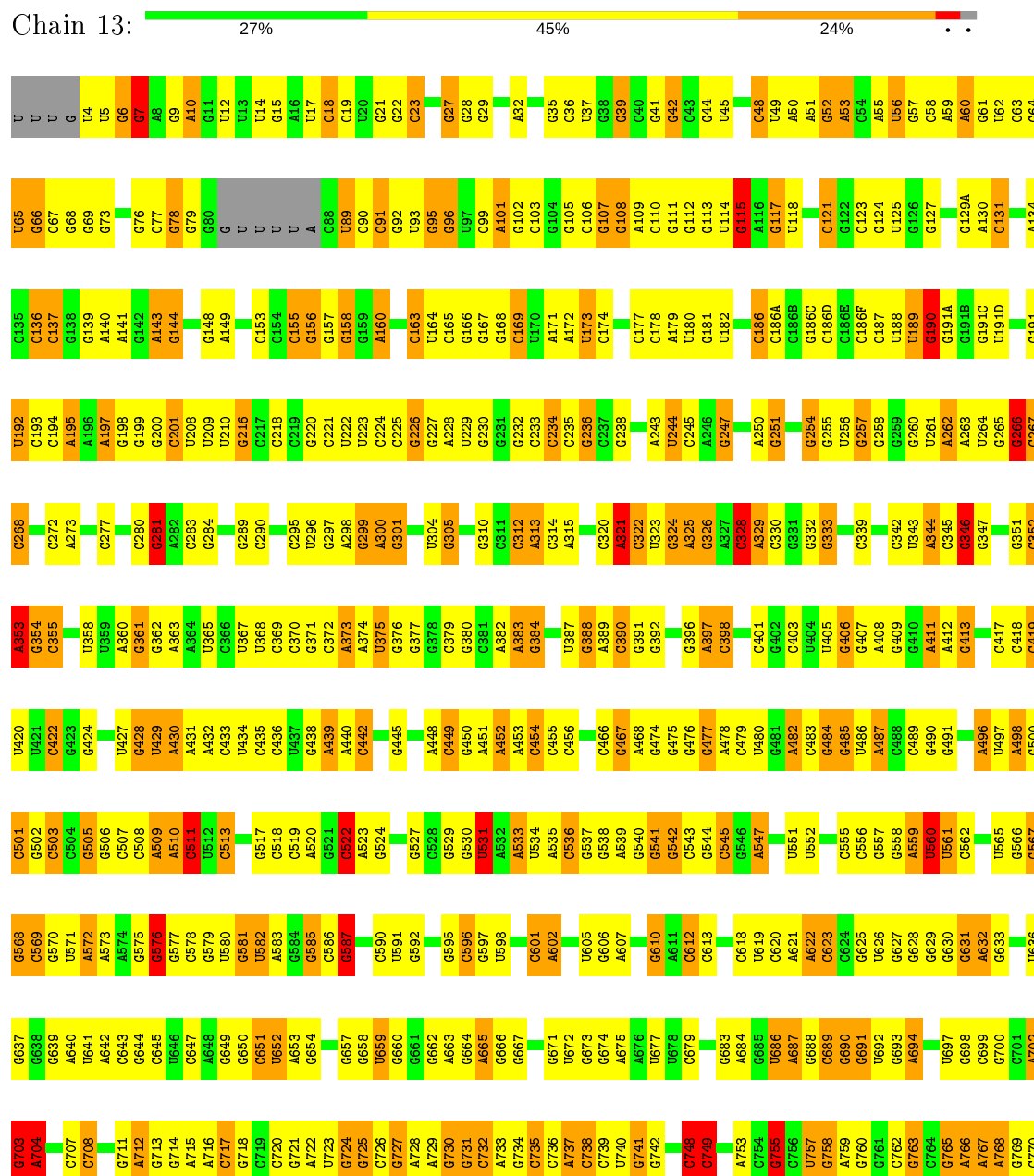
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
57	1J	22	Total 22	O 22	0	0
57	19	11	Total 11	O 11	0	0
57	39	3	Total 3	O 3	0	0
57	25	6	Total 6	O 6	0	0
57	35	1	Total 1	O 1	0	0
57	75	1	Total 1	O 1	0	0
57	85	4	Total 4	O 4	0	0
57	F5	1	Total 1	O 1	0	0
57	H5	2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

3 Residue-property plots

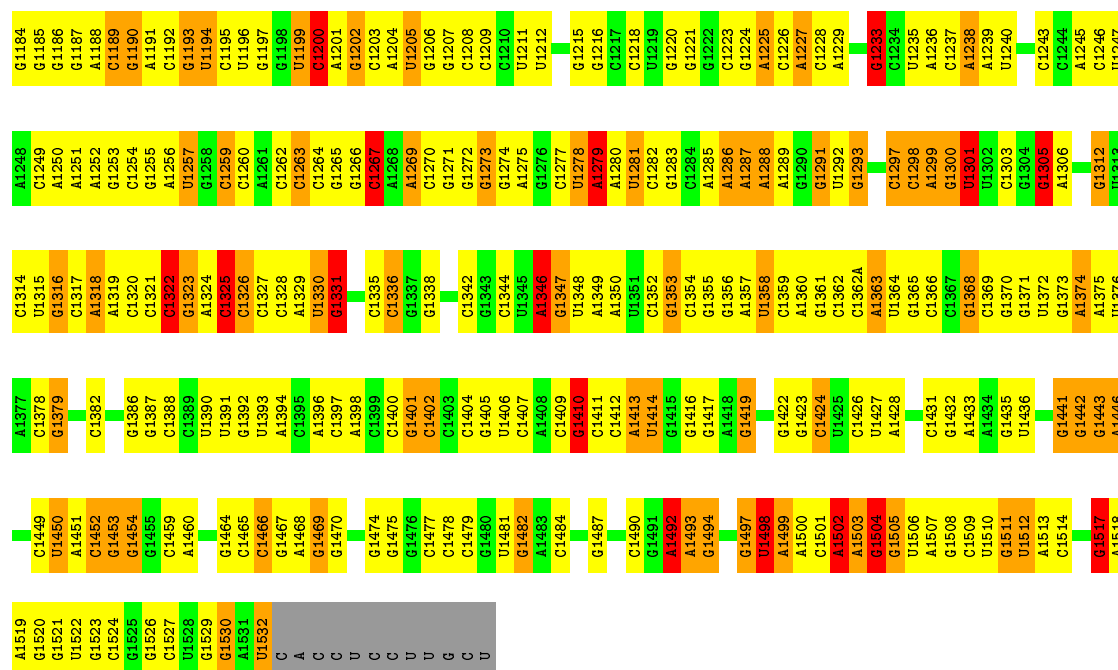
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are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

• Molecule 1: 16S ribosomal RNA

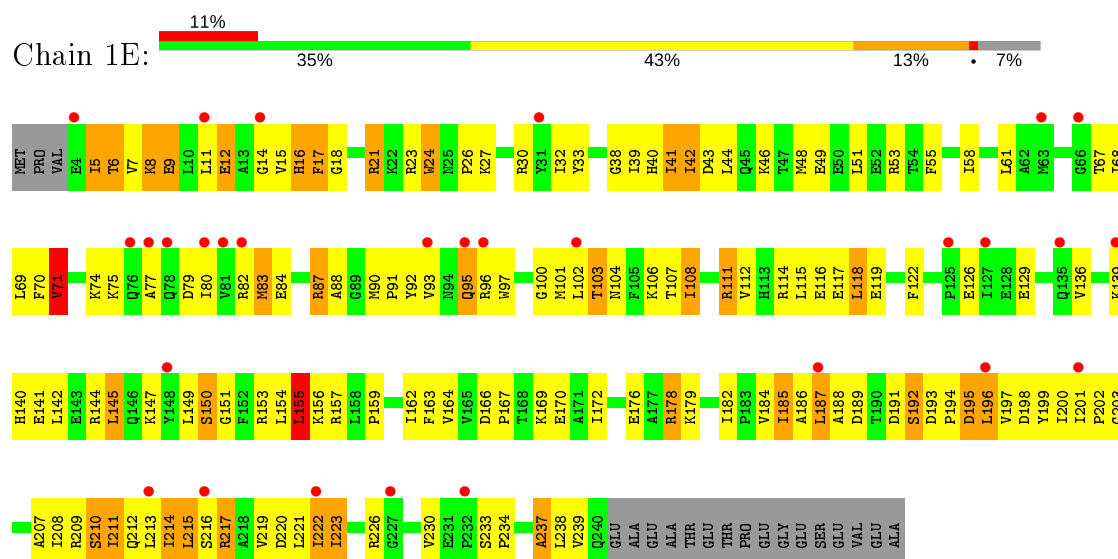




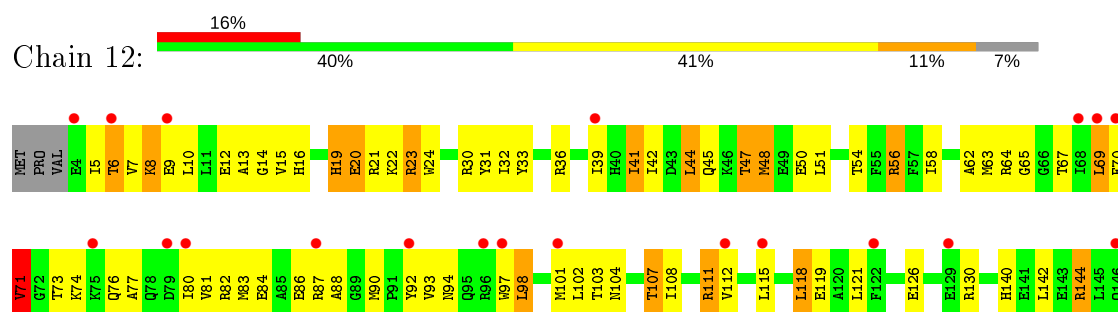
U1122	U1056	U992	G929	G861	A787	C719	C643	C569	G505	U427	A364	G289	C201	G138
A1123	G1057	G993	C932	C862	G791	C720	G644	G570	A509	G428	U365	C290	U208	G142
U1125	G1058	A994	G933	A863	A792	G721	C645	U571	A510	U429	U367	U296	U209	A143
U1126	C1059	C995	G934	A864	A793	C722	C646	A572	A511	A430	U368	A297	G216	G144
G1127	G1060	A996	C935	A865	A794	A723	C647	A573	C512	A431	U369	A298	G216	G145
G1128	G1061	U997	A935	C868	G724	A724	G650	G574	C513	A432	U370	A299	G220	G146
C1129	U1062	G998	A936	G869	G725	C725	C651	G575	C514	A433	U371	A300	U222	G147
A1130	C1063	A1000	A938	A872	G726	A726	C652	G576	G515	U434	A372	A301	G221	G148
G1131	U1065	G1001	G939	A873	G727	A727	A653	C577	U516	U435	A373	G306	U223	A149
C1132	C1066	G1002	G940	A874	G728	A728	G654	C578	C517	G438	U374	G305	G227	A151
G1133	A1067	G1003	G941	A875	G729	A729	U659	C579	C518	A439	A375	A304	A228	A152
G1134	U1068	A1004	G942	A876	G730	A730	G660	G580	C519	A440	G376	G306	U229	G153
U1135	C1069	A1005	G943	C877	G731	A731	G661	U582	A520	C442	G377	G309	G232	C154
C1136	G1070	G1006	G944	C878	G732	A732	G662	A583	C521	C443	G378	G310	G233	A160
G1137	U1071	G1007	G945	C879	G733	A733	A663	A584	C522	C444	G379	G311	C234	C163
G1138	G1072	G1008	A946	C880	G734	A734	A664	G585	A523	G445	G380	A313	C235	U164
C1139	U1073	G1009	G947	C881	G735	A735	A665	G586	C524	G446	G381	A314	G243	G165
G1140	C1074	G1010	A948	C882	G736	A736	A666	G587	C525	G447	A382	A315	U244	G166
C1141	U1075	G1011	A949	C883	G737	A737	G668	G588	C526	A448	A383	G316	C245	G167
G1142	G1076	A1014	G951	G884	G738	A738	U669	G589	G527	C449	A384	G317	G246	G168
G1143	U1077	A1015	G952	G885	G739	A739	G670	C590	G530	G450	G385	G318	A246	C169
C1144	G1078	A1016	G953	G886	U740	A740	G671	U591	U531	A452	U387	G319	G247	G170
G1145	U1079	G1017	G954	A889	G741	A741	U672	G595	A532	C457	U388	G320	G247	C182
C1146	G1080	C1018	U955	C893	A814	A742	G673	G596	A533	G458	A389	A321	A250	G183
G1147	U1081	G1021	U956	G894	A815	C747	G674	C597	A534	C459	G390	A322	G251	U173
U1148	U1082	G1022	U957	G895	A816	C748	A675	C601	A535	G460	G391	U323	U252	C174
C1149	G1083	G1023	A958	C896	A817	C749	A676	A602	C536	A465	G392	G324	U253	C175
U1150	U1084	G1024	U960	C897	G818	G750	U677	U603	G537	A466	A393	G327	G254	C176
A1151	G1085	U1025	U961	C898	G819	C751	U678	G604	G538	G467	A394	A328	G255	C177
C1152	U1086	G1026	C962	C899	U820	C752	C679	U605	A539	A468	C395	A329	U256	C178
G1153	G1087	C1027	G963	A900	G821	G755	G683	G606	A540	G474	G396	G330	G257	U182
U1154	U1088	U1028	A964	G901	C822	C756	A684	A607	G541	G475	A397	G331	G258	G184
G1155	G1089	C1029	A965	G902	G823	U757	G685	G612	C543	G477	C401	G332	U261	C186
C1156	U1090	C1030	G966	G903	C824	G758	G686	C613	G544	G481	G402	G333	A262	C186A
A1157	G1091	G1031	C967	C904	G825	A759	U687	C614	C545	A482	C403	G337	U263	C186B
U1158	U1092	U1032	A968	U905	G826	G760	A687	C615	G546	A483	U404	A338	G265	G186C
C1159	G1093	G1033	A969	G906	U827	G761	G688	C616	A547	G484	U405	C339	G266	G186D
G1160	U1094	G1034	G970	U907	A828	C762	C689	G617	C548	G485	G406	C341	G267	C186E
C1161	G1095	U1035	G971	C907	G831	A766	G691	C620	C553	A487	A403	C342	C268	C186F
U1162	U1096	G1036	C972	A908	G832	C767	U692	A621	A553	A488	G409	C345	C269	C187
C1163	G1097	U1037	G973	U909	G833	C768	G693	A622	C554	C489	G410	G346	A270	U189
G1164	U1098	G1038	C974	G910	U834	C769	A694	G623	C555	G490	A411	G347	G275	G190
U1165	G1099	C1039	A975	C911	U835	C770	U697	G624	C556	G491	A412	G348	A274	U191D
C1166	U1100	U1040	A976	C912	U836	C771	A695	G625	C557	G492	G413	G349	G276	G191E
G1167	A1101	G1041	C977	C913	G837	C772	G701	U626	G558	G493	A414	G350	C277	U191F
U1168	U1102	U1042	A978	U911	U838	C773	U692	U627	G559	U494	C418	G351	G278	G191G
C1169	G1103	G1043	G979	U912	U839	C774	A702	G628	A560	A495	C419	G352	A279	G191H
U1170	U1104	A1044	A980	U913	C840	C775	A706	G629	U561	A496	U420	G353	C280	G191I
G1171	G1105	G1045	G981	U914	U841	C776	A707	G630	C562	U497	U421	G354	G281	A195
C1172	U1106	U1046	G982	U915	U842	C777	A708	G631	A563	A498	U422	G355	G282	A196
U1173	G1107	A1047	U983	C914	C841	C778	A709	G632	C564	G500	C422	U359	G283	A197
G1174	U1108	C1048	U984	U916	U843	C779	G710	G633	U565	C501	G423	A360	G284	A198
C1175	G1109	A1049	A985	U917	U844	C780	G711	G634	U566	C502	G424	A361	G285	A199
U1176	U1110	G1050	U986	U918	U845	C781	G712	G635	G567	C503	G425	U362	G286	G199
G1177	A1111	A1051	C986	U919	U846	C782	G713	A640	G568	C504	G426	A363	A288	G200
C1178	C1112	G1052	G987	U920	U847	C783	G714	U641	G569					
U1179	U1113	U1053	G988	U921	U848	C784	G715	A642						
A1180	G1117	G1054	G989	U922	U849	C785	G716							
G1181	C1118	C1055	G990	U923	U850	C786	A716							
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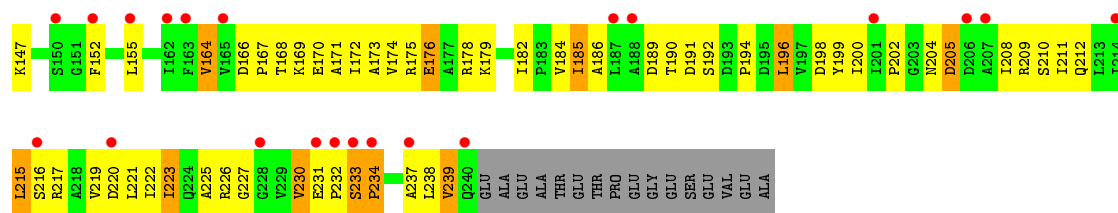


• Molecule 2: 30S ribosomal protein S2

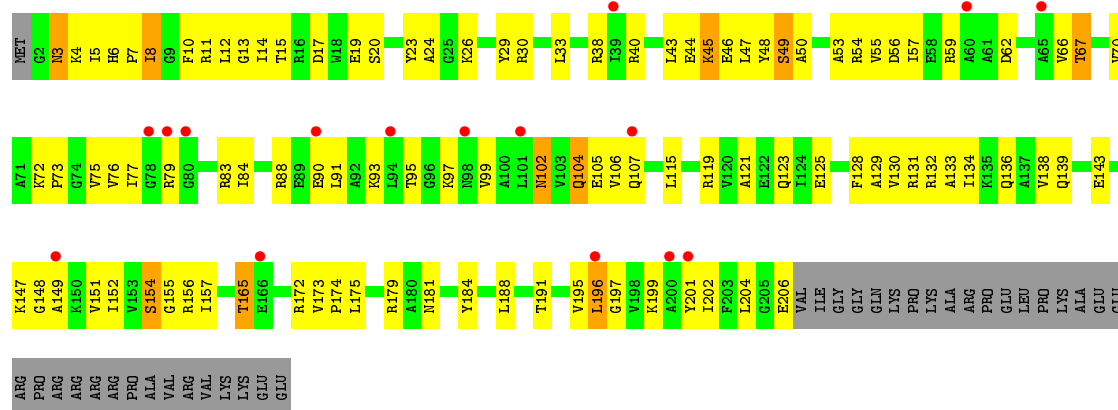
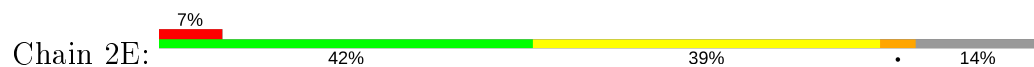


• Molecule 2: 30S ribosomal protein S2

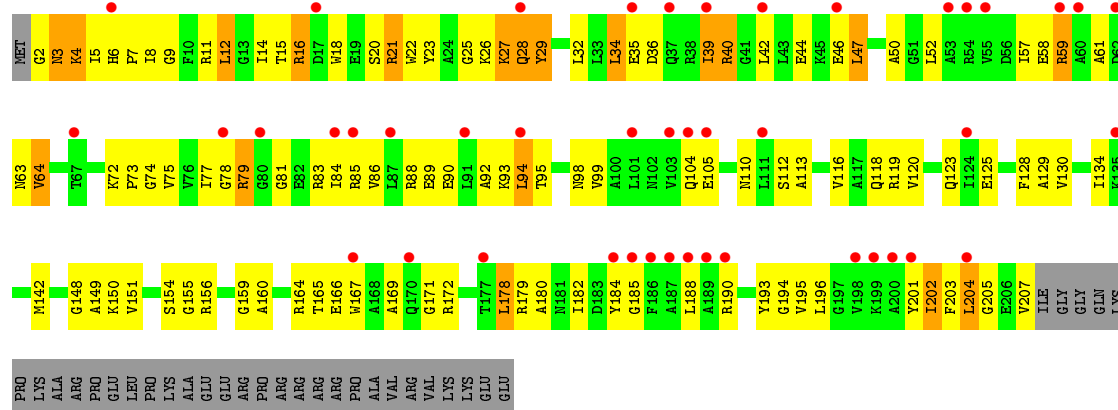




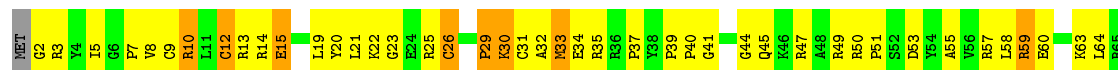
• Molecule 3: 30S ribosomal protein S3

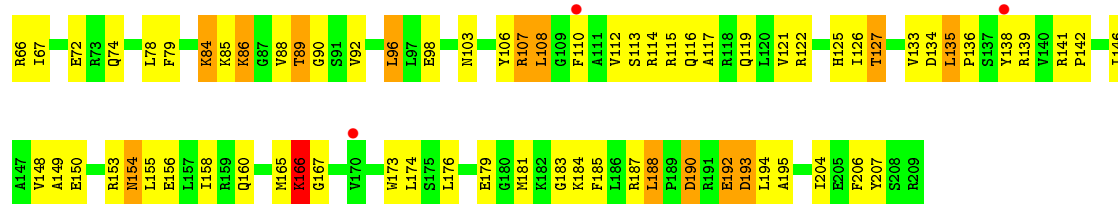


• Molecule 3: 30S ribosomal protein S3

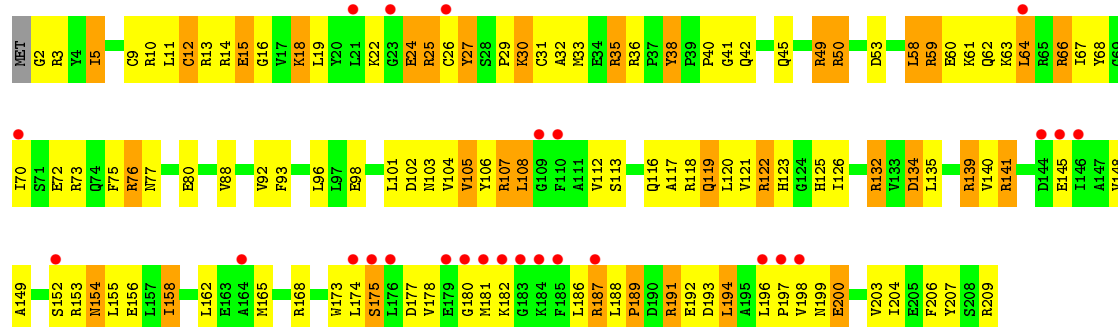
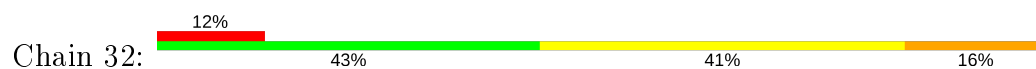


• Molecule 4: 30S ribosomal protein S4

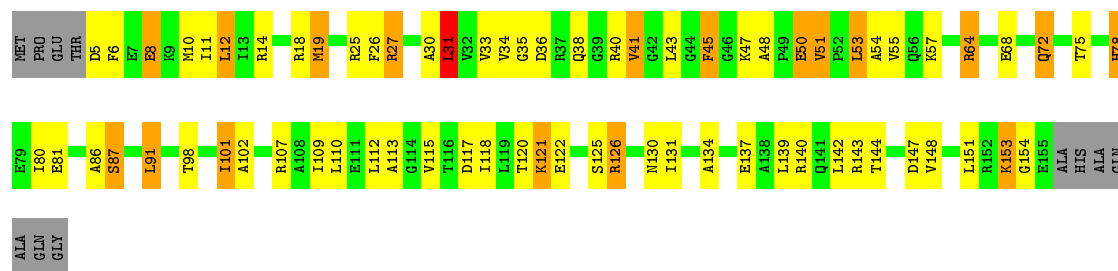




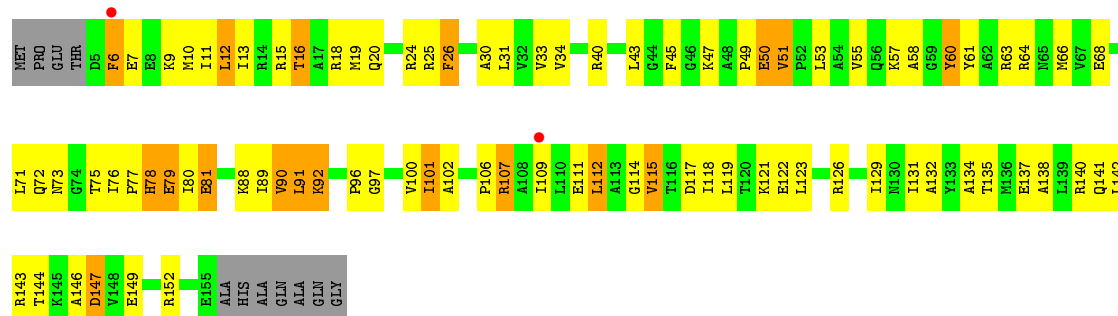
• Molecule 4: 30S ribosomal protein S4



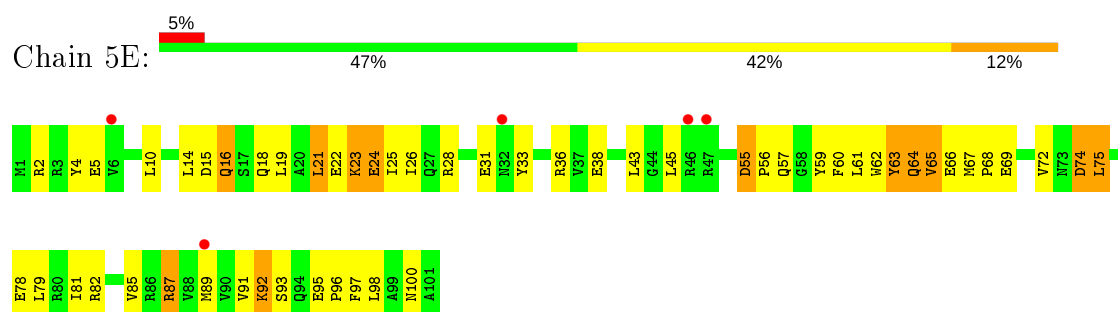
• Molecule 5: 30S ribosomal protein S5



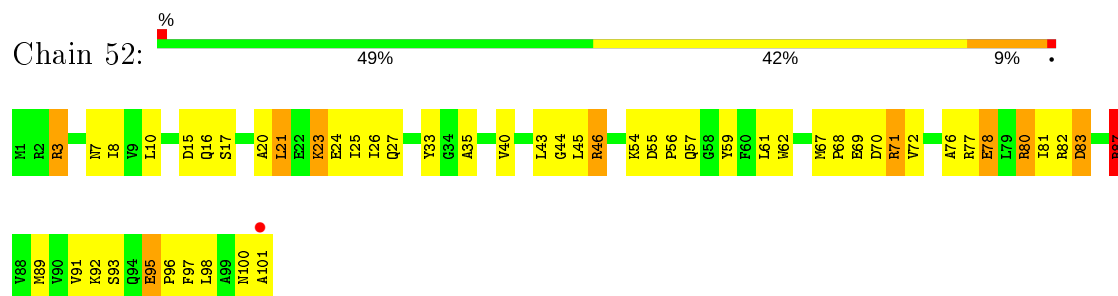
• Molecule 5: 30S ribosomal protein S5



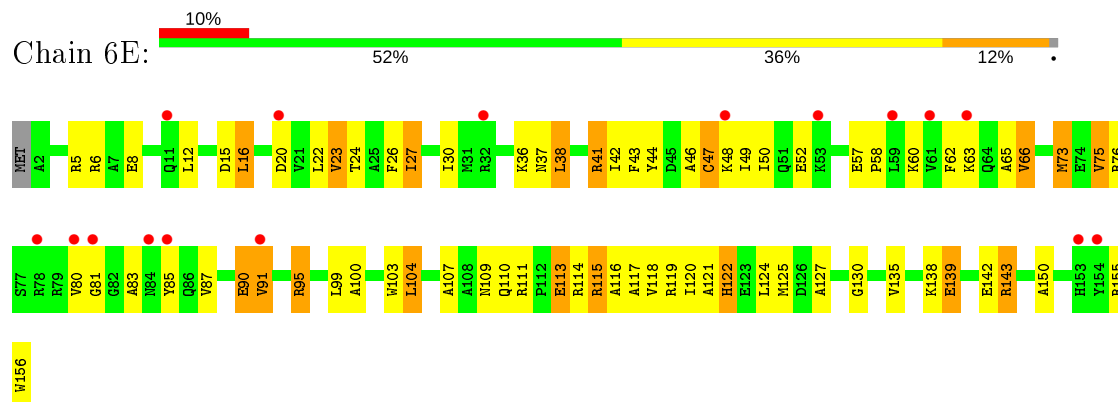
• Molecule 6: 30S ribosomal protein S6



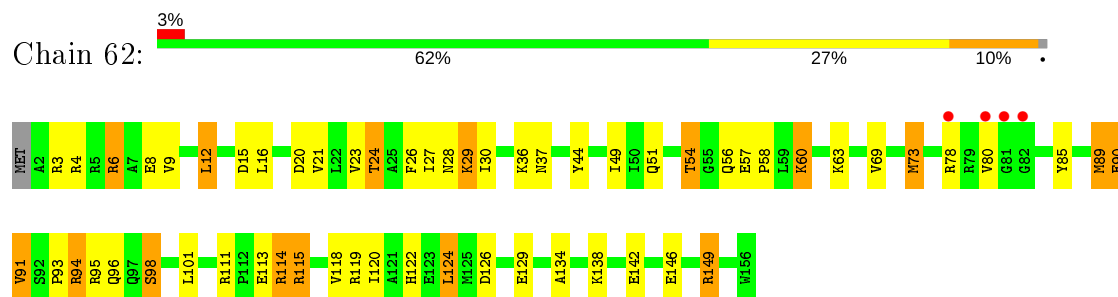
- Molecule 6: 30S ribosomal protein S6



- Molecule 7: 30S ribosomal protein S7

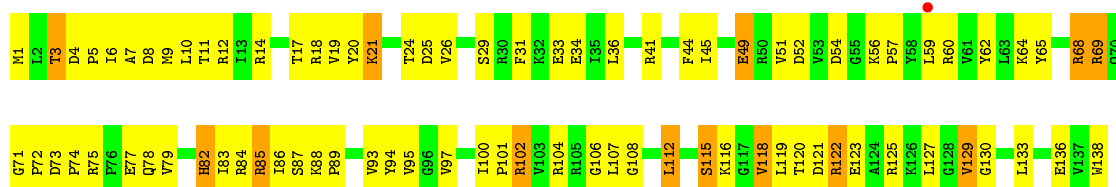


- Molecule 7: 30S ribosomal protein S7

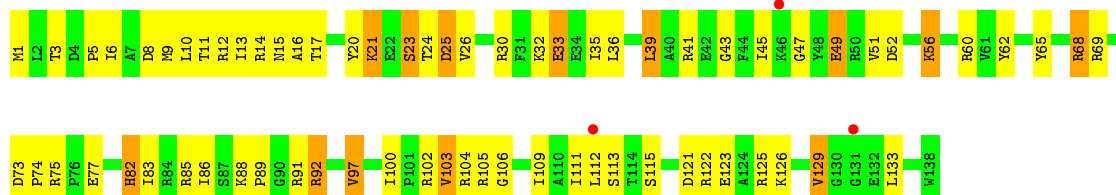


- Molecule 8: 30S ribosomal protein S8

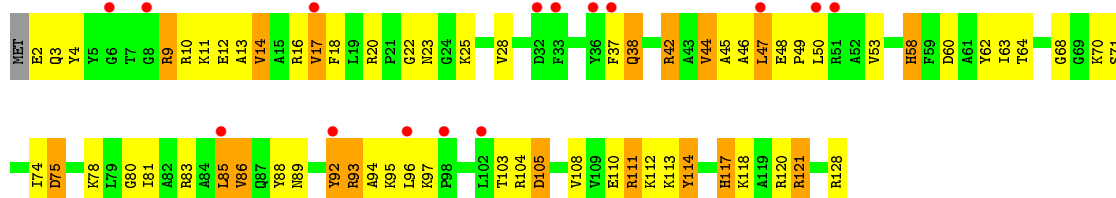




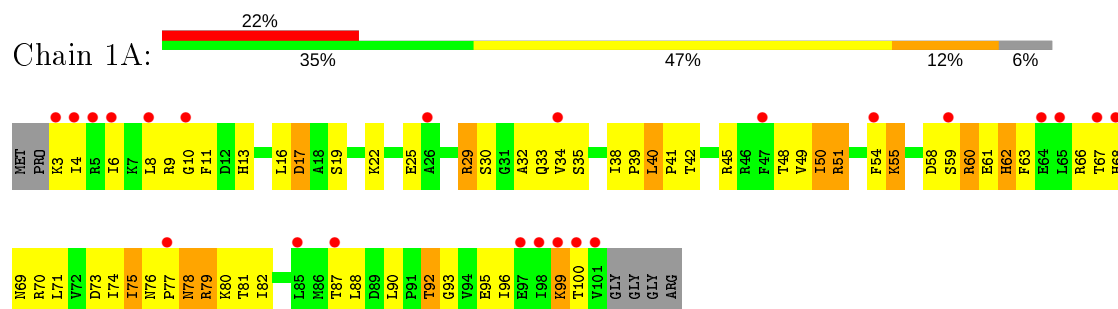
• Molecule 8: 30S ribosomal protein S8



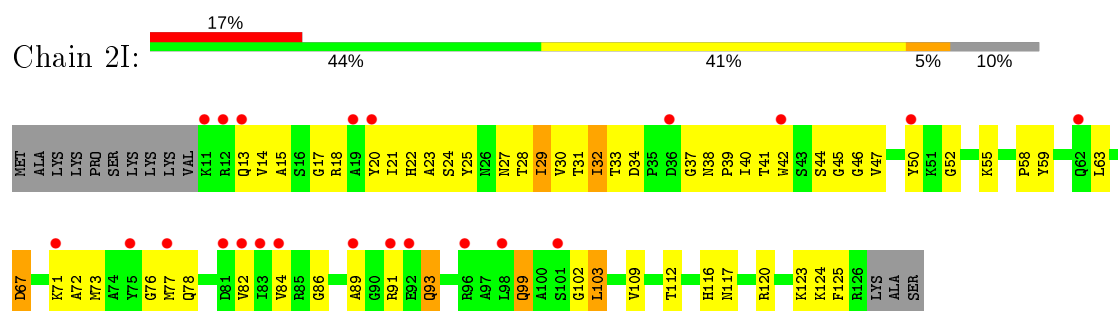
• Molecule 9: 30S ribosomal protein S9



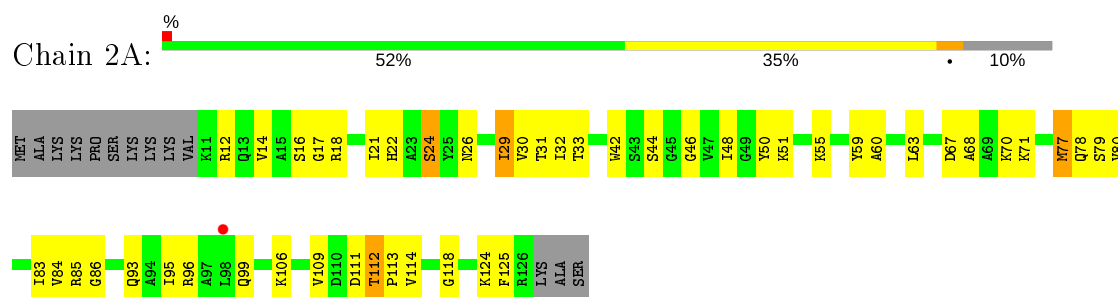
- Molecule 10: 30S ribosomal protein S10



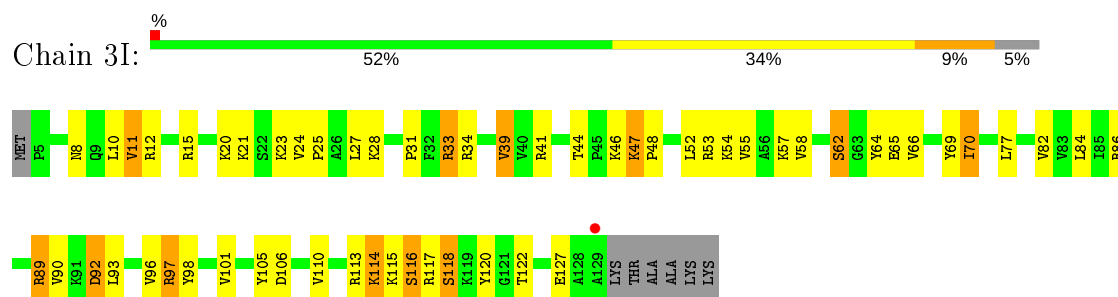
- Molecule 11: 30S ribosomal protein S11



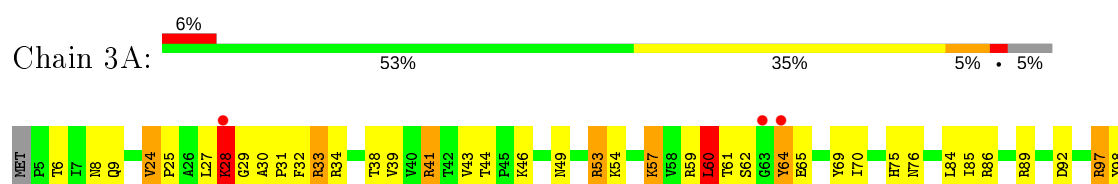
- Molecule 11: 30S ribosomal protein S11



- Molecule 12: 30S ribosomal protein S12

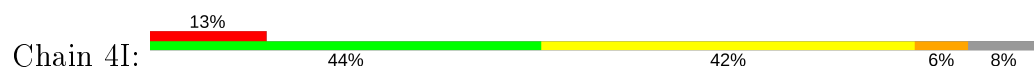


- Molecule 12: 30S ribosomal protein S12

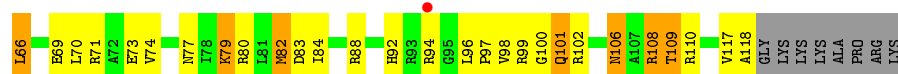
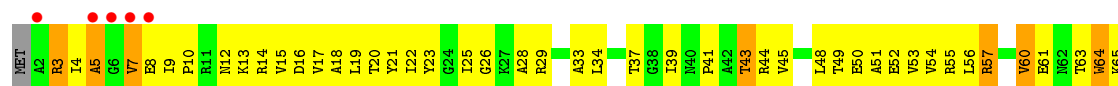




- Molecule 13: 30S ribosomal protein S13



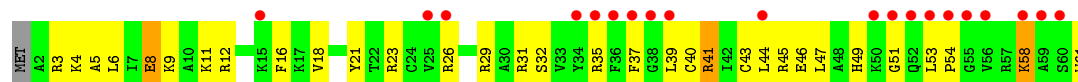
- Molecule 13: 30S ribosomal protein S13



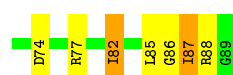
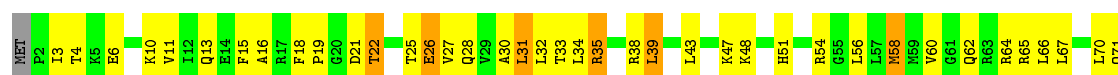
- Molecule 14: 30S ribosomal protein S14 type Z



- Molecule 14: 30S ribosomal protein S14 type Z



- Molecule 15: 30S ribosomal protein S15



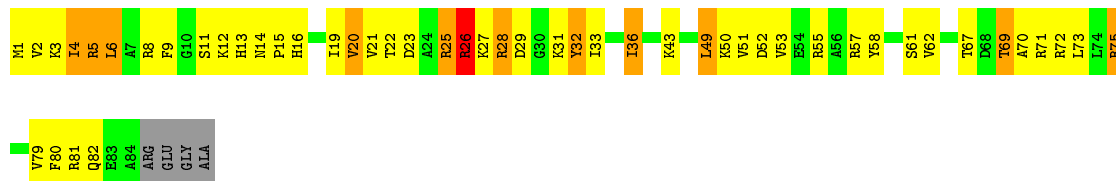
- Molecule 15: 30S ribosomal protein S15

Chain 6A: 



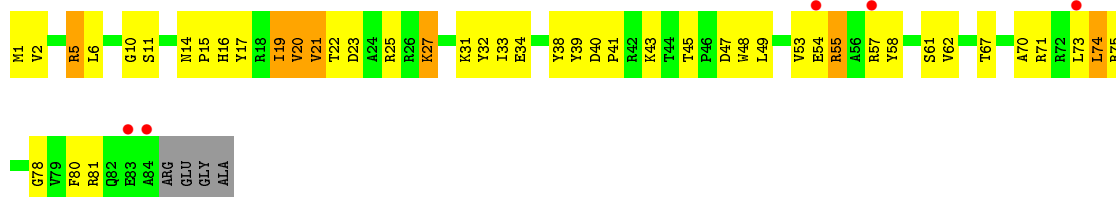
- Molecule 16: 30S ribosomal protein S16

Chain 7I: 



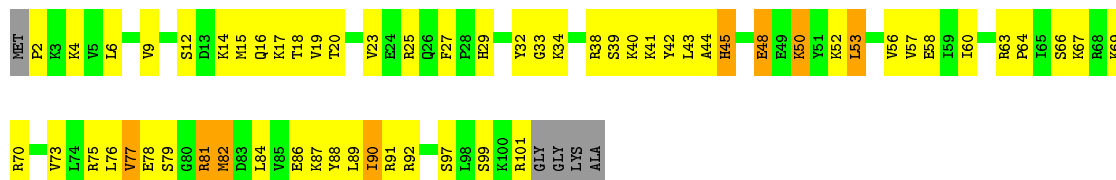
- Molecule 16: 30S ribosomal protein S16

Chain 7A: 



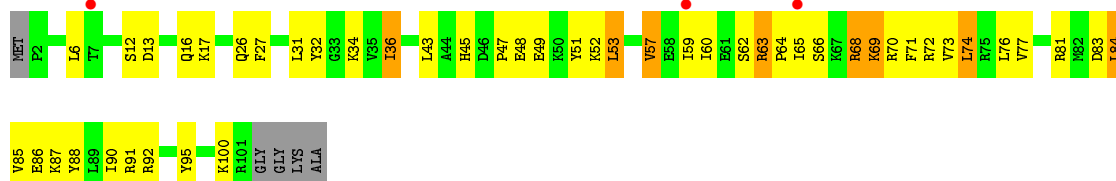
- Molecule 17: 30S ribosomal protein S17

Chain 8I: 

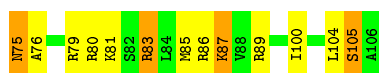


- Molecule 17: 30S ribosomal protein S17

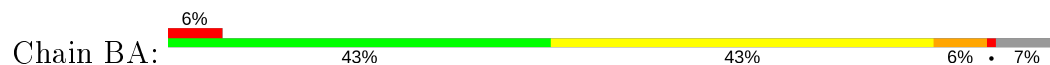
Chain 8A: 



- Molecule 18: 30S ribosomal protein S18



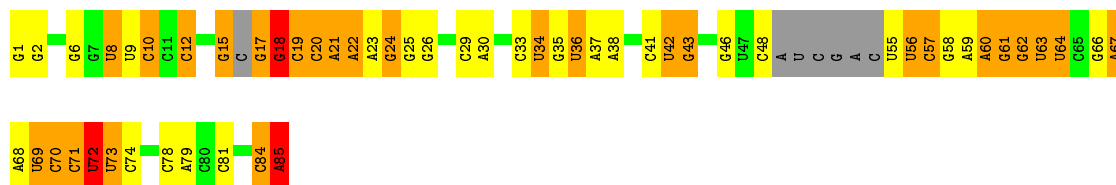
- Molecule 20: 30S ribosomal protein S20



- Molecule 21: 30S ribosomal protein Thx

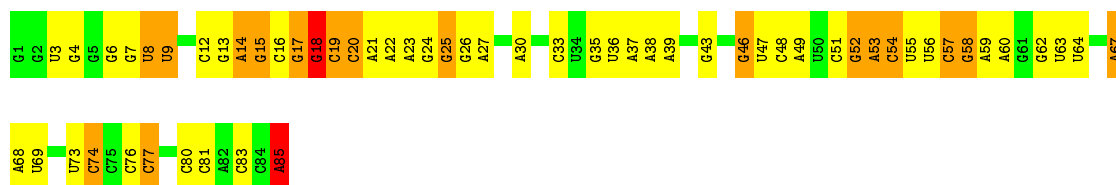


Chain 2L: 27% 29% 32% 8%



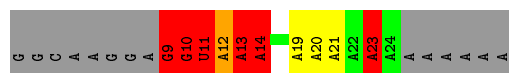
• Molecule 22: tRNA-Tyr

Chain 3L: 32% 46% 20%



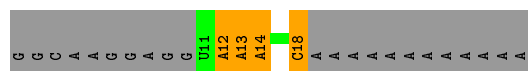
• Molecule 23: mRNA

Chain 4K: 20% 10% 20% 47%



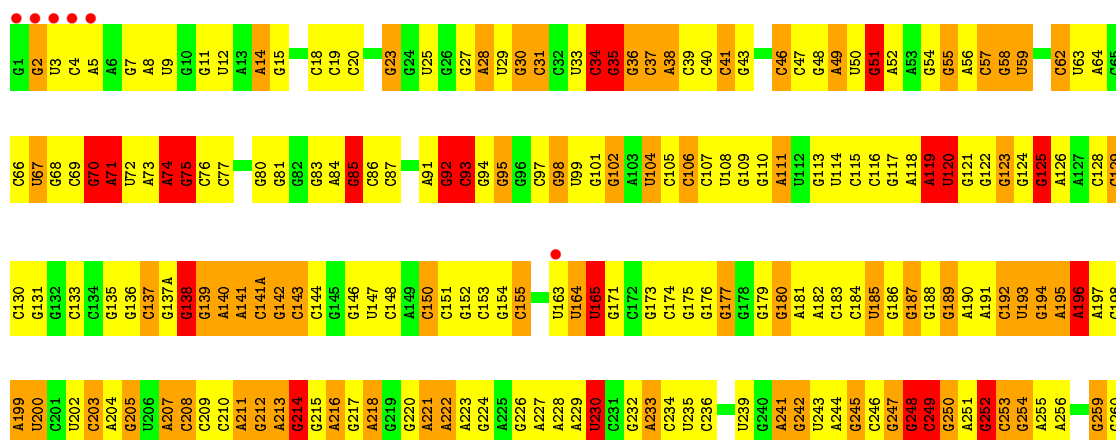
• Molecule 23: mRNA

Chain 4L: 13% 13% 73%



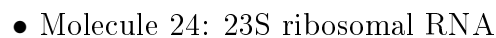
• Molecule 24: 23S ribosomal RNA

Chain 1H: 21% 42% 29% 7%





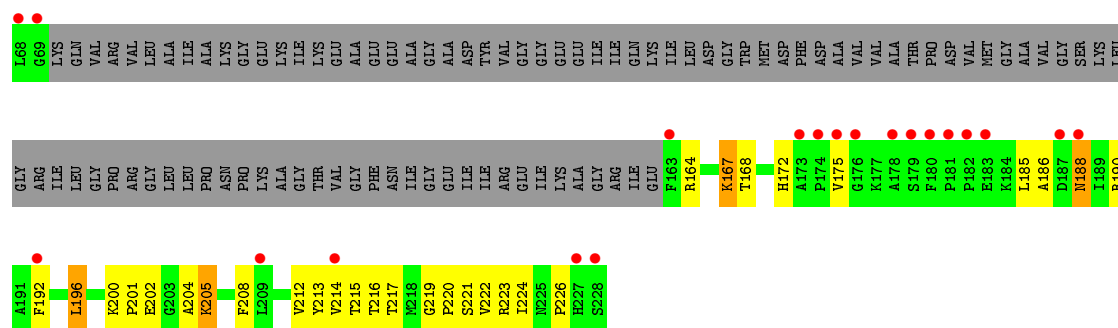
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C2058	G1186	G1246	G1310	C1375	G1436	C1506	A1570	G1637	G1696	G1788	A1853	A1937	G1998	C2058
A2059	G1187	U1249	G1311	G1376	C1437	A1507	A1571	A1638	A1698	A1789	G1854	A1938	A1999	A2059
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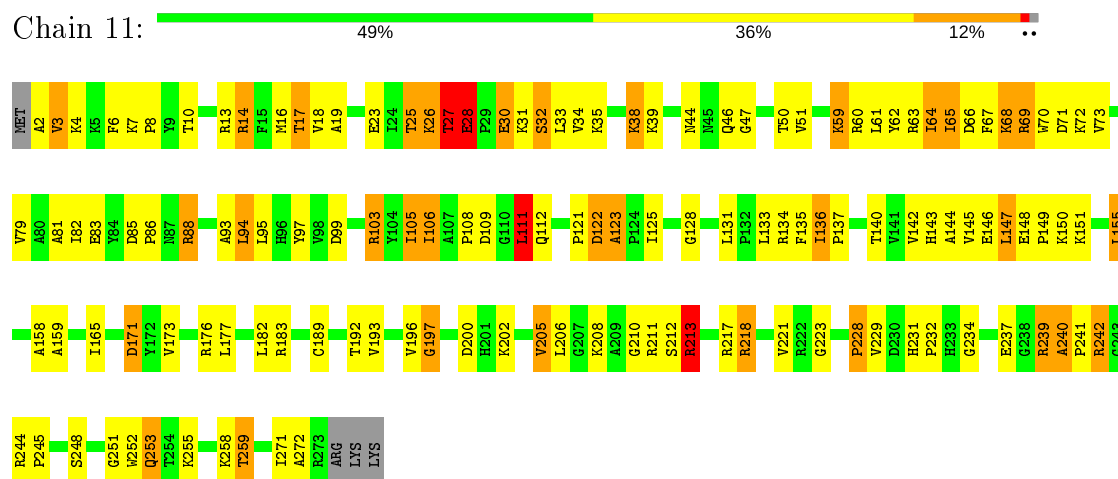




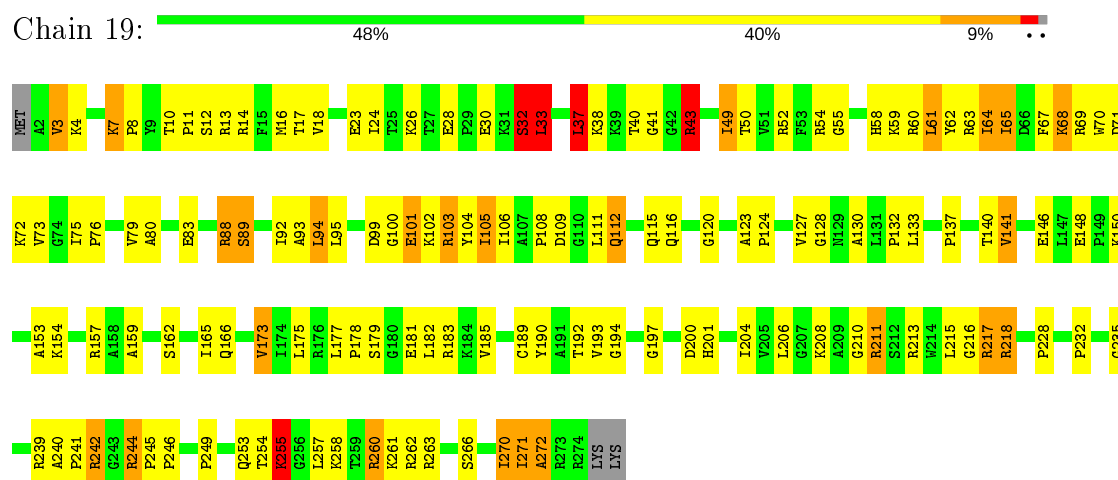
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	G2777	C2708	G2638	G2443	G2379	G2251	C2178	G2115	G2052	
G2845	G2778	C2709	G2639	G2444	C2380	G2252	C2179	G2116	G2053	G1984
G2846	U2779	C2710	G2640	G2445		G2253	C2180	G2117	G1985	
U2847	U2780	G2711		G2446	G2383	G2254	U2181	G2118	C2055	C1988
G2848	A2781	U2712	G2643	G2447	G2384	G2255	A2182	G2119	G2056	G1989
G2849	G2782	A2712A	G2644	A2448	C2385	G2256	G2183	G2120	A2057	C1990
U2850	G2783		G2645	U2449	C2386	U2257	C2184	G2121	A2058	U1991
U2851	C2784	C2715	C2646	A2450	G2387	G2258	G2185	G2122	A2059	G1992
G2852	C2785	G2716	U2647	G2451	C2388	G2259	C2186	G2123	A2060	U1993
G2853	U2786	G2717	U2648	C2452	G2389	G2260	G2187	G2124	G2061	C1994
G2854	C2787	G2718	U2649		U2390	G2261	C2188	G2125	A2062	U1995
	C2788	G2719	U2650	G2455	G2391	U2262	C2189	G2126	G2063	C1996
G2857	G2789	U2720	C2651	U2456	A2392	G2263	G2190	G2127	C2064	
G2858	A2790	A2721	C2652	U2457	C2393	C2264	C2191	G2128	C2065	C1999
G2859	C2791	G2722	U2653	G2458	C2394		G2192	C2129	C2066	G2000
A2860	G2792	C2723	G2654	U2460	C2395	A2267	G2193	U2130	G2067	A2001
G2861	G2793	C2724	G2655	G2461	G2396	A2268		G2131	U2068	G2002
G2862	C2794	A2725	U2656	U2462	G2400	A2269	A2198	G2132	G2069	C2006
C2863	G2795	U2726	A2657	C2463	U2401	G2270	A2199	G2133	A2071	
G2864	U2797		G2658		C2402	G2271	C2205	G2134	G2072	G2009
U2865	C2798	G2729	G2659	G2467	C2403	A2272	C2206	G2135	G2073	C2010
G2866	A2799	C2730	U2660	A2468	C2404	A2273	C2207	G2136	U2011	U2010
G2867	G2801	G2731	G2661	A2469	G2405	A2274		G2137	U2074	G2012
A2868	G2802	G2732	A2662	G2470	U2406	G2275		G2140	U2075	G2013
G2869	C2803	A2733	G2663	U2471	G2407	G2276		G2141	A2013	
C2870	G2804		G2664	U2472	U2408	A2277		G2142	A2014	A2015
G2871	G2805	A2741	A2665	C2473	U2409	A2278		G2143	U2016	U2017
G2872	C2807	C2742		C2474	G2410	G2279		G2144	G2080	U2017
A2873	U2808		G2669	A2475		G2280		G2145	G2081	G2018
C2874	A2809	C2743		U2476		G2281		G2146	G2082	
G2875	G2810	C2744	G2673	G2477		G2282		G2147	A2083	A2019
G2876	G2811	U2745	G2674	C2478		C2283			C2084	G2023
	G2812	U2746		C2479		G2284			C2085	G2024
	A2813	G2747	A2679	G2480		G2285			U2086	G2025
C2879	G2814	U2748	C2680	G2481		A2287			G2087	C2026
C2880	C2815	A2749	C2681	U2485		A2288				G2027
A2882	C2816	G2749	U2682	G2486		G2289			G2090	U2028
A2883	G2817	A2750	G2683	G2487		G2290			U2091	U2029
U2884	G2818	C2752	U2684	A2488	G2421	G2291			U2092	A2030
C2885	G2819	G2753	G2685	G2489	U2423	U2292			G2093	A2031
G2886	A2820	U2754	U2686	G2490	G2424	G2293				G2032
U2887	G2821	C2755	U2688	U2491	A2425	C2294			U2096	A2033
C2888	A2822	U2756	U2689	U2492	A2426	G2295			C2097	U2034
C2889	U2823	G2757	C2690	G2493	C2427	U2296			U2098	U2035
G2891	C2824			U2494	G2428	G2297			U2099	C2036
A2892	G2761		A2693	G2495	G2429	A2298			G2100	G2037
G2893	G2762		G2694	C2496	A2430				G2101	G2038
G2894	G2763		C2695	A2497	C2431	G2303			U2102	C2039
U2895	C2829	A2764		C2498	U2432	G2304			G2103	U2040
G2896	G2830	A2765	U2698	U2499	G2365	A2305			C2104	
U2897	G2831	G2766	C2699	U2500	A2366	C2306			G2168	



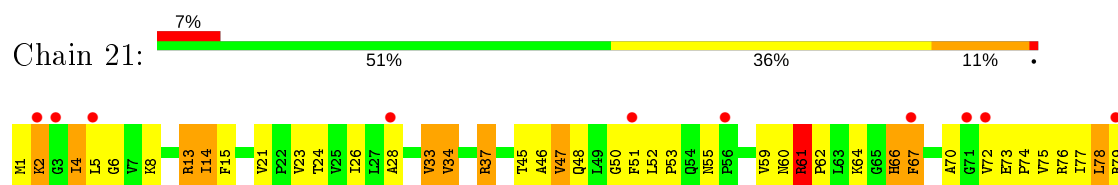
• Molecule 27: 50S ribosomal protein L2

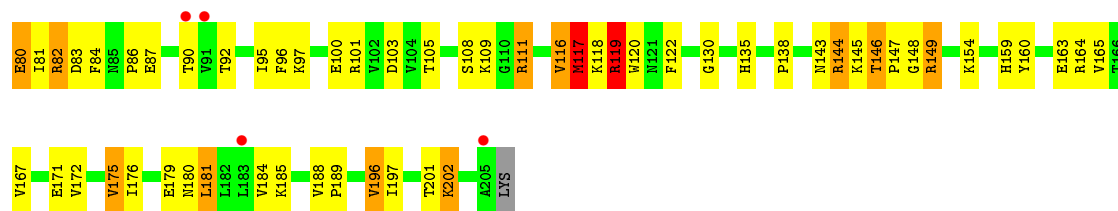


• Molecule 27: 50S ribosomal protein L2

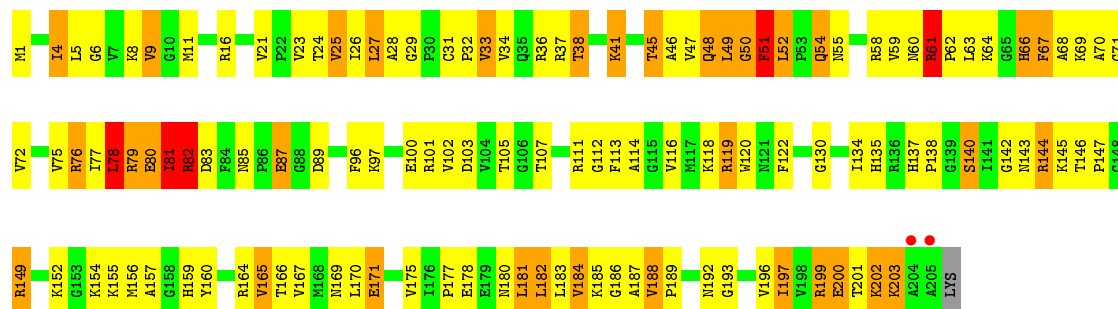


• Molecule 28: 50S ribosomal protein L3

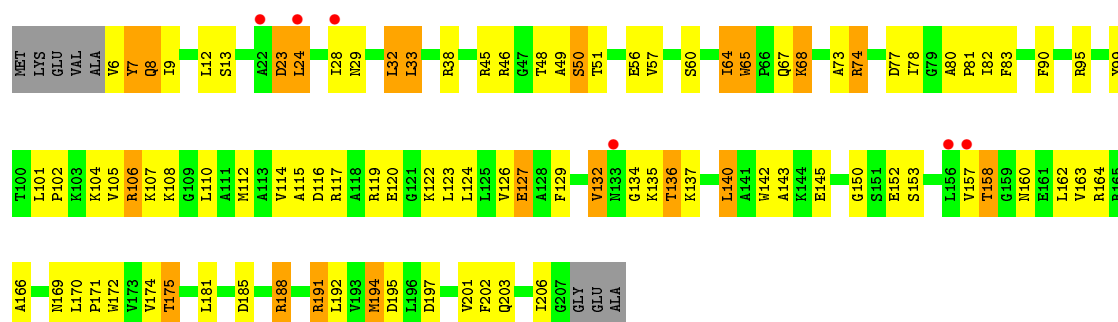




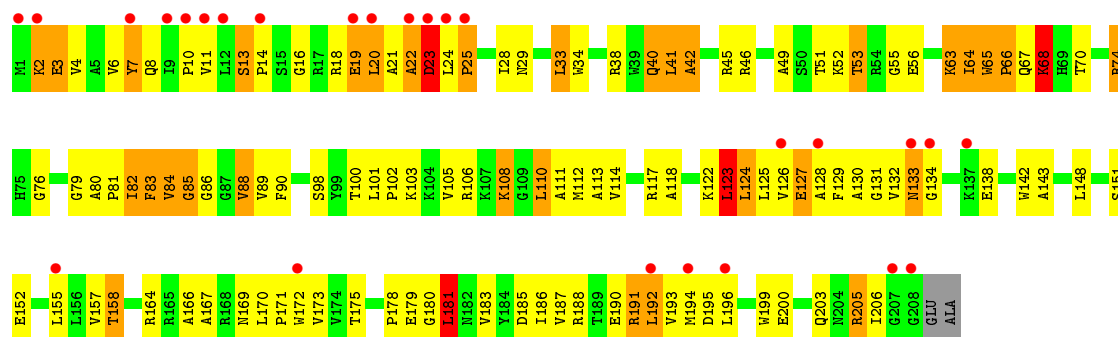
• Molecule 28: 50S ribosomal protein L3



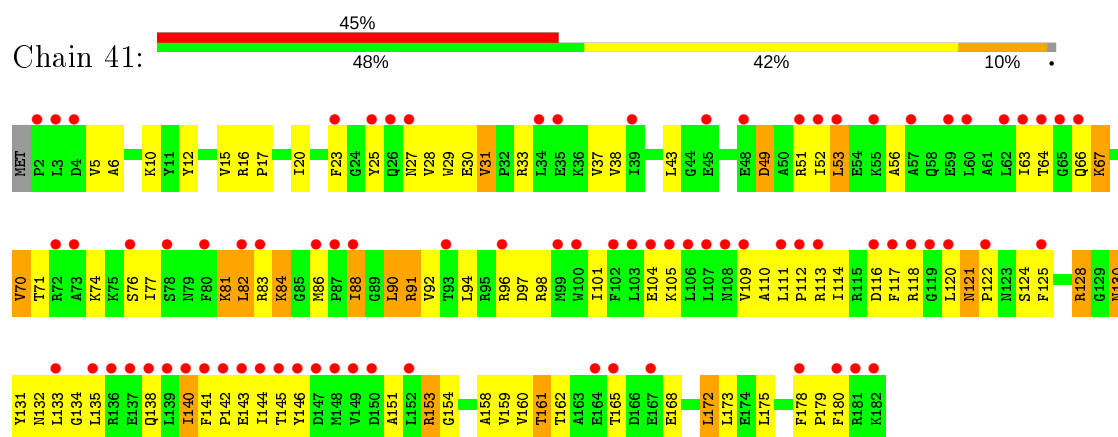
• Molecule 29: 50S ribosomal protein L4



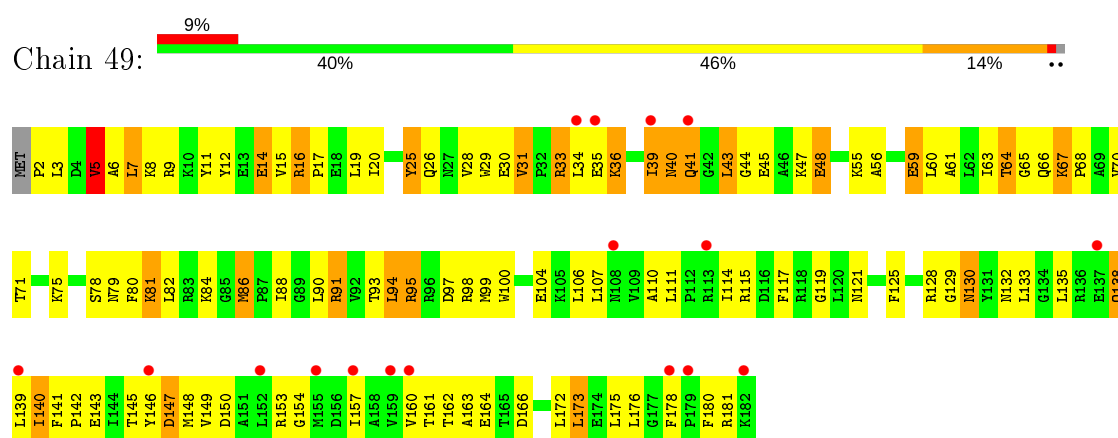
• Molecule 29: 50S ribosomal protein L4



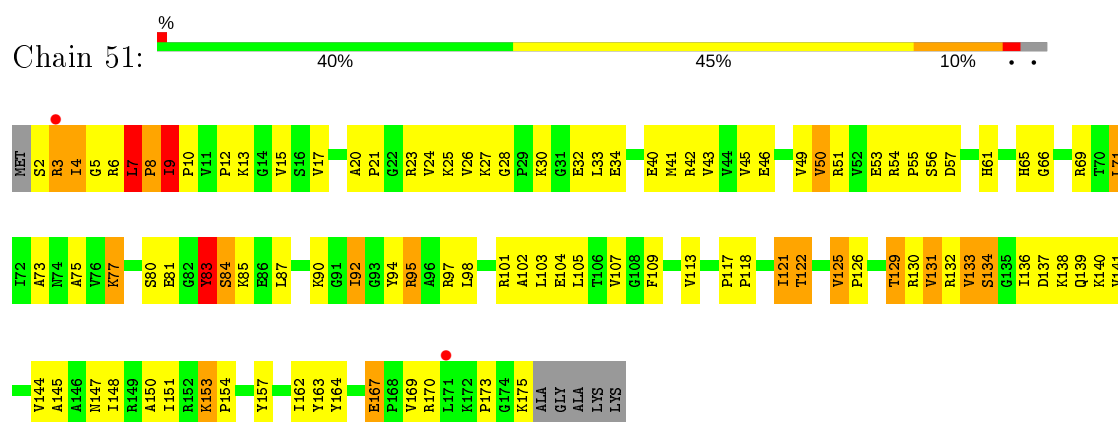
• Molecule 30: 50S ribosomal protein L5



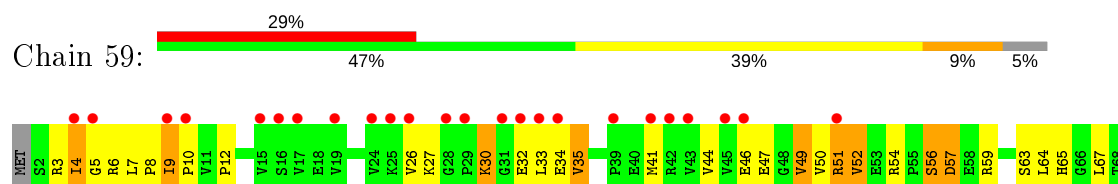
• Molecule 30: 50S ribosomal protein L5

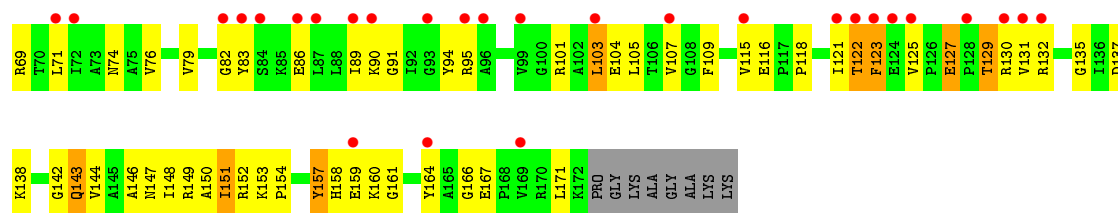


• Molecule 31: 50S ribosomal protein L6

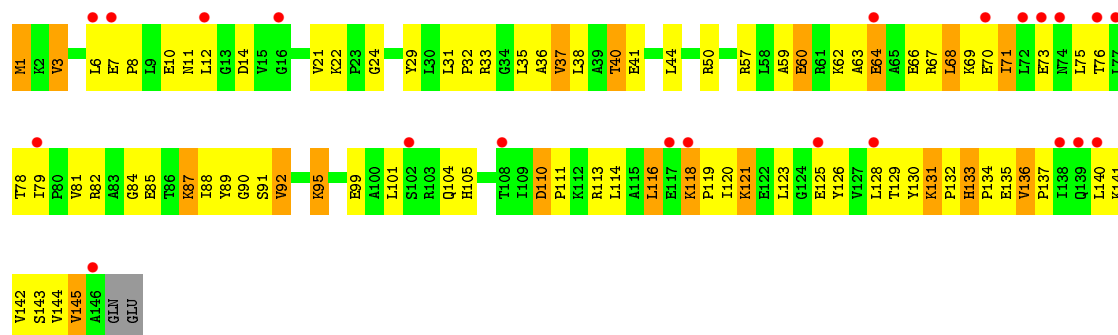
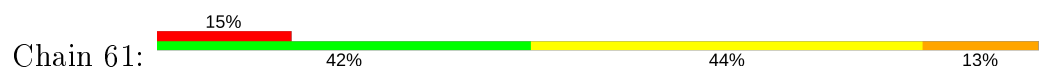


• Molecule 31: 50S ribosomal protein L6

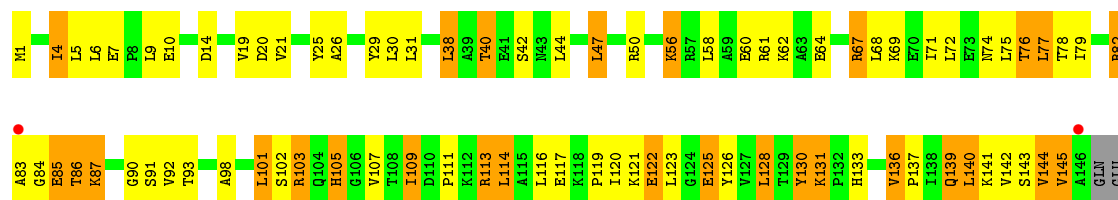
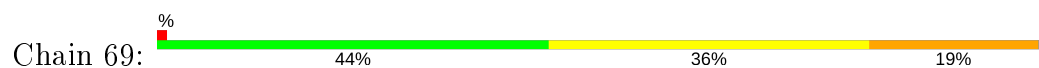




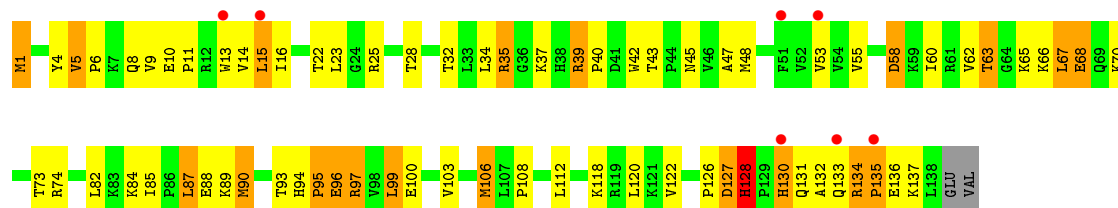
• Molecule 32: 50S ribosomal protein L9



• Molecule 32: 50S ribosomal protein L9



• Molecule 33: 50S ribosomal protein L13



• Molecule 33: 50S ribosomal protein L13





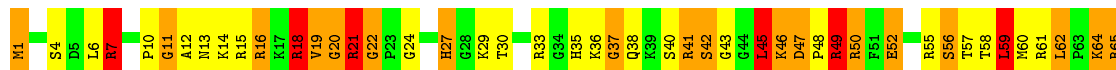
- Molecule 34: 50S ribosomal protein L14



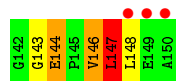
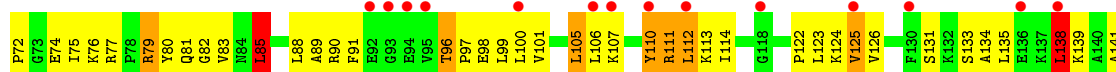
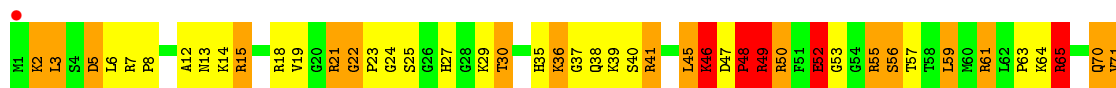
- Molecule 34: 50S ribosomal protein L14



- Molecule 35: 50S ribosomal protein L15

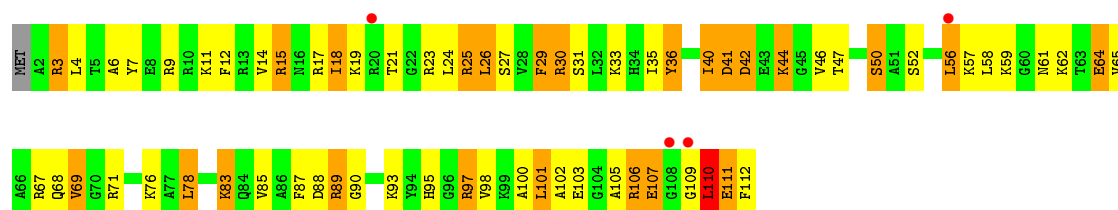


- Molecule 35: 50S ribosomal protein L15

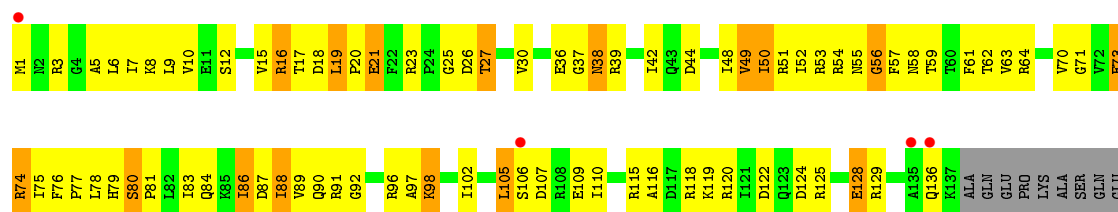


- Molecule 36: 50S ribosomal protein L16

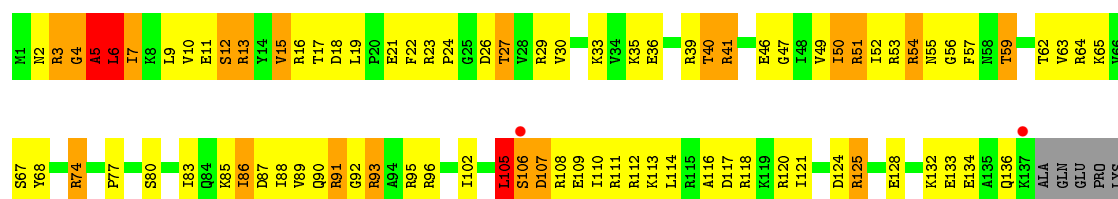
- Molecule 38: 50S ribosomal protein L18



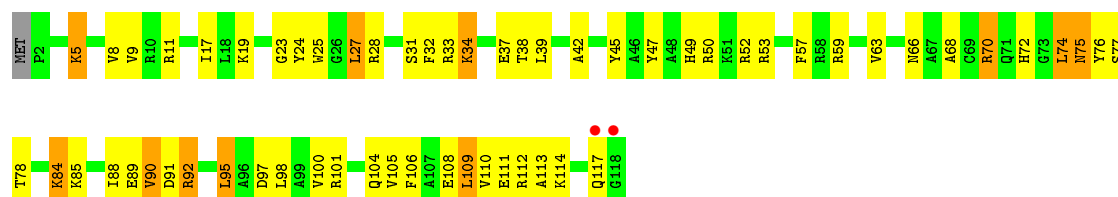
- Molecule 39: 50S ribosomal protein L19



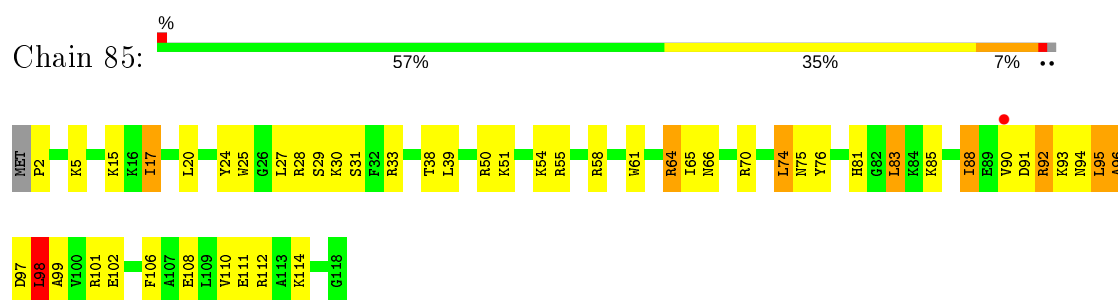
- Molecule 39: 50S ribosomal protein L19



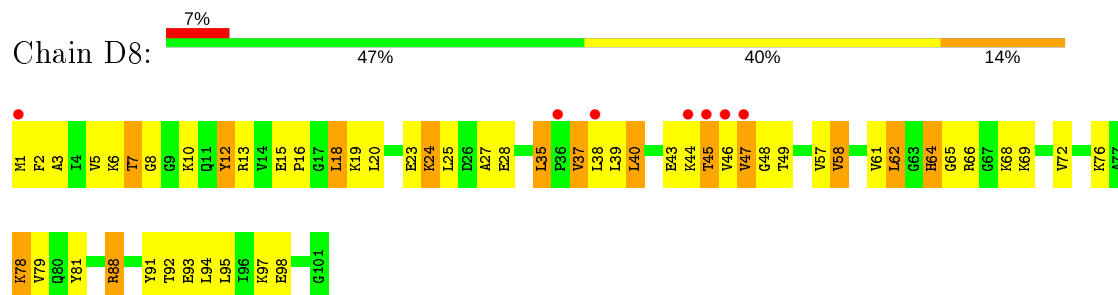
- Molecule 40: 50S ribosomal protein L20



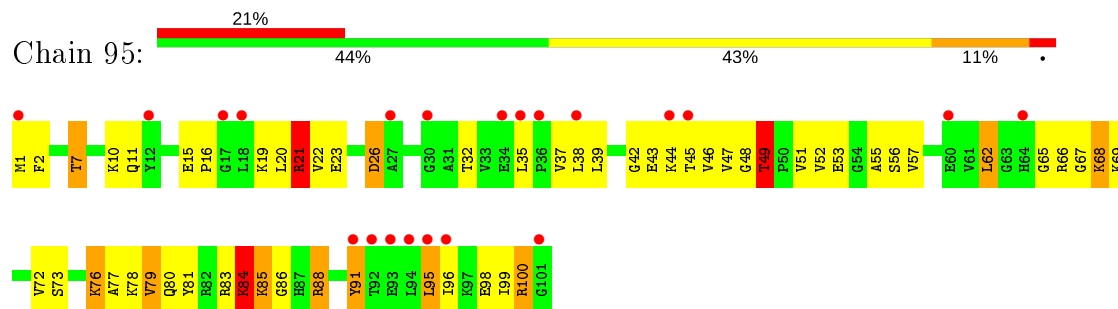
- Molecule 40: 50S ribosomal protein L20



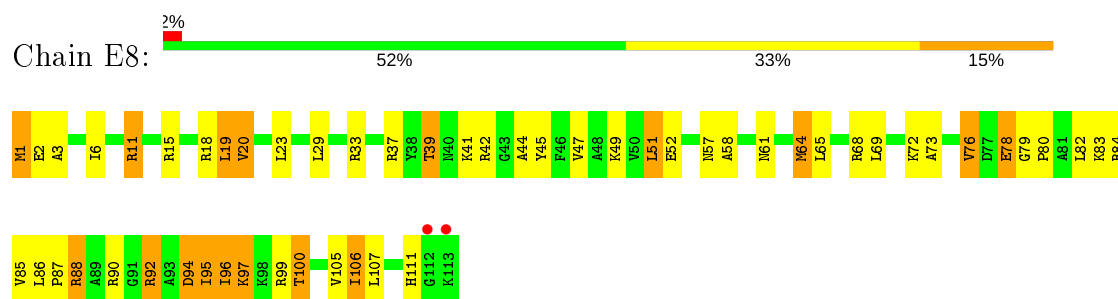
• Molecule 41: 50S ribosomal protein L21



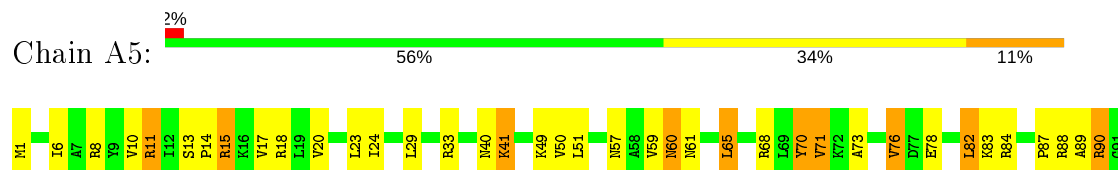
• Molecule 41: 50S ribosomal protein L21



• Molecule 42: 50S ribosomal protein L22



• Molecule 42: 50S ribosomal protein L22





- Molecule 43: 50S ribosomal protein L23



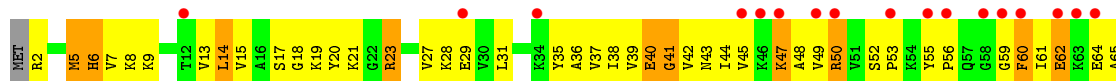
- Molecule 43: 50S ribosomal protein L23



- Molecule 44: 50S ribosomal protein L24

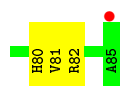


- Molecule 44: 50S ribosomal protein L24

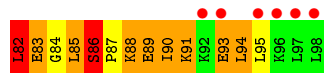
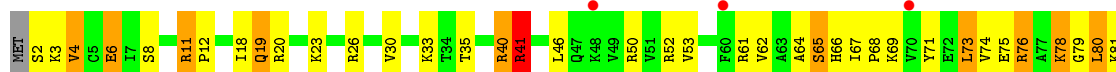


- Molecule 45: 50S ribosomal protein L25

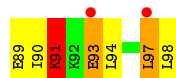
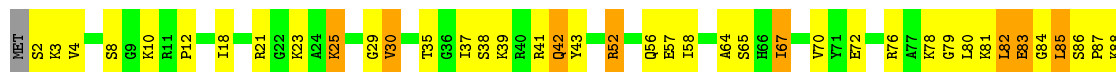




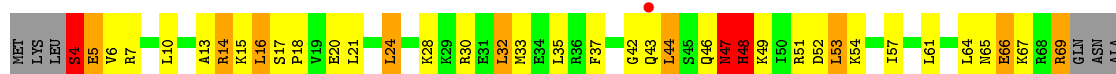
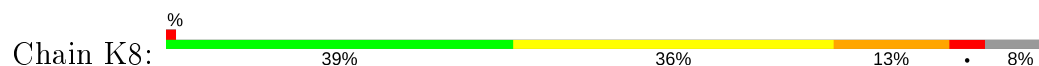
- Molecule 47: 50S ribosomal protein L28



- Molecule 47: 50S ribosomal protein L28



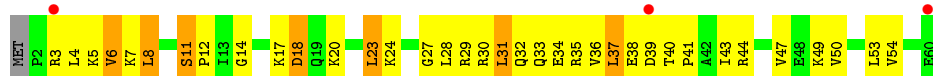
- Molecule 48: 50S ribosomal protein L29



- Molecule 48: 50S ribosomal protein L29

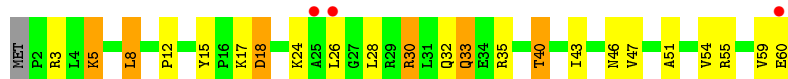


- Molecule 49: 50S ribosomal protein L30

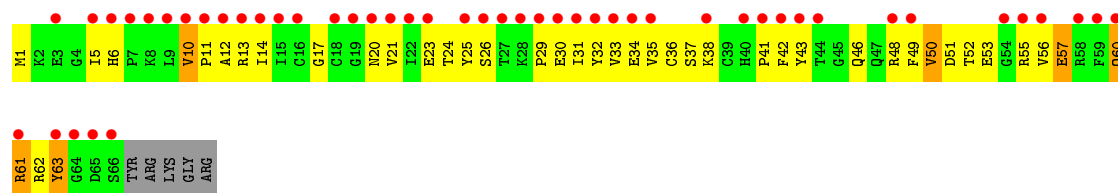


- Molecule 49: 50S ribosomal protein L30

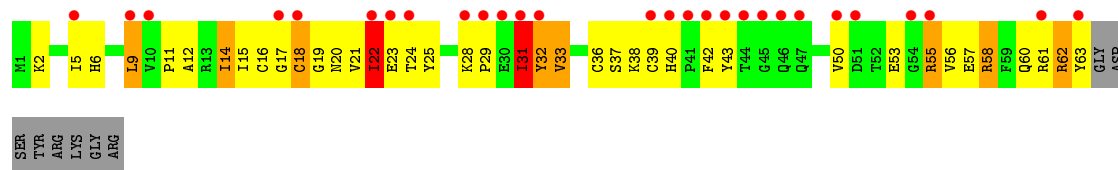




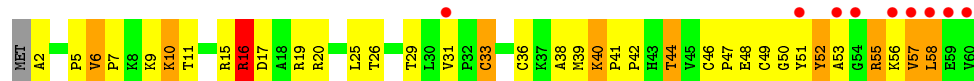
- Molecule 50: 50S ribosomal protein L31



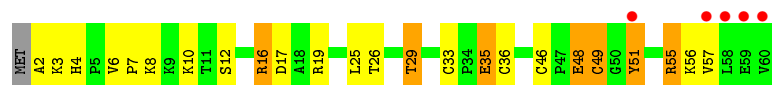
- Molecule 50: 50S ribosomal protein L31



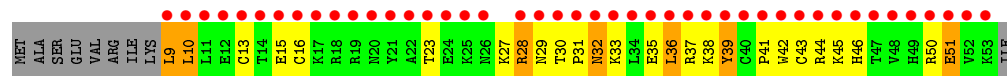
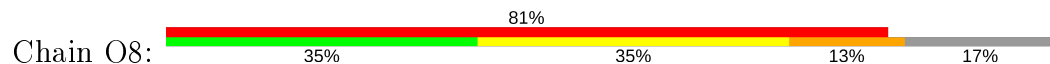
- Molecule 51: 50S ribosomal protein L32



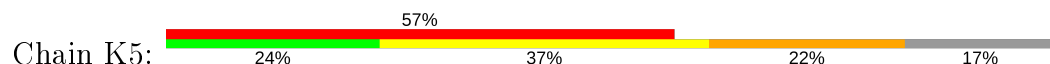
- Molecule 51: 50S ribosomal protein L32

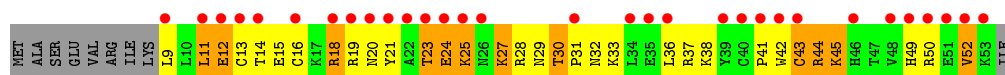


- Molecule 52: 50S ribosomal protein L33



- Molecule 52: 50S ribosomal protein L33

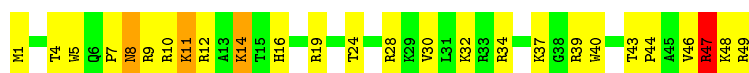




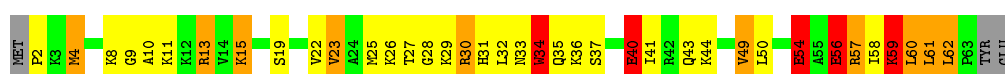
- Molecule 53: 50S ribosomal protein L34



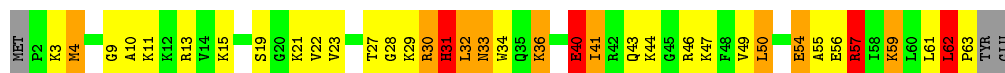
- Molecule 53: 50S ribosomal protein L34



- 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	210.70 Å 448.40 Å 616.30 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	153.54 – 3.10 253.96 – 3.10	Depositor EDS
% Data completeness (in resolution range)	99.8 (153.54-3.10) 91.1 (253.96-3.10)	Depositor EDS
R_{merge}	0.22	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.83 (at 3.07 Å)	Xtriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.227 , 0.193 0.193 , 0.229	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 , 81.2	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	0.94	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: 5MU, ZN, OMG, MIA, MG, 4SU, QUO, PSU

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	13	0.81	9/36199 (0.0%)	1.50	567/56498 (1.0%)
1	1G	0.81	7/36167 (0.0%)	1.49	517/56448 (0.9%)
2	12	0.39	0/1959	0.65	0/2642
2	1E	0.43	0/1959	0.67	1/2642 (0.0%)
3	22	0.47	0/1636	0.68	0/2205
3	2E	0.47	0/1629	0.63	0/2195
4	32	0.57	0/1732	0.80	1/2318 (0.0%)
4	3E	0.65	2/1732 (0.1%)	0.78	4/2318 (0.2%)
5	42	0.60	0/1171	0.78	0/1576
5	4E	0.59	0/1171	0.77	1/1576 (0.1%)
6	52	0.61	0/855	0.76	2/1154 (0.2%)
6	5E	0.57	0/855	0.72	0/1154
7	62	0.48	0/1275	0.65	0/1709
7	6E	0.47	0/1275	0.62	0/1709
8	72	0.52	0/1135	0.70	0/1527
8	7E	0.52	0/1135	0.78	1/1527 (0.1%)
9	82	0.46	0/1028	0.67	0/1379
9	8E	0.45	0/1028	0.65	1/1379 (0.1%)
10	1A	0.43	0/814	0.66	0/1095
10	1I	0.44	0/814	0.62	0/1095
11	2A	0.57	0/879	0.75	0/1187
11	2I	0.57	0/879	0.74	0/1187
12	3A	0.65	0/991	0.82	0/1327
12	3I	0.68	0/991	0.87	1/1327 (0.1%)
13	4A	0.40	0/943	0.62	0/1265
13	4I	0.40	0/938	0.70	0/1258
14	5A	0.53	0/500	0.74	0/664
14	5I	0.56	0/500	0.77	1/664 (0.2%)
15	6A	0.61	0/744	0.72	0/992
15	6I	0.59	0/744	0.78	0/992
16	7A	0.59	0/721	0.76	0/970
16	7I	0.51	0/721	0.80	1/970 (0.1%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
17	8A	0.62	0/847	0.76	0/1131
17	8I	0.55	0/847	0.74	0/1131
18	9A	0.58	0/595	0.79	2/790 (0.3%)
18	9I	0.52	0/595	0.73	1/790 (0.1%)
19	AA	0.43	0/647	0.71	0/871
19	AI	0.41	0/680	0.70	0/915
20	BA	0.57	0/764	0.80	1/1007 (0.1%)
20	BI	0.44	0/764	0.72	0/1007
21	1B	0.44	0/221	0.69	0/288
21	1F	0.43	0/221	0.65	0/288
22	2K	0.82	0/1784	1.60	34/2771 (1.2%)
22	2L	0.83	0/1686	1.53	26/2618 (1.0%)
22	3K	0.45	0/1850	1.08	5/2875 (0.2%)
22	3L	0.50	0/1851	1.15	10/2877 (0.3%)
23	4K	1.22	0/392	1.69	14/609 (2.3%)
23	4L	0.96	0/190	1.70	5/293 (1.7%)
24	14	1.10	158/70167 (0.2%)	1.83	2510/109541 (2.3%)
24	1H	1.18	231/70233 (0.3%)	1.95	3196/109643 (2.9%)
25	16	0.89	0/2928	1.59	63/4568 (1.4%)
25	1J	0.85	0/2928	1.68	64/4568 (1.4%)
26	71	0.29	0/1072	0.51	0/1447
26	79	0.29	0/1072	0.48	0/1447
27	11	0.97	2/2165 (0.1%)	1.12	8/2919 (0.3%)
27	19	0.88	1/2170 (0.0%)	1.05	8/2926 (0.3%)
28	21	0.73	0/1601	0.97	4/2160 (0.2%)
28	29	0.80	0/1601	1.01	5/2160 (0.2%)
29	31	0.86	0/1620	0.99	2/2194 (0.1%)
29	39	0.73	1/1662 (0.1%)	0.94	3/2249 (0.1%)
30	41	0.44	0/1498	0.65	0/2016
30	49	0.45	0/1498	0.67	0/2016
31	51	0.63	0/1362	0.89	1/1841 (0.1%)
31	59	0.37	0/1337	0.69	0/1809
32	61	0.56	0/1151	0.83	3/1558 (0.2%)
32	69	0.54	0/1151	0.76	1/1558 (0.1%)
33	15	0.61	0/1131	0.81	0/1525
33	58	0.67	0/1131	0.83	0/1525
34	25	0.82	0/942	0.89	1/1269 (0.1%)
34	68	0.76	0/942	0.84	0/1269
35	35	0.76	1/1161 (0.1%)	1.10	5/1544 (0.3%)
35	78	0.83	0/1161	1.19	8/1544 (0.5%)
36	45	0.71	0/1142	0.97	3/1527 (0.2%)
36	88	0.82	2/1142 (0.2%)	0.99	3/1527 (0.2%)
37	55	0.77	0/973	1.03	3/1302 (0.2%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
37	98	0.70	0/981	0.96	1/1312 (0.1%)
38	65	0.61	0/891	0.88	1/1187 (0.1%)
38	A8	0.62	0/891	0.88	2/1187 (0.2%)
39	75	0.76	0/1145	0.95	2/1531 (0.1%)
39	B8	0.71	0/1155	0.88	1/1542 (0.1%)
40	85	0.69	0/981	0.84	2/1306 (0.2%)
40	C8	0.78	0/981	0.84	0/1306
41	95	4.12	8/789 (1.0%)	1.45	6/1057 (0.6%)
41	D8	0.73	0/789	0.89	2/1057 (0.2%)
42	A5	0.75	0/910	0.89	1/1220 (0.1%)
42	E8	0.79	0/910	0.93	3/1220 (0.2%)
43	B5	0.88	1/744 (0.1%)	0.85	0/1000
43	F8	0.95	1/739 (0.1%)	0.89	0/993
44	C5	0.69	0/807	0.93	1/1076 (0.1%)
44	G8	0.90	1/804 (0.1%)	1.06	3/1073 (0.3%)
45	D5	0.47	0/1460	0.71	0/1982
45	H8	0.45	0/1427	0.73	2/1935 (0.1%)
46	E5	0.72	0/620	0.93	0/827
46	I8	0.83	0/665	1.01	3/885 (0.3%)
47	F5	0.74	0/769	0.92	1/1022 (0.1%)
47	J8	0.78	0/769	1.09	6/1022 (0.6%)
48	G5	0.68	2/582 (0.3%)	0.89	1/771 (0.1%)
48	K8	1.01	2/560 (0.4%)	0.97	0/741
49	H5	0.61	0/473	0.81	0/635
49	L8	0.70	0/473	0.91	0/635
50	I5	0.44	0/527	0.68	0/709
50	M8	0.36	0/545	0.59	0/733
51	J5	0.65	0/472	0.84	0/639
51	N8	0.80	0/472	0.98	2/639 (0.3%)
52	K5	0.57	0/396	0.77	0/529
52	O8	0.51	0/396	0.72	0/529
53	L5	0.84	0/437	1.05	3/575 (0.5%)
53	P8	1.01	0/417	1.18	3/550 (0.5%)
54	M5	0.97	1/502 (0.2%)	1.27	5/661 (0.8%)
54	Q8	1.08	1/488 (0.2%)	1.19	2/641 (0.3%)
All	All	0.95	431/321962 (0.1%)	1.56	7140/481589 (1.5%)

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

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

The worst 5 of 431 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
41	95	91	TYR	CD1-CE1	59.58	2.28	1.39
41	95	91	TYR	CD2-CE2	57.56	2.25	1.39
41	95	91	TYR	CE2-CZ	41.48	1.92	1.38
41	95	91	TYR	CE1-CZ	39.94	1.90	1.38
41	95	91	TYR	CG-CD2	31.31	1.79	1.39

The worst 5 of 7140 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	1H	1332	G	N3-C4-N9	-24.58	111.25	126.00
24	1H	1332	G	N3-C4-C5	23.29	140.25	128.60
41	95	21	ARG	CD-NE-CZ	23.04	155.86	123.60
24	1H	1899	G	N3-C4-N9	-22.45	112.53	126.00
41	95	21	ARG	NE-CZ-NH1	22.42	131.51	120.30

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	890	0
1	1G	32309	0	16307	834	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	12	1924	0	1975	95	0
2	1E	1924	0	1975	120	0
3	22	1612	0	1677	92	0
3	2E	1605	0	1668	72	0
4	32	1702	0	1763	112	1
4	3E	1702	0	1763	83	0
5	42	1155	0	1213	70	0
5	4E	1155	0	1213	52	0
6	52	842	0	857	38	0
6	5E	842	0	857	43	1
7	62	1256	0	1296	41	0
7	6E	1256	0	1296	55	0
8	72	1115	0	1177	50	0
8	7E	1115	0	1177	71	0
9	82	1009	0	1037	72	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	27	0
11	2I	864	0	881	39	0
12	3A	975	0	1062	39	0
12	3I	975	0	1062	43	0
13	4A	933	0	992	57	0
13	4I	928	0	987	50	0
14	5A	491	0	529	36	0
14	5I	491	0	529	45	0
15	6A	733	0	771	28	0
15	6I	733	0	771	36	0
16	7A	705	0	725	34	0
16	7I	705	0	725	47	0
17	8A	834	0	904	44	0
17	8I	834	0	904	47	0
18	9A	590	0	662	26	0
18	9I	590	0	662	20	0
19	AA	633	0	649	46	0
19	AI	665	0	686	36	0
20	BA	762	0	861	37	0
20	BI	762	0	861	54	0
21	1B	217	0	234	17	0
21	1F	217	0	234	12	0
22	2K	1765	0	916	65	0
22	2L	1678	0	872	64	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
22	3K	1824	0	945	58	0
22	3L	1825	0	946	52	0
23	4K	348	0	175	9	0
23	4L	170	0	87	3	0
24	14	62647	0	31572	1458	0
24	1H	62707	0	31606	1603	0
25	16	2617	0	1328	87	0
25	1J	2617	0	1328	93	0
26	71	1049	0	1071	31	0
26	79	1049	0	1071	42	0
27	11	2115	0	2195	134	0
27	19	2120	0	2197	114	0
28	21	1568	0	1634	95	0
28	29	1568	0	1634	121	0
29	31	1585	0	1632	79	0
29	39	1627	0	1680	103	0
30	41	1473	0	1535	72	0
30	49	1473	0	1535	89	0
31	51	1336	0	1418	89	0
31	59	1312	0	1384	64	0
32	61	1136	0	1223	55	0
32	69	1136	0	1223	65	0
33	15	1104	0	1180	47	0
33	58	1104	0	1180	51	0
34	25	932	0	996	39	0
34	68	932	0	996	32	0
35	35	1144	0	1228	81	0
35	78	1144	0	1228	90	0
36	45	1121	0	1179	71	0
36	88	1121	0	1179	84	0
37	55	959	0	1021	54	0
37	98	967	0	1033	68	0
38	65	881	0	943	77	0
38	A8	881	0	943	49	0
39	75	1131	0	1180	86	0
39	B8	1141	0	1202	58	0
40	85	963	0	1022	54	0
40	C8	963	0	1022	60	0
41	95	778	0	852	86	0
41	D8	778	0	852	32	0
42	A5	899	0	964	34	0
42	E8	899	0	964	40	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
43	B5	730	0	780	39	0
43	F8	725	0	778	46	0
44	C5	794	0	884	58	0
44	G8	791	0	880	67	0
45	D5	1428	0	1454	89	0
45	H8	1397	0	1430	86	0
46	E5	612	0	633	39	0
46	I8	656	0	683	55	0
47	F5	762	0	848	35	0
47	J8	762	0	848	47	0
48	G5	580	0	629	29	0
48	K8	558	0	610	30	0
49	H5	468	0	518	14	0
49	L8	468	0	518	36	0
50	I5	515	0	514	43	0
50	M8	533	0	526	40	0
51	J5	458	0	480	20	0
51	N8	458	0	480	36	0
52	K5	389	0	404	24	0
52	O8	389	0	404	27	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	42	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

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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

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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	9341	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 9341 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:CD1	41:95:91:TYR:CG	1.79	1.67
41:95:91:TYR:CD2	41:95:91:TYR:CG	1.79	1.65
41:95:91:TYR:CZ	41:95:91:TYR:CE1	1.90	1.56
41:95:91:TYR:CZ	41:95:91:TYR:CE2	1.92	1.55
22:2K:35:QUO:N3	22:2K:35:QUO:C4	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%)	9	36
2	1E	235/256 (92%)	199 (85%)	32 (14%)	4 (2%)	9	36
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%)	8	33
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%)	22	57
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%)	10	39
8	7E	136/138 (99%)	125 (92%)	11 (8%)	0	100	100
9	82	125/128 (98%)	112 (90%)	12 (10%)	1 (1%)	19	54
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%)	17	52
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	16
13	4I	114/126 (90%)	98 (86%)	16 (14%)	0	100	100
14	5A	58/61 (95%)	48 (83%)	10 (17%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
14	5I	58/61 (95%)	52 (90%)	5 (9%)	1 (2%)	9	36
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%)	13	44
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%)	15	49
18	9A	70/88 (80%)	65 (93%)	5 (7%)	0	100	100
18	9I	70/88 (80%)	63 (90%)	6 (9%)	1 (1%)	11	40
19	AA	77/93 (83%)	57 (74%)	17 (22%)	3 (4%)	3	18
19	AI	81/93 (87%)	66 (82%)	13 (16%)	2 (2%)	5	27
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	71	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%)	10	39
27	19	271/276 (98%)	253 (93%)	15 (6%)	3 (1%)	14	46
28	21	203/206 (98%)	174 (86%)	28 (14%)	1 (0%)	29	64
28	29	203/206 (98%)	160 (79%)	34 (17%)	9 (4%)	2	15
29	31	200/210 (95%)	189 (94%)	10 (5%)	1 (0%)	29	64
29	39	206/210 (98%)	176 (85%)	21 (10%)	9 (4%)	2	15
30	41	179/182 (98%)	154 (86%)	24 (13%)	1 (1%)	25	59
30	49	179/182 (98%)	151 (84%)	25 (14%)	3 (2%)	9	36
31	51	172/180 (96%)	146 (85%)	20 (12%)	6 (4%)	3	20
31	59	169/180 (94%)	133 (79%)	35 (21%)	1 (1%)	25	59
32	61	144/148 (97%)	120 (83%)	21 (15%)	3 (2%)	7	30
32	69	144/148 (97%)	122 (85%)	19 (13%)	3 (2%)	7	30
33	15	136/140 (97%)	128 (94%)	7 (5%)	1 (1%)	22	57
33	58	136/140 (97%)	116 (85%)	13 (10%)	7 (5%)	2	13

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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%)	19	54
35	35	148/150 (99%)	118 (80%)	24 (16%)	6 (4%)	3	16
35	78	148/150 (99%)	117 (79%)	28 (19%)	3 (2%)	7	31
36	45	139/141 (99%)	114 (82%)	20 (14%)	5 (4%)	3	20
36	88	139/141 (99%)	111 (80%)	23 (16%)	5 (4%)	3	20
37	55	115/118 (98%)	103 (90%)	11 (10%)	1 (1%)	17	52
37	98	116/118 (98%)	104 (90%)	10 (9%)	2 (2%)	9	36
38	65	109/112 (97%)	93 (85%)	14 (13%)	2 (2%)	8	34
38	A8	109/112 (97%)	94 (86%)	13 (12%)	2 (2%)	8	34
39	75	135/146 (92%)	113 (84%)	19 (14%)	3 (2%)	6	29
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%)	2	13
41	D8	99/101 (98%)	89 (90%)	9 (9%)	1 (1%)	15	49
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%)	14	46
43	F8	90/96 (94%)	84 (93%)	4 (4%)	2 (2%)	6	29
44	C5	102/110 (93%)	72 (71%)	27 (26%)	3 (3%)	4	24
44	G8	102/110 (93%)	84 (82%)	12 (12%)	6 (6%)	1	10
45	D5	177/206 (86%)	145 (82%)	25 (14%)	7 (4%)	3	17
45	H8	173/206 (84%)	134 (78%)	32 (18%)	7 (4%)	3	17
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%)	14	46
47	J8	95/98 (97%)	83 (87%)	10 (10%)	2 (2%)	7	30
48	G5	67/72 (93%)	56 (84%)	11 (16%)	0	100	100
48	K8	64/72 (89%)	61 (95%)	0	3 (5%)	2	14
49	H5	57/60 (95%)	55 (96%)	2 (4%)	0	100	100

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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	7
50	M8	64/71 (90%)	45 (70%)	17 (27%)	2 (3%)	4	23
51	J5	57/60 (95%)	48 (84%)	8 (14%)	1 (2%)	8	34
51	N8	57/60 (95%)	49 (86%)	6 (10%)	2 (4%)	3	20
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	15
54	M5	60/65 (92%)	51 (85%)	6 (10%)	3 (5%)	2	13
54	Q8	60/65 (92%)	51 (85%)	7 (12%)	2 (3%)	4	21
All	All	11616/12512 (93%)	10210 (88%)	1239 (11%)	167 (1%)	11	40

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%)	165 (80%)	40 (20%)	1	6
2	1E	205/220 (93%)	150 (73%)	55 (27%)	0	1
3	22	160/188 (85%)	123 (77%)	37 (23%)	1	3
3	2E	159/188 (85%)	135 (85%)	24 (15%)	3	12
4	32	180/181 (99%)	142 (79%)	38 (21%)	1	5

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	3E	180/181 (99%)	146 (81%)	34 (19%)	1	6
5	42	116/123 (94%)	89 (77%)	27 (23%)	1	3
5	4E	116/123 (94%)	89 (77%)	27 (23%)	1	3
6	52	90/90 (100%)	75 (83%)	15 (17%)	2	9
6	5E	90/90 (100%)	75 (83%)	15 (17%)	2	9
7	62	126/127 (99%)	100 (79%)	26 (21%)	1	5
7	6E	126/127 (99%)	98 (78%)	28 (22%)	1	4
8	72	119/119 (100%)	99 (83%)	20 (17%)	2	9
8	7E	119/119 (100%)	97 (82%)	22 (18%)	1	7
9	82	98/99 (99%)	77 (79%)	21 (21%)	1	4
9	8E	98/99 (99%)	78 (80%)	20 (20%)	1	5
10	1A	89/92 (97%)	68 (76%)	21 (24%)	1	2
10	1I	89/92 (97%)	74 (83%)	15 (17%)	2	9
11	2A	88/99 (89%)	73 (83%)	15 (17%)	2	9
11	2I	88/99 (89%)	74 (84%)	14 (16%)	2	11
12	3A	104/109 (95%)	89 (86%)	15 (14%)	3	14
12	3I	104/109 (95%)	87 (84%)	17 (16%)	2	10
13	4A	94/101 (93%)	75 (80%)	19 (20%)	1	5
13	4I	94/101 (93%)	76 (81%)	18 (19%)	1	6
14	5A	49/50 (98%)	42 (86%)	7 (14%)	3	14
14	5I	49/50 (98%)	36 (74%)	13 (26%)	0	1
15	6A	79/80 (99%)	68 (86%)	11 (14%)	3	15
15	6I	79/80 (99%)	66 (84%)	13 (16%)	2	10
16	7A	72/74 (97%)	58 (81%)	14 (19%)	1	6
16	7I	72/74 (97%)	53 (74%)	19 (26%)	0	1
17	8A	95/97 (98%)	79 (83%)	16 (17%)	2	9
17	8I	95/97 (98%)	77 (81%)	18 (19%)	1	6
18	9A	63/77 (82%)	54 (86%)	9 (14%)	3	14
18	9I	63/77 (82%)	54 (86%)	9 (14%)	3	14
19	AA	68/80 (85%)	53 (78%)	15 (22%)	1	4
19	AI	72/80 (90%)	59 (82%)	13 (18%)	1	7

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
20	BA	76/82 (93%)	64 (84%)	12 (16%)	2	11
20	BI	76/82 (93%)	60 (79%)	16 (21%)	1	5
21	1B	20/22 (91%)	16 (80%)	4 (20%)	1	5
21	1F	20/22 (91%)	19 (95%)	1 (5%)	24	57
26	71	111/181 (61%)	103 (93%)	8 (7%)	14	44
26	79	111/181 (61%)	99 (89%)	12 (11%)	6	25
27	11	214/218 (98%)	172 (80%)	42 (20%)	1	6
27	19	214/218 (98%)	176 (82%)	38 (18%)	2	8
28	21	165/166 (99%)	130 (79%)	35 (21%)	1	5
28	29	165/166 (99%)	132 (80%)	33 (20%)	1	5
29	31	161/166 (97%)	123 (76%)	38 (24%)	1	2
29	39	165/166 (99%)	126 (76%)	39 (24%)	1	2
30	41	155/156 (99%)	128 (83%)	27 (17%)	2	9
30	49	155/156 (99%)	116 (75%)	39 (25%)	0	1
31	51	145/148 (98%)	112 (77%)	33 (23%)	1	3
31	59	142/148 (96%)	112 (79%)	30 (21%)	1	5
32	61	122/124 (98%)	97 (80%)	25 (20%)	1	5
32	69	122/124 (98%)	85 (70%)	37 (30%)	0	0
33	15	117/119 (98%)	88 (75%)	29 (25%)	0	2
33	58	117/119 (98%)	84 (72%)	33 (28%)	0	1
34	25	100/100 (100%)	82 (82%)	18 (18%)	1	7
34	68	100/100 (100%)	85 (85%)	15 (15%)	3	12
35	35	116/116 (100%)	78 (67%)	38 (33%)	0	0
35	78	116/116 (100%)	75 (65%)	41 (35%)	0	0
36	45	111/111 (100%)	92 (83%)	19 (17%)	2	9
36	88	111/111 (100%)	88 (79%)	23 (21%)	1	5
37	55	100/101 (99%)	81 (81%)	19 (19%)	1	6
37	98	101/101 (100%)	84 (83%)	17 (17%)	2	9
38	65	87/88 (99%)	57 (66%)	30 (34%)	0	0
38	A8	87/88 (99%)	71 (82%)	16 (18%)	1	7
39	75	117/127 (92%)	89 (76%)	28 (24%)	0	2

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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%)	1	7
40	C8	93/94 (99%)	75 (81%)	18 (19%)	1	6
41	95	82/82 (100%)	65 (79%)	17 (21%)	1	5
41	D8	82/82 (100%)	57 (70%)	25 (30%)	0	0
42	A5	92/92 (100%)	71 (77%)	21 (23%)	1	3
42	E8	92/92 (100%)	68 (74%)	24 (26%)	0	1
43	B5	74/78 (95%)	59 (80%)	15 (20%)	1	5
43	F8	74/78 (95%)	57 (77%)	17 (23%)	1	3
44	C5	85/91 (93%)	64 (75%)	21 (25%)	0	2
44	G8	85/91 (93%)	66 (78%)	19 (22%)	1	3
45	D5	158/179 (88%)	122 (77%)	36 (23%)	1	3
45	H8	154/179 (86%)	116 (75%)	38 (25%)	0	2
46	E5	62/67 (92%)	51 (82%)	11 (18%)	2	8
46	I8	66/67 (98%)	52 (79%)	14 (21%)	1	5
47	F5	82/83 (99%)	62 (76%)	20 (24%)	0	2
47	J8	82/83 (99%)	58 (71%)	24 (29%)	0	1
48	G5	64/67 (96%)	51 (80%)	13 (20%)	1	5
48	K8	62/67 (92%)	47 (76%)	15 (24%)	0	2
49	H5	51/52 (98%)	42 (82%)	9 (18%)	2	8
49	L8	51/52 (98%)	41 (80%)	10 (20%)	1	6
50	I5	57/63 (90%)	44 (77%)	13 (23%)	1	3
50	M8	59/63 (94%)	51 (86%)	8 (14%)	3	16
51	J5	51/52 (98%)	39 (76%)	12 (24%)	1	3
51	N8	51/52 (98%)	35 (69%)	16 (31%)	0	0
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%)	0	2
53	P8	40/42 (95%)	32 (80%)	8 (20%)	1	5
54	M5	52/55 (94%)	39 (75%)	13 (25%)	0	2
54	Q8	50/55 (91%)	30 (60%)	20 (40%)	0	0

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	9806/10360 (95%)	7722 (79%)	2084 (21%)	1 4

5 of 2084 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
47	J8	46	LEU
5	42	24	ARG
44	C5	89	PHE
48	K8	53	LEU
2	12	48	MET

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 21 such sidechains are listed below:

Mol	Chain	Res	Type
50	M8	60	GLN
4	32	119	GLN
29	39	203	GLN
45	H8	54	HIS
40	85	81	HIS

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	13	1492/1522 (98%)	352 (23%)	26 (1%)
1	1G	1502/1522 (98%)	370 (24%)	39 (2%)
22	2K	77/85 (90%)	33 (42%)	5 (6%)
22	2L	74/85 (87%)	25 (33%)	8 (10%)
22	3K	81/85 (95%)	23 (28%)	3 (3%)
22	3L	82/85 (96%)	21 (25%)	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%)	685 (23%)	48 (1%)
24	1H	2911/2917 (99%)	698 (23%)	56 (1%)
25	16	121/122 (99%)	38 (31%)	0
25	1J	121/122 (99%)	34 (28%)	0
All	All	9392/9522 (98%)	2290 (24%)	192 (2%)

5 of 2290 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
24	1H	2422	A
1	1G	632	A
24	14	2166	G
24	1H	2566	A
1	1G	115	G

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	QUO	2L	35	22,23	28,35,36	5.66	9 (32%)	32,52,55	5.35	15 (46%)
22	OMG	2L	17	22	18,26,27	5.54	6 (33%)	20,38,41	5.52	7 (35%)
22	MIA	2L	38	22	24,31,32	2.27	2 (8%)	26,44,47	2.36	7 (26%)
22	QUO	3K	35	22	28,35,36	5.73	9 (32%)	32,52,55	5.67	12 (37%)
22	4SU	2L	8	22	14,21,22	3.08	2 (14%)	15,30,33	1.82	3 (20%)
22	PSU	2L	64	22	17,21,22	1.22	1 (5%)	20,30,33	3.68	7 (35%)
22	QUO	2K	35	22,23	28,35,36	5.48	10 (35%)	32,52,55	5.12	10 (31%)
22	PSU	2K	40	22	17,21,22	0.88	1 (5%)	20,30,33	3.09	5 (25%)
22	OMG	3L	17	22	18,26,27	5.77	7 (38%)	20,38,41	5.34	7 (35%)
22	PSU	2K	64	55,22	17,21,22	1.07	1 (5%)	20,30,33	3.14	8 (40%)
22	MIA	3K	38	22	24,31,32	2.44	4 (16%)	26,44,47	3.04	11 (42%)
22	MIA	2K	38	22	24,31,32	2.39	3 (12%)	26,44,47	3.78	8 (30%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
22	QUO	3L	35	22	28,35,36	5.61	10 (35%)	32,52,55	5.11	14 (43%)
22	5MU	2K	63	22	15,22,23	2.22	3 (20%)	16,32,35	1.76	2 (12%)
22	PSU	3K	64	22	17,21,22	1.03	1 (5%)	20,30,33	3.31	8 (40%)
22	5MU	2L	63	22	15,22,23	2.14	3 (20%)	16,32,35	1.68	2 (12%)
22	MIA	3L	38	22	24,31,32	2.43	3 (12%)	26,44,47	3.06	10 (38%)
22	OMG	3K	17	22	18,26,27	5.84	6 (33%)	20,38,41	5.65	7 (35%)
22	5MU	3L	63	22	15,22,23	2.18	3 (20%)	16,32,35	1.77	2 (12%)
22	PSU	3L	64	22	17,21,22	1.09	1 (5%)	20,30,33	3.55	7 (35%)
22	4SU	3L	8	55,22	14,21,22	3.51	2 (14%)	15,30,33	1.39	2 (13%)
22	PSU	2L	40	22	17,21,22	1.23	2 (11%)	20,30,33	3.41	5 (25%)
22	PSU	3K	40	22	17,21,22	1.01	1 (5%)	20,30,33	3.34	5 (25%)
22	4SU	3K	8	22	14,21,22	3.24	2 (14%)	15,30,33	0.95	1 (6%)
22	4SU	2K	8	22	14,21,22	3.60	2 (14%)	15,30,33	0.85	0
22	OMG	2K	17	22	18,26,27	5.68	6 (33%)	20,38,41	5.34	8 (40%)
22	5MU	3K	63	22	15,22,23	2.16	3 (20%)	16,32,35	1.82	2 (12%)
22	PSU	3L	40	22	17,21,22	1.12	1 (5%)	20,30,33	3.25	7 (35%)

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	QUO	2L	35	22,23	-	1/6/43/44	0/4/4/4
22	OMG	2L	17	22	-	2/5/27/28	0/3/3/3
22	MIA	2L	38	22	-	3/11/33/34	0/3/3/3
22	QUO	3K	35	22	-	3/6/43/44	0/4/4/4
22	4SU	2L	8	22	-	0/5/25/26	0/2/2/2
22	PSU	2L	64	22	-	0/7/25/26	0/2/2/2
22	QUO	2K	35	22,23	-	2/6/43/44	0/4/4/4
22	PSU	2K	40	22	-	0/7/25/26	0/2/2/2
22	OMG	3L	17	22	-	3/5/27/28	0/3/3/3
22	PSU	2K	64	55,22	-	5/7/25/26	0/2/2/2
22	MIA	3K	38	22	-	8/11/33/34	0/3/3/3
22	MIA	2K	38	22	-	5/11/33/34	0/3/3/3
22	QUO	3L	35	22	-	3/6/43/44	0/4/4/4
22	5MU	2K	63	22	-	4/5/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	PSU	3K	64	22	-	0/7/25/26	0/2/2/2
22	5MU	2L	63	22	-	3/5/25/26	0/2/2/2
22	MIA	3L	38	22	-	7/11/33/34	0/3/3/3
22	OMG	3K	17	22	-	2/5/27/28	0/3/3/3
22	5MU	3L	63	22	-	0/5/25/26	0/2/2/2
22	PSU	3L	64	22	-	2/7/25/26	0/2/2/2
22	4SU	3L	8	55,22	-	0/5/25/26	0/2/2/2
22	PSU	2L	40	22	-	0/7/25/26	0/2/2/2
22	PSU	3K	40	22	-	0/7/25/26	0/2/2/2
22	4SU	3K	8	22	-	0/5/25/26	0/2/2/2
22	4SU	2K	8	22	-	0/5/25/26	0/2/2/2
22	OMG	2K	17	22	-	3/5/27/28	0/3/3/3
22	5MU	3K	63	22	-	0/5/25/26	0/2/2/2
22	PSU	3L	40	22	-	0/7/25/26	0/2/2/2

The worst 5 of 104 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	2L	35	QUO	C4-N3	23.01	1.71	1.35
22	3L	35	QUO	C4-N3	22.94	1.71	1.35
22	3K	35	QUO	C4-N3	22.88	1.71	1.35
22	2K	35	QUO	C4-N3	21.22	1.68	1.35
22	3K	17	OMG	C4-N3	16.50	1.61	1.35

The worst 5 of 182 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	3K	35	QUO	C6-C5-C4	23.78	128.44	115.01
22	3L	35	QUO	C6-C5-C4	23.30	128.16	115.01
22	2K	35	QUO	C6-C5-C4	22.74	127.85	115.01
22	2L	35	QUO	C6-C5-C4	22.63	127.79	115.01
22	2L	17	OMG	C6-C5-C4	-16.00	105.53	120.80

There are no chirality outliers.

5 of 56 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
22	2L	17	OMG	C4'-C5'-O5'-P
22	2L	38	MIA	N1-C2-S10-C11
22	2L	38	MIA	N3-C2-S10-C11

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Mol	Chain	Res	Type	Atoms
22	2L	38	MIA	C12-C13-C14-C15
22	3K	35	QUO	O4'-C4'-C5'-O5'

There are no ring outliers.

22 monomers are involved in 45 short contacts:

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

5.5 Carbohydrates [i](#)

There are no carbohydrates 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

There are no such residues in this entry.

5.8 Polymer linkage issues

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%)	-0.56	1 (0%) 95 92	63, 117, 206, 445	0
1	1G	1503/1522 (98%)	-0.53	5 (0%) 94 88	68, 115, 190, 453	0
2	12	237/256 (92%)	0.90	41 (17%) 1 0	127, 170, 220, 245	0
2	1E	237/256 (92%)	0.72	29 (12%) 4 1	120, 163, 212, 246	0
3	22	206/239 (86%)	1.18	44 (21%) 0 0	120, 147, 179, 189	0
3	2E	205/239 (85%)	0.50	16 (7%) 13 5	111, 138, 196, 212	0
4	32	208/209 (99%)	0.84	26 (12%) 3 1	94, 119, 152, 172	0
4	3E	208/209 (99%)	-0.09	3 (1%) 75 56	87, 119, 147, 176	0
5	42	151/162 (93%)	0.21	2 (1%) 77 59	94, 113, 140, 210	0
5	4E	151/162 (93%)	0.02	0 100 100	87, 114, 139, 206	0
6	52	101/101 (100%)	-0.22	1 (0%) 82 67	85, 106, 127, 146	0
6	5E	101/101 (100%)	0.73	5 (4%) 28 13	95, 122, 138, 154	0
7	62	155/156 (99%)	-0.07	4 (2%) 56 33	111, 129, 145, 152	0
7	6E	155/156 (99%)	0.61	16 (10%) 6 2	106, 137, 161, 172	0
8	72	138/138 (100%)	0.32	3 (2%) 62 41	98, 117, 133, 158	0
8	7E	138/138 (100%)	0.07	1 (0%) 87 75	101, 121, 136, 150	0
9	82	127/128 (99%)	0.15	4 (3%) 49 26	111, 160, 187, 206	0
9	8E	127/128 (99%)	0.59	15 (11%) 4 2	104, 155, 177, 185	0
10	1A	99/105 (94%)	1.21	23 (23%) 0 0	121, 161, 193, 210	0
10	1I	99/105 (94%)	0.90	15 (15%) 2 1	105, 164, 206, 215	0
11	2A	116/129 (89%)	-0.05	1 (0%) 84 69	81, 110, 134, 164	0
11	2I	116/129 (89%)	1.12	22 (18%) 1 0	79, 114, 153, 224	0
12	3A	125/132 (94%)	0.45	8 (6%) 19 8	86, 102, 141, 189	0
12	3I	125/132 (94%)	-0.29	1 (0%) 86 72	79, 92, 125, 247	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
13	4A	117/126 (92%)	0.09	6 (5%) 28 13	122, 164, 193, 228	0
13	4I	116/126 (92%)	0.81	17 (14%) 2 1	117, 165, 186, 205	0
14	5A	60/61 (98%)	1.29	20 (33%) 0 0	131, 150, 178, 185	0
14	5I	60/61 (98%)	-0.07	1 (1%) 70 49	112, 128, 149, 170	0
15	6A	88/89 (98%)	0.11	0 100 100	84, 115, 134, 141	0
15	6I	88/89 (98%)	-0.11	0 100 100	92, 112, 133, 151	0
16	7A	84/88 (95%)	0.44	5 (5%) 21 10	94, 108, 132, 195	0
16	7I	84/88 (95%)	-0.43	0 100 100	107, 127, 154, 194	0
17	8A	100/105 (95%)	0.13	3 (3%) 50 27	91, 108, 126, 176	0
17	8I	100/105 (95%)	-0.46	0 100 100	97, 119, 133, 142	0
18	9A	72/88 (81%)	0.45	5 (6%) 16 7	91, 112, 166, 208	0
18	9I	72/88 (81%)	1.46	16 (22%) 0 0	100, 121, 150, 227	0
19	AA	79/93 (84%)	1.43	26 (32%) 0 0	144, 187, 220, 228	0
19	AI	83/93 (89%)	0.28	7 (8%) 11 4	142, 168, 204, 221	0
20	BA	99/106 (93%)	0.54	6 (6%) 21 9	86, 114, 153, 193	0
20	BI	99/106 (93%)	-0.23	1 (1%) 82 67	112, 138, 188, 193	0
21	1B	25/27 (92%)	0.20	1 (4%) 38 19	117, 140, 171, 190	0
21	1F	25/27 (92%)	0.37	0 100 100	125, 139, 170, 187	0
22	2K	75/85 (88%)	-0.39	0 100 100	74, 113, 195, 247	0
22	2L	71/85 (83%)	-0.59	0 100 100	73, 115, 176, 193	0
22	3K	78/85 (91%)	-0.03	6 (7%) 13 5	85, 189, 296, 344	0
22	3L	78/85 (91%)	-0.80	0 100 100	79, 195, 286, 321	0
23	4K	16/30 (53%)	-0.18	0 100 100	82, 126, 168, 170	0
23	4L	8/30 (26%)	-0.37	0 100 100	93, 107, 190, 231	0
24	14	2909/2917 (99%)	-0.38	39 (1%) 77 59	53, 84, 260, 407	0
24	1H	2912/2917 (99%)	-0.24	32 (1%) 80 64	48, 80, 247, 440	0
25	16	122/122 (100%)	-0.32	1 (0%) 86 72	85, 118, 144, 247	0
25	1J	122/122 (100%)	-0.70	0 100 100	86, 123, 143, 217	0
26	71	135/229 (58%)	3.72	103 (76%) 0 0	156, 219, 251, 258	0
26	79	135/229 (58%)	1.35	41 (30%) 0 0	152, 228, 253, 265	0
27	11	272/276 (98%)	0.06	0 100 100	48, 69, 90, 122	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
27	19	273/276 (98%)	-0.40	0 100 100	50, 73, 91, 122	0
28	21	205/206 (99%)	0.32	14 (6%) 17 7	54, 94, 152, 211	0
28	29	205/206 (99%)	-0.16	2 (0%) 82 67	57, 88, 164, 238	0
29	31	202/210 (96%)	0.23	6 (2%) 50 27	47, 81, 123, 148	0
29	39	208/210 (99%)	0.84	26 (12%) 3 1	60, 98, 174, 203	0
30	41	181/182 (99%)	2.25	81 (44%) 0 0	123, 154, 197, 210	0
30	49	181/182 (99%)	0.44	17 (9%) 8 3	120, 146, 190, 208	0
31	51	174/180 (96%)	0.09	2 (1%) 80 64	90, 117, 139, 161	0
31	59	171/180 (95%)	1.55	52 (30%) 0 0	141, 208, 248, 354	0
32	61	146/148 (98%)	1.05	22 (15%) 2 1	84, 128, 153, 169	0
32	69	146/148 (98%)	-0.23	2 (1%) 75 56	81, 137, 164, 177	0
33	15	138/140 (98%)	0.21	4 (2%) 51 28	72, 101, 143, 174	0
33	58	138/140 (98%)	0.36	7 (5%) 28 13	73, 98, 154, 181	0
34	25	122/122 (100%)	0.04	0 100 100	64, 82, 100, 110	0
34	68	122/122 (100%)	-0.18	0 100 100	58, 85, 103, 114	0
35	35	150/150 (100%)	0.68	18 (12%) 4 2	61, 105, 144, 203	0
35	78	150/150 (100%)	0.33	5 (3%) 46 24	55, 91, 117, 251	0
36	45	141/141 (100%)	0.13	7 (4%) 28 13	67, 104, 131, 154	0
36	88	141/141 (100%)	0.36	8 (5%) 23 11	64, 99, 134, 181	0
37	55	117/118 (99%)	-0.21	0 100 100	62, 82, 99, 121	0
37	98	118/118 (100%)	0.01	1 (0%) 86 72	68, 88, 107, 125	0
38	65	111/112 (99%)	0.17	4 (3%) 42 22	93, 119, 148, 171	0
38	A8	111/112 (99%)	1.79	46 (41%) 0 0	97, 119, 163, 218	0
39	75	137/146 (93%)	-0.22	2 (1%) 73 54	75, 91, 161, 227	0
39	B8	137/146 (93%)	-0.24	4 (2%) 51 28	84, 102, 165, 218	0
40	85	117/118 (99%)	0.08	1 (0%) 84 69	65, 95, 135, 167	0
40	C8	117/118 (99%)	0.10	2 (1%) 70 49	57, 83, 130, 183	0
41	95	101/101 (100%)	1.18	21 (20%) 1 0	67, 124, 148, 194	0
41	D8	101/101 (100%)	0.58	7 (6%) 16 7	58, 106, 160, 237	0
42	A5	113/113 (100%)	0.15	2 (1%) 68 47	63, 77, 110, 206	0
42	E8	113/113 (100%)	0.14	2 (1%) 68 47	61, 77, 109, 231	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
43	B5	93/96 (96%)	0.28	4 (4%) 35 17	73, 86, 119, 127	0
43	F8	92/96 (95%)	0.47	6 (6%) 18 8	64, 74, 98, 112	0
44	C5	104/110 (94%)	1.56	27 (25%) 0 0	89, 130, 221, 252	0
44	G8	104/110 (94%)	0.46	7 (6%) 17 7	71, 96, 149, 186	0
45	D5	179/206 (86%)	1.68	57 (31%) 0 0	111, 160, 262, 335	0
45	H8	175/206 (84%)	1.47	52 (29%) 0 0	105, 160, 274, 301	0
46	E5	77/85 (90%)	0.15	2 (2%) 56 33	74, 89, 109, 178	0
46	I8	83/85 (97%)	0.52	5 (6%) 21 10	70, 90, 112, 158	0
47	F5	97/98 (98%)	-0.19	2 (2%) 63 43	60, 83, 157, 204	0
47	J8	97/98 (98%)	0.82	9 (9%) 8 3	57, 82, 168, 218	0
48	G5	69/72 (95%)	0.68	5 (7%) 15 6	84, 109, 145, 187	0
48	K8	66/72 (91%)	0.32	1 (1%) 73 54	63, 82, 115, 177	0
49	H5	59/60 (98%)	0.49	3 (5%) 28 13	79, 97, 156, 188	0
49	L8	59/60 (98%)	0.35	3 (5%) 28 13	73, 91, 138, 151	0
50	I5	63/71 (88%)	2.56	28 (44%) 0 0	161, 233, 263, 283	0
50	M8	66/71 (92%)	4.31	49 (74%) 0 0	152, 233, 267, 285	0
51	J5	59/60 (98%)	0.14	5 (8%) 10 4	58, 87, 207, 244	0
51	N8	59/60 (98%)	0.84	9 (15%) 2 1	52, 92, 216, 240	0
52	K5	45/54 (83%)	3.25	31 (68%) 0 0	161, 210, 253, 272	0
52	O8	45/54 (83%)	6.27	44 (97%) 0 0	164, 213, 245, 256	0
53	L5	49/49 (100%)	-0.30	0 100 100	56, 61, 106, 147	0
53	P8	47/49 (95%)	-0.32	0 100 100	48, 54, 72, 121	0
54	M5	62/65 (95%)	-0.09	0 100 100	67, 77, 100, 127	0
54	Q8	62/65 (95%)	-0.06	0 100 100	62, 80, 108, 129	0
All	All	21209/22034 (96%)	0.13	1336 (6%) 20 8	47, 108, 216, 453	0

The worst 5 of 1336 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
31	59	96	ALA	26.6
26	71	1	PRO	21.7
24	14	654(K)	C	21.5
50	I5	42	PHE	18.1
24	14	654(L)	G	14.6

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	3L	64	20/21	0.67	0.15	180,200,211,213	0
22	PSU	3K	64	20/21	0.72	0.26	182,190,202,202	0
22	4SU	3L	8	20/21	0.73	0.14	184,194,207,207	0
22	PSU	2L	64	20/21	0.74	0.13	138,148,163,166	0
22	OMG	3K	17	24/25	0.75	0.18	194,212,234,239	0
22	4SU	3K	8	20/21	0.83	0.12	186,202,212,214	0
22	OMG	2L	17	24/25	0.84	0.15	136,152,154,155	0
22	OMG	3L	17	24/25	0.85	0.12	200,216,227,230	0
22	PSU	2K	64	20/21	0.85	0.15	133,144,150,155	0
22	5MU	3L	63	21/22	0.85	0.13	174,186,190,192	0
22	5MU	3K	63	21/22	0.86	0.19	176,183,187,190	0
22	OMG	2K	17	24/25	0.87	0.14	142,148,151,151	0
22	4SU	2K	8	20/21	0.91	0.13	106,112,119,121	0
22	PSU	3K	40	20/21	0.91	0.13	118,124,129,130	0
22	5MU	2K	63	21/22	0.91	0.12	135,139,149,156	0
22	5MU	2L	63	21/22	0.92	0.10	141,149,156,167	0
22	4SU	2L	8	20/21	0.92	0.11	112,122,128,139	0
22	QUO	3L	35	32/33	0.93	0.15	105,114,128,132	0
22	QUO	2L	35	32/33	0.94	0.18	91,112,118,124	0
22	QUO	3K	35	32/33	0.94	0.18	108,114,124,127	0
22	PSU	2L	40	20/21	0.94	0.15	89,100,105,105	0
22	MIA	3K	38	29/30	0.94	0.18	114,122,132,135	0
22	PSU	3L	40	20/21	0.94	0.12	107,122,124,127	0
22	MIA	3L	38	29/30	0.95	0.17	118,123,131,133	0
22	QUO	2K	35	32/33	0.95	0.18	84,96,115,117	6
22	MIA	2L	38	29/30	0.95	0.18	92,101,113,119	0
22	PSU	2K	40	20/21	0.96	0.17	83,91,99,105	0
22	MIA	2K	38	29/30	0.96	0.19	82,94,106,112	0

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 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	16	208	1/1	0.20	0.34	113,113,113,113	0
55	MG	1H	3220	1/1	0.20	0.27	92,92,92,92	0
55	MG	1H	3240	1/1	0.21	0.32	92,92,92,92	0
55	MG	1H	3301	1/1	0.24	0.37	79,79,79,79	0
55	MG	1H	3364	1/1	0.28	0.34	103,103,103,103	0
55	MG	1G	1685	1/1	0.30	0.26	116,116,116,116	0
55	MG	1H	3360	1/1	0.30	0.34	167,167,167,167	0
55	MG	1H	3379	1/1	0.33	0.13	245,245,245,245	0
55	MG	42	201	1/1	0.34	0.35	101,101,101,101	0
55	MG	14	3335	1/1	0.34	0.24	90,90,90,90	0
56	ZN	G8	202	1/1	0.36	0.32	203,203,203,203	0
55	MG	13	1689	1/1	0.37	0.45	116,116,116,116	0
55	MG	14	3329	1/1	0.39	0.27	101,101,101,101	0
55	MG	13	1700	1/1	0.40	0.34	97,97,97,97	0
55	MG	14	3287	1/1	0.41	0.32	98,98,98,98	0
55	MG	14	3258	1/1	0.41	0.32	70,70,70,70	0
55	MG	14	3331	1/1	0.42	0.33	138,138,138,138	0
55	MG	14	3132	1/1	0.42	0.29	120,120,120,120	0
55	MG	14	3367	1/1	0.44	0.17	72,72,72,72	0
55	MG	13	1656	1/1	0.44	0.25	120,120,120,120	0
55	MG	1H	3346	1/1	0.45	0.24	113,113,113,113	0
55	MG	1G	1702	1/1	0.47	0.21	95,95,95,95	0
55	MG	14	3159	1/1	0.47	0.38	85,85,85,85	0
55	MG	13	1699	1/1	0.49	0.46	109,109,109,109	0
55	MG	1H	3186	1/1	0.49	0.23	70,70,70,70	0
55	MG	1H	3312	1/1	0.50	0.28	81,81,81,81	0
55	MG	1G	1613	1/1	0.50	0.08	92,92,92,92	0
55	MG	1H	3396	1/1	0.51	0.25	104,104,104,104	0
55	MG	13	1684	1/1	0.51	0.30	94,94,94,94	0
55	MG	1H	3405	1/1	0.52	0.14	74,74,74,74	0
55	MG	1H	3209	1/1	0.54	0.49	99,99,99,99	0
55	MG	14	3301	1/1	0.54	0.40	82,82,82,82	0
55	MG	1G	1721	1/1	0.54	0.55	129,129,129,129	0
55	MG	14	3113	1/1	0.54	0.35	97,97,97,97	0
55	MG	14	3190	1/1	0.54	0.36	95,95,95,95	0
55	MG	14	3300	1/1	0.55	0.17	83,83,83,83	0
55	MG	1H	3190	1/1	0.55	0.58	101,101,101,101	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
55	MG	1H	3407	1/1	0.55	0.37	89,89,89,89	0
55	MG	13	1621	1/1	0.55	0.27	87,87,87,87	0
55	MG	1H	3377	1/1	0.56	0.35	81,81,81,81	0
55	MG	14	3318	1/1	0.56	0.13	80,80,80,80	0
55	MG	1H	3386	1/1	0.57	0.30	66,66,66,66	0
55	MG	14	3373	1/1	0.57	0.23	98,98,98,98	0
55	MG	1H	3286	1/1	0.57	0.33	82,82,82,82	0
55	MG	13	1688	1/1	0.58	0.49	91,91,91,91	0
55	MG	1G	1669	1/1	0.58	0.25	86,86,86,86	0
55	MG	13	1706	1/1	0.58	0.44	93,93,93,93	0
55	MG	14	3127	1/1	0.58	0.39	84,84,84,84	0
55	MG	14	3082	1/1	0.58	0.15	64,64,64,64	0
55	MG	16	204	1/1	0.58	0.19	99,99,99,99	0
55	MG	16	203	1/1	0.59	0.24	92,92,92,92	0
55	MG	1G	1691	1/1	0.60	0.27	132,132,132,132	0
55	MG	1H	3162	1/1	0.60	0.21	94,94,94,94	0
55	MG	3E	301	1/1	0.60	0.11	156,156,156,156	0
55	MG	14	3174	1/1	0.60	0.36	107,107,107,107	0
55	MG	1H	3282	1/1	0.60	0.44	90,90,90,90	0
55	MG	1G	1701	1/1	0.60	0.13	93,93,93,93	0
55	MG	1G	1620	1/1	0.60	0.41	96,96,96,96	0
55	MG	4K	101	1/1	0.61	0.29	111,111,111,111	0
55	MG	1H	3121	1/1	0.61	0.25	98,98,98,98	0
55	MG	14	3038	1/1	0.61	0.25	86,86,86,86	0
55	MG	1G	1739	1/1	0.61	0.09	154,154,154,154	0
55	MG	13	1738	1/1	0.62	0.08	138,138,138,138	0
55	MG	1H	3518	1/1	0.62	0.17	135,135,135,135	0
55	MG	1H	3387	1/1	0.62	0.31	75,75,75,75	0
55	MG	1H	3398	1/1	0.63	0.17	106,106,106,106	0
55	MG	1H	3315	1/1	0.63	0.24	88,88,88,88	0
55	MG	16	211	1/1	0.63	0.23	98,98,98,98	0
55	MG	1H	3218	1/1	0.64	0.51	82,82,82,82	0
55	MG	14	3292	1/1	0.64	0.27	90,90,90,90	0
55	MG	1H	3511	1/1	0.64	0.07	119,119,119,119	0
55	MG	1G	1703	1/1	0.64	0.28	99,99,99,99	0
55	MG	1G	1718	1/1	0.64	0.34	118,118,118,118	0
55	MG	14	3368	1/1	0.64	0.23	76,76,76,76	0
55	MG	13	1693	1/1	0.64	0.38	100,100,100,100	0
55	MG	13	1610	1/1	0.64	0.33	115,115,115,115	0
55	MG	1H	3203	1/1	0.64	0.46	99,99,99,99	0
55	MG	1G	1726	1/1	0.64	0.44	124,124,124,124	0
55	MG	1G	1653	1/1	0.65	0.36	103,103,103,103	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
55	MG	29	303	1/1	0.65	0.15	74,74,74,74	0
55	MG	1H	3370	1/1	0.65	0.33	73,73,73,73	0
55	MG	1H	3234	1/1	0.65	0.31	88,88,88,88	0
55	MG	14	3291	1/1	0.65	0.21	82,82,82,82	0
55	MG	1H	3027	1/1	0.66	0.34	86,86,86,86	0
55	MG	1H	3342	1/1	0.66	0.40	89,89,89,89	0
55	MG	14	3303	1/1	0.66	0.39	99,99,99,99	0
55	MG	1H	3375	1/1	0.67	0.36	85,85,85,85	0
55	MG	1H	3307	1/1	0.67	0.24	83,83,83,83	0
55	MG	2K	104	1/1	0.67	0.47	101,101,101,101	0
55	MG	13	1695	1/1	0.67	0.26	90,90,90,90	0
55	MG	1G	1699	1/1	0.67	0.46	101,101,101,101	0
55	MG	1G	1719	1/1	0.67	0.20	104,104,104,104	0
55	MG	1H	3043	1/1	0.67	0.26	92,92,92,92	0
55	MG	1H	3355	1/1	0.68	0.58	107,107,107,107	0
55	MG	1H	3336	1/1	0.68	0.43	83,83,83,83	0
55	MG	14	3282	1/1	0.68	0.23	87,87,87,87	0
55	MG	14	3309	1/1	0.68	0.34	84,84,84,84	0
55	MG	13	1644	1/1	0.68	0.44	116,116,116,116	0
55	MG	14	3128	1/1	0.69	0.43	76,76,76,76	0
55	MG	1H	3168	1/1	0.69	0.35	85,85,85,85	0
55	MG	1H	3330	1/1	0.69	0.51	90,90,90,90	0
55	MG	14	3286	1/1	0.69	0.20	100,100,100,100	0
55	MG	14	3255	1/1	0.69	0.36	92,92,92,92	0
55	MG	1H	3350	1/1	0.69	0.51	89,89,89,89	0
55	MG	13	1647	1/1	0.69	0.15	110,110,110,110	0
55	MG	14	3281	1/1	0.70	0.38	82,82,82,82	0
55	MG	14	3345	1/1	0.70	0.28	78,78,78,78	0
55	MG	14	3289	1/1	0.70	0.16	175,175,175,175	0
55	MG	1H	3185	1/1	0.70	0.53	91,91,91,91	0
55	MG	1G	1663	1/1	0.70	0.29	81,81,81,81	0
55	MG	13	1668	1/1	0.70	0.42	102,102,102,102	0
55	MG	13	1608	1/1	0.70	0.32	101,101,101,101	0
55	MG	13	1712	1/1	0.70	0.35	123,123,123,123	0
55	MG	1H	3283	1/1	0.70	0.41	104,104,104,104	0
56	ZN	C5	202	1/1	0.70	0.31	219,219,219,219	0
55	MG	13	1635	1/1	0.71	0.31	95,95,95,95	0
55	MG	1H	3352	1/1	0.71	0.35	97,97,97,97	0
55	MG	1H	3215	1/1	0.71	0.52	91,91,91,91	0
55	MG	1G	1639	1/1	0.71	0.46	97,97,97,97	0
55	MG	1H	3259	1/1	0.71	0.33	93,93,93,93	0
55	MG	3L	101	1/1	0.71	0.18	180,180,180,180	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
55	MG	14	3252	1/1	0.71	0.21	81,81,81,81	0
55	MG	1G	1638	1/1	0.71	0.43	88,88,88,88	0
55	MG	13	1611	1/1	0.71	0.26	83,83,83,83	0
55	MG	1H	3178	1/1	0.71	0.25	77,77,77,77	0
55	MG	1H	3120	1/1	0.71	0.23	69,69,69,69	0
55	MG	1G	1692	1/1	0.71	0.33	120,120,120,120	0
55	MG	1H	3232	1/1	0.72	0.24	103,103,103,103	0
55	MG	5E	201	1/1	0.72	0.20	106,106,106,106	0
55	MG	1H	3385	1/1	0.72	0.21	97,97,97,97	0
55	MG	1G	1741	1/1	0.72	0.09	112,112,112,112	0
55	MG	1H	3180	1/1	0.72	0.19	86,86,86,86	0
55	MG	1H	3039	1/1	0.72	0.22	68,68,68,68	0
55	MG	1G	1722	1/1	0.72	0.15	91,91,91,91	0
55	MG	14	3169	1/1	0.72	0.31	100,100,100,100	0
55	MG	14	3191	1/1	0.72	0.33	92,92,92,92	0
55	MG	14	3161	1/1	0.72	0.37	89,89,89,89	0
55	MG	13	1698	1/1	0.72	0.35	78,78,78,78	0
55	MG	14	3261	1/1	0.72	0.54	105,105,105,105	0
55	MG	14	3154	1/1	0.72	0.33	87,87,87,87	0
55	MG	1H	3167	1/1	0.72	0.25	66,66,66,66	0
55	MG	1G	1705	1/1	0.73	0.15	96,96,96,96	0
55	MG	2L	102	1/1	0.73	0.32	102,102,102,102	0
55	MG	14	3269	1/1	0.73	0.20	68,68,68,68	0
55	MG	14	3312	1/1	0.73	0.35	81,81,81,81	0
55	MG	1G	1686	1/1	0.73	0.11	95,95,95,95	0
55	MG	1H	3465	1/1	0.73	0.08	87,87,87,87	0
55	MG	29	304	1/1	0.73	0.45	89,89,89,89	0
55	MG	39	301	1/1	0.73	0.17	83,83,83,83	0
55	MG	1G	1636	1/1	0.73	0.32	80,80,80,80	0
55	MG	1H	3221	1/1	0.73	0.27	108,108,108,108	0
55	MG	14	3311	1/1	0.74	0.27	87,87,87,87	0
55	MG	13	1737	1/1	0.74	0.07	111,111,111,111	0
55	MG	14	3306	1/1	0.74	0.14	74,74,74,74	0
55	MG	14	3353	1/1	0.74	0.28	84,84,84,84	0
55	MG	14	3436	1/1	0.74	0.14	107,107,107,107	0
55	MG	1H	3366	1/1	0.74	0.29	84,84,84,84	0
55	MG	1H	3196	1/1	0.74	0.41	80,80,80,80	0
55	MG	16	209	1/1	0.74	0.25	80,80,80,80	0
55	MG	14	3283	1/1	0.74	0.32	87,87,87,87	0
55	MG	1H	3231	1/1	0.74	0.53	88,88,88,88	0
55	MG	13	1643	1/1	0.74	0.51	86,86,86,86	0
55	MG	14	3263	1/1	0.74	0.13	72,72,72,72	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
55	MG	13	1645	1/1	0.74	0.49	98,98,98,98	0
55	MG	52	201	1/1	0.74	0.17	84,84,84,84	0
55	MG	1H	3340	1/1	0.75	0.34	77,77,77,77	0
55	MG	4A	201	1/1	0.75	0.34	115,115,115,115	0
55	MG	14	3277	1/1	0.75	0.31	78,78,78,78	0
55	MG	1H	3253	1/1	0.75	0.30	71,71,71,71	0
55	MG	1H	3119	1/1	0.75	0.35	77,77,77,77	0
55	MG	13	1617	1/1	0.75	0.32	122,122,122,122	0
55	MG	14	3325	1/1	0.75	0.36	78,78,78,78	0
55	MG	1G	1683	1/1	0.75	0.31	103,103,103,103	0
55	MG	14	3119	1/1	0.75	0.33	70,70,70,70	0
55	MG	14	3186	1/1	0.75	0.33	113,113,113,113	0
55	MG	11	302	1/1	0.76	0.23	85,85,85,85	0
55	MG	14	3166	1/1	0.76	0.15	71,71,71,71	0
55	MG	1H	3193	1/1	0.76	0.39	77,77,77,77	0
55	MG	1G	1679	1/1	0.76	0.30	97,97,97,97	0
55	MG	14	3354	1/1	0.76	0.31	134,134,134,134	0
55	MG	14	3096	1/1	0.76	0.36	94,94,94,94	0
55	MG	1G	1694	1/1	0.76	0.18	118,118,118,118	0
55	MG	1G	1629	1/1	0.76	0.36	86,86,86,86	0
55	MG	14	3235	1/1	0.76	0.14	63,63,63,63	0
55	MG	14	3182	1/1	0.76	0.17	77,77,77,77	0
55	MG	1G	1708	1/1	0.76	0.22	133,133,133,133	0
55	MG	1H	3298	1/1	0.76	0.37	87,87,87,87	0
55	MG	14	3239	1/1	0.76	0.36	87,87,87,87	0
55	MG	14	3307	1/1	0.76	0.27	89,89,89,89	0
55	MG	13	1671	1/1	0.76	0.15	70,70,70,70	0
55	MG	1H	3351	1/1	0.76	0.25	90,90,90,90	0
55	MG	14	3330	1/1	0.76	0.24	81,81,81,81	0
55	MG	1H	3394	1/1	0.76	0.16	69,69,69,69	0
55	MG	13	1711	1/1	0.76	0.62	90,90,90,90	0
55	MG	1H	3353	1/1	0.76	0.32	83,83,83,83	0
55	MG	1H	3327	1/1	0.76	0.31	63,63,63,63	0
55	MG	14	3273	1/1	0.76	0.18	87,87,87,87	0
55	MG	14	3135	1/1	0.77	0.23	64,64,64,64	0
55	MG	1H	3096	1/1	0.77	0.43	71,71,71,71	0
55	MG	14	3357	1/1	0.77	0.19	76,76,76,76	0
55	MG	13	1731	1/1	0.77	0.14	153,153,153,153	0
55	MG	1H	3469	1/1	0.77	0.15	115,115,115,115	0
55	MG	1G	1709	1/1	0.77	0.21	96,96,96,96	0
55	MG	1H	3140	1/1	0.77	0.20	52,52,52,52	0
55	MG	13	1638	1/1	0.77	0.23	85,85,85,85	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
55	MG	1G	1740	1/1	0.77	0.05	140,140,140,140	0
55	MG	1G	1688	1/1	0.77	0.23	102,102,102,102	0
55	MG	1G	1610	1/1	0.77	0.32	99,99,99,99	0
55	MG	14	3079	1/1	0.77	0.30	82,82,82,82	0
55	MG	14	3218	1/1	0.77	0.39	88,88,88,88	0
55	MG	13	1734	1/1	0.77	0.06	178,178,178,178	0
55	MG	13	1640	1/1	0.77	0.23	89,89,89,89	0
55	MG	1G	1677	1/1	0.77	0.29	89,89,89,89	0
55	MG	14	3262	1/1	0.77	0.37	86,86,86,86	0
55	MG	1H	3406	1/1	0.77	0.53	91,91,91,91	0
55	MG	1H	3265	1/1	0.77	0.17	83,83,83,83	0
55	MG	14	3336	1/1	0.77	0.20	73,73,73,73	0
55	MG	14	3314	1/1	0.78	0.28	105,105,105,105	0
55	MG	13	1624	1/1	0.78	0.36	107,107,107,107	0
55	MG	1H	3356	1/1	0.78	0.53	91,91,91,91	0
55	MG	2K	103	1/1	0.78	0.32	94,94,94,94	0
55	MG	32	301	1/1	0.78	0.42	113,113,113,113	0
55	MG	1H	3105	1/1	0.78	0.36	90,90,90,90	0
55	MG	1H	3106	1/1	0.78	0.40	85,85,85,85	0
55	MG	13	1666	1/1	0.78	0.47	104,104,104,104	0
55	MG	1H	3116	1/1	0.78	0.50	74,74,74,74	0
55	MG	13	1649	1/1	0.78	0.45	84,84,84,84	0
55	MG	14	3206	1/1	0.78	0.23	76,76,76,76	0
55	MG	14	3272	1/1	0.78	0.39	94,94,94,94	0
55	MG	13	1657	1/1	0.78	0.31	74,74,74,74	0
55	MG	14	3228	1/1	0.78	0.25	84,84,84,84	0
55	MG	1H	3349	1/1	0.78	0.15	77,77,77,77	0
55	MG	1H	3297	1/1	0.78	0.33	81,81,81,81	0
55	MG	1J	206	1/1	0.78	0.36	96,96,96,96	0
55	MG	14	3168	1/1	0.78	0.35	76,76,76,76	0
55	MG	1H	3294	1/1	0.78	0.54	85,85,85,85	0
55	MG	1H	3293	1/1	0.78	0.34	95,95,95,95	0
55	MG	1H	3501	1/1	0.78	0.09	99,99,99,99	0
55	MG	1H	3152	1/1	0.78	0.48	80,80,80,80	0
55	MG	13	1709	1/1	0.78	0.27	78,78,78,78	0
55	MG	1H	3311	1/1	0.78	0.55	83,83,83,83	0
55	MG	1H	3134	1/1	0.79	0.33	65,65,65,65	0
55	MG	1H	3058	1/1	0.79	0.47	60,60,60,60	0
55	MG	1H	3149	1/1	0.79	0.46	82,82,82,82	0
55	MG	1H	3388	1/1	0.79	0.34	74,74,74,74	0
55	MG	1H	3088	1/1	0.79	0.21	52,52,52,52	0
55	MG	1H	3357	1/1	0.79	0.35	92,92,92,92	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
55	MG	14	3175	1/1	0.79	0.39	85,85,85,85	0
55	MG	1H	3292	1/1	0.79	0.44	82,82,82,82	0
55	MG	1H	3172	1/1	0.79	0.20	69,69,69,69	0
55	MG	13	1680	1/1	0.79	0.40	77,77,77,77	0
55	MG	1H	3495	1/1	0.79	0.11	79,79,79,79	0
55	MG	14	3449	1/1	0.79	0.08	108,108,108,108	0
55	MG	1H	3339	1/1	0.79	0.45	91,91,91,91	0
55	MG	13	1708	1/1	0.79	0.54	127,127,127,127	0
55	MG	1J	210	1/1	0.79	0.12	144,144,144,144	0
55	MG	1H	3363	1/1	0.79	0.39	104,104,104,104	0
55	MG	1G	1654	1/1	0.79	0.38	91,91,91,91	0
55	MG	14	3321	1/1	0.79	0.37	89,89,89,89	0
55	MG	1H	3033	1/1	0.79	0.20	83,83,83,83	0
55	MG	14	3150	1/1	0.79	0.38	107,107,107,107	0
55	MG	14	3143	1/1	0.80	0.42	87,87,87,87	0
55	MG	14	3230	1/1	0.80	0.28	75,75,75,75	0
55	MG	E5	101	1/1	0.80	0.39	88,88,88,88	0
55	MG	1H	3207	1/1	0.80	0.18	67,67,67,67	0
55	MG	1H	3135	1/1	0.80	0.19	72,72,72,72	0
55	MG	14	3156	1/1	0.80	0.17	75,75,75,75	0
55	MG	1H	3397	1/1	0.80	0.12	94,94,94,94	0
55	MG	1H	3076	1/1	0.80	0.23	77,77,77,77	0
55	MG	14	3147	1/1	0.80	0.39	83,83,83,83	0
55	MG	1H	3146	1/1	0.80	0.23	48,48,48,48	0
55	MG	14	3349	1/1	0.80	0.20	100,100,100,100	0
55	MG	1G	1748	1/1	0.80	0.25	90,90,90,90	0
55	MG	1H	3216	1/1	0.80	0.48	90,90,90,90	0
55	MG	1H	3276	1/1	0.80	0.23	88,88,88,88	0
55	MG	1H	3497	1/1	0.80	0.16	105,105,105,105	0
55	MG	1H	3303	1/1	0.80	0.24	63,63,63,63	0
55	MG	1G	1693	1/1	0.80	0.35	95,95,95,95	0
55	MG	1H	3523	1/1	0.80	0.10	78,78,78,78	0
55	MG	1H	3323	1/1	0.80	0.41	80,80,80,80	0
55	MG	14	3123	1/1	0.80	0.23	50,50,50,50	0
55	MG	1H	3205	1/1	0.80	0.59	103,103,103,103	0
55	MG	1G	1656	1/1	0.80	0.31	94,94,94,94	0
55	MG	14	3361	1/1	0.80	0.30	90,90,90,90	0
55	MG	14	3220	1/1	0.80	0.17	89,89,89,89	0
55	MG	I8	101	1/1	0.80	0.32	83,83,83,83	0
55	MG	1H	3244	1/1	0.80	0.28	55,55,55,55	0
55	MG	1H	3173	1/1	0.81	0.49	90,90,90,90	0
55	MG	13	1715	1/1	0.81	0.23	70,70,70,70	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
55	MG	14	3200	1/1	0.81	0.42	100,100,100,100	0
55	MG	1H	3159	1/1	0.81	0.34	66,66,66,66	0
55	MG	14	3219	1/1	0.81	0.20	67,67,67,67	0
55	MG	1H	3044	1/1	0.81	0.29	98,98,98,98	0
55	MG	13	1697	1/1	0.81	0.41	84,84,84,84	0
55	MG	13	1694	1/1	0.81	0.30	92,92,92,92	0
55	MG	14	3148	1/1	0.81	0.46	86,86,86,86	0
55	MG	14	3431	1/1	0.81	0.10	102,102,102,102	0
55	MG	1H	3325	1/1	0.81	0.39	97,97,97,97	0
55	MG	1G	1618	1/1	0.81	0.26	79,79,79,79	0
55	MG	14	3155	1/1	0.81	0.33	77,77,77,77	0
55	MG	1H	3488	1/1	0.81	0.11	66,66,66,66	0
55	MG	1H	3086	1/1	0.81	0.19	59,59,59,59	0
55	MG	1H	3452	1/1	0.81	0.13	58,58,58,58	0
55	MG	1G	1738	1/1	0.81	0.10	140,140,140,140	0
55	MG	14	3171	1/1	0.81	0.37	86,86,86,86	0
55	MG	1H	3313	1/1	0.81	0.22	91,91,91,91	0
55	MG	14	3459	1/1	0.81	0.05	130,130,130,130	0
55	MG	14	3134	1/1	0.81	0.30	80,80,80,80	0
55	MG	13	1733	1/1	0.81	0.08	141,141,141,141	0
55	MG	45	201	1/1	0.81	0.33	76,76,76,76	0
55	MG	1H	3457	1/1	0.81	0.07	102,102,102,102	0
55	MG	14	3141	1/1	0.81	0.41	85,85,85,85	0
55	MG	1H	3197	1/1	0.81	0.62	85,85,85,85	0
55	MG	1H	3333	1/1	0.82	0.34	81,81,81,81	0
55	MG	1H	3174	1/1	0.82	0.27	89,89,89,89	0
55	MG	1H	3188	1/1	0.82	0.42	81,81,81,81	0
55	MG	14	3142	1/1	0.82	0.30	72,72,72,72	0
55	MG	14	3244	1/1	0.82	0.33	86,86,86,86	0
55	MG	14	3158	1/1	0.82	0.27	97,97,97,97	0
55	MG	14	3297	1/1	0.82	0.26	78,78,78,78	0
55	MG	1G	1646	1/1	0.82	0.23	93,93,93,93	0
55	MG	14	3296	1/1	0.82	0.28	97,97,97,97	0
55	MG	1H	3519	1/1	0.82	0.09	103,103,103,103	0
55	MG	14	3236	1/1	0.82	0.44	94,94,94,94	0
55	MG	1H	3150	1/1	0.82	0.39	78,78,78,78	0
55	MG	1H	3322	1/1	0.82	0.26	92,92,92,92	0
55	MG	14	3157	1/1	0.82	0.40	80,80,80,80	0
55	MG	1J	208	1/1	0.82	0.07	97,97,97,97	0
55	MG	1G	1725	1/1	0.82	0.20	93,93,93,93	0
55	MG	1J	204	1/1	0.82	0.23	101,101,101,101	0
55	MG	14	3087	1/1	0.82	0.27	65,65,65,65	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
55	MG	1H	3514	1/1	0.82	0.10	109,109,109,109	0
55	MG	1H	3030	1/1	0.82	0.29	91,91,91,91	0
55	MG	14	3305	1/1	0.82	0.36	89,89,89,89	0
55	MG	1H	3139	1/1	0.82	0.58	69,69,69,69	0
55	MG	1H	3341	1/1	0.82	0.30	76,76,76,76	0
55	MG	14	3034	1/1	0.82	0.31	73,73,73,73	0
55	MG	14	3308	1/1	0.83	0.20	80,80,80,80	0
55	MG	13	1660	1/1	0.83	0.38	80,80,80,80	0
55	MG	1G	1676	1/1	0.83	0.39	98,98,98,98	0
55	MG	1H	3132	1/1	0.83	0.36	76,76,76,76	0
55	MG	13	1677	1/1	0.83	0.16	83,83,83,83	0
55	MG	13	1713	1/1	0.83	0.33	100,100,100,100	0
55	MG	1H	3263	1/1	0.83	0.46	84,84,84,84	0
55	MG	1G	1660	1/1	0.83	0.10	87,87,87,87	0
55	MG	1H	3493	1/1	0.83	0.08	103,103,103,103	0
55	MG	1H	3260	1/1	0.83	0.22	70,70,70,70	0
55	MG	1H	3075	1/1	0.83	0.53	87,87,87,87	0
55	MG	1H	3103	1/1	0.83	0.41	71,71,71,71	0
55	MG	1G	1664	1/1	0.83	0.28	104,104,104,104	0
55	MG	1H	3118	1/1	0.83	0.37	83,83,83,83	0
55	MG	14	3323	1/1	0.83	0.25	87,87,87,87	0
55	MG	C5	201	1/1	0.83	0.26	86,86,86,86	0
55	MG	1H	3284	1/1	0.83	0.42	73,73,73,73	0
55	MG	1G	1727	1/1	0.83	0.24	104,104,104,104	0
55	MG	14	3317	1/1	0.83	0.36	83,83,83,83	0
55	MG	13	1646	1/1	0.83	0.39	90,90,90,90	0
55	MG	13	1702	1/1	0.83	0.24	147,147,147,147	0
55	MG	14	3295	1/1	0.83	0.18	72,72,72,72	0
55	MG	13	1655	1/1	0.83	0.31	92,92,92,92	0
55	MG	1G	1624	1/1	0.83	0.33	78,78,78,78	0
55	MG	14	3302	1/1	0.83	0.26	91,91,91,91	0
55	MG	1H	3175	1/1	0.84	0.54	74,74,74,74	0
55	MG	1H	3182	1/1	0.84	0.12	70,70,70,70	0
55	MG	1H	3032	1/1	0.84	0.35	95,95,95,95	0
55	MG	1J	203	1/1	0.84	0.10	92,92,92,92	0
55	MG	1H	3520	1/1	0.84	0.06	103,103,103,103	0
55	MG	14	3338	1/1	0.84	0.17	78,78,78,78	0
55	MG	14	3088	1/1	0.84	0.35	70,70,70,70	0
55	MG	1H	3200	1/1	0.84	0.29	99,99,99,99	0
55	MG	1G	1627	1/1	0.84	0.46	93,93,93,93	0
55	MG	1G	1674	1/1	0.84	0.34	111,111,111,111	0
55	MG	1H	3517	1/1	0.84	0.06	113,113,113,113	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
55	MG	1G	1671	1/1	0.84	0.15	92,92,92,92	0
55	MG	1G	1689	1/1	0.84	0.26	90,90,90,90	0
55	MG	14	3298	1/1	0.84	0.32	69,69,69,69	0
55	MG	14	3103	1/1	0.84	0.25	58,58,58,58	0
55	MG	1G	1642	1/1	0.84	0.26	87,87,87,87	0
55	MG	14	3210	1/1	0.84	0.15	68,68,68,68	0
55	MG	1H	3510	1/1	0.84	0.05	111,111,111,111	0
55	MG	1G	1667	1/1	0.84	0.31	103,103,103,103	0
55	MG	1H	3344	1/1	0.84	0.32	84,84,84,84	0
55	MG	1H	3157	1/1	0.84	0.28	79,79,79,79	0
55	MG	1H	3376	1/1	0.84	0.46	94,94,94,94	0
55	MG	1H	3482	1/1	0.84	0.10	70,70,70,70	0
55	MG	1H	3391	1/1	0.84	0.37	92,92,92,92	0
55	MG	1H	3508	1/1	0.84	0.06	119,119,119,119	0
55	MG	14	3324	1/1	0.84	0.36	101,101,101,101	0
55	MG	14	3105	1/1	0.84	0.38	72,72,72,72	0
55	MG	1H	3281	1/1	0.84	0.52	80,80,80,80	0
55	MG	1H	3268	1/1	0.84	0.39	100,100,100,100	0
55	MG	13	1613	1/1	0.84	0.29	99,99,99,99	0
55	MG	14	3188	1/1	0.84	0.37	76,76,76,76	0
55	MG	13	1618	1/1	0.84	0.29	96,96,96,96	0
55	MG	14	3181	1/1	0.85	0.29	70,70,70,70	0
55	MG	1H	3124	1/1	0.85	0.33	59,59,59,59	0
55	MG	1H	3359	1/1	0.85	0.14	77,77,77,77	0
55	MG	7E	201	1/1	0.85	0.33	83,83,83,83	0
55	MG	14	3285	1/1	0.85	0.31	93,93,93,93	0
55	MG	1H	3269	1/1	0.85	0.33	82,82,82,82	0
55	MG	1G	1684	1/1	0.85	0.41	99,99,99,99	0
55	MG	14	3326	1/1	0.85	0.16	90,90,90,90	0
55	MG	14	3461	1/1	0.85	0.09	82,82,82,82	0
55	MG	14	3279	1/1	0.85	0.44	84,84,84,84	0
55	MG	13	1692	1/1	0.85	0.44	132,132,132,132	0
55	MG	14	3221	1/1	0.85	0.12	76,76,76,76	0
55	MG	1H	3477	1/1	0.85	0.12	74,74,74,74	0
55	MG	14	3288	1/1	0.85	0.07	171,171,171,171	0
55	MG	14	3360	1/1	0.85	0.19	74,74,74,74	0
55	MG	14	3121	1/1	0.85	0.20	54,54,54,54	0
55	MG	1G	1650	1/1	0.85	0.26	90,90,90,90	0
55	MG	1H	3499	1/1	0.85	0.09	111,111,111,111	0
55	MG	1H	3318	1/1	0.85	0.16	75,75,75,75	0
55	MG	13	1667	1/1	0.85	0.43	94,94,94,94	0
55	MG	1H	3266	1/1	0.85	0.33	101,101,101,101	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
55	MG	1G	1632	1/1	0.85	0.30	79,79,79,79	0
55	MG	1H	3199	1/1	0.85	0.19	72,72,72,72	0
55	MG	1H	3291	1/1	0.85	0.19	68,68,68,68	0
55	MG	13	1658	1/1	0.85	0.37	108,108,108,108	0
55	MG	1H	3164	1/1	0.85	0.46	90,90,90,90	0
55	MG	13	1637	1/1	0.85	0.50	90,90,90,90	0
55	MG	1H	3066	1/1	0.85	0.41	70,70,70,70	0
55	MG	14	3274	1/1	0.85	0.11	69,69,69,69	0
55	MG	14	3376	1/1	0.85	0.10	66,66,66,66	0
55	MG	1H	3256	1/1	0.85	0.19	78,78,78,78	0
55	MG	1H	3213	1/1	0.85	0.24	84,84,84,84	0
55	MG	1H	3065	1/1	0.85	0.34	64,64,64,64	0
55	MG	14	3356	1/1	0.85	0.23	195,195,195,195	0
55	MG	14	3093	1/1	0.85	0.24	84,84,84,84	0
55	MG	1G	1672	1/1	0.85	0.28	79,79,79,79	0
55	MG	14	3185	1/1	0.85	0.34	90,90,90,90	0
55	MG	14	3163	1/1	0.85	0.23	80,80,80,80	0
55	MG	14	3036	1/1	0.85	0.29	91,91,91,91	0
55	MG	1H	3399	1/1	0.85	0.22	77,77,77,77	0
55	MG	14	3304	1/1	0.85	0.45	99,99,99,99	0
55	MG	14	3106	1/1	0.85	0.44	75,75,75,75	0
55	MG	14	3420	1/1	0.85	0.07	89,89,89,89	0
55	MG	14	3343	1/1	0.86	0.30	86,86,86,86	0
55	MG	14	3265	1/1	0.86	0.38	76,76,76,76	0
55	MG	1G	1640	1/1	0.86	0.45	107,107,107,107	0
55	MG	13	1714	1/1	0.86	0.57	117,117,117,117	0
55	MG	14	3267	1/1	0.86	0.12	90,90,90,90	0
55	MG	14	3313	1/1	0.86	0.14	86,86,86,86	0
55	MG	13	1682	1/1	0.86	0.43	85,85,85,85	0
55	MG	1G	1707	1/1	0.86	0.42	90,90,90,90	0
55	MG	1H	3509	1/1	0.86	0.07	85,85,85,85	0
55	MG	14	3293	1/1	0.86	0.15	75,75,75,75	0
55	MG	16	210	1/1	0.86	0.15	96,96,96,96	0
55	MG	1H	3300	1/1	0.86	0.30	77,77,77,77	0
55	MG	13	1605	1/1	0.86	0.17	84,84,84,84	0
55	MG	13	1686	1/1	0.86	0.39	85,85,85,85	0
55	MG	1G	1658	1/1	0.86	0.14	99,99,99,99	0
55	MG	1H	3064	1/1	0.86	0.35	70,70,70,70	0
55	MG	1H	3069	1/1	0.86	0.28	51,51,51,51	0
55	MG	1G	1635	1/1	0.86	0.48	70,70,70,70	0
55	MG	13	1707	1/1	0.86	0.26	100,100,100,100	0
55	MG	14	3464	1/1	0.86	0.06	101,101,101,101	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
55	MG	1H	3239	1/1	0.86	0.32	74,74,74,74	0
55	MG	1H	3181	1/1	0.86	0.33	62,62,62,62	0
55	MG	14	3140	1/1	0.86	0.38	77,77,77,77	0
55	MG	1H	3369	1/1	0.86	0.14	94,94,94,94	0
55	MG	1H	3314	1/1	0.86	0.38	97,97,97,97	0
55	MG	14	3054	1/1	0.86	0.35	81,81,81,81	0
55	MG	11	301	1/1	0.86	0.21	54,54,54,54	0
55	MG	1J	209	1/1	0.86	0.09	128,128,128,128	0
55	MG	1H	3235	1/1	0.86	0.52	88,88,88,88	0
55	MG	14	3442	1/1	0.86	0.04	107,107,107,107	0
55	MG	13	1705	1/1	0.86	0.30	76,76,76,76	0
55	MG	14	3037	1/1	0.86	0.34	71,71,71,71	0
55	MG	19	301	1/1	0.86	0.21	67,67,67,67	0
55	MG	13	1661	1/1	0.86	0.42	95,95,95,95	0
55	MG	1H	3148	1/1	0.86	0.18	86,86,86,86	0
55	MG	1G	1704	1/1	0.86	0.23	117,117,117,117	0
55	MG	14	3310	1/1	0.86	0.49	75,75,75,75	0
55	MG	1G	1678	1/1	0.86	0.35	102,102,102,102	0
55	MG	14	3280	1/1	0.86	0.24	75,75,75,75	0
55	MG	14	3378	1/1	0.86	0.14	78,78,78,78	0
55	MG	1G	1700	1/1	0.87	0.35	94,94,94,94	0
55	MG	1H	3204	1/1	0.87	0.44	83,83,83,83	0
55	MG	1H	3038	1/1	0.87	0.20	59,59,59,59	0
55	MG	2L	104	1/1	0.87	0.07	93,93,93,93	0
55	MG	1G	1720	1/1	0.87	0.31	95,95,95,95	0
55	MG	1H	3227	1/1	0.87	0.28	76,76,76,76	0
55	MG	14	3179	1/1	0.87	0.33	88,88,88,88	0
55	MG	1H	3410	1/1	0.87	0.10	52,52,52,52	0
55	MG	13	1678	1/1	0.87	0.35	104,104,104,104	0
55	MG	14	3462	1/1	0.87	0.04	130,130,130,130	0
55	MG	1H	3329	1/1	0.87	0.40	85,85,85,85	0
55	MG	14	3199	1/1	0.87	0.23	60,60,60,60	0
55	MG	14	3085	1/1	0.87	0.31	72,72,72,72	0
55	MG	1H	3041	1/1	0.87	0.22	63,63,63,63	0
55	MG	1G	1710	1/1	0.87	0.23	101,101,101,101	0
55	MG	1H	3211	1/1	0.87	0.37	79,79,79,79	0
55	MG	14	3184	1/1	0.87	0.23	71,71,71,71	0
55	MG	14	3117	1/1	0.87	0.33	93,93,93,93	0
55	MG	1H	3068	1/1	0.87	0.25	61,61,61,61	0
55	MG	1G	1652	1/1	0.87	0.33	82,82,82,82	0
55	MG	14	3271	1/1	0.87	0.20	82,82,82,82	0
55	MG	13	1607	1/1	0.87	0.34	86,86,86,86	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
55	MG	I8	103	1/1	0.87	0.39	92,92,92,92	0
55	MG	14	3208	1/1	0.87	0.23	88,88,88,88	0
55	MG	1G	1609	1/1	0.87	0.37	99,99,99,99	0
55	MG	1H	3238	1/1	0.87	0.56	82,82,82,82	0
55	MG	2K	105	1/1	0.87	0.21	76,76,76,76	0
55	MG	1H	3309	1/1	0.87	0.24	85,85,85,85	0
55	MG	1H	3194	1/1	0.87	0.32	68,68,68,68	0
55	MG	1H	3374	1/1	0.87	0.31	67,67,67,67	0
55	MG	14	3268	1/1	0.87	0.38	85,85,85,85	0
55	MG	13	1614	1/1	0.87	0.24	95,95,95,95	0
55	MG	14	3438	1/1	0.87	0.08	83,83,83,83	0
55	MG	14	3126	1/1	0.87	0.32	83,83,83,83	0
55	MG	13	1710	1/1	0.88	0.13	103,103,103,103	0
55	MG	14	3234	1/1	0.88	0.16	51,51,51,51	0
55	MG	14	3284	1/1	0.88	0.23	95,95,95,95	0
55	MG	1H	3277	1/1	0.88	0.33	74,74,74,74	0
55	MG	1G	1673	1/1	0.88	0.22	88,88,88,88	0
55	MG	14	3342	1/1	0.88	0.45	94,94,94,94	0
55	MG	1H	3176	1/1	0.88	0.38	73,73,73,73	0
55	MG	1H	3078	1/1	0.88	0.30	71,71,71,71	0
55	MG	1H	3177	1/1	0.88	0.21	69,69,69,69	0
55	MG	1H	3092	1/1	0.88	0.43	62,62,62,62	0
55	MG	13	1685	1/1	0.88	0.12	89,89,89,89	0
55	MG	14	3205	1/1	0.88	0.40	70,70,70,70	0
55	MG	1H	3305	1/1	0.88	0.17	104,104,104,104	0
55	MG	1G	1614	1/1	0.88	0.28	92,92,92,92	0
55	MG	1H	3504	1/1	0.88	0.07	80,80,80,80	0
55	MG	14	3457	1/1	0.88	0.06	125,125,125,125	0
55	MG	14	3100	1/1	0.88	0.21	79,79,79,79	0
55	MG	14	3362	1/1	0.88	0.29	111,111,111,111	0
55	MG	1H	3502	1/1	0.88	0.06	148,148,148,148	0
55	MG	25	201	1/1	0.88	0.08	111,111,111,111	0
55	MG	14	3099	1/1	0.88	0.22	67,67,67,67	0
55	MG	14	3433	1/1	0.88	0.07	87,87,87,87	0
55	MG	14	3197	1/1	0.88	0.26	81,81,81,81	0
55	MG	14	3196	1/1	0.88	0.10	60,60,60,60	0
55	MG	14	3358	1/1	0.88	0.17	85,85,85,85	0
55	MG	1H	3491	1/1	0.88	0.14	52,52,52,52	0
55	MG	1G	1655	1/1	0.88	0.33	74,74,74,74	0
55	MG	1G	1607	1/1	0.88	0.28	95,95,95,95	0
55	MG	1H	3104	1/1	0.88	0.18	85,85,85,85	0
55	MG	15	201	1/1	0.88	0.16	99,99,99,99	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
55	MG	16	207	1/1	0.88	0.46	85,85,85,85	0
55	MG	13	1632	1/1	0.88	0.49	74,74,74,74	0
55	MG	1H	3170	1/1	0.88	0.42	89,89,89,89	0
55	MG	13	1615	1/1	0.88	0.37	98,98,98,98	0
55	MG	1G	1687	1/1	0.88	0.25	79,79,79,79	0
55	MG	13	1625	1/1	0.88	0.46	95,95,95,95	0
55	MG	14	3149	1/1	0.88	0.18	66,66,66,66	0
55	MG	1H	3401	1/1	0.88	0.26	67,67,67,67	0
55	MG	1H	3258	1/1	0.88	0.50	91,91,91,91	0
55	MG	1G	1615	1/1	0.88	0.19	78,78,78,78	0
55	MG	1H	3262	1/1	0.88	0.09	71,71,71,71	0
55	MG	14	3224	1/1	0.88	0.16	112,112,112,112	0
55	MG	13	1652	1/1	0.88	0.30	88,88,88,88	0
55	MG	14	3260	1/1	0.88	0.31	99,99,99,99	0
55	MG	1H	3029	1/1	0.89	0.24	71,71,71,71	0
55	MG	1G	1626	1/1	0.89	0.26	107,107,107,107	0
55	MG	16	212	1/1	0.89	0.13	85,85,85,85	0
55	MG	1H	3037	1/1	0.89	0.33	60,60,60,60	0
55	MG	16	213	1/1	0.89	0.15	113,113,113,113	0
55	MG	1H	3372	1/1	0.89	0.38	94,94,94,94	0
55	MG	1G	1662	1/1	0.89	0.41	84,84,84,84	0
55	MG	1H	3390	1/1	0.89	0.36	88,88,88,88	0
55	MG	1H	3316	1/1	0.89	0.23	61,61,61,61	0
55	MG	13	1674	1/1	0.89	0.36	106,106,106,106	0
55	MG	1H	3154	1/1	0.89	0.45	79,79,79,79	0
55	MG	1H	3332	1/1	0.89	0.47	87,87,87,87	0
55	MG	1H	3513	1/1	0.89	0.08	116,116,116,116	0
55	MG	13	1722	1/1	0.89	0.18	101,101,101,101	0
55	MG	14	3370	1/1	0.89	0.27	75,75,75,75	0
55	MG	1H	3008	1/1	0.89	0.30	44,44,44,44	0
55	MG	14	3152	1/1	0.89	0.31	72,72,72,72	0
55	MG	14	3020	1/1	0.89	0.33	72,72,72,72	0
55	MG	1H	3184	1/1	0.89	0.47	85,85,85,85	0
55	MG	1J	202	1/1	0.89	0.45	90,90,90,90	0
55	MG	1G	1668	1/1	0.89	0.27	82,82,82,82	0
55	MG	14	3081	1/1	0.89	0.32	70,70,70,70	0
55	MG	1H	3512	1/1	0.89	0.08	115,115,115,115	0
55	MG	14	3455	1/1	0.89	0.11	108,108,108,108	0
55	MG	13	1653	1/1	0.89	0.35	104,104,104,104	0
55	MG	13	1701	1/1	0.89	0.33	100,100,100,100	0
55	MG	14	3425	1/1	0.89	0.08	96,96,96,96	0
55	MG	14	3080	1/1	0.89	0.52	81,81,81,81	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
55	MG	14	3136	1/1	0.89	0.39	75,75,75,75	0
55	MG	1G	1724	1/1	0.89	0.21	99,99,99,99	0
55	MG	1H	3310	1/1	0.89	0.41	72,72,72,72	0
55	MG	1H	3381	1/1	0.89	0.61	62,62,62,62	0
55	MG	14	3187	1/1	0.89	0.41	94,94,94,94	0
55	MG	14	3350	1/1	0.89	0.29	77,77,77,77	0
55	MG	1G	1651	1/1	0.89	0.39	96,96,96,96	0
55	MG	14	3144	1/1	0.89	0.47	98,98,98,98	0
55	MG	1H	3273	1/1	0.89	0.39	103,103,103,103	0
55	MG	14	3167	1/1	0.89	0.20	83,83,83,83	0
55	MG	14	3463	1/1	0.89	0.11	130,130,130,130	0
55	MG	1H	3093	1/1	0.89	0.48	82,82,82,82	0
55	MG	1H	3201	1/1	0.89	0.41	66,66,66,66	0
55	MG	1H	3131	1/1	0.89	0.33	75,75,75,75	0
55	MG	1H	3280	1/1	0.89	0.18	70,70,70,70	0
55	MG	Q8	102	1/1	0.89	0.31	81,81,81,81	0
55	MG	1H	3393	1/1	0.89	0.14	62,62,62,62	0
55	MG	1H	3179	1/1	0.89	0.17	60,60,60,60	0
55	MG	13	1676	1/1	0.89	0.37	84,84,84,84	0
55	MG	13	1736	1/1	0.89	0.08	132,132,132,132	0
55	MG	14	3074	1/1	0.89	0.16	47,47,47,47	0
55	MG	13	1650	1/1	0.89	0.40	88,88,88,88	0
55	MG	1H	3443	1/1	0.89	0.09	75,75,75,75	0
55	MG	1H	3212	1/1	0.89	0.22	78,78,78,78	0
55	MG	14	3241	1/1	0.89	0.30	89,89,89,89	0
55	MG	13	1662	1/1	0.89	0.26	86,86,86,86	0
55	MG	13	1651	1/1	0.89	0.31	73,73,73,73	0
55	MG	1H	3500	1/1	0.89	0.06	65,65,65,65	0
55	MG	1H	3278	1/1	0.89	0.45	76,76,76,76	0
55	MG	14	3369	1/1	0.89	0.21	78,78,78,78	0
55	MG	14	3001	1/1	0.89	0.24	70,70,70,70	0
55	MG	14	3019	1/1	0.89	0.34	68,68,68,68	0
55	MG	I8	102	1/1	0.89	0.38	65,65,65,65	0
55	MG	1G	1723	1/1	0.89	0.24	98,98,98,98	0
55	MG	1H	3486	1/1	0.89	0.07	79,79,79,79	0
55	MG	14	3414	1/1	0.89	0.10	56,56,56,56	0
55	MG	1G	1733	1/1	0.90	0.09	93,93,93,93	0
55	MG	14	3315	1/1	0.90	0.38	85,85,85,85	0
55	MG	1H	3034	1/1	0.90	0.14	54,54,54,54	0
55	MG	1H	3165	1/1	0.90	0.40	74,74,74,74	0
55	MG	1H	3522	1/1	0.90	0.15	68,68,68,68	0
55	MG	14	3424	1/1	0.90	0.08	81,81,81,81	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
55	MG	14	3333	1/1	0.90	0.15	89,89,89,89	0
55	MG	1H	3163	1/1	0.90	0.29	82,82,82,82	0
55	MG	1H	3362	1/1	0.90	0.41	103,103,103,103	0
55	MG	1G	1675	1/1	0.90	0.26	99,99,99,99	0
55	MG	1G	1643	1/1	0.90	0.31	106,106,106,106	0
55	MG	14	3439	1/1	0.90	0.07	101,101,101,101	0
55	MG	1G	1744	1/1	0.90	0.08	128,128,128,128	0
55	MG	14	3246	1/1	0.90	0.21	83,83,83,83	0
55	MG	14	3138	1/1	0.90	0.29	58,58,58,58	0
55	MG	13	1696	1/1	0.90	0.19	86,86,86,86	0
55	MG	1H	3084	1/1	0.90	0.32	62,62,62,62	0
55	MG	1H	3063	1/1	0.90	0.32	63,63,63,63	0
55	MG	98	201	1/1	0.90	0.34	89,89,89,89	0
55	MG	14	3364	1/1	0.90	0.09	68,68,68,68	0
55	MG	1G	1696	1/1	0.90	0.11	92,92,92,92	0
55	MG	14	3217	1/1	0.90	0.26	55,55,55,55	0
55	MG	1H	3272	1/1	0.90	0.31	76,76,76,76	0
55	MG	16	205	1/1	0.90	0.09	109,109,109,109	0
55	MG	14	3056	1/1	0.90	0.29	75,75,75,75	0
55	MG	14	3341	1/1	0.90	0.18	95,95,95,95	0
55	MG	1H	3334	1/1	0.90	0.23	108,108,108,108	0
55	MG	1G	1630	1/1	0.90	0.42	81,81,81,81	0
55	MG	14	3328	1/1	0.90	0.42	115,115,115,115	0
55	MG	14	3227	1/1	0.90	0.23	80,80,80,80	0
55	MG	13	1665	1/1	0.90	0.10	90,90,90,90	0
55	MG	14	3290	1/1	0.90	0.33	77,77,77,77	0
55	MG	14	3017	1/1	0.90	0.25	83,83,83,83	0
55	MG	1H	3304	1/1	0.90	0.36	82,82,82,82	0
55	MG	88	201	1/1	0.90	0.25	98,98,98,98	0
55	MG	1G	1633	1/1	0.90	0.48	80,80,80,80	0
55	MG	1H	3254	1/1	0.90	0.20	69,69,69,69	0
55	MG	14	3242	1/1	0.90	0.33	86,86,86,86	0
55	MG	14	3172	1/1	0.90	0.19	85,85,85,85	0
55	MG	1H	3324	1/1	0.90	0.26	66,66,66,66	0
55	MG	14	3299	1/1	0.90	0.42	100,100,100,100	0
55	MG	14	3385	1/1	0.90	0.13	73,73,73,73	0
55	MG	1G	1734	1/1	0.90	0.07	81,81,81,81	0
55	MG	1H	3108	1/1	0.90	0.38	77,77,77,77	0
55	MG	14	3270	1/1	0.90	0.39	76,76,76,76	0
55	MG	1H	3335	1/1	0.90	0.41	70,70,70,70	0
55	MG	1H	3226	1/1	0.90	0.30	114,114,114,114	0
55	MG	14	3294	1/1	0.90	0.11	81,81,81,81	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
55	MG	13	1681	1/1	0.90	0.39	104,104,104,104	0
55	MG	1G	1706	1/1	0.90	0.35	86,86,86,86	0
55	MG	14	3319	1/1	0.90	0.09	89,89,89,89	0
55	MG	1H	3245	1/1	0.90	0.34	86,86,86,86	0
55	MG	1H	3368	1/1	0.91	0.45	72,72,72,72	0
55	MG	1G	1670	1/1	0.91	0.32	92,92,92,92	0
55	MG	14	3327	1/1	0.91	0.43	110,110,110,110	0
55	MG	14	3115	1/1	0.91	0.16	58,58,58,58	0
55	MG	14	3278	1/1	0.91	0.27	84,84,84,84	0
55	MG	1H	3296	1/1	0.91	0.33	84,84,84,84	0
55	MG	14	3363	1/1	0.91	0.14	61,61,61,61	0
55	MG	1H	3285	1/1	0.91	0.09	89,89,89,89	0
55	MG	1H	3247	1/1	0.91	0.28	51,51,51,51	0
55	MG	14	3372	1/1	0.91	0.37	96,96,96,96	0
55	MG	13	1616	1/1	0.91	0.22	141,141,141,141	0
55	MG	13	1727	1/1	0.91	0.12	108,108,108,108	0
55	MG	14	3125	1/1	0.91	0.42	88,88,88,88	0
55	MG	13	1628	1/1	0.91	0.35	71,71,71,71	0
55	MG	14	3023	1/1	0.91	0.13	72,72,72,72	0
55	MG	1H	3389	1/1	0.91	0.40	101,101,101,101	0
55	MG	1H	3169	1/1	0.91	0.46	83,83,83,83	0
55	MG	14	3355	1/1	0.91	0.24	73,73,73,73	0
55	MG	14	3253	1/1	0.91	0.24	105,105,105,105	0
55	MG	14	3402	1/1	0.91	0.07	82,82,82,82	0
55	MG	14	3131	1/1	0.91	0.18	66,66,66,66	0
55	MG	1H	3384	1/1	0.91	0.60	108,108,108,108	0
55	MG	14	3078	1/1	0.91	0.26	60,60,60,60	0
55	MG	1H	3255	1/1	0.91	0.21	92,92,92,92	0
55	MG	1G	1622	1/1	0.91	0.29	86,86,86,86	0
55	MG	1H	3109	1/1	0.91	0.29	76,76,76,76	0
55	MG	1H	3408	1/1	0.91	0.12	54,54,54,54	0
55	MG	13	1704	1/1	0.91	0.20	87,87,87,87	0
55	MG	1H	3400	1/1	0.91	0.34	84,84,84,84	0
55	MG	1H	3345	1/1	0.91	0.29	67,67,67,67	0
55	MG	14	3413	1/1	0.91	0.12	70,70,70,70	0
55	MG	14	3450	1/1	0.91	0.14	105,105,105,105	0
55	MG	1H	3252	1/1	0.91	0.34	98,98,98,98	0
55	MG	1H	3073	1/1	0.91	0.26	77,77,77,77	0
55	MG	1H	3022	1/1	0.91	0.14	60,60,60,60	0
55	MG	14	3109	1/1	0.91	0.36	85,85,85,85	0
55	MG	14	3177	1/1	0.91	0.38	76,76,76,76	0
55	MG	1H	3361	1/1	0.91	0.22	155,155,155,155	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
55	MG	1J	201	1/1	0.91	0.24	100,100,100,100	0
55	MG	1H	3141	1/1	0.91	0.24	65,65,65,65	0
55	MG	1H	3056	1/1	0.91	0.47	68,68,68,68	0
55	MG	14	3094	1/1	0.91	0.34	81,81,81,81	0
55	MG	14	3257	1/1	0.91	0.22	75,75,75,75	0
55	MG	14	3428	1/1	0.91	0.09	69,69,69,69	0
55	MG	1H	3094	1/1	0.91	0.32	60,60,60,60	0
55	MG	1H	3049	1/1	0.91	0.33	71,71,71,71	0
55	MG	14	3212	1/1	0.91	0.14	66,66,66,66	0
55	MG	14	3320	1/1	0.91	0.40	88,88,88,88	0
55	MG	14	3409	1/1	0.91	0.07	64,64,64,64	0
55	MG	1H	3290	1/1	0.91	0.41	80,80,80,80	0
55	MG	1H	3337	1/1	0.91	0.28	94,94,94,94	0
55	MG	14	3026	1/1	0.91	0.19	78,78,78,78	0
55	MG	1G	1665	1/1	0.91	0.15	69,69,69,69	0
55	MG	14	3366	1/1	0.91	0.43	99,99,99,99	0
55	MG	1G	1659	1/1	0.91	0.20	107,107,107,107	0
55	MG	14	3374	1/1	0.91	0.17	52,52,52,52	0
55	MG	14	3334	1/1	0.91	0.24	84,84,84,84	0
55	MG	14	3124	1/1	0.91	0.19	56,56,56,56	0
55	MG	13	1664	1/1	0.91	0.59	93,93,93,93	0
55	MG	14	3446	1/1	0.91	0.07	87,87,87,87	0
55	MG	1H	3160	1/1	0.92	0.43	68,68,68,68	0
55	MG	1H	3236	1/1	0.92	0.47	89,89,89,89	0
55	MG	13	1603	1/1	0.92	0.20	96,96,96,96	0
55	MG	14	3275	1/1	0.92	0.38	90,90,90,90	0
55	MG	1H	3343	1/1	0.92	0.16	90,90,90,90	0
55	MG	14	3434	1/1	0.92	0.11	98,98,98,98	0
55	MG	2L	103	1/1	0.92	0.09	130,130,130,130	0
55	MG	1G	1731	1/1	0.92	0.13	110,110,110,110	0
55	MG	1G	1745	1/1	0.92	0.15	93,93,93,93	0
55	MG	14	3176	1/1	0.92	0.26	63,63,63,63	0
55	MG	Q8	101	1/1	0.92	0.30	99,99,99,99	0
55	MG	1H	3246	1/1	0.92	0.13	48,48,48,48	0
55	MG	1H	3005	1/1	0.92	0.26	44,44,44,44	0
55	MG	1H	3122	1/1	0.92	0.12	82,82,82,82	0
55	MG	14	3276	1/1	0.92	0.18	73,73,73,73	0
55	MG	14	3248	1/1	0.92	0.34	78,78,78,78	0
55	MG	14	3014	1/1	0.92	0.29	84,84,84,84	0
55	MG	1H	3348	1/1	0.92	0.24	88,88,88,88	0
55	MG	13	1642	1/1	0.92	0.46	66,66,66,66	0
55	MG	1G	1698	1/1	0.92	0.26	96,96,96,96	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
55	MG	1H	3288	1/1	0.92	0.25	72,72,72,72	0
55	MG	1H	3138	1/1	0.92	0.50	87,87,87,87	0
55	MG	1H	3448	1/1	0.92	0.11	63,63,63,63	0
55	MG	14	3092	1/1	0.92	0.48	70,70,70,70	0
55	MG	1G	1641	1/1	0.92	0.41	83,83,83,83	0
55	MG	1G	1714	1/1	0.92	0.24	98,98,98,98	0
55	MG	1H	3219	1/1	0.92	0.32	72,72,72,72	0
55	MG	14	3233	1/1	0.92	0.26	67,67,67,67	0
55	MG	14	3432	1/1	0.92	0.12	100,100,100,100	0
55	MG	14	3225	1/1	0.92	0.21	75,75,75,75	0
55	MG	1H	3130	1/1	0.92	0.28	69,69,69,69	0
55	MG	1H	3210	1/1	0.92	0.41	79,79,79,79	0
55	MG	1G	1742	1/1	0.92	0.05	112,112,112,112	0
55	MG	14	3375	1/1	0.92	0.17	51,51,51,51	0
55	MG	1H	3048	1/1	0.92	0.23	58,58,58,58	0
55	MG	14	3120	1/1	0.92	0.43	54,54,54,54	0
55	MG	14	3139	1/1	0.92	0.39	69,69,69,69	0
55	MG	14	3021	1/1	0.92	0.12	63,63,63,63	0
55	MG	1H	3257	1/1	0.92	0.43	83,83,83,83	0
55	MG	1H	3143	1/1	0.92	0.28	73,73,73,73	0
55	MG	13	1620	1/1	0.92	0.36	66,66,66,66	0
55	MG	1J	205	1/1	0.92	0.36	122,122,122,122	0
55	MG	1G	1712	1/1	0.92	0.17	109,109,109,109	0
55	MG	14	3071	1/1	0.92	0.21	62,62,62,62	0
55	MG	16	206	1/1	0.92	0.09	101,101,101,101	0
55	MG	1H	3365	1/1	0.92	0.28	86,86,86,86	0
55	MG	1G	1644	1/1	0.92	0.25	115,115,115,115	0
55	MG	13	1721	1/1	0.92	0.11	88,88,88,88	0
55	MG	1H	3189	1/1	0.92	0.12	83,83,83,83	0
55	MG	13	1726	1/1	0.92	0.13	89,89,89,89	0
55	MG	1H	3373	1/1	0.92	0.47	79,79,79,79	0
55	MG	14	3160	1/1	0.92	0.21	74,74,74,74	0
55	MG	1H	3156	1/1	0.92	0.31	72,72,72,72	0
55	MG	1G	1608	1/1	0.92	0.23	85,85,85,85	0
55	MG	1H	3515	1/1	0.92	0.07	106,106,106,106	0
55	MG	1G	1746	1/1	0.92	0.13	134,134,134,134	0
55	MG	14	3352	1/1	0.92	0.45	93,93,93,93	0
55	MG	1H	3476	1/1	0.92	0.15	59,59,59,59	0
55	MG	14	3226	1/1	0.92	0.12	55,55,55,55	0
55	MG	1H	3224	1/1	0.92	0.50	83,83,83,83	0
55	MG	14	3437	1/1	0.92	0.06	85,85,85,85	0
55	MG	1H	3046	1/1	0.92	0.34	71,71,71,71	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
55	MG	14	3453	1/1	0.92	0.07	76,76,76,76	0
55	MG	14	3254	1/1	0.92	0.37	85,85,85,85	0
55	MG	1H	3117	1/1	0.92	0.35	75,75,75,75	0
55	MG	14	3346	1/1	0.92	0.29	84,84,84,84	0
55	MG	14	3401	1/1	0.92	0.06	82,82,82,82	0
55	MG	1H	3183	1/1	0.92	0.31	63,63,63,63	0
55	MG	14	3178	1/1	0.92	0.27	81,81,81,81	0
55	MG	14	3337	1/1	0.92	0.25	105,105,105,105	0
55	MG	14	3222	1/1	0.92	0.28	79,79,79,79	0
55	MG	13	1663	1/1	0.92	0.29	105,105,105,105	0
55	MG	21	301	1/1	0.92	0.31	58,58,58,58	0
55	MG	14	3322	1/1	0.92	0.09	70,70,70,70	0
55	MG	1H	3338	1/1	0.92	0.10	78,78,78,78	0
55	MG	1H	3434	1/1	0.92	0.11	60,60,60,60	0
55	MG	13	1633	1/1	0.92	0.31	79,79,79,79	0
55	MG	1H	3208	1/1	0.92	0.45	69,69,69,69	0
55	MG	1H	3358	1/1	0.92	0.12	98,98,98,98	0
55	MG	13	1673	1/1	0.92	0.26	109,109,109,109	0
55	MG	1H	3449	1/1	0.92	0.22	94,94,94,94	0
55	MG	1H	3347	1/1	0.93	0.32	72,72,72,72	0
55	MG	14	3213	1/1	0.93	0.32	68,68,68,68	0
55	MG	1H	3230	1/1	0.93	0.40	71,71,71,71	0
55	MG	13	1687	1/1	0.93	0.25	77,77,77,77	0
55	MG	13	1690	1/1	0.93	0.13	118,118,118,118	0
55	MG	14	3443	1/1	0.93	0.05	103,103,103,103	0
55	MG	55	201	1/1	0.93	0.26	68,68,68,68	0
55	MG	14	3042	1/1	0.93	0.29	67,67,67,67	0
55	MG	14	3214	1/1	0.93	0.24	66,66,66,66	0
55	MG	1H	3153	1/1	0.93	0.38	86,86,86,86	0
55	MG	14	3441	1/1	0.93	0.09	86,86,86,86	0
55	MG	1H	3326	1/1	0.93	0.11	78,78,78,78	0
55	MG	14	3421	1/1	0.93	0.05	82,82,82,82	0
55	MG	1H	3506	1/1	0.93	0.09	110,110,110,110	0
55	MG	1H	3414	1/1	0.93	0.15	59,59,59,59	0
55	MG	14	3351	1/1	0.93	0.24	87,87,87,87	0
55	MG	14	3089	1/1	0.93	0.39	71,71,71,71	0
55	MG	14	3430	1/1	0.93	0.10	67,67,67,67	0
55	MG	1H	3431	1/1	0.93	0.14	70,70,70,70	0
55	MG	1G	1737	1/1	0.93	0.07	114,114,114,114	0
55	MG	14	3051	1/1	0.93	0.27	62,62,62,62	0
55	MG	1H	3302	1/1	0.93	0.66	74,74,74,74	0
55	MG	14	3173	1/1	0.93	0.30	70,70,70,70	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
55	MG	1G	1648	1/1	0.93	0.25	89,89,89,89	0
55	MG	1H	3438	1/1	0.93	0.09	60,60,60,60	0
55	MG	13	1604	1/1	0.93	0.10	86,86,86,86	0
55	MG	1H	3271	1/1	0.93	0.09	90,90,90,90	0
55	MG	14	3195	1/1	0.93	0.25	65,65,65,65	0
55	MG	14	3365	1/1	0.93	0.19	78,78,78,78	0
55	MG	21	302	1/1	0.93	0.22	68,68,68,68	0
55	MG	1H	3320	1/1	0.93	0.61	109,109,109,109	0
55	MG	14	3256	1/1	0.93	0.35	67,67,67,67	0
55	MG	14	3129	1/1	0.93	0.39	70,70,70,70	0
55	MG	13	1634	1/1	0.93	0.35	73,73,73,73	0
55	MG	14	3130	1/1	0.93	0.20	72,72,72,72	0
55	MG	14	3162	1/1	0.93	0.42	71,71,71,71	0
55	MG	1H	3233	1/1	0.93	0.16	72,72,72,72	0
55	MG	1H	3250	1/1	0.93	0.09	73,73,73,73	0
55	MG	1H	3243	1/1	0.93	0.17	52,52,52,52	0
55	MG	1G	1645	1/1	0.93	0.12	79,79,79,79	0
55	MG	14	3394	1/1	0.93	0.06	89,89,89,89	0
55	MG	14	3059	1/1	0.93	0.30	60,60,60,60	0
55	MG	13	1672	1/1	0.93	0.23	119,119,119,119	0
55	MG	1H	3114	1/1	0.93	0.08	56,56,56,56	0
55	MG	13	1703	1/1	0.93	0.62	147,147,147,147	0
55	MG	1H	3110	1/1	0.93	0.24	47,47,47,47	0
55	MG	14	3456	1/1	0.93	0.06	102,102,102,102	0
55	MG	1H	3306	1/1	0.93	0.15	83,83,83,83	0
55	MG	14	3211	1/1	0.93	0.30	77,77,77,77	0
55	MG	14	3151	1/1	0.93	0.48	78,78,78,78	0
55	MG	14	3359	1/1	0.93	0.10	89,89,89,89	0
55	MG	1G	1604	1/1	0.93	0.15	78,78,78,78	0
55	MG	13	1623	1/1	0.93	0.21	107,107,107,107	0
55	MG	1H	3229	1/1	0.93	0.12	54,54,54,54	0
55	MG	1H	3042	1/1	0.93	0.12	95,95,95,95	0
55	MG	1H	3195	1/1	0.93	0.19	79,79,79,79	0
55	MG	1G	1680	1/1	0.93	0.39	88,88,88,88	0
55	MG	13	1622	1/1	0.93	0.42	74,74,74,74	0
55	MG	1H	3442	1/1	0.93	0.16	43,43,43,43	0
55	MG	1G	1605	1/1	0.93	0.21	92,92,92,92	0
55	MG	1H	3144	1/1	0.93	0.40	69,69,69,69	0
55	MG	14	3069	1/1	0.93	0.43	96,96,96,96	0
55	MG	1G	1617	1/1	0.93	0.38	71,71,71,71	0
55	MG	14	3435	1/1	0.93	0.07	95,95,95,95	0
55	MG	14	3198	1/1	0.93	0.23	70,70,70,70	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
55	MG	3I	201	1/1	0.93	0.20	80,80,80,80	0
55	MG	14	3416	1/1	0.93	0.12	52,52,52,52	0
55	MG	13	1691	1/1	0.93	0.49	83,83,83,83	0
55	MG	13	1732	1/1	0.93	0.13	128,128,128,128	0
55	MG	1G	1690	1/1	0.93	0.32	98,98,98,98	0
55	MG	1H	3060	1/1	0.94	0.26	80,80,80,80	0
55	MG	1H	3087	1/1	0.94	0.22	49,49,49,49	0
55	MG	1H	3127	1/1	0.94	0.41	60,60,60,60	0
55	MG	1H	3416	1/1	0.94	0.17	71,71,71,71	0
55	MG	14	3238	1/1	0.94	0.41	81,81,81,81	0
55	MG	1G	1637	1/1	0.94	0.35	71,71,71,71	0
55	MG	1H	3059	1/1	0.94	0.26	83,83,83,83	0
55	MG	1H	3380	1/1	0.94	0.45	88,88,88,88	0
55	MG	14	3266	1/1	0.94	0.43	88,88,88,88	0
55	MG	1H	3371	1/1	0.94	0.16	62,62,62,62	0
55	MG	14	3170	1/1	0.94	0.19	79,79,79,79	0
55	MG	1G	1695	1/1	0.94	0.10	86,86,86,86	0
55	MG	14	3018	1/1	0.94	0.08	64,64,64,64	0
55	MG	1H	3427	1/1	0.94	0.08	107,107,107,107	0
55	MG	14	3083	1/1	0.94	0.41	68,68,68,68	0
55	MG	14	3426	1/1	0.94	0.07	91,91,91,91	0
55	MG	1H	3016	1/1	0.94	0.29	56,56,56,56	0
55	MG	1H	3102	1/1	0.94	0.33	49,49,49,49	0
55	MG	14	3045	1/1	0.94	0.22	41,41,41,41	0
55	MG	1H	3331	1/1	0.94	0.23	84,84,84,84	0
55	MG	14	3145	1/1	0.94	0.28	78,78,78,78	0
55	MG	1G	1717	1/1	0.94	0.16	107,107,107,107	0
55	MG	1H	3490	1/1	0.94	0.06	89,89,89,89	0
55	MG	1H	3067	1/1	0.94	0.18	47,47,47,47	0
55	MG	1H	3248	1/1	0.94	0.33	61,61,61,61	0
55	MG	1H	3402	1/1	0.94	0.17	77,77,77,77	0
55	MG	14	3029	1/1	0.94	0.33	51,51,51,51	0
55	MG	1H	3079	1/1	0.94	0.38	66,66,66,66	0
55	MG	1H	3100	1/1	0.94	0.43	61,61,61,61	0
55	MG	14	3066	1/1	0.94	0.17	63,63,63,63	0
55	MG	14	3075	1/1	0.94	0.27	52,52,52,52	0
55	MG	14	3231	1/1	0.94	0.28	76,76,76,76	0
55	MG	13	1639	1/1	0.94	0.29	66,66,66,66	0
55	MG	13	1629	1/1	0.94	0.35	60,60,60,60	0
55	MG	14	3396	1/1	0.94	0.11	67,67,67,67	0
55	MG	1H	3378	1/1	0.94	0.09	91,91,91,91	0
55	MG	13	1717	1/1	0.94	0.12	66,66,66,66	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
55	MG	14	3400	1/1	0.94	0.13	65,65,65,65	0
55	MG	1H	3080	1/1	0.94	0.26	62,62,62,62	0
55	MG	1H	3126	1/1	0.94	0.42	61,61,61,61	0
55	MG	14	3451	1/1	0.94	0.13	74,74,74,74	0
55	MG	16	215	1/1	0.94	0.09	93,93,93,93	0
55	MG	1G	1729	1/1	0.94	0.05	93,93,93,93	0
55	MG	14	3458	1/1	0.94	0.10	108,108,108,108	0
55	MG	13	1679	1/1	0.94	0.34	80,80,80,80	0
55	MG	1H	3478	1/1	0.94	0.08	82,82,82,82	0
55	MG	14	3249	1/1	0.94	0.24	87,87,87,87	0
55	MG	1H	3429	1/1	0.94	0.11	71,71,71,71	0
55	MG	1G	1611	1/1	0.94	0.15	132,132,132,132	0
55	MG	14	3332	1/1	0.94	0.27	83,83,83,83	0
55	MG	14	3030	1/1	0.94	0.32	60,60,60,60	0
55	MG	1H	3484	1/1	0.94	0.06	118,118,118,118	0
55	MG	1H	3223	1/1	0.94	0.34	97,97,97,97	0
55	MG	F5	101	1/1	0.94	0.33	77,77,77,77	0
55	MG	1H	3145	1/1	0.94	0.26	46,46,46,46	0
55	MG	14	3090	1/1	0.94	0.37	70,70,70,70	0
55	MG	13	1735	1/1	0.94	0.04	106,106,106,106	0
55	MG	14	3460	1/1	0.94	0.06	112,112,112,112	0
55	MG	1G	1697	1/1	0.94	0.41	85,85,85,85	0
55	MG	1H	3437	1/1	0.94	0.12	66,66,66,66	0
55	MG	14	3153	1/1	0.94	0.44	82,82,82,82	0
55	MG	14	3052	1/1	0.94	0.37	65,65,65,65	0
55	MG	13	1720	1/1	0.94	0.09	129,129,129,129	0
55	MG	1H	3461	1/1	0.94	0.12	54,54,54,54	0
55	MG	1H	3392	1/1	0.94	0.29	73,73,73,73	0
55	MG	1H	3090	1/1	0.94	0.26	47,47,47,47	0
55	MG	1H	3107	1/1	0.94	0.46	81,81,81,81	0
55	MG	1H	3035	1/1	0.94	0.26	75,75,75,75	0
55	MG	1H	3001	1/1	0.94	0.40	50,50,50,50	0
55	MG	1H	3496	1/1	0.94	0.11	78,78,78,78	0
55	MG	1H	3136	1/1	0.94	0.56	85,85,85,85	0
55	MG	1H	3354	1/1	0.94	0.43	88,88,88,88	0
55	MG	1H	3483	1/1	0.94	0.05	84,84,84,84	0
55	MG	13	1641	1/1	0.94	0.29	67,67,67,67	0
55	MG	1H	3115	1/1	0.94	0.27	51,51,51,51	0
55	MG	1G	1735	1/1	0.94	0.08	96,96,96,96	0
55	MG	1G	1649	1/1	0.94	0.37	93,93,93,93	0
55	MG	13	1669	1/1	0.94	0.46	77,77,77,77	0
55	MG	14	3039	1/1	0.94	0.15	67,67,67,67	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
55	MG	14	3180	1/1	0.95	0.41	82,82,82,82	0
55	MG	13	1612	1/1	0.95	0.32	102,102,102,102	0
55	MG	1H	3466	1/1	0.95	0.15	59,59,59,59	0
55	MG	14	3348	1/1	0.95	0.18	65,65,65,65	0
55	MG	1G	1661	1/1	0.95	0.38	76,76,76,76	0
55	MG	1H	3472	1/1	0.95	0.07	82,82,82,82	0
55	MG	1G	1711	1/1	0.95	0.30	73,73,73,73	0
55	MG	1H	3007	1/1	0.95	0.33	62,62,62,62	0
55	MG	16	202	1/1	0.95	0.26	84,84,84,84	0
55	MG	14	3033	1/1	0.95	0.30	71,71,71,71	0
55	MG	1H	3460	1/1	0.95	0.06	87,87,87,87	0
55	MG	1H	3409	1/1	0.95	0.12	62,62,62,62	0
55	MG	1H	3054	1/1	0.95	0.39	51,51,51,51	0
55	MG	1H	3428	1/1	0.95	0.10	74,74,74,74	0
55	MG	1G	1657	1/1	0.95	0.29	87,87,87,87	0
55	MG	13	1718	1/1	0.95	0.12	85,85,85,85	0
55	MG	14	3247	1/1	0.95	0.07	79,79,79,79	0
55	MG	14	3204	1/1	0.95	0.36	70,70,70,70	0
55	MG	1H	3155	1/1	0.95	0.28	38,38,38,38	0
55	MG	1H	3321	1/1	0.95	0.48	79,79,79,79	0
55	MG	14	3041	1/1	0.95	0.32	58,58,58,58	0
55	MG	1H	3471	1/1	0.95	0.08	71,71,71,71	0
55	MG	1H	3055	1/1	0.95	0.47	77,77,77,77	0
55	MG	14	3118	1/1	0.95	0.22	84,84,84,84	0
55	MG	1H	3057	1/1	0.95	0.26	84,84,84,84	0
55	MG	1G	1612	1/1	0.95	0.06	84,84,84,84	0
55	MG	13	1659	1/1	0.95	0.33	102,102,102,102	0
55	MG	14	3229	1/1	0.95	0.21	64,64,64,64	0
55	MG	1H	3459	1/1	0.95	0.08	75,75,75,75	0
55	MG	1H	3287	1/1	0.95	0.38	78,78,78,78	0
55	MG	1H	3267	1/1	0.95	0.27	57,57,57,57	0
55	MG	14	3371	1/1	0.95	0.24	84,84,84,84	0
55	MG	1H	3028	1/1	0.95	0.17	53,53,53,53	0
55	MG	14	3245	1/1	0.95	0.40	64,64,64,64	0
55	MG	14	3070	1/1	0.95	0.34	66,66,66,66	0
55	MG	1G	1681	1/1	0.95	0.36	88,88,88,88	0
55	MG	14	3146	1/1	0.95	0.39	64,64,64,64	0
55	MG	14	3044	1/1	0.95	0.16	43,43,43,43	0
55	MG	14	3061	1/1	0.95	0.32	70,70,70,70	0
55	MG	1H	3439	1/1	0.95	0.09	92,92,92,92	0
55	MG	1G	1747	1/1	0.95	0.26	86,86,86,86	0
55	MG	1H	3251	1/1	0.95	0.32	56,56,56,56	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
55	MG	2K	101	1/1	0.95	0.25	118,118,118,118	0
55	MG	1H	3098	1/1	0.95	0.21	42,42,42,42	0
55	MG	13	1654	1/1	0.95	0.39	72,72,72,72	0
55	MG	14	3380	1/1	0.95	0.12	79,79,79,79	0
55	MG	1G	1621	1/1	0.95	0.20	91,91,91,91	0
55	MG	1H	3112	1/1	0.95	0.47	73,73,73,73	0
55	MG	1G	1603	1/1	0.95	0.35	76,76,76,76	0
55	MG	1G	1619	1/1	0.95	0.34	73,73,73,73	0
55	MG	14	3454	1/1	0.95	0.14	106,106,106,106	0
55	MG	1H	3077	1/1	0.95	0.28	59,59,59,59	0
55	MG	14	3046	1/1	0.95	0.27	75,75,75,75	0
55	MG	1H	3125	1/1	0.95	0.36	73,73,73,73	0
56	ZN	5A	101	1/1	0.95	0.11	133,133,133,133	0
55	MG	14	3028	1/1	0.95	0.25	77,77,77,77	0
55	MG	16	201	1/1	0.95	0.15	110,110,110,110	0
55	MG	13	1724	1/1	0.95	0.14	107,107,107,107	0
55	MG	14	3133	1/1	0.95	0.35	71,71,71,71	0
55	MG	1H	3289	1/1	0.95	0.16	78,78,78,78	0
55	MG	14	3137	1/1	0.95	0.30	69,69,69,69	0
55	MG	1H	3475	1/1	0.95	0.09	70,70,70,70	0
55	MG	13	1670	1/1	0.95	0.11	106,106,106,106	0
55	MG	14	3110	1/1	0.95	0.34	63,63,63,63	0
55	MG	14	3192	1/1	0.95	0.09	56,56,56,56	0
55	MG	14	3091	1/1	0.95	0.35	81,81,81,81	0
55	MG	14	3395	1/1	0.95	0.11	65,65,65,65	0
55	MG	14	3165	1/1	0.95	0.18	74,74,74,74	0
55	MG	1H	3425	1/1	0.95	0.13	61,61,61,61	0
55	MG	13	1601	1/1	0.95	0.21	103,103,103,103	0
55	MG	1H	3383	1/1	0.95	0.12	60,60,60,60	0
55	MG	14	3068	1/1	0.95	0.33	66,66,66,66	0
55	MG	14	3429	1/1	0.95	0.10	77,77,77,77	0
55	MG	14	3108	1/1	0.95	0.36	85,85,85,85	0
55	MG	1H	3404	1/1	0.95	0.30	80,80,80,80	0
55	MG	14	3025	1/1	0.95	0.35	86,86,86,86	0
55	MG	1H	3274	1/1	0.95	0.44	71,71,71,71	0
55	MG	1H	3129	1/1	0.95	0.14	63,63,63,63	0
55	MG	14	3264	1/1	0.95	0.28	84,84,84,84	0
55	MG	1H	3395	1/1	0.95	0.41	76,76,76,76	0
55	MG	2L	101	1/1	0.95	0.21	77,77,77,77	0
55	MG	1H	3006	1/1	0.95	0.27	67,67,67,67	0
55	MG	14	3101	1/1	0.95	0.24	65,65,65,65	0
55	MG	14	3379	1/1	0.95	0.11	53,53,53,53	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
55	MG	14	3098	1/1	0.95	0.33	46,46,46,46	0
56	ZN	32	302	1/1	0.95	0.33	111,111,111,111	0
55	MG	14	3215	1/1	0.95	0.28	76,76,76,76	0
55	MG	13	1627	1/1	0.95	0.48	65,65,65,65	0
55	MG	1H	3202	1/1	0.95	0.13	94,94,94,94	0
55	MG	1H	3433	1/1	0.96	0.12	54,54,54,54	0
55	MG	14	3383	1/1	0.96	0.08	81,81,81,81	0
55	MG	13	1675	1/1	0.96	0.42	85,85,85,85	0
55	MG	1H	3494	1/1	0.96	0.10	81,81,81,81	0
55	MG	1H	3435	1/1	0.96	0.12	76,76,76,76	0
55	MG	1H	3161	1/1	0.96	0.28	69,69,69,69	0
55	MG	14	3427	1/1	0.96	0.07	75,75,75,75	0
55	MG	1H	3214	1/1	0.96	0.31	64,64,64,64	0
55	MG	14	3194	1/1	0.96	0.13	46,46,46,46	0
55	MG	14	3251	1/1	0.96	0.26	67,67,67,67	0
55	MG	1H	3191	1/1	0.96	0.51	64,64,64,64	0
55	MG	1H	3074	1/1	0.96	0.34	82,82,82,82	0
55	MG	1H	3403	1/1	0.96	0.07	111,111,111,111	0
55	MG	14	3407	1/1	0.96	0.09	83,83,83,83	0
55	MG	14	3340	1/1	0.96	0.22	79,79,79,79	0
55	MG	14	3027	1/1	0.96	0.17	71,71,71,71	0
55	MG	1H	3097	1/1	0.96	0.39	70,70,70,70	0
55	MG	14	3408	1/1	0.96	0.11	56,56,56,56	0
55	MG	14	3024	1/1	0.96	0.23	49,49,49,49	0
55	MG	1G	1713	1/1	0.96	0.23	107,107,107,107	0
55	MG	14	3344	1/1	0.96	0.14	95,95,95,95	0
55	MG	1H	3299	1/1	0.96	0.22	57,57,57,57	0
55	MG	14	3022	1/1	0.96	0.26	60,60,60,60	0
55	MG	1H	3020	1/1	0.96	0.30	52,52,52,52	0
55	MG	3A	201	1/1	0.96	0.17	81,81,81,81	0
55	MG	1H	3308	1/1	0.96	0.23	106,106,106,106	0
55	MG	14	3202	1/1	0.96	0.48	74,74,74,74	0
55	MG	14	3111	1/1	0.96	0.10	54,54,54,54	0
55	MG	14	3040	1/1	0.96	0.34	69,69,69,69	0
55	MG	1H	3052	1/1	0.96	0.33	73,73,73,73	0
55	MG	14	3209	1/1	0.96	0.29	88,88,88,88	0
55	MG	1H	3317	1/1	0.96	0.33	63,63,63,63	0
55	MG	1H	3166	1/1	0.96	0.24	67,67,67,67	0
55	MG	14	3047	1/1	0.96	0.27	57,57,57,57	0
55	MG	1H	3275	1/1	0.96	0.26	69,69,69,69	0
55	MG	14	3393	1/1	0.96	0.12	53,53,53,53	0
55	MG	1H	3171	1/1	0.96	0.46	82,82,82,82	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
55	MG	1H	3328	1/1	0.96	0.45	85,85,85,85	0
55	MG	16	214	1/1	0.96	0.07	86,86,86,86	0
55	MG	1G	1616	1/1	0.96	0.12	62,62,62,62	0
55	MG	13	1729	1/1	0.96	0.07	112,112,112,112	0
55	MG	14	3250	1/1	0.96	0.26	70,70,70,70	0
55	MG	1H	3455	1/1	0.96	0.13	47,47,47,47	0
55	MG	1H	3444	1/1	0.96	0.14	59,59,59,59	0
55	MG	14	3447	1/1	0.96	0.04	102,102,102,102	0
55	MG	1H	3187	1/1	0.96	0.36	83,83,83,83	0
55	MG	1H	3489	1/1	0.96	0.13	67,67,67,67	0
55	MG	1H	3242	1/1	0.96	0.20	45,45,45,45	0
55	MG	14	3031	1/1	0.96	0.30	73,73,73,73	0
55	MG	1H	3498	1/1	0.96	0.07	77,77,77,77	0
55	MG	13	1730	1/1	0.96	0.10	115,115,115,115	0
55	MG	1G	1606	1/1	0.96	0.20	80,80,80,80	0
55	MG	1G	1625	1/1	0.96	0.30	85,85,85,85	0
55	MG	1H	3261	1/1	0.96	0.41	72,72,72,72	0
55	MG	13	1606	1/1	0.96	0.27	92,92,92,92	0
55	MG	1H	3507	1/1	0.96	0.19	62,62,62,62	0
55	MG	14	3193	1/1	0.96	0.21	56,56,56,56	0
55	MG	1H	3516	1/1	0.96	0.07	88,88,88,88	0
55	MG	14	3316	1/1	0.96	0.14	70,70,70,70	0
55	MG	14	3189	1/1	0.96	0.32	63,63,63,63	0
55	MG	1H	3432	1/1	0.96	0.14	68,68,68,68	0
55	MG	1H	3045	1/1	0.96	0.34	88,88,88,88	0
55	MG	13	1683	1/1	0.96	0.12	122,122,122,122	0
55	MG	14	3055	1/1	0.96	0.32	61,61,61,61	0
55	MG	1H	3128	1/1	0.96	0.42	63,63,63,63	0
55	MG	1H	3436	1/1	0.96	0.09	94,94,94,94	0
55	MG	1H	3021	1/1	0.96	0.29	51,51,51,51	0
55	MG	14	3201	1/1	0.96	0.21	61,61,61,61	0
55	MG	1H	3382	1/1	0.96	0.20	79,79,79,79	0
55	MG	1H	3441	1/1	0.96	0.08	63,63,63,63	0
55	MG	13	1648	1/1	0.96	0.37	105,105,105,105	0
55	MG	14	3399	1/1	0.96	0.07	82,82,82,82	0
55	MG	14	3440	1/1	0.96	0.05	101,101,101,101	0
55	MG	1G	1634	1/1	0.96	0.37	80,80,80,80	0
55	MG	1H	3222	1/1	0.96	0.37	65,65,65,65	0
55	MG	1H	3420	1/1	0.96	0.12	52,52,52,52	0
55	MG	1H	3225	1/1	0.96	0.46	77,77,77,77	0
55	MG	29	301	1/1	0.96	0.25	72,72,72,72	0
55	MG	1H	3479	1/1	0.96	0.17	58,58,58,58	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
55	MG	1H	3279	1/1	0.96	0.37	96,96,96,96	0
55	MG	1H	3147	1/1	0.96	0.45	60,60,60,60	0
55	MG	13	1719	1/1	0.96	0.07	94,94,94,94	0
55	MG	1H	3270	1/1	0.97	0.15	84,84,84,84	0
55	MG	14	3339	1/1	0.97	0.28	74,74,74,74	0
55	MG	1H	3295	1/1	0.97	0.31	87,87,87,87	0
55	MG	14	3084	1/1	0.97	0.10	73,73,73,73	0
55	MG	1H	3367	1/1	0.97	0.10	67,67,67,67	0
55	MG	14	3097	1/1	0.97	0.32	54,54,54,54	0
55	MG	1H	3047	1/1	0.97	0.27	76,76,76,76	0
55	MG	14	3067	1/1	0.97	0.29	71,71,71,71	0
55	MG	14	3387	1/1	0.97	0.12	58,58,58,58	0
55	MG	1H	3424	1/1	0.97	0.11	58,58,58,58	0
55	MG	1G	1666	1/1	0.97	0.38	72,72,72,72	0
55	MG	14	3397	1/1	0.97	0.15	70,70,70,70	0
55	MG	1H	3031	1/1	0.97	0.31	82,82,82,82	0
55	MG	14	3243	1/1	0.97	0.22	78,78,78,78	0
55	MG	14	3391	1/1	0.97	0.12	62,62,62,62	0
55	MG	1H	3454	1/1	0.97	0.09	49,49,49,49	0
55	MG	1J	207	1/1	0.97	0.07	88,88,88,88	0
55	MG	1G	1743	1/1	0.97	0.18	105,105,105,105	0
55	MG	1H	3198	1/1	0.97	0.42	77,77,77,77	0
55	MG	14	3444	1/1	0.97	0.04	90,90,90,90	0
55	MG	14	3448	1/1	0.97	0.06	87,87,87,87	0
55	MG	13	1626	1/1	0.97	0.39	65,65,65,65	0
55	MG	14	3004	1/1	0.97	0.25	57,57,57,57	0
55	MG	1H	3430	1/1	0.97	0.10	76,76,76,76	0
55	MG	14	3062	1/1	0.97	0.32	72,72,72,72	0
55	MG	14	3183	1/1	0.97	0.40	56,56,56,56	0
55	MG	1H	3217	1/1	0.97	0.65	92,92,92,92	0
55	MG	1H	3487	1/1	0.97	0.04	81,81,81,81	0
55	MG	14	3114	1/1	0.97	0.23	56,56,56,56	0
55	MG	14	3418	1/1	0.97	0.13	72,72,72,72	0
55	MG	1H	3015	1/1	0.97	0.38	46,46,46,46	0
55	MG	14	3382	1/1	0.97	0.12	55,55,55,55	0
55	MG	14	3452	1/1	0.97	0.07	100,100,100,100	0
55	MG	1H	3012	1/1	0.97	0.37	57,57,57,57	0
55	MG	14	3010	1/1	0.97	0.21	47,47,47,47	0
55	MG	1H	3036	1/1	0.97	0.27	70,70,70,70	0
55	MG	1H	3026	1/1	0.97	0.31	66,66,66,66	0
55	MG	1H	3023	1/1	0.97	0.35	55,55,55,55	0
55	MG	1H	3453	1/1	0.97	0.12	42,42,42,42	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
55	MG	14	3122	1/1	0.97	0.25	61,61,61,61	0
55	MG	14	3232	1/1	0.97	0.28	98,98,98,98	0
55	MG	14	3207	1/1	0.97	0.30	77,77,77,77	0
55	MG	13	1636	1/1	0.97	0.31	88,88,88,88	0
55	MG	1H	3237	1/1	0.97	0.38	67,67,67,67	0
55	MG	14	3060	1/1	0.97	0.35	64,64,64,64	0
55	MG	14	3116	1/1	0.97	0.36	49,49,49,49	0
55	MG	14	3104	1/1	0.97	0.31	59,59,59,59	0
55	MG	1H	3241	1/1	0.97	0.23	69,69,69,69	0
55	MG	1H	3445	1/1	0.97	0.13	59,59,59,59	0
55	MG	1H	3249	1/1	0.97	0.53	66,66,66,66	0
55	MG	14	3203	1/1	0.97	0.27	55,55,55,55	0
55	MG	1H	3470	1/1	0.97	0.08	74,74,74,74	0
55	MG	14	3240	1/1	0.97	0.16	95,95,95,95	0
55	MG	1G	1730	1/1	0.97	0.14	82,82,82,82	0
55	MG	1H	3081	1/1	0.97	0.37	73,73,73,73	0
55	MG	1G	1628	1/1	0.97	0.20	90,90,90,90	0
55	MG	14	3007	1/1	0.97	0.29	58,58,58,58	0
55	MG	14	3005	1/1	0.97	0.29	52,52,52,52	0
55	MG	1H	3192	1/1	0.97	0.29	87,87,87,87	0
55	MG	1H	3011	1/1	0.97	0.35	54,54,54,54	0
55	MG	29	302	1/1	0.97	0.26	51,51,51,51	0
55	MG	1G	1716	1/1	0.97	0.08	110,110,110,110	0
55	MG	14	3403	1/1	0.97	0.11	69,69,69,69	0
55	MG	1G	1682	1/1	0.97	0.15	87,87,87,87	0
55	MG	14	3237	1/1	0.97	0.34	74,74,74,74	0
55	MG	14	3415	1/1	0.97	0.06	62,62,62,62	0
55	MG	1H	3123	1/1	0.97	0.14	78,78,78,78	0
55	MG	1H	3264	1/1	0.97	0.40	100,100,100,100	0
55	MG	14	3043	1/1	0.97	0.36	62,62,62,62	0
55	MG	1H	3423	1/1	0.97	0.11	61,61,61,61	0
55	MG	14	3419	1/1	0.97	0.06	94,94,94,94	0
55	MG	1H	3413	1/1	0.97	0.10	44,44,44,44	0
55	MG	1H	3467	1/1	0.97	0.18	72,72,72,72	0
55	MG	1H	3040	1/1	0.97	0.34	71,71,71,71	0
55	MG	1H	3463	1/1	0.97	0.15	52,52,52,52	0
55	MG	1H	3082	1/1	0.97	0.38	72,72,72,72	0
56	ZN	5I	101	1/1	0.97	0.14	116,116,116,116	0
55	MG	1H	3418	1/1	0.97	0.10	63,63,63,63	0
55	MG	1G	1601	1/1	0.97	0.25	76,76,76,76	0
55	MG	1H	3142	1/1	0.97	0.25	74,74,74,74	0
55	MG	1H	3412	1/1	0.97	0.14	69,69,69,69	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
55	MG	14	3107	1/1	0.97	0.43	80,80,80,80	0
55	MG	1H	3456	1/1	0.97	0.15	51,51,51,51	0
55	MG	13	1619	1/1	0.97	0.40	74,74,74,74	0
55	MG	1H	3111	1/1	0.97	0.34	71,71,71,71	0
55	MG	1G	1715	1/1	0.97	0.21	106,106,106,106	0
55	MG	1G	1631	1/1	0.97	0.27	90,90,90,90	0
55	MG	14	3405	1/1	0.97	0.08	64,64,64,64	0
55	MG	14	3003	1/1	0.97	0.26	47,47,47,47	0
55	MG	14	3086	1/1	0.97	0.28	51,51,51,51	0
55	MG	1H	3083	1/1	0.97	0.33	58,58,58,58	0
55	MG	1H	3061	1/1	0.97	0.43	71,71,71,71	0
55	MG	1G	1732	1/1	0.97	0.05	113,113,113,113	0
55	MG	14	3008	1/1	0.97	0.31	53,53,53,53	0
55	MG	14	3388	1/1	0.97	0.13	61,61,61,61	0
55	MG	1H	3053	1/1	0.97	0.20	61,61,61,61	0
55	MG	13	1631	1/1	0.97	0.16	60,60,60,60	0
55	MG	1G	1736	1/1	0.97	0.11	94,94,94,94	0
55	MG	1H	3151	1/1	0.97	0.44	76,76,76,76	0
55	MG	13	1723	1/1	0.97	0.08	86,86,86,86	0
55	MG	1H	3451	1/1	0.98	0.09	54,54,54,54	0
55	MG	1H	3158	1/1	0.98	0.21	71,71,71,71	0
55	MG	1G	1602	1/1	0.98	0.41	75,75,75,75	0
55	MG	1H	3018	1/1	0.98	0.21	50,50,50,50	0
55	MG	1H	3419	1/1	0.98	0.14	48,48,48,48	0
55	MG	1H	3421	1/1	0.98	0.14	52,52,52,52	0
55	MG	14	3417	1/1	0.98	0.12	51,51,51,51	0
55	MG	14	3016	1/1	0.98	0.17	63,63,63,63	0
55	MG	13	1602	1/1	0.98	0.21	78,78,78,78	0
55	MG	1H	3101	1/1	0.98	0.14	50,50,50,50	0
55	MG	1H	3089	1/1	0.98	0.34	38,38,38,38	0
55	MG	14	3347	1/1	0.98	0.17	83,83,83,83	0
55	MG	14	3009	1/1	0.98	0.28	58,58,58,58	0
55	MG	14	3095	1/1	0.98	0.20	65,65,65,65	0
55	MG	14	3057	1/1	0.98	0.42	54,54,54,54	0
55	MG	14	3404	1/1	0.98	0.05	79,79,79,79	0
55	MG	13	1609	1/1	0.98	0.23	83,83,83,83	0
55	MG	1H	3492	1/1	0.98	0.11	83,83,83,83	0
55	MG	13	1716	1/1	0.98	0.17	74,74,74,74	0
55	MG	14	3006	1/1	0.98	0.33	56,56,56,56	0
55	MG	1H	3481	1/1	0.98	0.12	64,64,64,64	0
55	MG	1H	3002	1/1	0.98	0.33	53,53,53,53	0
55	MG	14	3058	1/1	0.98	0.20	63,63,63,63	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
55	MG	13	1728	1/1	0.98	0.07	76,76,76,76	0
55	MG	14	3423	1/1	0.98	0.09	84,84,84,84	0
55	MG	1H	3072	1/1	0.98	0.33	75,75,75,75	0
55	MG	1H	3206	1/1	0.98	0.44	72,72,72,72	0
55	MG	1H	3133	1/1	0.98	0.15	49,49,49,49	0
55	MG	1H	3010	1/1	0.98	0.40	66,66,66,66	0
55	MG	14	3072	1/1	0.98	0.35	54,54,54,54	0
55	MG	1H	3095	1/1	0.98	0.38	46,46,46,46	0
55	MG	14	3164	1/1	0.98	0.26	60,60,60,60	0
55	MG	13	1630	1/1	0.98	0.18	61,61,61,61	0
55	MG	1H	3440	1/1	0.98	0.07	91,91,91,91	0
56	ZN	3E	302	1/1	0.98	0.35	102,102,102,102	0
55	MG	14	3422	1/1	0.98	0.10	53,53,53,53	0
55	MG	2K	102	1/1	0.98	0.44	93,93,93,93	0
55	MG	1H	3062	1/1	0.98	0.18	48,48,48,48	0
55	MG	14	3012	1/1	0.98	0.30	53,53,53,53	0
55	MG	1H	3019	1/1	0.98	0.34	61,61,61,61	0
55	MG	14	3398	1/1	0.98	0.13	83,83,83,83	0
55	MG	14	3390	1/1	0.98	0.10	52,52,52,52	0
55	MG	1H	3017	1/1	0.98	0.33	47,47,47,47	0
55	MG	14	3216	1/1	0.98	0.29	72,72,72,72	0
55	MG	14	3381	1/1	0.98	0.13	52,52,52,52	0
55	MG	14	3050	1/1	0.98	0.15	65,65,65,65	0
55	MG	1H	3505	1/1	0.98	0.07	69,69,69,69	0
55	MG	1H	3411	1/1	0.98	0.14	67,67,67,67	0
55	MG	1H	3521	1/1	0.98	0.09	47,47,47,47	0
55	MG	1H	3099	1/1	0.98	0.47	52,52,52,52	0
55	MG	1H	3113	1/1	0.98	0.27	40,40,40,40	0
55	MG	1H	3464	1/1	0.98	0.14	52,52,52,52	0
55	MG	1H	3091	1/1	0.98	0.41	59,59,59,59	0
55	MG	14	3035	1/1	0.98	0.37	57,57,57,57	0
55	MG	14	3386	1/1	0.98	0.12	56,56,56,56	0
55	MG	14	3465	1/1	0.98	0.32	64,64,64,64	0
55	MG	1H	3485	1/1	0.98	0.15	75,75,75,75	0
55	MG	14	3112	1/1	0.98	0.33	68,68,68,68	0
55	MG	14	3063	1/1	0.98	0.35	51,51,51,51	0
55	MG	14	3011	1/1	0.98	0.33	47,47,47,47	0
55	MG	1H	3050	1/1	0.98	0.40	47,47,47,47	0
55	MG	1G	1623	1/1	0.98	0.28	87,87,87,87	0
55	MG	14	3015	1/1	0.98	0.17	64,64,64,64	0
55	MG	1H	3474	1/1	0.98	0.10	79,79,79,79	0
55	MG	14	3065	1/1	0.98	0.32	50,50,50,50	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
55	MG	1H	3473	1/1	0.98	0.06	64,64,64,64	0
55	MG	1H	3319	1/1	0.98	0.21	60,60,60,60	0
55	MG	14	3049	1/1	0.98	0.12	55,55,55,55	0
55	MG	1H	3447	1/1	0.98	0.09	62,62,62,62	0
55	MG	1H	3014	1/1	0.98	0.31	51,51,51,51	0
55	MG	1H	3228	1/1	0.98	0.32	63,63,63,63	0
55	MG	14	3392	1/1	0.98	0.10	54,54,54,54	0
55	MG	1H	3468	1/1	0.98	0.12	59,59,59,59	0
55	MG	14	3410	1/1	0.98	0.16	58,58,58,58	0
55	MG	1H	3446	1/1	0.98	0.10	52,52,52,52	0
55	MG	1H	3025	1/1	0.98	0.40	80,80,80,80	0
55	MG	14	3412	1/1	0.98	0.16	49,49,49,49	0
55	MG	14	3048	1/1	0.98	0.20	55,55,55,55	0
55	MG	14	3406	1/1	0.98	0.11	61,61,61,61	0
55	MG	14	3032	1/1	0.98	0.24	64,64,64,64	0
55	MG	1H	3009	1/1	0.98	0.38	44,44,44,44	0
55	MG	14	3411	1/1	0.98	0.10	63,63,63,63	0
55	MG	13	1725	1/1	0.98	0.11	99,99,99,99	0
55	MG	1H	3415	1/1	0.99	0.13	50,50,50,50	0
55	MG	1H	3462	1/1	0.99	0.14	49,49,49,49	0
55	MG	14	3013	1/1	0.99	0.23	56,56,56,56	0
55	MG	14	3102	1/1	0.99	0.21	61,61,61,61	0
55	MG	1H	3417	1/1	0.99	0.11	40,40,40,40	0
55	MG	1H	3137	1/1	0.99	0.26	60,60,60,60	0
55	MG	14	3002	1/1	0.99	0.23	67,67,67,67	0
55	MG	1H	3003	1/1	0.99	0.34	54,54,54,54	0
55	MG	1H	3480	1/1	0.99	0.12	47,47,47,47	0
55	MG	14	3389	1/1	0.99	0.17	53,53,53,53	0
55	MG	14	3259	1/1	0.99	0.29	82,82,82,82	0
55	MG	1G	1728	1/1	0.99	0.13	73,73,73,73	0
55	MG	14	3053	1/1	0.99	0.33	59,59,59,59	0
55	MG	1H	3071	1/1	0.99	0.36	51,51,51,51	0
55	MG	1H	3085	1/1	0.99	0.20	63,63,63,63	0
55	MG	1H	3070	1/1	0.99	0.27	60,60,60,60	0
55	MG	1H	3004	1/1	0.99	0.39	49,49,49,49	0
55	MG	14	3073	1/1	0.99	0.26	58,58,58,58	0
55	MG	1H	3458	1/1	0.99	0.15	70,70,70,70	0
55	MG	1H	3024	1/1	0.99	0.15	61,61,61,61	0
55	MG	14	3445	1/1	0.99	0.10	58,58,58,58	0
55	MG	1G	1647	1/1	0.99	0.25	80,80,80,80	0
55	MG	13	1739	1/1	0.99	0.22	90,90,90,90	0
55	MG	1H	3450	1/1	0.99	0.22	53,53,53,53	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
55	MG	14	3377	1/1	0.99	0.10	57,57,57,57	0
55	MG	14	3384	1/1	0.99	0.09	54,54,54,54	0
55	MG	14	3077	1/1	0.99	0.30	61,61,61,61	0
55	MG	1H	3013	1/1	0.99	0.30	47,47,47,47	0
55	MG	1H	3426	1/1	0.99	0.10	67,67,67,67	0
55	MG	14	3223	1/1	0.99	0.20	64,64,64,64	0
55	MG	G8	201	1/1	0.99	0.14	77,77,77,77	0
55	MG	14	3076	1/1	0.99	0.32	47,47,47,47	0
55	MG	1H	3422	1/1	0.99	0.07	56,56,56,56	0
55	MG	1H	3051	1/1	0.99	0.24	47,47,47,47	0
55	MG	14	3064	1/1	0.99	0.34	52,52,52,52	0
55	MG	1H	3503	1/1	1.00	0.10	57,57,57,57	0

6.5 Other polymers [i](#)

There are no such residues in this entry.