



wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 20, 2016 – 02:20 AM GMT

PDB ID : 4WR6
Title : Complex of 70S ribosome with tRNA-Tyr and mRNA with A-A mismatch in the first position in the A-site.
Authors : Rozov, A.; Demeshkina, N.; Yusupov, M.; Yusupova, G.
Deposited on : 2014-10-23
Resolution : 3.05 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 : 1.7.1 (RC1), CSD as537be (2016)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026982
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
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-20026982

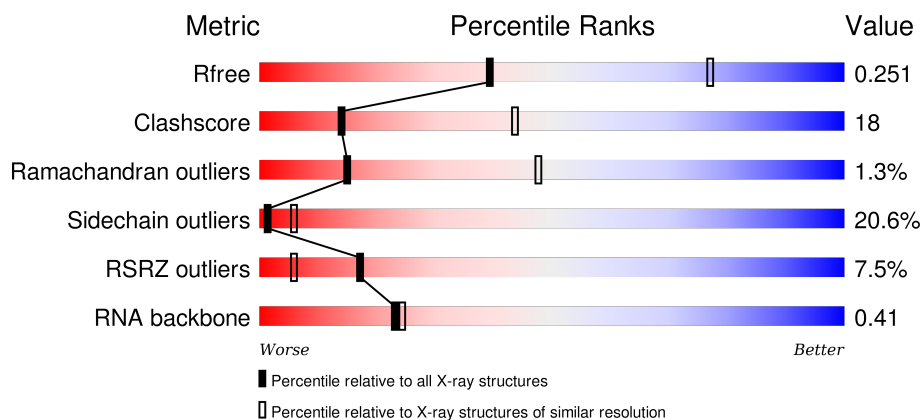
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.05 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}	91344	1191 (3.10-3.02)
Clashscore	102246	1303 (3.10-3.02)
Ramachandran outliers	100387	1254 (3.10-3.02)
Sidechain outliers	100360	1254 (3.10-3.02)
RSRZ outliers	91569	1197 (3.10-3.02)
RNA backbone	2183	1035 (3.50-2.62)

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>2%</div> <div>30% 46% 19% . .</div> </div>
2	12	256	<div> <div>3%</div> <div>37% 42% 14% 7%</div> </div>
2	1E	256	<div> <div>2%</div> <div>42% 40% 11% 7%</div> </div>
3	22	239	<div> <div>8%</div> <div>36% 41% 9% 14%</div> </div>

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Mol	Chain	Length	Quality of chain
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	
15	6I	89	

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Mol	Chain	Length	Quality of chain
16	7A	88	
16	7I	88	
17	8A	105	
17	8I	105	
18	9A	88	
18	9I	88	
19	AA	93	
19	AI	93	
20	BA	106	
20	BI	106	
21	1B	27	
21	1F	27	
22	1K	85	
22	3K	85	
23	2K	77	
24	4K	27	
25	14	2917	
25	1H	2917	
26	16	122	
26	1J	122	
27	11	276	
27	19	276	
28	21	206	
28	29	206	
29	31	210	

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Mol	Chain	Length	Quality of chain
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	
39	B8	146	
40	85	118	
40	C8	118	
41	95	101	
41	D8	101	

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Mol	Chain	Length	Quality of chain
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	
52	L5	49	
52	P8	49	
53	M5	65	
53	Q8	65	
54	1G	1522	

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Mol	Chain	Length	Quality of chain
55	1L	85	
55	3L	85	
56	2L	77	
57	4L	27	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
58	MG	13	1618	-	-	-	X
58	MG	13	1629	-	-	-	X
58	MG	13	1636	-	-	-	X
58	MG	13	1657	-	-	-	X
58	MG	13	1661	-	-	-	X
58	MG	13	1664	-	-	-	X
58	MG	13	1695	-	-	-	X
58	MG	13	1705	-	-	-	X
58	MG	13	1718	-	-	-	X
58	MG	14	3022	-	-	-	X
58	MG	14	3038	-	-	-	X
58	MG	14	3065	-	-	-	X
58	MG	14	3072	-	-	-	X
58	MG	14	3073	-	-	-	X
58	MG	14	3074	-	-	-	X
58	MG	14	3087	-	-	-	X
58	MG	14	3148	-	-	-	X
58	MG	14	3149	-	-	-	X
58	MG	14	3160	-	-	-	X
58	MG	14	3172	-	-	-	X
58	MG	14	3176	-	-	-	X
58	MG	14	3186	-	-	-	X
58	MG	14	3187	-	-	-	X
58	MG	14	3217	-	-	-	X
58	MG	14	3222	-	-	-	X
58	MG	14	3227	-	-	-	X
58	MG	14	3244	-	-	-	X
58	MG	14	3247	-	-	-	X
58	MG	14	3274	-	-	-	X
58	MG	14	3281	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
58	MG	14	3303	-	-	-	X
58	MG	14	3316	-	-	-	X
58	MG	14	3319	-	-	-	X
58	MG	16	201	-	-	-	X
58	MG	16	206	-	-	-	X
58	MG	16	211	-	-	-	X
58	MG	1G	1647	-	-	-	X
58	MG	1G	1665	-	-	-	X
58	MG	1H	3007	-	-	-	X
58	MG	1H	3016	-	-	-	X
58	MG	1H	3025	-	-	-	X
58	MG	1H	3043	-	-	-	X
58	MG	1H	3051	-	-	-	X
58	MG	1H	3053	-	-	-	X
58	MG	1H	3054	-	-	-	X
58	MG	1H	3055	-	-	-	X
58	MG	1H	3066	-	-	-	X
58	MG	1H	3070	-	-	-	X
58	MG	1H	3081	-	-	-	X
58	MG	1H	3085	-	-	-	X
58	MG	1H	3090	-	-	-	X
58	MG	1H	3100	-	-	-	X
58	MG	1H	3121	-	-	-	X
58	MG	1H	3154	-	-	-	X
58	MG	1H	3161	-	-	-	X
58	MG	1H	3162	-	-	-	X
58	MG	1H	3164	-	-	-	X
58	MG	1H	3166	-	-	-	X
58	MG	1H	3188	-	-	-	X
58	MG	1H	3197	-	-	-	X
58	MG	1H	3199	-	-	-	X
58	MG	1H	3204	-	-	-	X
58	MG	1H	3206	-	-	-	X
58	MG	1H	3220	-	-	-	X
58	MG	1H	3231	-	-	-	X
58	MG	1H	3238	-	-	-	X
58	MG	1H	3258	-	-	-	X
58	MG	1H	3261	-	-	-	X
58	MG	1H	3263	-	-	-	X
58	MG	1H	3288	-	-	-	X
58	MG	1H	3292	-	-	-	X
58	MG	1H	3299	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
58	MG	1H	3331	-	-	-	X
58	MG	1H	3338	-	-	-	X
58	MG	1H	3342	-	-	-	X
58	MG	1H	3347	-	-	-	X
58	MG	1H	3350	-	-	-	X
58	MG	1H	3356	-	-	-	X
58	MG	2K	103	-	-	-	X
59	ZN	3E	302	-	-	-	X

2 Entry composition

There are 60 unique types of molecules in this entry. The entry contains 299318 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	1498	Total	C	N	O	P	0	0	0
			32207	14334	5973	10402	1498			

- 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			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
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			
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	119	Total	C	N	O	S	0	0	0
			884	549	168	164	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.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
14	5I	61	Total	C	N	O	S	0	0	0
			498	316	105	72	5			
14	5A	58	Total	C	N	O	S	0	0	0
			475	303	99	69	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	69	Total	C	N	O		0	0	0
			564	361	110	93				

- 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	82	Total	C	N	O	S	0	0	0
			640	407	118	113	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	22	Total	C	N	O		0	0	0
			188	116	44	28				

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
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	1K	85	Total	C	N	O	P	S	0	0	0
			1825	822	323	593	85	2			
22	3K	85	Total	C	N	O	P	S	0	0	0
			1825	822	323	593	85	2			

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

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

- Molecule 24 is a RNA chain called mRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
24	4K	15	Total	C	N	O	P	0	1	0
			349	158	75	100	16			

- Molecule 25 is a RNA chain called 23S ribosomal RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
25	1H	2912	Total	C	N	O	P	0	0	0
			62707	27911	11722	20163	2911			
25	14	2907	Total	C	N	O	P	0	0	0
			62605	27865	11708	20126	2906			

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 26 is a RNA chain called 5S ribosomal RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
26	16	122	Total	C	N	O	P	0	0	0
			2617	1166	486	844	121			
26	1J	122	Total	C	N	O	P	0	0	0
			2617	1166	486	844	121			

- 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			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
31	59	171	Total	C	N	O	S	0	0	0
			1316	835	247	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			
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	138	Total	C	N	O	S	0	0	0
			1098	702	208	181	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	136	Total	C	N	O	0	0	0
			1133	705	233	195			
39	75	137	Total	C	N	O	S	0	0
			1141	710	234	196	1		

- 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	94	Total	C	N	O	S	0	0	0
			742	482	134	125	1			
43	B5	92	Total	C	N	O		0	0	0
			725	471	131	123				

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
44	G8	102	Total	C	N	O	S	0	0	0
			778	501	147	125	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	77	Total	C	N	O	S	0	0	0
			612	379	129	103	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	93	Total	C	N	O	S	0	0	0
			729	457	145	126	1			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
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	66	Total	C	N	O	S	0	0	0
			558	346	113	98	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	49	Total	C	N	O	S	0	0	0
			374	232	76	61	5			
51	J5	58	Total	C	N	O	S	0	0	0
			453	285	89	74	5			

- Molecule 52 is a protein called 50S ribosomal protein L34.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
52	P8	45	Total	C	N	O	S	0	0	0
			391	240	97	52	2			
52	L5	45	Total	C	N	O	S	0	0	0
			391	240	97	52	2			

- Molecule 53 is a protein called 50S ribosomal protein L35.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
53	Q8	62	Total	C	N	O	S	0	0	0
			448	284	86	76	2			
53	M5	60	Total	C	N	O	S	0	0	0
			480	306	98	74	2			

- Molecule 54 is a RNA chain called 16S ribosomal RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
54	1G	1498	Total	C	N	O	P	0	0	0
			32204	14334	5973	10400	1497			

- Molecule 55 is a RNA chain called tRNA-Tyr.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
55	1L	85	Total	C	N	O	P	0	0	0
			1807	807	323	592	85			
55	3L	85	Total	C	N	O	P	0	0	0
			1807	807	323	592	85			

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

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

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
2L	18	C	U	conflict	GB 675817920

- Molecule 57 is a RNA chain called mRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
57	4L	16	Total	C	N	O	P	0	0	0
			349	158	75	100	16			

- Molecule 58 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
58	98	2	Total	Mg	0	0
			2	2		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
58	45	1	Total 1	Mg 1	0	0
58	P8	1	Total 1	Mg 1	0	0
58	85	1	Total 1	Mg 1	0	0
58	C5	1	Total 1	Mg 1	0	0
58	13	138	Total 138	Mg 138	0	0
58	1J	6	Total 6	Mg 6	0	0
58	16	13	Total 13	Mg 13	0	0
58	25	1	Total 1	Mg 1	0	0
58	21	2	Total 2	Mg 2	0	0
58	31	4	Total 4	Mg 4	0	0
58	L8	2	Total 2	Mg 2	0	0
58	I8	2	Total 2	Mg 2	0	0
58	8E	1	Total 1	Mg 1	0	0
58	L5	1	Total 1	Mg 1	0	0
58	29	3	Total 3	Mg 3	0	0
58	2K	6	Total 6	Mg 6	0	0
58	1L	1	Total 1	Mg 1	0	0
58	39	1	Total 1	Mg 1	0	0
58	1G	90	Total 90	Mg 90	0	0
58	4E	1	Total 1	Mg 1	0	0
58	11	1	Total 1	Mg 1	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
58	1H	475	Total 475	Mg 475	0	0
58	3I	1	Total 1	Mg 1	0	0
58	14	398	Total 398	Mg 398	0	0
58	78	1	Total 1	Mg 1	0	0
58	3E	1	Total 1	Mg 1	0	0
58	3L	1	Total 1	Mg 1	0	0
58	1K	1	Total 1	Mg 1	0	0
58	2L	3	Total 3	Mg 3	0	0

- Molecule 59 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
59	32	1	Total 1	Zn 1	0	0
59	3E	1	Total 1	Zn 1	0	0
59	5I	1	Total 1	Zn 1	0	0
59	5A	1	Total 1	Zn 1	0	0
59	G8	1	Total 1	Zn 1	0	0
59	C5	1	Total 1	Zn 1	0	0

- Molecule 60 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
60	13	100	Total 100	O 100	0	0
60	3E	2	Total 2	O 2	0	0
60	3I	2	Total 2	O 2	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
60	5I	1	Total O 1 1	0	0
60	7I	1	Total O 1 1	0	0
60	1K	1	Total O 1 1	0	0
60	2K	6	Total O 6 6	0	0
60	4K	2	Total O 2 2	0	0
60	1H	538	Total O 538 538	0	0
60	16	11	Total O 11 11	0	0
60	11	4	Total O 4 4	0	0
60	21	2	Total O 2 2	0	0
60	31	4	Total O 4 4	0	0
60	78	4	Total O 4 4	0	0
60	D8	1	Total O 1 1	0	0
60	F8	1	Total O 1 1	0	0
60	L8	3	Total O 3 3	0	0
60	1G	51	Total O 51 51	0	0
60	32	1	Total O 1 1	0	0
60	BA	1	Total O 1 1	0	0
60	4L	1	Total O 1 1	0	0
60	14	409	Total O 409 409	0	0
60	19	7	Total O 7 7	0	0
60	29	2	Total O 2 2	0	0

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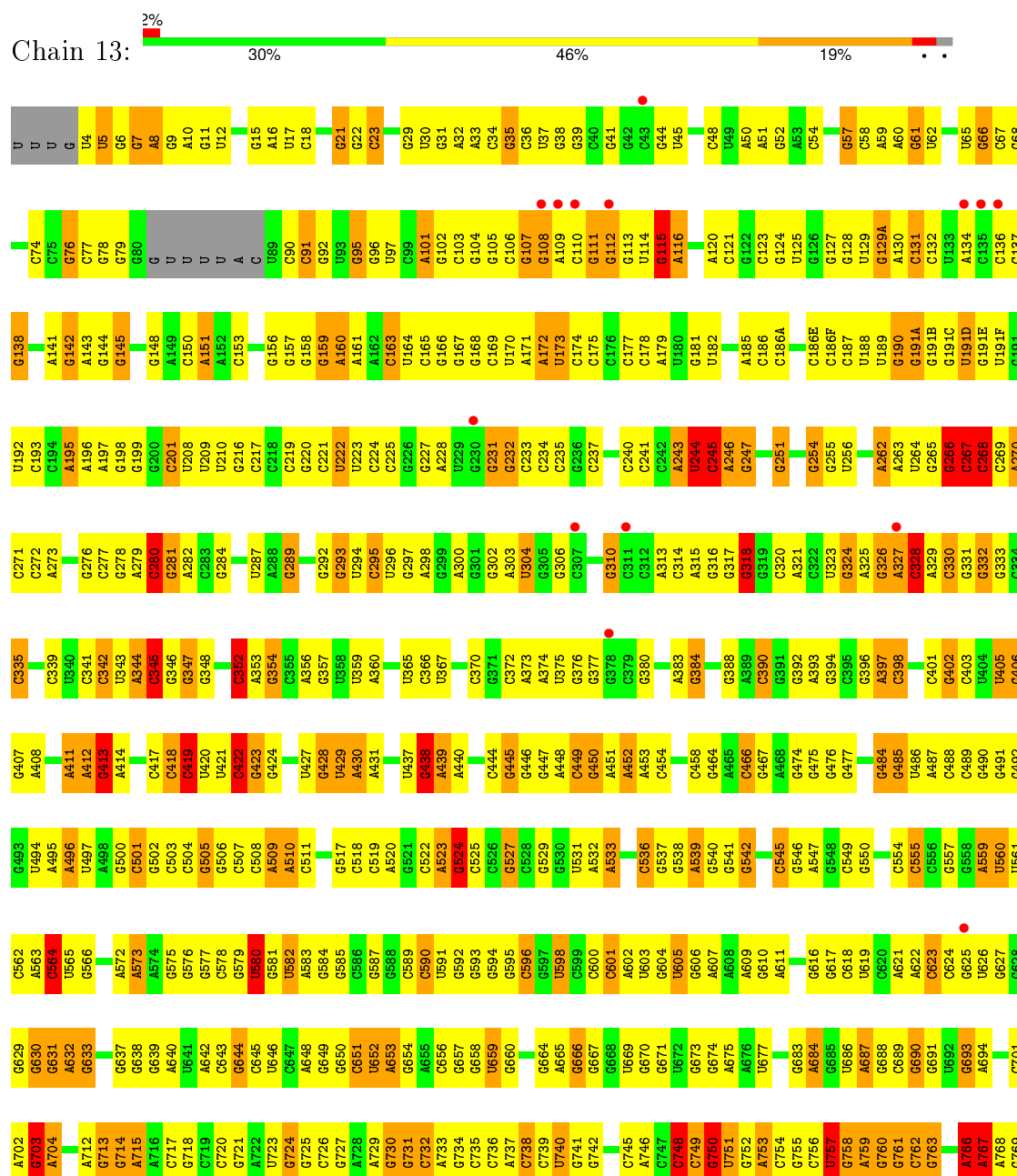
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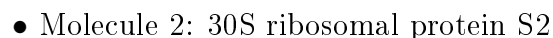
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
60	39	4	Total 4	O 4	0	0
60	35	1	Total 1	O 1	0	0
60	55	1	Total 1	O 1	0	0
60	75	1	Total 1	O 1	0	0
60	85	1	Total 1	O 1	0	0

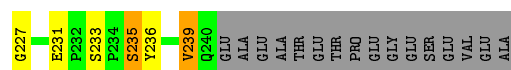
3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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 ($\text{RSRZ} > 2$). 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.

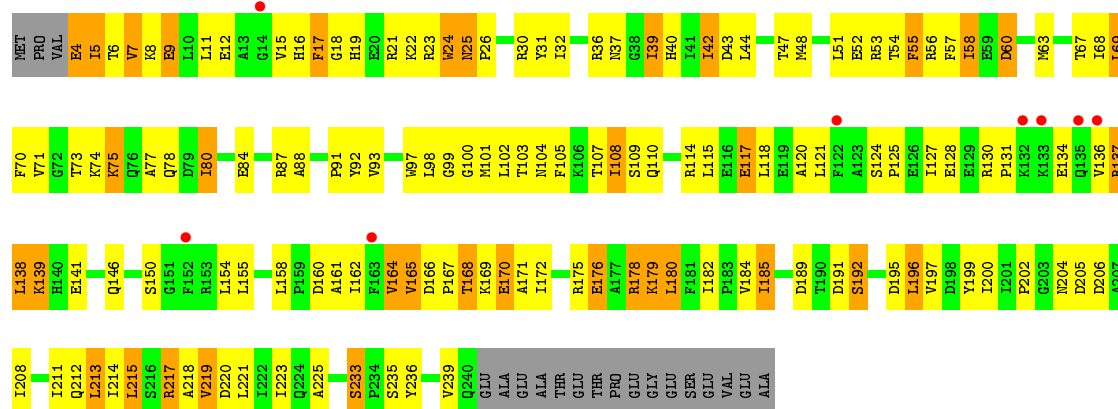
• Molecule 1: 16S ribosomal RNA



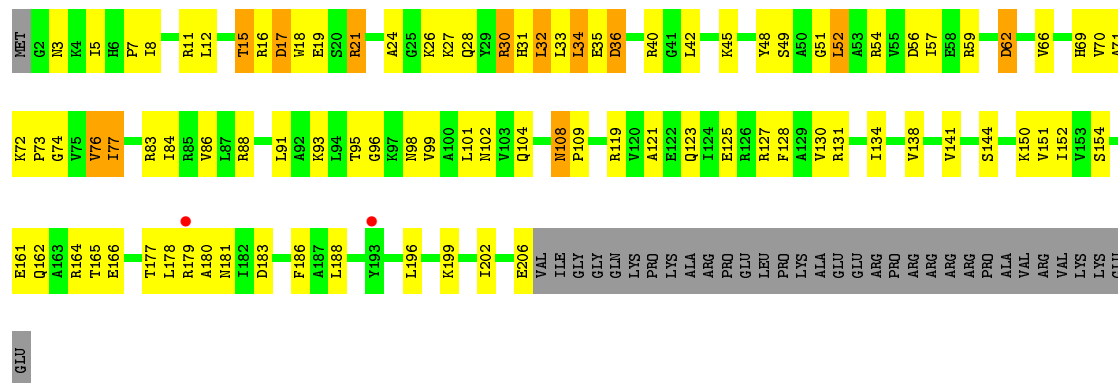




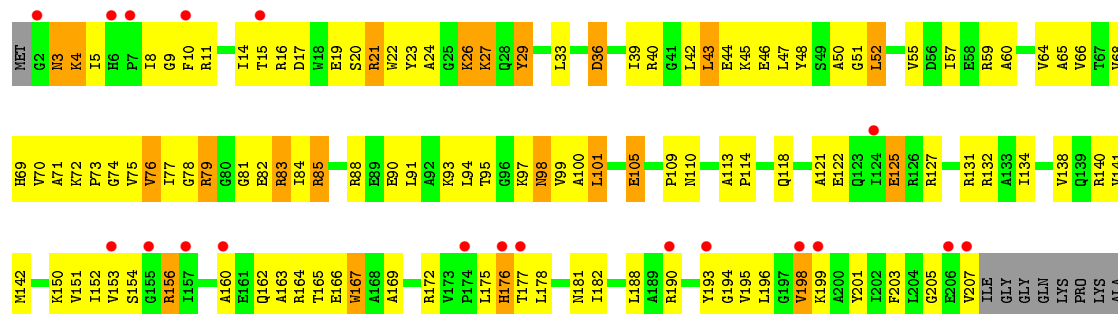
• Molecule 2: 30S ribosomal protein S2



• Molecule 3: 30S ribosomal protein S3

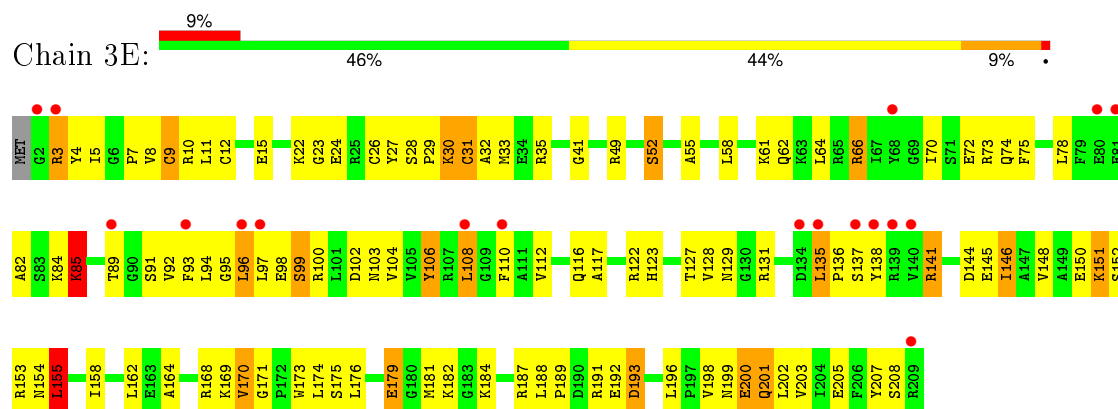


• Molecule 3: 30S ribosomal protein S3

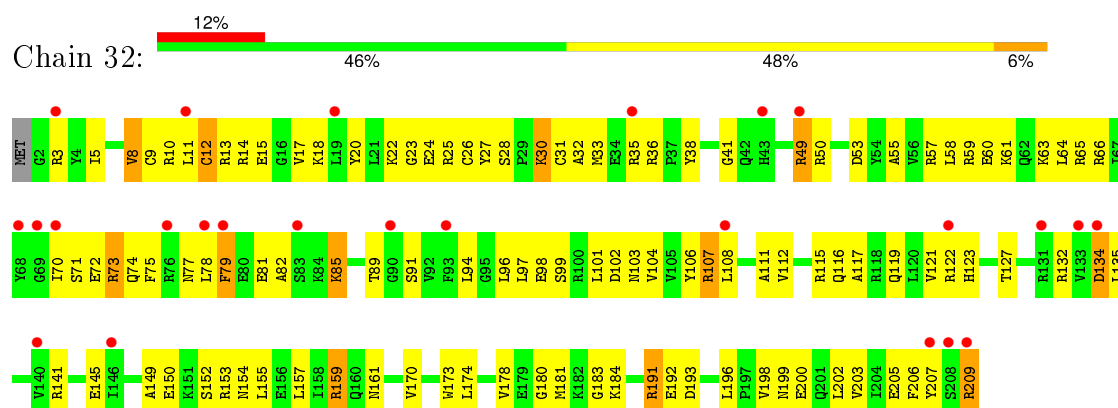


ARG
PRO
GLU
LEU
PRO
LYS
ALA
GLU
GLU
ARG
PRO
ARG
ARG
ARG
ARG
PRO
ALA
VAL
VAL
VAL
LYS
LYS
GLU
GLU

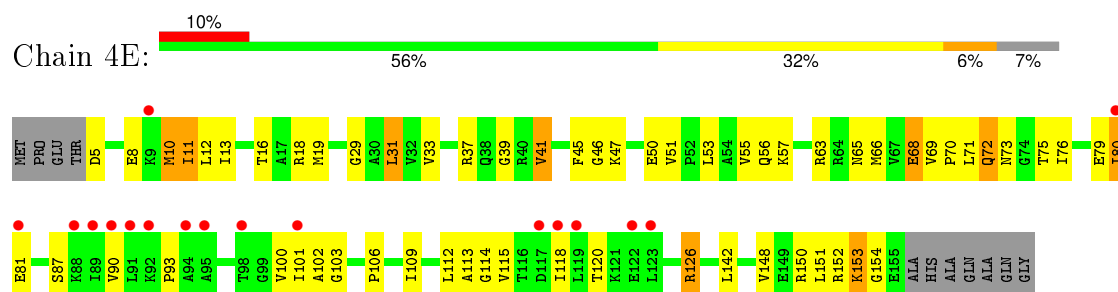
• Molecule 4: 30S ribosomal protein S4



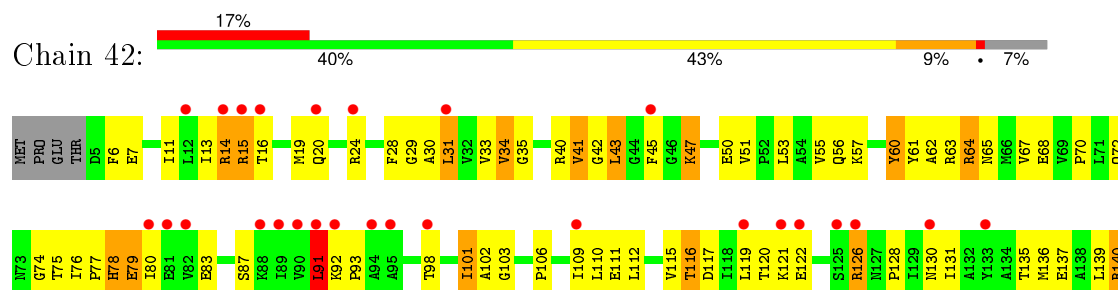
• Molecule 4: 30S ribosomal protein S4



• Molecule 5: 30S ribosomal protein S5

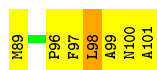
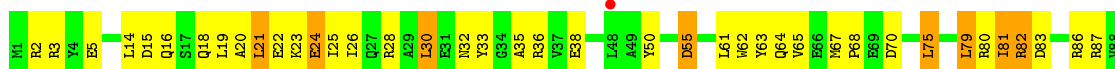


• Molecule 5: 30S ribosomal protein S5





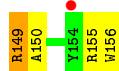
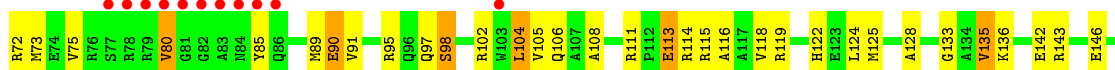
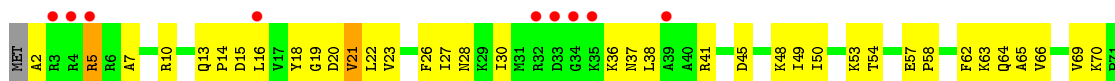
• Molecule 6: 30S ribosomal protein S6



• Molecule 6: 30S ribosomal protein S6



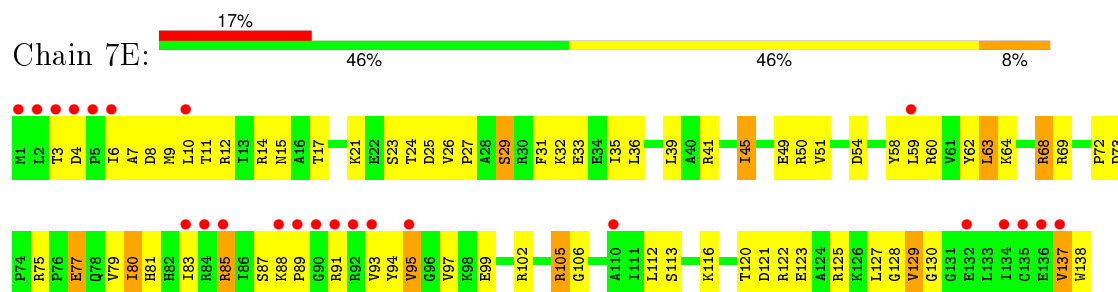
• Molecule 7: 30S ribosomal protein S7



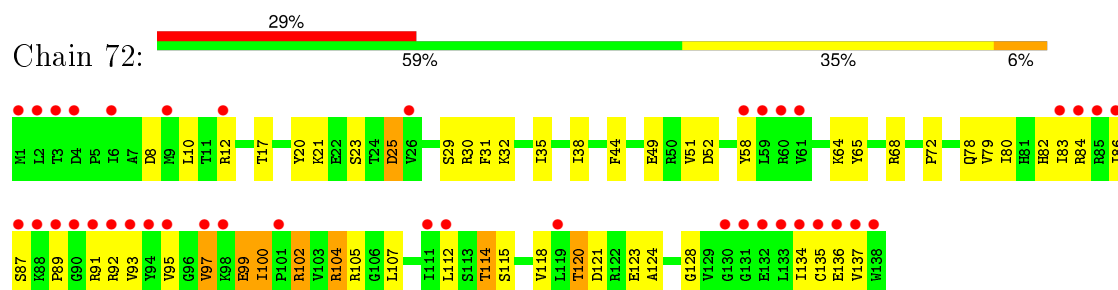
• Molecule 7: 30S ribosomal protein S7



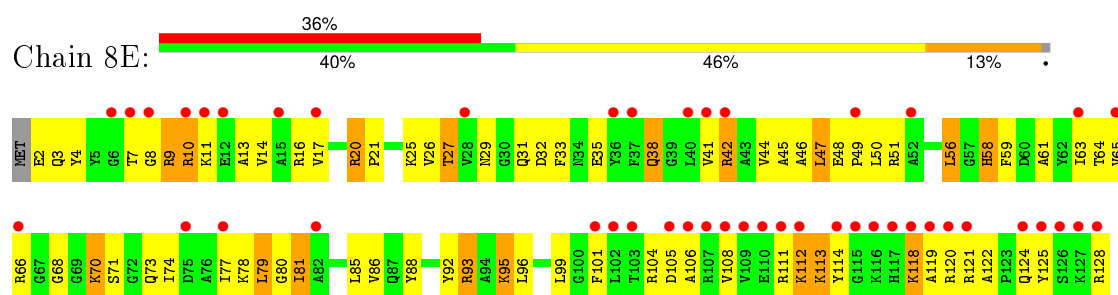
- Molecule 8: 30S ribosomal protein S8



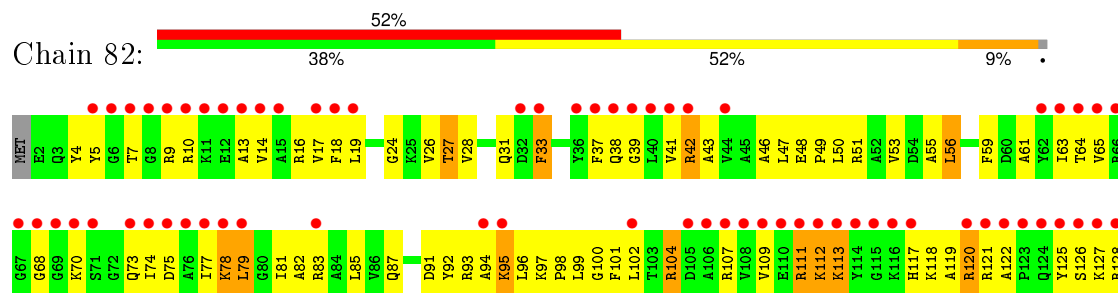
- Molecule 8: 30S ribosomal protein S8



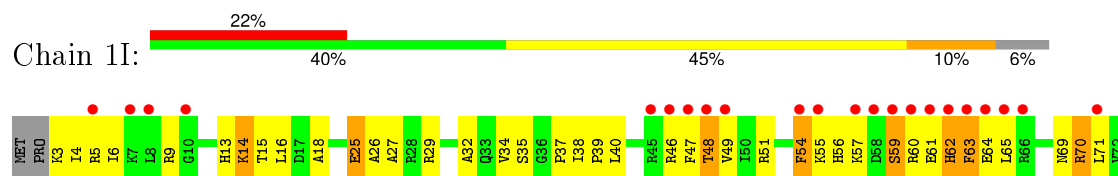
- Molecule 9: 30S ribosomal protein S9

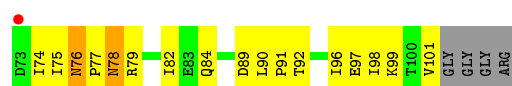


- Molecule 9: 30S ribosomal protein S9

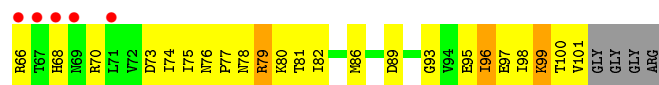
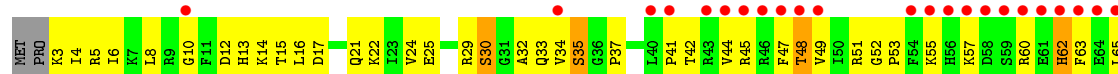


- Molecule 10: 30S ribosomal protein S10





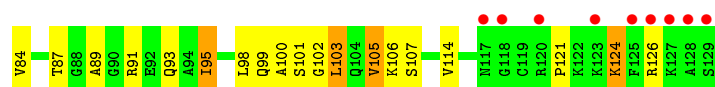
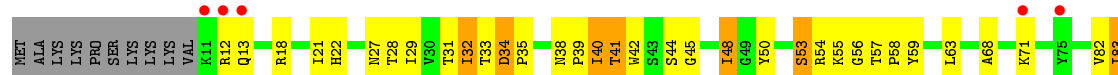
• Molecule 10: 30S ribosomal protein S10



• Molecule 11: 30S ribosomal protein S11



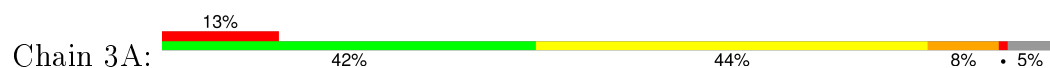
• Molecule 11: 30S ribosomal protein S11



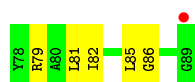
• Molecule 12: 30S ribosomal protein S12



• Molecule 12: 30S ribosomal protein S12



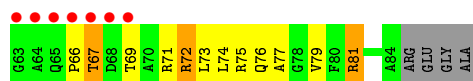
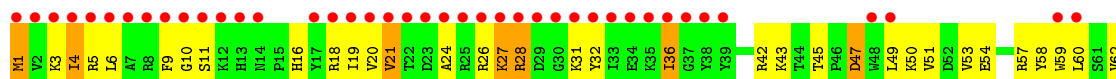




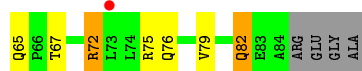
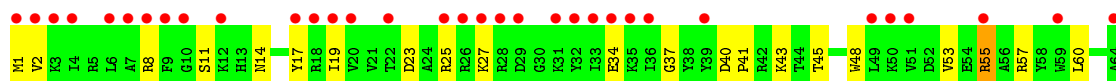
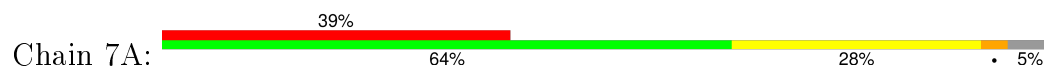
- Molecule 15: 30S ribosomal protein S15



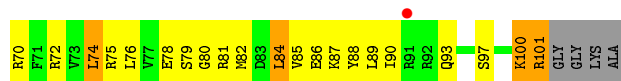
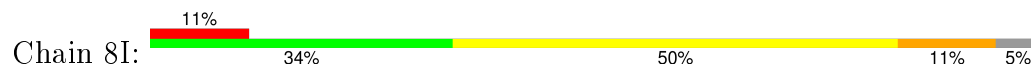
- Molecule 16: 30S ribosomal protein S16



- Molecule 16: 30S ribosomal protein S16

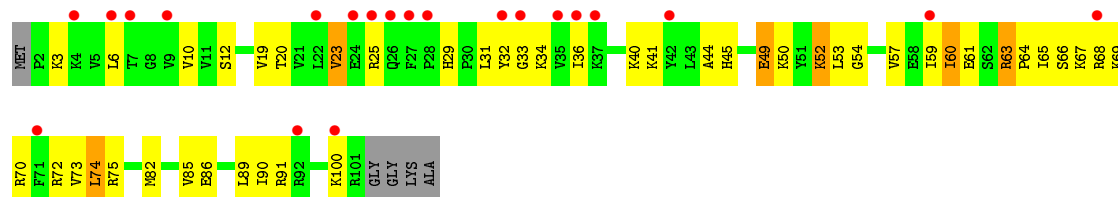


- Molecule 17: 30S ribosomal protein S17



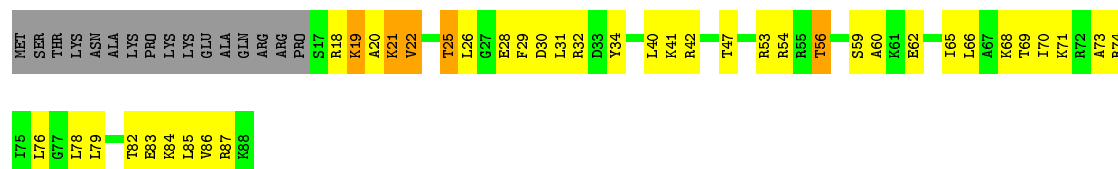
- Molecule 17: 30S ribosomal protein S17





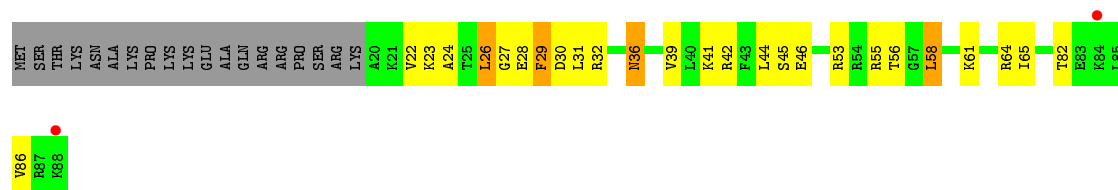
- Molecule 18: 30S ribosomal protein S18

Chain 9I: 36% 40% 6% 18%



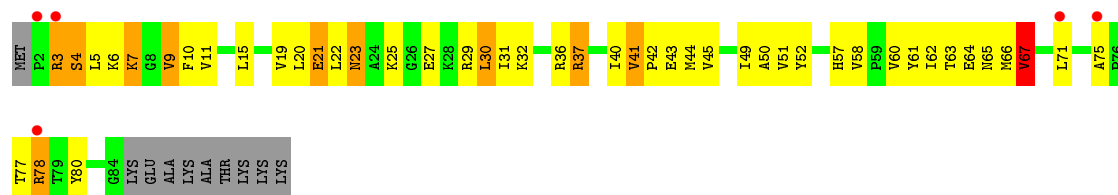
- Molecule 18: 30S ribosomal protein S18

Chain 9A: 2% 49% 25% 5% 22%



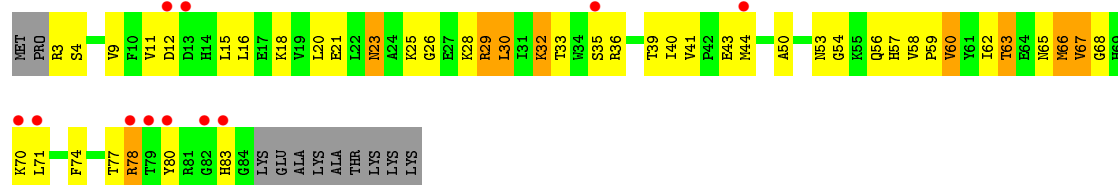
- Molecule 19: 30S ribosomal protein S19

Chain AI: 5% 39% 39% 11% 11%



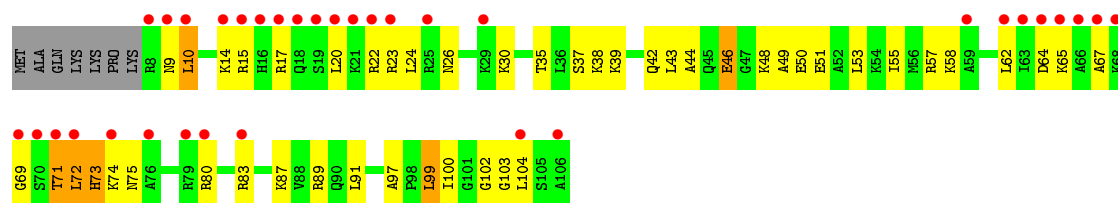
- Molecule 19: 30S ribosomal protein S19

Chain AA: 12% 39% 40% 10% 12%

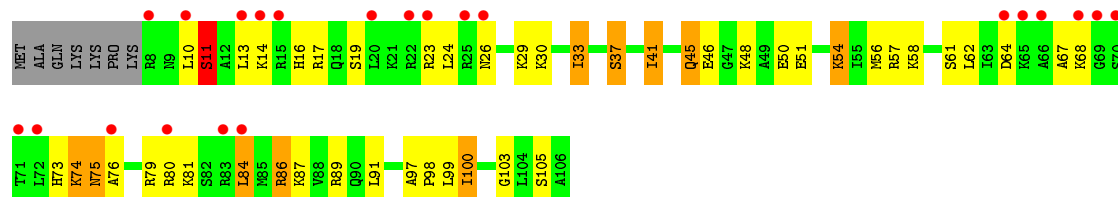


- Molecule 20: 30S ribosomal protein S20

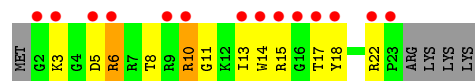
Chain BI: 32% 48% 40% 6% 7%



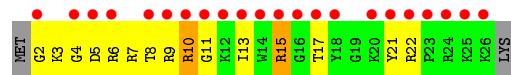
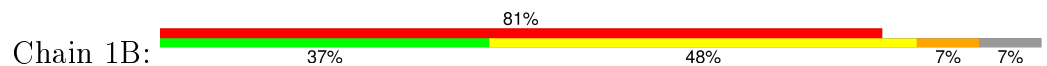
• Molecule 20: 30S ribosomal protein S20



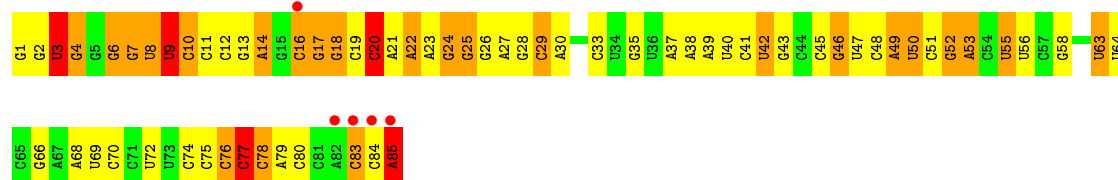
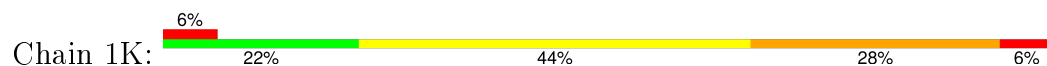
• Molecule 21: 30S ribosomal protein THX



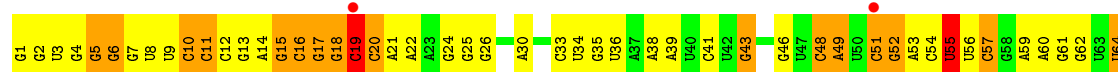
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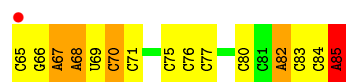


• Molecule 22: tRNA-Tyr

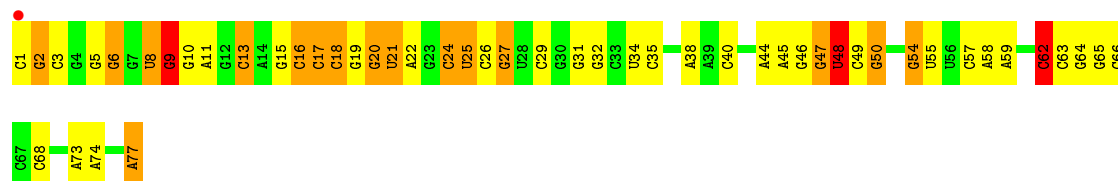


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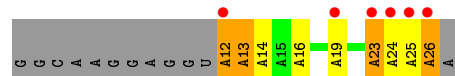




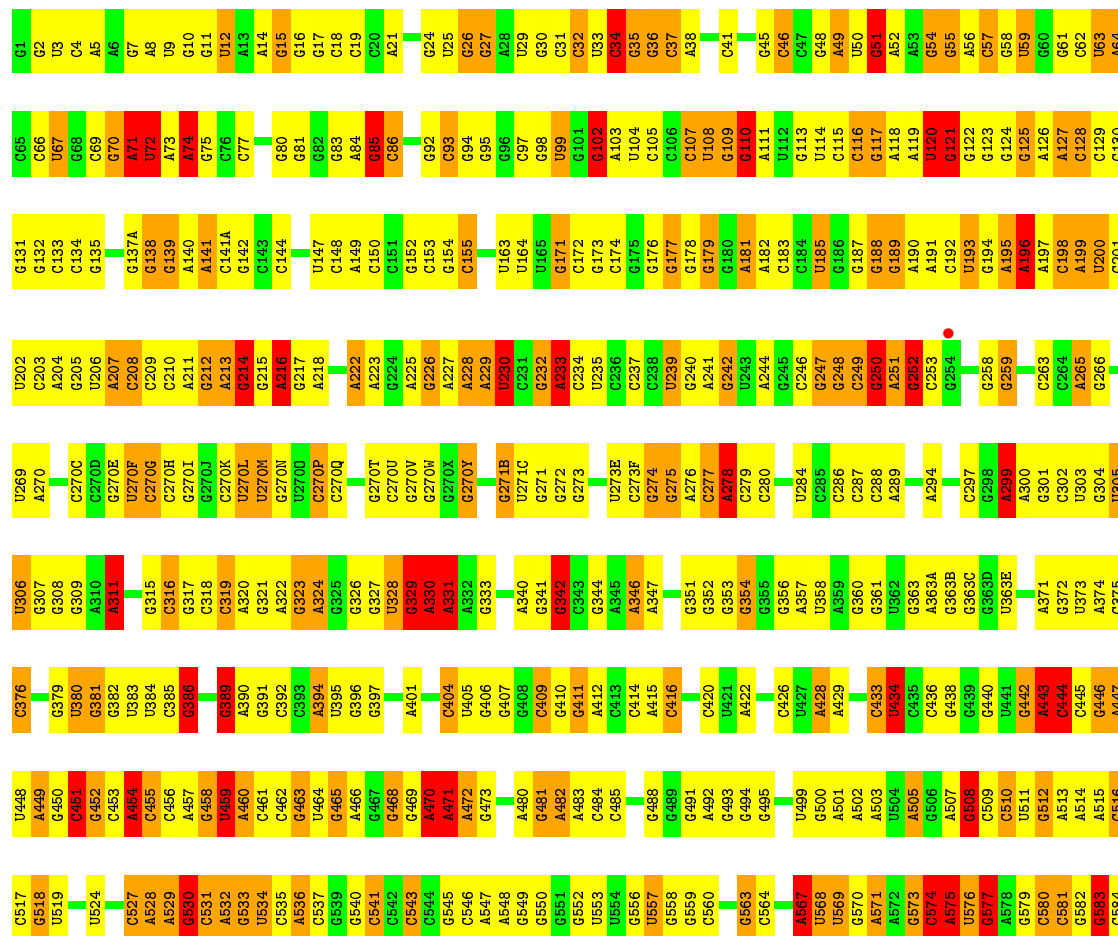
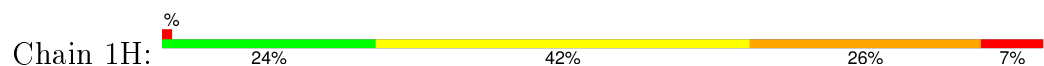
• Molecule 23: tRNA-fMet



• Molecule 24: mRNA

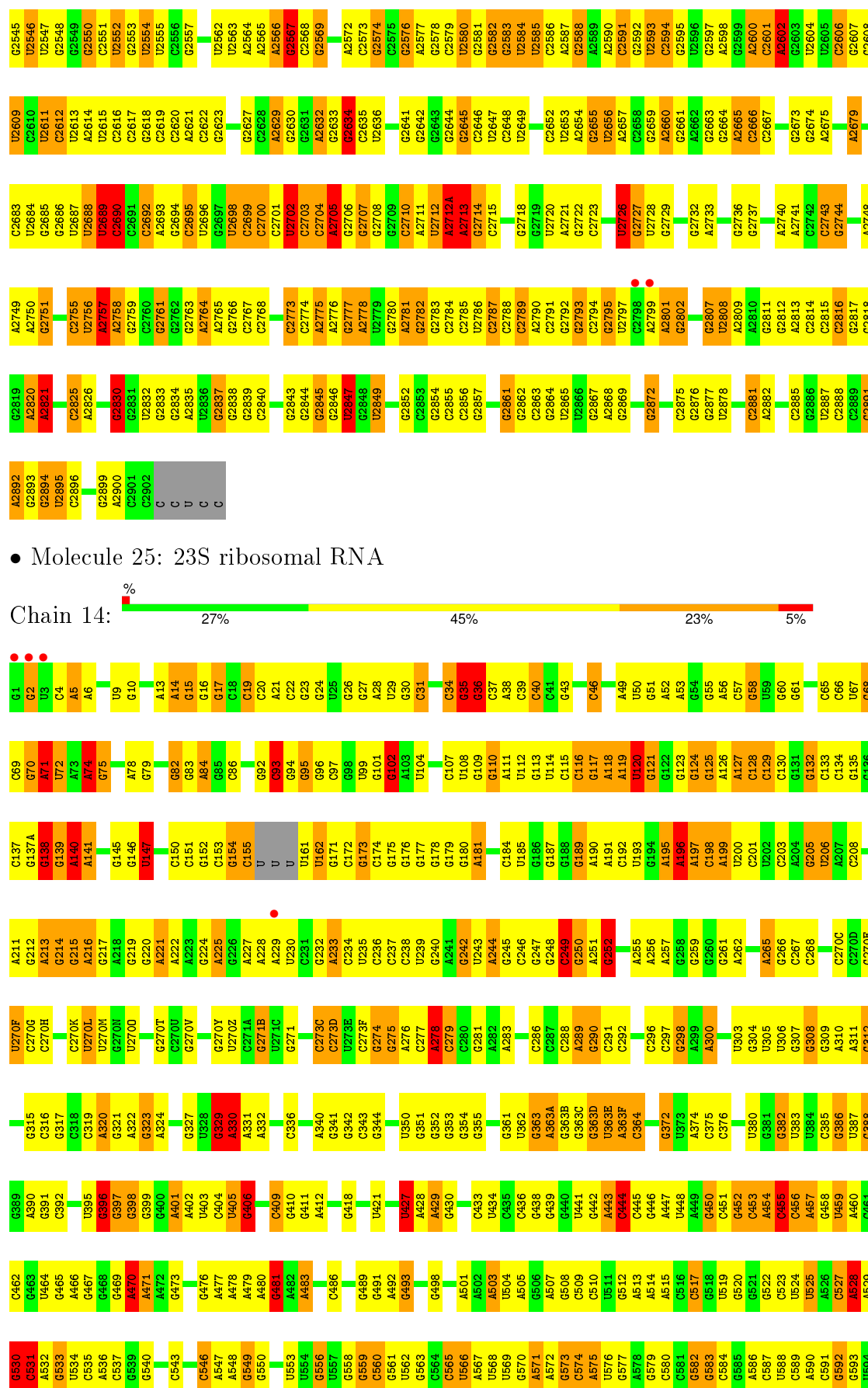


• Molecule 25: 23S ribosomal RNA



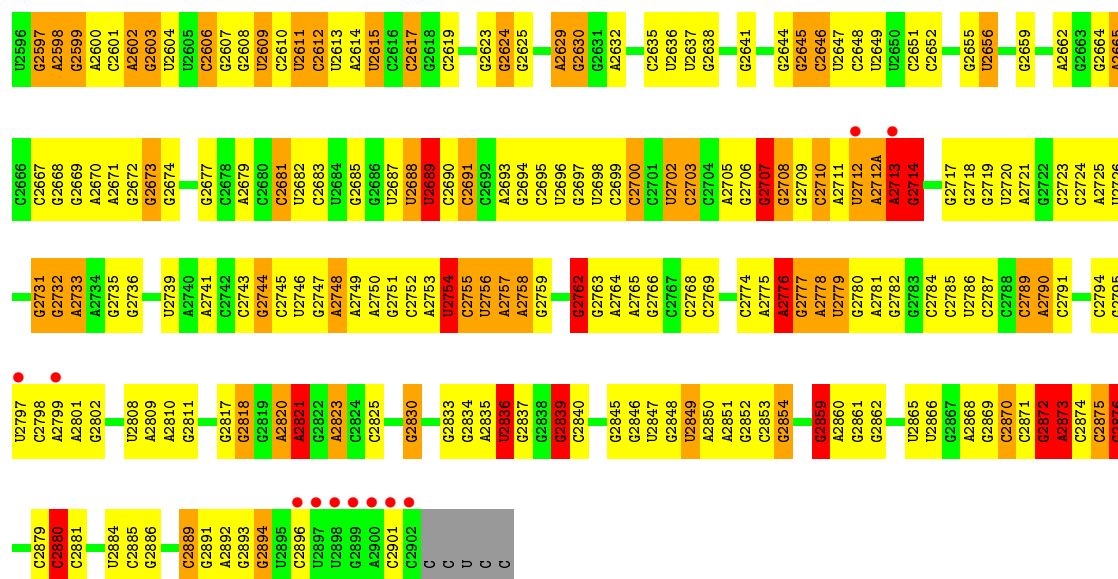
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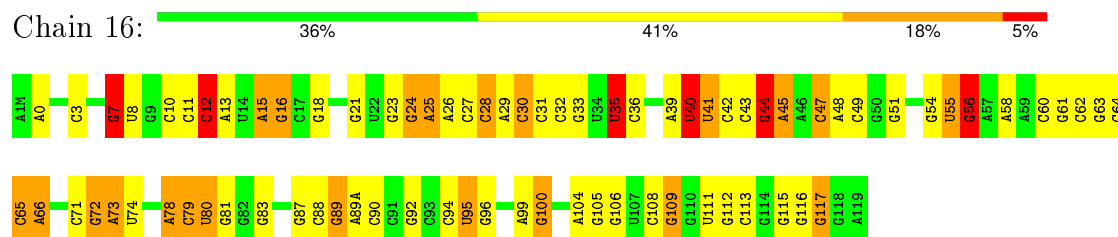


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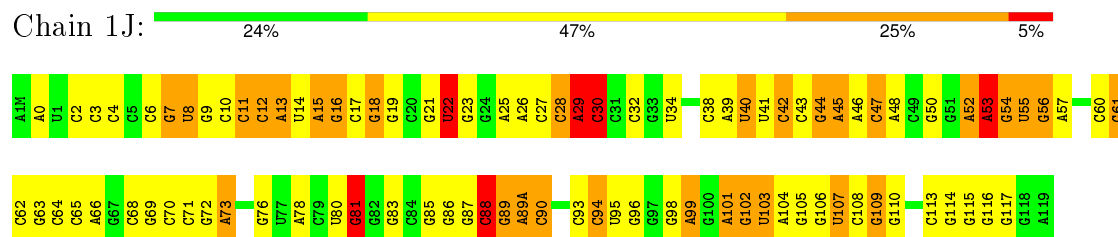




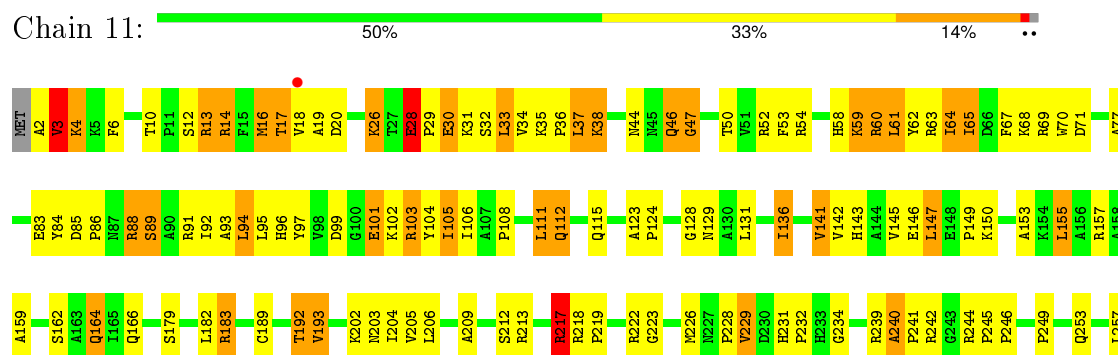
- Molecule 26: 5S ribosomal RNA

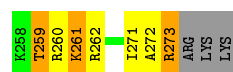


- Molecule 26: 5S ribosomal RNA

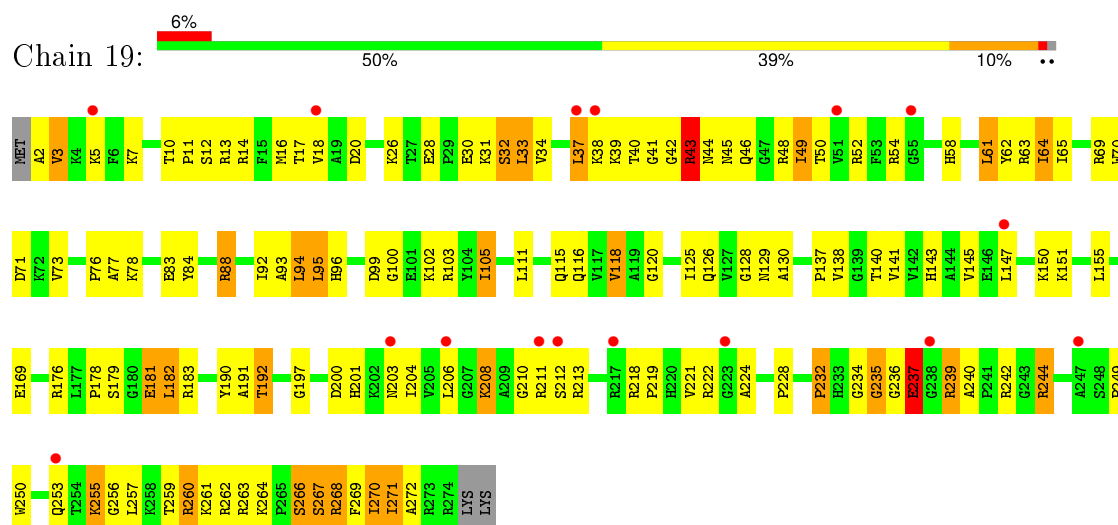


- Molecule 27: 50S ribosomal protein L2

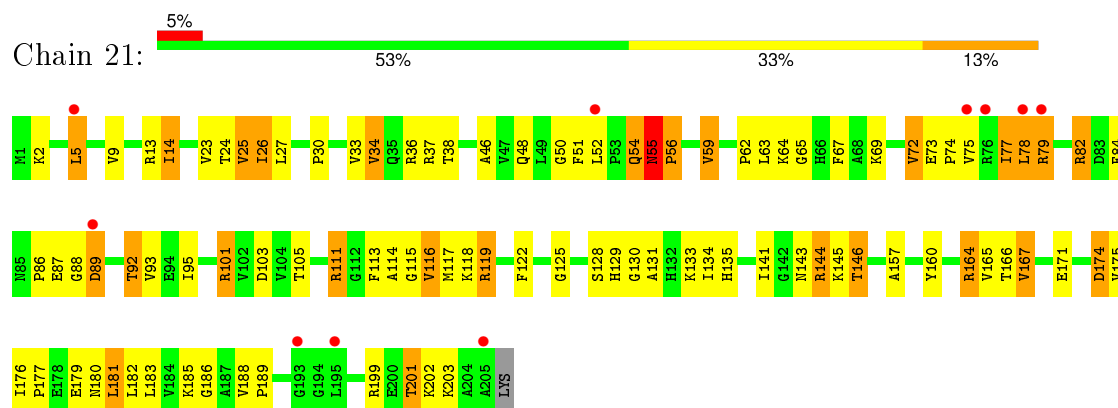




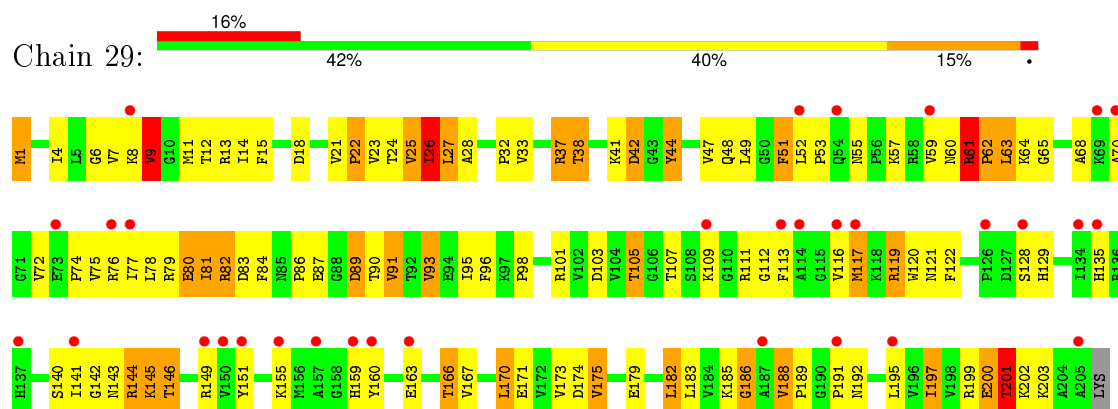
• Molecule 27: 50S ribosomal protein L2



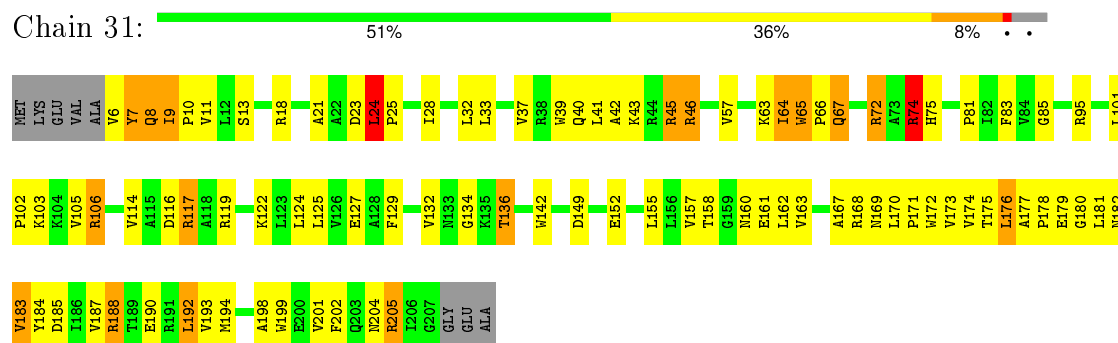
• Molecule 28: 50S ribosomal protein L3



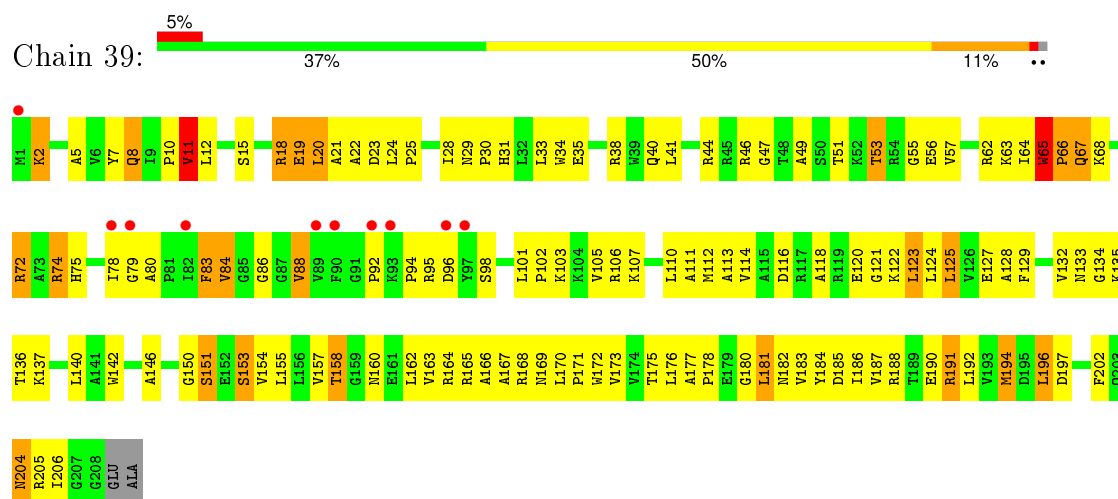
• Molecule 28: 50S ribosomal protein L3



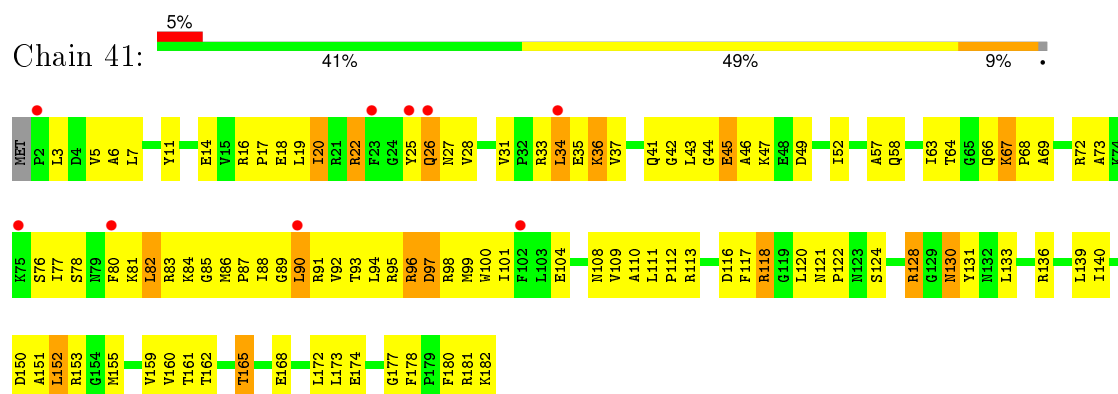
• Molecule 29: 50S ribosomal protein L4

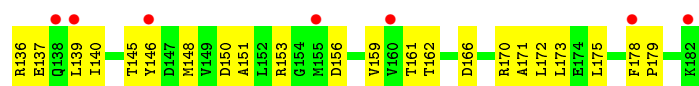


• Molecule 29: 50S ribosomal protein L4

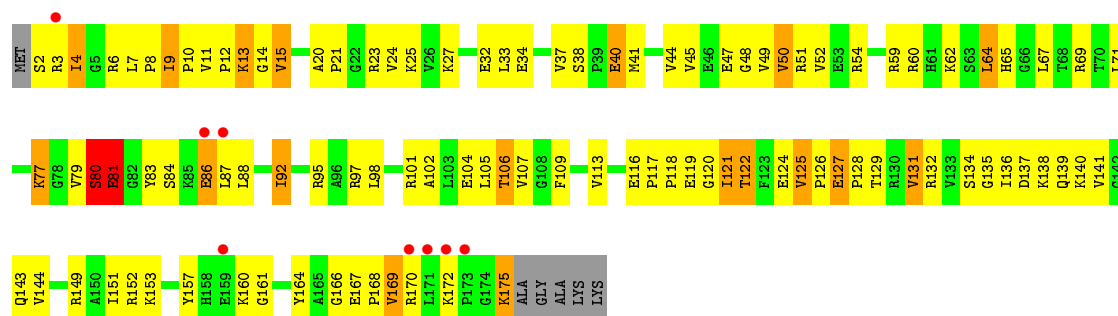


• Molecule 30: 50S ribosomal protein L5

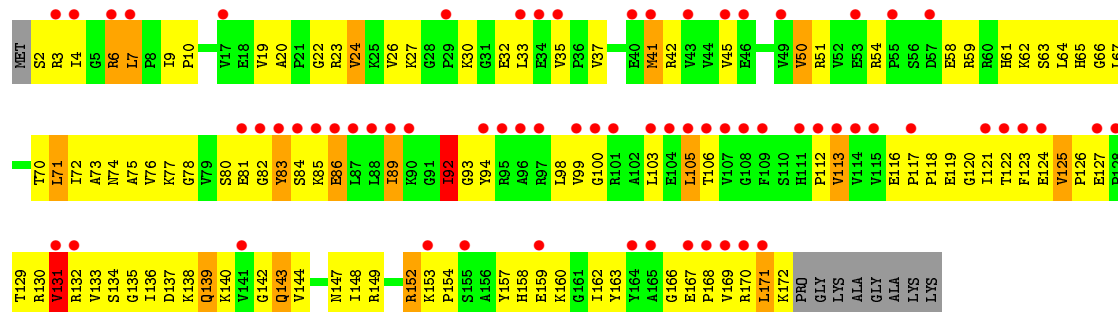




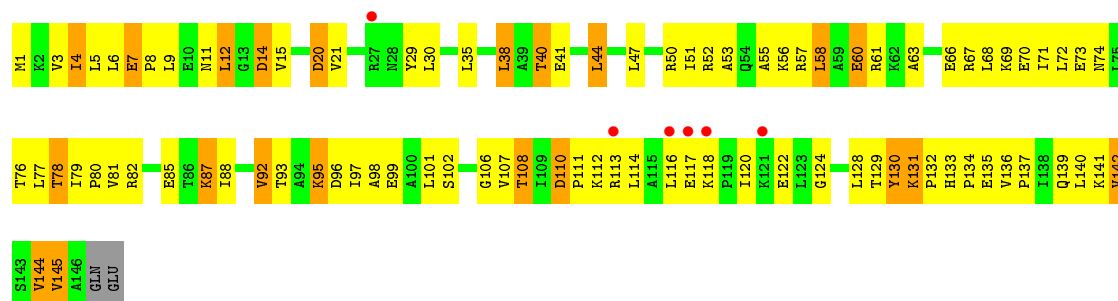
• Molecule 31: 50S ribosomal protein L6



• Molecule 31: 50S ribosomal protein L6

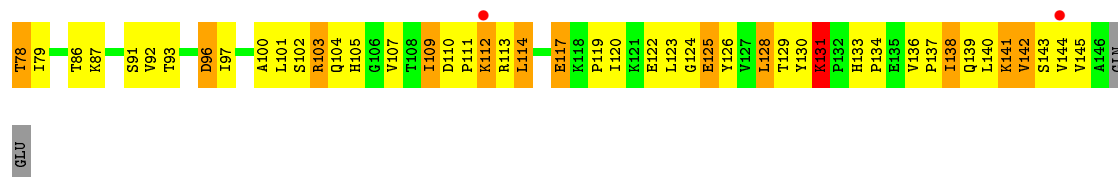


• Molecule 32: 50S ribosomal protein L9

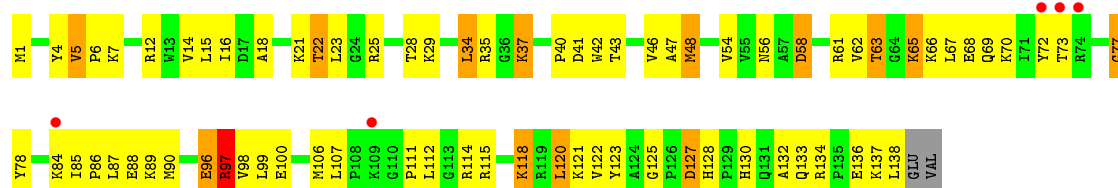


• Molecule 32: 50S ribosomal protein L9

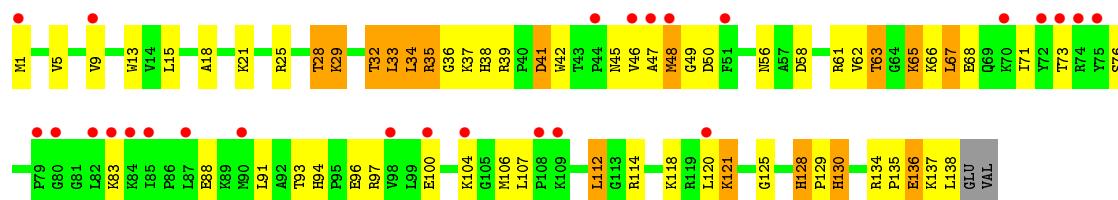




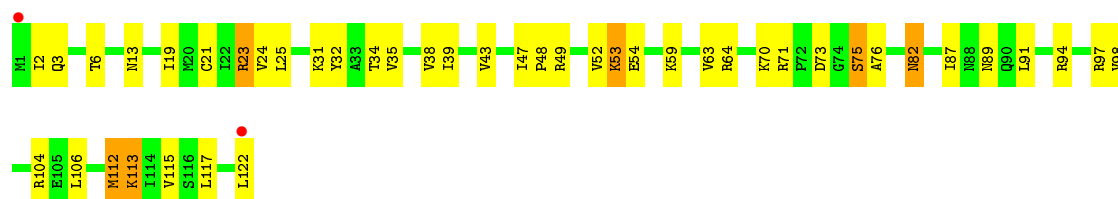
- Molecule 33: 50S ribosomal protein L13



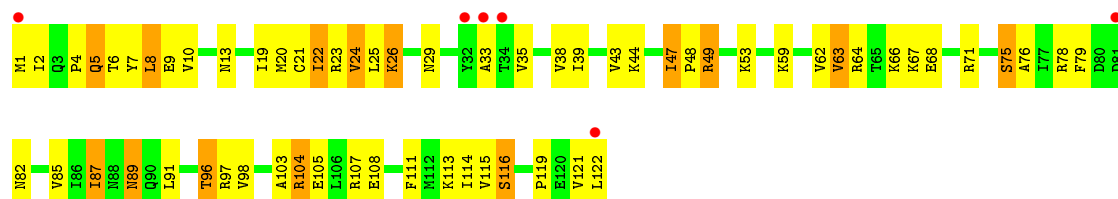
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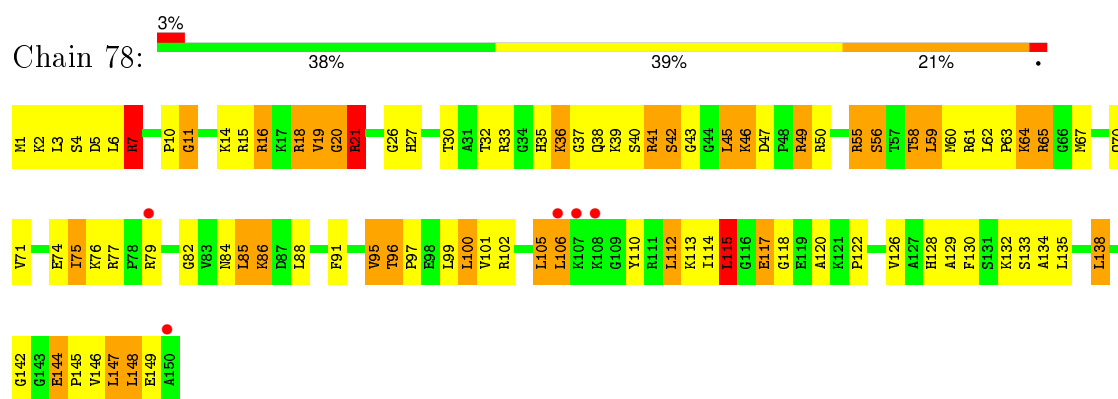
- Molecule 34: 50S ribosomal protein L14



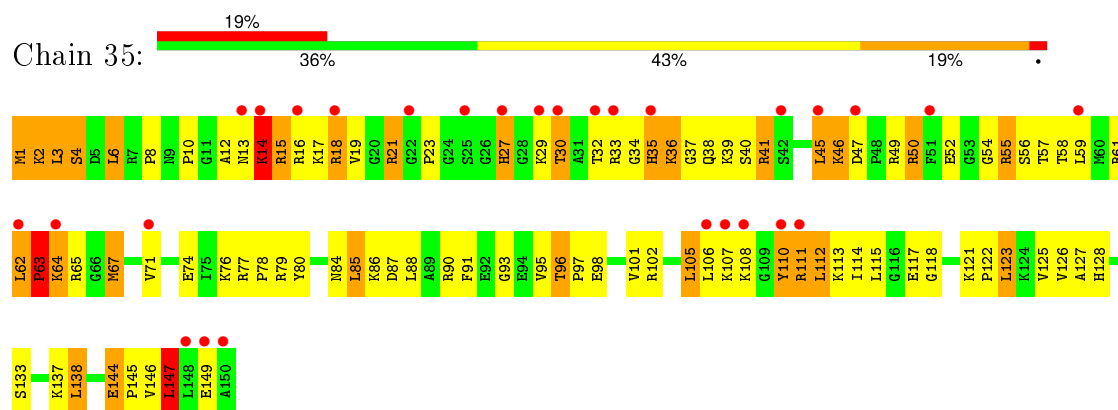
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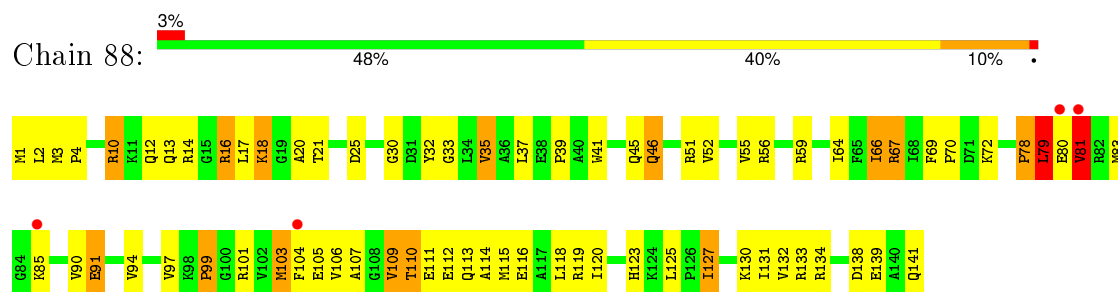
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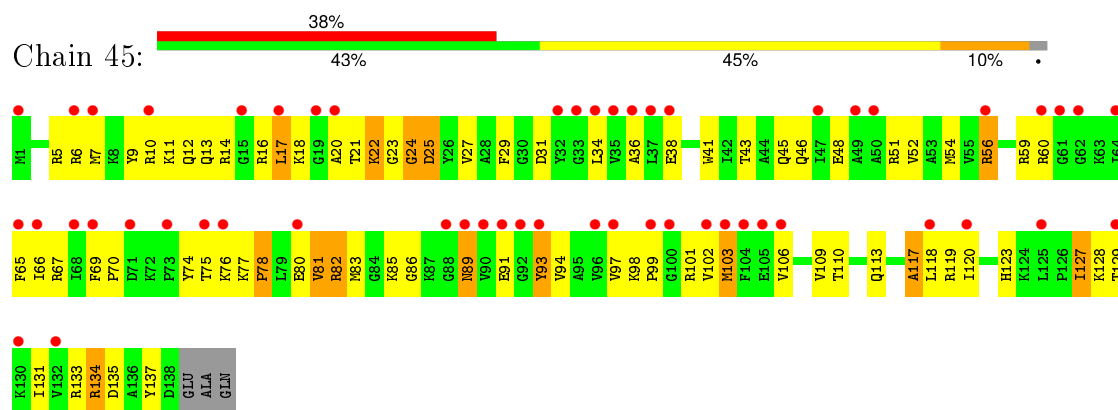
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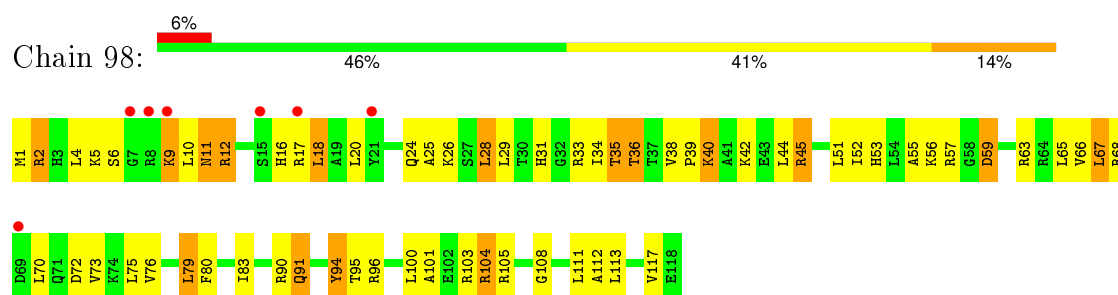
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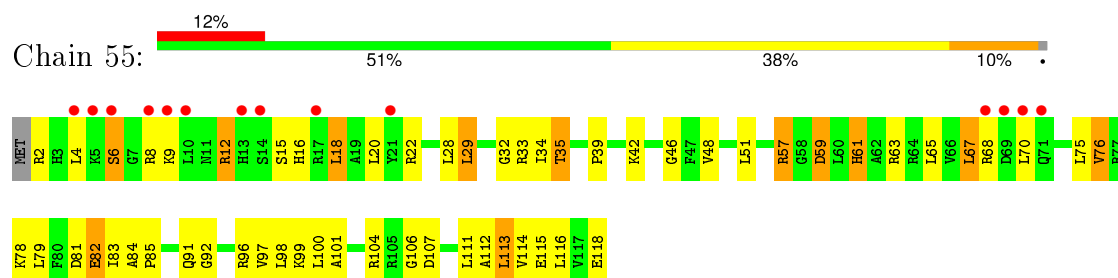
• Molecule 36: 50S ribosomal protein L16



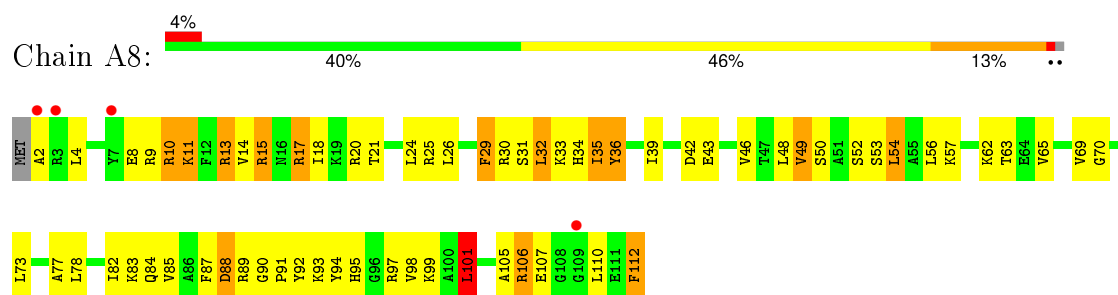
• Molecule 37: 50S ribosomal protein L17



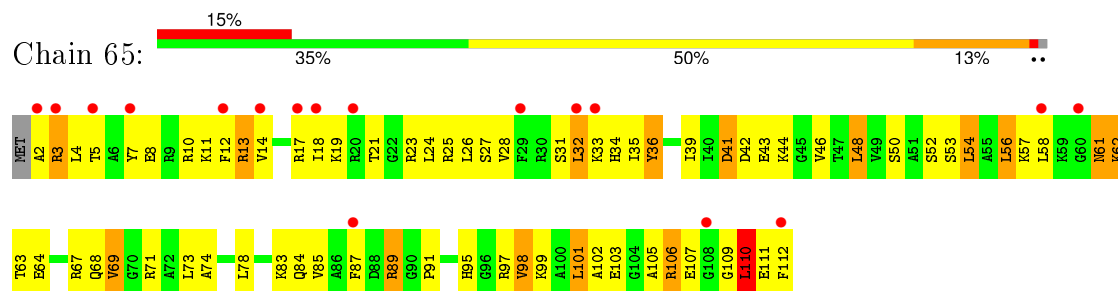
- Molecule 37: 50S ribosomal protein L17



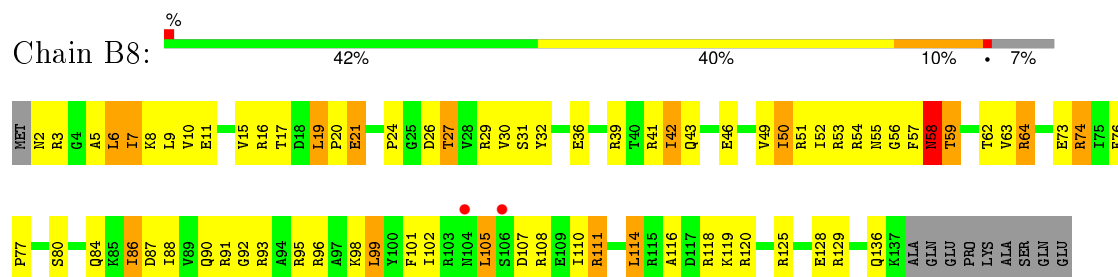
- Molecule 38: 50S ribosomal protein L18



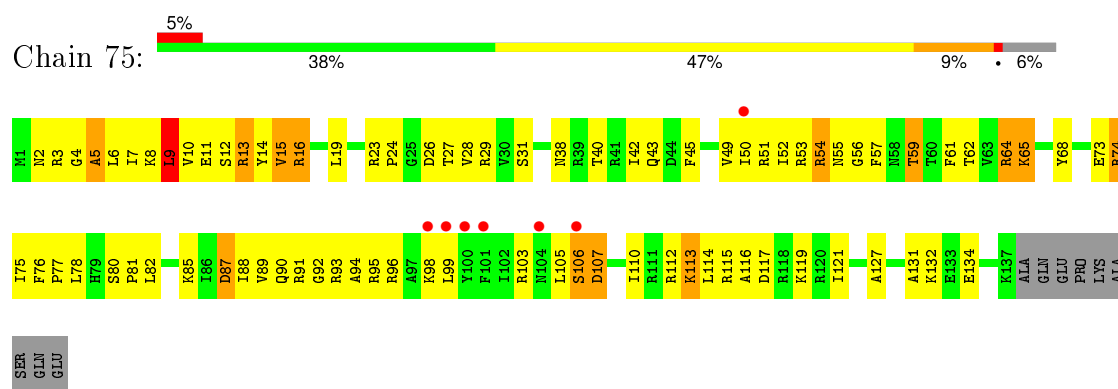
- Molecule 38: 50S ribosomal protein L18



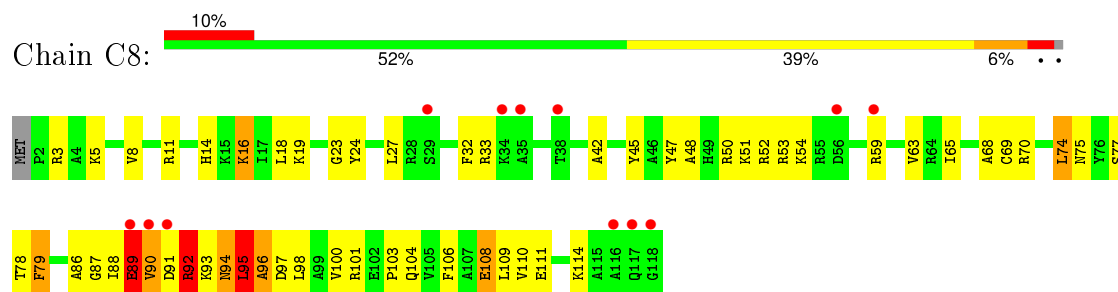
- Molecule 39: 50S ribosomal protein L19



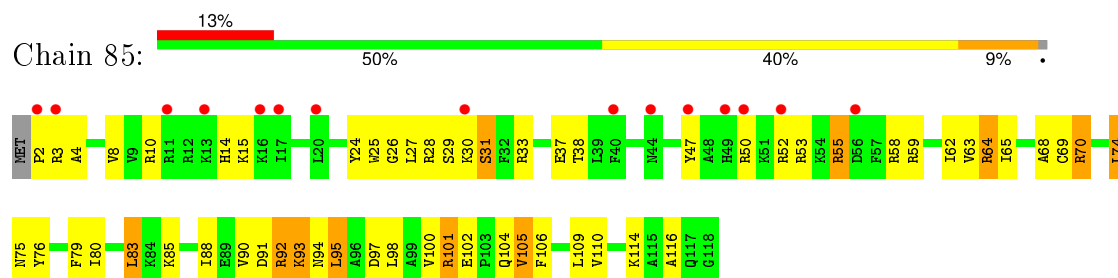
- Molecule 39: 50S ribosomal protein L19



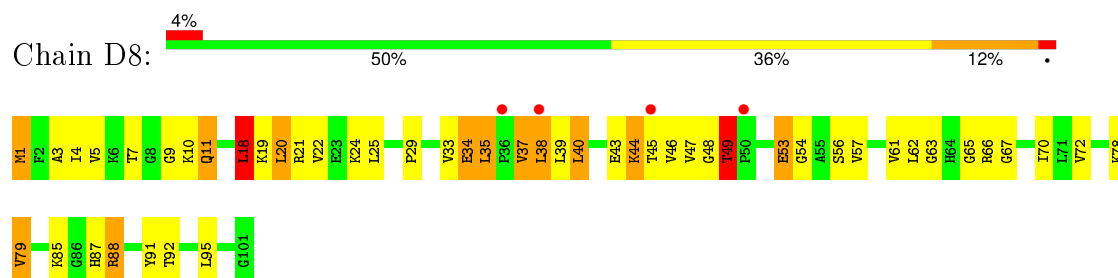
- Molecule 40: 50S ribosomal protein L20



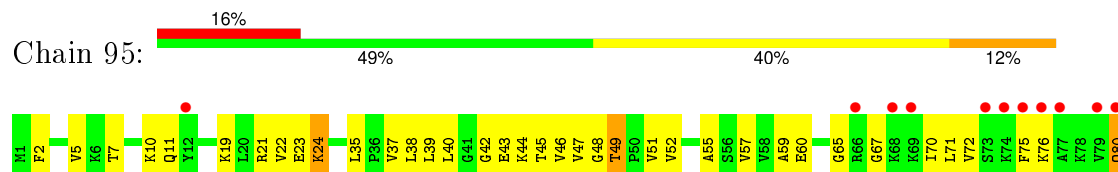
- Molecule 40: 50S ribosomal protein L20

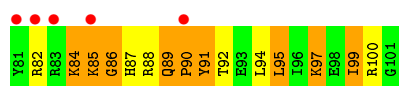


- Molecule 41: 50S ribosomal protein L21

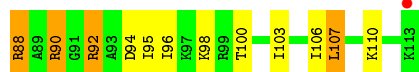


- Molecule 41: 50S ribosomal protein L21





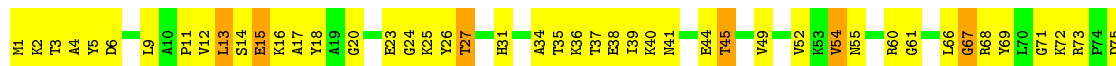
- Molecule 42: 50S ribosomal protein L22



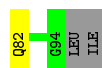
- Molecule 42: 50S ribosomal protein L22



- Molecule 43: 50S ribosomal protein L23

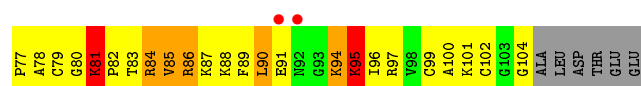


- Molecule 43: 50S ribosomal protein L23

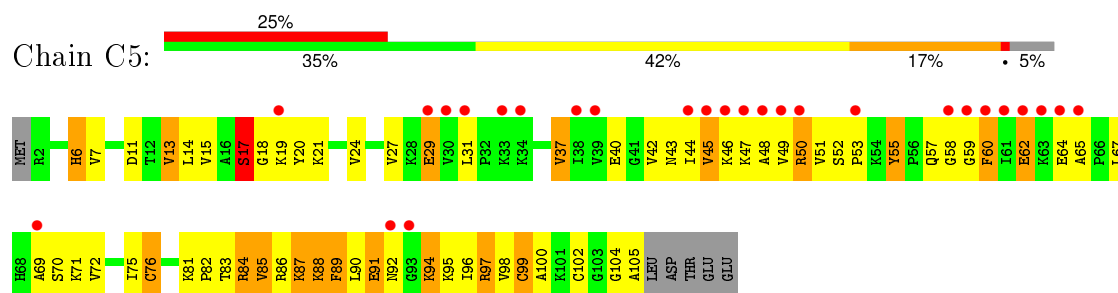


- Molecule 44: 50S ribosomal protein L24

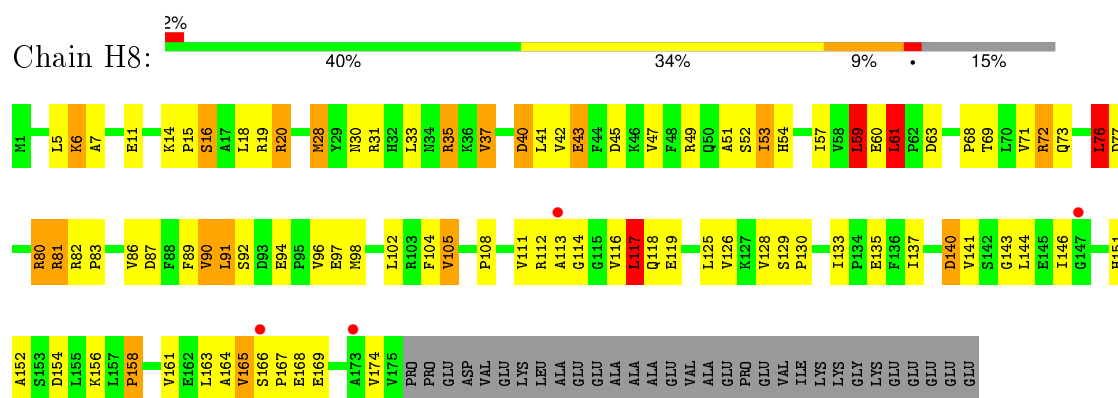




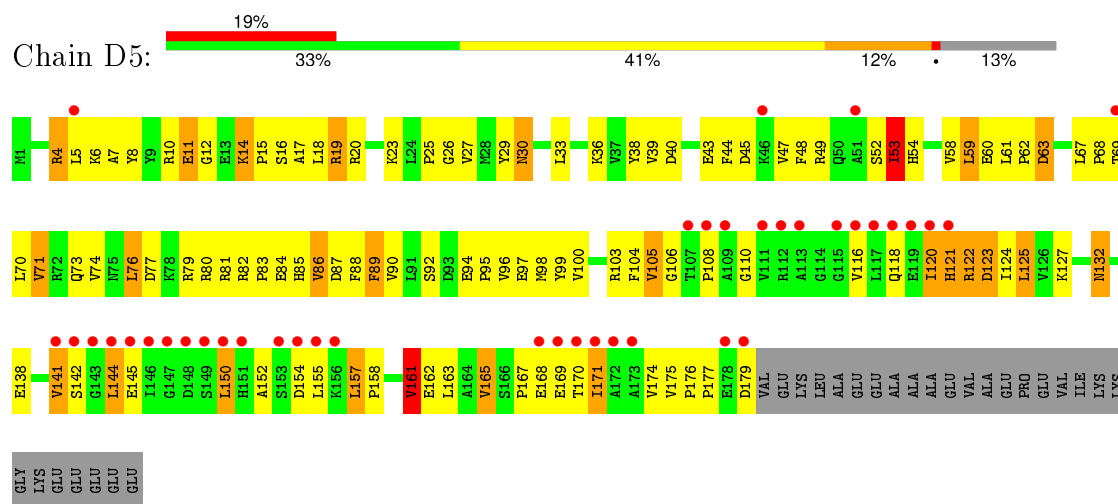
• Molecule 44: 50S ribosomal protein L24



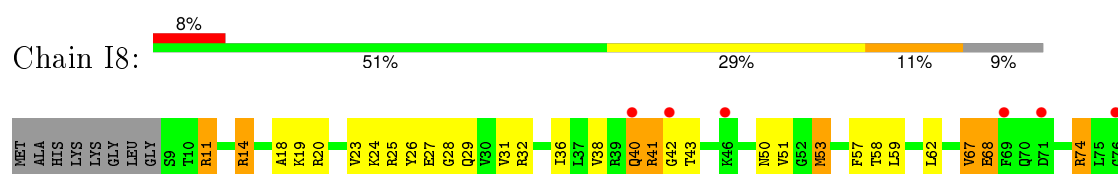
• Molecule 45: 50S ribosomal protein L25

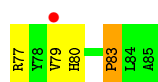


• Molecule 45: 50S ribosomal protein L25

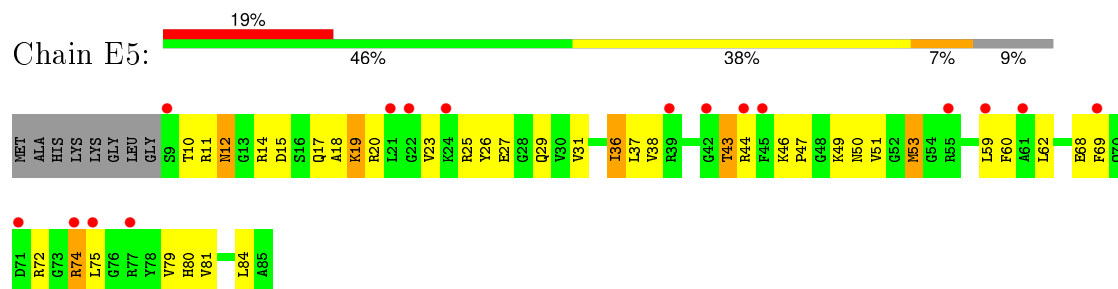


• Molecule 46: 50S ribosomal protein L27

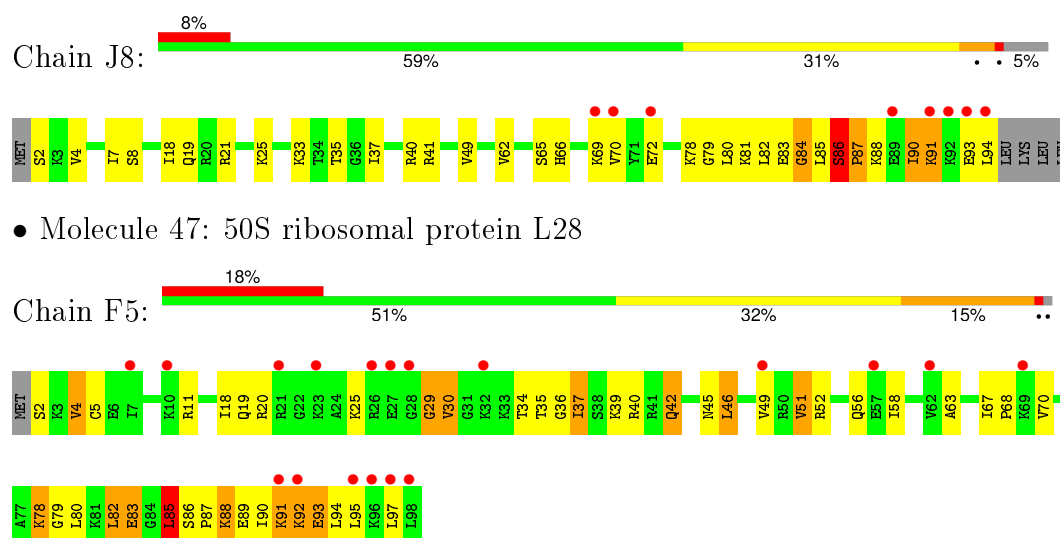




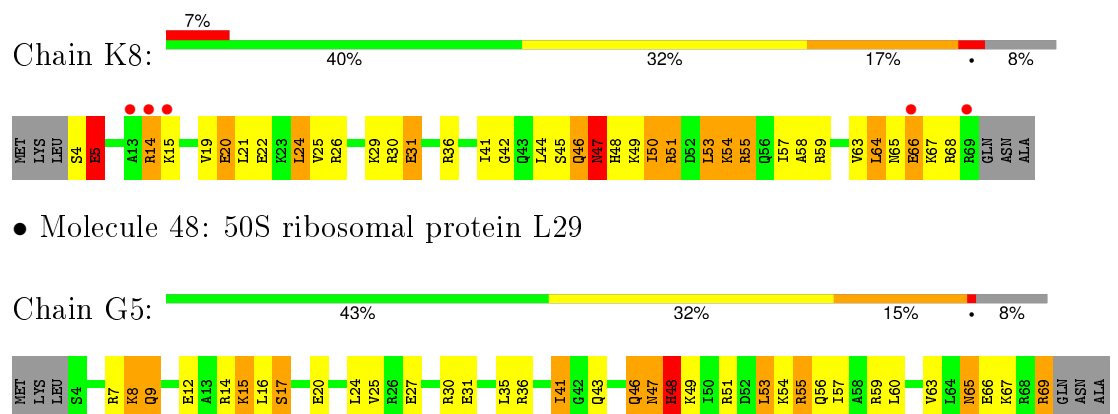
- Molecule 46: 50S ribosomal protein L27



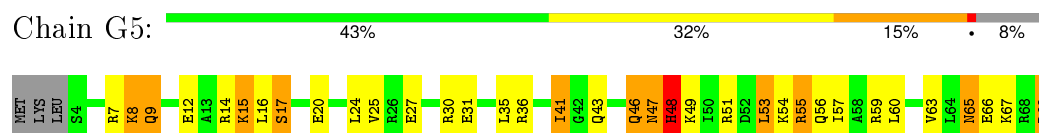
- Molecule 47: 50S ribosomal protein L28



- Molecule 48: 50S ribosomal protein L29



- Molecule 48: 50S ribosomal protein L29

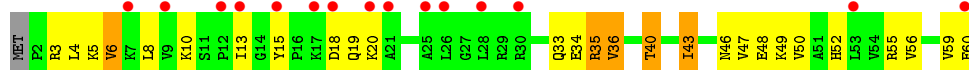


- Molecule 49: 50S ribosomal protein L30





- Molecule 49: 50S ribosomal protein L30

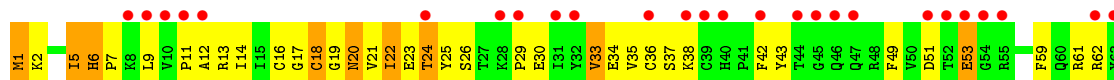


- Molecule 50: 50S ribosomal protein L31



GLY
ARG

- Molecule 50: 50S ribosomal protein L31



GLY
ASP
SER
TYR
ARG
LYS
GLY
ARG

- Molecule 51: 50S ribosomal protein L32



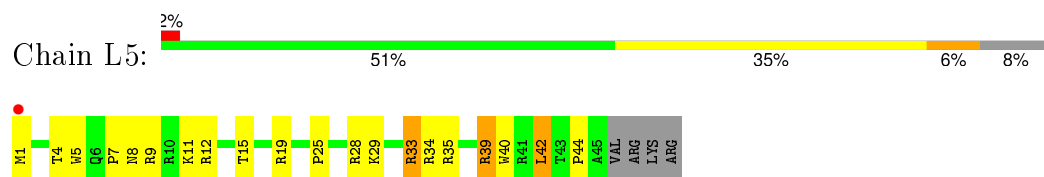
- Molecule 51: 50S ribosomal protein L32



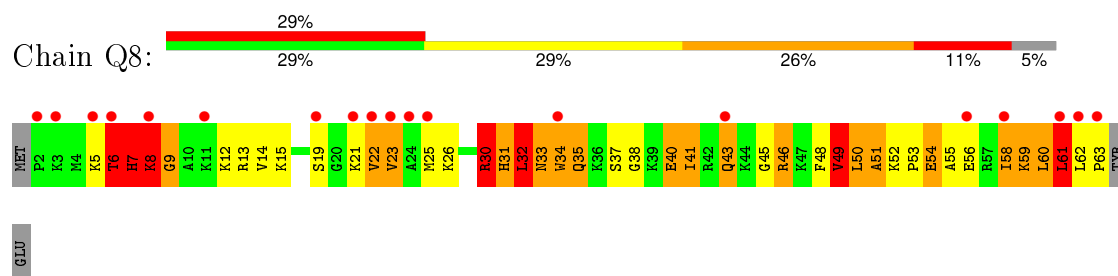
- Molecule 52: 50S ribosomal protein L34



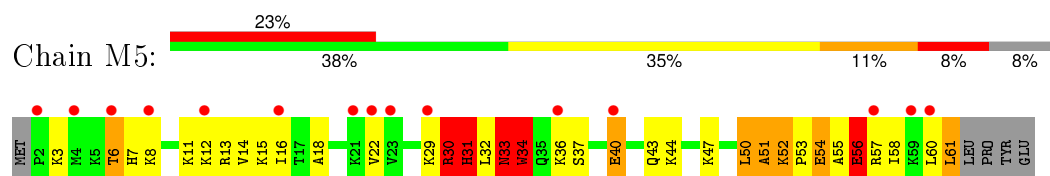
- Molecule 52: 50S ribosomal protein L34



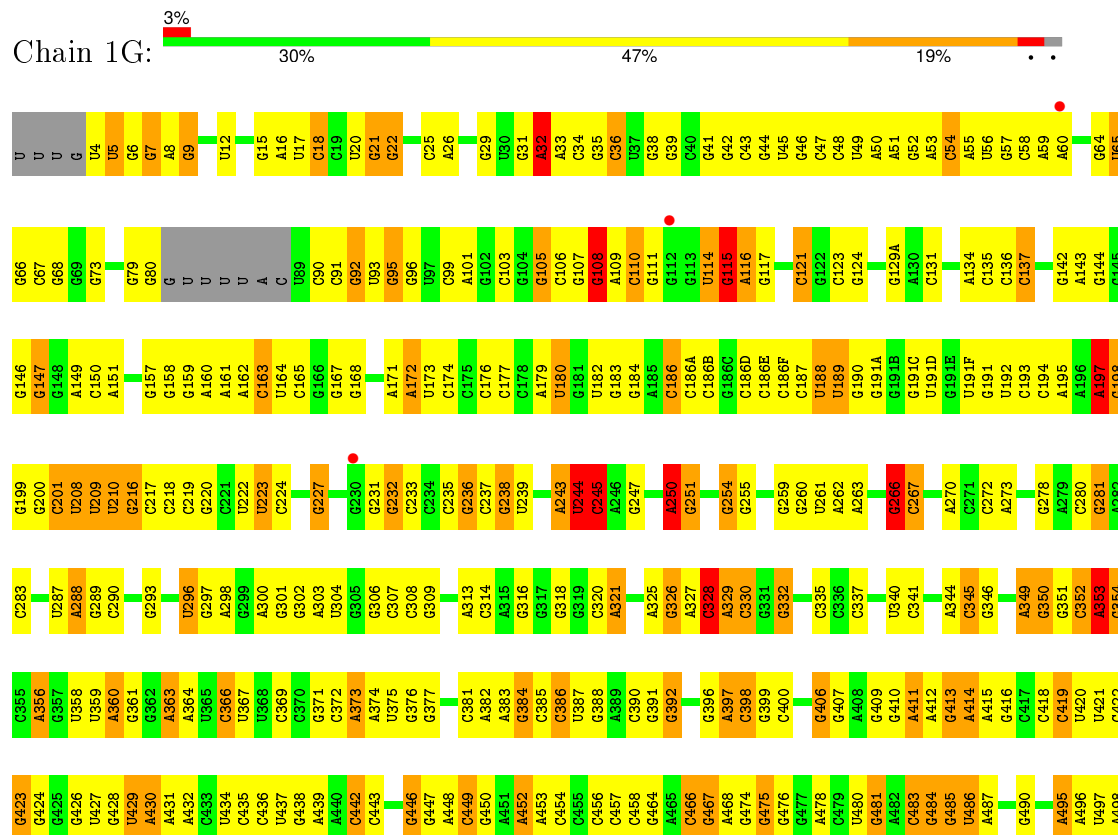
- Molecule 53: 50S ribosomal protein L35



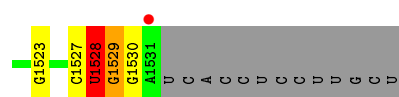
- Molecule 53: 50S ribosomal protein L35



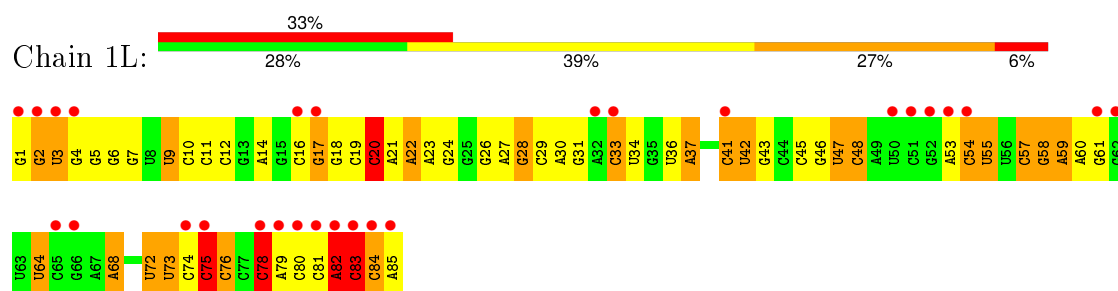
- Molecule 54: 16S ribosomal RNA



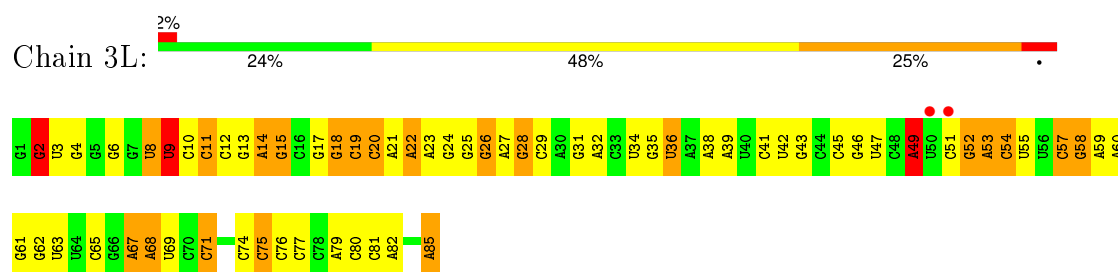
G1442	G1443	A1446	G1449	G1450	A1451	G1452	G1453	G1454	G1465	G1466	G1469	G1470	A1473	G1478	G1479	G1480	G1481	G1482	A1483	G1484	G1487	G1488	G1489	G1490	G1491	A1492	A1493	G1494	G1495	G1496	G1497	G1498	A1499	A1502	A1503	G1504	G1505	A1506	A1507	G1508	G1509	G1510	G1511	G1512	A1513	G1514	G1515	G1516	G1517	A1518	G1519																			
U1313	C1314	U1315	G1316	C1317	A1318	G1319	C1320	C1321	G1385	G1386	G1387	G1388	C1389	U1390	U1391	G1392	U1393	A1394	C1395	A1396	C1397	C1398	C1399	G1400	G1401	C1402	G1410	C1411	C1412	A1413	U1414	G1415	G1416	G1417	A1418	G1419	G1422	G1423	G1424	U1425	C1426	U1427	A1428	C1429	U1510	C1430	C1431	A1432	A1433	C1367	G1368	C1369	G1370	G1371	C1372	G1373														
U1247	A1248	C1249	A1250	G1251	A1252	G1253	C1254	G1255	A1256	G1257	G1258	C1259	C1260	A1261	G1267	A1268	A1269	G1272	G1273	G1274	G1275	A1276	G1277	U1278	C1403	C1404	A1279	U1211	U1212	A1213	U1281	G1282	A1285	A1286	A1287	A1288	A1289	G1290	G1291	U1292	A1293	G1294	G1295	C1296	C1297	C1298	A1299	G1300	U1301	U1302	G1303	G1304	G1305	A1306	U1307	G1308	C1362	C1362A	A1363	U1364	C1365	A1366	C1367	G1434	G1435	G1436	U1437	C1438	G1439	G1440
U1184	G1185	G1186	G1187	U1188	G1189	G1190	A1191	C1192	G1193	G1194	G1195	U1196	G1197	G1198	U1199	G1200	A1201	G1202	A1203	A1204	U1205	G1206	G1207	C1146	C1147	U1148	G1154	G1155	G1156	C1157	C1158	U1159	G1160	C1161	C1162	C1163	G1164	G1165	G1166	A1167	A1169	A1170	G1171	G1172	G1173	G1174	G1175	A1176	U1177	G1178	A1179	U1180	C1181	G1182	A1183															
C1059	C1060	G1064	U1065	U1066	U1067	A1068	C1069	U1070	U1071	G1072	U1073	G1074	C1075	C1076	U1077	U1078	G1079	A1080	G1081	U1082	U1083	C1084	U1085	U1086	C1087	G1088	U1089	C1090	U1091	A1092	A1093	G1094	U1095	C1096	C1097	G1098	G1099	A1035	G1036	A1101	C1037	G1038	C1039	G1042	C1043	A1044	C1045	A1046	G1047	G1048	U1049	G1050	G1053	C1054	A1055	U1056	G1057	G1058												
C998A	U999	A1000	G1001	G1002	G1003	A1004	A1005	C1006	C1007	C1008	G1009	U1012	G1013	A1014	A1015	A1016	G1017	C1018	C1019	G1022	G1023	G1024	U1025	C1028	C1028A	C1028B	A1151	A1152	G1153	A1094	A1095	A1032	G1032A	G1032B	G1033	G1034	G1035	G1036	A1101	C1037	G1038	C1039	G1042	C1043	A1044	C1045	A1046	G1047	G1048	U1049	G1050	G1053	C1054	A1055	U1056	G1057	G1058													
A855	C936	A937	A938	G939	G940	G941	G942	U943	G944	G947	G948	A949	U952	G953	G954	U955	U956	U957	A958	A959	U960	U961	C962	G963	G964	G965	G966	G967	A968	A969	C970	G971	G972	G973	A974	A975	G976	A977	A978	C979	C980	U981	U982	A983	A984	C985	A986	G987	G988	C989	C990	G991	G992	G993	U992	G994	C995	G994												
C862	U863	A864	A865	C866	G867	C868	G869	A872	A873	G876	C877	G878	C880	G881	U882	U883	U884	G885	G888	A889	G890	C893	C894	G895	C896	C897	G898	A901	A902	C904	U905	G906	A909	C910	U911	C912	A913	A914	A915	A918	A919	C984	U921	C949	U922	A923	C924	G853	C854	G855	G926	G927	C928	C857	G858	A859	C930	C934												
G776	A777	C778	C779	A780	G786	A787	A790	A792	U793	A794	G796	G800	U801	A802	U803	A804	A805	A807	C808	C809	C810	C811	C812	C736	G660	G661	C738	G664	A665	G666	G667	G742	U743	C745	A746	C747	A675	A676	U677	U751	G678	G679	G683	A684	C685	U686	A687	G688	C889	G690	U692	G693	A694	A695	G700	C701														
G501	G502	G503	C504	G505	G506	G507	C508	A509	C510	C511	U512	C513	U516	A517	U518	C519	A520	G521	C522	A523	C526	C527	C528	G529	G530	G531	A532	A533	U534	C535	C536	G537	C600	A601	A602	U603	G604	U605	C542	C543	C544	A607	A608	A609	A614	C615	C549	G616	G617	C618	U619	C620	A621	C622	G623	A624	U625	U561	C562											



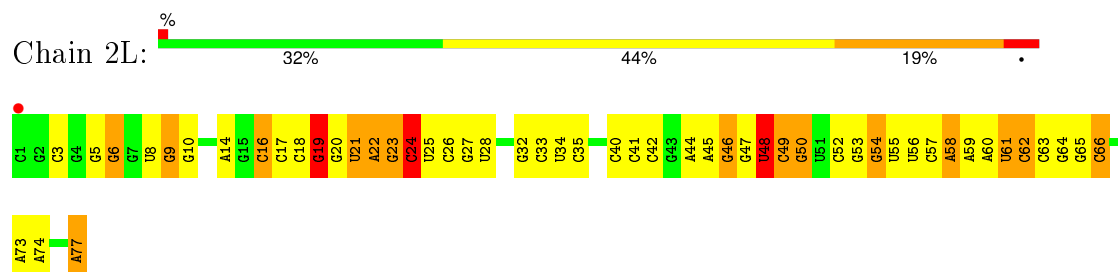
• Molecule 55: tRNA-Tyr



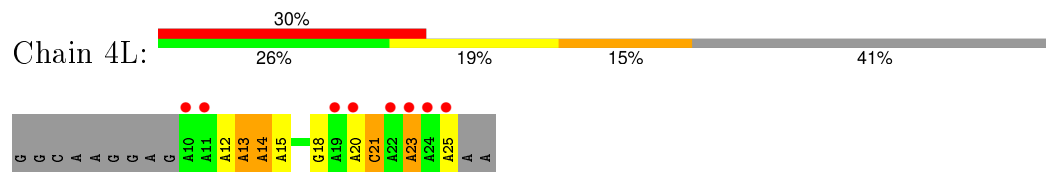
• Molecule 55: tRNA-Tyr



• Molecule 56: tRNA-fMet



• Molecule 57: mRNA



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	209.90Å 450.30Å 619.50Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	225.15 – 3.05 255.20 – 3.05	Depositor EDS
% Data completeness (in resolution range)	99.9 (225.15-3.05) 93.6 (255.20-3.05)	Depositor EDS
R_{merge}	0.42	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.64 (at 3.07Å)	Xtriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.205 , 0.249 0.206 , 0.251	Depositor DCC
R_{free} test set	2000 reflections (0.19%)	DCC
Wilson B-factor (Å ²)	74.3	Xtriage
Anisotropy	0.273	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.26 , 75.5	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.41$, $\langle L^2 \rangle = 0.23$	Xtriage
Outliers	0 of 1100882 reflections	Xtriage
F_o, F_c correlation	0.89	EDS
Total number of atoms	299318	wwPDB-VP
Average B, all atoms (Å ²)	104.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.41% 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, 0.375 respectively for untwinned datasets, and 0.333, 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, OMC, ZN, OMG, MIA, MG, H2U, 4SU, 7MG, 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	0.78	10/36053 (0.0%)	1.46	488/56270 (0.9%)
2	12	0.35	0/1959	0.61	0/2642
2	1E	0.42	0/1959	0.66	1/2642 (0.0%)
3	22	0.40	0/1636	0.60	0/2205
3	2E	0.51	0/1629	0.66	0/2195
4	32	0.48	0/1732	0.71	0/2318
4	3E	0.65	3/1732 (0.2%)	0.80	2/2318 (0.1%)
5	42	0.45	0/1171	0.70	1/1576 (0.1%)
5	4E	0.55	0/1171	0.70	0/1576
6	52	0.50	0/855	0.70	0/1154
6	5E	0.56	0/855	0.74	0/1154
7	62	0.43	0/1275	0.59	0/1709
7	6E	0.46	0/1275	0.61	0/1709
8	72	0.42	0/1135	0.64	0/1527
8	7E	0.53	0/1135	0.71	0/1527
9	82	0.42	0/1028	0.63	0/1379
9	8E	0.45	0/1028	0.66	0/1379
10	1A	0.36	0/814	0.60	0/1095
10	1I	0.46	0/814	0.67	0/1095
11	2A	0.46	0/899	0.69	0/1213
11	2I	0.53	0/879	0.72	1/1187 (0.1%)
12	3A	0.52	0/991	0.81	2/1327 (0.2%)
12	3I	0.71	0/991	0.85	0/1327
13	4A	0.37	0/943	0.60	0/1265
13	4I	0.47	0/938	0.72	1/1258 (0.1%)
14	5A	0.43	0/484	0.72	0/643
14	5I	0.59	0/507	0.92	1/672 (0.1%)
15	6A	0.45	0/744	0.62	1/992 (0.1%)
15	6I	0.57	0/744	0.77	0/992
16	7A	0.51	0/721	0.71	0/970
16	7I	0.47	0/721	0.72	0/970
17	8A	0.52	1/847 (0.1%)	0.64	0/1131

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
17	8I	0.55	0/847	0.74	0/1131
18	9A	0.50	0/569	0.69	0/757
18	9I	0.50	0/595	0.73	0/790
19	AA	0.41	0/654	0.70	0/884
19	AI	0.51	0/680	0.77	0/915
20	BA	0.48	0/764	0.76	0/1007
20	BI	0.43	0/764	0.68	0/1007
21	1B	0.48	0/221	0.65	0/288
21	1F	0.55	0/192	0.74	0/252
22	1K	0.76	0/1851	1.36	18/2877 (0.6%)
22	3K	0.64	0/1851	1.17	10/2877 (0.3%)
23	2K	0.90	1/1699 (0.1%)	1.64	40/2648 (1.5%)
24	4K	0.93	0/394	1.31	2/612 (0.3%)
25	14	0.95	72/70119 (0.1%)	1.66	1690/109464 (1.5%)
25	1H	1.12	193/70233 (0.3%)	1.89	2816/109643 (2.6%)
26	16	0.86	0/2928	1.60	51/4568 (1.1%)
26	1J	0.76	0/2928	1.48	37/4568 (0.8%)
27	11	0.83	0/2165	1.00	3/2919 (0.1%)
27	19	0.77	0/2170	0.98	6/2926 (0.2%)
28	21	0.66	0/1601	0.93	1/2160 (0.0%)
28	29	0.66	0/1601	0.89	1/2160 (0.0%)
29	31	0.79	1/1620 (0.1%)	0.90	2/2194 (0.1%)
29	39	0.62	1/1662 (0.1%)	0.84	2/2249 (0.1%)
30	41	0.55	0/1498	0.74	0/2016
30	49	0.42	0/1498	0.69	0/2016
31	51	0.60	0/1362	0.88	2/1841 (0.1%)
31	59	0.38	0/1341	0.67	1/1813 (0.1%)
32	61	0.50	0/1151	0.76	0/1558
32	69	0.47	0/1151	0.74	2/1558 (0.1%)
33	15	0.50	0/1131	0.69	0/1525
33	58	0.61	0/1131	0.84	0/1525
34	25	0.65	0/942	0.81	1/1269 (0.1%)
34	68	0.70	0/942	0.81	0/1269
35	35	0.65	0/1161	1.09	3/1544 (0.2%)
35	78	0.75	0/1161	1.06	1/1544 (0.1%)
36	45	0.68	0/1119	0.92	2/1496 (0.1%)
36	88	0.88	2/1142 (0.2%)	1.01	1/1527 (0.1%)
37	55	0.65	0/973	0.83	0/1302
37	98	0.64	0/981	0.85	0/1312
38	65	0.55	0/891	0.92	3/1187 (0.3%)
38	A8	0.65	0/891	0.89	2/1187 (0.2%)
39	75	0.60	0/1155	0.81	1/1542 (0.1%)
39	B8	0.66	0/1147	0.80	0/1532

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
40	85	0.61	0/981	0.76	0/1306
40	C8	0.72	0/981	0.93	3/1306 (0.2%)
41	95	0.59	0/789	0.81	0/1057
41	D8	0.61	0/789	0.85	2/1057 (0.2%)
42	A5	0.74	0/910	0.82	0/1220
42	E8	0.70	0/910	0.93	3/1220 (0.2%)
43	B5	0.78	0/739	0.86	0/993
43	F8	0.82	0/756	0.95	1/1014 (0.1%)
44	C5	0.60	0/807	0.82	0/1076
44	G8	0.76	1/791 (0.1%)	0.98	3/1055 (0.3%)
45	D5	0.41	0/1460	0.67	0/1982
45	H8	0.50	0/1427	0.82	2/1935 (0.1%)
46	E5	0.64	0/620	0.85	0/827
46	I8	0.85	0/620	0.94	0/827
47	F5	0.63	0/769	0.85	0/1022
47	J8	0.77	0/736	0.93	0/978
48	G5	0.60	0/560	0.79	0/741
48	K8	0.85	1/560 (0.2%)	0.92	0/741
49	H5	0.53	0/473	0.70	0/635
49	L8	0.57	0/473	0.70	0/635
50	I5	0.43	0/527	0.73	0/709
50	M8	0.45	0/545	0.70	0/733
51	J5	0.62	0/467	0.80	0/632
51	N8	0.65	0/386	0.84	0/523
52	L5	0.82	0/399	0.94	0/526
52	P8	0.96	0/399	0.98	0/526
53	M5	0.83	1/486 (0.2%)	1.13	2/638 (0.3%)
53	Q8	1.03	0/454	1.44	4/607 (0.7%)
54	1G	0.68	1/36049 (0.0%)	1.34	271/56262 (0.5%)
55	1L	0.85	1/2018 (0.0%)	1.32	24/3142 (0.8%)
55	3L	0.67	2/2018 (0.1%)	1.25	12/3142 (0.4%)
56	2L	0.73	0/1725	1.37	12/2689 (0.4%)
57	4L	0.81	0/394	1.29	2/612 (0.3%)
All	All	0.85	291/322559 (0.1%)	1.47	5537/483244 (1.1%)

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	1E	0	2

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Mol	Chain	#Chirality outliers	#Planarity outliers
3	2E	0	1
4	3E	0	2
6	5E	0	1
11	2A	0	1
12	3I	0	1
13	4I	0	1
14	5A	0	1
14	5I	0	1
17	8I	0	1
19	AI	0	1
20	BA	0	1
20	BI	0	1
27	11	0	5
27	19	0	5
28	21	0	3
28	29	0	4
29	39	0	2
30	41	0	1
31	51	0	1
31	59	0	1
32	61	0	4
32	69	0	1
33	58	0	1
35	35	0	2
35	78	0	5
36	45	0	5
36	88	0	4
39	75	0	1
39	B8	0	1
40	85	0	2
40	C8	0	1
41	95	0	2
41	D8	0	1
43	B5	0	2
44	C5	0	2
44	G8	0	5
45	D5	0	1
45	H8	0	3
47	F5	0	2
47	J8	0	2
48	G5	0	3
50	M8	0	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
53	M5	0	3
53	Q8	0	4
All	All	0	95

The worst 5 of 291 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	1H	783	A	N3-C4	-12.01	1.27	1.34
25	1H	774	A	N9-C4	-10.83	1.31	1.37
25	1H	2430	A	N9-C4	-10.39	1.31	1.37
25	14	783	A	N9-C4	-9.88	1.31	1.37
25	14	774	A	N9-C4	-9.74	1.32	1.37

The worst 5 of 5537 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	1H	1899	G	N3-C4-N9	-19.08	114.55	126.00
25	1H	676	A	C2-N3-C4	-18.37	101.42	110.60
25	1H	945	A	C6-C5-N7	-18.34	119.46	132.30
25	1H	945	A	N1-C6-N6	17.84	129.30	118.60
25	1H	783	A	C2-N3-C4	-17.75	101.73	110.60

There are no chirality outliers.

5 of 95 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	1E	15	VAL	Peptide
2	1E	71	VAL	Peptide
3	2E	166	GLU	Peptide
4	3E	29	PRO	Peptide
4	3E	85	LYS	Peptide

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	13	32207	0	16254	795	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	12	1924	0	1975	105	0
2	1E	1924	0	1975	91	0
3	22	1612	0	1677	104	0
3	2E	1605	0	1668	46	0
4	32	1702	0	1763	103	0
4	3E	1702	0	1763	79	0
5	42	1155	0	1213	75	0
5	4E	1155	0	1213	37	0
6	52	842	0	857	28	0
6	5E	842	0	857	44	0
7	62	1256	0	1296	57	0
7	6E	1256	0	1296	60	0
8	72	1115	0	1177	46	0
8	7E	1115	0	1177	56	0
9	82	1009	0	1037	65	0
9	8E	1009	0	1037	63	0
10	1A	801	0	849	52	0
10	1I	801	0	849	52	0
11	2A	884	0	904	39	0
11	2I	864	0	881	35	0
12	3A	975	0	1062	57	0
12	3I	975	0	1062	37	0
13	4A	933	0	992	61	0
13	4I	928	0	987	56	0
14	5A	475	0	511	31	0
14	5I	498	0	537	38	0
15	6A	733	0	771	28	0
15	6I	733	0	771	30	0
16	7A	705	0	725	15	0
16	7I	705	0	725	46	0
17	8A	834	0	904	35	0
17	8I	834	0	904	54	0
18	9A	564	0	631	21	0
18	9I	590	0	662	33	0
19	AA	640	0	633	37	0
19	AI	665	0	686	41	0
20	BA	762	0	861	36	0
20	BI	762	0	861	38	0
21	1B	217	0	234	20	0
21	1F	188	0	195	9	0
22	1K	1825	0	946	59	0
22	3K	1825	0	946	49	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
23	2K	1646	0	847	33	0
24	4K	349	0	176	13	0
25	14	62605	0	31561	1396	0
25	1H	62707	0	31610	1456	1
26	16	2617	0	1328	68	0
26	1J	2617	0	1328	93	0
27	11	2115	0	2195	124	0
27	19	2120	0	2197	103	0
28	21	1568	0	1634	94	0
28	29	1568	0	1634	108	0
29	31	1585	0	1632	81	0
29	39	1627	0	1680	101	0
30	41	1473	0	1535	86	0
30	49	1473	0	1535	74	0
31	51	1336	0	1418	82	0
31	59	1316	0	1395	79	0
32	61	1136	0	1223	61	0
32	69	1136	0	1223	62	0
33	15	1104	0	1180	50	0
33	58	1104	0	1180	66	0
34	25	932	0	996	54	0
34	68	932	0	996	26	0
35	35	1144	0	1228	108	0
35	78	1144	0	1228	99	0
36	45	1098	0	1160	66	0
36	88	1121	0	1179	56	0
37	55	959	0	1021	44	0
37	98	967	0	1033	55	0
38	65	881	0	943	67	0
38	A8	881	0	943	47	0
39	75	1141	0	1202	64	0
39	B8	1133	0	1190	64	0
40	85	963	0	1022	55	0
40	C8	963	0	1022	65	0
41	95	778	0	852	60	0
41	D8	778	0	852	34	0
42	A5	899	0	964	40	0
42	E8	899	0	964	27	0
43	B5	725	0	778	29	0
43	F8	742	0	803	44	0
44	C5	794	0	883	64	0
44	G8	778	0	863	61	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
45	D5	1428	0	1454	82	0
45	H8	1397	0	1430	57	0
46	E5	612	0	633	35	0
46	I8	612	0	633	31	0
47	F5	762	0	848	42	0
47	J8	729	0	802	23	0
48	G5	558	0	610	24	0
48	K8	558	0	610	33	0
49	H5	468	0	518	16	0
49	L8	468	0	518	20	0
50	I5	515	0	514	30	0
50	M8	533	0	526	34	0
51	J5	453	0	475	18	0
51	N8	374	0	393	22	0
52	L5	391	0	432	22	0
52	P8	391	0	432	15	0
53	M5	480	0	549	44	0
53	Q8	448	0	463	60	0
54	1G	32204	0	16256	845	1
55	1L	1807	0	920	33	0
55	3L	1807	0	920	54	0
56	2L	1645	0	843	44	0
57	4L	349	0	176	10	0
58	11	1	0	0	0	0
58	13	138	0	0	0	0
58	14	398	0	0	0	0
58	16	13	0	0	0	0
58	1G	90	0	0	0	0
58	1H	475	0	0	0	0
58	1J	6	0	0	0	0
58	1K	1	0	0	0	0
58	1L	1	0	0	0	0
58	21	2	0	0	0	0
58	25	1	0	0	0	0
58	29	3	0	0	0	0
58	2K	6	0	0	0	0
58	2L	3	0	0	0	0
58	31	4	0	0	0	0
58	39	1	0	0	0	0
58	3E	1	0	0	0	0
58	3I	1	0	0	0	0
58	3L	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
58	45	1	0	0	0	0
58	4E	1	0	0	0	0
58	78	1	0	0	0	0
58	85	1	0	0	0	0
58	8E	1	0	0	0	0
58	98	2	0	0	0	0
58	C5	1	0	0	0	0
58	I8	2	0	0	0	0
58	L5	1	0	0	0	0
58	L8	2	0	0	0	0
58	P8	1	0	0	0	0
59	32	1	0	0	0	0
59	3E	1	0	0	0	0
59	5A	1	0	0	0	0
59	5I	1	0	0	0	0
59	C5	1	0	0	0	0
59	G8	1	0	0	0	0
60	11	4	0	0	0	0
60	13	100	0	0	20	0
60	14	409	0	0	100	0
60	16	11	0	0	1	0
60	19	7	0	0	1	0
60	1G	51	0	0	14	0
60	1H	538	0	0	157	0
60	1K	1	0	0	0	0
60	21	2	0	0	0	0
60	29	2	0	0	1	0
60	2K	6	0	0	0	0
60	31	4	0	0	0	0
60	32	1	0	0	0	0
60	35	1	0	0	0	0
60	39	4	0	0	0	0
60	3E	2	0	0	0	0
60	3I	2	0	0	1	0
60	4K	2	0	0	0	0
60	4L	1	0	0	0	0
60	55	1	0	0	2	0
60	5I	1	0	0	0	0
60	75	1	0	0	0	0
60	78	4	0	0	2	0
60	7I	1	0	0	0	0
60	85	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
60	BA	1	0	0	0	0
60	D8	1	0	0	0	0
60	F8	1	0	0	0	0
60	L8	3	0	0	0	0
All	All	299318	0	199912	8796	1

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

The worst 5 of 8796 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)
22:1K:35:QUO:N3	22:1K:35:QUO:C4	1.70	1.51
22:3K:35:QUO:C4	22:3K:35:QUO:N3	1.72	1.48
25:14:2057:A:OP2	60:14:3437:HOH:O	1.73	1.07
25:14:2032:G:N7	60:14:3594:HOH:O	1.91	1.04
25:14:2711:A:OP2	60:14:3464:HOH:O	1.72	1.04

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)
25:1H:2137:C:OP1	54:1G:999:U:O2'[4_555]	2.16	0.04

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
2	12	235/256 (92%)	201 (86%)	32 (14%)	2 (1%)	21 58
2	1E	235/256 (92%)	202 (86%)	31 (13%)	2 (1%)	21 58

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	22	204/239 (85%)	187 (92%)	17 (8%)	0	100	100
3	2E	203/239 (85%)	191 (94%)	12 (6%)	0	100	100
4	32	206/209 (99%)	181 (88%)	25 (12%)	0	100	100
4	3E	206/209 (99%)	191 (93%)	14 (7%)	1 (0%)	34	70
5	42	149/162 (92%)	141 (95%)	8 (5%)	0	100	100
5	4E	149/162 (92%)	145 (97%)	3 (2%)	1 (1%)	26	64
6	52	99/101 (98%)	97 (98%)	2 (2%)	0	100	100
6	5E	99/101 (98%)	94 (95%)	5 (5%)	0	100	100
7	62	153/156 (98%)	146 (95%)	7 (5%)	0	100	100
7	6E	153/156 (98%)	145 (95%)	8 (5%)	0	100	100
8	72	136/138 (99%)	127 (93%)	8 (6%)	1 (1%)	26	64
8	7E	136/138 (99%)	130 (96%)	6 (4%)	0	100	100
9	82	125/128 (98%)	116 (93%)	9 (7%)	0	100	100
9	8E	125/128 (98%)	109 (87%)	16 (13%)	0	100	100
10	1A	97/105 (92%)	90 (93%)	7 (7%)	0	100	100
10	1I	97/105 (92%)	86 (89%)	11 (11%)	0	100	100
11	2A	117/129 (91%)	106 (91%)	11 (9%)	0	100	100
11	2I	114/129 (88%)	98 (86%)	14 (12%)	2 (2%)	11	39
12	3A	123/132 (93%)	106 (86%)	14 (11%)	3 (2%)	7	31
12	3I	123/132 (93%)	106 (86%)	17 (14%)	0	100	100
13	4A	115/126 (91%)	99 (86%)	15 (13%)	1 (1%)	21	58
13	4I	114/126 (90%)	98 (86%)	16 (14%)	0	100	100
14	5A	56/61 (92%)	48 (86%)	8 (14%)	0	100	100
14	5I	59/61 (97%)	49 (83%)	9 (15%)	1 (2%)	11	41
15	6A	86/89 (97%)	78 (91%)	8 (9%)	0	100	100
15	6I	86/89 (97%)	77 (90%)	9 (10%)	0	100	100
16	7A	82/88 (93%)	73 (89%)	9 (11%)	0	100	100
16	7I	82/88 (93%)	78 (95%)	4 (5%)	0	100	100
17	8A	98/105 (93%)	91 (93%)	7 (7%)	0	100	100
17	8I	98/105 (93%)	92 (94%)	6 (6%)	0	100	100
18	9A	67/88 (76%)	61 (91%)	6 (9%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
18	9I	70/88 (80%)	63 (90%)	6 (9%)	1 (1%)	14	46
19	AA	80/93 (86%)	64 (80%)	14 (18%)	2 (2%)	7	30
19	AI	81/93 (87%)	69 (85%)	9 (11%)	3 (4%)	4	22
20	BA	97/106 (92%)	88 (91%)	9 (9%)	0	100	100
20	BI	97/106 (92%)	84 (87%)	13 (13%)	0	100	100
21	1B	23/27 (85%)	19 (83%)	4 (17%)	0	100	100
21	1F	20/27 (74%)	18 (90%)	2 (10%)	0	100	100
27	11	270/276 (98%)	249 (92%)	18 (7%)	3 (1%)	17	53
27	19	271/276 (98%)	249 (92%)	17 (6%)	5 (2%)	11	39
28	21	203/206 (98%)	175 (86%)	24 (12%)	4 (2%)	9	36
28	29	203/206 (98%)	162 (80%)	32 (16%)	9 (4%)	3	17
29	31	200/210 (95%)	178 (89%)	21 (10%)	1 (0%)	34	70
29	39	206/210 (98%)	171 (83%)	29 (14%)	6 (3%)	6	27
30	41	179/182 (98%)	158 (88%)	18 (10%)	3 (2%)	11	41
30	49	179/182 (98%)	160 (89%)	18 (10%)	1 (1%)	30	66
31	51	172/180 (96%)	139 (81%)	28 (16%)	5 (3%)	6	27
31	59	169/180 (94%)	137 (81%)	29 (17%)	3 (2%)	11	39
32	61	144/148 (97%)	117 (81%)	23 (16%)	4 (3%)	6	28
32	69	144/148 (97%)	120 (83%)	20 (14%)	4 (3%)	6	28
33	15	136/140 (97%)	122 (90%)	13 (10%)	1 (1%)	26	64
33	58	136/140 (97%)	118 (87%)	15 (11%)	3 (2%)	8	34
34	25	120/122 (98%)	113 (94%)	7 (6%)	0	100	100
34	68	120/122 (98%)	113 (94%)	7 (6%)	0	100	100
35	35	148/150 (99%)	110 (74%)	31 (21%)	7 (5%)	3	16
35	78	148/150 (99%)	119 (80%)	24 (16%)	5 (3%)	5	23
36	45	136/141 (96%)	114 (84%)	21 (15%)	1 (1%)	26	64
36	88	139/141 (99%)	113 (81%)	25 (18%)	1 (1%)	26	64
37	55	115/118 (98%)	107 (93%)	8 (7%)	0	100	100
37	98	116/118 (98%)	106 (91%)	8 (7%)	2 (2%)	11	41
38	65	109/112 (97%)	89 (82%)	19 (17%)	1 (1%)	21	58
38	A8	109/112 (97%)	89 (82%)	19 (17%)	1 (1%)	21	58

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
39	75	135/146 (92%)	116 (86%)	17 (13%)	2 (2%)	13	44
39	B8	134/146 (92%)	122 (91%)	12 (9%)	0	100	100
40	85	115/118 (98%)	106 (92%)	8 (7%)	1 (1%)	21	58
40	C8	115/118 (98%)	105 (91%)	8 (7%)	2 (2%)	11	41
41	95	99/101 (98%)	80 (81%)	17 (17%)	2 (2%)	9	36
41	D8	99/101 (98%)	95 (96%)	2 (2%)	2 (2%)	9	36
42	A5	111/113 (98%)	103 (93%)	7 (6%)	1 (1%)	21	58
42	E8	111/113 (98%)	105 (95%)	6 (5%)	0	100	100
43	B5	90/96 (94%)	87 (97%)	3 (3%)	0	100	100
43	F8	92/96 (96%)	83 (90%)	7 (8%)	2 (2%)	8	34
44	C5	102/110 (93%)	75 (74%)	24 (24%)	3 (3%)	6	27
44	G8	100/110 (91%)	81 (81%)	14 (14%)	5 (5%)	3	15
45	D5	177/206 (86%)	138 (78%)	30 (17%)	9 (5%)	2	14
45	H8	173/206 (84%)	143 (83%)	22 (13%)	8 (5%)	3	16
46	E5	75/85 (88%)	73 (97%)	1 (1%)	1 (1%)	15	48
46	I8	75/85 (88%)	63 (84%)	11 (15%)	1 (1%)	15	48
47	F5	95/98 (97%)	87 (92%)	6 (6%)	2 (2%)	9	35
47	J8	91/98 (93%)	85 (93%)	4 (4%)	2 (2%)	8	34
48	G5	64/72 (89%)	60 (94%)	2 (3%)	2 (3%)	5	25
48	K8	64/72 (89%)	59 (92%)	4 (6%)	1 (2%)	12	42
49	H5	57/60 (95%)	55 (96%)	2 (4%)	0	100	100
49	L8	57/60 (95%)	55 (96%)	2 (4%)	0	100	100
50	I5	61/71 (86%)	35 (57%)	24 (39%)	2 (3%)	5	24
50	M8	64/71 (90%)	44 (69%)	18 (28%)	2 (3%)	5	25
51	J5	56/60 (93%)	50 (89%)	5 (9%)	1 (2%)	11	39
51	N8	47/60 (78%)	43 (92%)	4 (8%)	0	100	100
52	L5	43/49 (88%)	41 (95%)	2 (5%)	0	100	100
52	P8	43/49 (88%)	41 (95%)	2 (5%)	0	100	100
53	M5	58/65 (89%)	46 (79%)	10 (17%)	2 (3%)	5	23
53	Q8	60/65 (92%)	41 (68%)	12 (20%)	7 (12%)	0	2
All	All	11230/11946 (94%)	9889 (88%)	1191 (11%)	150 (1%)	15	48

5 of 150 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
14	5I	25	VAL
18	9I	22	VAL
44	G8	81	LYS
45	H8	53	ILE
53	Q8	51	ALA

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%)	159 (78%)	46 (22%)	1	4
2	1E	205/220 (93%)	161 (78%)	44 (22%)	1	5
3	22	160/188 (85%)	124 (78%)	36 (22%)	1	4
3	2E	159/188 (85%)	124 (78%)	35 (22%)	1	4
4	32	180/181 (99%)	150 (83%)	30 (17%)	3	10
4	3E	180/181 (99%)	148 (82%)	32 (18%)	2	9
5	42	116/123 (94%)	93 (80%)	23 (20%)	1	6
5	4E	116/123 (94%)	97 (84%)	19 (16%)	3	11
6	52	90/90 (100%)	73 (81%)	17 (19%)	2	7
6	5E	90/90 (100%)	77 (86%)	13 (14%)	4	16
7	62	126/127 (99%)	102 (81%)	24 (19%)	2	7
7	6E	126/127 (99%)	107 (85%)	19 (15%)	3	14
8	72	119/119 (100%)	106 (89%)	13 (11%)	8	29
8	7E	119/119 (100%)	97 (82%)	22 (18%)	2	8
9	82	98/99 (99%)	78 (80%)	20 (20%)	1	6
9	8E	98/99 (99%)	76 (78%)	22 (22%)	1	4
10	1A	89/92 (97%)	70 (79%)	19 (21%)	1	5
10	1I	89/92 (97%)	73 (82%)	16 (18%)	2	9
11	2A	90/99 (91%)	74 (82%)	16 (18%)	2	9

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
11	2I	88/99 (89%)	73 (83%)	15 (17%)	2	10
12	3A	104/109 (95%)	85 (82%)	19 (18%)	2	8
12	3I	104/109 (95%)	88 (85%)	16 (15%)	3	13
13	4A	94/101 (93%)	77 (82%)	17 (18%)	2	9
13	4I	94/101 (93%)	76 (81%)	18 (19%)	2	7
14	5A	48/50 (96%)	39 (81%)	9 (19%)	2	7
14	5I	50/50 (100%)	36 (72%)	14 (28%)	0	1
15	6A	79/80 (99%)	70 (89%)	9 (11%)	7	26
15	6I	79/80 (99%)	67 (85%)	12 (15%)	3	14
16	7A	72/74 (97%)	62 (86%)	10 (14%)	4	18
16	7I	72/74 (97%)	56 (78%)	16 (22%)	1	4
17	8A	95/97 (98%)	82 (86%)	13 (14%)	4	18
17	8I	95/97 (98%)	77 (81%)	18 (19%)	2	7
18	9A	60/77 (78%)	50 (83%)	10 (17%)	3	10
18	9I	63/77 (82%)	52 (82%)	11 (18%)	2	9
19	AA	66/80 (82%)	55 (83%)	11 (17%)	3	10
19	AI	72/80 (90%)	55 (76%)	17 (24%)	1	3
20	BA	76/82 (93%)	58 (76%)	18 (24%)	1	3
20	BI	76/82 (93%)	66 (87%)	10 (13%)	5	19
21	1B	20/22 (91%)	17 (85%)	3 (15%)	3	14
21	1F	17/22 (77%)	14 (82%)	3 (18%)	2	9
27	11	214/218 (98%)	164 (77%)	50 (23%)	1	3
27	19	214/218 (98%)	170 (79%)	44 (21%)	1	6
28	21	165/166 (99%)	131 (79%)	34 (21%)	1	6
28	29	165/166 (99%)	124 (75%)	41 (25%)	1	2
29	31	161/166 (97%)	133 (83%)	28 (17%)	2	10
29	39	165/166 (99%)	129 (78%)	36 (22%)	1	5
30	41	155/156 (99%)	123 (79%)	32 (21%)	1	6
30	49	155/156 (99%)	127 (82%)	28 (18%)	2	9
31	51	145/148 (98%)	111 (77%)	34 (23%)	1	3
31	59	143/148 (97%)	114 (80%)	29 (20%)	1	6

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
32	61	122/124 (98%)	91 (75%)	31 (25%)	1	2
32	69	122/124 (98%)	89 (73%)	33 (27%)	0	1
33	15	117/119 (98%)	91 (78%)	26 (22%)	1	4
33	58	117/119 (98%)	96 (82%)	21 (18%)	2	9
34	25	100/100 (100%)	77 (77%)	23 (23%)	1	4
34	68	100/100 (100%)	84 (84%)	16 (16%)	3	12
35	35	116/116 (100%)	81 (70%)	35 (30%)	0	1
35	78	116/116 (100%)	73 (63%)	43 (37%)	0	0
36	45	109/111 (98%)	87 (80%)	22 (20%)	1	6
36	88	111/111 (100%)	89 (80%)	22 (20%)	1	6
37	55	100/101 (99%)	78 (78%)	22 (22%)	1	4
37	98	101/101 (100%)	78 (77%)	23 (23%)	1	4
38	65	87/88 (99%)	61 (70%)	26 (30%)	0	1
38	A8	87/88 (99%)	59 (68%)	28 (32%)	0	0
39	75	120/127 (94%)	94 (78%)	26 (22%)	1	5
39	B8	119/127 (94%)	89 (75%)	30 (25%)	1	2
40	85	93/94 (99%)	81 (87%)	12 (13%)	5	20
40	C8	93/94 (99%)	78 (84%)	15 (16%)	3	12
41	95	82/82 (100%)	65 (79%)	17 (21%)	1	6
41	D8	82/82 (100%)	63 (77%)	19 (23%)	1	3
42	A5	92/92 (100%)	75 (82%)	17 (18%)	2	8
42	E8	92/92 (100%)	66 (72%)	26 (28%)	0	1
43	B5	74/78 (95%)	60 (81%)	14 (19%)	2	7
43	F8	76/78 (97%)	66 (87%)	10 (13%)	5	19
44	C5	85/91 (93%)	59 (69%)	26 (31%)	0	1
44	G8	84/91 (92%)	68 (81%)	16 (19%)	2	7
45	D5	158/179 (88%)	123 (78%)	35 (22%)	1	4
45	H8	154/179 (86%)	120 (78%)	34 (22%)	1	4
46	E5	62/67 (92%)	51 (82%)	11 (18%)	2	9
46	I8	62/67 (92%)	51 (82%)	11 (18%)	2	9
47	F5	82/83 (99%)	63 (77%)	19 (23%)	1	3

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
47	J8	78/83 (94%)	66 (85%)	12 (15%)	3	13
48	G5	62/67 (92%)	49 (79%)	13 (21%)	1	5
48	K8	62/67 (92%)	42 (68%)	20 (32%)	0	0
49	H5	51/52 (98%)	40 (78%)	11 (22%)	1	5
49	L8	51/52 (98%)	42 (82%)	9 (18%)	2	9
50	I5	57/63 (90%)	43 (75%)	14 (25%)	1	2
50	M8	59/63 (94%)	47 (80%)	12 (20%)	1	6
51	J5	51/52 (98%)	45 (88%)	6 (12%)	6	24
51	N8	43/52 (83%)	34 (79%)	9 (21%)	1	5
52	L5	38/42 (90%)	33 (87%)	5 (13%)	5	19
52	P8	38/42 (90%)	30 (79%)	8 (21%)	1	5
53	M5	50/55 (91%)	37 (74%)	13 (26%)	0	2
53	Q8	42/55 (76%)	22 (52%)	20 (48%)	0	0
All	All	9458/9894 (96%)	7506 (79%)	1952 (21%)	1	6

5 of 1952 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
45	H8	168	GLU
4	32	184	LYS
44	C5	31	LEU
48	K8	14	ARG
2	12	25	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 23 such sidechains are listed below:

Mol	Chain	Res	Type
7	62	28	ASN
11	2A	26	ASN
46	E5	29	GLN
9	82	23	ASN
13	4A	77	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	13	1496/1522 (98%)	355 (23%)	31 (2%)
22	1K	82/85 (96%)	39 (47%)	4 (4%)
22	3K	82/85 (96%)	31 (37%)	3 (3%)
23	2K	76/77 (98%)	20 (26%)	3 (3%)
24	4K	13/27 (48%)	4 (30%)	0
25	14	2905/2917 (99%)	766 (26%)	39 (1%)
25	1H	2911/2917 (99%)	766 (26%)	56 (1%)
26	16	121/122 (99%)	26 (21%)	0
26	1J	121/122 (99%)	30 (24%)	2 (1%)
54	1G	1495/1522 (98%)	393 (26%)	37 (2%)
55	1L	84/85 (98%)	37 (44%)	4 (4%)
55	3L	84/85 (98%)	28 (33%)	3 (3%)
56	2L	76/77 (98%)	17 (22%)	2 (2%)
57	4L	15/27 (55%)	5 (33%)	1 (6%)
All	All	9561/9670 (98%)	2517 (26%)	185 (1%)

5 of 2517 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	31	G

5 of 185 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
25	1H	1992	G
54	1G	266	G
25	14	2212	A
25	1H	2171	A
25	1H	2566	A

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

25 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	1K	17	22	18,26,27	5.58	6 (33%)	21,38,41	6.02	10 (47%)
22	QUO	1K	35	24,22	27,35,36	5.75	8 (29%)	30,52,55	3.83	9 (30%)
22	MIA	1K	38	22	22,31,32	1.10	1 (4%)	26,44,47	1.97	3 (11%)
22	PSU	1K	40	22	15,21,22	1.02	1 (6%)	16,30,33	2.08	4 (25%)
22	5MU	1K	63	22	13,22,23	1.68	2 (15%)	16,32,35	1.55	1 (6%)
22	PSU	1K	64	22	15,21,22	0.96	1 (6%)	16,30,33	2.09	2 (12%)
22	4SU	1K	8	22	12,21,22	3.33	2 (16%)	15,30,33	1.24	1 (6%)
23	H2U	2K	21	23	17,21,22	2.62	4 (23%)	23,30,33	2.92	6 (26%)
23	OMC	2K	33	23	15,22,23	1.98	4 (26%)	20,31,34	1.89	3 (15%)
23	7MG	2K	47	23	20,26,27	3.24	6 (30%)	23,39,42	2.11	6 (26%)
23	5MU	2K	55	23	13,22,23	1.66	2 (15%)	16,32,35	1.43	2 (12%)
23	PSU	2K	56	23	15,21,22	1.10	2 (13%)	16,30,33	1.89	2 (12%)
23	4SU	2K	8	23	12,21,22	3.28	2 (16%)	15,30,33	0.75	1 (6%)
56	H2U	2L	21	56	17,21,22	2.43	4 (23%)	23,30,33	3.03	6 (26%)
56	OMC	2L	33	56	15,22,23	2.27	4 (26%)	20,31,34	1.63	2 (10%)
56	5MU	2L	55	56	13,22,23	1.67	2 (15%)	16,32,35	1.34	1 (6%)
56	PSU	2L	56	56	15,21,22	1.09	1 (6%)	16,30,33	1.87	3 (18%)
56	4SU	2L	8	56	12,21,22	3.41	2 (16%)	15,30,33	1.02	1 (6%)
22	OMG	3K	17	22	18,26,27	5.65	6 (33%)	21,38,41	6.12	7 (33%)
22	QUO	3K	35	22	27,35,36	6.00	9 (33%)	30,52,55	4.08	10 (33%)
22	MIA	3K	38	22	22,31,32	1.46	2 (9%)	26,44,47	1.78	5 (19%)
22	PSU	3K	40	22	15,21,22	1.13	1 (6%)	16,30,33	2.37	4 (25%)
22	5MU	3K	63	22	13,22,23	1.66	2 (15%)	16,32,35	1.53	1 (6%)
22	PSU	3K	64	22	15,21,22	1.21	1 (6%)	16,30,33	1.99	3 (18%)
22	4SU	3K	8	22	12,21,22	3.12	2 (16%)	15,30,33	1.21	1 (6%)

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	1K	17	22	-	0/5/27/28	0/3/3/3
22	QUO	1K	35	24,22	-	0/6/43/44	0/4/4/4

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	MIA	1K	38	22	-	0/11/33/34	0/3/3/3
22	PSU	1K	40	22	-	0/7/25/26	0/2/2/2
22	5MU	1K	63	22	-	0/3/25/26	0/2/2/2
22	PSU	1K	64	22	-	0/7/25/26	0/2/2/2
22	4SU	1K	8	22	-	0/3/25/26	0/2/2/2
23	H2U	2K	21	23	-	0/7/38/39	0/2/2/2
23	OMC	2K	33	23	-	0/5/27/28	0/2/2/2
23	7MG	2K	47	23	-	0/7/37/38	0/3/3/3
23	5MU	2K	55	23	-	0/3/25/26	0/2/2/2
23	PSU	2K	56	23	-	0/7/25/26	0/2/2/2
23	4SU	2K	8	23	-	0/3/25/26	0/2/2/2
56	H2U	2L	21	56	-	0/7/38/39	0/2/2/2
56	OMC	2L	33	56	-	0/5/27/28	0/2/2/2
56	5MU	2L	55	56	-	0/3/25/26	0/2/2/2
56	PSU	2L	56	56	-	0/7/25/26	0/2/2/2
56	4SU	2L	8	56	-	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
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

The worst 5 of 77 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	1K	17	OMG	C8-N7	-13.51	1.08	1.34
22	3K	17	OMG	C8-N7	-13.35	1.09	1.34
22	1K	35	QUO	C8-N9	-10.11	1.23	1.38
22	3K	35	QUO	C8-N9	-9.86	1.24	1.38
22	1K	35	QUO	C6-N1	-9.77	1.15	1.33

The worst 5 of 94 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	1K	35	QUO	C8-N9-C1'	-13.43	114.96	125.45
22	1K	17	OMG	C6-C5-C4	-12.27	106.83	120.86
22	3K	17	OMG	C6-C5-C4	-12.03	107.11	120.86
22	3K	35	QUO	C1'-N9-C4	-10.84	114.70	126.81
22	3K	35	QUO	C8-N9-C1'	-10.84	116.98	125.45

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

20 monomers are involved in 43 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
22	1K	17	OMG	3	0
22	1K	35	QUO	6	0
22	1K	38	MIA	5	0
22	1K	63	5MU	2	0
22	1K	64	PSU	2	0
22	1K	8	4SU	1	0
23	2K	21	H2U	1	0
23	2K	47	7MG	3	0
23	2K	55	5MU	3	0
23	2K	8	4SU	1	0
56	2L	21	H2U	1	0
56	2L	33	OMC	1	0
56	2L	55	5MU	2	0
56	2L	56	PSU	1	0
56	2L	8	4SU	1	0
22	3K	17	OMG	3	0
22	3K	35	QUO	2	0
22	3K	38	MIA	4	0
22	3K	64	PSU	1	0
22	3K	8	4SU	2	0

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 1166 ligands modelled in this entry, 1166 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
54	1G	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	1G	1530:G	O3'	1531:A	P	3.04

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	1498/1522 (98%)	0.03	24 (1%) 74 52	53, 97, 184, 399	0
2	12	237/256 (92%)	-0.05	8 (3%) 49 23	130, 169, 209, 225	0
2	1E	237/256 (92%)	-0.03	5 (2%) 67 42	106, 143, 183, 208	0
3	22	206/239 (86%)	0.31	19 (9%) 11 4	131, 148, 178, 208	0
3	2E	205/239 (85%)	-0.10	2 (0%) 84 66	84, 106, 147, 160	0
4	32	208/209 (99%)	0.96	25 (12%) 6 2	94, 116, 145, 163	0
4	3E	208/209 (99%)	0.56	18 (8%) 13 4	78, 104, 133, 148	0
5	42	151/162 (93%)	0.76	27 (17%) 2 1	104, 129, 145, 174	0
5	4E	151/162 (93%)	0.59	17 (11%) 7 2	73, 99, 121, 159	0
6	52	101/101 (100%)	-0.35	0 100 100	86, 101, 124, 148	0
6	5E	101/101 (100%)	0.11	1 (0%) 84 66	82, 104, 122, 147	0
7	62	155/156 (99%)	0.61	21 (13%) 4 1	107, 125, 147, 172	0
7	6E	155/156 (99%)	0.55	21 (13%) 4 1	99, 117, 150, 172	0
8	72	138/138 (100%)	1.45	40 (28%) 1 0	103, 129, 141, 146	0
8	7E	138/138 (100%)	0.70	24 (17%) 2 1	86, 107, 122, 130	0
9	82	127/128 (99%)	2.63	67 (52%) 0 0	112, 160, 189, 195	0
9	8E	127/128 (99%)	1.73	46 (36%) 0 0	87, 138, 174, 191	0
10	1A	99/105 (94%)	1.38	28 (28%) 1 0	125, 160, 189, 204	0
10	1I	99/105 (94%)	0.87	23 (23%) 1 0	84, 135, 166, 180	0
11	2A	119/129 (92%)	1.00	14 (11%) 6 2	90, 112, 142, 222	0
11	2I	116/129 (89%)	0.54	8 (6%) 20 7	75, 106, 136, 169	0
12	3A	125/132 (94%)	0.51	17 (13%) 4 1	84, 106, 150, 179	0
12	3I	125/132 (94%)	0.36	11 (8%) 12 4	65, 74, 119, 207	0
13	4A	117/126 (92%)	0.84	23 (19%) 1 0	113, 148, 183, 198	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
13	4I	116/126 (92%)	0.30	9 (7%) 16 5	82, 125, 146, 160	0
14	5A	58/61 (95%)	3.45	41 (70%) 0 0	130, 150, 162, 165	0
14	5I	61/61 (100%)	0.89	9 (14%) 3 1	85, 96, 116, 139	0
15	6A	88/89 (98%)	0.37	5 (5%) 27 11	82, 113, 134, 140	0
15	6I	88/89 (98%)	0.47	4 (4%) 37 17	78, 99, 119, 132	0
16	7A	84/88 (95%)	1.87	34 (40%) 0 0	88, 105, 134, 165	0
16	7I	84/88 (95%)	2.61	48 (57%) 0 0	97, 113, 152, 171	0
17	8A	100/105 (95%)	0.86	21 (21%) 1 0	92, 111, 131, 172	0
17	8I	100/105 (95%)	0.61	12 (12%) 6 2	85, 103, 119, 129	0
18	9A	69/88 (78%)	0.02	2 (2%) 55 29	94, 116, 143, 162	0
18	9I	72/88 (81%)	0.14	0 100 100	87, 108, 156, 177	0
19	AA	82/93 (88%)	0.86	11 (13%) 4 1	144, 164, 200, 218	0
19	AI	83/93 (89%)	0.28	5 (6%) 25 10	93, 125, 162, 185	0
20	BA	99/106 (93%)	1.10	22 (22%) 1 0	85, 108, 139, 170	0
20	BI	99/106 (93%)	1.20	34 (34%) 0 0	107, 121, 164, 171	0
21	1B	25/27 (92%)	5.68	22 (88%) 0 0	114, 135, 154, 180	0
21	1F	22/27 (81%)	3.17	14 (63%) 0 0	96, 108, 115, 122	0
22	1K	78/85 (91%)	0.14	5 (6%) 23 8	84, 149, 162, 175	0
22	3K	78/85 (91%)	-0.27	3 (3%) 44 20	68, 166, 190, 197	0
23	2K	71/77 (92%)	-0.09	1 (1%) 78 57	65, 89, 122, 126	0
24	4K	15/27 (55%)	1.95	6 (40%) 0 0	68, 100, 173, 180	0
25	14	2907/2917 (99%)	0.05	40 (1%) 78 57	46, 81, 243, 482	0
25	1H	2912/2917 (99%)	0.08	20 (0%) 89 75	35, 69, 228, 380	0
26	16	122/122 (100%)	-0.31	0 100 100	64, 90, 115, 254	0
26	1J	122/122 (100%)	-0.43	0 100 100	79, 115, 142, 216	0
27	11	272/276 (98%)	0.19	1 (0%) 93 84	38, 61, 80, 92	0
27	19	273/276 (98%)	0.54	16 (5%) 26 10	43, 70, 87, 100	0
28	21	205/206 (99%)	0.52	10 (4%) 33 14	46, 86, 143, 168	0
28	29	205/206 (99%)	0.84	32 (15%) 3 1	56, 90, 162, 204	0
29	31	202/210 (96%)	0.08	0 100 100	41, 75, 128, 144	0
29	39	208/210 (99%)	0.20	10 (4%) 34 15	56, 99, 181, 218	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
30	41	181/182 (99%)	0.43	9 (4%) 32 13	81, 107, 149, 173	0
30	49	181/182 (99%)	0.48	19 (10%) 8 3	110, 135, 175, 194	0
31	51	174/180 (96%)	0.25	8 (4%) 36 16	80, 105, 120, 146	0
31	59	171/180 (95%)	1.96	67 (39%) 0 0	138, 195, 241, 262	0
32	61	146/148 (98%)	0.11	6 (4%) 41 18	72, 128, 153, 163	0
32	69	146/148 (98%)	0.37	14 (9%) 10 3	77, 127, 159, 170	0
33	15	138/140 (98%)	0.97	26 (18%) 2 0	72, 103, 140, 162	0
33	58	138/140 (98%)	0.31	5 (3%) 46 21	62, 87, 134, 151	0
34	25	122/122 (100%)	0.35	6 (4%) 33 14	62, 84, 103, 109	0
34	68	122/122 (100%)	0.11	2 (1%) 74 52	53, 73, 90, 105	0
35	35	150/150 (100%)	0.93	28 (18%) 2 0	57, 105, 148, 199	0
35	78	150/150 (100%)	0.37	5 (3%) 50 24	43, 80, 110, 179	0
36	45	138/141 (97%)	1.83	53 (38%) 0 0	72, 104, 132, 153	0
36	88	141/141 (100%)	0.58	4 (2%) 56 30	55, 77, 101, 124	0
37	55	117/118 (99%)	0.62	14 (11%) 6 2	56, 76, 93, 114	0
37	98	118/118 (100%)	0.47	7 (5%) 26 10	56, 80, 99, 114	0
38	65	111/112 (99%)	0.81	17 (15%) 3 1	88, 112, 136, 157	0
38	A8	111/112 (99%)	0.15	4 (3%) 46 21	72, 87, 122, 145	0
39	75	137/146 (93%)	0.35	7 (5%) 32 13	75, 92, 156, 208	0
39	B8	136/146 (93%)	0.16	2 (1%) 76 55	70, 91, 146, 166	0
40	85	117/118 (99%)	0.82	15 (12%) 5 2	61, 89, 141, 183	0
40	C8	117/118 (99%)	0.74	12 (10%) 9 3	49, 77, 129, 152	0
41	95	101/101 (100%)	0.66	16 (15%) 3 1	59, 129, 145, 163	0
41	D8	101/101 (100%)	0.30	4 (3%) 42 19	52, 106, 146, 167	0
42	A5	113/113 (100%)	0.56	6 (5%) 30 12	58, 71, 109, 189	0
42	E8	113/113 (100%)	0.36	1 (0%) 85 69	51, 69, 100, 167	0
43	B5	92/96 (95%)	0.18	4 (4%) 39 17	64, 79, 106, 118	0
43	F8	94/96 (97%)	-0.08	0 100 100	52, 68, 95, 109	0
44	C5	104/110 (94%)	1.30	27 (25%) 1 0	90, 118, 184, 206	0
44	G8	102/110 (92%)	0.63	4 (3%) 43 20	64, 93, 138, 169	0
45	D5	179/206 (86%)	1.13	40 (22%) 1 0	111, 159, 253, 266	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
45	H8	175/206 (84%)	-0.01	4 (2%) 64 38	83, 130, 215, 234	0
46	E5	77/85 (90%)	1.19	16 (20%) 1 0	64, 85, 108, 157	0
46	I8	77/85 (90%)	0.68	7 (9%) 11 4	53, 69, 93, 148	0
47	F5	97/98 (98%)	1.45	18 (18%) 2 0	57, 80, 139, 192	0
47	J8	93/98 (94%)	0.85	8 (8%) 13 4	48, 68, 134, 163	0
48	G5	66/72 (91%)	0.08	0 100 100	78, 100, 122, 175	0
48	K8	66/72 (91%)	0.56	5 (7%) 17 6	54, 78, 98, 148	0
49	H5	59/60 (98%)	1.42	15 (25%) 1 0	77, 97, 153, 166	0
49	L8	59/60 (98%)	0.41	1 (1%) 73 49	58, 77, 114, 136	0
50	I5	63/71 (88%)	1.99	26 (41%) 0 0	153, 212, 237, 256	0
50	M8	66/71 (92%)	0.71	8 (12%) 6 2	111, 171, 226, 241	0
51	J5	58/60 (96%)	0.32	2 (3%) 49 23	55, 84, 168, 218	0
51	N8	49/60 (81%)	0.44	0 100 100	45, 64, 135, 149	0
52	L5	45/49 (91%)	0.52	1 (2%) 65 40	47, 56, 67, 77	0
52	P8	45/49 (91%)	0.17	1 (2%) 65 40	38, 45, 58, 78	0
53	M5	60/65 (92%)	1.42	15 (25%) 1 0	66, 77, 112, 129	0
53	Q8	62/65 (95%)	1.51	19 (30%) 1 0	56, 70, 96, 108	0
54	1G	1498/1522 (98%)	0.07	40 (2%) 58 32	69, 115, 181, 370	0
55	1L	85/85 (100%)	1.93	28 (32%) 0 0	124, 157, 168, 180	0
55	3L	85/85 (100%)	0.08	2 (2%) 62 37	75, 171, 201, 208	0
56	2L	72/77 (93%)	-0.28	1 (1%) 78 57	74, 105, 136, 141	0
57	4L	16/27 (59%)	2.46	8 (50%) 0 0	93, 136, 209, 217	0
All	All	20977/21616 (97%)	0.39	1583 (7%) 17 6	35, 99, 186, 482	0

The worst 5 of 1583 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
11	2A	129	SER	23.9
47	F5	98	LEU	19.3
31	59	100	GLY	15.5
11	2A	128	ALA	15.0
47	F5	97	LEU	12.2

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
23	7MG	2K	47	24/25	0.95	0.14	-	91,98,108,113	0
56	PSU	2L	56	20/21	0.90	0.10	-	110,113,122,124	0
22	OMG	1K	17	24/25	0.79	0.19	-	131,142,162,173	0
22	PSU	3K	64	20/21	0.81	0.17	-	152,161,169,173	0
22	OMG	3K	17	24/25	0.85	0.16	-	155,167,174,174	0
22	MIA	3K	38	29/30	0.94	0.18	-	107,114,119,123	0
56	5MU	2L	55	21/22	0.95	0.10	-	109,115,121,126	0
22	5MU	1K	63	21/22	0.89	0.18	-	115,124,133,139	0
56	4SU	2L	8	20/21	0.91	0.12	-	108,114,119,122	0
56	OMC	2L	33	21/22	0.96	0.23	-	96,98,101,111	0
22	PSU	1K	40	20/21	0.93	0.17	-	75,99,107,110	0
23	5MU	2K	55	21/22	0.97	0.15	-	92,101,109,115	0
22	4SU	1K	8	20/21	0.86	0.14	-	137,141,150,153	0
22	PSU	3K	40	20/21	0.96	0.11	-	104,112,115,117	0
22	MIA	1K	38	29/30	0.94	0.32	-	76,87,107,110	0
22	5MU	3K	63	21/22	0.80	0.20	-	141,157,163,170	0
23	4SU	2K	8	20/21	0.96	0.15	-	87,91,95,95	0
23	PSU	2K	56	20/21	0.95	0.13	-	92,97,108,110	0
23	H2U	2K	21	20/21	0.86	0.19	-	113,120,123,125	0
22	PSU	1K	64	20/21	0.90	0.17	-	116,128,135,140	0
22	4SU	3K	8	20/21	0.83	0.12	-	159,163,169,172	0
56	H2U	2L	21	20/21	0.72	0.21	-	126,132,139,144	0
22	QUO	1K	35	32/33	0.93	0.35	-	71,90,101,103	0
23	OMC	2K	33	21/22	0.96	0.27	-	70,76,81,84	0
22	QUO	3K	35	32/33	0.91	0.26	-	107,114,128,136	0

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. 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
58	MG	13	1657	1/1	0.93	0.23	33.48	74,74,74,74	0
58	MG	1H	3154	1/1	0.96	0.32	25.09	52,52,52,52	0
58	MG	1H	3231	1/1	0.82	0.31	19.32	110,110,110,110	0
58	MG	1H	3055	1/1	0.99	0.36	18.87	41,41,41,41	0
58	MG	1H	3292	1/1	0.93	0.90	17.03	50,50,50,50	0
58	MG	1H	3081	1/1	0.94	0.37	13.49	67,67,67,67	0
58	MG	1H	3347	1/1	0.88	0.31	12.98	64,64,64,64	0
58	MG	1H	3090	1/1	0.98	0.27	12.28	45,45,45,45	0
58	MG	14	3247	1/1	0.93	0.47	11.99	64,64,64,64	0
58	MG	13	1618	1/1	0.96	0.31	11.70	92,92,92,92	0
58	MG	1H	3350	1/1	0.97	0.35	10.70	62,62,62,62	0
58	MG	14	3319	1/1	0.83	0.34	10.70	96,96,96,96	0
58	MG	1H	3356	1/1	0.98	0.34	10.59	55,55,55,55	0
58	MG	1H	3299	1/1	0.90	0.34	9.69	60,60,60,60	0
58	MG	14	3187	1/1	0.76	0.48	9.62	88,88,88,88	0
58	MG	1H	3007	1/1	0.98	0.34	9.43	45,45,45,45	0
58	MG	14	3217	1/1	0.97	0.39	9.35	79,79,79,79	0
58	MG	13	1629	1/1	0.98	0.32	9.15	45,45,45,45	0
58	MG	1H	3338	1/1	0.79	0.31	8.48	80,80,80,80	0
58	MG	13	1718	1/1	0.89	0.29	8.40	113,113,113,113	0
58	MG	1H	3288	1/1	0.86	0.28	8.22	76,76,76,76	0
58	MG	1H	3331	1/1	0.93	0.28	8.06	72,72,72,72	0
58	MG	1H	3188	1/1	0.91	0.29	7.86	60,60,60,60	0
58	MG	13	1664	1/1	0.95	0.26	7.33	71,71,71,71	0
58	MG	1H	3051	1/1	0.99	0.38	7.31	57,57,57,57	0
58	MG	14	3274	1/1	0.92	0.47	7.18	77,77,77,77	0
58	MG	14	3244	1/1	0.96	0.42	7.04	61,61,61,61	0
58	MG	1H	3043	1/1	0.96	0.26	6.94	62,62,62,62	0
58	MG	14	3303	1/1	0.87	0.40	6.91	73,73,73,73	0
58	MG	14	3074	1/1	0.99	0.28	6.74	41,41,41,41	0
58	MG	14	3149	1/1	0.97	0.23	6.56	69,69,69,69	0
58	MG	1H	3100	1/1	0.90	0.38	6.42	46,46,46,46	0
58	MG	1H	3238	1/1	0.83	0.31	6.35	67,67,67,67	0
58	MG	14	3172	1/1	0.95	0.21	6.33	64,64,64,64	0
58	MG	1H	3197	1/1	0.87	0.23	6.11	61,61,61,61	0
58	MG	1H	3161	1/1	0.88	0.28	5.65	68,68,68,68	0
58	MG	1H	3166	1/1	0.94	0.25	5.64	58,58,58,58	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
58	MG	1G	1665	1/1	0.90	0.27	5.53	77,77,77,77	0
58	MG	14	3316	1/1	0.63	0.28	5.49	96,96,96,96	0
58	MG	13	1695	1/1	0.93	0.30	5.42	75,75,75,75	0
58	MG	14	3038	1/1	0.95	0.29	5.19	71,71,71,71	0
58	MG	16	211	1/1	0.91	0.26	5.19	80,80,80,80	0
58	MG	1H	3220	1/1	0.94	0.22	5.18	64,64,64,64	0
58	MG	16	201	1/1	0.95	0.23	5.05	75,75,75,75	0
58	MG	14	3186	1/1	0.95	0.27	4.78	65,65,65,65	0
58	MG	14	3160	1/1	0.97	0.19	4.66	80,80,80,80	0
58	MG	13	1705	1/1	0.92	0.32	4.62	127,127,127,127	0
58	MG	14	3281	1/1	0.94	0.63	4.57	67,67,67,67	0
58	MG	1H	3085	1/1	0.95	0.33	4.52	48,48,48,48	0
58	MG	16	206	1/1	0.93	0.18	4.46	78,78,78,78	0
58	MG	14	3227	1/1	0.97	0.29	4.24	51,51,51,51	0
58	MG	14	3073	1/1	0.98	0.30	4.12	37,37,37,37	0
58	MG	14	3176	1/1	0.88	0.20	4.08	71,71,71,71	0
58	MG	1H	3263	1/1	0.77	0.20	3.82	61,61,61,61	0
58	MG	2K	103	1/1	0.51	0.22	3.54	80,80,80,80	0
58	MG	14	3022	1/1	0.95	0.28	3.51	80,80,80,80	0
58	MG	1H	3025	1/1	0.97	0.28	3.50	47,47,47,47	0
58	MG	1H	3016	1/1	0.99	0.29	3.47	45,45,45,45	0
58	MG	1H	3070	1/1	0.92	0.26	3.46	55,55,55,55	0
58	MG	1H	3121	1/1	0.97	0.26	3.37	41,41,41,41	0
58	MG	14	3148	1/1	0.90	0.20	3.28	79,79,79,79	0
58	MG	1H	3199	1/1	0.93	0.26	3.22	63,63,63,63	0
58	MG	1G	1647	1/1	0.87	0.27	3.09	83,83,83,83	0
58	MG	14	3072	1/1	0.97	0.30	3.02	56,56,56,56	0
59	ZN	3E	302	1/1	0.98	0.37	2.94	89,89,89,89	0
58	MG	1H	3162	1/1	0.97	0.39	2.93	57,57,57,57	0
58	MG	1H	3054	1/1	0.99	0.27	2.93	57,57,57,57	0
58	MG	1H	3164	1/1	0.88	0.23	2.91	78,78,78,78	0
58	MG	1H	3261	1/1	0.70	0.24	2.87	66,66,66,66	0
58	MG	1H	3342	1/1	0.84	0.23	2.65	70,70,70,70	0
58	MG	14	3065	1/1	0.99	0.29	2.58	39,39,39,39	0
58	MG	1H	3053	1/1	0.95	0.28	2.57	33,33,33,33	0
58	MG	14	3222	1/1	0.91	0.26	2.55	58,58,58,58	0
58	MG	13	1636	1/1	0.98	0.22	2.44	65,65,65,65	0
58	MG	1H	3206	1/1	0.95	0.22	2.41	65,65,65,65	0
58	MG	1H	3204	1/1	0.93	0.24	2.16	72,72,72,72	0
58	MG	1H	3066	1/1	0.89	0.23	2.12	71,71,71,71	0
58	MG	1H	3258	1/1	0.90	0.25	2.02	55,55,55,55	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
58	MG	14	3087	1/1	0.92	0.23	2.01	41,41,41,41	0
58	MG	13	1661	1/1	0.97	0.29	2.00	82,82,82,82	0
58	MG	14	3122	1/1	0.97	0.24	1.96	54,54,54,54	0
58	MG	1H	3074	1/1	0.84	0.25	1.84	58,58,58,58	0
58	MG	1H	3117	1/1	0.95	0.30	1.79	54,54,54,54	0
58	MG	1H	3052	1/1	0.92	0.24	1.72	63,63,63,63	0
58	MG	1H	3015	1/1	0.99	0.27	1.71	46,46,46,46	0
59	ZN	32	301	1/1	0.99	0.34	1.33	103,103,103,103	0
58	MG	14	3032	1/1	0.98	0.22	1.29	54,54,54,54	0
58	MG	16	205	1/1	0.80	0.19	1.22	87,87,87,87	0
58	MG	1G	1651	1/1	0.97	0.25	1.19	71,71,71,71	0
58	MG	13	1625	1/1	0.94	0.25	1.15	58,58,58,58	0
58	MG	1H	3125	1/1	0.93	0.24	1.12	46,46,46,46	0
58	MG	14	3306	1/1	0.71	0.23	1.04	66,66,66,66	0
58	MG	14	3002	1/1	0.97	0.21	1.04	43,43,43,43	0
58	MG	1H	3133	1/1	0.94	0.21	1.02	43,43,43,43	0
58	MG	14	3109	1/1	0.97	0.21	1.02	60,60,60,60	0
58	MG	1H	3101	1/1	0.96	0.25	0.99	30,30,30,30	0
58	MG	1H	3031	1/1	0.97	0.23	0.94	60,60,60,60	0
58	MG	14	3322	1/1	0.89	0.18	0.92	73,73,73,73	0
58	MG	14	3246	1/1	0.97	0.21	0.91	76,76,76,76	0
58	MG	14	3224	1/1	0.92	0.28	0.89	59,59,59,59	0
58	MG	31	301	1/1	0.87	0.23	0.86	56,56,56,56	0
58	MG	13	1688	1/1	0.89	0.19	0.83	101,101,101,101	0
58	MG	13	1643	1/1	0.99	0.22	0.83	50,50,50,50	0
58	MG	1H	3116	1/1	0.95	0.21	0.79	52,52,52,52	0
58	MG	14	3108	1/1	0.92	0.20	0.76	55,55,55,55	0
58	MG	1H	3037	1/1	0.94	0.20	0.76	47,47,47,47	0
58	MG	1H	3215	1/1	0.91	0.20	0.73	52,52,52,52	0
58	MG	14	3103	1/1	0.99	0.22	0.68	36,36,36,36	0
58	MG	1H	3073	1/1	0.93	0.26	0.59	52,52,52,52	0
58	MG	13	1623	1/1	0.98	0.26	0.52	56,56,56,56	0
58	MG	1H	3137	1/1	0.86	0.21	0.51	49,49,49,49	0
58	MG	13	1638	1/1	0.92	0.22	0.50	78,78,78,78	0
58	MG	14	3088	1/1	0.97	0.20	0.49	47,47,47,47	0
58	MG	1H	3077	1/1	0.96	0.22	0.48	47,47,47,47	0
58	MG	1H	3144	1/1	0.97	0.26	0.45	47,47,47,47	0
58	MG	13	1650	1/1	0.85	0.30	0.41	76,76,76,76	0
58	MG	1H	3349	1/1	0.90	0.20	0.38	62,62,62,62	0
58	MG	13	1607	1/1	0.97	0.23	0.37	69,69,69,69	0
58	MG	14	3104	1/1	0.97	0.26	0.36	42,42,42,42	0
58	MG	85	201	1/1	0.93	0.29	0.36	64,64,64,64	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
59	ZN	G8	201	1/1	0.73	0.33	0.36	185,185,185,185	0
58	MG	1H	3131	1/1	0.94	0.21	0.32	60,60,60,60	0
58	MG	14	3396	1/1	0.95	0.29	0.31	75,75,75,75	0
58	MG	1H	3139	1/1	0.94	0.19	0.24	48,48,48,48	0
58	MG	1G	1644	1/1	0.96	0.20	0.22	83,83,83,83	0
58	MG	1G	1619	1/1	0.97	0.18	0.21	88,88,88,88	0
58	MG	1H	3286	1/1	0.94	0.25	0.21	67,67,67,67	0
58	MG	14	3254	1/1	0.76	0.21	0.19	94,94,94,94	0
58	MG	3E	301	1/1	0.70	0.24	0.18	115,115,115,115	0
58	MG	14	3083	1/1	0.97	0.22	0.14	58,58,58,58	0
58	MG	1H	3018	1/1	0.96	0.29	0.09	48,48,48,48	0
58	MG	1G	1677	1/1	0.80	0.18	0.07	99,99,99,99	0
58	MG	14	3028	1/1	0.95	0.15	0.07	76,76,76,76	0
58	MG	14	3094	1/1	0.98	0.21	0.02	40,40,40,40	0
58	MG	1H	3096	1/1	0.98	0.21	-0.03	40,40,40,40	0
58	MG	1H	3124	1/1	0.99	0.20	-0.03	43,43,43,43	0
58	MG	13	1601	1/1	0.98	0.21	-0.04	59,59,59,59	0
58	MG	13	1617	1/1	0.98	0.27	-0.04	87,87,87,87	0
58	MG	1H	3165	1/1	0.93	0.20	-0.17	68,68,68,68	0
58	MG	1G	1601	1/1	0.98	0.22	-0.20	77,77,77,77	0
58	MG	1H	3058	1/1	0.98	0.23	-0.23	50,50,50,50	0
58	MG	13	1622	1/1	0.82	0.17	-0.28	64,64,64,64	0
58	MG	1H	3036	1/1	0.79	0.17	-0.30	67,67,67,67	0
58	MG	14	3282	1/1	0.96	0.25	-0.30	62,62,62,62	0
58	MG	14	3077	1/1	0.94	0.21	-0.34	68,68,68,68	0
58	MG	1J	206	1/1	0.93	0.14	-0.36	109,109,109,109	0
58	MG	98	202	1/1	0.92	0.20	-0.37	90,90,90,90	0
58	MG	14	3025	1/1	0.94	0.20	-0.40	79,79,79,79	0
58	MG	14	3079	1/1	0.97	0.20	-0.42	55,55,55,55	0
58	MG	14	3085	1/1	0.67	0.32	-0.43	59,59,59,59	0
58	MG	29	303	1/1	0.86	0.25	-0.49	63,63,63,63	0
58	MG	14	3018	1/1	0.98	0.16	-0.51	79,79,79,79	0
58	MG	1G	1655	1/1	0.90	0.18	-0.51	112,112,112,112	0
58	MG	14	3067	1/1	0.98	0.20	-0.53	54,54,54,54	0
58	MG	1H	3009	1/1	0.97	0.23	-0.54	42,42,42,42	0
58	MG	2L	101	1/1	0.95	0.19	-0.56	69,69,69,69	0
58	MG	29	302	1/1	0.61	0.26	-0.56	68,68,68,68	0
58	MG	1H	3034	1/1	0.98	0.22	-0.58	71,71,71,71	0
58	MG	1H	3091	1/1	0.92	0.21	-0.59	62,62,62,62	0
58	MG	1H	3149	1/1	0.97	0.21	-0.60	42,42,42,42	0
58	MG	1H	3418	1/1	0.91	0.19	-0.61	52,52,52,52	0
58	MG	1G	1666	1/1	0.74	0.21	-0.63	117,117,117,117	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
58	MG	1H	3147	1/1	0.99	0.20	-0.64	57,57,57,57	0
58	MG	14	3011	1/1	0.94	0.18	-0.65	48,48,48,48	0
58	MG	1J	201	1/1	0.97	0.16	-0.66	100,100,100,100	0
59	ZN	5I	101	1/1	0.99	0.18	-0.71	88,88,88,88	0
58	MG	1H	3038	1/1	0.96	0.16	-0.71	46,46,46,46	0
58	MG	13	1639	1/1	0.89	0.17	-0.71	69,69,69,69	0
58	MG	13	1710	1/1	0.82	0.20	-0.74	77,77,77,77	0
59	ZN	C5	202	1/1	0.80	0.15	-0.77	194,194,194,194	0
58	MG	13	1698	1/1	0.76	0.17	-0.79	83,83,83,83	0
58	MG	1H	3213	1/1	0.92	0.18	-0.81	63,63,63,63	0
58	MG	13	1606	1/1	0.96	0.17	-0.83	70,70,70,70	0
58	MG	14	3003	1/1	0.98	0.19	-0.83	49,49,49,49	0
58	MG	14	3191	1/1	0.98	0.22	-0.86	66,66,66,66	0
58	MG	14	3334	1/1	0.95	0.18	-0.86	48,48,48,48	0
58	MG	1H	3020	1/1	0.97	0.22	-0.87	38,38,38,38	0
58	MG	1H	3241	1/1	0.93	0.18	-0.88	65,65,65,65	0
58	MG	1G	1646	1/1	0.95	0.20	-0.90	117,117,117,117	0
58	MG	14	3066	1/1	0.98	0.18	-0.95	54,54,54,54	0
58	MG	14	3155	1/1	0.93	0.17	-0.96	57,57,57,57	0
58	MG	1G	1642	1/1	0.94	0.12	-0.96	80,80,80,80	0
58	MG	1G	1687	1/1	0.83	0.08	-0.97	106,106,106,106	0
58	MG	14	3293	1/1	0.90	0.13	-0.98	71,71,71,71	0
58	MG	14	3092	1/1	0.96	0.16	-0.99	59,59,59,59	0
58	MG	13	1686	1/1	0.95	0.17	-1.01	89,89,89,89	0
58	MG	14	3218	1/1	0.97	0.16	-1.02	89,89,89,89	0
58	MG	2K	101	1/1	0.99	0.21	-1.03	55,55,55,55	0
58	MG	14	3121	1/1	0.98	0.16	-1.04	64,64,64,64	0
58	MG	14	3033	1/1	0.98	0.15	-1.04	56,56,56,56	0
58	MG	1H	3028	1/1	0.98	0.18	-1.04	51,51,51,51	0
58	MG	1G	1617	1/1	0.97	0.16	-1.05	96,96,96,96	0
58	MG	14	3236	1/1	0.95	0.11	-1.05	71,71,71,71	0
58	MG	13	1694	1/1	0.86	0.15	-1.05	82,82,82,82	0
58	MG	1H	3021	1/1	0.97	0.20	-1.06	43,43,43,43	0
58	MG	14	3061	1/1	0.97	0.23	-1.06	43,43,43,43	0
58	MG	13	1723	1/1	0.77	0.14	-1.06	77,77,77,77	0
58	MG	1H	3087	1/1	0.93	0.16	-1.07	61,61,61,61	0
58	MG	14	3219	1/1	0.95	0.13	-1.07	68,68,68,68	0
59	ZN	5A	101	1/1	0.93	0.13	-1.08	132,132,132,132	0
58	MG	14	3315	1/1	0.92	0.16	-1.10	67,67,67,67	0
58	MG	14	3253	1/1	0.94	0.14	-1.12	83,83,83,83	0
58	MG	14	3382	1/1	0.94	0.14	-1.14	60,60,60,60	0
58	MG	1H	3169	1/1	0.91	0.17	-1.15	58,58,58,58	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
58	MG	14	3152	1/1	0.98	0.18	-1.16	72,72,72,72	0
58	MG	14	3045	1/1	0.97	0.16	-1.16	44,44,44,44	0
58	MG	14	3263	1/1	0.92	0.12	-1.17	84,84,84,84	0
58	MG	1H	3190	1/1	0.94	0.16	-1.20	50,50,50,50	0
58	MG	14	3137	1/1	0.98	0.19	-1.22	65,65,65,65	0
58	MG	1H	3041	1/1	0.94	0.14	-1.22	51,51,51,51	0
58	MG	1G	1654	1/1	0.77	0.16	-1.24	110,110,110,110	0
58	MG	1G	1625	1/1	0.87	0.20	-1.24	90,90,90,90	0
58	MG	1H	3175	1/1	0.62	0.17	-1.24	58,58,58,58	0
58	MG	14	3183	1/1	0.94	0.13	-1.27	60,60,60,60	0
58	MG	14	3359	1/1	0.84	0.19	-1.28	73,73,73,73	0
58	MG	1G	1620	1/1	0.80	0.14	-1.29	91,91,91,91	0
58	MG	1H	3194	1/1	0.92	0.20	-1.30	55,55,55,55	0
58	MG	14	3211	1/1	0.94	0.16	-1.31	60,60,60,60	0
58	MG	2I	302	1/1	0.88	0.18	-1.32	69,69,69,69	0
58	MG	1H	3150	1/1	0.92	0.17	-1.34	48,48,48,48	0
58	MG	13	1728	1/1	0.83	0.06	-1.35	101,101,101,101	0
58	MG	1H	3227	1/1	0.95	0.15	-1.38	63,63,63,63	0
58	MG	13	1662	1/1	0.88	0.09	-1.42	81,81,81,81	0
58	MG	1H	3098	1/1	0.91	0.17	-1.43	44,44,44,44	0
58	MG	13	1605	1/1	0.98	0.11	-1.44	77,77,77,77	0
58	MG	14	3114	1/1	0.97	0.20	-1.44	65,65,65,65	0
58	MG	14	3013	1/1	0.99	0.18	-1.46	56,56,56,56	0
58	MG	14	3024	1/1	0.96	0.14	-1.49	70,70,70,70	0
58	MG	14	3285	1/1	0.95	0.18	-1.51	74,74,74,74	0
58	MG	1H	3262	1/1	0.80	0.17	-1.52	56,56,56,56	0
58	MG	14	3054	1/1	0.99	0.15	-1.58	48,48,48,48	0
58	MG	13	1609	1/1	0.98	0.19	-1.58	72,72,72,72	0
58	MG	1H	3064	1/1	0.87	0.18	-1.58	55,55,55,55	0
58	MG	1H	3002	1/1	0.99	0.19	-1.59	38,38,38,38	0
58	MG	14	3245	1/1	0.86	0.14	-1.60	69,69,69,69	0
58	MG	1H	3141	1/1	0.90	0.10	-1.66	70,70,70,70	0
58	MG	1H	3193	1/1	0.94	0.18	-1.68	52,52,52,52	0
58	MG	1H	3014	1/1	0.95	0.18	-1.69	33,33,33,33	0
58	MG	1I	301	1/1	0.89	0.22	-1.69	39,39,39,39	0
58	MG	1H	3432	1/1	0.89	0.12	-1.73	77,77,77,77	0
58	MG	14	3133	1/1	0.90	0.13	-1.73	58,58,58,58	0
58	MG	1H	3395	1/1	0.98	0.17	-1.76	40,40,40,40	0
58	MG	1G	1616	1/1	0.86	0.14	-1.79	56,56,56,56	0
58	MG	1G	1602	1/1	0.96	0.21	-1.80	64,64,64,64	0
58	MG	3I	303	1/1	0.81	0.15	-1.81	63,63,63,63	0
58	MG	14	3250	1/1	0.89	0.15	-1.82	70,70,70,70	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
58	MG	14	3042	1/1	0.98	0.18	-1.82	46,46,46,46	0
58	MG	14	3041	1/1	0.98	0.12	-1.82	35,35,35,35	0
58	MG	39	301	1/1	0.80	0.12	-1.88	60,60,60,60	0
58	MG	1G	1607	1/1	0.95	0.08	-1.90	92,92,92,92	0
58	MG	14	3203	1/1	0.96	0.23	-1.90	47,47,47,47	0
58	MG	14	3238	1/1	0.87	0.14	-1.94	83,83,83,83	0
58	MG	16	204	1/1	0.81	0.12	-1.97	75,75,75,75	0
58	MG	1H	3123	1/1	0.95	0.10	-1.98	32,32,32,32	0
58	MG	14	3053	1/1	0.94	0.12	-2.08	57,57,57,57	0
58	MG	14	3362	1/1	0.94	0.17	-2.10	70,70,70,70	0
58	MG	1H	3433	1/1	0.83	0.12	-2.11	53,53,53,53	0
58	MG	14	3208	1/1	0.92	0.16	-2.14	58,58,58,58	0
58	MG	1H	3274	1/1	0.95	0.14	-2.15	59,59,59,59	0
58	MG	13	1724	1/1	0.95	0.07	-2.15	87,87,87,87	0
58	MG	14	3016	1/1	0.97	0.15	-2.16	53,53,53,53	0
58	MG	14	3332	1/1	0.95	0.14	-2.17	62,62,62,62	0
58	MG	14	3336	1/1	0.92	0.11	-2.18	48,48,48,48	0
58	MG	13	1633	1/1	0.91	0.16	-2.19	54,54,54,54	0
58	MG	14	3329	1/1	0.92	0.10	-2.19	56,56,56,56	0
58	MG	14	3207	1/1	0.96	0.17	-2.19	53,53,53,53	0
58	MG	1H	3371	1/1	0.97	0.16	-2.23	59,59,59,59	0
58	MG	14	3387	1/1	0.74	0.09	-2.26	86,86,86,86	0
58	MG	14	3351	1/1	0.98	0.17	-2.27	60,60,60,60	0
58	MG	1H	3118	1/1	0.98	0.17	-2.27	36,36,36,36	0
58	MG	14	3142	1/1	0.83	0.17	-2.27	62,62,62,62	0
58	MG	1H	3146	1/1	0.93	0.16	-2.27	62,62,62,62	0
58	MG	13	1719	1/1	0.88	0.11	-2.28	89,89,89,89	0
58	MG	14	3043	1/1	0.99	0.21	-2.29	47,47,47,47	0
58	MG	14	3178	1/1	0.92	0.10	-2.29	85,85,85,85	0
58	MG	1H	3102	1/1	0.95	0.18	-2.29	44,44,44,44	0
58	MG	16	210	1/1	0.97	0.14	-2.32	63,63,63,63	0
58	MG	13	1691	1/1	0.98	0.14	-2.34	71,71,71,71	0
58	MG	14	3140	1/1	0.77	0.13	-2.37	61,61,61,61	0
58	MG	14	3204	1/1	0.88	0.14	-2.39	48,48,48,48	0
58	MG	1H	3156	1/1	0.96	0.16	-2.41	44,44,44,44	0
58	MG	1H	3449	1/1	0.97	0.08	-2.41	74,74,74,74	0
58	MG	14	3369	1/1	0.96	0.12	-2.41	69,69,69,69	0
58	MG	14	3075	1/1	0.99	0.19	-2.43	53,53,53,53	0
58	MG	14	3328	1/1	0.97	0.16	-2.48	55,55,55,55	0
58	MG	1H	3275	1/1	0.91	0.14	-2.52	53,53,53,53	0
58	MG	1H	3273	1/1	0.94	0.12	-2.52	66,66,66,66	0
58	MG	1G	1614	1/1	0.97	0.17	-2.53	73,73,73,73	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
58	MG	14	3124	1/1	0.93	0.15	-2.55	43,43,43,43	0
58	MG	14	3230	1/1	0.94	0.12	-2.55	63,63,63,63	0
58	MG	13	1656	1/1	0.91	0.13	-2.59	72,72,72,72	0
58	MG	13	1644	1/1	0.98	0.14	-2.71	56,56,56,56	0
58	MG	14	3350	1/1	0.95	0.13	-2.71	61,61,61,61	0
58	MG	1H	3417	1/1	0.94	0.12	-2.75	51,51,51,51	0
58	MG	1H	3076	1/1	0.98	0.15	-2.75	53,53,53,53	0
58	MG	14	3384	1/1	0.83	0.10	-2.79	71,71,71,71	0
58	MG	1H	3112	1/1	0.86	0.14	-2.81	33,33,33,33	0
58	MG	31	304	1/1	0.91	0.11	-2.83	48,48,48,48	0
58	MG	1H	3389	1/1	0.97	0.10	-2.83	49,49,49,49	0
58	MG	1G	1686	1/1	0.92	0.09	-2.88	83,83,83,83	0
58	MG	1H	3006	1/1	0.95	0.14	-2.91	42,42,42,42	0
58	MG	1G	1641	1/1	0.91	0.09	-2.92	94,94,94,94	0
58	MG	1H	3067	1/1	0.99	0.15	-2.92	53,53,53,53	0
58	MG	1H	3168	1/1	0.88	0.17	-2.92	64,64,64,64	0
58	MG	14	3209	1/1	0.94	0.12	-2.94	63,63,63,63	0
58	MG	1H	3253	1/1	0.78	0.15	-2.95	47,47,47,47	0
58	MG	14	3029	1/1	0.92	0.11	-2.96	77,77,77,77	0
58	MG	1H	3042	1/1	0.98	0.17	-2.97	48,48,48,48	0
58	MG	13	1645	1/1	0.94	0.14	-2.97	65,65,65,65	0
58	MG	1G	1609	1/1	0.95	0.14	-2.98	81,81,81,81	0
58	MG	1H	3348	1/1	0.90	0.15	-2.99	64,64,64,64	0
58	MG	1H	3011	1/1	0.97	0.19	-3.01	50,50,50,50	0
58	MG	14	3050	1/1	0.94	0.16	-3.04	55,55,55,55	0
58	MG	1G	1689	1/1	0.71	0.08	-3.05	108,108,108,108	0
58	MG	14	3040	1/1	0.96	0.17	-3.06	61,61,61,61	0
58	MG	13	1697	1/1	0.93	0.13	-3.11	90,90,90,90	0
58	MG	1H	3128	1/1	0.85	0.17	-3.17	46,46,46,46	0
58	MG	14	3358	1/1	0.95	0.12	-3.21	51,51,51,51	0
58	MG	1H	3319	1/1	0.92	0.19	-3.23	50,50,50,50	0
58	MG	13	1733	1/1	0.98	0.10	-3.27	61,61,61,61	0
58	MG	14	3019	1/1	0.97	0.13	-3.28	69,69,69,69	0
58	MG	1H	3095	1/1	0.92	0.15	-3.33	47,47,47,47	0
58	MG	14	3339	1/1	0.97	0.09	-3.34	60,60,60,60	0
58	MG	1H	3114	1/1	0.99	0.16	-3.36	40,40,40,40	0
58	MG	14	3132	1/1	0.83	0.08	-3.38	64,64,64,64	0
58	MG	1H	3386	1/1	0.96	0.16	-3.40	39,39,39,39	0
58	MG	13	1729	1/1	0.93	0.08	-3.47	85,85,85,85	0
58	MG	14	3280	1/1	0.94	0.13	-3.48	51,51,51,51	0
58	MG	14	3380	1/1	0.90	0.09	-3.49	90,90,90,90	0
58	MG	1H	3384	1/1	0.95	0.13	-3.55	38,38,38,38	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
58	MG	1G	1683	1/1	0.96	0.11	-3.63	81,81,81,81	0
58	MG	14	3232	1/1	0.93	0.13	-3.65	73,73,73,73	0
58	MG	14	3333	1/1	0.98	0.21	-3.71	54,54,54,54	0
58	MG	3I	201	1/1	0.86	0.09	-3.75	59,59,59,59	0
58	MG	1H	3455	1/1	0.94	0.13	-3.84	58,58,58,58	0
58	MG	13	1721	1/1	0.81	0.12	-3.91	59,59,59,59	0
58	MG	1G	1684	1/1	0.95	0.08	-3.94	81,81,81,81	0
58	MG	14	3058	1/1	0.99	0.20	-4.08	61,61,61,61	0
58	MG	1H	3404	1/1	0.86	0.12	-4.15	56,56,56,56	0
58	MG	14	3242	1/1	0.98	0.12	-4.19	55,55,55,55	0
58	MG	14	3348	1/1	0.97	0.07	-4.20	42,42,42,42	0
58	MG	14	3117	1/1	0.94	0.11	-4.24	52,52,52,52	0
58	MG	1H	3420	1/1	0.99	0.14	-4.30	37,37,37,37	0
58	MG	13	1682	1/1	0.82	0.11	-4.35	78,78,78,78	0
58	MG	1H	3388	1/1	0.96	0.14	-4.40	39,39,39,39	0
58	MG	1H	3421	1/1	0.98	0.10	-4.50	43,43,43,43	0
58	MG	1H	3099	1/1	0.94	0.15	-4.53	37,37,37,37	0
58	MG	14	3312	1/1	0.97	0.09	-4.56	89,89,89,89	0
58	MG	14	3089	1/1	0.87	0.08	-4.58	72,72,72,72	0
58	MG	14	3213	1/1	0.94	0.13	-4.61	55,55,55,55	0
58	MG	14	3364	1/1	0.98	0.11	-4.62	45,45,45,45	0
58	MG	14	3039	1/1	0.97	0.14	-4.63	45,45,45,45	0
58	MG	1H	3394	1/1	0.94	0.15	-4.72	47,47,47,47	0
58	MG	14	3372	1/1	0.97	0.08	-4.72	59,59,59,59	0
58	MG	1H	3109	1/1	0.94	0.15	-4.87	37,37,37,37	0
58	MG	14	3036	1/1	0.86	0.12	-4.99	74,74,74,74	0
58	MG	1H	3434	1/1	0.98	0.12	-5.09	42,42,42,42	0
58	MG	13	1674	1/1	0.89	0.09	-5.10	81,81,81,81	0
58	MG	1H	3392	1/1	0.96	0.10	-5.13	60,60,60,60	0
58	MG	14	3340	1/1	0.95	0.15	-5.16	60,60,60,60	0
58	MG	14	3113	1/1	0.97	0.10	-5.22	46,46,46,46	0
58	MG	1H	3447	1/1	0.89	0.14	-5.23	47,47,47,47	0
58	MG	1H	3368	1/1	0.96	0.15	-5.28	72,72,72,72	0
58	MG	1H	3307	1/1	0.97	0.12	-5.37	64,64,64,64	0
58	MG	14	3006	1/1	0.97	0.13	-5.46	46,46,46,46	0
58	MG	13	1677	1/1	0.73	0.11	-5.52	59,59,59,59	0
58	MG	1H	3414	1/1	0.93	0.10	-5.61	50,50,50,50	0
58	MG	1H	3405	1/1	0.95	0.10	-5.62	41,41,41,41	0
58	MG	14	3371	1/1	0.96	0.08	-5.74	59,59,59,59	0
58	MG	14	3353	1/1	0.97	0.06	-5.75	57,57,57,57	0
58	MG	1H	3221	1/1	0.76	0.15	-5.78	69,69,69,69	0
58	MG	1H	3453	1/1	0.86	0.13	-5.78	51,51,51,51	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
58	MG	14	3136	1/1	0.95	0.11	-5.78	50,50,50,50	0
58	MG	1H	3466	1/1	0.98	0.12	-5.83	51,51,51,51	0
58	MG	1H	3448	1/1	0.99	0.12	-5.84	50,50,50,50	0
58	MG	14	3237	1/1	0.96	0.11	-5.87	48,48,48,48	0
58	MG	14	3395	1/1	0.96	0.08	-5.89	64,64,64,64	0
58	MG	1H	3465	1/1	0.84	0.09	-5.96	87,87,87,87	0
58	MG	1H	3180	1/1	0.92	0.14	-6.06	63,63,63,63	0
58	MG	1H	3001	1/1	0.97	0.15	-6.07	44,44,44,44	0
58	MG	1H	3452	1/1	0.89	0.07	-6.18	71,71,71,71	0
58	MG	14	3361	1/1	0.97	0.08	-6.55	52,52,52,52	0
58	MG	13	1632	1/1	0.94	0.10	-6.74	45,45,45,45	0
58	MG	14	3342	1/1	0.95	0.10	-6.77	51,51,51,51	0
58	MG	14	3360	1/1	0.98	0.07	-6.79	55,55,55,55	0
58	MG	1H	3413	1/1	0.96	0.07	-6.81	40,40,40,40	0
58	MG	1G	1603	1/1	0.91	0.12	-6.91	71,71,71,71	0
58	MG	1H	3443	1/1	0.99	0.12	-7.09	55,55,55,55	0
58	MG	1H	3424	1/1	0.98	0.08	-7.29	48,48,48,48	0
58	MG	1H	3412	1/1	0.97	0.10	-7.30	48,48,48,48	0
58	MG	1H	3255	1/1	0.96	0.12	-7.34	40,40,40,40	0
58	MG	1H	3252	1/1	0.97	0.11	-7.51	36,36,36,36	0
58	MG	1H	3445	1/1	0.99	0.11	-7.86	40,40,40,40	0
58	MG	14	3331	1/1	0.98	0.09	-8.01	53,53,53,53	0
58	MG	13	1689	1/1	0.98	0.10	-8.19	70,70,70,70	0
58	MG	1H	3390	1/1	0.95	0.09	-8.35	41,41,41,41	0
58	MG	1H	3401	1/1	0.97	0.10	-8.44	71,71,71,71	0
58	MG	1H	3430	1/1	0.95	0.06	-8.47	69,69,69,69	0
58	MG	14	3311	1/1	0.95	0.14	-8.80	66,66,66,66	0
58	MG	14	3335	1/1	0.90	0.11	-8.94	71,71,71,71	0
58	MG	13	1726	1/1	0.96	0.10	-9.38	75,75,75,75	0
58	MG	1H	3402	1/1	0.94	0.07	-9.69	58,58,58,58	0
58	MG	13	1651	1/1	0.89	0.11	-10.48	63,63,63,63	0
58	MG	1H	3460	1/1	0.95	0.12	-10.62	53,53,53,53	0
58	MG	1H	3044	1/1	0.93	0.15	-10.87	50,50,50,50	0
58	MG	14	3389	1/1	0.87	0.09	-11.26	73,73,73,73	0
58	MG	1H	3422	1/1	0.95	0.13	-11.73	63,63,63,63	0
58	MG	14	3343	1/1	0.97	0.08	-13.42	49,49,49,49	0
58	MG	1H	3459	1/1	0.99	0.07	-14.63	65,65,65,65	0
58	MG	1H	3472	1/1	0.98	0.07	-16.89	75,75,75,75	0
58	MG	14	3059	1/1	0.90	0.40	-	65,65,65,65	0
58	MG	1H	3235	1/1	0.97	0.12	-	53,53,53,53	0
58	MG	1H	3071	1/1	0.89	0.27	-	52,52,52,52	0
58	MG	1H	3446	1/1	0.94	0.07	-	60,60,60,60	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
58	MG	1H	3191	1/1	0.91	0.14	-	68,68,68,68	0
58	MG	13	1670	1/1	0.83	0.19	-	86,86,86,86	0
58	MG	1H	3357	1/1	0.78	0.38	-	86,86,86,86	0
58	MG	1G	1667	1/1	0.90	0.14	-	84,84,84,84	0
58	MG	14	3081	1/1	0.97	0.18	-	52,52,52,52	0
58	MG	1H	3259	1/1	0.96	0.19	-	46,46,46,46	0
58	MG	16	203	1/1	0.81	0.36	-	77,77,77,77	0
58	MG	1H	3475	1/1	0.84	0.13	-	95,95,95,95	0
58	MG	14	3266	1/1	0.91	0.22	-	72,72,72,72	0
58	MG	14	3295	1/1	0.80	0.19	-	80,80,80,80	0
58	MG	14	3177	1/1	0.93	0.13	-	70,70,70,70	0
58	MG	1G	1610	1/1	0.90	0.17	-	95,95,95,95	0
58	MG	13	1714	1/1	0.81	0.36	-	95,95,95,95	0
58	MG	14	3168	1/1	0.86	0.28	-	79,79,79,79	0
58	MG	1H	3271	1/1	0.89	0.35	-	77,77,77,77	0
58	MG	14	3116	1/1	0.97	0.12	-	57,57,57,57	0
58	MG	13	1653	1/1	0.81	0.15	-	84,84,84,84	0
58	MG	1H	3093	1/1	0.98	0.39	-	38,38,38,38	0
58	MG	14	3095	1/1	0.93	0.11	-	52,52,52,52	0
58	MG	1H	3065	1/1	0.96	0.19	-	72,72,72,72	0
58	MG	1H	3171	1/1	0.89	0.43	-	89,89,89,89	0
58	MG	1H	3195	1/1	0.84	0.28	-	80,80,80,80	0
58	MG	1G	1636	1/1	0.84	0.24	-	85,85,85,85	0
58	MG	1H	3391	1/1	0.95	0.08	-	47,47,47,47	0
58	MG	1H	3427	1/1	0.92	0.10	-	55,55,55,55	0
58	MG	13	1727	1/1	0.95	0.14	-	69,69,69,69	0
58	MG	1H	3113	1/1	0.94	0.31	-	37,37,37,37	0
58	MG	13	1738	1/1	0.90	0.08	-	112,112,112,112	0
58	MG	1H	3201	1/1	0.84	0.44	-	87,87,87,87	0
58	MG	13	1646	1/1	0.95	0.12	-	63,63,63,63	0
58	MG	13	1679	1/1	0.91	0.34	-	96,96,96,96	0
58	MG	1H	3324	1/1	0.87	0.42	-	86,86,86,86	0
58	MG	14	3397	1/1	0.79	0.10	-	86,86,86,86	0
58	MG	14	3341	1/1	0.95	0.04	-	71,71,71,71	0
58	MG	1H	3381	1/1	0.92	0.26	-	90,90,90,90	0
58	MG	14	3145	1/1	0.91	0.17	-	65,65,65,65	0
58	MG	14	3048	1/1	0.94	0.22	-	66,66,66,66	0
58	MG	1H	3428	1/1	0.98	0.10	-	38,38,38,38	0
58	MG	1J	202	1/1	0.95	0.43	-	84,84,84,84	0
58	MG	14	3064	1/1	0.68	0.54	-	63,63,63,63	0
58	MG	1H	3103	1/1	0.94	0.29	-	47,47,47,47	0
58	MG	1H	3170	1/1	0.90	0.28	-	65,65,65,65	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
58	MG	1H	3325	1/1	0.91	0.22	-	67,67,67,67	0
58	MG	1H	3153	1/1	0.94	0.29	-	58,58,58,58	0
58	MG	1H	3062	1/1	0.98	0.21	-	66,66,66,66	0
58	MG	1G	1608	1/1	0.93	0.24	-	81,81,81,81	0
58	MG	1H	3282	1/1	0.90	0.51	-	85,85,85,85	0
58	MG	14	3392	1/1	0.93	0.11	-	61,61,61,61	0
58	MG	1H	3343	1/1	0.95	0.28	-	62,62,62,62	0
58	MG	1G	1682	1/1	0.96	0.10	-	75,75,75,75	0
58	MG	1H	3322	1/1	0.99	0.23	-	39,39,39,39	0
58	MG	1G	1657	1/1	0.81	0.39	-	110,110,110,110	0
58	MG	1H	3178	1/1	0.88	0.49	-	69,69,69,69	0
58	MG	1G	1627	1/1	0.79	0.26	-	77,77,77,77	0
58	MG	14	3126	1/1	0.95	0.29	-	78,78,78,78	0
58	MG	1H	3382	1/1	0.87	0.21	-	80,80,80,80	0
58	MG	3L	101	1/1	0.94	0.30	-	81,81,81,81	0
58	MG	14	3190	1/1	0.97	0.21	-	65,65,65,65	0
58	MG	14	3210	1/1	0.88	0.32	-	79,79,79,79	0
58	MG	1H	3264	1/1	0.97	0.19	-	47,47,47,47	0
58	MG	14	3070	1/1	0.96	0.19	-	62,62,62,62	0
58	MG	1H	3415	1/1	0.95	0.12	-	48,48,48,48	0
58	MG	1H	3029	1/1	0.99	0.21	-	50,50,50,50	0
58	MG	14	3363	1/1	0.86	0.07	-	77,77,77,77	0
58	MG	14	3255	1/1	0.89	0.35	-	69,69,69,69	0
58	MG	1H	3339	1/1	0.88	0.42	-	78,78,78,78	0
58	MG	14	3202	1/1	0.49	0.23	-	70,70,70,70	0
58	MG	1G	1628	1/1	0.89	0.21	-	64,64,64,64	0
58	MG	13	1616	1/1	0.97	0.18	-	59,59,59,59	0
58	MG	13	1620	1/1	0.98	0.12	-	64,64,64,64	0
58	MG	14	3166	1/1	0.74	0.25	-	76,76,76,76	0
58	MG	14	3182	1/1	0.90	0.23	-	61,61,61,61	0
58	MG	16	202	1/1	0.92	0.30	-	63,63,63,63	0
58	MG	14	3120	1/1	0.94	0.10	-	84,84,84,84	0
58	MG	13	1630	1/1	0.91	0.30	-	70,70,70,70	0
58	MG	1G	1612	1/1	0.74	0.24	-	78,78,78,78	0
58	MG	14	3046	1/1	0.91	0.24	-	73,73,73,73	0
58	MG	14	3275	1/1	0.87	0.15	-	70,70,70,70	0
58	MG	1H	3326	1/1	0.96	0.16	-	92,92,92,92	0
58	MG	1H	3205	1/1	0.90	0.34	-	71,71,71,71	0
58	MG	1H	3105	1/1	0.86	0.15	-	59,59,59,59	0
58	MG	1H	3312	1/1	0.86	0.27	-	68,68,68,68	0
58	MG	13	1717	1/1	0.70	0.32	-	93,93,93,93	0
58	MG	1H	3439	1/1	0.99	0.06	-	70,70,70,70	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
58	MG	1H	3362	1/1	0.93	0.20	-	105,105,105,105	0
58	MG	14	3198	1/1	0.90	0.31	-	84,84,84,84	0
58	MG	14	3037	1/1	0.96	0.08	-	72,72,72,72	0
58	MG	1H	3287	1/1	0.89	0.37	-	62,62,62,62	0
58	MG	13	1631	1/1	0.93	0.20	-	64,64,64,64	0
58	MG	14	3378	1/1	0.98	0.08	-	73,73,73,73	0
58	MG	1H	3245	1/1	0.89	0.25	-	69,69,69,69	0
58	MG	1H	3355	1/1	0.97	0.21	-	73,73,73,73	0
58	MG	13	1702	1/1	0.82	0.23	-	77,77,77,77	0
58	MG	13	1603	1/1	0.98	0.12	-	61,61,61,61	0
58	MG	1G	1634	1/1	0.90	0.24	-	87,87,87,87	0
58	MG	1H	3409	1/1	0.69	0.14	-	46,46,46,46	0
58	MG	14	3393	1/1	0.97	0.07	-	71,71,71,71	0
58	MG	14	3309	1/1	0.86	0.24	-	83,83,83,83	0
58	MG	1H	3294	1/1	0.93	0.22	-	70,70,70,70	0
58	MG	14	3106	1/1	0.95	0.13	-	57,57,57,57	0
58	MG	1G	1618	1/1	0.97	0.20	-	86,86,86,86	0
58	MG	14	3005	1/1	0.99	0.24	-	49,49,49,49	0
58	MG	14	3205	1/1	0.96	0.14	-	44,44,44,44	0
58	MG	14	3180	1/1	0.96	0.26	-	75,75,75,75	0
58	MG	1G	1652	1/1	0.94	0.20	-	91,91,91,91	0
58	MG	14	3165	1/1	0.93	0.19	-	65,65,65,65	0
58	MG	1H	3228	1/1	0.89	0.33	-	83,83,83,83	0
58	MG	1G	1604	1/1	0.98	0.12	-	84,84,84,84	0
58	MG	1H	3004	1/1	0.97	0.35	-	33,33,33,33	0
58	MG	1H	3239	1/1	0.84	0.37	-	76,76,76,76	0
58	MG	14	3161	1/1	0.86	0.27	-	88,88,88,88	0
58	MG	1H	3363	1/1	0.87	0.46	-	98,98,98,98	0
58	MG	1G	1605	1/1	0.95	0.12	-	78,78,78,78	0
58	MG	14	3374	1/1	0.75	0.15	-	87,87,87,87	0
58	MG	14	3234	1/1	0.90	0.07	-	56,56,56,56	0
58	MG	14	3139	1/1	0.96	0.36	-	68,68,68,68	0
58	MG	13	1713	1/1	0.74	0.24	-	83,83,83,83	0
58	MG	13	1654	1/1	0.63	0.24	-	76,76,76,76	0
58	MG	1L	101	1/1	0.98	0.17	-	71,71,71,71	0
58	MG	1H	3373	1/1	0.76	0.48	-	72,72,72,72	0
58	MG	13	1709	1/1	0.85	0.33	-	87,87,87,87	0
58	MG	1H	3182	1/1	0.93	0.49	-	73,73,73,73	0
58	MG	1H	3336	1/1	0.88	0.34	-	66,66,66,66	0
58	MG	13	1660	1/1	0.82	0.20	-	87,87,87,87	0
58	MG	2K	106	1/1	0.93	0.07	-	87,87,87,87	0
58	MG	1H	3358	1/1	0.89	0.44	-	92,92,92,92	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
58	MG	14	3366	1/1	0.93	0.12	-	76,76,76,76	0
58	MG	14	3049	1/1	0.98	0.13	-	47,47,47,47	0
58	MG	14	3102	1/1	0.86	0.48	-	81,81,81,81	0
58	MG	1H	3211	1/1	0.92	0.36	-	59,59,59,59	0
58	MG	1H	3232	1/1	0.90	0.26	-	70,70,70,70	0
58	MG	1H	3406	1/1	0.93	0.16	-	53,53,53,53	0
58	MG	14	3398	1/1	0.65	0.21	-	107,107,107,107	0
58	MG	14	3153	1/1	0.92	0.30	-	104,104,104,104	0
58	MG	14	3383	1/1	0.95	0.12	-	70,70,70,70	0
58	MG	14	3159	1/1	0.94	0.21	-	63,63,63,63	0
58	MG	14	3125	1/1	0.94	0.14	-	42,42,42,42	0
58	MG	1H	3243	1/1	0.96	0.28	-	50,50,50,50	0
58	MG	14	3144	1/1	0.94	0.27	-	75,75,75,75	0
58	MG	1G	1668	1/1	0.82	0.24	-	76,76,76,76	0
58	MG	1H	3157	1/1	0.92	0.20	-	48,48,48,48	0
58	MG	1H	3249	1/1	0.97	0.18	-	53,53,53,53	0
58	MG	1H	3456	1/1	0.90	0.09	-	87,87,87,87	0
58	MG	1H	3134	1/1	0.98	0.21	-	45,45,45,45	0
58	MG	1H	3385	1/1	0.93	0.14	-	49,49,49,49	0
58	MG	1G	1623	1/1	0.93	0.16	-	96,96,96,96	0
58	MG	1H	3244	1/1	0.87	0.42	-	75,75,75,75	0
58	MG	1H	3186	1/1	0.92	0.33	-	52,52,52,52	0
58	MG	1H	3260	1/1	0.96	0.32	-	48,48,48,48	0
58	MG	14	3269	1/1	0.97	0.16	-	78,78,78,78	0
58	MG	1H	3026	1/1	0.97	0.19	-	45,45,45,45	0
58	MG	1G	1664	1/1	0.87	0.34	-	88,88,88,88	0
58	MG	14	3325	1/1	0.80	0.30	-	86,86,86,86	0
58	MG	14	3174	1/1	0.86	0.11	-	78,78,78,78	0
58	MG	14	3385	1/1	0.96	0.15	-	71,71,71,71	0
58	MG	1H	3361	1/1	0.95	0.33	-	112,112,112,112	0
58	MG	13	1676	1/1	0.86	0.25	-	76,76,76,76	0
58	MG	13	1619	1/1	0.52	0.23	-	99,99,99,99	0
58	MG	14	3256	1/1	0.96	0.27	-	80,80,80,80	0
58	MG	1H	3111	1/1	0.98	0.11	-	53,53,53,53	0
58	MG	1H	3145	1/1	0.97	0.33	-	53,53,53,53	0
58	MG	1H	3303	1/1	0.76	0.26	-	75,75,75,75	0
58	MG	1H	3010	1/1	0.99	0.33	-	33,33,33,33	0
58	MG	13	1711	1/1	0.85	0.35	-	89,89,89,89	0
58	MG	14	3277	1/1	0.88	0.18	-	73,73,73,73	0
58	MG	1H	3270	1/1	0.93	0.34	-	76,76,76,76	0
58	MG	1H	3468	1/1	0.97	0.07	-	59,59,59,59	0
58	MG	1H	3039	1/1	0.98	0.31	-	76,76,76,76	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
58	MG	1H	3122	1/1	0.78	0.35	-	74,74,74,74	0
58	MG	13	1699	1/1	0.87	0.45	-	71,71,71,71	0
58	MG	14	3157	1/1	0.95	0.35	-	63,63,63,63	0
58	MG	14	3349	1/1	0.99	0.12	-	57,57,57,57	0
58	MG	14	3192	1/1	0.97	0.18	-	74,74,74,74	0
58	MG	14	3228	1/1	0.49	0.38	-	79,79,79,79	0
58	MG	1H	3229	1/1	0.89	0.21	-	61,61,61,61	0
58	MG	1H	3092	1/1	0.98	0.26	-	65,65,65,65	0
58	MG	1H	3280	1/1	0.94	0.14	-	44,44,44,44	0
58	MG	14	3017	1/1	0.98	0.22	-	49,49,49,49	0
58	MG	1H	3019	1/1	0.97	0.28	-	38,38,38,38	0
58	MG	14	3259	1/1	0.78	0.21	-	66,66,66,66	0
58	MG	14	3249	1/1	0.88	0.62	-	49,49,49,49	0
58	MG	14	3150	1/1	0.85	0.37	-	70,70,70,70	0
58	MG	4E	201	1/1	0.89	0.29	-	76,76,76,76	0
58	MG	14	3119	1/1	0.97	0.32	-	75,75,75,75	0
58	MG	1H	3321	1/1	0.96	0.27	-	80,80,80,80	0
58	MG	16	213	1/1	0.88	0.13	-	82,82,82,82	0
58	MG	1H	3233	1/1	0.90	0.27	-	65,65,65,65	0
58	MG	1H	3187	1/1	0.95	0.24	-	64,64,64,64	0
58	MG	14	3004	1/1	0.97	0.15	-	50,50,50,50	0
58	MG	1H	3089	1/1	0.92	0.14	-	68,68,68,68	0
58	MG	14	3196	1/1	0.85	0.31	-	82,82,82,82	0
58	MG	P8	101	1/1	0.68	0.34	-	70,70,70,70	0
58	MG	14	3289	1/1	0.79	0.41	-	75,75,75,75	0
58	MG	14	3220	1/1	0.95	0.15	-	66,66,66,66	0
58	MG	14	3012	1/1	0.97	0.27	-	66,66,66,66	0
58	MG	1H	3297	1/1	0.82	0.22	-	59,59,59,59	0
58	MG	1G	1633	1/1	0.58	0.20	-	80,80,80,80	0
58	MG	14	3355	1/1	0.97	0.12	-	43,43,43,43	0
58	MG	1H	3383	1/1	0.86	0.23	-	113,113,113,113	0
58	MG	1H	3214	1/1	0.96	0.27	-	53,53,53,53	0
58	MG	14	3216	1/1	0.88	0.20	-	83,83,83,83	0
58	MG	14	3030	1/1	0.86	0.18	-	91,91,91,91	0
58	MG	14	3135	1/1	0.97	0.14	-	67,67,67,67	0
58	MG	1G	1685	1/1	0.77	0.07	-	111,111,111,111	0
58	MG	1H	3234	1/1	0.92	0.45	-	85,85,85,85	0
58	MG	1H	3225	1/1	0.85	0.34	-	68,68,68,68	0
58	MG	14	3287	1/1	0.89	0.43	-	112,112,112,112	0
58	MG	14	3197	1/1	0.86	0.17	-	85,85,85,85	0
58	MG	14	3225	1/1	0.96	0.15	-	68,68,68,68	0
58	MG	21	301	1/1	0.94	0.14	-	46,46,46,46	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
58	MG	1H	3354	1/1	0.94	0.29	-	80,80,80,80	0
58	MG	13	1675	1/1	0.97	0.22	-	63,63,63,63	0
58	MG	14	3226	1/1	0.93	0.17	-	74,74,74,74	0
58	MG	14	3007	1/1	0.96	0.13	-	42,42,42,42	0
58	MG	1H	3056	1/1	0.98	0.19	-	59,59,59,59	0
58	MG	1H	3463	1/1	0.84	0.25	-	92,92,92,92	0
58	MG	1H	3317	1/1	0.89	0.27	-	73,73,73,73	0
58	MG	1G	1632	1/1	0.93	0.28	-	64,64,64,64	0
58	MG	1H	3328	1/1	0.86	0.31	-	63,63,63,63	0
58	MG	14	3337	1/1	0.98	0.10	-	49,49,49,49	0
58	MG	1H	3387	1/1	0.98	0.12	-	38,38,38,38	0
58	MG	14	3184	1/1	0.94	0.26	-	60,60,60,60	0
58	MG	14	3302	1/1	0.73	0.25	-	131,131,131,131	0
58	MG	14	3260	1/1	0.99	0.12	-	57,57,57,57	0
58	MG	14	3324	1/1	0.93	0.17	-	83,83,83,83	0
58	MG	14	3273	1/1	0.96	0.11	-	64,64,64,64	0
58	MG	13	1637	1/1	0.88	0.40	-	73,73,73,73	0
58	MG	1G	1670	1/1	0.92	0.18	-	86,86,86,86	0
58	MG	1H	3209	1/1	0.94	0.18	-	57,57,57,57	0
58	MG	13	1690	1/1	0.92	0.18	-	66,66,66,66	0
58	MG	1H	3431	1/1	0.95	0.08	-	57,57,57,57	0
58	MG	1H	3458	1/1	0.91	0.14	-	68,68,68,68	0
58	MG	1H	3045	1/1	0.95	0.20	-	90,90,90,90	0
58	MG	14	3300	1/1	0.94	0.09	-	81,81,81,81	0
58	MG	1H	3410	1/1	0.92	0.08	-	59,59,59,59	0
58	MG	1H	3080	1/1	0.96	0.25	-	67,67,67,67	0
58	MG	1H	3078	1/1	0.98	0.22	-	41,41,41,41	0
58	MG	1H	3411	1/1	0.98	0.11	-	43,43,43,43	0
58	MG	1H	3226	1/1	0.81	0.48	-	66,66,66,66	0
58	MG	13	1642	1/1	0.86	0.17	-	59,59,59,59	0
58	MG	1H	3359	1/1	0.62	0.56	-	97,97,97,97	0
58	MG	1H	3250	1/1	0.98	0.20	-	41,41,41,41	0
58	MG	1H	3176	1/1	0.91	0.28	-	70,70,70,70	0
58	MG	14	3101	1/1	0.97	0.18	-	60,60,60,60	0
58	MG	13	1706	1/1	0.86	0.18	-	98,98,98,98	0
58	MG	14	3297	1/1	0.98	0.11	-	60,60,60,60	0
58	MG	14	3354	1/1	0.98	0.11	-	57,57,57,57	0
58	MG	14	3080	1/1	0.84	0.19	-	45,45,45,45	0
58	MG	14	3127	1/1	0.94	0.17	-	55,55,55,55	0
58	MG	14	3233	1/1	0.92	0.19	-	66,66,66,66	0
58	MG	13	1673	1/1	0.90	0.26	-	70,70,70,70	0
58	MG	1H	3330	1/1	0.92	0.16	-	74,74,74,74	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
58	MG	13	1668	1/1	0.94	0.29	-	69,69,69,69	0
58	MG	14	3386	1/1	0.89	0.09	-	83,83,83,83	0
58	MG	1H	3397	1/1	0.97	0.10	-	51,51,51,51	0
58	MG	1H	3159	1/1	0.84	0.38	-	64,64,64,64	0
58	MG	1G	1622	1/1	0.96	0.12	-	113,113,113,113	0
58	MG	14	3279	1/1	0.96	0.09	-	67,67,67,67	0
58	MG	1H	3198	1/1	0.76	0.16	-	79,79,79,79	0
58	MG	1H	3200	1/1	0.93	0.25	-	73,73,73,73	0
58	MG	14	3123	1/1	0.98	0.15	-	59,59,59,59	0
58	MG	1H	3172	1/1	0.93	0.37	-	56,56,56,56	0
58	MG	1J	204	1/1	0.92	0.28	-	88,88,88,88	0
58	MG	1G	1648	1/1	0.92	0.30	-	95,95,95,95	0
58	MG	1H	3435	1/1	0.93	0.08	-	70,70,70,70	0
58	MG	L8	101	1/1	0.78	0.24	-	84,84,84,84	0
58	MG	14	3076	1/1	0.94	0.13	-	59,59,59,59	0
58	MG	14	3111	1/1	0.98	0.19	-	63,63,63,63	0
58	MG	1H	3407	1/1	0.93	0.12	-	60,60,60,60	0
58	MG	14	3107	1/1	0.78	0.24	-	64,64,64,64	0
58	MG	14	3096	1/1	0.96	0.11	-	61,61,61,61	0
58	MG	13	1640	1/1	0.93	0.19	-	65,65,65,65	0
58	MG	14	3031	1/1	0.97	0.25	-	56,56,56,56	0
58	MG	14	3206	1/1	0.93	0.18	-	56,56,56,56	0
58	MG	1H	3257	1/1	0.96	0.17	-	55,55,55,55	0
58	MG	14	3188	1/1	0.87	0.25	-	79,79,79,79	0
58	MG	1H	3346	1/1	0.85	0.28	-	78,78,78,78	0
58	MG	14	3015	1/1	0.92	0.14	-	76,76,76,76	0
58	MG	14	3173	1/1	0.97	0.12	-	78,78,78,78	0
58	MG	14	3298	1/1	0.80	0.57	-	80,80,80,80	0
58	MG	14	3100	1/1	0.95	0.47	-	62,62,62,62	0
58	MG	14	3014	1/1	0.99	0.19	-	61,61,61,61	0
58	MG	2L	102	1/1	0.77	0.19	-	76,76,76,76	0
58	MG	14	3170	1/1	0.85	0.12	-	69,69,69,69	0
58	MG	14	3060	1/1	0.95	0.17	-	67,67,67,67	0
58	MG	14	3056	1/1	0.94	0.12	-	73,73,73,73	0
58	MG	14	3252	1/1	0.94	0.11	-	71,71,71,71	0
58	MG	13	1612	1/1	0.82	0.15	-	74,74,74,74	0
58	MG	1H	3163	1/1	0.75	0.38	-	78,78,78,78	0
58	MG	13	1602	1/1	0.96	0.22	-	71,71,71,71	0
58	MG	1H	3208	1/1	0.95	0.43	-	70,70,70,70	0
58	MG	14	3344	1/1	0.94	0.09	-	60,60,60,60	0
58	MG	1H	3040	1/1	0.87	0.16	-	62,62,62,62	0
58	MG	14	3185	1/1	0.70	0.15	-	63,63,63,63	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
58	MG	1G	1653	1/1	0.92	0.13	-	77,77,77,77	0
58	MG	13	1665	1/1	0.96	0.20	-	82,82,82,82	0
58	MG	C5	201	1/1	0.89	0.29	-	105,105,105,105	0
58	MG	1G	1649	1/1	0.95	0.19	-	78,78,78,78	0
58	MG	14	3138	1/1	0.82	0.19	-	69,69,69,69	0
58	MG	1H	3130	1/1	0.96	0.31	-	67,67,67,67	0
58	MG	1G	1631	1/1	0.76	0.26	-	73,73,73,73	0
58	MG	1G	1645	1/1	0.79	0.23	-	78,78,78,78	0
58	MG	13	1704	1/1	0.93	0.20	-	130,130,130,130	0
58	MG	1H	3035	1/1	0.83	0.34	-	83,83,83,83	0
58	MG	1H	3068	1/1	0.92	0.31	-	63,63,63,63	0
58	MG	1H	3370	1/1	0.72	0.45	-	83,83,83,83	0
58	MG	1H	3283	1/1	0.97	0.20	-	59,59,59,59	0
58	MG	14	3086	1/1	0.86	0.19	-	69,69,69,69	0
58	MG	13	1658	1/1	0.93	0.29	-	73,73,73,73	0
58	MG	14	3212	1/1	0.70	0.28	-	68,68,68,68	0
58	MG	1H	3306	1/1	0.96	0.23	-	54,54,54,54	0
58	MG	14	3321	1/1	0.92	0.38	-	86,86,86,86	0
58	MG	13	1667	1/1	0.89	0.33	-	59,59,59,59	0
58	MG	13	1734	1/1	0.99	0.09	-	76,76,76,76	0
58	MG	1H	3202	1/1	0.93	0.33	-	60,60,60,60	0
58	MG	1H	3369	1/1	0.95	0.33	-	54,54,54,54	0
58	MG	14	3189	1/1	0.83	0.25	-	71,71,71,71	0
58	MG	13	1655	1/1	0.89	0.28	-	78,78,78,78	0
58	MG	14	3317	1/1	0.93	0.30	-	65,65,65,65	0
58	MG	2K	104	1/1	0.95	0.21	-	72,72,72,72	0
58	MG	1H	3316	1/1	0.71	0.24	-	80,80,80,80	0
58	MG	1H	3017	1/1	0.99	0.17	-	52,52,52,52	0
58	MG	14	3110	1/1	0.99	0.17	-	44,44,44,44	0
58	MG	13	1692	1/1	0.73	0.39	-	80,80,80,80	0
58	MG	1H	3372	1/1	0.94	0.21	-	78,78,78,78	0
58	MG	1G	1629	1/1	0.78	0.26	-	85,85,85,85	0
58	MG	78	201	1/1	0.88	0.21	-	53,53,53,53	0
58	MG	1H	3174	1/1	0.94	0.14	-	51,51,51,51	0
58	MG	13	1615	1/1	0.86	0.18	-	86,86,86,86	0
58	MG	1H	3345	1/1	0.96	0.19	-	75,75,75,75	0
58	MG	1H	3301	1/1	0.76	0.21	-	75,75,75,75	0
58	MG	1G	1672	1/1	0.94	0.10	-	91,91,91,91	0
58	MG	1H	3470	1/1	0.97	0.10	-	64,64,64,64	0
58	MG	1H	3300	1/1	0.86	0.30	-	63,63,63,63	0
58	MG	14	3283	1/1	0.85	0.28	-	88,88,88,88	0
58	MG	14	3307	1/1	0.92	0.08	-	62,62,62,62	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
58	MG	14	3051	1/1	0.99	0.09	-	52,52,52,52	0
58	MG	14	3292	1/1	0.94	0.17	-	109,109,109,109	0
58	MG	14	3265	1/1	0.97	0.19	-	55,55,55,55	0
58	MG	14	3026	1/1	0.94	0.09	-	76,76,76,76	0
58	MG	1H	3063	1/1	0.95	0.25	-	45,45,45,45	0
58	MG	1H	3184	1/1	0.80	0.16	-	87,87,87,87	0
58	MG	1H	3008	1/1	0.98	0.30	-	37,37,37,37	0
58	MG	1H	3473	1/1	0.94	0.07	-	99,99,99,99	0
58	MG	14	3235	1/1	0.85	0.19	-	87,87,87,87	0
58	MG	1H	3400	1/1	0.93	0.14	-	58,58,58,58	0
58	MG	13	1701	1/1	0.97	0.21	-	74,74,74,74	0
58	MG	14	3323	1/1	0.91	0.20	-	85,85,85,85	0
58	MG	1H	3107	1/1	0.98	0.32	-	54,54,54,54	0
58	MG	1H	3237	1/1	0.97	0.12	-	44,44,44,44	0
58	MG	1H	3094	1/1	0.92	0.24	-	53,53,53,53	0
58	MG	14	3105	1/1	0.93	0.12	-	65,65,65,65	0
58	MG	1H	3360	1/1	0.93	0.34	-	73,73,73,73	0
58	MG	14	3320	1/1	0.93	0.14	-	61,61,61,61	0
58	MG	13	1684	1/1	0.87	0.27	-	96,96,96,96	0
58	MG	14	3084	1/1	0.97	0.21	-	54,54,54,54	0
58	MG	14	3008	1/1	0.98	0.21	-	55,55,55,55	0
58	MG	1H	3398	1/1	0.83	0.12	-	50,50,50,50	0
58	MG	1G	1626	1/1	0.81	0.18	-	80,80,80,80	0
58	MG	1H	3329	1/1	0.94	0.37	-	74,74,74,74	0
58	MG	1G	1679	1/1	0.79	0.22	-	157,157,157,157	0
58	MG	1H	3167	1/1	0.94	0.26	-	65,65,65,65	0
58	MG	14	3034	1/1	0.85	0.30	-	57,57,57,57	0
58	MG	1H	3097	1/1	0.96	0.22	-	47,47,47,47	0
58	MG	L8	102	1/1	0.89	0.23	-	67,67,67,67	0
58	MG	1H	3152	1/1	0.93	0.19	-	62,62,62,62	0
58	MG	1H	3217	1/1	0.83	0.34	-	77,77,77,77	0
58	MG	14	3390	1/1	0.85	0.14	-	70,70,70,70	0
58	MG	1H	3203	1/1	0.97	0.14	-	68,68,68,68	0
58	MG	14	3128	1/1	0.93	0.41	-	79,79,79,79	0
58	MG	1H	3050	1/1	0.96	0.29	-	59,59,59,59	0
58	MG	14	3129	1/1	0.82	0.36	-	73,73,73,73	0
58	MG	1G	1613	1/1	0.91	0.33	-	81,81,81,81	0
58	MG	14	3130	1/1	0.87	0.28	-	68,68,68,68	0
58	MG	1H	3069	1/1	0.98	0.43	-	69,69,69,69	0
58	MG	1H	3281	1/1	0.95	0.21	-	65,65,65,65	0
58	MG	16	209	1/1	0.87	0.27	-	59,59,59,59	0
58	MG	1H	3296	1/1	0.69	0.24	-	66,66,66,66	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
58	MG	1G	1606	1/1	0.93	0.07	-	92,92,92,92	0
58	MG	1H	3284	1/1	0.94	0.10	-	72,72,72,72	0
58	MG	13	1700	1/1	0.68	0.33	-	96,96,96,96	0
58	MG	14	3071	1/1	0.98	0.27	-	38,38,38,38	0
58	MG	14	3299	1/1	0.84	0.22	-	53,53,53,53	0
58	MG	14	3346	1/1	0.91	0.07	-	63,63,63,63	0
58	MG	14	3286	1/1	0.84	0.30	-	84,84,84,84	0
58	MG	1H	3075	1/1	0.93	0.13	-	41,41,41,41	0
58	MG	1H	3290	1/1	0.88	0.18	-	66,66,66,66	0
58	MG	1G	1680	1/1	0.97	0.12	-	83,83,83,83	0
58	MG	1H	3084	1/1	0.89	0.14	-	59,59,59,59	0
58	MG	1H	3425	1/1	0.99	0.10	-	43,43,43,43	0
58	MG	14	3271	1/1	0.97	0.11	-	58,58,58,58	0
58	MG	1H	3024	1/1	0.98	0.21	-	40,40,40,40	0
58	MG	1H	3471	1/1	0.98	0.11	-	54,54,54,54	0
58	MG	1H	3327	1/1	0.93	0.34	-	80,80,80,80	0
58	MG	1H	3441	1/1	0.94	0.12	-	40,40,40,40	0
58	MG	14	3270	1/1	0.47	0.26	-	84,84,84,84	0
58	MG	1H	3461	1/1	0.79	0.16	-	103,103,103,103	0
58	MG	14	3258	1/1	0.95	0.40	-	68,68,68,68	0
58	MG	14	3391	1/1	0.97	0.11	-	93,93,93,93	0
58	MG	13	1708	1/1	0.82	0.24	-	81,81,81,81	0
58	MG	1H	3308	1/1	0.90	0.34	-	82,82,82,82	0
58	MG	14	3175	1/1	0.94	0.32	-	64,64,64,64	0
58	MG	1G	1673	1/1	0.91	0.35	-	94,94,94,94	0
58	MG	14	3154	1/1	0.98	0.17	-	80,80,80,80	0
58	MG	13	1732	1/1	0.96	0.08	-	79,79,79,79	0
58	MG	1H	3061	1/1	0.94	0.20	-	51,51,51,51	0
58	MG	1H	3310	1/1	0.99	0.16	-	79,79,79,79	0
58	MG	1H	3335	1/1	0.99	0.16	-	47,47,47,47	0
58	MG	1H	3047	1/1	0.95	0.43	-	84,84,84,84	0
58	MG	14	3200	1/1	0.72	0.21	-	85,85,85,85	0
58	MG	13	1627	1/1	0.94	0.44	-	72,72,72,72	0
58	MG	14	3240	1/1	0.93	0.17	-	71,71,71,71	0
58	MG	45	201	1/1	0.91	0.15	-	59,59,59,59	0
58	MG	1H	3365	1/1	0.63	0.46	-	84,84,84,84	0
58	MG	13	1659	1/1	0.91	0.27	-	85,85,85,85	0
58	MG	14	3151	1/1	0.57	0.24	-	82,82,82,82	0
58	MG	1H	3352	1/1	0.92	0.36	-	81,81,81,81	0
58	MG	14	3373	1/1	0.96	0.06	-	65,65,65,65	0
58	MG	1H	3106	1/1	0.63	0.25	-	78,78,78,78	0
58	MG	1G	1676	1/1	0.90	0.31	-	105,105,105,105	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
58	MG	14	3345	1/1	0.91	0.13	-	63,63,63,63	0
58	MG	1H	3289	1/1	0.94	0.18	-	63,63,63,63	0
58	MG	14	3118	1/1	0.94	0.19	-	40,40,40,40	0
58	MG	1G	1638	1/1	0.92	0.31	-	80,80,80,80	0
58	MG	14	3377	1/1	0.97	0.15	-	66,66,66,66	0
58	MG	14	3313	1/1	0.95	0.17	-	81,81,81,81	0
58	MG	1H	3367	1/1	0.73	0.50	-	88,88,88,88	0
58	MG	14	3381	1/1	0.86	0.08	-	70,70,70,70	0
58	MG	13	1669	1/1	0.93	0.21	-	70,70,70,70	0
58	MG	1H	3438	1/1	0.95	0.06	-	71,71,71,71	0
58	MG	1H	3132	1/1	0.90	0.21	-	63,63,63,63	0
58	MG	1H	3023	1/1	0.99	0.25	-	40,40,40,40	0
58	MG	1H	3060	1/1	0.95	0.39	-	59,59,59,59	0
58	MG	14	3370	1/1	0.90	0.06	-	75,75,75,75	0
58	MG	1H	3277	1/1	0.95	0.18	-	70,70,70,70	0
58	MG	1H	3374	1/1	0.67	0.34	-	78,78,78,78	0
58	MG	14	3027	1/1	0.94	0.23	-	76,76,76,76	0
58	MG	13	1696	1/1	0.96	0.35	-	81,81,81,81	0
58	MG	14	3169	1/1	0.95	0.29	-	91,91,91,91	0
58	MG	14	3276	1/1	0.91	0.25	-	75,75,75,75	0
58	MG	1H	3332	1/1	0.77	0.17	-	62,62,62,62	0
58	MG	13	1681	1/1	0.94	0.06	-	71,71,71,71	0
58	MG	1H	3083	1/1	0.92	0.26	-	71,71,71,71	0
58	MG	1H	3295	1/1	0.97	0.27	-	51,51,51,51	0
58	MG	14	3294	1/1	0.96	0.31	-	90,90,90,90	0
58	MG	1H	3177	1/1	0.92	0.20	-	47,47,47,47	0
58	MG	14	3248	1/1	0.91	0.10	-	65,65,65,65	0
58	MG	18	102	1/1	0.95	0.24	-	49,49,49,49	0
58	MG	1H	3236	1/1	0.99	0.12	-	52,52,52,52	0
58	MG	14	3251	1/1	0.91	0.18	-	80,80,80,80	0
58	MG	1H	3219	1/1	0.96	0.26	-	61,61,61,61	0
58	MG	1H	3285	1/1	0.85	0.26	-	62,62,62,62	0
58	MG	14	3044	1/1	0.97	0.14	-	40,40,40,40	0
58	MG	1H	3179	1/1	0.93	0.31	-	71,71,71,71	0
58	MG	1G	1659	1/1	0.96	0.10	-	76,76,76,76	0
58	MG	14	3146	1/1	0.69	0.52	-	88,88,88,88	0
58	MG	1H	3302	1/1	0.80	0.55	-	92,92,92,92	0
58	MG	14	3010	1/1	0.95	0.18	-	48,48,48,48	0
58	MG	14	3278	1/1	0.73	0.17	-	67,67,67,67	0
58	MG	13	1672	1/1	0.98	0.29	-	56,56,56,56	0
58	MG	13	1735	1/1	0.80	0.12	-	93,93,93,93	0
58	MG	1H	3240	1/1	0.92	0.62	-	86,86,86,86	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
58	MG	14	3264	1/1	0.94	0.24	-	69,69,69,69	0
58	MG	13	1707	1/1	0.58	0.27	-	83,83,83,83	0
58	MG	13	1635	1/1	0.80	0.32	-	77,77,77,77	0
58	MG	1H	3027	1/1	0.97	0.28	-	36,36,36,36	0
58	MG	14	3231	1/1	0.92	0.27	-	75,75,75,75	0
58	MG	1J	203	1/1	0.85	0.23	-	75,75,75,75	0
58	MG	1H	3256	1/1	0.93	0.17	-	57,57,57,57	0
58	MG	14	3090	1/1	0.97	0.23	-	65,65,65,65	0
58	MG	16	212	1/1	0.83	0.11	-	78,78,78,78	0
58	MG	1H	3140	1/1	0.89	0.25	-	59,59,59,59	0
58	MG	14	3262	1/1	0.83	0.21	-	86,86,86,86	0
58	MG	1H	3138	1/1	0.97	0.44	-	62,62,62,62	0
58	MG	1H	3366	1/1	0.78	0.42	-	83,83,83,83	0
58	MG	1H	3267	1/1	0.90	0.15	-	57,57,57,57	0
58	MG	1H	3408	1/1	0.88	0.11	-	47,47,47,47	0
58	MG	1H	3108	1/1	0.93	0.49	-	56,56,56,56	0
58	MG	1G	1624	1/1	0.86	0.31	-	89,89,89,89	0
58	MG	1H	3173	1/1	0.93	0.23	-	68,68,68,68	0
58	MG	14	3167	1/1	0.94	0.17	-	61,61,61,61	0
58	MG	1H	3393	1/1	0.95	0.11	-	47,47,47,47	0
58	MG	14	3021	1/1	0.98	0.16	-	51,51,51,51	0
58	MG	1H	3440	1/1	0.98	0.07	-	59,59,59,59	0
58	MG	98	201	1/1	0.95	0.29	-	64,64,64,64	0
58	MG	14	3156	1/1	0.84	0.33	-	70,70,70,70	0
58	MG	14	3388	1/1	0.91	0.12	-	88,88,88,88	0
58	MG	13	1614	1/1	0.89	0.22	-	65,65,65,65	0
58	MG	1H	3298	1/1	0.98	0.36	-	94,94,94,94	0
58	MG	1H	3276	1/1	0.84	0.45	-	76,76,76,76	0
58	MG	13	1666	1/1	0.97	0.34	-	81,81,81,81	0
58	MG	13	1621	1/1	0.98	0.23	-	59,59,59,59	0
58	MG	1H	3315	1/1	0.75	0.26	-	67,67,67,67	0
58	MG	14	3063	1/1	0.94	0.20	-	51,51,51,51	0
58	MG	1H	3155	1/1	0.95	0.14	-	41,41,41,41	0
58	MG	1G	1656	1/1	0.76	0.17	-	92,92,92,92	0
58	MG	14	3304	1/1	0.92	0.34	-	63,63,63,63	0
58	MG	13	1648	1/1	0.80	0.30	-	75,75,75,75	0
58	MG	13	1687	1/1	0.89	0.20	-	82,82,82,82	0
58	MG	1G	1643	1/1	0.98	0.09	-	83,83,83,83	0
58	MG	1H	3059	1/1	0.97	0.34	-	55,55,55,55	0
58	MG	1G	1658	1/1	0.70	0.30	-	104,104,104,104	0
58	MG	1H	3126	1/1	0.98	0.24	-	46,46,46,46	0
58	MG	1H	3254	1/1	0.89	0.22	-	73,73,73,73	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
58	MG	1H	3423	1/1	0.85	0.11	-	71,71,71,71	0
58	MG	1H	3419	1/1	0.96	0.11	-	37,37,37,37	0
58	MG	1H	3337	1/1	0.94	0.40	-	67,67,67,67	0
58	MG	1H	3379	1/1	0.94	0.21	-	85,85,85,85	0
58	MG	14	3068	1/1	0.95	0.20	-	54,54,54,54	0
58	MG	1H	3192	1/1	0.80	0.23	-	58,58,58,58	0
58	MG	13	1703	1/1	0.88	0.27	-	71,71,71,71	0
58	MG	14	3338	1/1	0.95	0.07	-	61,61,61,61	0
58	MG	14	3347	1/1	0.94	0.09	-	49,49,49,49	0
58	MG	1H	3320	1/1	0.87	0.23	-	59,59,59,59	0
58	MG	1H	3222	1/1	0.87	0.36	-	82,82,82,82	0
58	MG	1H	3403	1/1	0.98	0.11	-	69,69,69,69	0
58	MG	1H	3046	1/1	0.86	0.31	-	82,82,82,82	0
58	MG	1G	1674	1/1	0.93	0.22	-	136,136,136,136	0
58	MG	1G	1637	1/1	0.83	0.17	-	75,75,75,75	0
58	MG	14	3163	1/1	0.87	0.43	-	71,71,71,71	0
58	MG	13	1683	1/1	0.94	0.10	-	94,94,94,94	0
58	MG	14	3301	1/1	0.45	0.23	-	87,87,87,87	0
58	MG	1G	1661	1/1	0.55	0.21	-	100,100,100,100	0
58	MG	L5	400	1/1	0.91	0.15	-	70,70,70,70	0
58	MG	13	1649	1/1	0.90	0.45	-	83,83,83,83	0
58	MG	1H	3230	1/1	0.98	0.23	-	47,47,47,47	0
58	MG	1H	3013	1/1	0.98	0.28	-	46,46,46,46	0
58	MG	13	1611	1/1	0.86	0.29	-	64,64,64,64	0
58	MG	14	3164	1/1	0.71	0.12	-	76,76,76,76	0
58	MG	1G	1639	1/1	0.96	0.24	-	110,110,110,110	0
58	MG	14	3368	1/1	0.92	0.10	-	64,64,64,64	0
58	MG	14	3091	1/1	0.99	0.26	-	50,50,50,50	0
58	MG	1H	3380	1/1	0.84	0.22	-	69,69,69,69	0
58	MG	13	1715	1/1	0.98	0.08	-	78,78,78,78	0
58	MG	14	3290	1/1	0.90	0.18	-	74,74,74,74	0
58	MG	1G	1681	1/1	0.97	0.40	-	85,85,85,85	0
58	MG	1H	3030	1/1	0.97	0.19	-	40,40,40,40	0
58	MG	1H	3212	1/1	0.97	0.32	-	80,80,80,80	0
58	MG	14	3069	1/1	0.99	0.26	-	75,75,75,75	0
58	MG	14	3131	1/1	0.86	0.23	-	71,71,71,71	0
58	MG	1G	1635	1/1	0.88	0.21	-	86,86,86,86	0
58	MG	14	3093	1/1	0.99	0.11	-	63,63,63,63	0
58	MG	1H	3272	1/1	0.94	0.46	-	88,88,88,88	0
58	MG	1H	3088	1/1	0.90	0.30	-	56,56,56,56	0
58	MG	14	3001	1/1	0.98	0.27	-	50,50,50,50	0
58	MG	13	1678	1/1	0.95	0.28	-	92,92,92,92	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
58	MG	1H	3048	1/1	0.98	0.18	-	52,52,52,52	0
58	MG	1H	3248	1/1	0.91	0.20	-	88,88,88,88	0
58	MG	14	3288	1/1	0.88	0.15	-	66,66,66,66	0
58	MG	1H	3399	1/1	0.98	0.08	-	58,58,58,58	0
58	MG	14	3112	1/1	0.94	0.26	-	86,86,86,86	0
58	MG	14	3078	1/1	0.84	0.26	-	87,87,87,87	0
58	MG	1H	3110	1/1	0.68	0.30	-	58,58,58,58	0
58	MG	13	1722	1/1	0.88	0.11	-	101,101,101,101	0
58	MG	1G	1615	1/1	0.96	0.19	-	82,82,82,82	0
58	MG	14	3326	1/1	0.84	0.13	-	90,90,90,90	0
58	MG	1H	3313	1/1	0.69	0.40	-	82,82,82,82	0
58	MG	31	302	1/1	0.98	0.08	-	57,57,57,57	0
58	MG	25	201	1/1	0.71	0.26	-	88,88,88,88	0
58	MG	8E	201	1/1	0.82	0.22	-	95,95,95,95	0
58	MG	1H	3375	1/1	0.89	0.55	-	94,94,94,94	0
58	MG	1G	1675	1/1	0.89	0.25	-	83,83,83,83	0
58	MG	1H	3251	1/1	0.97	0.18	-	33,33,33,33	0
58	MG	1H	3344	1/1	0.93	0.35	-	71,71,71,71	0
58	MG	14	3239	1/1	0.89	0.15	-	64,64,64,64	0
58	MG	1H	3049	1/1	0.89	0.24	-	56,56,56,56	0
58	MG	1K	101	1/1	0.88	0.21	-	84,84,84,84	0
58	MG	13	1647	1/1	0.96	0.30	-	47,47,47,47	0
58	MG	1H	3129	1/1	0.91	0.32	-	58,58,58,58	0
58	MG	1H	3022	1/1	0.99	0.17	-	39,39,39,39	0
58	MG	1H	3437	1/1	0.82	0.13	-	66,66,66,66	0
58	MG	1H	3291	1/1	0.73	0.25	-	70,70,70,70	0
58	MG	13	1730	1/1	0.92	0.09	-	88,88,88,88	0
58	MG	1H	3143	1/1	0.79	0.29	-	66,66,66,66	0
58	MG	14	3097	1/1	0.95	0.22	-	51,51,51,51	0
58	MG	14	3023	1/1	0.97	0.12	-	46,46,46,46	0
58	MG	1G	1640	1/1	0.83	0.27	-	78,78,78,78	0
58	MG	13	1671	1/1	0.80	0.20	-	138,138,138,138	0
58	MG	14	3055	1/1	0.95	0.18	-	55,55,55,55	0
58	MG	1G	1690	1/1	0.91	0.31	-	98,98,98,98	0
58	MG	13	1736	1/1	0.95	0.14	-	97,97,97,97	0
58	MG	2L	103	1/1	0.88	0.12	-	102,102,102,102	0
58	MG	13	1716	1/1	0.77	0.16	-	80,80,80,80	0
58	MG	1H	3442	1/1	0.99	0.06	-	60,60,60,60	0
58	MG	1G	1669	1/1	0.94	0.28	-	131,131,131,131	0
58	MG	1H	3279	1/1	0.91	0.21	-	77,77,77,77	0
58	MG	14	3147	1/1	0.74	0.15	-	73,73,73,73	0
58	MG	13	1634	1/1	0.97	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
58	MG	14	3181	1/1	0.93	0.24	-	81,81,81,81	0
58	MG	1G	1630	1/1	0.89	0.19	-	71,71,71,71	0
58	MG	14	3134	1/1	0.94	0.14	-	54,54,54,54	0
58	MG	14	3047	1/1	0.97	0.17	-	71,71,71,71	0
58	MG	1H	3082	1/1	0.84	0.36	-	60,60,60,60	0
58	MG	1H	3216	1/1	0.94	0.22	-	68,68,68,68	0
58	MG	1H	3377	1/1	0.70	0.29	-	68,68,68,68	0
58	MG	14	3062	1/1	0.93	0.17	-	51,51,51,51	0
58	MG	1H	3469	1/1	0.80	0.10	-	106,106,106,106	0
58	MG	1G	1662	1/1	0.94	0.18	-	78,78,78,78	0
58	MG	1H	3135	1/1	0.98	0.27	-	52,52,52,52	0
58	MG	16	208	1/1	0.78	0.31	-	80,80,80,80	0
58	MG	1G	1660	1/1	0.86	0.41	-	82,82,82,82	0
58	MG	18	101	1/1	0.83	0.19	-	63,63,63,63	0
58	MG	14	3115	1/1	0.76	0.20	-	71,71,71,71	0
58	MG	13	1731	1/1	0.98	0.11	-	85,85,85,85	0
58	MG	1H	3311	1/1	0.95	0.18	-	58,58,58,58	0
58	MG	13	1712	1/1	0.85	0.17	-	74,74,74,74	0
58	MG	14	3314	1/1	0.92	0.26	-	59,59,59,59	0
58	MG	14	3352	1/1	0.92	0.11	-	73,73,73,73	0
58	MG	14	3394	1/1	0.97	0.07	-	94,94,94,94	0
58	MG	1H	3467	1/1	0.82	0.09	-	68,68,68,68	0
58	MG	1H	3309	1/1	0.53	0.28	-	83,83,83,83	0
58	MG	13	1652	1/1	0.91	0.21	-	60,60,60,60	0
58	MG	1G	1678	1/1	0.91	0.32	-	92,92,92,92	0
58	MG	14	3296	1/1	0.57	0.37	-	97,97,97,97	0
58	MG	1H	3104	1/1	0.94	0.16	-	47,47,47,47	0
58	MG	13	1613	1/1	0.96	0.14	-	66,66,66,66	0
58	MG	1H	3464	1/1	0.90	0.08	-	88,88,88,88	0
58	MG	14	3195	1/1	0.87	0.33	-	81,81,81,81	0
58	MG	14	3158	1/1	0.94	0.14	-	72,72,72,72	0
58	MG	1H	3396	1/1	0.96	0.13	-	55,55,55,55	0
58	MG	1H	3207	1/1	0.85	0.21	-	57,57,57,57	0
58	MG	1J	205	1/1	0.93	0.27	-	75,75,75,75	0
58	MG	13	1626	1/1	0.94	0.24	-	80,80,80,80	0
58	MG	1H	3185	1/1	0.88	0.45	-	77,77,77,77	0
58	MG	1H	3278	1/1	0.96	0.14	-	75,75,75,75	0
58	MG	1G	1621	1/1	0.87	0.15	-	81,81,81,81	0
58	MG	14	3179	1/1	0.95	0.45	-	63,63,63,63	0
58	MG	14	3291	1/1	0.85	0.15	-	77,77,77,77	0
58	MG	1H	3247	1/1	0.93	0.48	-	73,73,73,73	0
58	MG	1H	3246	1/1	0.93	0.46	-	79,79,79,79	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
58	MG	14	3201	1/1	0.95	0.42	-	49,49,49,49	0
58	MG	14	3009	1/1	0.99	0.16	-	49,49,49,49	0
58	MG	2K	105	1/1	0.83	0.30	-	87,87,87,87	0
58	MG	13	1624	1/1	0.99	0.26	-	85,85,85,85	0
58	MG	1H	3158	1/1	0.88	0.26	-	69,69,69,69	0
58	MG	1H	3119	1/1	0.94	0.20	-	55,55,55,55	0
58	MG	1G	1650	1/1	0.92	0.27	-	68,68,68,68	0
58	MG	14	3257	1/1	0.93	0.18	-	63,63,63,63	0
58	MG	14	3099	1/1	0.95	0.41	-	75,75,75,75	0
58	MG	1H	3120	1/1	0.96	0.18	-	63,63,63,63	0
58	MG	14	3305	1/1	0.89	0.19	-	59,59,59,59	0
58	MG	14	3267	1/1	0.80	0.12	-	74,74,74,74	0
58	MG	14	3223	1/1	0.97	0.19	-	44,44,44,44	0
58	MG	13	1610	1/1	0.80	0.32	-	94,94,94,94	0
58	MG	1H	3127	1/1	0.96	0.30	-	75,75,75,75	0
58	MG	14	3020	1/1	0.89	0.17	-	63,63,63,63	0
58	MG	1H	3341	1/1	0.88	0.51	-	86,86,86,86	0
58	MG	13	1604	1/1	0.98	0.14	-	65,65,65,65	0
58	MG	14	3082	1/1	0.95	0.18	-	54,54,54,54	0
58	MG	14	3193	1/1	0.96	0.23	-	60,60,60,60	0
58	MG	1H	3266	1/1	0.83	0.14	-	43,43,43,43	0
58	MG	1H	3218	1/1	0.91	0.28	-	57,57,57,57	0
58	MG	1H	3323	1/1	0.88	0.16	-	61,61,61,61	0
58	MG	1H	3142	1/1	0.90	0.23	-	59,59,59,59	0
58	MG	1H	3012	1/1	0.96	0.22	-	58,58,58,58	0
58	MG	1H	3293	1/1	0.97	0.12	-	56,56,56,56	0
58	MG	1H	3057	1/1	0.95	0.23	-	60,60,60,60	0
58	MG	1H	3210	1/1	0.70	0.27	-	86,86,86,86	0
58	MG	1H	3318	1/1	0.99	0.10	-	50,50,50,50	0
58	MG	1H	3451	1/1	0.91	0.11	-	84,84,84,84	0
58	MG	14	3310	1/1	0.81	0.30	-	76,76,76,76	0
58	MG	13	1628	1/1	0.97	0.25	-	43,43,43,43	0
58	MG	14	3143	1/1	0.84	0.21	-	64,64,64,64	0
58	MG	1H	3072	1/1	0.88	0.20	-	62,62,62,62	0
58	MG	1H	3160	1/1	0.98	0.18	-	64,64,64,64	0
58	MG	14	3367	1/1	0.94	0.08	-	49,49,49,49	0
58	MG	1H	3457	1/1	0.94	0.09	-	81,81,81,81	0
58	MG	14	3141	1/1	0.79	0.17	-	75,75,75,75	0
58	MG	14	3215	1/1	0.95	0.27	-	60,60,60,60	0
58	MG	14	3318	1/1	0.97	0.06	-	81,81,81,81	0
58	MG	13	1680	1/1	0.74	0.25	-	71,71,71,71	0
58	MG	1H	3224	1/1	0.80	0.38	-	79,79,79,79	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
58	MG	1H	3353	1/1	0.94	0.20	-	93,93,93,93	0
58	MG	1H	3032	1/1	0.90	0.26	-	71,71,71,71	0
58	MG	14	3376	1/1	0.96	0.11	-	87,87,87,87	0
58	MG	1G	1663	1/1	0.95	0.20	-	105,105,105,105	0
58	MG	14	3379	1/1	0.96	0.10	-	51,51,51,51	0
58	MG	14	3375	1/1	0.94	0.07	-	65,65,65,65	0
58	MG	14	3221	1/1	0.97	0.17	-	66,66,66,66	0
58	MG	16	207	1/1	0.90	0.40	-	76,76,76,76	0
58	MG	14	3194	1/1	0.79	0.14	-	57,57,57,57	0
58	MG	1H	3429	1/1	0.88	0.13	-	49,49,49,49	0
58	MG	1H	3450	1/1	0.99	0.05	-	79,79,79,79	0
58	MG	1H	3462	1/1	0.82	0.07	-	76,76,76,76	0
58	MG	14	3171	1/1	0.92	0.17	-	65,65,65,65	0
58	MG	14	3268	1/1	0.87	0.25	-	88,88,88,88	0
58	MG	1H	3136	1/1	0.94	0.24	-	53,53,53,53	0
58	MG	13	1693	1/1	0.73	0.30	-	87,87,87,87	0
58	MG	1H	3364	1/1	0.90	0.56	-	90,90,90,90	0
58	MG	1H	3086	1/1	0.97	0.40	-	52,52,52,52	0
58	MG	1H	3378	1/1	0.88	0.21	-	68,68,68,68	0
58	MG	2K	102	1/1	0.94	0.20	-	78,78,78,78	0
58	MG	14	3365	1/1	0.87	0.12	-	67,67,67,67	0
58	MG	14	3243	1/1	0.96	0.14	-	68,68,68,68	0
58	MG	1H	3314	1/1	0.90	0.36	-	86,86,86,86	0
58	MG	13	1663	1/1	0.85	0.20	-	68,68,68,68	0
58	MG	1H	3268	1/1	0.95	0.25	-	65,65,65,65	0
58	MG	14	3162	1/1	0.54	0.34	-	100,100,100,100	0
58	MG	29	301	1/1	0.98	0.19	-	46,46,46,46	0
58	MG	1H	3416	1/1	0.99	0.12	-	51,51,51,51	0
58	MG	14	3057	1/1	0.96	0.23	-	62,62,62,62	0
58	MG	1H	3242	1/1	0.92	0.34	-	66,66,66,66	0
58	MG	14	3098	1/1	0.91	0.39	-	67,67,67,67	0
58	MG	1H	3426	1/1	0.89	0.09	-	39,39,39,39	0
58	MG	14	3272	1/1	0.99	0.14	-	72,72,72,72	0
58	MG	1H	3376	1/1	0.92	0.28	-	78,78,78,78	0
58	MG	1H	3436	1/1	0.91	0.11	-	87,87,87,87	0
58	MG	14	3357	1/1	0.96	0.16	-	48,48,48,48	0
58	MG	14	3229	1/1	0.76	0.54	-	82,82,82,82	0
58	MG	1H	3003	1/1	0.97	0.35	-	30,30,30,30	0
58	MG	1H	3005	1/1	0.96	0.23	-	53,53,53,53	0
58	MG	1H	3340	1/1	0.93	0.23	-	51,51,51,51	0
58	MG	1G	1611	1/1	0.85	0.23	-	89,89,89,89	0
58	MG	13	1737	1/1	0.80	0.14	-	132,132,132,132	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
58	MG	1H	3148	1/1	0.95	0.28	-	57,57,57,57	0
58	MG	13	1608	1/1	0.95	0.20	-	77,77,77,77	0
58	MG	14	3214	1/1	0.94	0.22	-	54,54,54,54	0
58	MG	1H	3183	1/1	0.94	0.23	-	56,56,56,56	0
58	MG	14	3356	1/1	0.94	0.17	-	78,78,78,78	0
58	MG	14	3052	1/1	0.96	0.15	-	52,52,52,52	0
58	MG	1H	3334	1/1	0.95	0.14	-	55,55,55,55	0
58	MG	1H	3474	1/1	0.62	0.07	-	84,84,84,84	0
58	MG	14	3261	1/1	0.87	0.39	-	68,68,68,68	0
58	MG	14	3241	1/1	0.94	0.10	-	72,72,72,72	0
58	MG	1H	3333	1/1	0.93	0.20	-	63,63,63,63	0
58	MG	14	3035	1/1	0.96	0.20	-	76,76,76,76	0
58	MG	1H	3265	1/1	0.96	0.15	-	66,66,66,66	0
58	MG	1H	3181	1/1	0.98	0.30	-	71,71,71,71	0
58	MG	13	1685	1/1	0.90	0.26	-	65,65,65,65	0
58	MG	14	3330	1/1	0.96	0.14	-	58,58,58,58	0
58	MG	14	3327	1/1	0.87	0.29	-	86,86,86,86	0
58	MG	13	1725	1/1	0.90	0.07	-	85,85,85,85	0
58	MG	1H	3033	1/1	0.89	0.41	-	82,82,82,82	0
58	MG	1H	3151	1/1	0.77	0.27	-	56,56,56,56	0
58	MG	1H	3196	1/1	0.76	0.39	-	71,71,71,71	0
58	MG	1G	1688	1/1	0.94	0.17	-	105,105,105,105	0
58	MG	13	1641	1/1	0.83	0.26	-	68,68,68,68	0
58	MG	14	3199	1/1	0.97	0.22	-	66,66,66,66	0
58	MG	14	3284	1/1	0.74	0.18	-	70,70,70,70	0
58	MG	1H	3115	1/1	0.88	0.20	-	48,48,48,48	0
58	MG	1H	3454	1/1	0.88	0.08	-	65,65,65,65	0
58	MG	1H	3444	1/1	0.91	0.08	-	90,90,90,90	0
58	MG	1H	3305	1/1	0.76	0.24	-	66,66,66,66	0
58	MG	1H	3223	1/1	0.85	0.25	-	63,63,63,63	0
58	MG	1H	3304	1/1	0.84	0.39	-	77,77,77,77	0
58	MG	1H	3269	1/1	0.73	0.25	-	55,55,55,55	0
58	MG	1H	3079	1/1	0.98	0.32	-	55,55,55,55	0
58	MG	14	3308	1/1	0.74	0.53	-	79,79,79,79	0
58	MG	13	1720	1/1	0.72	0.26	-	89,89,89,89	0
58	MG	1G	1671	1/1	0.95	0.13	-	85,85,85,85	0
58	MG	1H	3351	1/1	0.93	0.19	-	62,62,62,62	0
58	MG	1H	3189	1/1	0.90	0.35	-	73,73,73,73	0

6.5 Other polymers ⓘ

There are no such residues in this entry.