



wwPDB X-ray Structure Validation Summary Report ⓘ

Nov 14, 2017 – 03:09 AM EST

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 : unknown
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

<http://wwpdb.org/validation/2016/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 : 1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20030345
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : rb-20030345

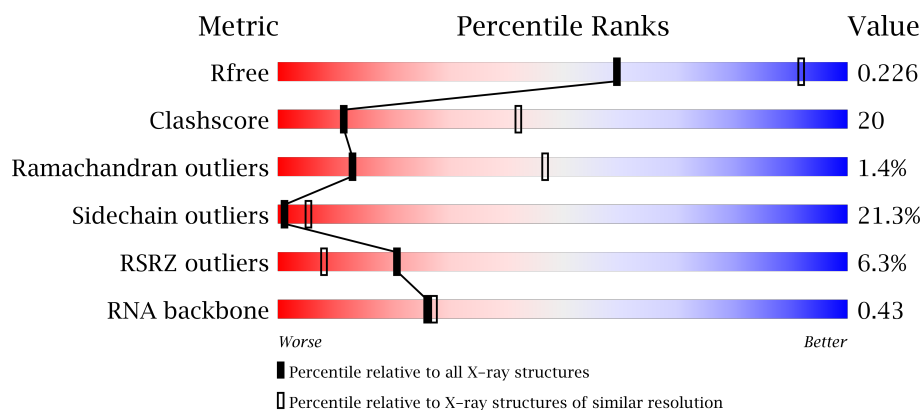
1 Overall quality at a glance

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}	100719	1001 (3.12-3.08)
Clashscore	112137	1099 (3.12-3.08)
Ramachandran outliers	110173	1057 (3.12-3.08)
Sidechain outliers	110143	1057 (3.12-3.08)
RSRZ outliers	101464	1006 (3.12-3.08)
RNA backbone	2435	1112 (3.50-2.70)

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. 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	<div> <div>27%</div> <div>45%</div> <div>24%</div> <div>• •</div> </div>
1	1G	1522	<div> <div>29%</div> <div>46%</div> <div>20%</div> <div>• •</div> </div>
2	12	256	<div> <div>16%</div> <div>40%</div> <div>41%</div> <div>11%</div> <div>7%</div> </div>
2	1E	256	<div> <div>12%</div> <div>35%</div> <div>43%</div> <div>13%</div> <div>• 7%</div> </div>




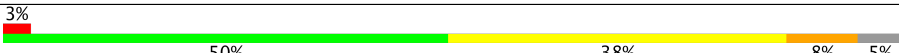
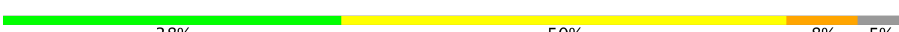
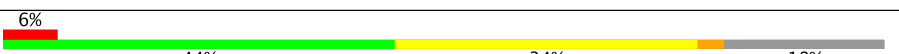
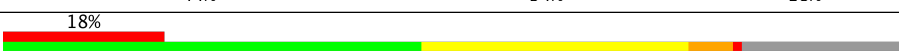
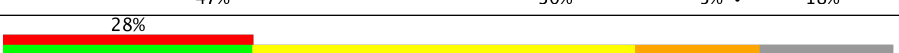
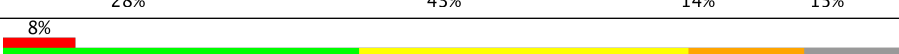
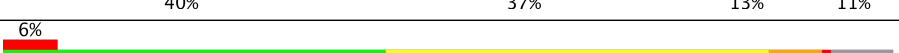

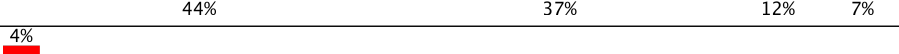




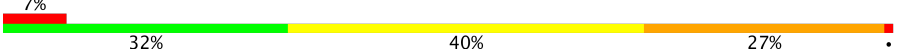



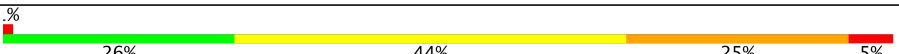
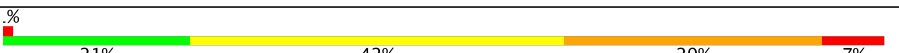
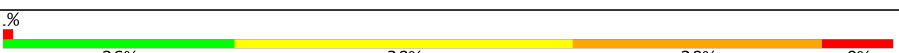
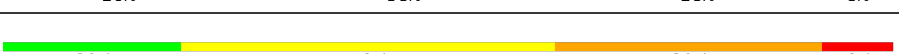
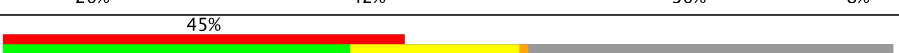
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Mol	Chain	Length	Quality of chain
3	22	239	
3	2E	239	
4	32	209	
4	3E	209	
5	42	162	
5	4E	162	
6	52	101	
6	5E	101	
7	62	156	
7	6E	156	
8	72	138	
8	7E	138	
9	82	128	
9	8E	128	
10	1A	105	
10	1I	105	
11	2A	129	
11	2I	129	
12	3A	132	
12	3I	132	
13	4A	126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




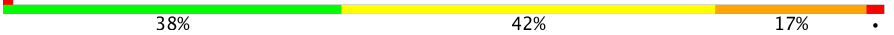

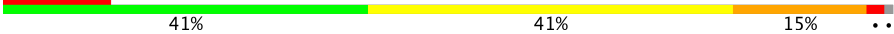

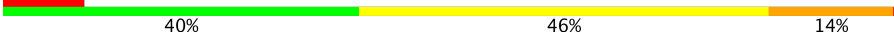
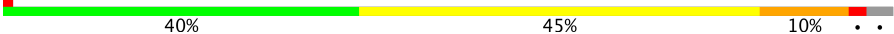
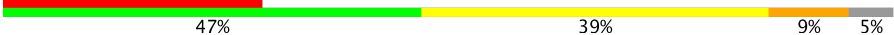
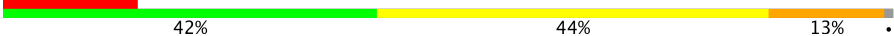
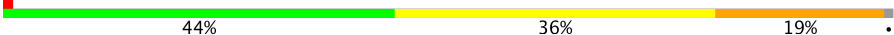

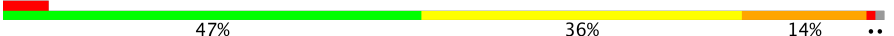











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Mol	Chain	Length	Quality of chain
15	6I	89	
16	7A	88	
16	7I	88	
17	8A	105	
17	8I	105	
18	9A	88	
18	9I	88	
19	AA	93	
19	AI	93	
20	BA	106	
20	BI	106	
21	1B	27	
21	1F	27	
22	2K	85	
22	2L	85	
22	3K	85	
22	3L	85	
23	4K	30	
23	4L	30	
24	14	2917	
24	1H	2917	
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	1606	-	-	-	X
55	MG	13	1609	-	-	-	X
55	MG	13	1611	-	-	-	X
55	MG	13	1621	-	-	-	X
55	MG	13	1622	-	-	-	X
55	MG	13	1627	-	-	-	X
55	MG	13	1633	-	-	-	X
55	MG	13	1636	-	-	-	X
55	MG	13	1639	-	-	-	X
55	MG	13	1640	-	-	-	X
55	MG	13	1646	-	-	-	X
55	MG	13	1654	-	-	-	X
55	MG	13	1655	-	-	-	X
55	MG	13	1659	-	-	-	X
55	MG	13	1671	-	-	-	X
55	MG	13	1673	-	-	-	X
55	MG	13	1675	-	-	-	X
55	MG	13	1681	-	-	-	X
55	MG	13	1687	-	-	-	X
55	MG	13	1691	-	-	-	X
55	MG	13	1692	-	-	-	X
55	MG	13	1704	-	-	-	X
55	MG	13	1705	-	-	-	X
55	MG	13	1708	-	-	-	X
55	MG	13	1709	-	-	-	X
55	MG	14	3004	-	-	-	X
55	MG	14	3007	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
55	MG	14	3011	-	-	-	X
55	MG	14	3013	-	-	-	X
55	MG	14	3019	-	-	-	X
55	MG	14	3022	-	-	-	X
55	MG	14	3027	-	-	-	X
55	MG	14	3031	-	-	-	X
55	MG	14	3032	-	-	-	X
55	MG	14	3033	-	-	-	X
55	MG	14	3038	-	-	-	X
55	MG	14	3041	-	-	-	X
55	MG	14	3042	-	-	-	X
55	MG	14	3045	-	-	-	X
55	MG	14	3048	-	-	-	X
55	MG	14	3052	-	-	-	X
55	MG	14	3055	-	-	-	X
55	MG	14	3058	-	-	-	X
55	MG	14	3059	-	-	-	X
55	MG	14	3064	-	-	-	X
55	MG	14	3068	-	-	-	X
55	MG	14	3070	-	-	-	X
55	MG	14	3071	-	-	-	X
55	MG	14	3075	-	-	-	X
55	MG	14	3076	-	-	-	X
55	MG	14	3078	-	-	-	X
55	MG	14	3081	-	-	-	X
55	MG	14	3086	-	-	-	X
55	MG	14	3093	-	-	-	X
55	MG	14	3097	-	-	-	X
55	MG	14	3101	-	-	-	X
55	MG	14	3102	-	-	-	X
55	MG	14	3103	-	-	-	X
55	MG	14	3112	-	-	-	X
55	MG	14	3119	-	-	-	X
55	MG	14	3121	-	-	-	X
55	MG	14	3123	-	-	-	X
55	MG	14	3130	-	-	-	X
55	MG	14	3131	-	-	-	X
55	MG	14	3135	-	-	-	X
55	MG	14	3143	-	-	-	X
55	MG	14	3145	-	-	-	X
55	MG	14	3152	-	-	-	X
55	MG	14	3156	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
55	MG	14	3172	-	-	-	X
55	MG	14	3176	-	-	-	X
55	MG	14	3179	-	-	-	X
55	MG	14	3193	-	-	-	X
55	MG	14	3197	-	-	-	X
55	MG	14	3198	-	-	-	X
55	MG	14	3199	-	-	-	X
55	MG	14	3202	-	-	-	X
55	MG	14	3203	-	-	-	X
55	MG	14	3206	-	-	-	X
55	MG	14	3209	-	-	-	X
55	MG	14	3215	-	-	-	X
55	MG	14	3217	-	-	-	X
55	MG	14	3219	-	-	-	X
55	MG	14	3227	-	-	-	X
55	MG	14	3229	-	-	-	X
55	MG	14	3231	-	-	-	X
55	MG	14	3233	-	-	-	X
55	MG	14	3239	-	-	-	X
55	MG	14	3255	-	-	-	X
55	MG	14	3258	-	-	-	X
55	MG	14	3269	-	-	-	X
55	MG	14	3271	-	-	-	X
55	MG	14	3273	-	-	-	X
55	MG	14	3276	-	-	-	X
55	MG	14	3281	-	-	-	X
55	MG	14	3283	-	-	-	X
55	MG	14	3293	-	-	-	X
55	MG	14	3295	-	-	-	X
55	MG	14	3297	-	-	-	X
55	MG	14	3298	-	-	-	X
55	MG	14	3315	-	-	-	X
55	MG	14	3320	-	-	-	X
55	MG	14	3321	-	-	-	X
55	MG	14	3323	-	-	-	X
55	MG	14	3326	-	-	-	X
55	MG	14	3328	-	-	-	X
55	MG	14	3335	-	-	-	X
55	MG	14	3338	-	-	-	X
55	MG	14	3339	-	-	-	X
55	MG	14	3365	-	-	-	X
55	MG	14	3373	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
55	MG	14	3465	-	-	-	X
55	MG	1G	1601	-	-	-	X
55	MG	1G	1602	-	-	-	X
55	MG	1G	1603	-	-	-	X
55	MG	1G	1605	-	-	-	X
55	MG	1G	1608	-	-	-	X
55	MG	1G	1610	-	-	-	X
55	MG	1G	1615	-	-	-	X
55	MG	1G	1619	-	-	-	X
55	MG	1G	1621	-	-	-	X
55	MG	1G	1623	-	-	-	X
55	MG	1G	1624	-	-	-	X
55	MG	1G	1632	-	-	-	X
55	MG	1G	1644	-	-	-	X
55	MG	1G	1646	-	-	-	X
55	MG	1G	1647	-	-	-	X
55	MG	1G	1649	-	-	-	X
55	MG	1G	1651	-	-	-	X
55	MG	1G	1653	-	-	-	X
55	MG	1G	1661	-	-	-	X
55	MG	1G	1664	-	-	-	X
55	MG	1G	1689	-	-	-	X
55	MG	1G	1711	-	-	-	X
55	MG	1G	1713	-	-	-	X
55	MG	1G	1714	-	-	-	X
55	MG	1G	1717	-	-	-	X
55	MG	1G	1719	-	-	-	X
55	MG	1H	3001	-	-	-	X
55	MG	1H	3002	-	-	-	X
55	MG	1H	3004	-	-	-	X
55	MG	1H	3007	-	-	-	X
55	MG	1H	3011	-	-	-	X
55	MG	1H	3013	-	-	-	X
55	MG	1H	3015	-	-	-	X
55	MG	1H	3016	-	-	-	X
55	MG	1H	3017	-	-	-	X
55	MG	1H	3021	-	-	-	X
55	MG	1H	3029	-	-	-	X
55	MG	1H	3031	-	-	-	X
55	MG	1H	3035	-	-	-	X
55	MG	1H	3039	-	-	-	X
55	MG	1H	3040	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
55	MG	1H	3041	-	-	-	X
55	MG	1H	3047	-	-	-	X
55	MG	1H	3049	-	-	-	X
55	MG	1H	3052	-	-	-	X
55	MG	1H	3053	-	-	-	X
55	MG	1H	3057	-	-	-	X
55	MG	1H	3061	-	-	-	X
55	MG	1H	3063	-	-	-	X
55	MG	1H	3065	-	-	-	X
55	MG	1H	3066	-	-	-	X
55	MG	1H	3068	-	-	-	X
55	MG	1H	3069	-	-	-	X
55	MG	1H	3071	-	-	-	X
55	MG	1H	3074	-	-	-	X
55	MG	1H	3078	-	-	-	X
55	MG	1H	3080	-	-	-	X
55	MG	1H	3085	-	-	-	X
55	MG	1H	3087	-	-	-	X
55	MG	1H	3088	-	-	-	X
55	MG	1H	3089	-	-	-	X
55	MG	1H	3090	-	-	-	X
55	MG	1H	3091	-	-	-	X
55	MG	1H	3095	-	-	-	X
55	MG	1H	3099	-	-	-	X
55	MG	1H	3104	-	-	-	X
55	MG	1H	3106	-	-	-	X
55	MG	1H	3109	-	-	-	X
55	MG	1H	3113	-	-	-	X
55	MG	1H	3127	-	-	-	X
55	MG	1H	3137	-	-	-	X
55	MG	1H	3143	-	-	-	X
55	MG	1H	3144	-	-	-	X
55	MG	1H	3146	-	-	-	X
55	MG	1H	3148	-	-	-	X
55	MG	1H	3151	-	-	-	X
55	MG	1H	3153	-	-	-	X
55	MG	1H	3155	-	-	-	X
55	MG	1H	3158	-	-	-	X
55	MG	1H	3159	-	-	-	X
55	MG	1H	3160	-	-	-	X
55	MG	1H	3167	-	-	-	X
55	MG	1H	3168	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
55	MG	1H	3172	-	-	-	X
55	MG	1H	3177	-	-	-	X
55	MG	1H	3183	-	-	-	X
55	MG	1H	3186	-	-	-	X
55	MG	1H	3192	-	-	-	X
55	MG	1H	3195	-	-	-	X
55	MG	1H	3207	-	-	-	X
55	MG	1H	3212	-	-	-	X
55	MG	1H	3213	-	-	-	X
55	MG	1H	3219	-	-	-	X
55	MG	1H	3226	-	-	-	X
55	MG	1H	3241	-	-	-	X
55	MG	1H	3244	-	-	-	X
55	MG	1H	3248	-	-	-	X
55	MG	1H	3260	-	-	-	X
55	MG	1H	3297	-	-	-	X
55	MG	1H	3302	-	-	-	X
55	MG	1H	3309	-	-	-	X
55	MG	1H	3315	-	-	-	X
55	MG	1H	3319	-	-	-	X
55	MG	1H	3322	-	-	-	X
55	MG	1H	3324	-	-	-	X
55	MG	1H	3330	-	-	-	X
55	MG	1H	3331	-	-	-	X
55	MG	1H	3339	-	-	-	X
55	MG	1H	3345	-	-	-	X
55	MG	1H	3356	-	-	-	X
55	MG	1H	3364	-	-	-	X
55	MG	1H	3370	-	-	-	X
55	MG	1H	3374	-	-	-	X
55	MG	1H	3381	-	-	-	X
55	MG	1H	3401	-	-	-	X
55	MG	1H	3450	-	-	-	X
55	MG	1J	201	-	-	-	X
55	MG	2I	302	-	-	-	X
55	MG	2K	105	-	-	-	X
55	MG	2L	101	-	-	-	X
55	MG	98	201	-	-	-	X
55	MG	F5	101	-	-	-	X
55	MG	I8	101	-	-	-	X

2 Entry composition [i](#)

There are 57 unique types of molecules in this entry. The entry contains 299705 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	13	1499	Total	C	N	O	P	0	5	0
			32337	14392	5999	10442	1504			
1	1G	1503	Total	C	N	O	P	0	0	0
			32309	14381	5990	10436	1502			

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	2E	205	Total	C	N	O	S	0	0	0
			1605	1011	313	280	1			
3	22	206	Total	C	N	O	S	0	0	0
			1612	1016	314	281	1			

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	4E	151	Total	C	N	O	S	0	0	0
			1155	729	218	204	4			
5	42	151	Total	C	N	O	S	0	0	0
			1155	729	218	204	4			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	5E	101	Total	C	N	O	S	0	0	0
			842	531	155	153	3			
6	52	101	Total	C	N	O	S	0	0	0
			842	531	155	153	3			

- Molecule 7 is a protein called 30S ribosomal protein S7.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	6E	155	Total	C	N	O	S	0	0	0
			1256	781	252	217	6			
7	62	155	Total	C	N	O	S	0	0	0
			1256	781	252	217	6			

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	8E	127	Total	C	N	O		0	0	0
			1009	639	197	173				
9	82	127	Total	C	N	O		0	0	0
			1009	639	197	173				

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

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

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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 1	Mg 1	0	0
55	14	465	Total 465	Mg 465	0	0
55	3E	1	Total 1	Mg 1	0	0
55	19	1	Total 1	Mg 1	0	0
55	3L	1	Total 1	Mg 1	0	0
55	4K	1	Total 1	Mg 1	0	0
55	3A	1	Total 1	Mg 1	0	0
55	G8	1	Total 1	Mg 1	0	0
55	2L	4	Total 4	Mg 4	0	0

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

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

- Molecule 57 is water.

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

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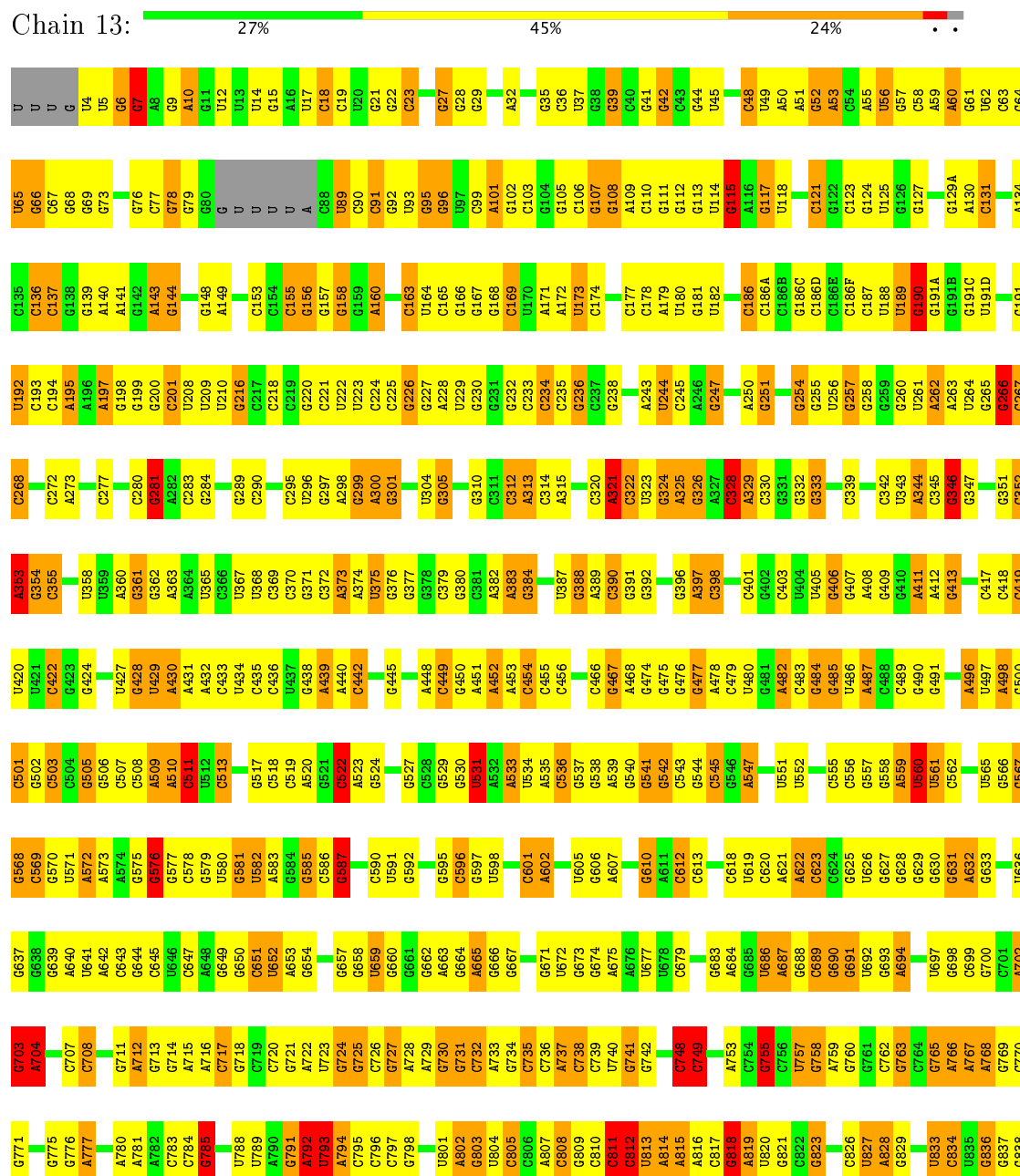
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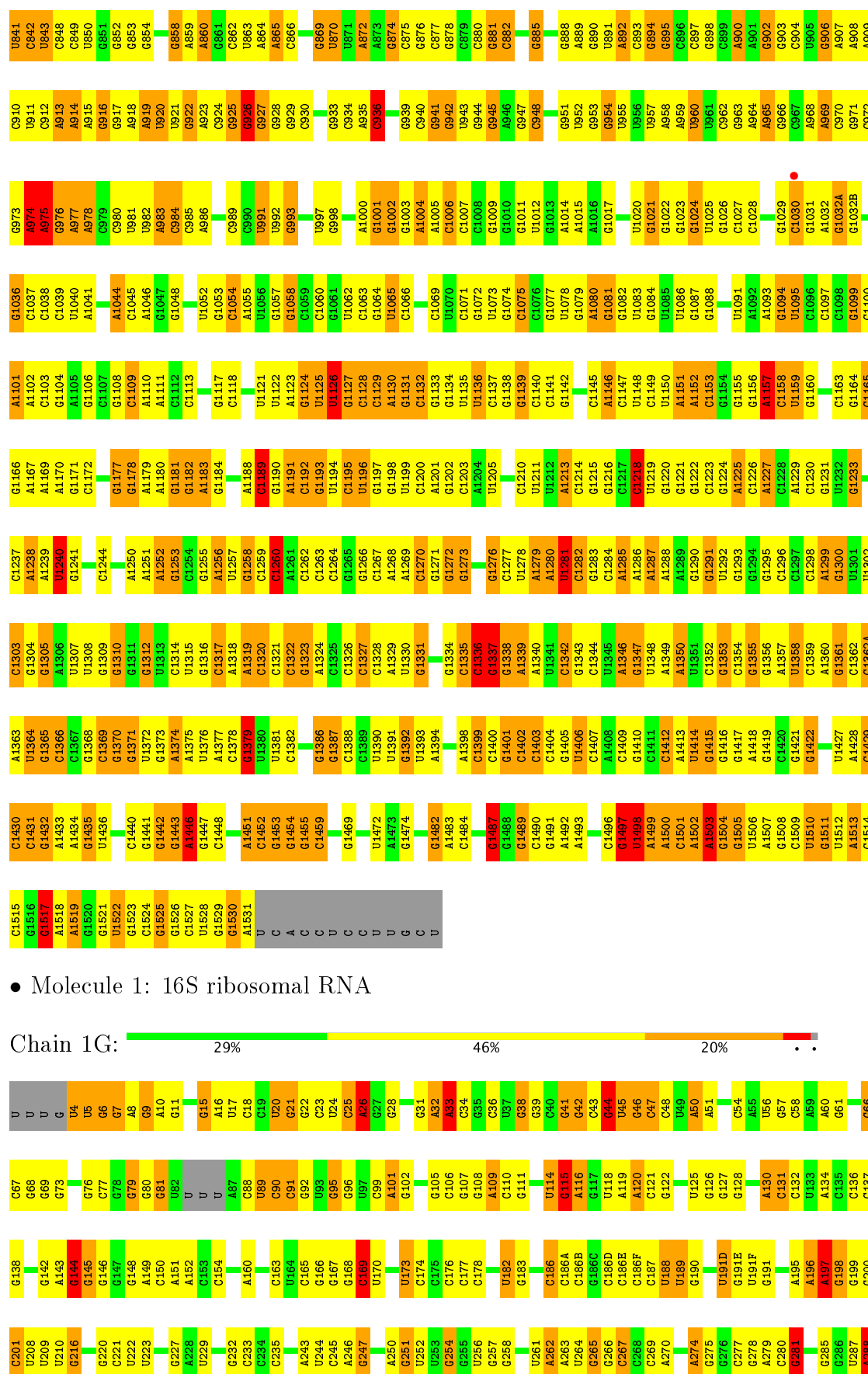
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
57	1J	22	Total 22	O 22	0	0
57	19	11	Total 11	O 11	0	0
57	39	3	Total 3	O 3	0	0
57	25	6	Total 6	O 6	0	0
57	35	1	Total 1	O 1	0	0
57	75	1	Total 1	O 1	0	0
57	85	4	Total 4	O 4	0	0
57	F5	1	Total 1	O 1	0	0
57	H5	2	Total 2	O 2	0	0

3 Residue-property plots

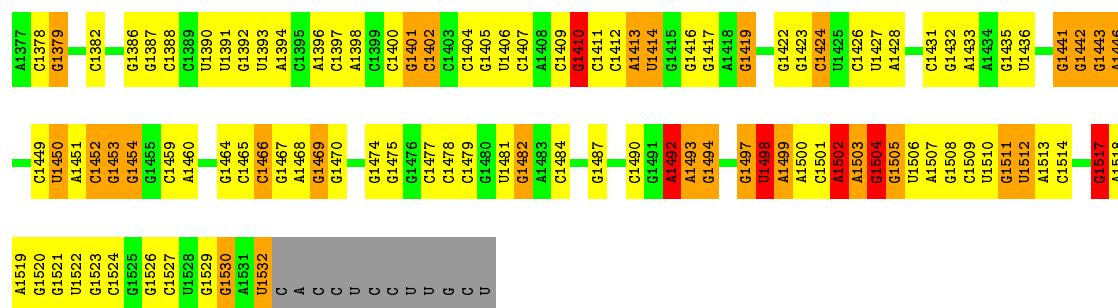
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are 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

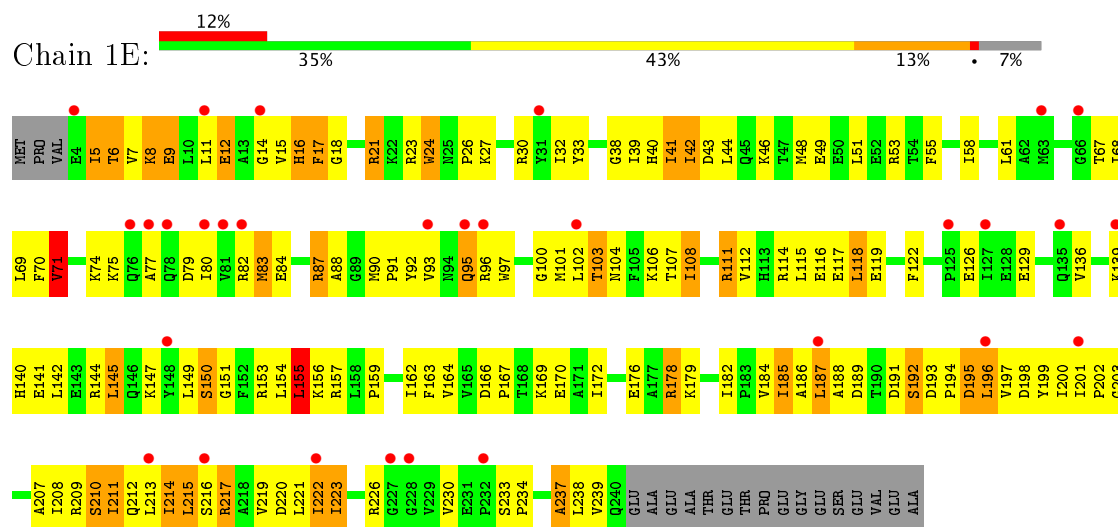




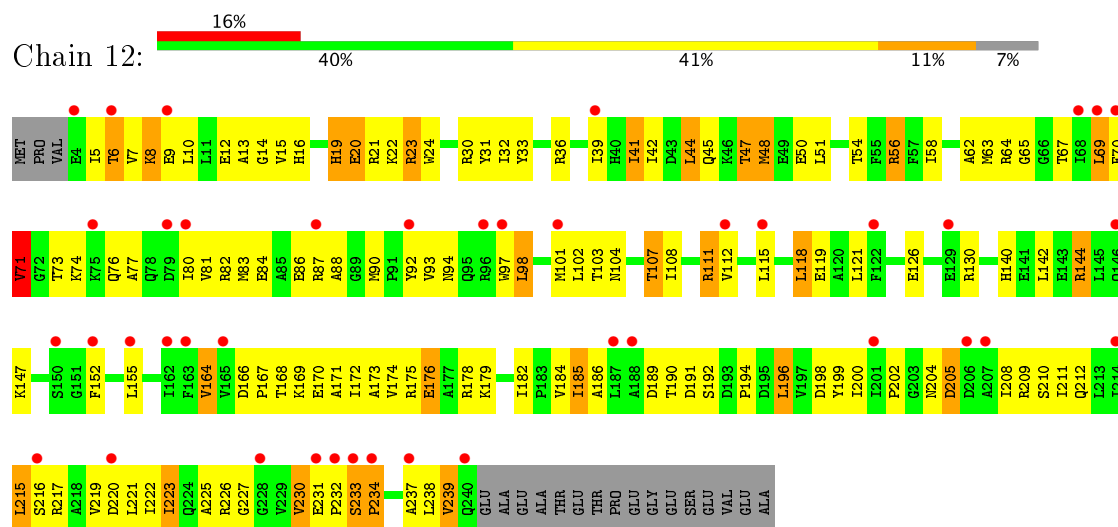




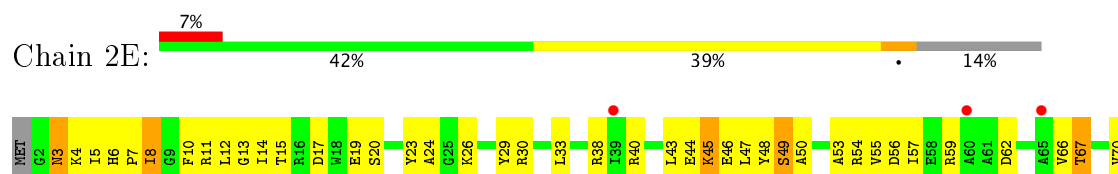
• Molecule 2: 30S ribosomal protein S2

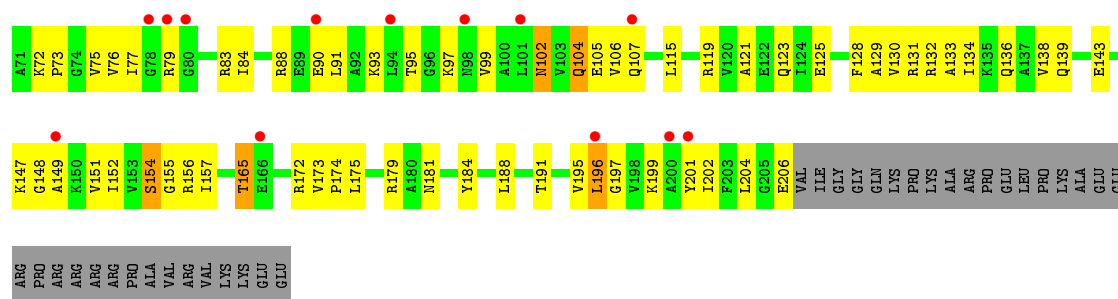


• Molecule 2: 30S ribosomal protein S2



• Molecule 3: 30S ribosomal protein S3

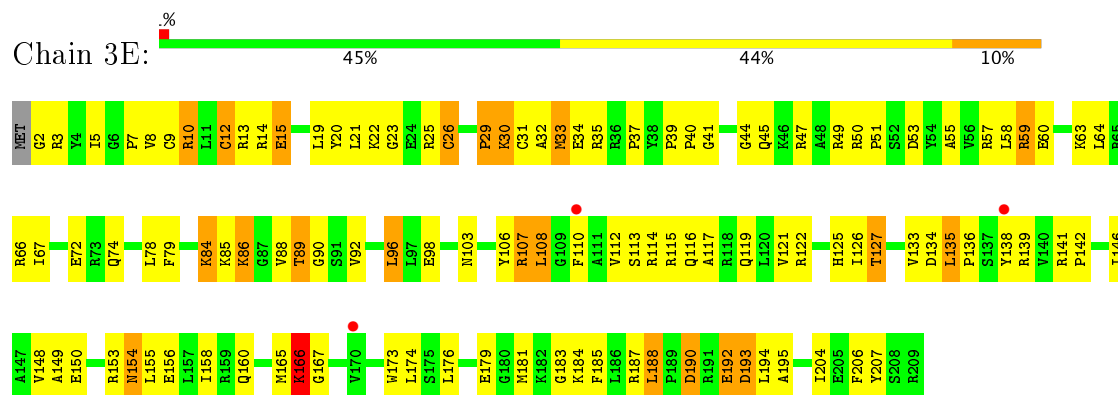




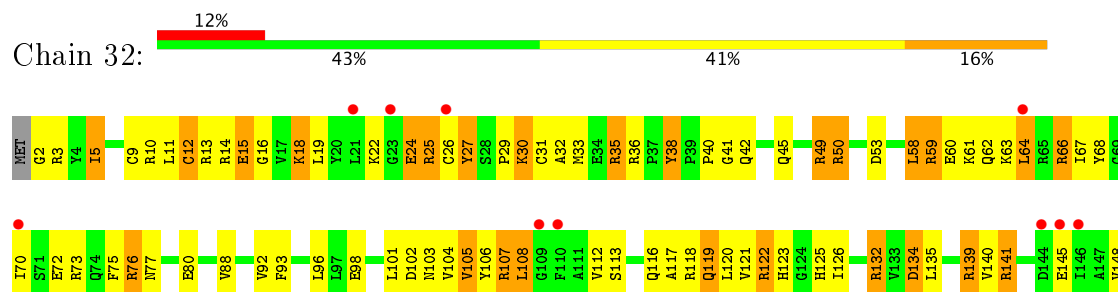
• Molecule 3: 30S ribosomal protein S3

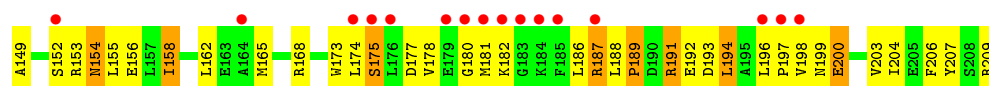


• Molecule 4: 30S ribosomal protein S4



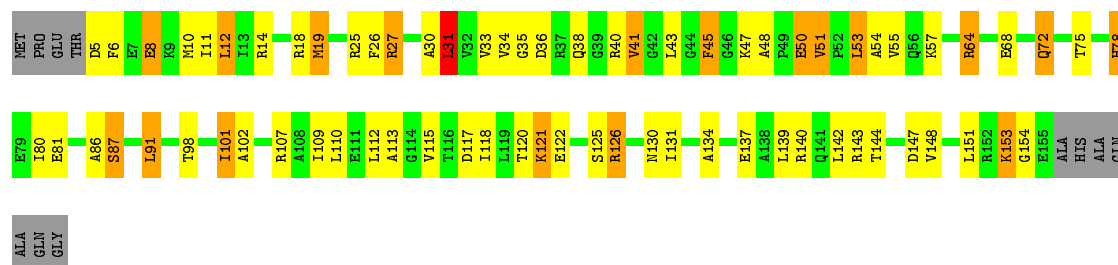
• Molecule 4: 30S ribosomal protein S4





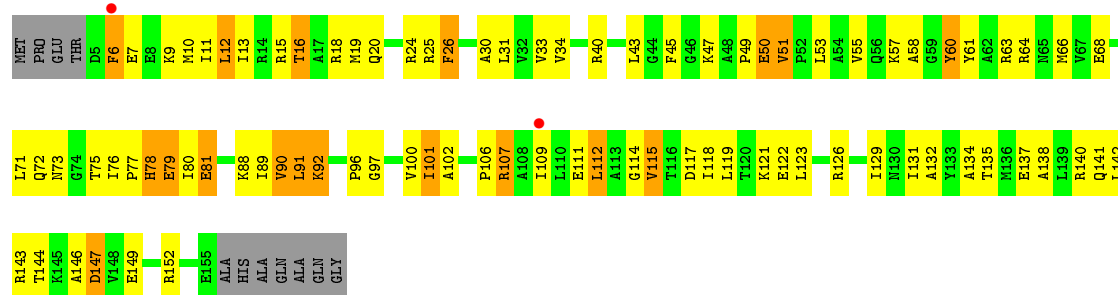
- Molecule 5: 30S ribosomal protein S5

Chain 4E: 49% 32% 11% 7%



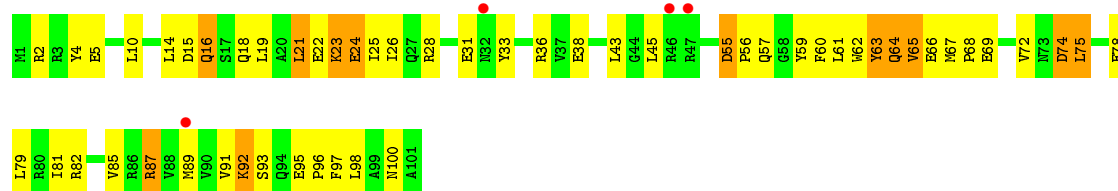
- Molecule 5: 30S ribosomal protein S5

Chain 42: 40% 42% 11% 7%



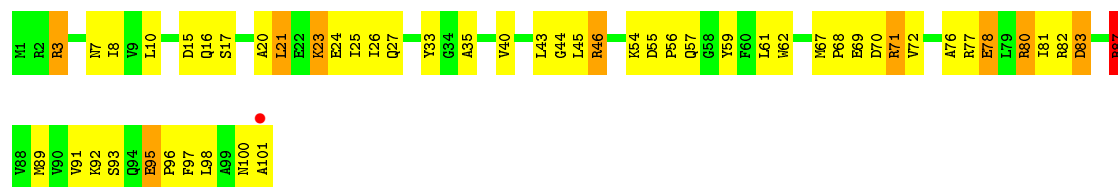
- Molecule 6: 30S ribosomal protein S6

Chain 5E: 47% 42% 12%

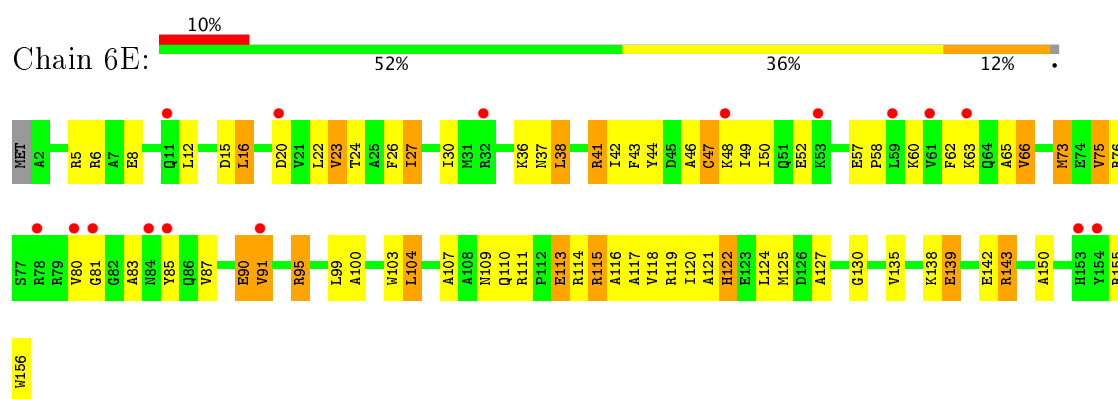


- Molecule 6: 30S ribosomal protein S6

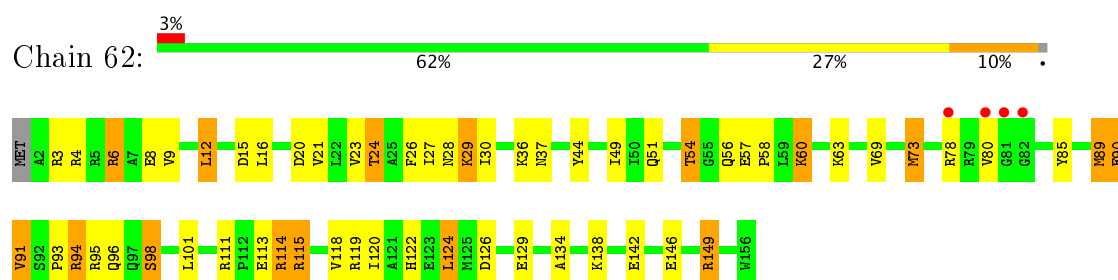
Chain 52: 49% 42% 9%



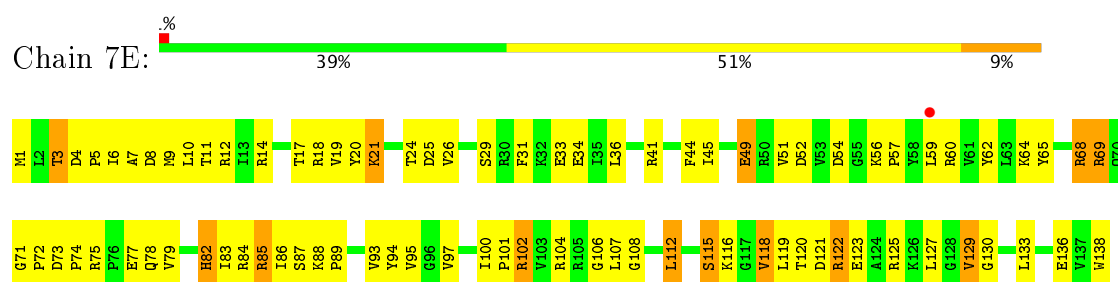
- Molecule 7: 30S ribosomal protein S7



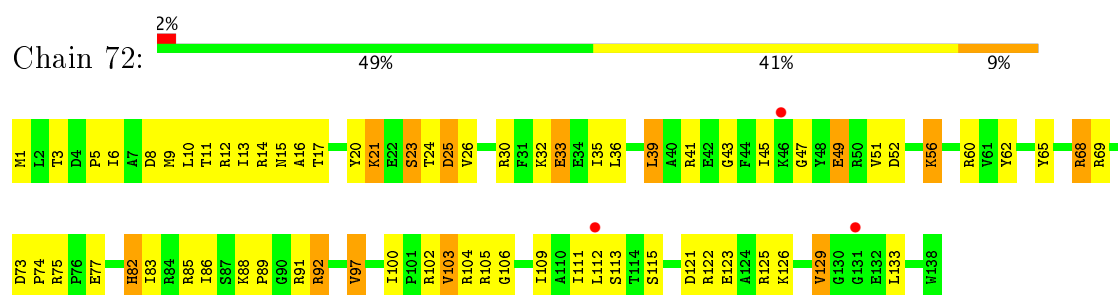
• Molecule 7: 30S ribosomal protein S7



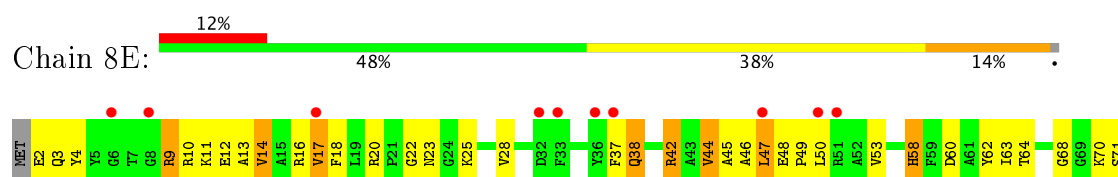
• Molecule 8: 30S ribosomal protein S8

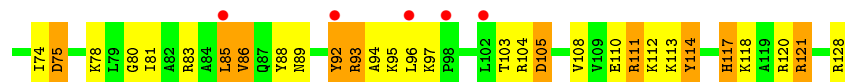


• Molecule 8: 30S ribosomal protein S8

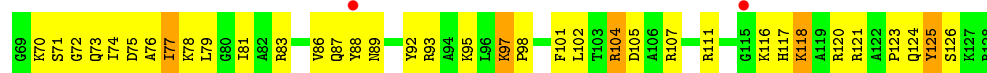
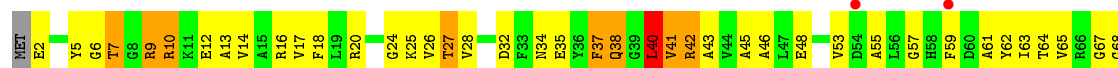


• Molecule 9: 30S ribosomal protein S9

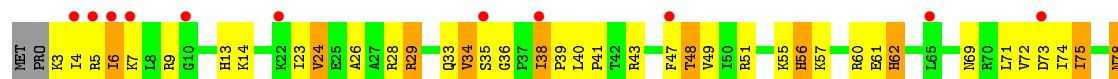




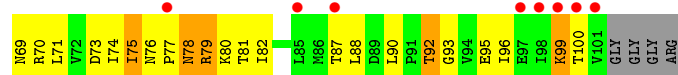
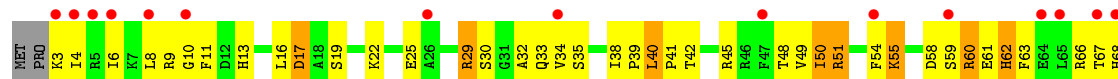
- Molecule 9: 30S ribosomal protein S9



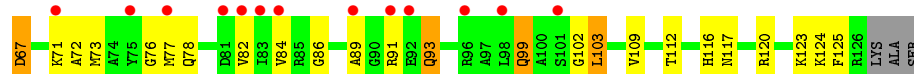
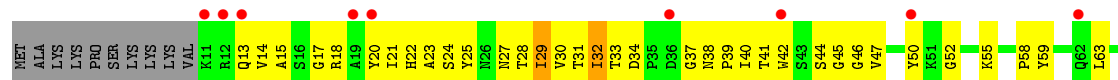
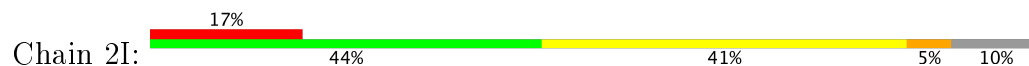
- Molecule 10: 30S ribosomal protein S10



- Molecule 10: 30S ribosomal protein S10

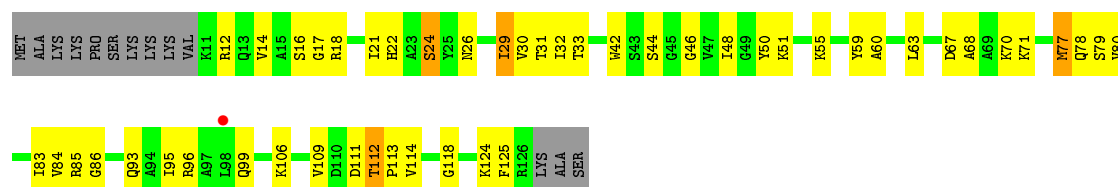


- Molecule 11: 30S ribosomal protein S11

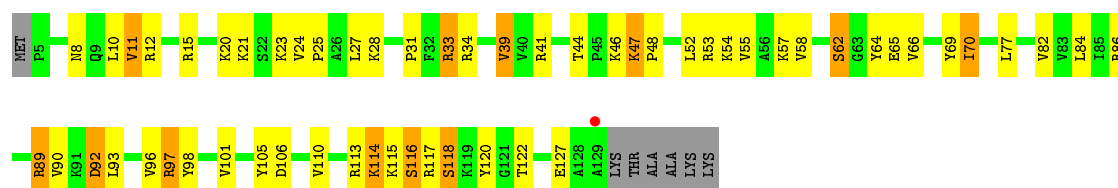


- Molecule 11: 30S ribosomal protein S11

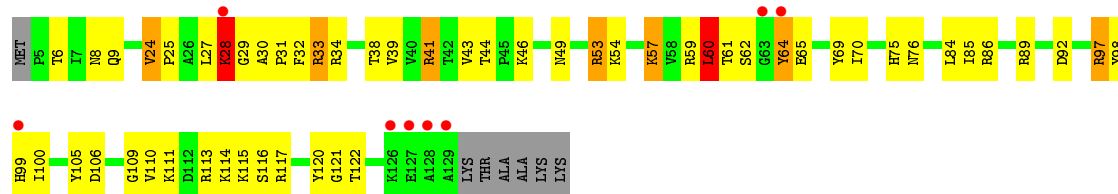




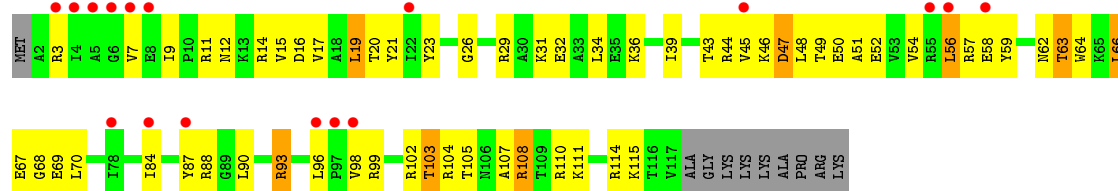
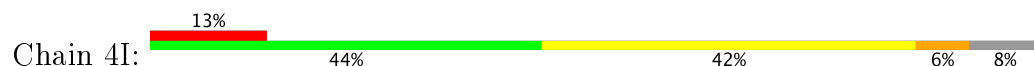
• Molecule 12: 30S ribosomal protein S12



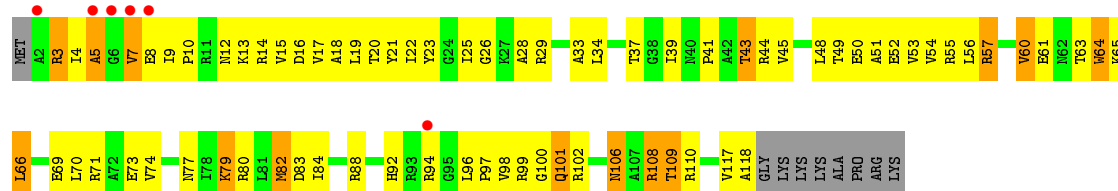
• Molecule 12: 30S ribosomal protein S12



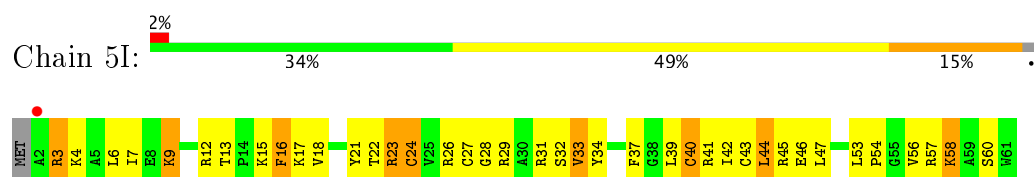
• Molecule 13: 30S ribosomal protein S13



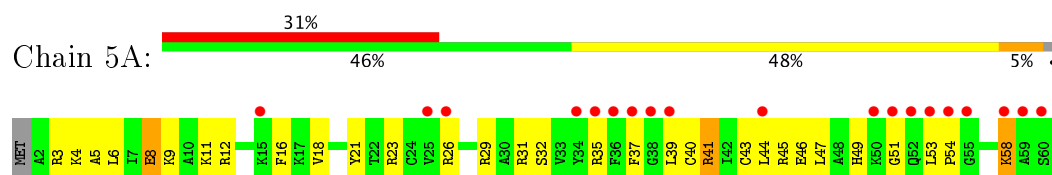
• Molecule 13: 30S ribosomal protein S13



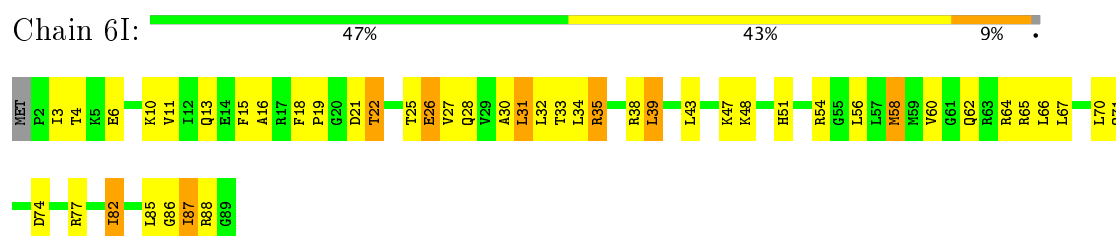
• Molecule 14: 30S ribosomal protein S14 type Z



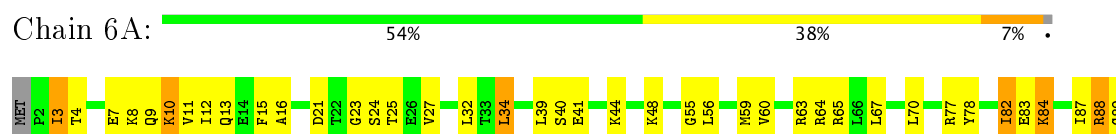
- Molecule 14: 30S ribosomal protein S14 type Z



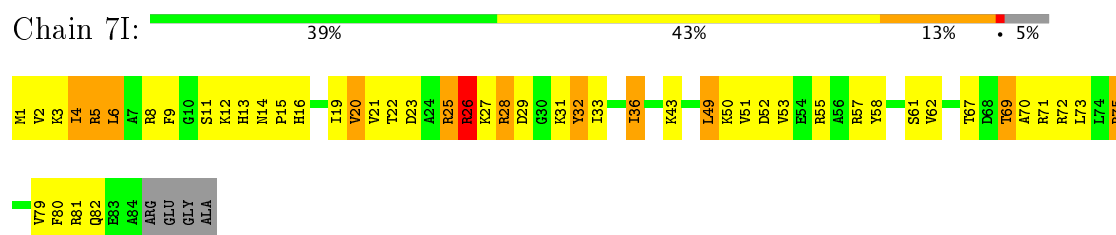
- Molecule 15: 30S ribosomal protein S15



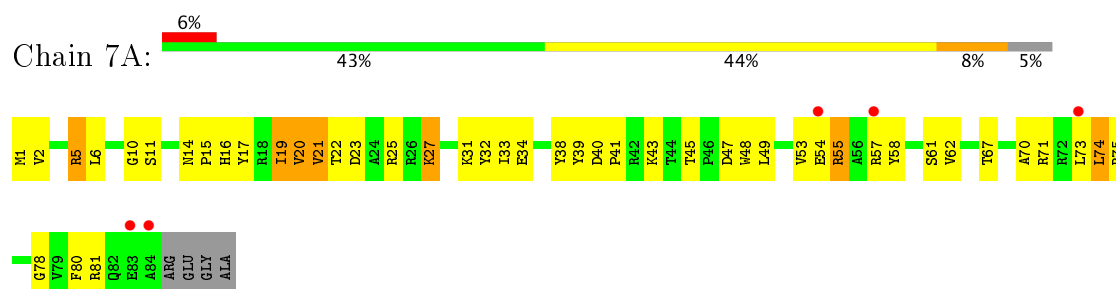
- Molecule 15: 30S ribosomal protein S15



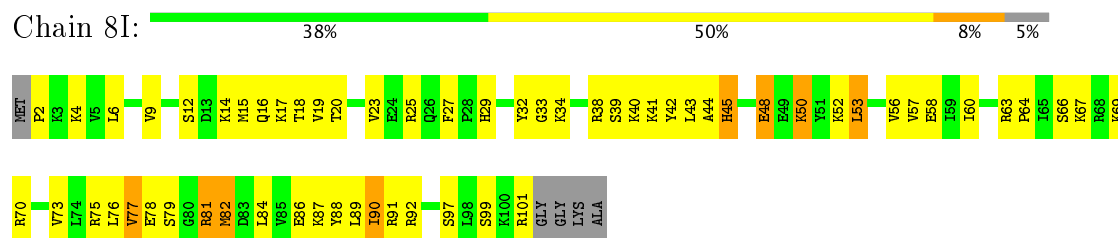
- Molecule 16: 30S ribosomal protein S16



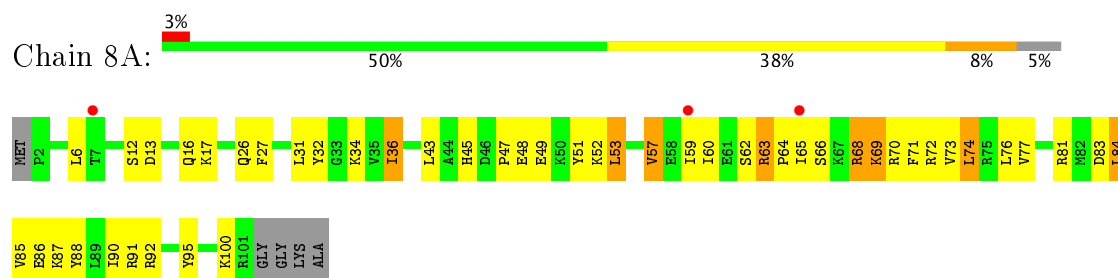
- Molecule 16: 30S ribosomal protein S16



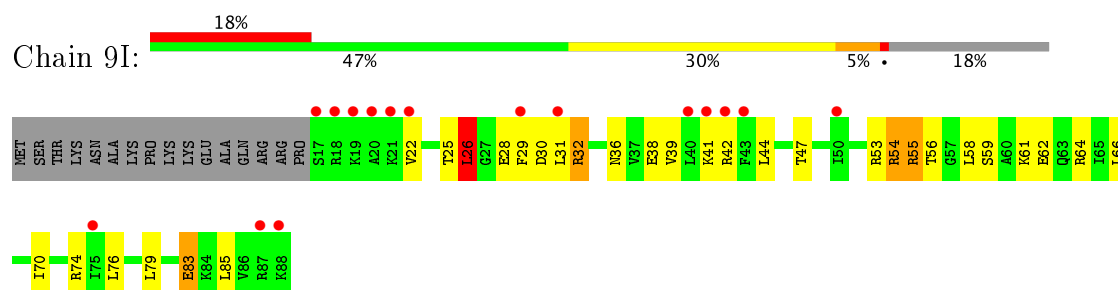
- Molecule 17: 30S ribosomal protein S17



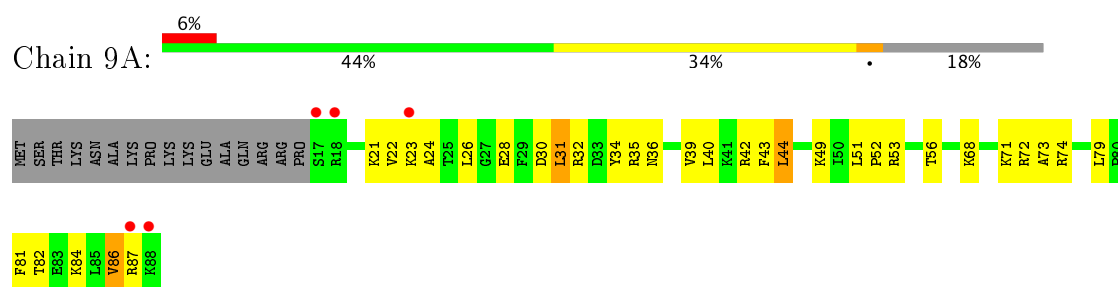
• Molecule 17: 30S ribosomal protein S17



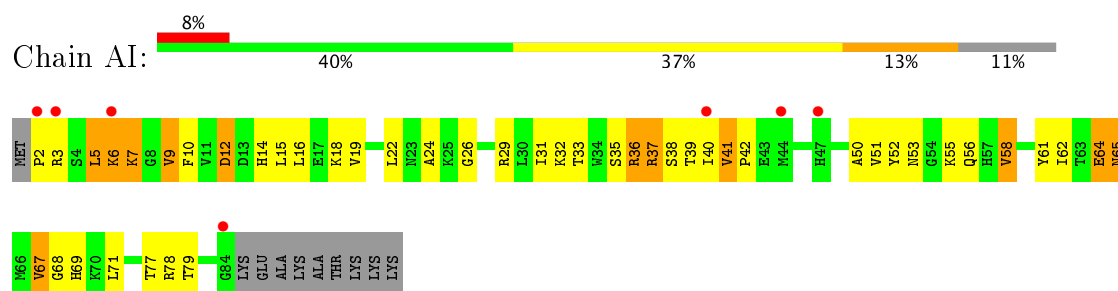
• Molecule 18: 30S ribosomal protein S18



• Molecule 18: 30S ribosomal protein S18



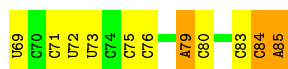
• Molecule 19: 30S ribosomal protein S19



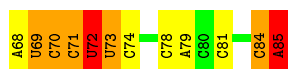
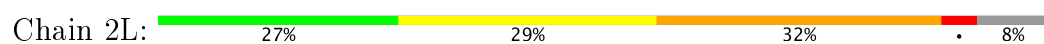
• Molecule 19: 30S ribosomal protein S19



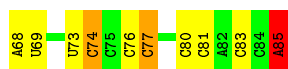
- Molecule 22: tRNA-Tyr



- Molecule 22: tRNA-Tyr



- Molecule 22: tRNA-Tyr



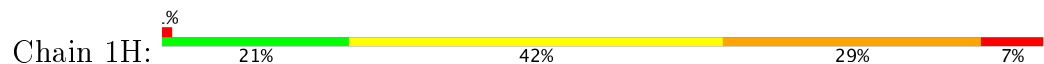
- Molecule 23: mRNA



- Molecule 23: mRNA



- Molecule 24: 23S ribosomal RNA





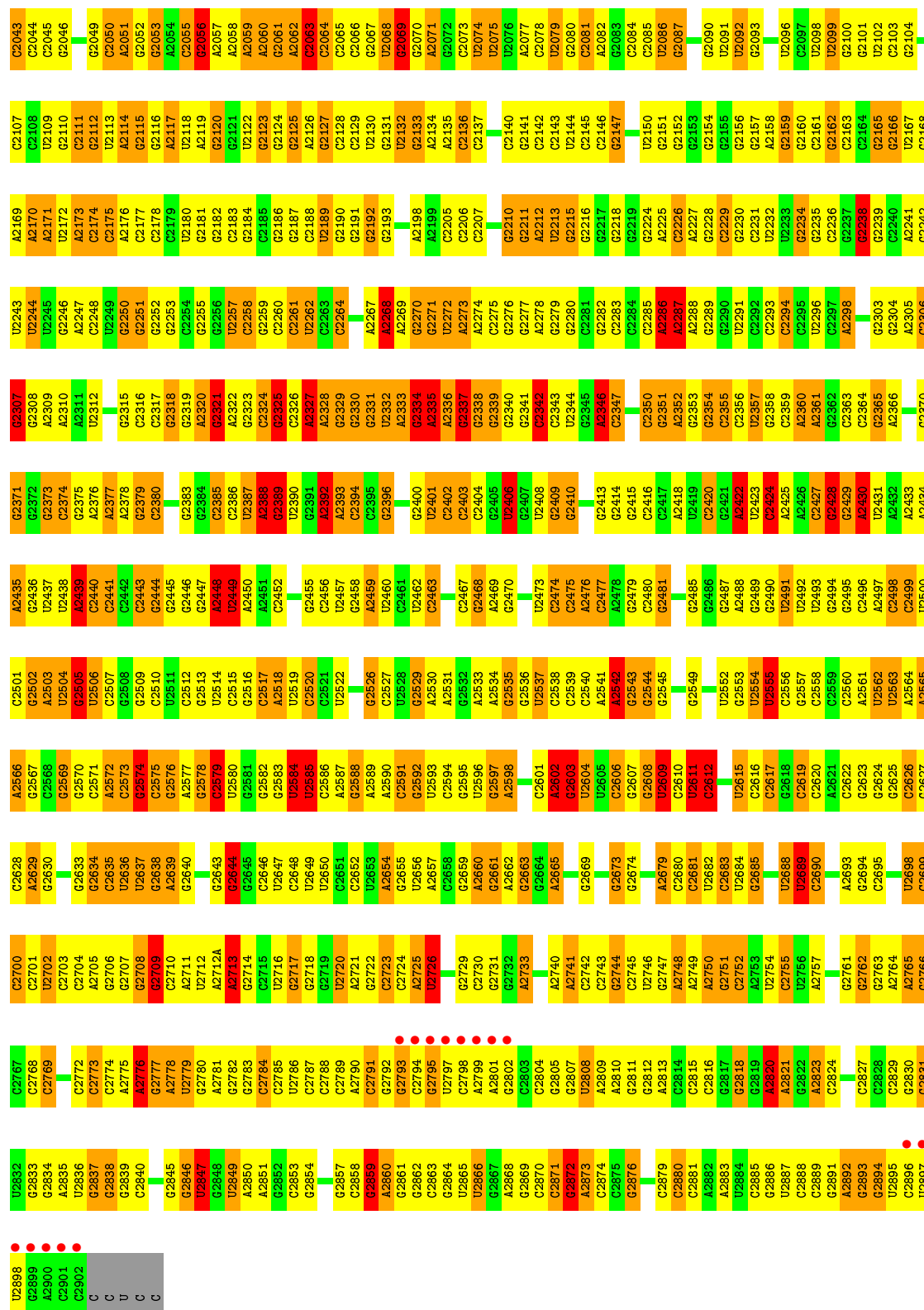


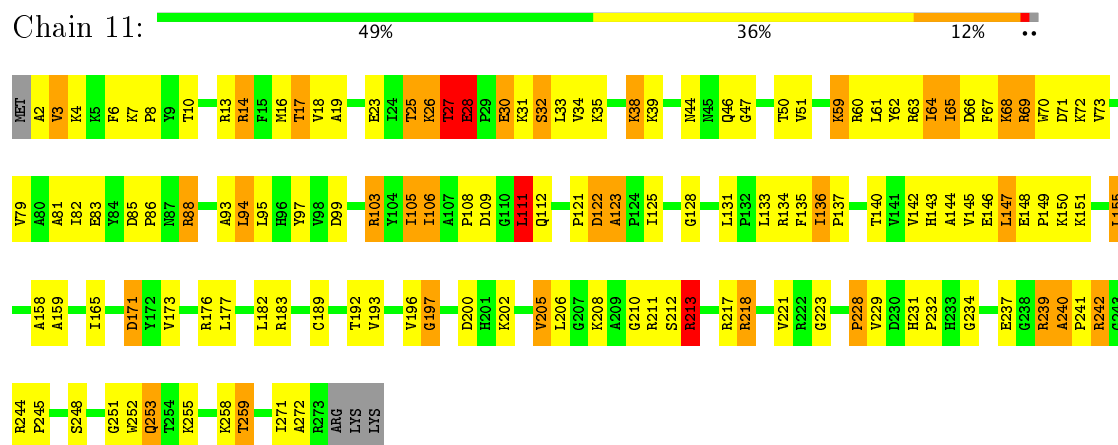
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C	G2842	G2771	G2707	A2640	U2511	G2447	C2385	G2325	U2261	U2189	G2123	C1997
	G2845	C2773	G2708	G2641	C2512	A2448	C2386	G2326	U2262	G2124	G2125	G1998
	G2846	C2774	G2709	G2642	C2513	U2449	U2387	C2327	G2263	G2125	G2126	G1999
	U2847	A2775	G2710	G2643	U2514	A2450	A2388	A2328	G2264	G2126	A2126	G2000
	U2848	G2776	G2711	G2644	C2515	A2451	G2389	A2329	U2265	G2127	G2127	A2001
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	U2850	G2778	A2713	G2646	C2517	A2453	G2391	G2331	A2267	C2128	C2063	G2003
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	G2852	G2780	G2715	U2653	C2520	G2455	A2393	U2333	A2269	U2130	C2065	A2005
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	G2854	G2782	U2717	A2654	U2522	G2458	G2397	A2335	U2272	U2132	G2067	G2007
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		C2785	U2720	A2657	C2525	U2462	U2401	G2338	G2275	A2135	G2070	G2010
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		A2809	A2744	U2682	G2549	U2484	U2423	A2360	C2297	G2163	G2094	G2032
		C2815	U2745	C2683	C2550	A2485	C2424	A2361	C2298	C2164	U2096	A2033
		G2816	G2746	U2684	C2551	U2486	A2425	C2362	A2299	G2165	C2097	U2034
		G2817	G2747	G2685	G2552	G2487	A2426	C2363	G2299	G2166	C2035	G2035
		U2818	U2748	U2686	G2553	U2488	G2427	C2364	C2240	G2167	U2099	C2036
		G2819	A2749	U2688	U2554	U2489	G2428	A2365	G2303	U2167	G2037	G2037
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		G2827	G2761	C2696	A2564	U2497	A2436	A2373	A2311	C2175	U2109	C2045
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		U2830	A2764	A2699	G2567	G2502	U2439	A2376	C2314	C2178	G2112	G2048
		G2831	U2765	C2700	C2568	U2503	A2439	A2377	G2315	C2179	G2113	G2049
		U2833	G2766	C2701	G2569	U2504	C2440	A2378	C2316	U2180	A2114	C2050
		A2834	U2767	U2695	G2570	G2505	C2441	G2379	C2317	G2181	G2115	A2051
		C2835	C2768	U2696	C2571	U2506	C2442	C2380	G2318	G2116	G2116	G2052
		G2836	C2769	U2697	A2572	C2507	C2443	C2381	G2319	A2117	G2117	G2053
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- Molecule 24: 23S ribosomal RNA

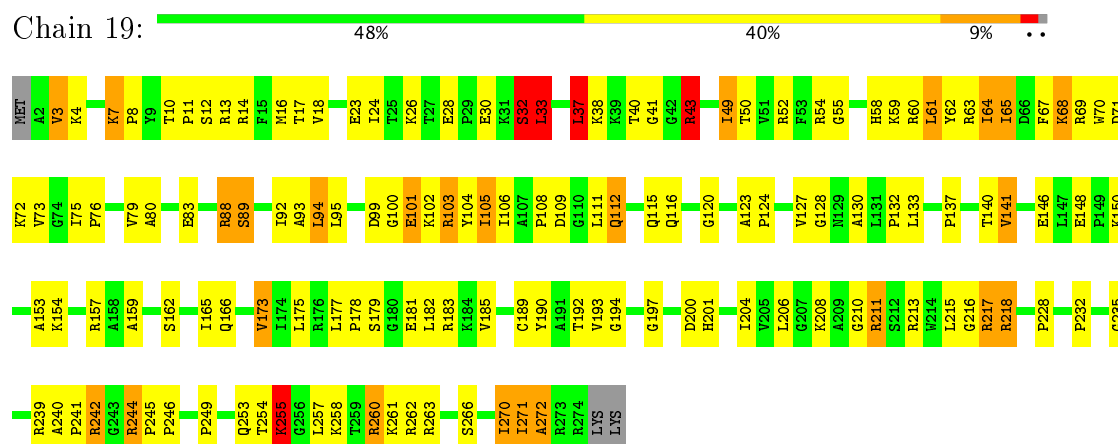


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C1979	G1908	C1832	G1772	U1687	A1558	U1489	G1424	C1358	C1293	G1231	G1161	U1098	U1035
G1980	C1909	G1833	A1773	U1688	G1559	A1490	G1425	A1359	U1294	G1232	G1162	G1099	G1036
G1981	G1910	U1834	C1774	A1899	G1560	G1491	G1426	A1360	C1295	G1233	G1163	U1037	G1037
C1982	U1911	G1835	U1775	A1690		G1492	A1427		G1296	U1234	G1164	G1104	
G1983	A1912	C1836	G1776	C1891	C1564	C1493	G1428	G1364	C1297		U1165	U1105	C1040
G1984	A1913	G1837	U1777	U1692	A1566	A1494	G1429	A1365	G1298	A1237	C1166	G1106	C1041
G1985	C1914	C1838	U1778	U1693	A1567	A1495	C1430	A1366	G1299	G1238		G1107	G1042
	U1915	G1839	U1779	C1694	A1567	A1496	C1431	A1367	U1300	G1239	G1170	U1108	C1043
	A1916	G1840	A1780	G1695	G1568	U1497	C1432	G1368	A1301	U1240	G1171	G1109	G1044
	U1917		C1781	G1696	A1569	G1498	U1433		G1302	A1241	G1173	G1110	A1045
C1988	G1918	G1845	G1782	G1697	A1570	G1499	A1434	G1371	G1303	A1242	A1174	A1111	A1046
G1989		G1846	A1783	C1698	A1571	G1500		U1372	G1304	G1243	U1175	G1112	G1047
G1990	G1924	A1847	A1784	A1699	A1572		C1437	A1373	C1305	G1244	G1176	U1113	A1048
U1991	C1925	A1848	A1785	U1700	G1573	U1503	U1438	G1374	C1306	G1245	A1177	G1114	C1049
U1992	G1926	G1849	A1786	A1701	C1574	C1504	A1439	C1375	A1307	A1246	C1178	G1115	A1050
U1993	G1927	G1850	A1787	G1702	C1575	C1505	G1440	C1376	A1308	A1247	G1179	G1116	G1051
U1995	A1928	U1851	G1788	G1703	U1576	C1506	G1441	G1377	G1309	G1248	C1180	G1117	C1052
G1996	G1929	C1852	A1789	G1704	C1577	A1507	G1442	A1378	C1310	U1249	C1181	G1118	C1053
	C1930	G1853	C1790	G1705	U1578	A1508		A1379	G1250	G1250	A1182	C1119	A1054
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G2002	G1934	G1857	U1794	C1711	C1582	U1514		U1316	G1316	A1254	G1186	C1123	U1058
	G1935	G1858	C1795	C1712		C1515	G1448	A1384	A1317	U1255	G1187	G1124	G1059
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G2009	A1937	G1860	G1650	G1717	A1587	G1517	G1459	C1386	C1319	G1257	A1189	A1126	U1061
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U1939	U1939	A1652	G1652	G1725		C1519	C1451	C1388	G1321	G1259	G1191	A1128	G1064
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A2014	U1944	A1872	C1856	U1730	A1596	G1524	A1460	A1393	U1326	A1265	U1198	U1133	G1068
G2015	G1945	G1878	C1857	G1731	A1597	G1525	A1461	U1394	C1327	G1266	G1199	G1135	A1069
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U2017	C1947	C1880	U1659	G1733	C1599	G1527	C1462	U1397	U1329	A1268	C1201	G1137	C1071
G2018	G1948	G1881	C1860		C1600	A1528	C1463	U1398	C1330	G1269	C1202	G1138	C1072
A2019	G1949	C1882	G1661	C1742	G1601	A1529	G1465	C1399	G1332	C1270	A1204	G1139	A1073
G2020	G1950	A1883	C1662	G1746	A1602	G1530	G1466	C1400	G1333	G1271	U1141	U1140	G1074
G2021	U1951	A1884	A1664		A1603	C1531	C1467	G1401		A1272	U1142	U1141	C1075
G2022	A1952	A1885	A1665	C1751	C1604	G1532		C1402		U1273		A1142	C1076
G2023	G1953	C1887	G1666	C1752	C1605	C1533		A1336	G1209	A1274	G1209	A1142A	
G2024	G1954	G1888	G1667	G1753	G1606	G1534	G1470	C1403	A1210	A1275	A1143	A1143	C1079
G2025	U1955	A1889	C1668	C1754	C1607	U1535	A1471	G1338	U1211	A1276	G1144	G1144	A1080
G2026		A1890	A1669	A1755	A1608	A1536	A1472	U1405	G1212	C1145	C1145	C1145	U1081
G2027	C1961	C1891	C1670	G1756	A1609	C1537	G1473	U1406	G1213	A1277	C1146	C1146	U1082
A2031	U1963	U1671	U1671		A1610	G1538	C1474	C1407	A1213	G1278	C1147	C1147	U1083
G2032	G1964	C1672	C1672	A1759	C1611	G1539	G1475	C1408	A1342	G1279	A1148	A1148	U1084
A2033	C1965	U1673	U1673		C1612	G1540	C1476	C1409	C1345	G1281	G1216	G1216	A1085
G2034	G1966	G1674	G1674	A1760	G1613	U1541	C1477	G1410	G1346	U1282	G1149	G1149	A1086
G2035	C1967	C1675	C1675	C1761	A1614	G1542	A1478	G1347	G1283	A1278	A1220	G1150	A1087
G2036	U1968	A1676	A1676	G1763	C1615	G1479	C1479	C1348	A1284	G1284	C1152	C1152	G1087
A1969	G1969	G1677	G1677		A1616	A1543	G1480	A1349	G1285	G1285	G1224	C1153	G1088
G2037	G1970	A1678	A1678	C1765	C1617	U1482	U1482	G1416	C1350	A1286	G1225	G1154	G1089
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G2039	G1972	C1680	C1680	U1766	G1619	C1548	G1483	A1519	G1288	A1227	A1156	G1156	G1093
U2041	G1973	G1681	G1681	U1768	G1620	A1554	G1485	U1420	C1289	G1289	G1157	G1157	U1094
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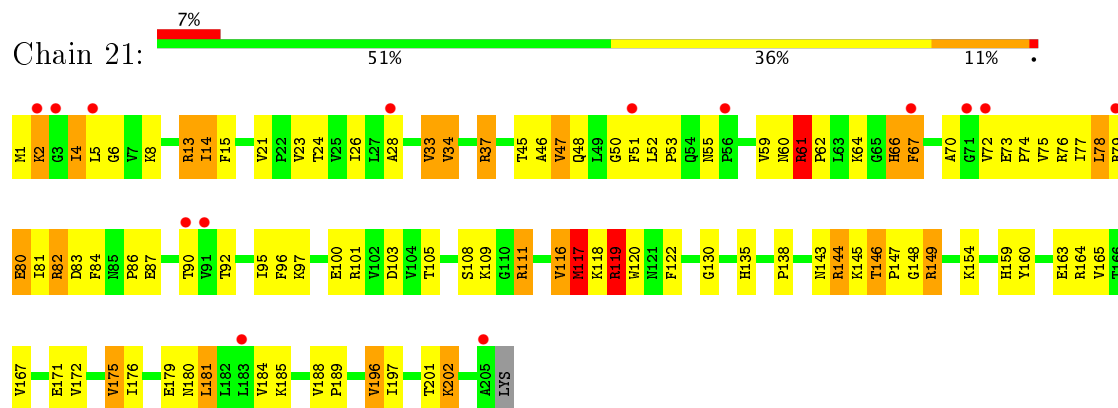




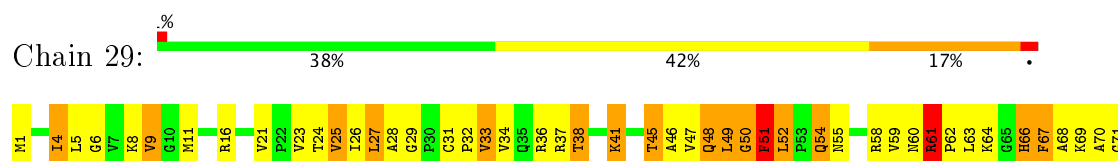
• Molecule 27: 50S ribosomal protein L2

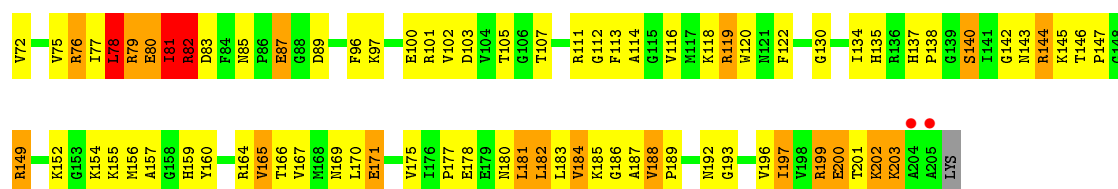


• Molecule 28: 50S ribosomal protein L3

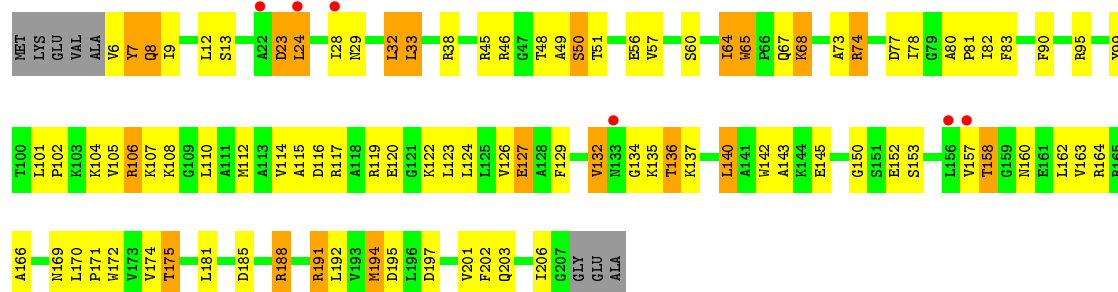


• Molecule 28: 50S ribosomal protein L3

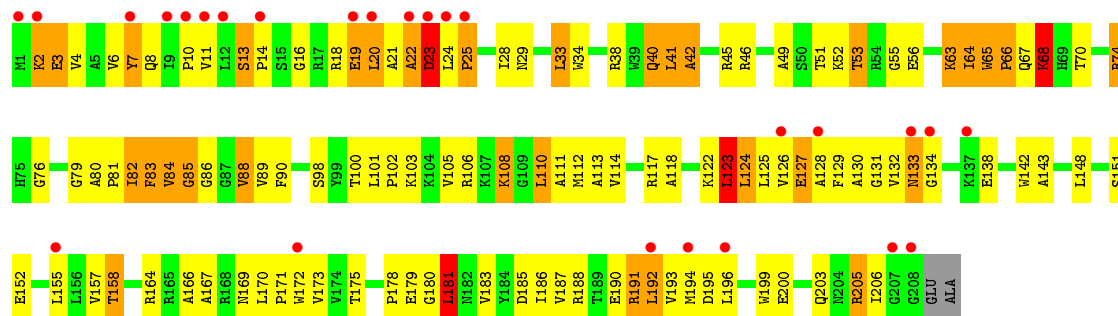




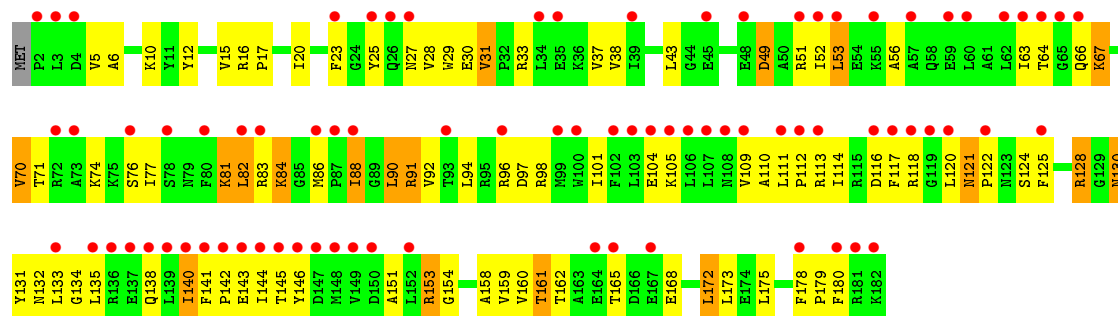
• Molecule 29: 50S ribosomal protein L4



• Molecule 29: 50S ribosomal protein L4

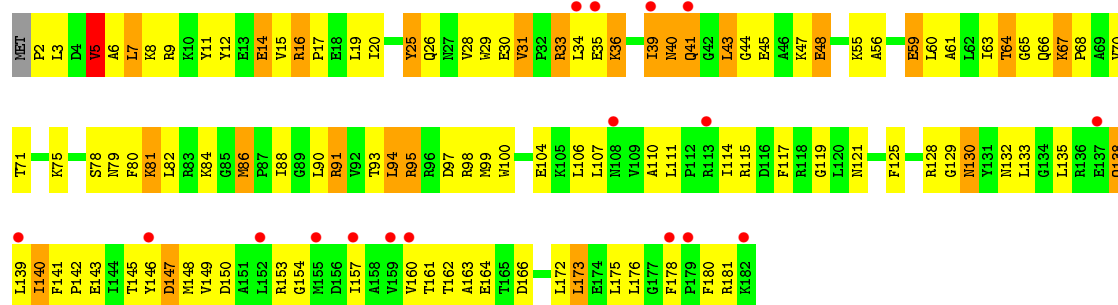


• Molecule 30: 50S ribosomal protein L5



• Molecule 30: 50S ribosomal protein L5

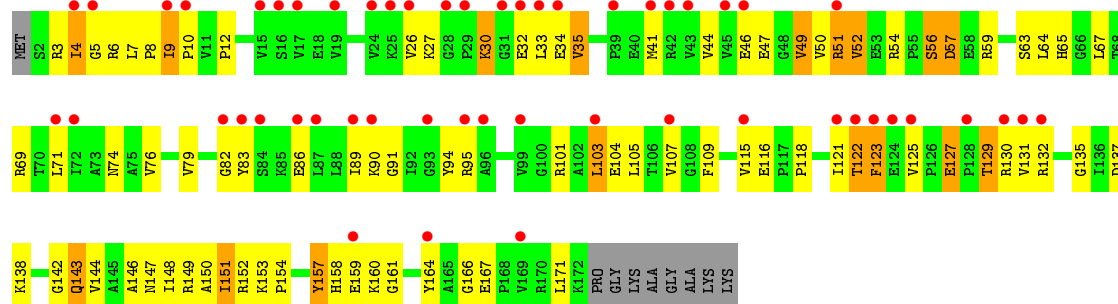




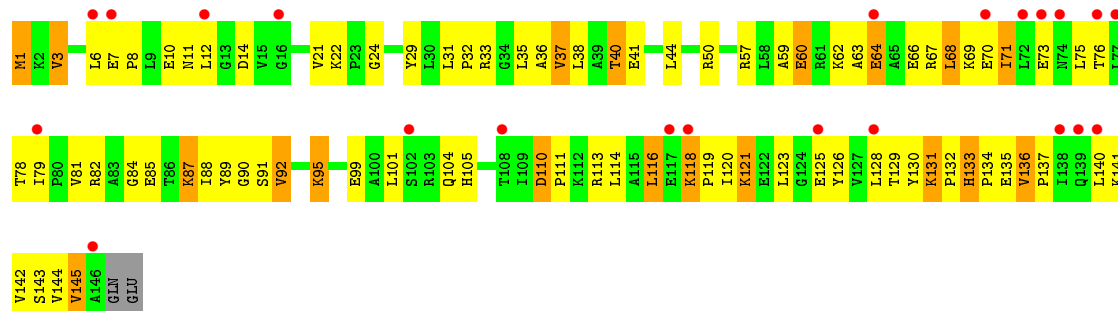
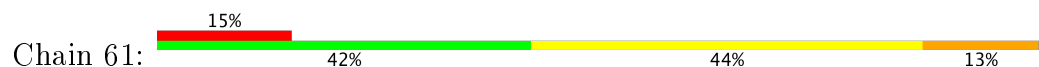
- Molecule 31: 50S ribosomal protein L6



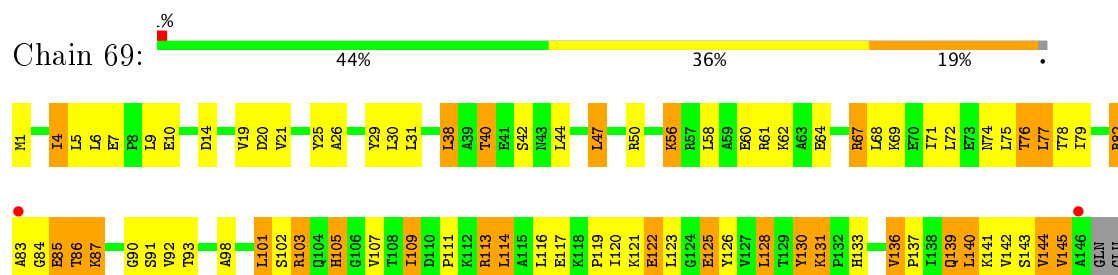
- Molecule 31: 50S ribosomal protein L6



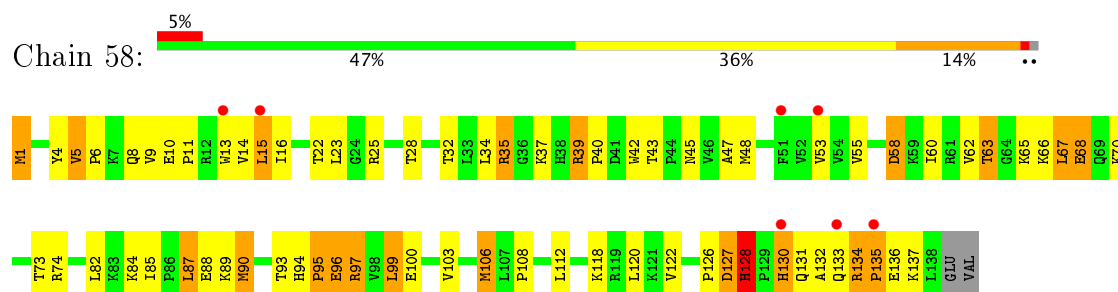
- Molecule 32: 50S ribosomal protein L9



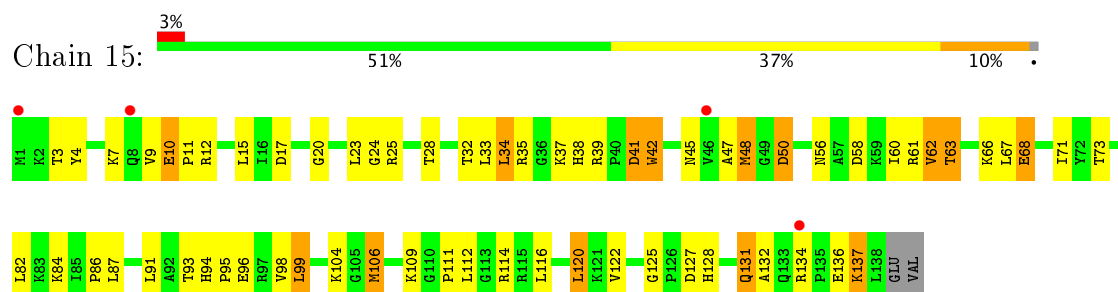
- Molecule 32: 50S ribosomal protein L9



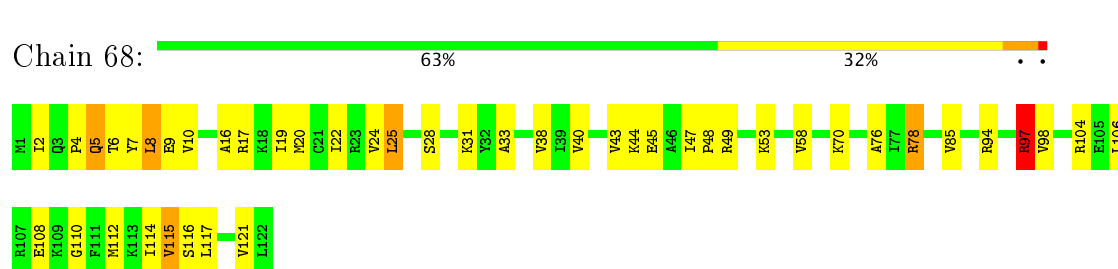
- Molecule 33: 50S ribosomal protein L13



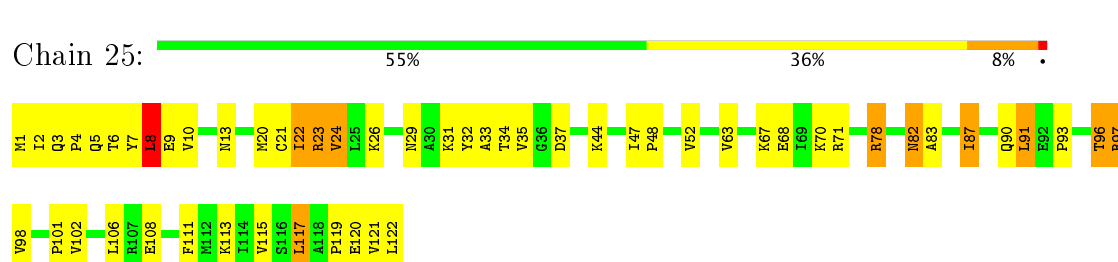
- Molecule 33: 50S ribosomal protein L13



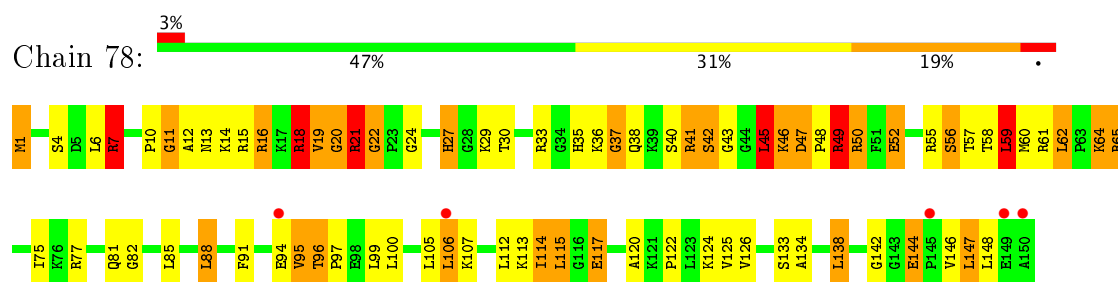
- Molecule 34: 50S ribosomal protein L14



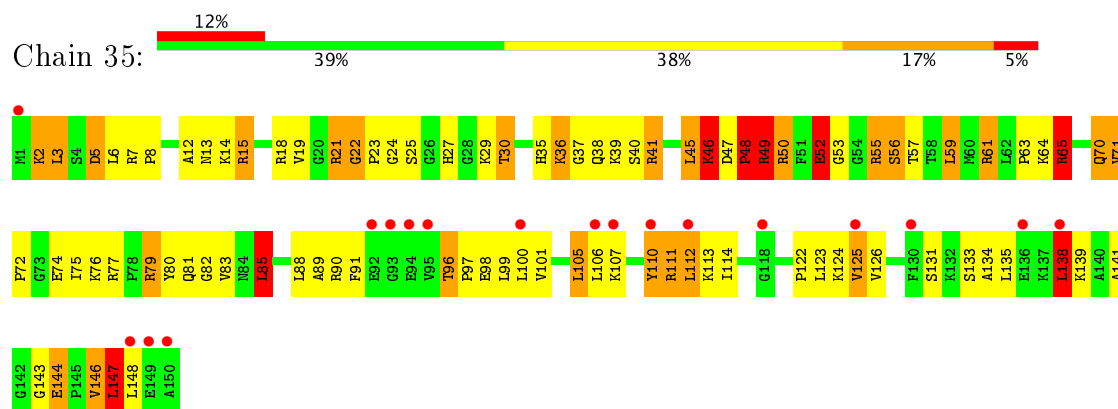
- Molecule 34: 50S ribosomal protein L14



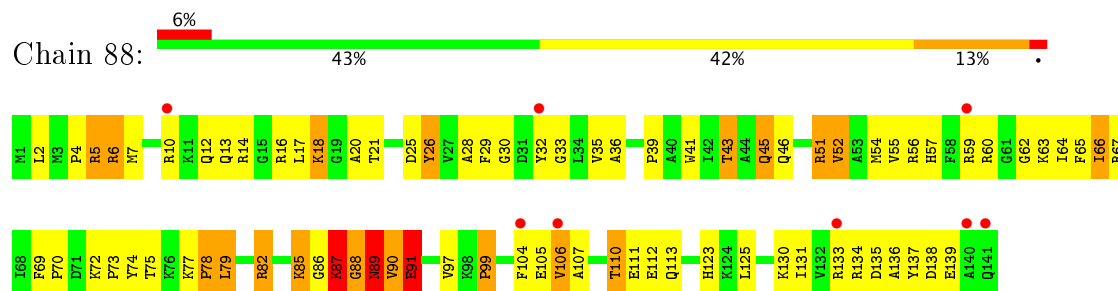
- Molecule 35: 50S ribosomal protein L15



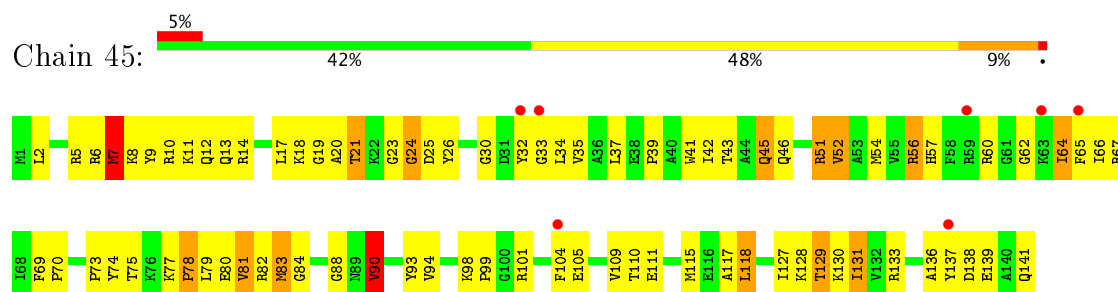
- Molecule 35: 50S ribosomal protein L15



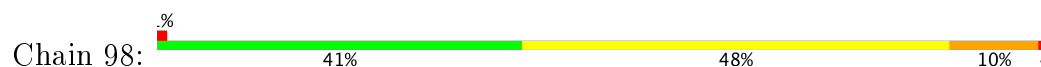
- Molecule 36: 50S ribosomal protein L16

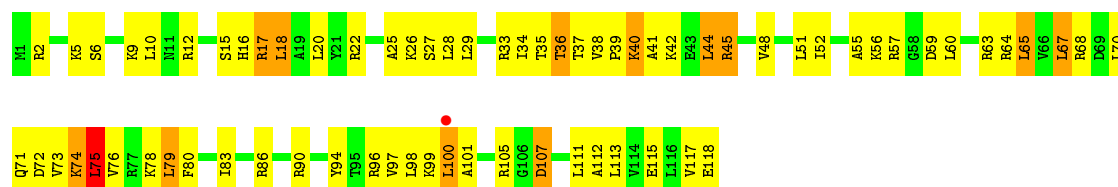


- Molecule 36: 50S ribosomal protein L16



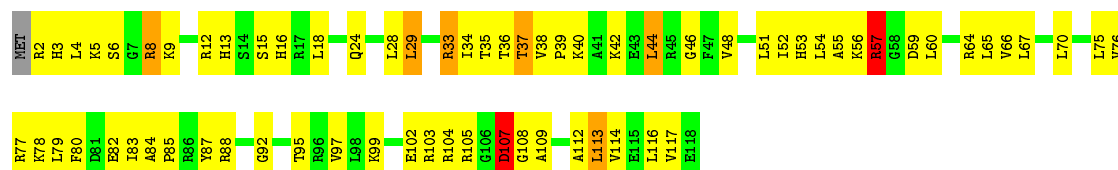
- Molecule 37: 50S ribosomal protein L17





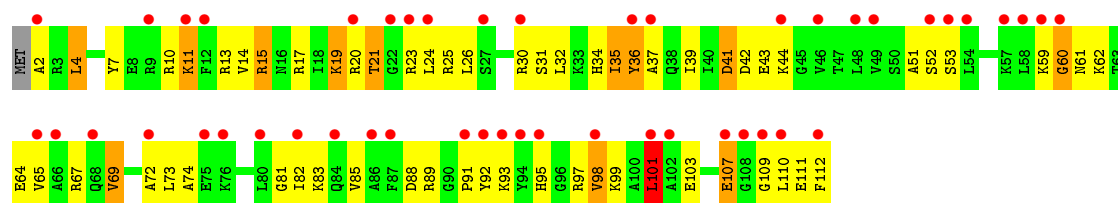
• Molecule 37: 50S ribosomal protein L17

Chain 55: 41% 52% 5% ..



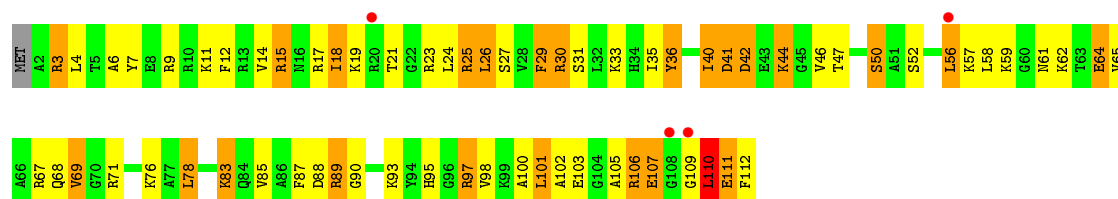
• Molecule 38: 50S ribosomal protein L18

Chain A8: 42% 44% 44% 11% ..



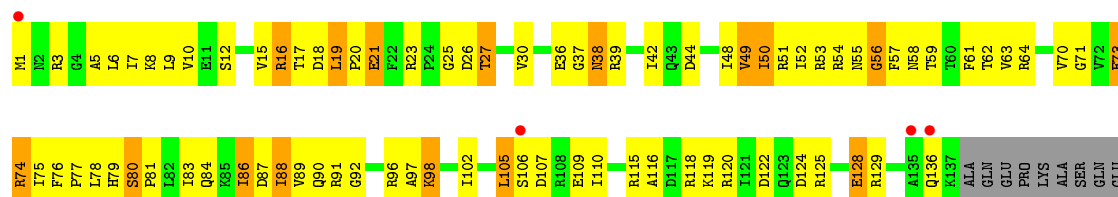
• Molecule 38: 50S ribosomal protein L18

Chain 65: 4% 39% 38% 21% ..



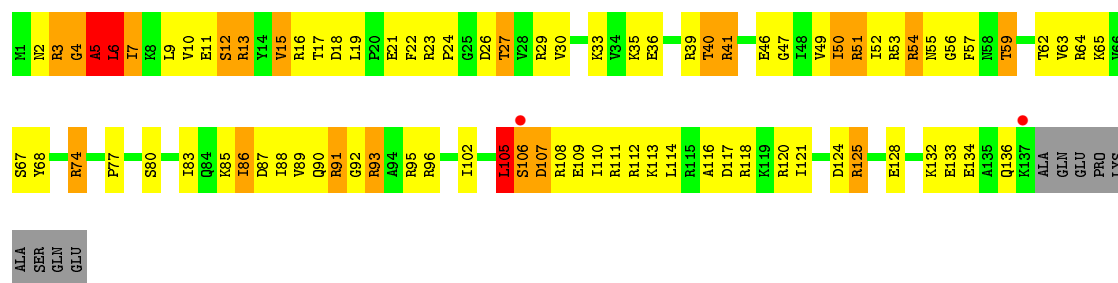
• Molecule 39: 50S ribosomal protein L19

Chain B8: 3% 37% 46% 11% 6%

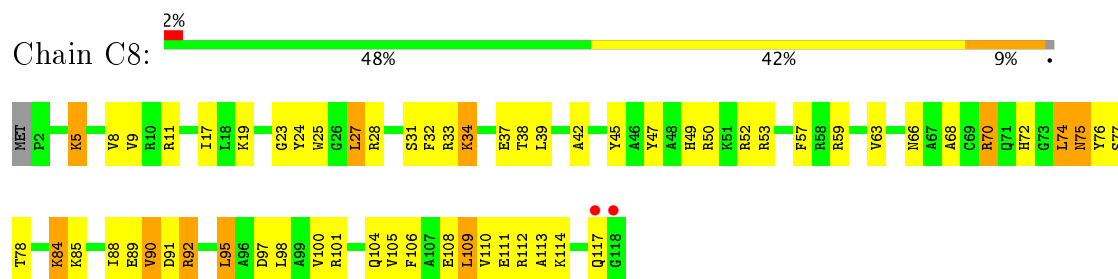


• Molecule 39: 50S ribosomal protein L19

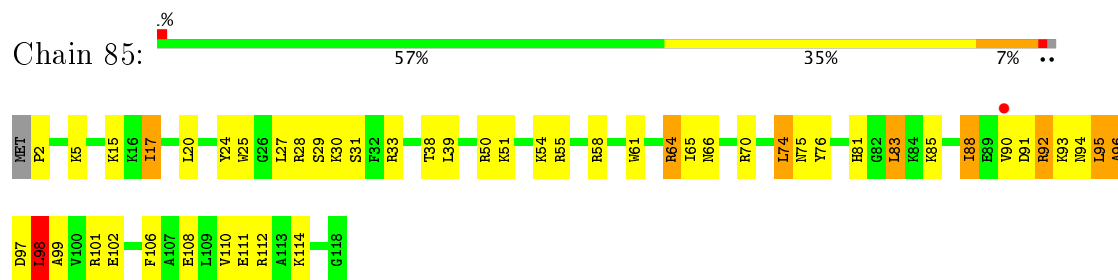
Chain 75: % 35% 43% 14% 6%



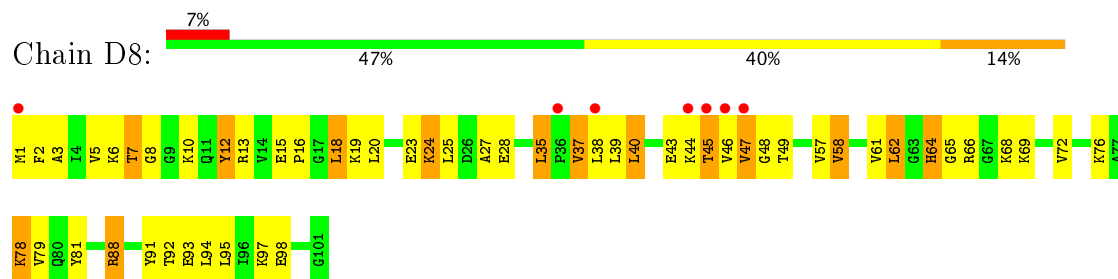
- Molecule 40: 50S ribosomal protein L20



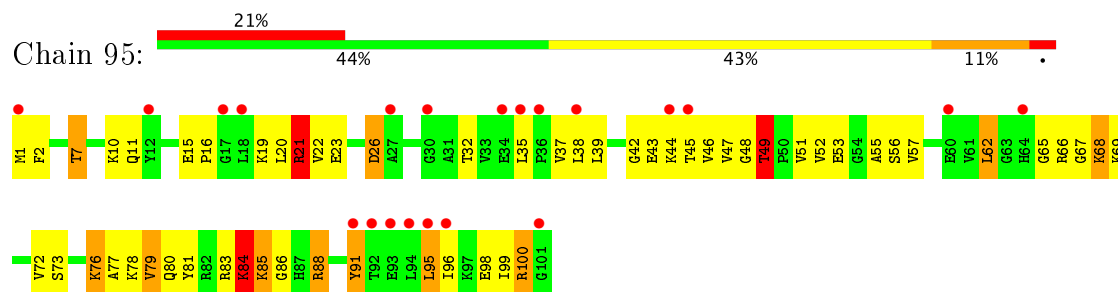
- Molecule 40: 50S ribosomal protein L20



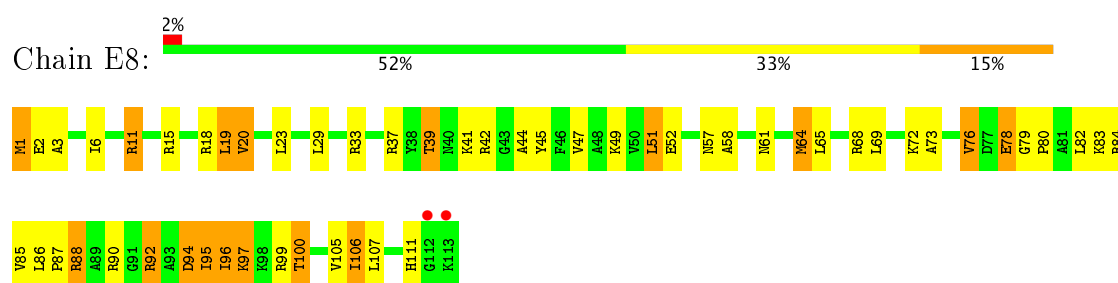
- Molecule 41: 50S ribosomal protein L21



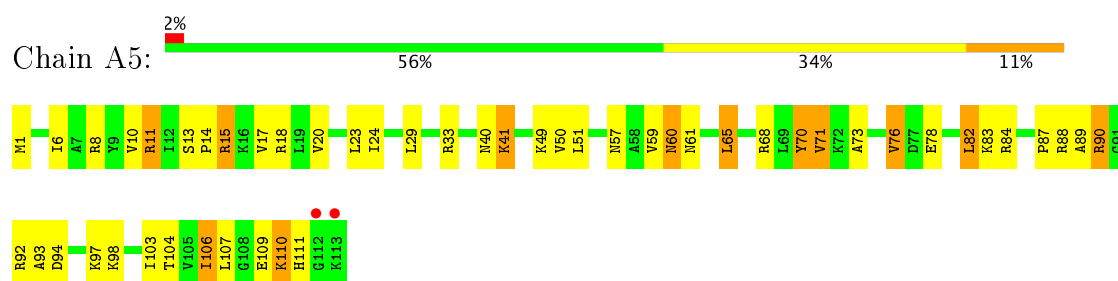
- Molecule 41: 50S ribosomal protein L21



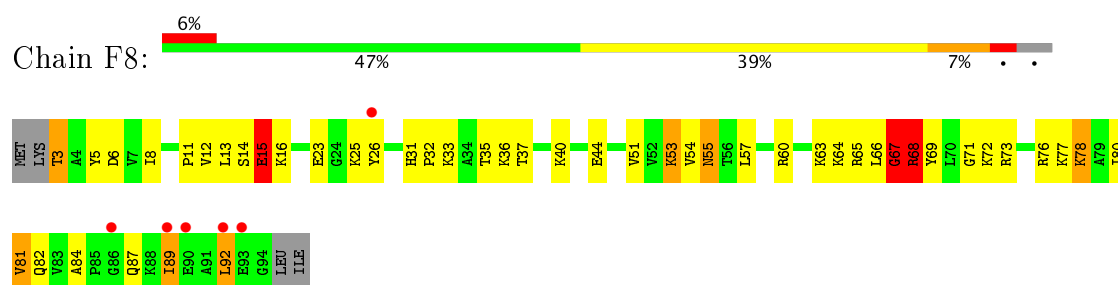
- Molecule 42: 50S ribosomal protein L22



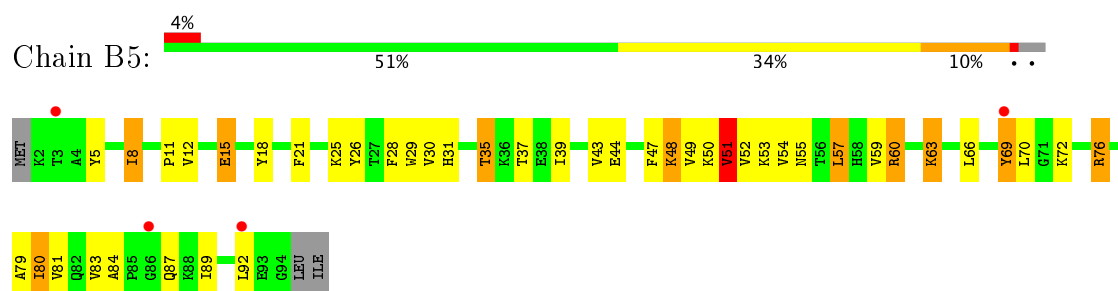
- Molecule 42: 50S ribosomal protein L22



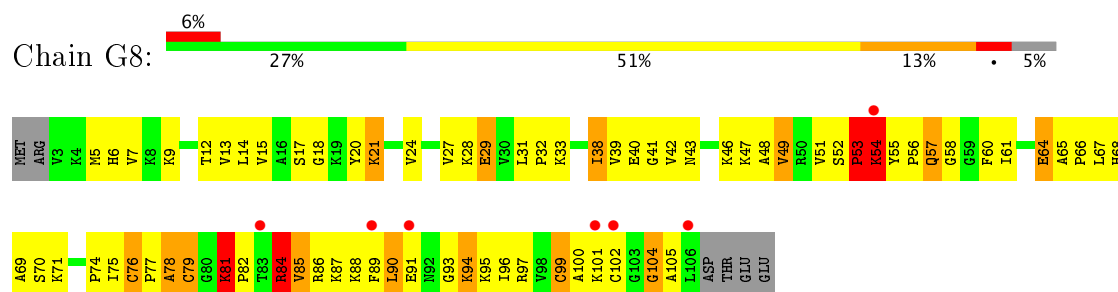
- Molecule 43: 50S ribosomal protein L23



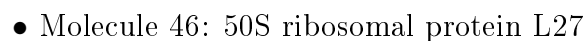
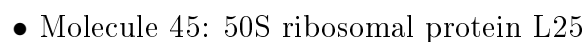
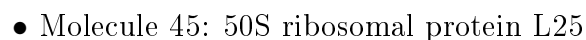
- Molecule 43: 50S ribosomal protein L23

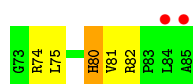


- Molecule 44: 50S ribosomal protein L24

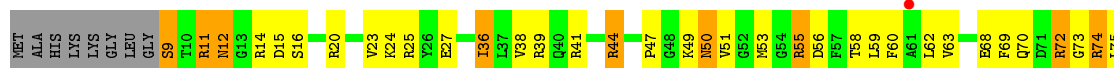


- Molecule 44: 50S ribosomal protein L24

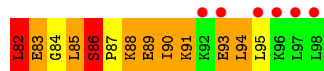
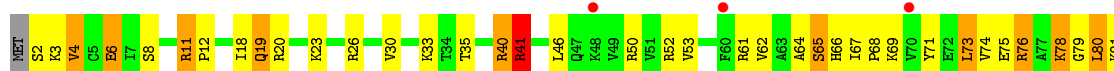




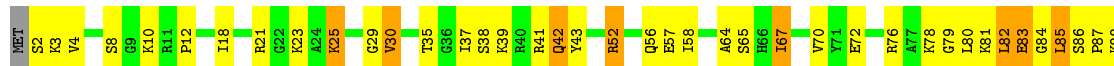
- Molecule 46: 50S ribosomal protein L27



- Molecule 47: 50S ribosomal protein L28



- Molecule 47: 50S ribosomal protein L28



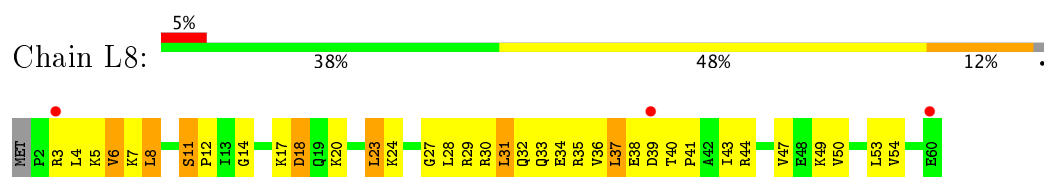
- Molecule 48: 50S ribosomal protein L29



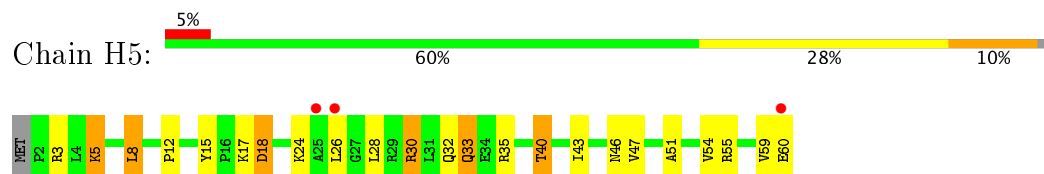
- Molecule 48: 50S ribosomal protein L29



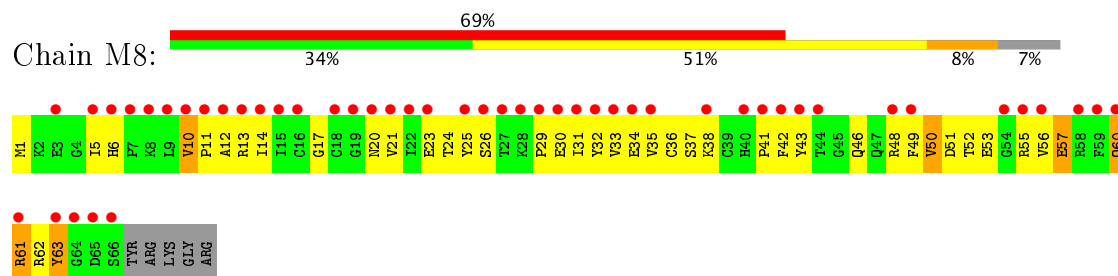
- Molecule 49: 50S ribosomal protein L30



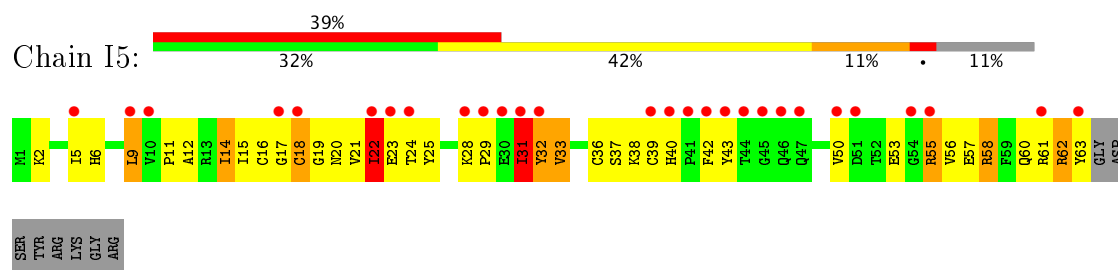
- Molecule 49: 50S ribosomal protein L30



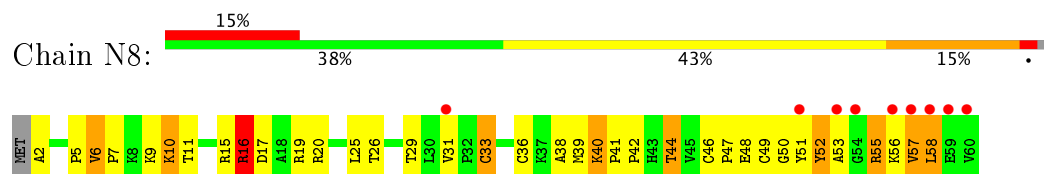
- Molecule 50: 50S ribosomal protein L31



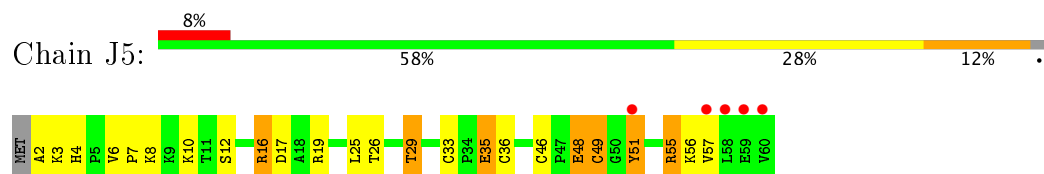
- Molecule 50: 50S ribosomal protein L31



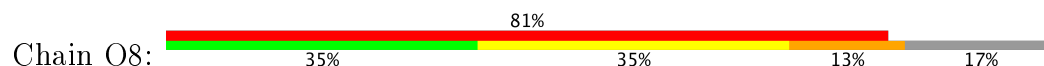
- Molecule 51: 50S ribosomal protein L32

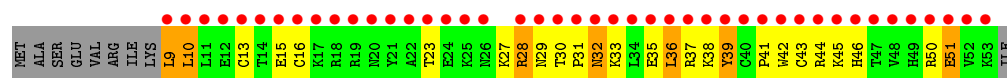


- Molecule 51: 50S ribosomal protein L32

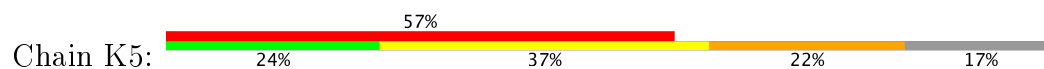


- Molecule 52: 50S ribosomal protein L33





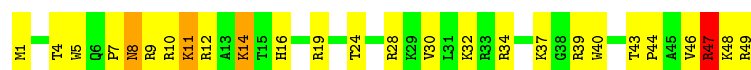
- Molecule 52: 50S ribosomal protein L33



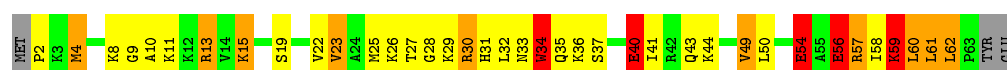
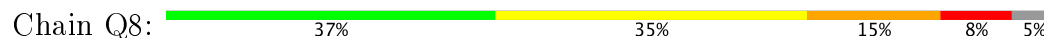
- Molecule 53: 50S ribosomal protein L34



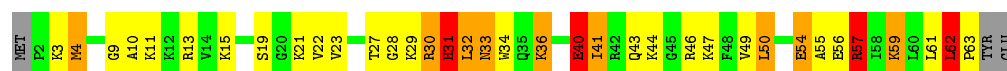
- Molecule 53: 50S ribosomal protein L34



- Molecule 54: 50S ribosomal protein L35



- Molecule 54: 50S ribosomal protein L35



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	210.70 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	1.64 (at 3.07 Å)	Xtriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.227 , 0.193 0.193 , 0.226	Depositor DCC
R_{free} test set	1805 reflections (0.19%)	DCC
Wilson B-factor (Å ²)	83.9	Xtriage
Anisotropy	0.112	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 81.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	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%)	11	42
2	1E	235/256 (92%)	199 (85%)	32 (14%)	4 (2%)	11	42
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%)	9	39
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%)	25	64
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%)	12	45
8	7E	136/138 (99%)	125 (92%)	11 (8%)	0	100	100
9	82	125/128 (98%)	112 (90%)	12 (10%)	1 (1%)	22	62
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%)	20	60
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%)	3	18
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%)	11	42
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%)	15	51
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%)	18	57
18	9A	70/88 (80%)	65 (93%)	5 (7%)	0	100	100
18	9I	70/88 (80%)	63 (90%)	6 (9%)	1 (1%)	13	47
19	AA	77/93 (83%)	57 (74%)	17 (22%)	3 (4%)	3	21
19	AI	81/93 (87%)	66 (82%)	13 (16%)	2 (2%)	6	31
20	BA	97/106 (92%)	83 (86%)	14 (14%)	0	100	100
20	BI	97/106 (92%)	84 (87%)	13 (13%)	0	100	100
21	1B	23/27 (85%)	22 (96%)	1 (4%)	0	100	100
21	1F	23/27 (85%)	21 (91%)	2 (9%)	0	100	100
26	7I	131/229 (57%)	130 (99%)	1 (1%)	0	100	100
26	79	131/229 (57%)	129 (98%)	2 (2%)	0	100	100
27	11	270/276 (98%)	254 (94%)	12 (4%)	4 (2%)	12	45
27	19	271/276 (98%)	253 (93%)	15 (6%)	3 (1%)	17	54
28	21	203/206 (98%)	174 (86%)	28 (14%)	1 (0%)	32	71
28	29	203/206 (98%)	160 (79%)	34 (17%)	9 (4%)	3	18
29	31	200/210 (95%)	189 (94%)	10 (5%)	1 (0%)	32	71
29	39	206/210 (98%)	176 (85%)	21 (10%)	9 (4%)	3	18
30	41	179/182 (98%)	154 (86%)	24 (13%)	1 (1%)	28	67
30	49	179/182 (98%)	151 (84%)	25 (14%)	3 (2%)	11	42
31	51	172/180 (96%)	146 (85%)	20 (12%)	6 (4%)	4	23
31	59	169/180 (94%)	133 (79%)	35 (21%)	1 (1%)	28	67
32	61	144/148 (97%)	120 (83%)	21 (15%)	3 (2%)	8	36
32	69	144/148 (97%)	122 (85%)	19 (13%)	3 (2%)	8	36
33	15	136/140 (97%)	128 (94%)	7 (5%)	1 (1%)	25	64
33	58	136/140 (97%)	116 (85%)	13 (10%)	7 (5%)	2	15

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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%)	22	62
35	35	148/150 (99%)	118 (80%)	24 (16%)	6 (4%)	3	19
35	78	148/150 (99%)	117 (79%)	28 (19%)	3 (2%)	9	37
36	45	139/141 (99%)	114 (82%)	20 (14%)	5 (4%)	4	23
36	88	139/141 (99%)	111 (80%)	23 (16%)	5 (4%)	4	23
37	55	115/118 (98%)	103 (90%)	11 (10%)	1 (1%)	20	60
37	98	116/118 (98%)	104 (90%)	10 (9%)	2 (2%)	11	42
38	65	109/112 (97%)	93 (85%)	14 (13%)	2 (2%)	10	40
38	A8	109/112 (97%)	94 (86%)	13 (12%)	2 (2%)	10	40
39	75	135/146 (92%)	113 (84%)	19 (14%)	3 (2%)	8	35
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	15
41	D8	99/101 (98%)	89 (90%)	9 (9%)	1 (1%)	18	57
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%)	17	54
43	F8	90/96 (94%)	84 (93%)	4 (4%)	2 (2%)	8	35
44	C5	102/110 (93%)	72 (71%)	27 (26%)	3 (3%)	5	28
44	G8	102/110 (93%)	84 (82%)	12 (12%)	6 (6%)	2	12
45	D5	177/206 (86%)	145 (82%)	25 (14%)	7 (4%)	3	20
45	H8	173/206 (84%)	134 (78%)	32 (18%)	7 (4%)	3	20
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%)	17	54
47	J8	95/98 (97%)	83 (87%)	10 (10%)	2 (2%)	8	36
48	G5	67/72 (93%)	56 (84%)	11 (16%)	0	100	100
48	K8	64/72 (89%)	61 (95%)	0	3 (5%)	3	17
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	9
50	M8	64/71 (90%)	45 (70%)	17 (27%)	2 (3%)	5	26
51	J5	57/60 (95%)	48 (84%)	8 (14%)	1 (2%)	10	40
51	N8	57/60 (95%)	49 (86%)	6 (10%)	2 (4%)	4	23
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%)	3	18
54	M5	60/65 (92%)	51 (85%)	6 (10%)	3 (5%)	2	16
54	Q8	60/65 (92%)	51 (85%)	7 (12%)	2 (3%)	4	25
All	All	11616/12512 (93%)	10210 (88%)	1239 (11%)	167 (1%)	13	47

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	7
2	1E	205/220 (93%)	150 (73%)	55 (27%)	0	1
3	22	160/188 (85%)	123 (77%)	37 (23%)	1	4
3	2E	159/188 (85%)	135 (85%)	24 (15%)	3	15
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%)	2	7
5	42	116/123 (94%)	89 (77%)	27 (23%)	1	4
5	4E	116/123 (94%)	89 (77%)	27 (23%)	1	4
6	52	90/90 (100%)	75 (83%)	15 (17%)	2	11
6	5E	90/90 (100%)	75 (83%)	15 (17%)	2	11
7	62	126/127 (99%)	100 (79%)	26 (21%)	1	6
7	6E	126/127 (99%)	98 (78%)	28 (22%)	1	4
8	72	119/119 (100%)	99 (83%)	20 (17%)	2	11
8	7E	119/119 (100%)	97 (82%)	22 (18%)	2	8
9	82	98/99 (99%)	77 (79%)	21 (21%)	1	5
9	8E	98/99 (99%)	78 (80%)	20 (20%)	1	6
10	1A	89/92 (97%)	68 (76%)	21 (24%)	1	3
10	1I	89/92 (97%)	74 (83%)	15 (17%)	2	11
11	2A	88/99 (89%)	73 (83%)	15 (17%)	2	11
11	2I	88/99 (89%)	74 (84%)	14 (16%)	3	13
12	3A	104/109 (95%)	89 (86%)	15 (14%)	4	16
12	3I	104/109 (95%)	87 (84%)	17 (16%)	3	12
13	4A	94/101 (93%)	75 (80%)	19 (20%)	1	6
13	4I	94/101 (93%)	76 (81%)	18 (19%)	2	7
14	5A	49/50 (98%)	42 (86%)	7 (14%)	4	17
14	5I	49/50 (98%)	36 (74%)	13 (26%)	0	1
15	6A	79/80 (99%)	68 (86%)	11 (14%)	4	18
15	6I	79/80 (99%)	66 (84%)	13 (16%)	2	12
16	7A	72/74 (97%)	58 (81%)	14 (19%)	1	7
16	7I	72/74 (97%)	53 (74%)	19 (26%)	0	1
17	8A	95/97 (98%)	79 (83%)	16 (17%)	2	11
17	8I	95/97 (98%)	77 (81%)	18 (19%)	2	7
18	9A	63/77 (82%)	54 (86%)	9 (14%)	4	17
18	9I	63/77 (82%)	54 (86%)	9 (14%)	4	17
19	AA	68/80 (85%)	53 (78%)	15 (22%)	1	4
19	AI	72/80 (90%)	59 (82%)	13 (18%)	2	9

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
20	BA	76/82 (93%)	64 (84%)	12 (16%)	3	13
20	BI	76/82 (93%)	60 (79%)	16 (21%)	1	5
21	1B	20/22 (91%)	16 (80%)	4 (20%)	1	6
21	1F	20/22 (91%)	19 (95%)	1 (5%)	28	65
26	71	111/181 (61%)	103 (93%)	8 (7%)	17	51
26	79	111/181 (61%)	99 (89%)	12 (11%)	7	30
27	11	214/218 (98%)	172 (80%)	42 (20%)	1	7
27	19	214/218 (98%)	176 (82%)	38 (18%)	2	9
28	21	165/166 (99%)	130 (79%)	35 (21%)	1	5
28	29	165/166 (99%)	132 (80%)	33 (20%)	1	6
29	31	161/166 (97%)	123 (76%)	38 (24%)	1	3
29	39	165/166 (99%)	126 (76%)	39 (24%)	1	3
30	41	155/156 (99%)	128 (83%)	27 (17%)	2	10
30	49	155/156 (99%)	116 (75%)	39 (25%)	0	2
31	51	145/148 (98%)	112 (77%)	33 (23%)	1	4
31	59	142/148 (96%)	112 (79%)	30 (21%)	1	5
32	61	122/124 (98%)	97 (80%)	25 (20%)	1	6
32	69	122/124 (98%)	85 (70%)	37 (30%)	0	1
33	15	117/119 (98%)	88 (75%)	29 (25%)	1	2
33	58	117/119 (98%)	84 (72%)	33 (28%)	0	1
34	25	100/100 (100%)	82 (82%)	18 (18%)	2	9
34	68	100/100 (100%)	85 (85%)	15 (15%)	3	15
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	11
36	88	111/111 (100%)	88 (79%)	23 (21%)	1	6
37	55	100/101 (99%)	81 (81%)	19 (19%)	2	7
37	98	101/101 (100%)	84 (83%)	17 (17%)	2	11
38	65	87/88 (99%)	57 (66%)	30 (34%)	0	0
38	A8	87/88 (99%)	71 (82%)	16 (18%)	2	9
39	75	117/127 (92%)	89 (76%)	28 (24%)	1	3

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
39	B8	120/127 (94%)	83 (69%)	37 (31%)	0	1
40	85	93/94 (99%)	76 (82%)	17 (18%)	2	9
40	C8	93/94 (99%)	75 (81%)	18 (19%)	1	7
41	95	82/82 (100%)	65 (79%)	17 (21%)	1	6
41	D8	82/82 (100%)	57 (70%)	25 (30%)	0	1
42	A5	92/92 (100%)	71 (77%)	21 (23%)	1	4
42	E8	92/92 (100%)	68 (74%)	24 (26%)	0	2
43	B5	74/78 (95%)	59 (80%)	15 (20%)	1	6
43	F8	74/78 (95%)	57 (77%)	17 (23%)	1	4
44	C5	85/91 (93%)	64 (75%)	21 (25%)	1	2
44	G8	85/91 (93%)	66 (78%)	19 (22%)	1	4
45	D5	158/179 (88%)	122 (77%)	36 (23%)	1	4
45	H8	154/179 (86%)	116 (75%)	38 (25%)	1	2
46	E5	62/67 (92%)	51 (82%)	11 (18%)	2	10
46	I8	66/67 (98%)	52 (79%)	14 (21%)	1	5
47	F5	82/83 (99%)	62 (76%)	20 (24%)	1	3
47	J8	82/83 (99%)	58 (71%)	24 (29%)	0	1
48	G5	64/67 (96%)	51 (80%)	13 (20%)	1	6
48	K8	62/67 (92%)	47 (76%)	15 (24%)	1	3
49	H5	51/52 (98%)	42 (82%)	9 (18%)	2	10
49	L8	51/52 (98%)	41 (80%)	10 (20%)	1	7
50	I5	57/63 (90%)	44 (77%)	13 (23%)	1	4
50	M8	59/63 (94%)	51 (86%)	8 (14%)	4	19
51	J5	51/52 (98%)	39 (76%)	12 (24%)	1	3
51	N8	51/52 (98%)	35 (69%)	16 (31%)	0	1
52	K5	44/52 (85%)	27 (61%)	17 (39%)	0	0
52	O8	44/52 (85%)	33 (75%)	11 (25%)	1	2
53	L5	42/42 (100%)	32 (76%)	10 (24%)	1	3
53	P8	40/42 (95%)	32 (80%)	8 (20%)	1	6
54	M5	52/55 (94%)	39 (75%)	13 (25%)	1	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 5

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	OMG	2K	17	22	18,26,27	5.61	6 (33%)	22,38,41	5.14	8 (36%)
22	QUO	2K	35	22,23	28,35,36	5.49	11 (39%)	33,52,55	5.08	11 (33%)
22	MIA	2K	38	22	23,31,32	1.10	2 (8%)	25,44,47	3.27	5 (20%)
22	PSU	2K	40	22	16,21,22	0.92	1 (6%)	20,30,33	3.47	5 (25%)
22	5MU	2K	63	22	14,22,23	1.83	3 (21%)	16,32,35	1.73	2 (12%)
22	PSU	2K	64	55,22	16,21,22	0.99	1 (6%)	20,30,33	3.52	8 (40%)
22	4SU	2K	8	22	14,21,22	3.34	2 (14%)	15,30,33	0.83	0
22	OMG	2L	17	22	18,26,27	5.46	6 (33%)	22,38,41	5.28	7 (31%)
22	QUO	2L	35	22,23	28,35,36	5.67	10 (35%)	33,52,55	5.32	16 (48%)
22	MIA	2L	38	22	23,31,32	0.96	1 (4%)	25,44,47	1.15	4 (16%)
22	PSU	2L	40	22	16,21,22	1.25	2 (12%)	20,30,33	3.77	6 (30%)
22	5MU	2L	63	22	14,22,23	1.80	2 (14%)	16,32,35	1.70	2 (12%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
22	PSU	2L	64	22	16,21,22	1.28	2 (12%)	20,30,33	3.97	7 (35%)
22	4SU	2L	8	22	14,21,22	2.91	3 (21%)	15,30,33	1.84	3 (20%)
22	OMG	3K	17	22	18,26,27	5.77	6 (33%)	22,38,41	5.45	8 (36%)
22	QUO	3K	35	22	28,35,36	5.72	9 (32%)	33,52,55	5.63	13 (39%)
22	MIA	3K	38	22	23,31,32	1.22	2 (8%)	25,44,47	2.38	5 (20%)
22	PSU	3K	40	22	16,21,22	1.03	1 (6%)	20,30,33	3.69	6 (30%)
22	5MU	3K	63	22	14,22,23	1.72	2 (14%)	16,32,35	1.77	2 (12%)
22	PSU	3K	64	22	16,21,22	1.06	1 (6%)	20,30,33	3.63	8 (40%)
22	4SU	3K	8	22	14,21,22	3.01	2 (14%)	15,30,33	0.96	1 (6%)
22	OMG	3L	17	22	18,26,27	5.70	7 (38%)	22,38,41	5.16	7 (31%)
22	QUO	3L	35	22	28,35,36	5.58	9 (32%)	33,52,55	5.08	14 (42%)
22	MIA	3L	38	22	23,31,32	1.16	2 (8%)	25,44,47	2.30	6 (24%)
22	PSU	3L	40	22	16,21,22	1.17	1 (6%)	20,30,33	3.59	7 (35%)
22	5MU	3L	63	22	14,22,23	1.78	2 (14%)	16,32,35	1.76	2 (12%)
22	PSU	3L	64	22	16,21,22	1.16	2 (12%)	20,30,33	3.91	8 (40%)
22	4SU	3L	8	55,22	14,21,22	3.25	2 (14%)	15,30,33	1.42	2 (13%)

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

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	MIA	3K	38	22	-	0/11/33/34	0/3/3/3
22	PSU	3K	40	22	-	0/7/25/26	0/2/2/2
22	5MU	3K	63	22	-	0/3/25/26	0/2/2/2
22	PSU	3K	64	22	-	0/7/25/26	0/2/2/2
22	4SU	3K	8	22	-	0/3/25/26	0/2/2/2
22	OMG	3L	17	22	-	0/5/27/28	0/3/3/3
22	QUO	3L	35	22	-	0/6/43/44	0/4/4/4
22	MIA	3L	38	22	-	0/11/33/34	0/3/3/3
22	PSU	3L	40	22	-	0/7/25/26	0/2/2/2
22	5MU	3L	63	22	-	0/3/25/26	0/2/2/2
22	PSU	3L	64	22	-	0/7/25/26	0/2/2/2
22	4SU	3L	8	55,22	-	0/3/25/26	0/2/2/2

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	3K	17	OMG	C8-N7	-14.28	1.07	1.34
22	2L	17	OMG	C8-N7	-14.20	1.08	1.34
22	3L	17	OMG	C8-N7	-13.92	1.08	1.34
22	2K	17	OMG	C8-N7	-13.80	1.08	1.34
22	3K	35	QUO	C8-N9	-10.53	1.22	1.38

The worst 5 of 173 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	3K	35	QUO	C8-N9-C1'	-16.12	111.35	125.49
22	2L	17	OMG	C6-C5-C4	-15.40	105.53	120.84
22	2L	64	PSU	N1-C2-N3	-14.50	117.97	128.40
22	2K	17	OMG	C6-C5-C4	-14.23	106.69	120.84
22	2L	35	QUO	C8-N9-C1'	-13.69	113.48	125.49

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

22 monomers are involved in 45 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
22	2K	17	OMG	6	0
22	2K	35	QUO	2	0
22	2K	38	MIA	1	0
22	2K	64	PSU	4	0

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

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 90	63, 117, 206, 445	0
1	1G	1503/1522 (98%)	-0.53	5 (0%) 93 86	68, 115, 190, 453	0
2	12	237/256 (92%)	0.90	41 (17%) 2 1	127, 170, 220, 245	0
2	1E	237/256 (92%)	0.72	30 (12%) 4 2	120, 163, 212, 246	0
3	22	206/239 (86%)	1.17	43 (20%) 1 0	120, 147, 179, 189	0
3	2E	205/239 (85%)	0.50	16 (7%) 14 5	111, 138, 196, 212	0
4	32	208/209 (99%)	0.84	26 (12%) 4 2	94, 119, 152, 172	0
4	3E	208/209 (99%)	-0.09	3 (1%) 75 57	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%)	0.72	4 (3%) 39 19	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%) 7 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%) 5 2	104, 155, 177, 185	0
10	1A	99/105 (94%)	1.21	23 (23%) 1 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%) 20 7	86, 102, 141, 189	0
12	3I	125/132 (94%)	-0.29	1 (0%) 86 71	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%) 29 13	122, 164, 193, 228	0
13	4I	116/126 (92%)	0.81	17 (14%) 3 1	117, 165, 186, 205	0
14	5A	60/61 (98%)	1.29	19 (31%) 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%) 23 9	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%) 51 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%) 18 7	91, 112, 166, 208	0
18	9I	72/88 (81%)	1.46	16 (22%) 1 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%) 12 4	142, 168, 204, 221	0
20	BA	99/106 (93%)	0.54	6 (6%) 22 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%) 39 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%) 14 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 65	48, 80, 247, 440	0
25	16	122/122 (100%)	-0.32	1 (0%) 86 71	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%)	1.34	40 (29%) 1 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%)	-0.41	0 100 100	50, 73, 91, 122	0
28	21	205/206 (99%)	0.32	14 (6%) 18 7	54, 94, 152, 211	0
28	29	205/206 (99%)	-0.17	2 (0%) 82 67	57, 88, 164, 238	0
29	31	202/210 (96%)	0.23	6 (2%) 51 27	47, 81, 123, 148	0
29	39	208/210 (99%)	0.84	26 (12%) 4 2	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%) 9 3	120, 146, 190, 208	0
31	51	174/180 (96%)	0.09	2 (1%) 80 65	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%) 3 1	84, 128, 153, 169	0
32	69	146/148 (98%)	-0.23	2 (1%) 75 57	81, 137, 164, 177	0
33	15	138/140 (98%)	0.21	4 (2%) 52 28	72, 101, 143, 174	0
33	58	138/140 (98%)	0.36	7 (5%) 29 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%) 5 2	61, 105, 144, 203	0
35	78	150/150 (100%)	0.33	5 (3%) 47 24	55, 91, 117, 251	0
36	45	141/141 (100%)	0.13	7 (4%) 30 13	67, 104, 131, 154	0
36	88	141/141 (100%)	0.35	8 (5%) 24 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 71	68, 88, 107, 125	0
38	65	111/112 (99%)	0.17	4 (3%) 43 21	93, 119, 148, 171	0
38	A8	111/112 (99%)	1.79	47 (42%) 0 0	97, 119, 163, 218	0
39	75	137/146 (93%)	-0.22	2 (1%) 74 54	75, 91, 161, 227	0
39	B8	137/146 (93%)	-0.24	4 (2%) 52 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%) 18 7	58, 106, 160, 237	0
42	A5	113/113 (100%)	0.15	2 (1%) 69 47	63, 77, 110, 206	0
42	E8	113/113 (100%)	0.14	2 (1%) 69 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%) 36 17	73, 86, 119, 127	0
43	F8	92/96 (95%)	0.47	6 (6%) 20 7	64, 74, 98, 112	0
44	C5	104/110 (94%)	1.56	26 (25%) 1 0	89, 130, 221, 252	0
44	G8	104/110 (94%)	0.45	7 (6%) 19 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%) 1 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%) 23 9	70, 90, 112, 158	0
47	F5	97/98 (98%)	-0.19	2 (2%) 64 43	60, 83, 157, 204	0
47	J8	97/98 (98%)	0.82	9 (9%) 9 3	57, 82, 168, 218	0
48	G5	69/72 (95%)	0.68	5 (7%) 16 6	84, 109, 145, 187	0
48	K8	66/72 (91%)	0.32	1 (1%) 74 54	63, 82, 115, 177	0
49	H5	59/60 (98%)	0.49	3 (5%) 29 13	79, 97, 156, 188	0
49	L8	59/60 (98%)	0.35	3 (5%) 29 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%) 11 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%)	6.28	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	1333 (6%) 21 8	47, 108, 216, 453	0

The worst 5 of 1333 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
31	59	96	ALA	26.7
26	71	1	PRO	21.7
24	14	654(K)	C	21.5
50	I5	42	PHE	18.2
24	14	654(L)	G	14.6

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

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(Å ²)	Q<0.9
22	QUO	2L	35	32/33	0.94	0.18	-	91,112,118,124	0
22	OMG	2L	17	24/25	0.84	0.15	-	136,152,154,155	0
22	MIA	2L	38	29/30	0.95	0.18	-	92,101,113,119	0
22	QUO	3K	35	32/33	0.94	0.18	-	108,114,124,127	0
22	4SU	2L	8	20/21	0.92	0.11	-	112,122,128,139	0
22	PSU	2L	64	20/21	0.74	0.12	-	138,148,163,166	0
22	QUO	2K	35	32/33	0.95	0.18	-	84,96,115,117	6
22	PSU	2K	40	20/21	0.96	0.17	-	83,91,99,105	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	MIA	3K	38	29/30	0.94	0.18	-	114,122,132,135	0
22	MIA	2K	38	29/30	0.96	0.19	-	82,94,106,112	0
22	QUO	3L	35	32/33	0.93	0.15	-	105,114,128,132	0
22	5MU	2K	63	21/22	0.91	0.12	-	135,139,149,156	0
22	PSU	3K	64	20/21	0.72	0.26	-	182,190,202,202	0
22	5MU	2L	63	21/22	0.92	0.10	-	141,149,156,167	0
22	MIA	3L	38	29/30	0.95	0.17	-	118,123,131,133	0
22	OMG	3K	17	24/25	0.75	0.18	-	194,212,234,239	0
22	5MU	3L	63	21/22	0.85	0.13	-	174,186,190,192	0
22	PSU	3L	64	20/21	0.67	0.15	-	180,200,211,213	0
22	4SU	3L	8	20/21	0.73	0.14	-	184,194,207,207	0
22	PSU	2L	40	20/21	0.94	0.15	-	89,100,105,105	0
22	PSU	3K	40	20/21	0.91	0.13	-	118,124,129,130	0
22	4SU	3K	8	20/21	0.83	0.12	-	186,202,212,214	0
22	4SU	2K	8	20/21	0.91	0.13	-	106,112,119,121	0
22	OMG	2K	17	24/25	0.87	0.14	-	142,148,151,151	0
22	5MU	3K	63	21/22	0.86	0.19	-	176,183,187,190	0
22	PSU	3L	40	20/21	0.94	0.12	-	107,122,124,127	0

6.3 Carbohydrates [i](#)

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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(Å ²)	Q<0.9
55	MG	1H	3381	1/1	0.89	0.61	92.20	62,62,62,62	0
55	MG	14	3143	1/1	0.80	0.42	46.78	87,87,87,87	0
55	MG	1H	3091	1/1	0.98	0.41	42.98	59,59,59,59	0
55	MG	1H	3066	1/1	0.85	0.41	42.49	70,70,70,70	0
55	MG	13	1691	1/1	0.93	0.49	42.48	83,83,83,83	0
55	MG	14	3255	1/1	0.69	0.36	36.37	92,92,92,92	0
55	MG	1H	3099	1/1	0.98	0.47	35.79	52,52,52,52	0
55	MG	13	1692	1/1	0.85	0.44	35.71	132,132,132,132	0
55	MG	1H	3356	1/1	0.78	0.54	34.98	91,91,91,91	0
55	MG	14	3281	1/1	0.70	0.38	34.53	82,82,82,82	0
55	MG	1H	3106	1/1	0.78	0.40	32.36	85,85,85,85	0
55	MG	13	1627	1/1	0.95	0.48	32.12	65,65,65,65	0
55	MG	14	3042	1/1	0.93	0.29	32.08	67,67,67,67	0
55	MG	13	1675	1/1	0.96	0.42	29.00	85,85,85,85	0
55	MG	13	1633	1/1	0.92	0.31	27.84	79,79,79,79	0
55	MG	1H	3330	1/1	0.69	0.50	25.51	90,90,90,90	0
55	MG	1G	1603	1/1	0.95	0.35	25.16	76,76,76,76	0
55	MG	13	1708	1/1	0.79	0.54	25.01	127,127,127,127	0
55	MG	1H	3160	1/1	0.92	0.43	23.63	68,68,68,68	0
55	MG	1H	3074	1/1	0.96	0.34	23.47	82,82,82,82	0
55	MG	14	3239	1/1	0.76	0.36	23.25	87,87,87,87	0
55	MG	14	3179	1/1	0.87	0.33	22.82	88,88,88,88	0
55	MG	1H	3004	1/1	0.99	0.39	21.49	49,49,49,49	0
55	MG	1G	1711	1/1	0.95	0.30	20.98	73,73,73,73	0
55	MG	1H	3144	1/1	0.93	0.40	20.77	69,69,69,69	0
55	MG	1H	3095	1/1	0.98	0.38	20.60	46,46,46,46	0
55	MG	13	1654	1/1	0.95	0.39	20.36	72,72,72,72	0
55	MG	1H	3339	1/1	0.79	0.45	19.02	91,91,91,91	0
55	MG	13	1659	1/1	0.95	0.33	18.92	102,102,102,102	0
55	MG	13	1655	1/1	0.83	0.31	18.92	92,92,92,92	0
55	MG	1G	1602	1/1	0.98	0.41	18.65	75,75,75,75	0
55	MG	1H	3127	1/1	0.94	0.41	18.47	60,60,60,60	0
55	MG	14	3202	1/1	0.96	0.48	18.46	74,74,74,74	0
55	MG	1H	3071	1/1	0.99	0.36	18.09	51,51,51,51	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
55	MG	14	3283	1/1	0.74	0.32	18.07	87,87,87,87	0
55	MG	14	3097	1/1	0.97	0.32	17.57	54,54,54,54	0
55	MG	1H	3302	1/1	0.93	0.66	17.42	74,74,74,74	0
55	MG	14	3321	1/1	0.79	0.37	17.36	89,89,89,89	0
55	MG	1H	3089	1/1	0.98	0.34	17.27	38,38,38,38	0
55	MG	14	3059	1/1	0.93	0.30	17.24	60,60,60,60	0
55	MG	14	3068	1/1	0.95	0.33	16.46	66,66,66,66	0
55	MG	14	3064	1/1	0.99	0.34	16.21	52,52,52,52	0
55	MG	14	3081	1/1	0.89	0.32	16.17	70,70,70,70	0
55	MG	14	3022	1/1	0.96	0.26	16.16	60,60,60,60	0
55	MG	1H	3345	1/1	0.91	0.29	15.90	67,67,67,67	0
55	MG	1H	3001	1/1	0.94	0.40	15.78	50,50,50,50	0
55	MG	1H	3370	1/1	0.65	0.33	15.59	73,73,73,73	0
55	MG	1H	3159	1/1	0.81	0.34	15.48	66,66,66,66	0
55	MG	13	1622	1/1	0.93	0.42	15.31	74,74,74,74	0
55	MG	14	3011	1/1	0.98	0.33	15.16	47,47,47,47	0
55	MG	14	3033	1/1	0.95	0.30	15.06	71,71,71,71	0
55	MG	1G	1623	1/1	0.98	0.28	15.03	87,87,87,87	0
55	MG	1H	3040	1/1	0.97	0.34	14.79	71,71,71,71	0
55	MG	14	3328	1/1	0.90	0.42	14.71	115,115,115,115	0
55	MG	13	1611	1/1	0.71	0.26	14.66	83,83,83,83	0
55	MG	14	3315	1/1	0.90	0.38	14.12	85,85,85,85	0
55	MG	1H	3021	1/1	0.96	0.29	14.06	51,51,51,51	0
55	MG	1H	3063	1/1	0.90	0.32	14.01	63,63,63,63	0
55	MG	18	101	1/1	0.80	0.32	13.77	83,83,83,83	0
55	MG	1H	3183	1/1	0.92	0.31	13.69	63,63,63,63	0
55	MG	1H	3168	1/1	0.69	0.35	13.52	85,85,85,85	0
55	MG	14	3215	1/1	0.95	0.28	13.51	76,76,76,76	0
55	MG	14	3076	1/1	0.99	0.32	13.34	47,47,47,47	0
55	MG	1H	3186	1/1	0.49	0.23	13.25	70,70,70,70	0
55	MG	1H	3047	1/1	0.97	0.27	13.25	76,76,76,76	0
55	MG	14	3041	1/1	0.95	0.32	13.13	58,58,58,58	0
55	MG	14	3055	1/1	0.96	0.32	12.80	61,61,61,61	0
55	MG	14	3335	1/1	0.34	0.24	12.69	90,90,90,90	0
55	MG	14	3058	1/1	0.98	0.20	12.41	63,63,63,63	0
55	MG	13	1636	1/1	0.97	0.31	12.35	88,88,88,88	0
55	MG	14	3112	1/1	0.98	0.33	12.20	68,68,68,68	0
55	MG	14	3199	1/1	0.87	0.23	12.10	60,60,60,60	0
55	MG	1H	3061	1/1	0.97	0.43	11.96	71,71,71,71	0
55	MG	1H	3153	1/1	0.93	0.38	11.94	86,86,86,86	0
55	MG	14	3019	1/1	0.89	0.34	11.86	68,68,68,68	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
55	MG	1G	1649	1/1	0.94	0.37	11.82	93,93,93,93	0
55	MG	1G	1619	1/1	0.95	0.34	11.80	73,73,73,73	0
55	MG	1H	3155	1/1	0.95	0.28	11.73	38,38,38,38	0
55	MG	1H	3226	1/1	0.90	0.29	11.72	114,114,114,114	0
55	MG	13	1681	1/1	0.90	0.39	11.57	104,104,104,104	0
55	MG	14	3070	1/1	0.95	0.34	11.55	66,66,66,66	0
55	MG	14	3373	1/1	0.57	0.23	11.54	98,98,98,98	0
55	MG	14	3031	1/1	0.96	0.30	11.54	73,73,73,73	0
55	MG	1G	1651	1/1	0.89	0.39	11.48	96,96,96,96	0
55	MG	14	3152	1/1	0.89	0.31	11.37	72,72,72,72	0
55	MG	1H	3016	1/1	0.94	0.29	11.34	56,56,56,56	0
55	MG	13	1673	1/1	0.92	0.26	11.21	109,109,109,109	0
55	MG	1H	3002	1/1	0.98	0.33	11.14	53,53,53,53	0
55	MG	1H	3052	1/1	0.96	0.33	11.07	73,73,73,73	0
55	MG	13	1709	1/1	0.78	0.27	10.93	78,78,78,78	0
55	MG	1G	1624	1/1	0.83	0.33	10.74	78,78,78,78	0
55	MG	1H	3011	1/1	0.97	0.35	10.70	54,54,54,54	0
55	MG	1G	1653	1/1	0.65	0.36	10.67	103,103,103,103	0
55	MG	1H	3035	1/1	0.94	0.26	10.67	75,75,75,75	0
55	MG	1H	3065	1/1	0.85	0.34	10.66	64,64,64,64	0
55	MG	14	3007	1/1	0.97	0.29	10.64	58,58,58,58	0
55	MG	1H	3015	1/1	0.97	0.38	10.63	46,46,46,46	0
55	MG	1H	3167	1/1	0.72	0.25	10.60	66,66,66,66	0
55	MG	1G	1689	1/1	0.84	0.26	10.57	90,90,90,90	0
55	MG	1H	3049	1/1	0.91	0.33	10.53	71,71,71,71	0
55	MG	1H	3013	1/1	0.99	0.30	10.35	47,47,47,47	0
55	MG	1H	3248	1/1	0.94	0.33	10.26	61,61,61,61	0
55	MG	1H	3017	1/1	0.98	0.33	10.19	47,47,47,47	0
55	MG	14	3203	1/1	0.97	0.27	10.14	55,55,55,55	0
55	MG	14	3298	1/1	0.84	0.32	10.08	69,69,69,69	0
55	MG	1H	3069	1/1	0.86	0.28	10.07	51,51,51,51	0
55	MG	1G	1644	1/1	0.92	0.25	9.94	115,115,115,115	0
55	MG	1H	3146	1/1	0.80	0.23	9.93	48,48,48,48	0
55	MG	1H	3322	1/1	0.82	0.26	9.90	92,92,92,92	0
55	MG	1H	3315	1/1	0.63	0.24	9.85	88,88,88,88	0
55	MG	14	3206	1/1	0.78	0.23	9.82	76,76,76,76	0
55	MG	14	3231	1/1	0.94	0.28	9.78	76,76,76,76	0
55	MG	13	1705	1/1	0.86	0.30	9.72	76,76,76,76	0
55	MG	1G	1664	1/1	0.83	0.28	9.61	104,104,104,104	0
55	MG	14	3258	1/1	0.41	0.32	9.60	70,70,70,70	0
55	MG	1G	1601	1/1	0.97	0.25	9.49	76,76,76,76	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
55	MG	14	3004	1/1	0.97	0.25	9.49	57,57,57,57	0
55	MG	14	3052	1/1	0.94	0.37	9.42	65,65,65,65	0
55	MG	1H	3078	1/1	0.88	0.30	9.42	71,71,71,71	0
55	MG	1H	3364	1/1	0.27	0.34	9.42	103,103,103,103	0
55	MG	1G	1610	1/1	0.77	0.32	9.34	99,99,99,99	0
55	MG	1H	3401	1/1	0.88	0.26	9.29	67,67,67,67	0
55	MG	1H	3260	1/1	0.83	0.22	9.27	70,70,70,70	0
55	MG	1G	1661	1/1	0.95	0.38	9.24	76,76,76,76	0
55	MG	1H	3007	1/1	0.95	0.33	9.14	62,62,62,62	0
55	MG	13	1646	1/1	0.83	0.39	9.09	90,90,90,90	0
55	MG	1H	3192	1/1	0.97	0.29	9.01	87,87,87,87	0
55	MG	14	3078	1/1	0.91	0.26	8.96	60,60,60,60	0
55	MG	13	1621	1/1	0.55	0.27	8.67	87,87,87,87	0
55	MG	13	1639	1/1	0.94	0.29	8.53	66,66,66,66	0
55	MG	1H	3219	1/1	0.92	0.32	8.47	72,72,72,72	0
55	MG	1H	3241	1/1	0.97	0.23	8.42	69,69,69,69	0
55	MG	98	201	1/1	0.90	0.34	8.34	89,89,89,89	0
55	MG	14	3145	1/1	0.94	0.28	8.04	78,78,78,78	0
55	MG	14	3227	1/1	0.90	0.23	8.00	80,80,80,80	0
55	MG	1H	3031	1/1	0.97	0.31	7.87	82,82,82,82	0
55	MG	14	3323	1/1	0.83	0.25	7.83	87,87,87,87	0
55	MG	1H	3151	1/1	0.97	0.44	7.72	76,76,76,76	0
55	MG	14	3217	1/1	0.90	0.26	7.70	55,55,55,55	0
55	MG	14	3135	1/1	0.77	0.23	7.46	64,64,64,64	0
55	MG	13	1687	1/1	0.93	0.25	7.45	77,77,77,77	0
55	MG	14	3038	1/1	0.62	0.25	7.30	86,86,86,86	0
55	MG	1H	3068	1/1	0.87	0.25	7.23	61,61,61,61	0
55	MG	13	1606	1/1	0.96	0.27	7.18	92,92,92,92	0
55	MG	1G	1632	1/1	0.85	0.30	7.11	79,79,79,79	0
55	MG	14	3198	1/1	0.93	0.23	7.02	70,70,70,70	0
55	MG	14	3086	1/1	0.97	0.28	6.89	51,51,51,51	0
55	MG	14	3101	1/1	0.95	0.24	6.85	65,65,65,65	0
55	MG	14	3075	1/1	0.94	0.27	6.70	52,52,52,52	0
55	MG	1H	3057	1/1	0.95	0.26	6.62	84,84,84,84	0
55	MG	1H	3143	1/1	0.92	0.28	6.58	73,73,73,73	0
55	MG	1G	1605	1/1	0.93	0.21	6.54	92,92,92,92	0
55	MG	1H	3309	1/1	0.87	0.24	6.38	85,85,85,85	0
55	MG	14	3130	1/1	0.93	0.20	6.27	72,72,72,72	0
55	MG	1H	3324	1/1	0.90	0.26	6.16	66,66,66,66	0
55	MG	1H	3244	1/1	0.80	0.28	6.13	55,55,55,55	0
55	MG	1H	3213	1/1	0.85	0.24	6.02	84,84,84,84	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
55	MG	1J	201	1/1	0.91	0.24	5.97	100,100,100,100	0
55	MG	1H	3297	1/1	0.78	0.33	5.96	81,81,81,81	0
55	MG	14	3233	1/1	0.93	0.26	5.84	67,67,67,67	0
55	MG	14	3297	1/1	0.82	0.26	5.79	78,78,78,78	0
55	MG	14	3339	1/1	0.97	0.28	5.72	74,74,74,74	0
55	MG	14	3269	1/1	0.73	0.20	5.66	68,68,68,68	0
55	MG	14	3071	1/1	0.92	0.21	5.59	62,62,62,62	0
55	MG	13	1609	1/1	0.98	0.23	5.57	83,83,83,83	0
55	MG	1H	3207	1/1	0.80	0.18	5.46	67,67,67,67	0
55	MG	1H	3080	1/1	0.94	0.26	5.45	62,62,62,62	0
55	MG	14	3027	1/1	0.95	0.17	5.39	71,71,71,71	0
55	MG	14	3276	1/1	0.92	0.18	5.23	73,73,73,73	0
55	MG	1G	1713	1/1	0.96	0.23	5.21	107,107,107,107	0
55	MG	14	3295	1/1	0.83	0.18	5.14	72,72,72,72	0
55	MG	1H	3053	1/1	0.97	0.20	5.10	61,61,61,61	0
55	MG	F5	101	1/1	0.94	0.33	5.05	77,77,77,77	0
55	MG	1H	3090	1/1	0.94	0.26	4.94	47,47,47,47	0
55	MG	14	3229	1/1	0.95	0.21	4.93	64,64,64,64	0
55	MG	13	1640	1/1	0.77	0.23	4.92	89,89,89,89	0
55	MG	14	3176	1/1	0.92	0.26	4.73	63,63,63,63	0
55	MG	1G	1646	1/1	0.82	0.23	4.72	93,93,93,93	0
55	MG	14	3123	1/1	0.80	0.23	4.69	50,50,50,50	0
55	MG	14	3103	1/1	0.84	0.25	4.67	58,58,58,58	0
55	MG	14	3365	1/1	0.93	0.19	4.55	78,78,78,78	0
55	MG	1H	3041	1/1	0.87	0.22	4.52	63,63,63,63	0
55	MG	14	3093	1/1	0.85	0.24	4.30	84,84,84,84	0
55	MG	1H	3212	1/1	0.89	0.22	4.30	78,78,78,78	0
55	MG	1G	1647	1/1	0.99	0.25	4.22	80,80,80,80	0
55	MG	1H	3319	1/1	0.98	0.21	4.22	60,60,60,60	0
55	MG	14	3032	1/1	0.98	0.24	4.21	64,64,64,64	0
55	MG	1H	3331	1/1	0.94	0.23	4.10	84,84,84,84	0
55	MG	14	3219	1/1	0.81	0.20	4.06	67,67,67,67	0
55	MG	14	3197	1/1	0.88	0.26	4.03	81,81,81,81	0
55	MG	13	1704	1/1	0.91	0.20	3.96	87,87,87,87	0
55	MG	1G	1615	1/1	0.88	0.19	3.86	78,78,78,78	0
55	MG	1H	3374	1/1	0.87	0.31	3.85	67,67,67,67	0
55	MG	1H	3039	1/1	0.72	0.22	3.82	68,68,68,68	0
55	MG	1H	3158	1/1	0.98	0.21	3.77	71,71,71,71	0
55	MG	1H	3450	1/1	0.99	0.22	3.74	53,53,53,53	0
55	MG	14	3193	1/1	0.96	0.21	3.71	56,56,56,56	0
55	MG	1G	1608	1/1	0.92	0.23	3.69	85,85,85,85	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
55	MG	14	3465	1/1	0.98	0.32	3.66	64,64,64,64	0
55	MG	1H	3104	1/1	0.88	0.18	3.52	85,85,85,85	0
55	MG	14	3271	1/1	0.87	0.20	3.49	82,82,82,82	0
55	MG	1H	3177	1/1	0.88	0.21	3.48	69,69,69,69	0
55	MG	1H	3029	1/1	0.89	0.24	3.48	71,71,71,71	0
55	MG	14	3013	1/1	0.99	0.23	3.46	56,56,56,56	0
55	MG	14	3338	1/1	0.84	0.17	3.46	78,78,78,78	0
55	MG	1H	3137	1/1	0.99	0.26	3.38	60,60,60,60	0
55	MG	14	3293	1/1	0.86	0.15	3.36	75,75,75,75	0
55	MG	14	3172	1/1	0.90	0.19	3.30	85,85,85,85	0
55	MG	1H	3087	1/1	0.94	0.22	3.21	49,49,49,49	0
55	MG	14	3048	1/1	0.98	0.20	3.20	55,55,55,55	0
55	MG	1G	1717	1/1	0.94	0.16	3.18	107,107,107,107	0
55	MG	2K	105	1/1	0.86	0.21	3.17	76,76,76,76	0
55	MG	1H	3109	1/1	0.91	0.29	3.13	76,76,76,76	0
55	MG	1H	3172	1/1	0.79	0.20	3.04	69,69,69,69	0
55	MG	14	3119	1/1	0.75	0.33	3.01	70,70,70,70	0
55	MG	14	3121	1/1	0.85	0.20	2.96	54,54,54,54	0
55	MG	1H	3085	1/1	0.99	0.20	2.94	63,63,63,63	0
55	MG	1G	1621	1/1	0.95	0.20	2.86	91,91,91,91	0
55	MG	2L	101	1/1	0.95	0.21	2.84	77,77,77,77	0
55	MG	14	3102	1/1	0.99	0.21	2.83	61,61,61,61	0
55	MG	1H	3113	1/1	0.98	0.27	2.80	40,40,40,40	0
55	MG	1G	1719	1/1	0.67	0.20	2.80	104,104,104,104	0
55	MG	1G	1714	1/1	0.92	0.24	2.75	98,98,98,98	0
55	MG	1H	3088	1/1	0.79	0.21	2.56	52,52,52,52	0
55	MG	1H	3195	1/1	0.93	0.19	2.50	79,79,79,79	0
55	MG	14	3045	1/1	0.94	0.22	2.45	41,41,41,41	0
55	MG	14	3209	1/1	0.96	0.29	2.44	88,88,88,88	0
55	MG	14	3326	1/1	0.85	0.16	2.40	90,90,90,90	0
55	MG	14	3320	1/1	0.91	0.40	2.32	88,88,88,88	0
55	MG	2I	302	1/1	0.93	0.22	2.32	68,68,68,68	0
55	MG	13	1671	1/1	0.75	0.15	2.31	70,70,70,70	0
55	MG	1H	3148	1/1	0.86	0.18	2.27	86,86,86,86	0
55	MG	14	3273	1/1	0.76	0.18	2.27	87,87,87,87	0
55	MG	14	3156	1/1	0.80	0.17	2.19	75,75,75,75	0
55	MG	14	3131	1/1	0.91	0.18	2.01	66,66,66,66	0
55	MG	4A	201	1/1	0.75	0.34	1.83	115,115,115,115	0
55	MG	14	3318	1/1	0.56	0.13	1.82	80,80,80,80	0
55	MG	1H	3497	1/1	0.80	0.16	1.80	105,105,105,105	0
55	MG	13	1630	1/1	0.98	0.18	1.72	61,61,61,61	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
55	MG	13	1716	1/1	0.98	0.17	1.71	74,74,74,74	0
55	MG	1H	3033	1/1	0.79	0.20	1.65	83,83,83,83	0
55	MG	1G	1669	1/1	0.58	0.25	1.52	86,86,86,86	0
55	MG	55	201	1/1	0.93	0.26	1.50	68,68,68,68	0
55	MG	1G	1682	1/1	0.97	0.15	1.40	87,87,87,87	0
55	MG	19	301	1/1	0.86	0.21	1.34	67,67,67,67	0
55	MG	14	3367	1/1	0.44	0.17	1.25	72,72,72,72	0
55	MG	11	301	1/1	0.86	0.21	1.25	54,54,54,54	0
55	MG	1H	3098	1/1	0.95	0.21	1.20	42,42,42,42	0
56	ZN	3E	302	1/1	0.98	0.35	1.15	102,102,102,102	0
55	MG	13	1605	1/1	0.86	0.17	1.13	84,84,84,84	0
55	MG	14	3259	1/1	0.99	0.29	1.11	82,82,82,82	0
55	MG	1H	3306	1/1	0.93	0.15	1.06	83,83,83,83	0
55	MG	1H	3280	1/1	0.89	0.18	0.99	70,70,70,70	0
55	MG	14	3115	1/1	0.91	0.16	0.97	58,58,58,58	0
55	MG	1H	3479	1/1	0.96	0.18	0.95	58,58,58,58	0
55	MG	Q8	102	1/1	0.89	0.31	0.91	81,81,81,81	0
55	MG	13	1731	1/1	0.76	0.14	0.89	153,153,153,153	0
55	MG	1H	3135	1/1	0.80	0.19	0.84	72,72,72,72	0
56	ZN	32	302	1/1	0.95	0.33	0.78	111,111,111,111	0
55	MG	14	3114	1/1	0.97	0.23	0.65	56,56,56,56	0
55	MG	13	1656	1/1	0.44	0.25	0.58	120,120,120,120	0
55	MG	1H	3199	1/1	0.85	0.19	0.52	72,72,72,72	0
55	MG	1G	1705	1/1	0.73	0.15	0.50	96,96,96,96	0
55	MG	1H	3062	1/1	0.98	0.18	0.48	48,48,48,48	0
55	MG	14	3039	1/1	0.94	0.15	0.46	67,67,67,67	0
55	MG	14	3169	1/1	0.72	0.31	0.45	100,100,100,100	0
55	MG	14	3225	1/1	0.92	0.21	0.45	75,75,75,75	0
55	MG	1H	3467	1/1	0.97	0.18	0.39	72,72,72,72	0
55	MG	13	1616	1/1	0.91	0.22	0.30	141,141,141,141	0
55	MG	14	3375	1/1	0.92	0.17	0.29	51,51,51,51	0
55	MG	14	3015	1/1	0.98	0.17	0.29	64,64,64,64	0
55	MG	1H	3038	1/1	0.87	0.20	0.20	59,59,59,59	0
55	MG	14	3066	1/1	0.94	0.17	0.20	63,63,63,63	0
55	MG	14	3082	1/1	0.58	0.15	0.18	64,64,64,64	0
55	MG	16	204	1/1	0.58	0.19	0.08	99,99,99,99	0
55	MG	1H	3398	1/1	0.62	0.17	0.03	106,106,106,106	0
55	MG	88	201	1/1	0.90	0.25	0.01	98,98,98,98	0
56	ZN	G8	202	1/1	0.36	0.32	0.01	203,203,203,203	0
55	MG	16	201	1/1	0.95	0.15	-0.02	110,110,110,110	0
55	MG	1G	1611	1/1	0.94	0.15	-0.05	132,132,132,132	0
55	MG	1H	3318	1/1	0.85	0.16	-0.05	75,75,75,75	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
55	MG	1G	1658	1/1	0.86	0.14	-0.06	99,99,99,99	0
55	MG	1H	3243	1/1	0.93	0.17	-0.13	52,52,52,52	0
55	MG	14	3306	1/1	0.74	0.14	-0.17	74,74,74,74	0
55	MG	1H	3256	1/1	0.85	0.19	-0.18	78,78,78,78	0
55	MG	1H	3289	1/1	0.95	0.16	-0.23	78,78,78,78	0
55	MG	1G	1671	1/1	0.84	0.15	-0.23	92,92,92,92	0
55	MG	1H	3371	1/1	0.94	0.16	-0.25	62,62,62,62	0
56	ZN	C5	202	1/1	0.70	0.31	-0.25	219,219,219,219	0
55	MG	14	3044	1/1	0.95	0.16	-0.34	43,43,43,43	0
55	MG	1G	1745	1/1	0.92	0.15	-0.38	93,93,93,93	0
55	MG	13	1718	1/1	0.95	0.12	-0.42	85,85,85,85	0
55	MG	14	3410	1/1	0.98	0.16	-0.42	58,58,58,58	0
55	MG	1H	3361	1/1	0.91	0.22	-0.45	155,155,155,155	0
55	MG	14	3023	1/1	0.91	0.13	-0.47	72,72,72,72	0
55	MG	13	1683	1/1	0.96	0.12	-0.54	122,122,122,122	0
55	MG	1G	1730	1/1	0.97	0.14	-0.57	82,82,82,82	0
55	MG	29	303	1/1	0.65	0.15	-0.59	74,74,74,74	0
56	ZN	5I	101	1/1	0.97	0.14	-0.68	116,116,116,116	0
55	MG	1H	3233	1/1	0.93	0.16	-0.80	72,72,72,72	0
55	MG	1H	3416	1/1	0.94	0.17	-0.81	71,71,71,71	0
55	MG	14	3412	1/1	0.98	0.16	-0.82	49,49,49,49	0
55	MG	1H	3431	1/1	0.93	0.14	-0.84	70,70,70,70	0
55	MG	14	3454	1/1	0.95	0.14	-0.85	106,106,106,106	0
55	MG	14	3234	1/1	0.88	0.16	-0.86	51,51,51,51	0
56	ZN	5A	101	1/1	0.95	0.11	-0.87	133,133,133,133	0
55	MG	1G	1738	1/1	0.82	0.10	-0.88	140,140,140,140	0
55	MG	1G	1746	1/1	0.92	0.13	-0.96	134,134,134,134	0
55	MG	G8	201	1/1	0.99	0.14	-0.98	77,77,77,77	0
55	MG	13	1647	1/1	0.70	0.15	-0.99	110,110,110,110	0
55	MG	1H	3432	1/1	0.96	0.14	-1.09	68,68,68,68	0
55	MG	14	3267	1/1	0.86	0.12	-1.10	90,90,90,90	0
55	MG	14	3363	1/1	0.91	0.14	-1.11	61,61,61,61	0
55	MG	16	212	1/1	0.89	0.13	-1.14	85,85,85,85	0
55	MG	14	3212	1/1	0.91	0.14	-1.21	66,66,66,66	0
55	MG	14	3263	1/1	0.74	0.13	-1.30	72,72,72,72	0
55	MG	1H	3358	1/1	0.92	0.12	-1.36	98,98,98,98	0
55	MG	14	3418	1/1	0.97	0.13	-1.50	72,72,72,72	0
55	MG	13	1604	1/1	0.93	0.10	-1.51	86,86,86,86	0
55	MG	14	3221	1/1	0.85	0.13	-1.51	76,76,76,76	0
55	MG	1H	3414	1/1	0.93	0.15	-1.54	59,59,59,59	0
55	MG	15	201	1/1	0.88	0.16	-1.56	99,99,99,99	0
55	MG	1H	3034	1/1	0.90	0.14	-1.61	54,54,54,54	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
55	MG	13	1685	1/1	0.88	0.11	-1.63	89,89,89,89	0
55	MG	14	3385	1/1	0.90	0.13	-1.68	73,73,73,73	0
55	MG	1H	3463	1/1	0.97	0.15	-1.73	52,52,52,52	0
55	MG	13	1725	1/1	0.98	0.11	-1.73	99,99,99,99	0
55	MG	39	301	1/1	0.73	0.17	-1.75	83,83,83,83	0
55	MG	1H	3369	1/1	0.86	0.14	-1.77	94,94,94,94	0
55	MG	13	1720	1/1	0.94	0.09	-1.77	129,129,129,129	0
55	MG	14	3274	1/1	0.85	0.11	-1.80	69,69,69,69	0
55	MG	14	3393	1/1	0.96	0.12	-1.81	53,53,53,53	0
55	MG	1G	1728	1/1	0.99	0.13	-1.82	73,73,73,73	0
55	MG	14	3386	1/1	0.98	0.12	-1.85	56,56,56,56	0
55	MG	1H	3523	1/1	0.80	0.10	-1.87	78,78,78,78	0
55	MG	1H	3408	1/1	0.91	0.12	-1.92	54,54,54,54	0
55	MG	1G	1660	1/1	0.83	0.10	-1.95	87,87,87,87	0
55	MG	14	3378	1/1	0.86	0.14	-2.02	78,78,78,78	0
55	MG	13	1717	1/1	0.94	0.12	-2.07	66,66,66,66	0
55	MG	1H	3397	1/1	0.80	0.12	-2.09	94,94,94,94	0
55	MG	16	205	1/1	0.90	0.09	-2.10	109,109,109,109	0
55	MG	1G	1616	1/1	0.96	0.12	-2.12	62,62,62,62	0
55	MG	13	1690	1/1	0.93	0.13	-2.17	118,118,118,118	0
55	MG	1H	3466	1/1	0.95	0.15	-2.17	59,59,59,59	0
55	MG	14	3226	1/1	0.92	0.12	-2.20	55,55,55,55	0
55	MG	14	3388	1/1	0.97	0.13	-2.21	61,61,61,61	0
55	MG	14	3383	1/1	0.96	0.08	-2.22	81,81,81,81	0
55	MG	14	3391	1/1	0.97	0.12	-2.24	62,62,62,62	0
55	MG	1H	3271	1/1	0.93	0.09	-2.32	90,90,90,90	0
55	MG	1H	3423	1/1	0.97	0.11	-2.32	61,61,61,61	0
55	MG	1H	3489	1/1	0.96	0.13	-2.36	67,67,67,67	0
55	MG	14	3400	1/1	0.94	0.13	-2.36	65,65,65,65	0
55	MG	1H	3133	1/1	0.98	0.15	-2.36	49,49,49,49	0
55	MG	1H	3285	1/1	0.91	0.09	-2.37	89,89,89,89	0
55	MG	1H	3438	1/1	0.93	0.09	-2.38	60,60,60,60	0
55	MG	1H	3488	1/1	0.81	0.11	-2.41	66,66,66,66	0
55	MG	1H	3129	1/1	0.95	0.14	-2.44	63,63,63,63	0
55	MG	14	3390	1/1	0.98	0.10	-2.46	52,52,52,52	0
55	MG	1H	3122	1/1	0.92	0.12	-2.49	82,82,82,82	0
55	MG	1H	3419	1/1	0.98	0.14	-2.58	48,48,48,48	0
55	MG	1H	3101	1/1	0.98	0.14	-2.60	50,50,50,50	0
55	MG	16	206	1/1	0.92	0.09	-2.62	101,101,101,101	0
55	MG	1H	3451	1/1	0.98	0.09	-2.67	54,54,54,54	0
55	MG	14	3430	1/1	0.93	0.10	-2.71	67,67,67,67	0
55	MG	14	3413	1/1	0.91	0.12	-2.76	70,70,70,70	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
55	MG	1H	3458	1/1	0.99	0.15	-2.76	70,70,70,70	0
55	MG	3E	301	1/1	0.60	0.11	-2.77	156,156,156,156	0
55	MG	14	3021	1/1	0.92	0.12	-2.81	63,63,63,63	0
55	MG	1H	3421	1/1	0.98	0.14	-2.83	52,52,52,52	0
55	MG	1H	3456	1/1	0.97	0.15	-2.86	51,51,51,51	0
55	MG	14	3448	1/1	0.97	0.06	-2.87	87,87,87,87	0
55	MG	14	3428	1/1	0.91	0.09	-2.99	69,69,69,69	0
55	MG	14	3403	1/1	0.97	0.11	-3.17	69,69,69,69	0
55	MG	1H	3448	1/1	0.92	0.11	-3.22	63,63,63,63	0
55	MG	1H	3383	1/1	0.95	0.12	-3.30	60,60,60,60	0
55	MG	1H	3246	1/1	0.92	0.13	-3.33	48,48,48,48	0
55	MG	14	3429	1/1	0.95	0.10	-3.41	77,77,77,77	0
55	MG	1H	3452	1/1	0.81	0.13	-3.43	58,58,58,58	0
55	MG	1H	3405	1/1	0.53	0.14	-3.46	74,74,74,74	0
55	MG	14	3434	1/1	0.92	0.11	-3.46	98,98,98,98	0
55	MG	1H	3429	1/1	0.94	0.11	-3.46	71,71,71,71	0
55	MG	14	3381	1/1	0.97	0.13	-3.48	52,52,52,52	0
55	MG	1H	3445	1/1	0.97	0.13	-3.50	59,59,59,59	0
55	MG	1H	3418	1/1	0.97	0.10	-3.63	63,63,63,63	0
55	MG	1H	3420	1/1	0.96	0.12	-3.86	52,52,52,52	0
55	MG	1H	3182	1/1	0.84	0.12	-3.90	70,70,70,70	0
55	MG	1J	203	1/1	0.84	0.10	-3.92	92,92,92,92	0
55	MG	1H	3435	1/1	0.96	0.12	-3.98	76,76,76,76	0
55	MG	14	3018	1/1	0.94	0.08	-4.01	64,64,64,64	0
55	MG	1H	3495	1/1	0.79	0.11	-4.01	79,79,79,79	0
55	MG	14	3459	1/1	0.81	0.05	-4.04	130,130,130,130	0
55	MG	1H	3262	1/1	0.88	0.09	-4.04	71,71,71,71	0
55	MG	1H	3114	1/1	0.93	0.08	-4.11	56,56,56,56	0
55	MG	1H	3428	1/1	0.95	0.10	-4.13	74,74,74,74	0
55	MG	1H	3434	1/1	0.92	0.11	-4.21	60,60,60,60	0
55	MG	1H	3441	1/1	0.96	0.08	-4.26	63,63,63,63	0
55	MG	14	3408	1/1	0.96	0.11	-4.31	56,56,56,56	0
55	MG	14	3422	1/1	0.98	0.10	-4.36	53,53,53,53	0
55	MG	14	3392	1/1	0.98	0.10	-4.47	54,54,54,54	0
55	MG	1H	3455	1/1	0.96	0.13	-4.52	47,47,47,47	0
55	MG	14	3396	1/1	0.94	0.11	-4.55	67,67,67,67	0
55	MG	1H	3433	1/1	0.96	0.12	-4.63	54,54,54,54	0
55	MG	14	3379	1/1	0.95	0.11	-4.66	53,53,53,53	0
55	MG	14	3411	1/1	0.98	0.10	-4.77	63,63,63,63	0
55	MG	1H	3425	1/1	0.95	0.13	-4.84	61,61,61,61	0
55	MG	1H	3482	1/1	0.84	0.10	-4.85	70,70,70,70	0
55	MG	1H	3496	1/1	0.94	0.11	-4.92	78,78,78,78	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
55	MG	14	3427	1/1	0.96	0.07	-5.14	75,75,75,75	0
55	MG	1H	3509	1/1	0.86	0.07	-5.20	85,85,85,85	0
55	MG	14	3414	1/1	0.89	0.10	-5.20	56,56,56,56	0
55	MG	1H	3480	1/1	0.99	0.12	-5.22	47,47,47,47	0
55	MG	1H	3468	1/1	0.98	0.12	-5.28	59,59,59,59	0
55	MG	1H	3461	1/1	0.94	0.12	-5.31	54,54,54,54	0
55	MG	1H	3503	1/1	1.00	0.10	-5.53	57,57,57,57	0
55	MG	14	3416	1/1	0.93	0.12	-5.69	52,52,52,52	0
55	MG	14	3460	1/1	0.94	0.06	-5.69	112,112,112,112	0
55	MG	1H	3411	1/1	0.98	0.14	-5.76	67,67,67,67	0
55	MG	1H	3446	1/1	0.98	0.10	-5.76	52,52,52,52	0
55	MG	14	3441	1/1	0.94	0.09	-5.81	86,86,86,86	0
55	MG	14	3453	1/1	0.92	0.07	-5.90	76,76,76,76	0
55	MG	1H	3338	1/1	0.92	0.10	-6.02	78,78,78,78	0
55	MG	1G	1613	1/1	0.50	0.08	-6.05	92,92,92,92	0
55	MG	1H	3250	1/1	0.93	0.09	-6.11	73,73,73,73	0
55	MG	14	3415	1/1	0.97	0.06	-6.13	62,62,62,62	0
55	MG	14	3426	1/1	0.94	0.07	-6.27	91,91,91,91	0
55	MG	1H	3501	1/1	0.78	0.09	-6.33	99,99,99,99	0
55	MG	14	3445	1/1	0.99	0.10	-6.47	58,58,58,58	0
55	MG	1H	3410	1/1	0.87	0.10	-6.78	52,52,52,52	0
55	MG	1H	3500	1/1	0.89	0.06	-6.90	65,65,65,65	0
55	MG	14	3437	1/1	0.92	0.06	-6.98	85,85,85,85	0
55	MG	14	3404	1/1	0.98	0.05	-7.17	79,79,79,79	0
55	MG	1H	3486	1/1	0.89	0.07	-7.18	79,79,79,79	0
55	MG	14	3111	1/1	0.96	0.10	-7.56	54,54,54,54	0
55	MG	14	3192	1/1	0.95	0.09	-7.57	56,56,56,56	0
55	MG	14	3377	1/1	0.99	0.10	-7.57	57,57,57,57	0
55	MG	1H	3367	1/1	0.97	0.10	-7.59	67,67,67,67	0
55	MG	14	3380	1/1	0.95	0.12	-7.64	79,79,79,79	0
55	MG	1H	3521	1/1	0.98	0.09	-8.26	47,47,47,47	0
55	MG	1H	3465	1/1	0.73	0.08	-8.88	87,87,87,87	0
55	MG	14	3420	1/1	0.85	0.07	-8.94	89,89,89,89	0
55	MG	1H	3413	1/1	0.97	0.10	-9.05	44,44,44,44	0
55	MG	14	3401	1/1	0.92	0.06	-10.18	82,82,82,82	0
55	MG	1H	3454	1/1	0.97	0.09	-10.35	49,49,49,49	0
55	MG	14	3447	1/1	0.96	0.04	-10.71	102,102,102,102	0
55	MG	14	3444	1/1	0.97	0.04	-13.34	90,90,90,90	0
55	MG	1H	3473	1/1	0.98	0.06	-13.34	64,64,64,64	0
55	MG	7E	201	1/1	0.85	0.33	-	83,83,83,83	0
55	MG	1H	3366	1/1	0.74	0.29	-	84,84,84,84	0
55	MG	1H	3138	1/1	0.92	0.50	-	87,87,87,87	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	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	3084	1/1	0.90	0.32	-	62,62,62,62	0
55	MG	13	1734	1/1	0.77	0.06	-	178,178,178,178	0
55	MG	1H	3475	1/1	0.95	0.09	-	70,70,70,70	0
55	MG	13	1714	1/1	0.86	0.57	-	117,117,117,117	0
55	MG	1H	3083	1/1	0.97	0.33	-	58,58,58,58	0
55	MG	1G	1720	1/1	0.87	0.31	-	95,95,95,95	0
55	MG	1H	3516	1/1	0.96	0.07	-	88,88,88,88	0
55	MG	1H	3045	1/1	0.96	0.34	-	88,88,88,88	0
55	MG	14	3305	1/1	0.82	0.36	-	89,89,89,89	0
55	MG	13	1723	1/1	0.97	0.08	-	86,86,86,86	0
55	MG	1H	3056	1/1	0.91	0.47	-	68,68,68,68	0
55	MG	1H	3464	1/1	0.98	0.14	-	52,52,52,52	0
55	MG	1H	3048	1/1	0.92	0.23	-	58,58,58,58	0
55	MG	1H	3196	1/1	0.75	0.41	-	80,80,80,80	0
55	MG	1H	3424	1/1	0.97	0.11	-	58,58,58,58	0
55	MG	1H	3442	1/1	0.93	0.16	-	43,43,43,43	0
55	MG	1H	3470	1/1	0.97	0.08	-	74,74,74,74	0
55	MG	1H	3010	1/1	0.98	0.40	-	66,66,66,66	0
55	MG	1J	207	1/1	0.97	0.07	-	88,88,88,88	0
55	MG	1H	3430	1/1	0.97	0.10	-	76,76,76,76	0
55	MG	1H	3392	1/1	0.94	0.29	-	73,73,73,73	0
55	MG	14	3361	1/1	0.80	0.30	-	90,90,90,90	0
55	MG	1G	1652	1/1	0.87	0.33	-	82,82,82,82	0
55	MG	1H	3304	1/1	0.90	0.36	-	82,82,82,82	0
55	MG	14	3149	1/1	0.88	0.18	-	66,66,66,66	0
55	MG	14	3054	1/1	0.86	0.35	-	81,81,81,81	0
55	MG	1H	3247	1/1	0.91	0.28	-	51,51,51,51	0
55	MG	14	3232	1/1	0.97	0.28	-	98,98,98,98	0
55	MG	16	210	1/1	0.86	0.15	-	96,96,96,96	0
55	MG	13	1680	1/1	0.79	0.40	-	77,77,77,77	0
55	MG	1H	3169	1/1	0.91	0.46	-	83,83,83,83	0
55	MG	14	3098	1/1	0.95	0.33	-	46,46,46,46	0
55	MG	1H	3303	1/1	0.81	0.24	-	63,63,63,63	0
55	MG	14	3154	1/1	0.72	0.32	-	87,87,87,87	0
55	MG	1H	3175	1/1	0.84	0.54	-	74,74,74,74	0
55	MG	14	3050	1/1	0.98	0.15	-	65,65,65,65	0
55	MG	14	3180	1/1	0.95	0.41	-	82,82,82,82	0
55	MG	14	3157	1/1	0.82	0.40	-	80,80,80,80	0
55	MG	1H	3402	1/1	0.94	0.17	-	77,77,77,77	0
55	MG	1G	1706	1/1	0.90	0.35	-	86,86,86,86	0
55	MG	14	3264	1/1	0.95	0.28	-	84,84,84,84	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
55	MG	16	208	1/1	0.20	0.34	-	113,113,113,113	0
55	MG	14	3200	1/1	0.81	0.42	-	100,100,100,100	0
55	MG	1G	1715	1/1	0.97	0.21	-	106,106,106,106	0
55	MG	1G	1609	1/1	0.87	0.36	-	99,99,99,99	0
55	MG	1H	3363	1/1	0.79	0.39	-	104,104,104,104	0
55	MG	14	3248	1/1	0.92	0.34	-	78,78,78,78	0
55	MG	1H	3258	1/1	0.88	0.50	-	91,91,91,91	0
55	MG	1H	3166	1/1	0.96	0.24	-	67,67,67,67	0
55	MG	1H	3094	1/1	0.91	0.32	-	60,60,60,60	0
55	MG	13	1719	1/1	0.96	0.07	-	94,94,94,94	0
55	MG	14	3251	1/1	0.96	0.26	-	67,67,67,67	0
55	MG	1H	3353	1/1	0.76	0.32	-	83,83,83,83	0
55	MG	14	3374	1/1	0.91	0.17	-	52,52,52,52	0
55	MG	14	3436	1/1	0.74	0.14	-	107,107,107,107	0
55	MG	1H	3054	1/1	0.95	0.39	-	51,51,51,51	0
55	MG	14	3277	1/1	0.75	0.31	-	78,78,78,78	0
55	MG	14	3069	1/1	0.93	0.43	-	96,96,96,96	0
55	MG	1H	3060	1/1	0.94	0.26	-	80,80,80,80	0
55	MG	14	3003	1/1	0.97	0.26	-	47,47,47,47	0
55	MG	1H	3404	1/1	0.95	0.30	-	80,80,80,80	0
55	MG	14	3302	1/1	0.83	0.26	-	91,91,91,91	0
55	MG	1G	1743	1/1	0.97	0.18	-	105,105,105,105	0
55	MG	1H	3014	1/1	0.98	0.31	-	51,51,51,51	0
55	MG	1H	3354	1/1	0.94	0.43	-	88,88,88,88	0
55	MG	1G	1690	1/1	0.93	0.32	-	98,98,98,98	0
55	MG	1H	3025	1/1	0.98	0.39	-	80,80,80,80	0
55	MG	1G	1612	1/1	0.95	0.06	-	84,84,84,84	0
55	MG	1H	3215	1/1	0.71	0.52	-	91,91,91,91	0
55	MG	1H	3147	1/1	0.96	0.45	-	60,60,60,60	0
55	MG	14	3457	1/1	0.88	0.06	-	125,125,125,125	0
55	MG	1H	3012	1/1	0.97	0.37	-	57,57,57,57	0
55	MG	14	3371	1/1	0.95	0.24	-	84,84,84,84	0
55	MG	14	3314	1/1	0.78	0.28	-	105,105,105,105	0
55	MG	1H	3272	1/1	0.90	0.31	-	76,76,76,76	0
55	MG	14	3228	1/1	0.78	0.25	-	84,84,84,84	0
55	MG	13	1648	1/1	0.96	0.37	-	105,105,105,105	0
55	MG	14	3351	1/1	0.93	0.24	-	87,87,87,87	0
55	MG	14	3104	1/1	0.97	0.31	-	59,59,59,59	0
55	MG	14	3037	1/1	0.86	0.34	-	71,71,71,71	0
55	MG	13	1710	1/1	0.88	0.13	-	103,103,103,103	0
55	MG	13	1726	1/1	0.92	0.13	-	89,89,89,89	0
55	MG	1H	3181	1/1	0.86	0.33	-	62,62,62,62	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
55	MG	14	3043	1/1	0.97	0.36	-	62,62,62,62	0
55	MG	14	3191	1/1	0.72	0.33	-	92,92,92,92	0
55	MG	13	1632	1/1	0.88	0.49	-	74,74,74,74	0
55	MG	14	3091	1/1	0.95	0.35	-	81,81,81,81	0
55	MG	14	3407	1/1	0.96	0.09	-	83,83,83,83	0
55	MG	14	3256	1/1	0.93	0.35	-	67,67,67,67	0
55	MG	I8	102	1/1	0.89	0.38	-	65,65,65,65	0
55	MG	14	3162	1/1	0.93	0.42	-	71,71,71,71	0
55	MG	13	1619	1/1	0.97	0.40	-	74,74,74,74	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	1H	3274	1/1	0.95	0.44	-	71,71,71,71	0
55	MG	14	3040	1/1	0.96	0.34	-	69,69,69,69	0
55	MG	1H	3510	1/1	0.84	0.05	-	111,111,111,111	0
55	MG	1H	3317	1/1	0.96	0.33	-	63,63,63,63	0
55	MG	14	3008	1/1	0.97	0.31	-	53,53,53,53	0
55	MG	1H	3157	1/1	0.84	0.28	-	79,79,79,79	0
55	MG	14	3216	1/1	0.98	0.28	-	72,72,72,72	0
55	MG	1H	3484	1/1	0.94	0.06	-	118,118,118,118	0
55	MG	13	1703	1/1	0.93	0.62	-	147,147,147,147	0
55	MG	14	3280	1/1	0.86	0.24	-	75,75,75,75	0
55	MG	13	1660	1/1	0.83	0.38	-	80,80,80,80	0
55	MG	1G	1622	1/1	0.91	0.29	-	86,86,86,86	0
55	MG	1H	3216	1/1	0.80	0.48	-	90,90,90,90	0
55	MG	1G	1673	1/1	0.88	0.22	-	88,88,88,88	0
55	MG	14	3310	1/1	0.86	0.49	-	75,75,75,75	0
55	MG	1H	3236	1/1	0.92	0.47	-	89,89,89,89	0
55	MG	14	3275	1/1	0.92	0.38	-	90,90,90,90	0
55	MG	1H	3227	1/1	0.87	0.28	-	76,76,76,76	0
55	MG	1H	3044	1/1	0.81	0.29	-	98,98,98,98	0
55	MG	1H	3119	1/1	0.75	0.35	-	77,77,77,77	0
55	MG	Q8	101	1/1	0.92	0.30	-	99,99,99,99	0
55	MG	1H	3407	1/1	0.55	0.37	-	89,89,89,89	0
55	MG	14	3257	1/1	0.91	0.22	-	75,75,75,75	0
55	MG	1G	1693	1/1	0.80	0.35	-	95,95,95,95	0
55	MG	5E	201	1/1	0.72	0.20	-	106,106,106,106	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	3117	1/1	0.87	0.33	-	93,93,93,93	0
55	MG	14	3350	1/1	0.89	0.29	-	77,77,77,77	0
55	MG	1H	3333	1/1	0.82	0.34	-	81,81,81,81	0
55	MG	14	3345	1/1	0.70	0.28	-	78,78,78,78	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
55	MG	1G	1679	1/1	0.76	0.30	-	97,97,97,97	0
55	MG	1H	3097	1/1	0.96	0.39	-	70,70,70,70	0
55	MG	2L	102	1/1	0.73	0.32	-	102,102,102,102	0
55	MG	13	1694	1/1	0.81	0.30	-	92,92,92,92	0
55	MG	14	3331	1/1	0.42	0.33	-	138,138,138,138	0
55	MG	1H	3020	1/1	0.96	0.30	-	52,52,52,52	0
55	MG	1G	1666	1/1	0.97	0.38	-	72,72,72,72	0
55	MG	13	1658	1/1	0.85	0.37	-	108,108,108,108	0
55	MG	13	1707	1/1	0.86	0.26	-	100,100,100,100	0
55	MG	1H	3005	1/1	0.92	0.26	-	44,44,44,44	0
55	MG	14	3224	1/1	0.88	0.16	-	112,112,112,112	0
55	MG	13	1677	1/1	0.83	0.16	-	83,83,83,83	0
55	MG	1H	3019	1/1	0.98	0.34	-	61,61,61,61	0
55	MG	1H	3328	1/1	0.96	0.45	-	85,85,85,85	0
55	MG	1H	3082	1/1	0.98	0.38	-	72,72,72,72	0
55	MG	1H	3173	1/1	0.81	0.49	-	90,90,90,90	0
55	MG	1H	3234	1/1	0.65	0.31	-	88,88,88,88	0
55	MG	14	3207	1/1	0.97	0.30	-	77,77,77,77	0
55	MG	1J	208	1/1	0.82	0.07	-	97,97,97,97	0
55	MG	52	201	1/1	0.74	0.17	-	84,84,84,84	0
55	MG	1H	3224	1/1	0.92	0.50	-	83,83,83,83	0
55	MG	14	3073	1/1	0.99	0.26	-	58,58,58,58	0
55	MG	1H	3118	1/1	0.83	0.37	-	83,83,83,83	0
55	MG	1G	1731	1/1	0.92	0.13	-	110,110,110,110	0
55	MG	1H	3287	1/1	0.95	0.38	-	78,78,78,78	0
55	MG	14	3346	1/1	0.92	0.29	-	84,84,84,84	0
55	MG	1J	202	1/1	0.89	0.45	-	90,90,90,90	0
55	MG	13	1738	1/1	0.62	0.08	-	138,138,138,138	0
55	MG	1H	3340	1/1	0.75	0.34	-	77,77,77,77	0
55	MG	1H	3270	1/1	0.97	0.15	-	84,84,84,84	0
55	MG	1H	3185	1/1	0.70	0.52	-	91,91,91,91	0
55	MG	1H	3202	1/1	0.95	0.13	-	94,94,94,94	0
55	MG	14	3325	1/1	0.75	0.35	-	78,78,78,78	0
55	MG	13	1663	1/1	0.92	0.29	-	105,105,105,105	0
55	MG	14	3348	1/1	0.95	0.18	-	65,65,65,65	0
55	MG	1H	3180	1/1	0.72	0.19	-	86,86,86,86	0
55	MG	1H	3051	1/1	0.99	0.24	-	47,47,47,47	0
55	MG	14	3397	1/1	0.97	0.15	-	70,70,70,70	0
55	MG	1G	1724	1/1	0.89	0.21	-	99,99,99,99	0
55	MG	1H	3276	1/1	0.81	0.22	-	88,88,88,88	0
55	MG	1H	3437	1/1	0.94	0.12	-	66,66,66,66	0
55	MG	14	3133	1/1	0.95	0.35	-	71,71,71,71	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
55	MG	14	3300	1/1	0.55	0.17	-	83,83,83,83	0
55	MG	13	1625	1/1	0.88	0.46	-	95,95,95,95	0
55	MG	1H	3311	1/1	0.78	0.55	-	83,83,83,83	0
55	MG	1G	1700	1/1	0.87	0.35	-	94,94,94,94	0
55	MG	1H	3093	1/1	0.89	0.48	-	82,82,82,82	0
55	MG	1G	1650	1/1	0.85	0.26	-	90,90,90,90	0
55	MG	1H	3107	1/1	0.94	0.46	-	81,81,81,81	0
55	MG	13	1610	1/1	0.64	0.33	-	115,115,115,115	0
55	MG	1H	3240	1/1	0.21	0.32	-	92,92,92,92	0
55	MG	1G	1680	1/1	0.93	0.39	-	88,88,88,88	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	1H	3288	1/1	0.92	0.25	-	72,72,72,72	0
55	MG	1G	1725	1/1	0.82	0.20	-	93,93,93,93	0
55	MG	14	3241	1/1	0.89	0.30	-	89,89,89,89	0
55	MG	14	3089	1/1	0.93	0.39	-	71,71,71,71	0
55	MG	14	3061	1/1	0.95	0.32	-	70,70,70,70	0
55	MG	1H	3059	1/1	0.94	0.26	-	83,83,83,83	0
55	MG	14	3340	1/1	0.96	0.22	-	79,79,79,79	0
55	MG	14	3240	1/1	0.97	0.16	-	95,95,95,95	0
55	MG	14	3308	1/1	0.83	0.20	-	80,80,80,80	0
55	MG	1H	3251	1/1	0.95	0.32	-	56,56,56,56	0
55	MG	1H	3081	1/1	0.97	0.37	-	73,73,73,73	0
55	MG	1H	3347	1/1	0.93	0.32	-	72,72,72,72	0
55	MG	1H	3384	1/1	0.91	0.60	-	108,108,108,108	0
55	MG	13	1662	1/1	0.89	0.26	-	86,86,86,86	0
55	MG	14	3046	1/1	0.95	0.27	-	75,75,75,75	0
55	MG	1H	3436	1/1	0.96	0.09	-	94,94,94,94	0
55	MG	1H	3277	1/1	0.88	0.33	-	74,74,74,74	0
55	MG	1H	3210	1/1	0.92	0.41	-	79,79,79,79	0
55	MG	13	1612	1/1	0.95	0.32	-	102,102,102,102	0
55	MG	14	3342	1/1	0.88	0.45	-	94,94,94,94	0
55	MG	13	1686	1/1	0.86	0.39	-	85,85,85,85	0
55	MG	14	3261	1/1	0.72	0.53	-	105,105,105,105	0
55	MG	13	1634	1/1	0.93	0.35	-	73,73,73,73	0
55	MG	E5	101	1/1	0.80	0.39	-	88,88,88,88	0
55	MG	16	202	1/1	0.95	0.26	-	84,84,84,84	0
55	MG	1G	1701	1/1	0.60	0.13	-	93,93,93,93	0
55	MG	1H	3161	1/1	0.96	0.28	-	69,69,69,69	0
55	MG	1G	1662	1/1	0.89	0.41	-	84,84,84,84	0
55	MG	1G	1614	1/1	0.88	0.28	-	92,92,92,92	0
55	MG	14	3370	1/1	0.89	0.27	-	75,75,75,75	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
55	MG	1G	1712	1/1	0.92	0.16	-	109,109,109,109	0
55	MG	1H	3026	1/1	0.97	0.31	-	66,66,66,66	0
55	MG	1H	3139	1/1	0.82	0.58	-	69,69,69,69	0
55	MG	1H	3188	1/1	0.82	0.42	-	81,81,81,81	0
55	MG	14	3151	1/1	0.93	0.48	-	78,78,78,78	0
55	MG	1G	1729	1/1	0.94	0.05	-	93,93,93,93	0
55	MG	14	3409	1/1	0.91	0.07	-	64,64,64,64	0
55	MG	1H	3295	1/1	0.97	0.31	-	87,87,87,87	0
55	MG	1H	3350	1/1	0.69	0.51	-	89,89,89,89	0
55	MG	14	3387	1/1	0.97	0.12	-	58,58,58,58	0
55	MG	1H	3030	1/1	0.82	0.29	-	91,91,91,91	0
55	MG	14	3341	1/1	0.90	0.18	-	95,95,95,95	0
55	MG	29	304	1/1	0.73	0.45	-	89,89,89,89	0
55	MG	1J	206	1/1	0.78	0.36	-	96,96,96,96	0
55	MG	14	3099	1/1	0.88	0.22	-	67,67,67,67	0
55	MG	14	3268	1/1	0.87	0.38	-	85,85,85,85	0
55	MG	1H	3117	1/1	0.92	0.35	-	75,75,75,75	0
55	MG	1H	3377	1/1	0.56	0.35	-	81,81,81,81	0
55	MG	1G	1667	1/1	0.84	0.31	-	103,103,103,103	0
55	MG	1H	3313	1/1	0.81	0.22	-	91,91,91,91	0
55	MG	14	3360	1/1	0.85	0.19	-	74,74,74,74	0
55	MG	1H	3444	1/1	0.96	0.14	-	59,59,59,59	0
55	MG	14	3290	1/1	0.90	0.33	-	77,77,77,77	0
55	MG	14	3062	1/1	0.97	0.32	-	72,72,72,72	0
55	MG	14	3288	1/1	0.85	0.07	-	171,171,171,171	0
55	MG	21	301	1/1	0.92	0.31	-	58,58,58,58	0
55	MG	14	3424	1/1	0.90	0.08	-	81,81,81,81	0
55	MG	1H	3229	1/1	0.93	0.12	-	54,54,54,54	0
55	MG	1H	3449	1/1	0.92	0.22	-	94,94,94,94	0
55	MG	1H	3292	1/1	0.80	0.44	-	82,82,82,82	0
55	MG	14	3443	1/1	0.93	0.05	-	103,103,103,103	0
55	MG	1G	1740	1/1	0.77	0.05	-	140,140,140,140	0
55	MG	1H	3326	1/1	0.93	0.11	-	78,78,78,78	0
55	MG	13	1603	1/1	0.92	0.20	-	96,96,96,96	0
55	MG	1H	3190	1/1	0.56	0.58	-	101,101,101,101	0
55	MG	1H	3394	1/1	0.76	0.16	-	69,69,69,69	0
55	MG	2K	104	1/1	0.67	0.47	-	101,101,101,101	0
55	MG	1G	1638	1/1	0.70	0.43	-	88,88,88,88	0
55	MG	14	3138	1/1	0.90	0.29	-	58,58,58,58	0
55	MG	14	3074	1/1	0.89	0.16	-	47,47,47,47	0
55	MG	1H	3511	1/1	0.64	0.07	-	119,119,119,119	0
55	MG	1H	3176	1/1	0.88	0.38	-	73,73,73,73	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
55	MG	14	3270	1/1	0.90	0.39	-	76,76,76,76	0
55	MG	14	3322	1/1	0.92	0.09	-	70,70,70,70	0
55	MG	14	3262	1/1	0.78	0.37	-	86,86,86,86	0
55	MG	14	3087	1/1	0.82	0.27	-	65,65,65,65	0
55	MG	14	3349	1/1	0.80	0.20	-	100,100,100,100	0
55	MG	1G	1733	1/1	0.90	0.09	-	93,93,93,93	0
55	MG	14	3205	1/1	0.87	0.40	-	70,70,70,70	0
55	MG	1G	1698	1/1	0.92	0.26	-	96,96,96,96	0
55	MG	14	3402	1/1	0.91	0.07	-	82,82,82,82	0
55	MG	13	1698	1/1	0.72	0.35	-	78,78,78,78	0
55	MG	14	3148	1/1	0.81	0.46	-	86,86,86,86	0
55	MG	13	1670	1/1	0.95	0.11	-	106,106,106,106	0
55	MG	14	3289	1/1	0.70	0.16	-	175,175,175,175	0
55	MG	13	1737	1/1	0.74	0.07	-	111,111,111,111	0
55	MG	13	1689	1/1	0.37	0.45	-	116,116,116,116	0
55	MG	14	3432	1/1	0.92	0.12	-	100,100,100,100	0
55	MG	1H	3305	1/1	0.88	0.17	-	104,104,104,104	0
55	MG	1H	3517	1/1	0.84	0.06	-	113,113,113,113	0
55	MG	1H	3154	1/1	0.90	0.45	-	79,79,79,79	0
55	MG	1H	3376	1/1	0.84	0.46	-	94,94,94,94	0
55	MG	3L	101	1/1	0.71	0.18	-	180,180,180,180	0
55	MG	13	1664	1/1	0.91	0.59	-	93,93,93,93	0
55	MG	13	1623	1/1	0.92	0.21	-	107,107,107,107	0
55	MG	14	3368	1/1	0.64	0.23	-	76,76,76,76	0
55	MG	1H	3351	1/1	0.76	0.25	-	90,90,90,90	0
55	MG	1H	3296	1/1	0.91	0.33	-	84,84,84,84	0
55	MG	16	215	1/1	0.94	0.09	-	93,93,93,93	0
55	MG	1G	1686	1/1	0.73	0.10	-	95,95,95,95	0
55	MG	14	3376	1/1	0.85	0.10	-	66,66,66,66	0
55	MG	14	3285	1/1	0.85	0.31	-	93,93,93,93	0
55	MG	1H	3105	1/1	0.78	0.36	-	90,90,90,90	0
55	MG	13	1721	1/1	0.92	0.11	-	88,88,88,88	0
55	MG	1H	3235	1/1	0.86	0.52	-	88,88,88,88	0
55	MG	1H	3128	1/1	0.96	0.42	-	63,63,63,63	0
55	MG	1H	3156	1/1	0.92	0.31	-	72,72,72,72	0
55	MG	1H	3515	1/1	0.92	0.07	-	106,106,106,106	0
55	MG	1H	3417	1/1	0.99	0.11	-	40,40,40,40	0
55	MG	1H	3382	1/1	0.96	0.20	-	79,79,79,79	0
55	MG	13	1653	1/1	0.89	0.35	-	104,104,104,104	0
55	MG	14	3406	1/1	0.98	0.11	-	61,61,61,61	0
55	MG	1H	3498	1/1	0.96	0.07	-	77,77,77,77	0
55	MG	13	1701	1/1	0.89	0.33	-	100,100,100,100	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
55	MG	1H	3457	1/1	0.81	0.07	-	102,102,102,102	0
55	MG	1H	3385	1/1	0.72	0.21	-	97,97,97,97	0
55	MG	1H	3279	1/1	0.96	0.37	-	96,96,96,96	0
55	MG	14	3183	1/1	0.97	0.40	-	56,56,56,56	0
55	MG	14	3056	1/1	0.90	0.29	-	75,75,75,75	0
55	MG	1G	1708	1/1	0.76	0.22	-	133,133,133,133	0
55	MG	13	1693	1/1	0.64	0.38	-	100,100,100,100	0
55	MG	14	3336	1/1	0.77	0.20	-	73,73,73,73	0
55	MG	14	3284	1/1	0.88	0.23	-	95,95,95,95	0
55	MG	1H	3231	1/1	0.74	0.53	-	88,88,88,88	0
55	MG	14	3072	1/1	0.98	0.35	-	54,54,54,54	0
55	MG	14	3127	1/1	0.58	0.38	-	84,84,84,84	0
55	MG	14	3311	1/1	0.74	0.27	-	87,87,87,87	0
55	MG	1H	3220	1/1	0.20	0.27	-	92,92,92,92	0
55	MG	14	3253	1/1	0.91	0.24	-	105,105,105,105	0
55	MG	1G	1707	1/1	0.86	0.42	-	90,90,90,90	0
55	MG	13	1607	1/1	0.87	0.34	-	86,86,86,86	0
55	MG	13	1682	1/1	0.86	0.43	-	85,85,85,85	0
55	MG	14	3421	1/1	0.93	0.05	-	82,82,82,82	0
55	MG	14	3352	1/1	0.92	0.45	-	93,93,93,93	0
55	MG	1H	3200	1/1	0.84	0.29	-	99,99,99,99	0
55	MG	1H	3298	1/1	0.76	0.37	-	87,87,87,87	0
55	MG	2K	101	1/1	0.95	0.25	-	118,118,118,118	0
55	MG	1H	3086	1/1	0.81	0.19	-	59,59,59,59	0
55	MG	13	1650	1/1	0.89	0.40	-	88,88,88,88	0
55	MG	1H	3327	1/1	0.76	0.31	-	63,63,63,63	0
55	MG	1H	3396	1/1	0.52	0.24	-	104,104,104,104	0
55	MG	1G	1716	1/1	0.97	0.08	-	110,110,110,110	0
55	MG	1H	3460	1/1	0.95	0.06	-	87,87,87,87	0
55	MG	14	3236	1/1	0.82	0.44	-	94,94,94,94	0
55	MG	14	3254	1/1	0.92	0.37	-	85,85,85,85	0
55	MG	14	3108	1/1	0.95	0.36	-	85,85,85,85	0
55	MG	1H	3134	1/1	0.79	0.33	-	65,65,65,65	0
55	MG	1H	3443	1/1	0.89	0.09	-	75,75,75,75	0
55	MG	13	1638	1/1	0.77	0.23	-	85,85,85,85	0
55	MG	14	3218	1/1	0.77	0.39	-	88,88,88,88	0
55	MG	14	3136	1/1	0.89	0.39	-	75,75,75,75	0
55	MG	14	3140	1/1	0.86	0.38	-	77,77,77,77	0
55	MG	14	3107	1/1	0.97	0.42	-	80,80,80,80	0
55	MG	14	3014	1/1	0.92	0.29	-	84,84,84,84	0
55	MG	1G	1604	1/1	0.93	0.15	-	78,78,78,78	0
55	MG	14	3272	1/1	0.78	0.39	-	94,94,94,94	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
55	MG	1H	3389	1/1	0.91	0.40	-	101,101,101,101	0
55	MG	1G	1688	1/1	0.77	0.23	-	102,102,102,102	0
55	MG	14	3245	1/1	0.95	0.40	-	64,64,64,64	0
55	MG	1H	3316	1/1	0.89	0.23	-	61,61,61,61	0
55	MG	1G	1742	1/1	0.92	0.05	-	112,112,112,112	0
55	MG	13	1629	1/1	0.94	0.35	-	60,60,60,60	0
55	MG	1H	3422	1/1	0.99	0.07	-	56,56,56,56	0
55	MG	14	3252	1/1	0.71	0.21	-	81,81,81,81	0
55	MG	1H	3205	1/1	0.80	0.59	-	103,103,103,103	0
55	MG	14	3440	1/1	0.96	0.05	-	101,101,101,101	0
55	MG	14	3166	1/1	0.76	0.15	-	71,71,71,71	0
55	MG	1H	3222	1/1	0.96	0.37	-	65,65,65,65	0
55	MG	1H	3299	1/1	0.96	0.22	-	57,57,57,57	0
55	MG	1G	1676	1/1	0.83	0.39	-	98,98,98,98	0
55	MG	1H	3391	1/1	0.84	0.37	-	92,92,92,92	0
55	MG	1H	3393	1/1	0.89	0.14	-	62,62,62,62	0
55	MG	14	3120	1/1	0.92	0.43	-	54,54,54,54	0
55	MG	14	3187	1/1	0.89	0.41	-	94,94,94,94	0
55	MG	1H	3478	1/1	0.94	0.08	-	82,82,82,82	0
55	MG	1H	3334	1/1	0.90	0.23	-	108,108,108,108	0
55	MG	13	1631	1/1	0.97	0.16	-	60,60,60,60	0
55	MG	13	1645	1/1	0.74	0.49	-	98,98,98,98	0
55	MG	1H	3281	1/1	0.84	0.52	-	80,80,80,80	0
55	MG	1G	1699	1/1	0.67	0.46	-	101,101,101,101	0
55	MG	14	3150	1/1	0.79	0.38	-	107,107,107,107	0
55	MG	13	1666	1/1	0.78	0.47	-	104,104,104,104	0
55	MG	14	3223	1/1	0.99	0.20	-	64,64,64,64	0
55	MG	14	3184	1/1	0.87	0.23	-	71,71,71,71	0
55	MG	1H	3365	1/1	0.92	0.28	-	86,86,86,86	0
55	MG	14	3462	1/1	0.87	0.04	-	130,130,130,130	0
55	MG	1H	3336	1/1	0.68	0.43	-	83,83,83,83	0
55	MG	14	3195	1/1	0.93	0.25	-	65,65,65,65	0
55	MG	14	3237	1/1	0.97	0.34	-	74,74,74,74	0
55	MG	1G	1709	1/1	0.77	0.21	-	96,96,96,96	0
55	MG	1H	3320	1/1	0.93	0.61	-	109,109,109,109	0
55	MG	14	3213	1/1	0.93	0.32	-	68,68,68,68	0
55	MG	14	3144	1/1	0.89	0.47	-	98,98,98,98	0
55	MG	1H	3036	1/1	0.97	0.27	-	70,70,70,70	0
55	MG	14	3182	1/1	0.76	0.17	-	77,77,77,77	0
55	MG	1H	3267	1/1	0.95	0.27	-	57,57,57,57	0
55	MG	16	203	1/1	0.59	0.24	-	92,92,92,92	0
55	MG	14	3230	1/1	0.80	0.28	-	75,75,75,75	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
55	MG	13	1608	1/1	0.70	0.32	-	101,101,101,101	0
55	MG	1H	3380	1/1	0.94	0.46	-	88,88,88,88	0
55	MG	14	3449	1/1	0.79	0.08	-	108,108,108,108	0
55	MG	1H	3255	1/1	0.91	0.21	-	92,92,92,92	0
55	MG	1H	3055	1/1	0.95	0.47	-	77,77,77,77	0
55	MG	14	3167	1/1	0.89	0.20	-	83,83,83,83	0
55	MG	1H	3046	1/1	0.92	0.34	-	71,71,71,71	0
55	MG	1H	3290	1/1	0.91	0.41	-	80,80,80,80	0
55	MG	13	1672	1/1	0.93	0.23	-	119,119,119,119	0
55	MG	1H	3261	1/1	0.96	0.41	-	72,72,72,72	0
55	MG	1H	3165	1/1	0.90	0.40	-	74,74,74,74	0
55	MG	1H	3201	1/1	0.89	0.41	-	66,66,66,66	0
55	MG	14	3439	1/1	0.90	0.07	-	101,101,101,101	0
55	MG	1H	3283	1/1	0.70	0.41	-	104,104,104,104	0
55	MG	14	3278	1/1	0.91	0.27	-	84,84,84,84	0
55	MG	1H	3269	1/1	0.85	0.33	-	82,82,82,82	0
55	MG	1H	3294	1/1	0.78	0.54	-	85,85,85,85	0
55	MG	13	1696	1/1	0.90	0.19	-	86,86,86,86	0
55	MG	1H	3490	1/1	0.94	0.06	-	89,89,89,89	0
55	MG	1G	1687	1/1	0.88	0.25	-	79,79,79,79	0
55	MG	14	3287	1/1	0.41	0.32	-	98,98,98,98	0
55	MG	14	3282	1/1	0.68	0.23	-	87,87,87,87	0
55	MG	14	3246	1/1	0.90	0.21	-	83,83,83,83	0
55	MG	1G	1642	1/1	0.84	0.26	-	87,87,87,87	0
55	MG	14	3095	1/1	0.98	0.20	-	65,65,65,65	0
55	MG	14	3188	1/1	0.84	0.37	-	76,76,76,76	0
55	MG	1H	3307	1/1	0.67	0.24	-	83,83,83,83	0
55	MG	1H	3259	1/1	0.71	0.33	-	93,93,93,93	0
55	MG	13	1728	1/1	0.98	0.07	-	76,76,76,76	0
55	MG	1H	3072	1/1	0.98	0.33	-	75,75,75,75	0
55	MG	13	1651	1/1	0.89	0.31	-	73,73,73,73	0
55	MG	1H	3278	1/1	0.89	0.45	-	76,76,76,76	0
55	MG	14	3384	1/1	0.99	0.09	-	54,54,54,54	0
55	MG	14	3356	1/1	0.85	0.23	-	195,195,195,195	0
55	MG	1H	3346	1/1	0.45	0.24	-	113,113,113,113	0
55	MG	1H	3075	1/1	0.83	0.53	-	87,87,87,87	0
55	MG	1G	1723	1/1	0.89	0.24	-	98,98,98,98	0
55	MG	13	1678	1/1	0.88	0.35	-	104,104,104,104	0
55	MG	1H	3027	1/1	0.66	0.33	-	86,86,86,86	0
55	MG	14	3185	1/1	0.84	0.34	-	90,90,90,90	0
55	MG	1H	3187	1/1	0.96	0.36	-	83,83,83,83	0
55	MG	1G	1607	1/1	0.88	0.28	-	95,95,95,95	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
55	MG	1G	1710	1/1	0.87	0.23	-	101,101,101,101	0
55	MG	14	3357	1/1	0.77	0.19	-	76,76,76,76	0
55	MG	42	201	1/1	0.34	0.35	-	101,101,101,101	0
55	MG	16	213	1/1	0.89	0.15	-	113,113,113,113	0
55	MG	13	1735	1/1	0.94	0.04	-	106,106,106,106	0
55	MG	1G	1657	1/1	0.95	0.29	-	87,87,87,87	0
55	MG	1G	1633	1/1	0.90	0.48	-	80,80,80,80	0
55	MG	14	3084	1/1	0.97	0.10	-	73,73,73,73	0
55	MG	14	3134	1/1	0.81	0.30	-	80,80,80,80	0
55	MG	14	3304	1/1	0.85	0.45	-	99,99,99,99	0
55	MG	1H	3390	1/1	0.89	0.36	-	88,88,88,88	0
55	MG	1H	3184	1/1	0.89	0.47	-	85,85,85,85	0
55	MG	1G	1737	1/1	0.93	0.07	-	114,114,114,114	0
55	MG	1H	3136	1/1	0.94	0.56	-	85,85,85,85	0
55	MG	13	1684	1/1	0.51	0.30	-	94,94,94,94	0
55	MG	14	3299	1/1	0.90	0.42	-	100,100,100,100	0
55	MG	14	3047	1/1	0.96	0.27	-	57,57,57,57	0
55	MG	1G	1656	1/1	0.80	0.31	-	94,94,94,94	0
55	MG	1H	3171	1/1	0.96	0.46	-	82,82,82,82	0
55	MG	1H	3221	1/1	0.74	0.27	-	108,108,108,108	0
55	MG	1H	3387	1/1	0.62	0.31	-	75,75,75,75	0
55	MG	1H	3024	1/1	0.99	0.15	-	61,61,61,61	0
55	MG	13	1626	1/1	0.97	0.39	-	65,65,65,65	0
55	MG	14	3065	1/1	0.98	0.32	-	50,50,50,50	0
55	MG	14	3026	1/1	0.91	0.19	-	78,78,78,78	0
55	MG	14	3238	1/1	0.94	0.41	-	81,81,81,81	0
55	MG	1H	3513	1/1	0.89	0.08	-	116,116,116,116	0
55	MG	14	3190	1/1	0.54	0.36	-	95,95,95,95	0
55	MG	14	3382	1/1	0.97	0.12	-	55,55,55,55	0
55	MG	1H	3043	1/1	0.67	0.26	-	92,92,92,92	0
55	MG	14	3100	1/1	0.88	0.21	-	79,79,79,79	0
55	MG	1G	1670	1/1	0.91	0.32	-	92,92,92,92	0
55	MG	16	214	1/1	0.96	0.08	-	86,86,86,86	0
55	MG	1H	3239	1/1	0.86	0.32	-	74,74,74,74	0
55	MG	1H	3028	1/1	0.95	0.17	-	53,53,53,53	0
55	MG	1H	3245	1/1	0.90	0.34	-	86,86,86,86	0
55	MG	14	3020	1/1	0.89	0.33	-	72,72,72,72	0
55	MG	1G	1727	1/1	0.83	0.24	-	104,104,104,104	0
55	MG	1H	3102	1/1	0.94	0.33	-	49,49,49,49	0
55	MG	14	3009	1/1	0.98	0.28	-	58,58,58,58	0
55	MG	1H	3018	1/1	0.98	0.21	-	50,50,50,50	0
55	MG	13	1614	1/1	0.87	0.24	-	95,95,95,95	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
55	MG	14	3006	1/1	0.98	0.33	-	56,56,56,56	0
55	MG	1G	1645	1/1	0.93	0.12	-	79,79,79,79	0
55	MG	1G	1684	1/1	0.85	0.41	-	99,99,99,99	0
55	MG	1H	3321	1/1	0.95	0.48	-	79,79,79,79	0
55	MG	1H	3447	1/1	0.98	0.09	-	62,62,62,62	0
55	MG	14	3125	1/1	0.91	0.42	-	88,88,88,88	0
55	MG	14	3423	1/1	0.98	0.09	-	84,84,84,84	0
55	MG	1G	1732	1/1	0.97	0.05	-	113,113,113,113	0
55	MG	14	3029	1/1	0.94	0.33	-	51,51,51,51	0
55	MG	1H	3112	1/1	0.95	0.47	-	73,73,73,73	0
55	MG	1H	3268	1/1	0.84	0.39	-	100,100,100,100	0
55	MG	1H	3058	1/1	0.79	0.47	-	60,60,60,60	0
55	MG	14	3394	1/1	0.93	0.06	-	89,89,89,89	0
55	MG	1H	3282	1/1	0.60	0.44	-	90,90,90,90	0
55	MG	13	1715	1/1	0.81	0.23	-	70,70,70,70	0
55	MG	4K	101	1/1	0.61	0.29	-	111,111,111,111	0
55	MG	1H	3477	1/1	0.85	0.12	-	74,74,74,74	0
55	MG	14	3137	1/1	0.95	0.30	-	69,69,69,69	0
55	MG	14	3105	1/1	0.84	0.38	-	72,72,72,72	0
55	MG	14	3389	1/1	0.99	0.17	-	53,53,53,53	0
55	MG	1H	3481	1/1	0.98	0.12	-	64,64,64,64	0
55	MG	1H	3494	1/1	0.96	0.10	-	81,81,81,81	0
55	MG	1H	3189	1/1	0.92	0.12	-	83,83,83,83	0
55	MG	1H	3232	1/1	0.72	0.24	-	103,103,103,103	0
55	MG	1H	3073	1/1	0.91	0.26	-	77,77,77,77	0
55	MG	1H	3373	1/1	0.92	0.47	-	79,79,79,79	0
55	MG	1H	3439	1/1	0.95	0.09	-	92,92,92,92	0
55	MG	1H	3263	1/1	0.83	0.45	-	84,84,84,84	0
55	MG	13	1739	1/1	0.99	0.22	-	90,90,90,90	0
55	MG	14	3034	1/1	0.82	0.31	-	73,73,73,73	0
55	MG	14	3244	1/1	0.82	0.33	-	86,86,86,86	0
55	MG	1H	3412	1/1	0.97	0.14	-	69,69,69,69	0
55	MG	1H	3360	1/1	0.29	0.34	-	167,167,167,167	0
55	MG	1H	3440	1/1	0.98	0.07	-	91,91,91,91	0
55	MG	1H	3518	1/1	0.62	0.17	-	135,135,135,135	0
55	MG	14	3063	1/1	0.98	0.35	-	51,51,51,51	0
55	MG	1G	1677	1/1	0.77	0.29	-	89,89,89,89	0
55	MG	14	3286	1/1	0.69	0.20	-	100,100,100,100	0
55	MG	14	3024	1/1	0.96	0.23	-	49,49,49,49	0
55	MG	1H	3178	1/1	0.71	0.25	-	77,77,77,77	0
55	MG	1H	3042	1/1	0.93	0.13	-	95,95,95,95	0
55	MG	13	1679	1/1	0.94	0.34	-	80,80,80,80	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
55	MG	1H	3252	1/1	0.91	0.34	-	98,98,98,98	0
55	MG	14	3309	1/1	0.68	0.33	-	84,84,84,84	0
55	MG	1H	3308	1/1	0.96	0.23	-	106,106,106,106	0
55	MG	14	3109	1/1	0.91	0.36	-	85,85,85,85	0
55	MG	1H	3162	1/1	0.60	0.21	-	94,94,94,94	0
55	MG	I8	103	1/1	0.87	0.39	-	92,92,92,92	0
55	MG	13	1661	1/1	0.86	0.42	-	95,95,95,95	0
55	MG	1H	3323	1/1	0.80	0.41	-	80,80,80,80	0
55	MG	C5	201	1/1	0.83	0.26	-	86,86,86,86	0
55	MG	14	3214	1/1	0.93	0.24	-	66,66,66,66	0
55	MG	1H	3009	1/1	0.98	0.38	-	44,44,44,44	0
55	MG	14	3158	1/1	0.82	0.27	-	97,97,97,97	0
55	MG	14	3163	1/1	0.85	0.23	-	80,80,80,80	0
55	MG	13	1711	1/1	0.76	0.62	-	90,90,90,90	0
55	MG	14	3067	1/1	0.97	0.29	-	71,71,71,71	0
55	MG	14	3116	1/1	0.97	0.36	-	49,49,49,49	0
55	MG	1H	3266	1/1	0.85	0.33	-	101,101,101,101	0
55	MG	14	3250	1/1	0.96	0.26	-	70,70,70,70	0
55	MG	14	3294	1/1	0.90	0.11	-	81,81,81,81	0
55	MG	13	1649	1/1	0.78	0.45	-	84,84,84,84	0
55	MG	14	3243	1/1	0.97	0.22	-	78,78,78,78	0
55	MG	1H	3110	1/1	0.93	0.24	-	47,47,47,47	0
55	MG	1H	3257	1/1	0.92	0.43	-	83,83,83,83	0
55	MG	25	201	1/1	0.88	0.08	-	111,111,111,111	0
55	MG	1H	3337	1/1	0.91	0.28	-	94,94,94,94	0
55	MG	1G	1626	1/1	0.89	0.27	-	107,107,107,107	0
55	MG	1G	1734	1/1	0.90	0.07	-	81,81,81,81	0
55	MG	13	1730	1/1	0.96	0.10	-	115,115,115,115	0
55	MG	14	3126	1/1	0.87	0.32	-	83,83,83,83	0
55	MG	14	3118	1/1	0.95	0.22	-	84,84,84,84	0
55	MG	14	3313	1/1	0.86	0.14	-	86,86,86,86	0
55	MG	1H	3427	1/1	0.94	0.08	-	107,107,107,107	0
55	MG	14	3083	1/1	0.95	0.41	-	68,68,68,68	0
55	MG	1G	1655	1/1	0.88	0.33	-	74,74,74,74	0
55	MG	1H	3037	1/1	0.89	0.33	-	60,60,60,60	0
55	MG	2L	103	1/1	0.92	0.09	-	130,130,130,130	0
55	MG	1H	3368	1/1	0.91	0.45	-	72,72,72,72	0
55	MG	1H	3375	1/1	0.67	0.36	-	85,85,85,85	0
55	MG	14	3036	1/1	0.85	0.29	-	91,91,91,91	0
55	MG	14	3327	1/1	0.91	0.43	-	110,110,110,110	0
55	MG	13	1733	1/1	0.81	0.08	-	141,141,141,141	0
55	MG	14	3319	1/1	0.90	0.09	-	89,89,89,89	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
55	MG	14	3353	1/1	0.74	0.28	-	84,84,84,84	0
55	MG	1H	3237	1/1	0.97	0.37	-	67,67,67,67	0
55	MG	14	3060	1/1	0.97	0.35	-	64,64,64,64	0
55	MG	14	3464	1/1	0.86	0.06	-	101,101,101,101	0
55	MG	1H	3399	1/1	0.85	0.22	-	77,77,77,77	0
55	MG	1H	3193	1/1	0.76	0.39	-	77,77,77,77	0
55	MG	14	3242	1/1	0.90	0.33	-	86,86,86,86	0
55	MG	13	1727	1/1	0.91	0.12	-	108,108,108,108	0
55	MG	1H	3372	1/1	0.89	0.38	-	94,94,94,94	0
55	MG	1H	3355	1/1	0.68	0.58	-	107,107,107,107	0
55	MG	1H	3504	1/1	0.88	0.07	-	80,80,80,80	0
55	MG	1H	3163	1/1	0.90	0.29	-	82,82,82,82	0
55	MG	14	3181	1/1	0.85	0.29	-	70,70,70,70	0
55	MG	14	3129	1/1	0.93	0.39	-	70,70,70,70	0
55	MG	1G	1641	1/1	0.92	0.40	-	83,83,83,83	0
55	MG	1H	3125	1/1	0.95	0.36	-	73,73,73,73	0
55	MG	1H	3067	1/1	0.94	0.18	-	47,47,47,47	0
55	MG	1H	3214	1/1	0.96	0.31	-	64,64,64,64	0
55	MG	13	1674	1/1	0.89	0.36	-	106,106,106,106	0
55	MG	1H	3191	1/1	0.96	0.51	-	64,64,64,64	0
55	MG	1H	3064	1/1	0.86	0.34	-	70,70,70,70	0
55	MG	1H	3403	1/1	0.96	0.07	-	111,111,111,111	0
55	MG	32	301	1/1	0.78	0.42	-	113,113,113,113	0
55	MG	14	3303	1/1	0.66	0.39	-	99,99,99,99	0
55	MG	13	1713	1/1	0.83	0.33	-	100,100,100,100	0
55	MG	1H	3228	1/1	0.98	0.32	-	63,63,63,63	0
55	MG	14	3168	1/1	0.78	0.35	-	76,76,76,76	0
55	MG	13	1722	1/1	0.89	0.18	-	101,101,101,101	0
55	MG	1H	3197	1/1	0.81	0.62	-	85,85,85,85	0
55	MG	1H	3493	1/1	0.83	0.08	-	103,103,103,103	0
55	MG	14	3030	1/1	0.94	0.32	-	60,60,60,60	0
55	MG	13	1601	1/1	0.95	0.21	-	103,103,103,103	0
55	MG	14	3296	1/1	0.82	0.28	-	97,97,97,97	0
55	MG	1G	1634	1/1	0.96	0.37	-	80,80,80,80	0
55	MG	1H	3145	1/1	0.94	0.26	-	46,46,46,46	0
55	MG	14	3164	1/1	0.98	0.26	-	60,60,60,60	0
55	MG	1H	3111	1/1	0.97	0.34	-	71,71,71,71	0
55	MG	1H	3152	1/1	0.78	0.48	-	80,80,80,80	0
55	MG	1H	3203	1/1	0.64	0.46	-	99,99,99,99	0
55	MG	1H	3238	1/1	0.87	0.56	-	82,82,82,82	0
55	MG	1H	3314	1/1	0.86	0.38	-	97,97,97,97	0
55	MG	14	3455	1/1	0.89	0.11	-	108,108,108,108	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
55	MG	14	3128	1/1	0.69	0.43	-	76,76,76,76	0
55	MG	1H	3459	1/1	0.95	0.08	-	75,75,75,75	0
55	MG	1H	3378	1/1	0.94	0.09	-	91,91,91,91	0
55	MG	1H	3273	1/1	0.89	0.39	-	103,103,103,103	0
55	MG	14	3456	1/1	0.93	0.06	-	102,102,102,102	0
55	MG	1G	1694	1/1	0.76	0.18	-	118,118,118,118	0
55	MG	1J	204	1/1	0.83	0.23	-	101,101,101,101	0
55	MG	13	1624	1/1	0.78	0.36	-	107,107,107,107	0
55	MG	14	3442	1/1	0.86	0.04	-	107,107,107,107	0
55	MG	1G	1629	1/1	0.75	0.36	-	86,86,86,86	0
55	MG	14	3446	1/1	0.91	0.07	-	87,87,87,87	0
55	MG	1H	3223	1/1	0.94	0.34	-	97,97,97,97	0
55	MG	1H	3472	1/1	0.95	0.07	-	82,82,82,82	0
55	MG	16	211	1/1	0.63	0.23	-	98,98,98,98	0
55	MG	14	3178	1/1	0.92	0.27	-	81,81,81,81	0
55	MG	14	3160	1/1	0.92	0.21	-	74,74,74,74	0
55	MG	13	1643	1/1	0.75	0.51	-	86,86,86,86	0
55	MG	1H	3409	1/1	0.95	0.12	-	62,62,62,62	0
55	MG	14	3372	1/1	0.91	0.36	-	96,96,96,96	0
55	MG	1G	1637	1/1	0.94	0.35	-	71,71,71,71	0
55	MG	1G	1639	1/1	0.71	0.46	-	97,97,97,97	0
55	MG	13	1688	1/1	0.58	0.49	-	91,91,91,91	0
55	MG	13	1667	1/1	0.85	0.43	-	94,94,94,94	0
55	MG	1H	3506	1/1	0.93	0.09	-	110,110,110,110	0
55	MG	1G	1695	1/1	0.94	0.10	-	86,86,86,86	0
55	MG	1H	3218	1/1	0.64	0.51	-	82,82,82,82	0
55	MG	14	3366	1/1	0.91	0.43	-	99,99,99,99	0
55	MG	14	3398	1/1	0.98	0.13	-	83,83,83,83	0
55	MG	14	3220	1/1	0.80	0.17	-	89,89,89,89	0
55	MG	14	3344	1/1	0.96	0.14	-	95,95,95,95	0
55	MG	14	3312	1/1	0.73	0.35	-	81,81,81,81	0
55	MG	1H	3170	1/1	0.88	0.42	-	89,89,89,89	0
55	MG	3A	201	1/1	0.96	0.17	-	81,81,81,81	0
55	MG	1H	3505	1/1	0.98	0.07	-	69,69,69,69	0
55	MG	13	1615	1/1	0.88	0.37	-	98,98,98,98	0
55	MG	1H	3023	1/1	0.97	0.35	-	55,55,55,55	0
55	MG	1J	210	1/1	0.79	0.12	-	144,144,144,144	0
55	MG	1H	3179	1/1	0.89	0.17	-	60,60,60,60	0
55	MG	14	3085	1/1	0.87	0.31	-	72,72,72,72	0
55	MG	1H	3291	1/1	0.85	0.19	-	68,68,68,68	0
55	MG	1H	3406	1/1	0.77	0.53	-	91,91,91,91	0
55	MG	14	3049	1/1	0.98	0.12	-	55,55,55,55	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
55	MG	13	1641	1/1	0.94	0.29	-	67,67,67,67	0
55	MG	14	3324	1/1	0.84	0.36	-	101,101,101,101	0
55	MG	1H	3211	1/1	0.87	0.37	-	79,79,79,79	0
55	MG	14	3337	1/1	0.92	0.25	-	105,105,105,105	0
55	MG	1G	1685	1/1	0.30	0.26	-	116,116,116,116	0
55	MG	14	3141	1/1	0.81	0.41	-	85,85,85,85	0
55	MG	1H	3453	1/1	0.97	0.12	-	42,42,42,42	0
55	MG	13	1637	1/1	0.85	0.50	-	90,90,90,90	0
55	MG	1H	3301	1/1	0.24	0.37	-	79,79,79,79	0
55	MG	14	3431	1/1	0.81	0.10	-	102,102,102,102	0
55	MG	14	3355	1/1	0.91	0.24	-	73,73,73,73	0
55	MG	1H	3070	1/1	0.99	0.27	-	60,60,60,60	0
55	MG	1H	3242	1/1	0.96	0.20	-	45,45,45,45	0
55	MG	14	3461	1/1	0.85	0.09	-	82,82,82,82	0
55	MG	1H	3522	1/1	0.90	0.15	-	68,68,68,68	0
55	MG	1H	3329	1/1	0.87	0.40	-	85,85,85,85	0
55	MG	13	1618	1/1	0.84	0.29	-	96,96,96,96	0
55	MG	1H	3349	1/1	0.79	0.15	-	77,77,77,77	0
55	MG	1H	3103	1/1	0.83	0.41	-	71,71,71,71	0
55	MG	1H	3520	1/1	0.84	0.06	-	103,103,103,103	0
55	MG	1H	3386	1/1	0.57	0.30	-	66,66,66,66	0
55	MG	1H	3284	1/1	0.83	0.42	-	73,73,73,73	0
55	MG	13	1635	1/1	0.71	0.31	-	95,95,95,95	0
55	MG	1G	1718	1/1	0.65	0.34	-	118,118,118,118	0
55	MG	14	3201	1/1	0.96	0.21	-	61,61,61,61	0
55	MG	1H	3357	1/1	0.79	0.35	-	92,92,92,92	0
55	MG	14	3079	1/1	0.77	0.30	-	82,82,82,82	0
55	MG	14	3210	1/1	0.84	0.15	-	68,68,68,68	0
55	MG	14	3110	1/1	0.95	0.34	-	63,63,63,63	0
55	MG	14	3211	1/1	0.93	0.30	-	77,77,77,77	0
55	MG	1H	3164	1/1	0.85	0.46	-	90,90,90,90	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	1G	1620	1/1	0.60	0.41	-	96,96,96,96	0
55	MG	14	3292	1/1	0.64	0.27	-	90,90,90,90	0
55	MG	1H	3502	1/1	0.88	0.06	-	148,148,148,148	0
55	MG	14	3364	1/1	0.90	0.09	-	68,68,68,68	0
55	MG	14	3057	1/1	0.98	0.42	-	54,54,54,54	0
55	MG	14	3090	1/1	0.94	0.37	-	70,70,70,70	0
55	MG	1H	3400	1/1	0.91	0.34	-	84,84,84,84	0
55	MG	1H	3204	1/1	0.87	0.44	-	83,83,83,83	0
55	MG	2K	102	1/1	0.98	0.44	-	93,93,93,93	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
55	MG	16	209	1/1	0.74	0.25	-	80,80,80,80	0
55	MG	1J	205	1/1	0.92	0.36	-	122,122,122,122	0
55	MG	1G	1635	1/1	0.86	0.48	-	70,70,70,70	0
55	MG	1G	1630	1/1	0.90	0.42	-	81,81,81,81	0
55	MG	14	3433	1/1	0.88	0.07	-	87,87,87,87	0
55	MG	14	3358	1/1	0.88	0.17	-	85,85,85,85	0
55	MG	1H	3006	1/1	0.95	0.27	-	67,67,67,67	0
55	MG	1H	3206	1/1	0.98	0.44	-	72,72,72,72	0
55	MG	13	1642	1/1	0.92	0.46	-	66,66,66,66	0
55	MG	13	1665	1/1	0.90	0.10	-	90,90,90,90	0
55	MG	1H	3341	1/1	0.82	0.30	-	76,76,76,76	0
55	MG	1H	3312	1/1	0.50	0.28	-	81,81,81,81	0
55	MG	14	3106	1/1	0.85	0.44	-	75,75,75,75	0
55	MG	14	3435	1/1	0.93	0.07	-	95,95,95,95	0
55	MG	13	1706	1/1	0.58	0.44	-	93,93,93,93	0
55	MG	3I	201	1/1	0.93	0.20	-	80,80,80,80	0
55	MG	14	3142	1/1	0.82	0.30	-	72,72,72,72	0
55	MG	1H	3310	1/1	0.89	0.40	-	72,72,72,72	0
55	MG	14	3354	1/1	0.76	0.31	-	134,134,134,134	0
55	MG	1H	3483	1/1	0.94	0.05	-	84,84,84,84	0
55	MG	14	3171	1/1	0.81	0.37	-	86,86,86,86	0
55	MG	1G	1735	1/1	0.94	0.08	-	96,96,96,96	0
55	MG	1H	3507	1/1	0.96	0.19	-	62,62,62,62	0
55	MG	1H	3132	1/1	0.83	0.36	-	76,76,76,76	0
55	MG	1G	1721	1/1	0.54	0.55	-	129,129,129,129	0
55	MG	1H	3286	1/1	0.57	0.33	-	82,82,82,82	0
55	MG	1H	3342	1/1	0.66	0.40	-	89,89,89,89	0
55	MG	1G	1668	1/1	0.89	0.27	-	82,82,82,82	0
55	MG	1H	3230	1/1	0.93	0.40	-	71,71,71,71	0
55	MG	1H	3130	1/1	0.92	0.28	-	69,69,69,69	0
55	MG	1H	3050	1/1	0.98	0.39	-	47,47,47,47	0
55	MG	1H	3512	1/1	0.89	0.08	-	115,115,115,115	0
55	MG	1G	1674	1/1	0.84	0.34	-	111,111,111,111	0
55	MG	2K	103	1/1	0.78	0.32	-	94,94,94,94	0
55	MG	14	3247	1/1	0.95	0.07	-	79,79,79,79	0
55	MG	14	3266	1/1	0.94	0.43	-	88,88,88,88	0
55	MG	1G	1654	1/1	0.79	0.38	-	91,91,91,91	0
55	MG	1H	3485	1/1	0.98	0.15	-	75,75,75,75	0
55	MG	14	3170	1/1	0.94	0.19	-	79,79,79,79	0
55	MG	1H	3471	1/1	0.95	0.08	-	71,71,71,71	0
55	MG	14	3265	1/1	0.86	0.38	-	76,76,76,76	0
55	MG	14	3438	1/1	0.87	0.08	-	83,83,83,83	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
55	MG	14	3080	1/1	0.89	0.52	-	81,81,81,81	0
55	MG	1H	3096	1/1	0.77	0.43	-	71,71,71,71	0
55	MG	1G	1741	1/1	0.72	0.09	-	112,112,112,112	0
55	MG	14	3279	1/1	0.85	0.44	-	84,84,84,84	0
55	MG	1H	3343	1/1	0.92	0.17	-	90,90,90,90	0
55	MG	1H	3379	1/1	0.33	0.13	-	245,245,245,245	0
55	MG	14	3260	1/1	0.88	0.31	-	99,99,99,99	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	1H	3514	1/1	0.82	0.10	-	109,109,109,109	0
55	MG	1G	1640	1/1	0.86	0.45	-	107,107,107,107	0
55	MG	1H	3469	1/1	0.78	0.15	-	115,115,115,115	0
55	MG	1H	3149	1/1	0.79	0.46	-	82,82,82,82	0
55	MG	13	1699	1/1	0.49	0.46	-	109,109,109,109	0
55	MG	1H	3348	1/1	0.92	0.24	-	88,88,88,88	0
55	MG	14	3463	1/1	0.89	0.11	-	130,130,130,130	0
55	MG	1H	3194	1/1	0.87	0.32	-	68,68,68,68	0
55	MG	1H	3300	1/1	0.86	0.30	-	77,77,77,77	0
55	MG	1H	3388	1/1	0.78	0.34	-	74,74,74,74	0
55	MG	1G	1744	1/1	0.90	0.08	-	128,128,128,128	0
55	MG	14	3088	1/1	0.84	0.35	-	70,70,70,70	0
55	MG	1H	3092	1/1	0.88	0.43	-	62,62,62,62	0
55	MG	1G	1663	1/1	0.70	0.29	-	81,81,81,81	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	1G	1703	1/1	0.64	0.28	-	99,99,99,99	0
55	MG	13	1697	1/1	0.81	0.41	-	84,84,84,84	0
55	MG	1H	3491	1/1	0.88	0.14	-	52,52,52,52	0
55	MG	13	1602	1/1	0.98	0.21	-	78,78,78,78	0
55	MG	1G	1696	1/1	0.90	0.11	-	92,92,92,92	0
55	MG	13	1657	1/1	0.78	0.31	-	74,74,74,74	0
55	MG	1G	1691	1/1	0.60	0.27	-	132,132,132,132	0
55	MG	1H	3008	1/1	0.89	0.30	-	44,44,44,44	0
55	MG	14	3330	1/1	0.76	0.24	-	81,81,81,81	0
55	MG	14	3362	1/1	0.88	0.29	-	111,111,111,111	0
55	MG	14	3028	1/1	0.95	0.25	-	77,77,77,77	0
55	MG	1G	1739	1/1	0.61	0.09	-	154,154,154,154	0
55	MG	13	1724	1/1	0.95	0.14	-	107,107,107,107	0
55	MG	14	3005	1/1	0.97	0.29	-	52,52,52,52	0
55	MG	13	1732	1/1	0.93	0.13	-	128,128,128,128	0
55	MG	13	1712	1/1	0.70	0.35	-	123,123,123,123	0
55	MG	14	3001	1/1	0.90	0.24	-	70,70,70,70	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
55	MG	1H	3275	1/1	0.96	0.26	-	69,69,69,69	0
55	MG	14	3450	1/1	0.91	0.14	-	105,105,105,105	0
55	MG	14	3132	1/1	0.42	0.29	-	120,120,120,120	0
55	MG	13	1617	1/1	0.75	0.32	-	122,122,122,122	0
55	MG	1H	3022	1/1	0.91	0.14	-	60,60,60,60	0
55	MG	1H	3076	1/1	0.80	0.23	-	77,77,77,77	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	1G	1672	1/1	0.85	0.28	-	79,79,79,79	0
55	MG	14	3017	1/1	0.90	0.25	-	83,83,83,83	0
55	MG	1H	3208	1/1	0.92	0.45	-	69,69,69,69	0
55	MG	14	3329	1/1	0.39	0.27	-	101,101,101,101	0
55	MG	14	3161	1/1	0.72	0.37	-	89,89,89,89	0
55	MG	11	302	1/1	0.76	0.23	-	85,85,85,85	0
55	MG	1H	3254	1/1	0.90	0.20	-	69,69,69,69	0
55	MG	1H	3142	1/1	0.97	0.25	-	74,74,74,74	0
55	MG	14	3025	1/1	0.95	0.35	-	86,86,86,86	0
55	MG	1G	1606	1/1	0.96	0.20	-	80,80,80,80	0
55	MG	13	1700	1/1	0.40	0.34	-	97,97,97,97	0
55	MG	14	3291	1/1	0.65	0.21	-	82,82,82,82	0
55	MG	1H	3265	1/1	0.77	0.17	-	83,83,83,83	0
55	MG	1G	1631	1/1	0.97	0.27	-	90,90,90,90	0
55	MG	14	3405	1/1	0.97	0.07	-	64,64,64,64	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	3150	1/1	0.82	0.39	-	78,78,78,78	0
55	MG	45	201	1/1	0.81	0.33	-	76,76,76,76	0
55	MG	1G	1617	1/1	0.93	0.38	-	71,71,71,71	0
55	MG	1H	3352	1/1	0.71	0.35	-	97,97,97,97	0
55	MG	1H	3124	1/1	0.85	0.33	-	59,59,59,59	0
55	MG	13	1613	1/1	0.84	0.29	-	99,99,99,99	0
55	MG	1H	3108	1/1	0.90	0.38	-	77,77,77,77	0
55	MG	13	1620	1/1	0.92	0.36	-	66,66,66,66	0
55	MG	1H	3115	1/1	0.94	0.27	-	51,51,51,51	0
55	MG	1G	1736	1/1	0.97	0.11	-	94,94,94,94	0
55	MG	1H	3335	1/1	0.90	0.40	-	70,70,70,70	0
55	MG	14	3012	1/1	0.98	0.30	-	53,53,53,53	0
55	MG	13	1669	1/1	0.94	0.46	-	77,77,77,77	0
55	MG	14	3399	1/1	0.96	0.07	-	82,82,82,82	0
55	MG	1G	1659	1/1	0.91	0.20	-	107,107,107,107	0
55	MG	14	3359	1/1	0.93	0.10	-	89,89,89,89	0
55	MG	1H	3426	1/1	0.99	0.10	-	67,67,67,67	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
55	MG	1J	209	1/1	0.86	0.09	-	128,128,128,128	0
55	MG	14	3334	1/1	0.91	0.24	-	84,84,84,84	0
55	MG	29	301	1/1	0.96	0.25	-	72,72,72,72	0
55	MG	13	1668	1/1	0.70	0.42	-	102,102,102,102	0
55	MG	1G	1704	1/1	0.86	0.23	-	117,117,117,117	0
55	MG	1G	1636	1/1	0.73	0.32	-	80,80,80,80	0
55	MG	1G	1748	1/1	0.80	0.25	-	90,90,90,90	0
55	MG	1H	3359	1/1	0.85	0.14	-	77,77,77,77	0
55	MG	13	1652	1/1	0.88	0.30	-	88,88,88,88	0
55	MG	14	3177	1/1	0.91	0.38	-	76,76,76,76	0
55	MG	14	3343	1/1	0.86	0.30	-	86,86,86,86	0
55	MG	14	3092	1/1	0.92	0.48	-	70,70,70,70	0
55	MG	14	3204	1/1	0.95	0.36	-	70,70,70,70	0
55	MG	14	3035	1/1	0.98	0.37	-	57,57,57,57	0
55	MG	1H	3198	1/1	0.97	0.42	-	77,77,77,77	0
55	MG	14	3174	1/1	0.60	0.36	-	107,107,107,107	0
55	MG	14	3194	1/1	0.96	0.13	-	46,46,46,46	0
55	MG	1G	1726	1/1	0.64	0.44	-	124,124,124,124	0
55	MG	14	3173	1/1	0.93	0.30	-	70,70,70,70	0
55	MG	14	3113	1/1	0.54	0.35	-	97,97,97,97	0
55	MG	14	3235	1/1	0.76	0.14	-	63,63,63,63	0
55	MG	14	3333	1/1	0.90	0.15	-	89,89,89,89	0
55	MG	1H	3116	1/1	0.78	0.51	-	74,74,74,74	0
55	MG	14	3452	1/1	0.97	0.07	-	100,100,100,100	0
55	MG	13	1628	1/1	0.91	0.35	-	71,71,71,71	0
55	MG	14	3051	1/1	0.93	0.27	-	62,62,62,62	0
55	MG	1H	3032	1/1	0.84	0.35	-	95,95,95,95	0
55	MG	14	3146	1/1	0.95	0.39	-	64,64,64,64	0
55	MG	14	3347	1/1	0.98	0.17	-	83,83,83,83	0
55	MG	1G	1648	1/1	0.93	0.25	-	89,89,89,89	0
55	MG	1H	3174	1/1	0.82	0.27	-	89,89,89,89	0
55	MG	14	3139	1/1	0.92	0.39	-	69,69,69,69	0
55	MG	14	3147	1/1	0.80	0.39	-	83,83,83,83	0
55	MG	1G	1665	1/1	0.91	0.15	-	69,69,69,69	0
55	MG	1H	3492	1/1	0.98	0.11	-	83,83,83,83	0
55	MG	1G	1681	1/1	0.95	0.36	-	88,88,88,88	0
55	MG	14	3425	1/1	0.89	0.08	-	96,96,96,96	0
55	MG	1H	3415	1/1	0.99	0.13	-	50,50,50,50	0
55	MG	14	3122	1/1	0.97	0.25	-	61,61,61,61	0
55	MG	2L	104	1/1	0.87	0.07	-	93,93,93,93	0
55	MG	1H	3474	1/1	0.98	0.10	-	79,79,79,79	0
55	MG	1H	3140	1/1	0.77	0.20	-	52,52,52,52	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
55	MG	1G	1747	1/1	0.95	0.26	-	86,86,86,86	0
55	MG	1H	3499	1/1	0.85	0.09	-	111,111,111,111	0
55	MG	1G	1683	1/1	0.75	0.31	-	103,103,103,103	0
55	MG	1H	3462	1/1	0.99	0.14	-	49,49,49,49	0
55	MG	1G	1722	1/1	0.72	0.15	-	91,91,91,91	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	3519	1/1	0.82	0.09	-	103,103,103,103	0
55	MG	13	1695	1/1	0.67	0.26	-	90,90,90,90	0
55	MG	1H	3121	1/1	0.61	0.25	-	98,98,98,98	0
55	MG	14	3458	1/1	0.94	0.10	-	108,108,108,108	0
55	MG	13	1729	1/1	0.96	0.07	-	112,112,112,112	0
55	MG	1G	1628	1/1	0.97	0.20	-	90,90,90,90	0
55	MG	1H	3077	1/1	0.95	0.28	-	59,59,59,59	0
55	MG	14	3010	1/1	0.97	0.21	-	47,47,47,47	0
55	MG	14	3307	1/1	0.76	0.27	-	89,89,89,89	0
55	MG	14	3249	1/1	0.94	0.24	-	87,87,87,87	0
55	MG	29	302	1/1	0.97	0.26	-	51,51,51,51	0
55	MG	1H	3003	1/1	0.99	0.34	-	54,54,54,54	0
55	MG	1H	3131	1/1	0.89	0.33	-	75,75,75,75	0
55	MG	14	3332	1/1	0.94	0.26	-	83,83,83,83	0
55	MG	14	3196	1/1	0.88	0.10	-	60,60,60,60	0
55	MG	14	3159	1/1	0.47	0.38	-	85,85,85,85	0
55	MG	1H	3123	1/1	0.97	0.14	-	78,78,78,78	0
55	MG	1H	3476	1/1	0.92	0.16	-	59,59,59,59	0
55	MG	14	3096	1/1	0.76	0.36	-	94,94,94,94	0
55	MG	1G	1625	1/1	0.96	0.30	-	85,85,85,85	0
55	MG	14	3419	1/1	0.97	0.06	-	94,94,94,94	0
55	MG	1H	3344	1/1	0.84	0.32	-	84,84,84,84	0
55	MG	1H	3141	1/1	0.90	0.24	-	65,65,65,65	0
55	MG	1H	3253	1/1	0.75	0.30	-	71,71,71,71	0
55	MG	14	3094	1/1	0.91	0.34	-	81,81,81,81	0
55	MG	1G	1697	1/1	0.94	0.41	-	85,85,85,85	0
55	MG	14	3002	1/1	0.99	0.23	-	67,67,67,67	0
55	MG	14	3222	1/1	0.92	0.28	-	79,79,79,79	0
55	MG	14	3153	1/1	0.94	0.44	-	82,82,82,82	0
55	MG	14	3369	1/1	0.89	0.21	-	78,78,78,78	0
55	MG	13	1644	1/1	0.68	0.44	-	116,116,116,116	0
55	MG	16	207	1/1	0.88	0.46	-	85,85,85,85	0
55	MG	14	3053	1/1	0.99	0.33	-	59,59,59,59	0
55	MG	1H	3264	1/1	0.97	0.40	-	100,100,100,100	0
55	MG	1H	3293	1/1	0.78	0.34	-	95,95,95,95	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
55	MG	14	3301	1/1	0.54	0.40	-	82,82,82,82	0
55	MG	14	3208	1/1	0.87	0.23	-	88,88,88,88	0
55	MG	1H	3508	1/1	0.84	0.06	-	119,119,119,119	0
55	MG	14	3317	1/1	0.83	0.36	-	83,83,83,83	0
55	MG	1H	3362	1/1	0.90	0.41	-	103,103,103,103	0
55	MG	1G	1627	1/1	0.84	0.46	-	93,93,93,93	0
55	MG	1H	3249	1/1	0.97	0.53	-	66,66,66,66	0
55	MG	13	1702	1/1	0.83	0.24	-	147,147,147,147	0
55	MG	1H	3325	1/1	0.81	0.39	-	97,97,97,97	0
55	MG	1G	1702	1/1	0.48	0.21	-	95,95,95,95	0
55	MG	1H	3120	1/1	0.71	0.23	-	69,69,69,69	0
55	MG	14	3077	1/1	0.99	0.30	-	61,61,61,61	0
55	MG	1H	3209	1/1	0.54	0.49	-	99,99,99,99	0
55	MG	1G	1692	1/1	0.71	0.33	-	120,120,120,120	0
55	MG	1H	3225	1/1	0.96	0.46	-	77,77,77,77	0
55	MG	1G	1678	1/1	0.86	0.35	-	102,102,102,102	0
55	MG	14	3124	1/1	0.91	0.19	-	56,56,56,56	0
55	MG	14	3186	1/1	0.75	0.33	-	113,113,113,113	0
55	MG	1H	3332	1/1	0.88	0.47	-	87,87,87,87	0
55	MG	1H	3395	1/1	0.95	0.41	-	76,76,76,76	0

6.5 Other polymers

There are no such residues in this entry.