



# wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 19, 2016 – 11:04 PM GMT

PDB ID : 4WQ1  
Title : Complex of 70S ribosome with tRNA-Tyr and mRNA with C-A mismatch in the first position in the A-site.  
Authors : Rozov, A.; Demeshkina, N.; Yusupov, M.; Yusupova, G.  
Deposited on : 2014-10-21  
Resolution : 3.10 Å(reported)

This is a wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.  
We welcome your comments at [validation@mail.wwpdb.org](mailto: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.

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

MolProbity : 4.02b-467  
Mogul : 1.7.1 (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

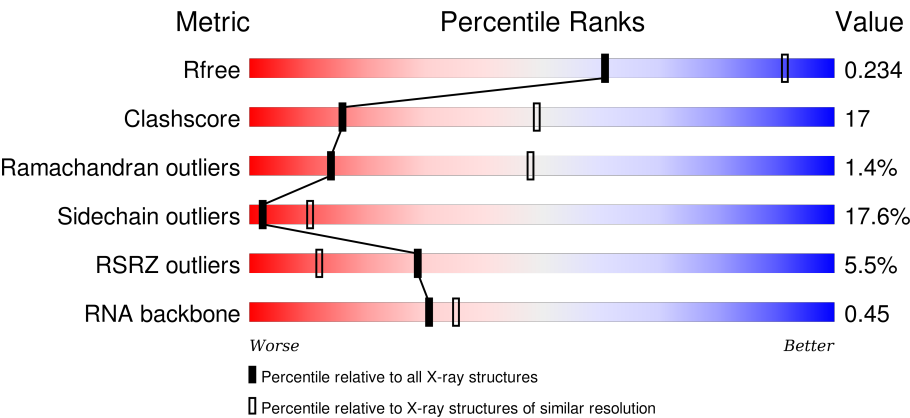
# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.10 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	91344	1114 (3.14-3.06)
Clashscore	102246	1222 (3.14-3.06)
Ramachandran outliers	100387	1174 (3.14-3.06)
Sidechain outliers	100360	1174 (3.14-3.06)
RSRZ outliers	91569	1119 (3.14-3.06)
RNA backbone	2183	1010 (3.52-2.68)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. 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></div><div><div></div><div>30%</div><div>45%</div><div>20%</div><div>• •</div></div></div>
2	12	256	<div><div>5%</div><div>48%</div><div>38%</div><div>7%</div><div>7%</div></div>
2	1E	256	<div><div></div><div><div></div><div>47%</div><div>39%</div><div>5%</div><div>7%</div></div></div>
3	22	239	<div><div>12%</div><div>49%</div><div>31%</div><div>6%</div><div>14%</div></div>

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Mol	Chain	Length	Quality of chain
3	2E	239	
4	32	208	
4	3E	208	
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	1L	85	
22	3K	85	
22	3L	85	
23	2K	77	
23	2L	77	
24	4K	30	
24	4L	30	
25	14	2912	
25	1H	2912	
26	16	122	
26	1J	122	
27	11	272	

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Mol	Chain	Length	Quality of chain
28	21	205	
28	29	205	
29	31	202	
30	41	181	
30	49	181	
31	51	180	
31	59	180	
32	61	146	
32	69	146	
33	15	138	
33	58	138	
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	111	
38	A8	111	
39	75	137	
39	B8	137	
40	85	117	
40	C8	117	

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Mol	Chain	Length	Quality of chain
41	95	101	
41	D8	101	
42	A5	113	
42	E8	113	
43	B5	94	
43	F8	94	
44	C5	110	
44	G8	110	
45	H8	175	
46	E5	85	
46	I8	85	
47	F5	98	
47	J8	98	
48	G5	66	
48	K8	66	
49	H5	59	
49	L8	59	
50	I5	66	
50	M8	66	
51	J5	59	
51	N8	59	
52	K5	45	
52	O8	45	
53	L5	49	
53	P8	49	

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Mol	Chain	Length	Quality of chain
54	Q8	65	
55	1G	1522	
56	19	276	
57	39	210	
58	D5	206	
59	M5	61	

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
60	MG	13	1604	-	-	-	X
60	MG	13	1605	-	-	-	X
60	MG	13	1608	-	-	-	X
60	MG	13	1617	-	-	-	X
60	MG	13	1621	-	-	-	X
60	MG	13	1627	-	-	-	X
60	MG	13	1642	-	-	-	X
60	MG	13	1648	-	-	-	X
60	MG	13	1650	-	-	-	X
60	MG	13	1651	-	-	-	X
60	MG	13	1660	-	-	-	X
60	MG	13	1664	-	-	-	X
60	MG	13	1668	-	-	-	X
60	MG	13	1672	-	-	-	X
60	MG	13	1692	-	-	-	X
60	MG	13	1710	-	-	-	X
60	MG	14	3004	-	-	-	X
60	MG	14	3010	-	-	-	X
60	MG	14	3011	-	-	-	X
60	MG	14	3012	-	-	-	X
60	MG	14	3023	-	-	-	X
60	MG	14	3028	-	-	-	X
60	MG	14	3034	-	-	-	X
60	MG	14	3035	-	-	-	X
60	MG	14	3036	-	-	-	X
60	MG	14	3042	-	-	-	X
60	MG	14	3052	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
60	MG	14	3054	-	-	-	X
60	MG	14	3058	-	-	-	X
60	MG	14	3061	-	-	-	X
60	MG	14	3064	-	-	-	X
60	MG	14	3066	-	-	-	X
60	MG	14	3068	-	-	-	X
60	MG	14	3074	-	-	-	X
60	MG	14	3079	-	-	-	X
60	MG	14	3082	-	-	-	X
60	MG	14	3083	-	-	-	X
60	MG	14	3086	-	-	-	X
60	MG	14	3088	-	-	-	X
60	MG	14	3090	-	-	-	X
60	MG	14	3092	-	-	-	X
60	MG	14	3094	-	-	-	X
60	MG	14	3095	-	-	-	X
60	MG	14	3097	-	-	-	X
60	MG	14	3098	-	-	-	X
60	MG	14	3100	-	-	-	X
60	MG	14	3102	-	-	-	X
60	MG	14	3112	-	-	-	X
60	MG	14	3115	-	-	-	X
60	MG	14	3118	-	-	-	X
60	MG	14	3119	-	-	-	X
60	MG	14	3127	-	-	-	X
60	MG	14	3130	-	-	-	X
60	MG	14	3134	-	-	-	X
60	MG	14	3137	-	-	-	X
60	MG	14	3139	-	-	-	X
60	MG	14	3147	-	-	-	X
60	MG	14	3151	-	-	-	X
60	MG	14	3153	-	-	-	X
60	MG	14	3156	-	-	-	X
60	MG	14	3157	-	-	-	X
60	MG	14	3161	-	-	-	X
60	MG	14	3163	-	-	-	X
60	MG	14	3176	-	-	-	X
60	MG	14	3177	-	-	-	X
60	MG	14	3179	-	-	-	X
60	MG	14	3192	-	-	-	X
60	MG	14	3203	-	-	-	X
60	MG	14	3206	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
60	MG	14	3208	-	-	-	X
60	MG	14	3214	-	-	-	X
60	MG	14	3219	-	-	-	X
60	MG	14	3221	-	-	-	X
60	MG	14	3223	-	-	-	X
60	MG	14	3225	-	-	-	X
60	MG	14	3229	-	-	-	X
60	MG	14	3231	-	-	-	X
60	MG	14	3232	-	-	-	X
60	MG	14	3233	-	-	-	X
60	MG	14	3235	-	-	-	X
60	MG	14	3237	-	-	-	X
60	MG	14	3238	-	-	-	X
60	MG	14	3245	-	-	-	X
60	MG	14	3246	-	-	-	X
60	MG	14	3258	-	-	-	X
60	MG	14	3270	-	-	-	X
60	MG	14	3279	-	-	-	X
60	MG	14	3281	-	-	-	X
60	MG	14	3284	-	-	-	X
60	MG	14	3286	-	-	-	X
60	MG	14	3288	-	-	-	X
60	MG	14	3289	-	-	-	X
60	MG	14	3290	-	-	-	X
60	MG	14	3294	-	-	-	X
60	MG	14	3299	-	-	-	X
60	MG	14	3305	-	-	-	X
60	MG	14	3306	-	-	-	X
60	MG	14	3386	-	-	-	X
60	MG	16	201	-	-	-	X
60	MG	16	204	-	-	-	X
60	MG	16	205	-	-	-	X
60	MG	1G	1601	-	-	-	X
60	MG	1G	1611	-	-	-	X
60	MG	1G	1614	-	-	-	X
60	MG	1G	1625	-	-	-	X
60	MG	1G	1631	-	-	-	X
60	MG	1G	1632	-	-	-	X
60	MG	1G	1644	-	-	-	X
60	MG	1G	1656	-	-	-	X
60	MG	1G	1657	-	-	-	X
60	MG	1G	1667	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
60	MG	1G	1673	-	-	-	X
60	MG	1G	1674	-	-	-	X
60	MG	1G	1678	-	-	-	X
60	MG	1G	1684	-	-	-	X
60	MG	1G	1688	-	-	-	X
60	MG	1H	3002	-	-	-	X
60	MG	1H	3010	-	-	-	X
60	MG	1H	3012	-	-	-	X
60	MG	1H	3014	-	-	-	X
60	MG	1H	3016	-	-	-	X
60	MG	1H	3020	-	-	-	X
60	MG	1H	3021	-	-	-	X
60	MG	1H	3023	-	-	-	X
60	MG	1H	3024	-	-	-	X
60	MG	1H	3030	-	-	-	X
60	MG	1H	3033	-	-	-	X
60	MG	1H	3034	-	-	-	X
60	MG	1H	3037	-	-	-	X
60	MG	1H	3042	-	-	-	X
60	MG	1H	3044	-	-	-	X
60	MG	1H	3048	-	-	-	X
60	MG	1H	3050	-	-	-	X
60	MG	1H	3051	-	-	-	X
60	MG	1H	3054	-	-	-	X
60	MG	1H	3058	-	-	-	X
60	MG	1H	3060	-	-	-	X
60	MG	1H	3062	-	-	-	X
60	MG	1H	3066	-	-	-	X
60	MG	1H	3067	-	-	-	X
60	MG	1H	3069	-	-	-	X
60	MG	1H	3075	-	-	-	X
60	MG	1H	3076	-	-	-	X
60	MG	1H	3083	-	-	-	X
60	MG	1H	3087	-	-	-	X
60	MG	1H	3096	-	-	-	X
60	MG	1H	3099	-	-	-	X
60	MG	1H	3107	-	-	-	X
60	MG	1H	3110	-	-	-	X
60	MG	1H	3115	-	-	-	X
60	MG	1H	3122	-	-	-	X
60	MG	1H	3127	-	-	-	X
60	MG	1H	3132	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
60	MG	1H	3142	-	-	-	X
60	MG	1H	3143	-	-	-	X
60	MG	1H	3147	-	-	-	X
60	MG	1H	3157	-	-	-	X
60	MG	1H	3164	-	-	-	X
60	MG	1H	3169	-	-	-	X
60	MG	1H	3173	-	-	-	X
60	MG	1H	3175	-	-	-	X
60	MG	1H	3184	-	-	-	X
60	MG	1H	3187	-	-	-	X
60	MG	1H	3191	-	-	-	X
60	MG	1H	3199	-	-	-	X
60	MG	1H	3202	-	-	-	X
60	MG	1H	3207	-	-	-	X
60	MG	1H	3221	-	-	-	X
60	MG	1H	3223	-	-	-	X
60	MG	1H	3229	-	-	-	X
60	MG	1H	3239	-	-	-	X
60	MG	1H	3242	-	-	-	X
60	MG	1H	3246	-	-	-	X
60	MG	1H	3256	-	-	-	X
60	MG	1H	3259	-	-	-	X
60	MG	1H	3265	-	-	-	X
60	MG	1H	3268	-	-	-	X
60	MG	1H	3270	-	-	-	X
60	MG	1H	3287	-	-	-	X
60	MG	1H	3294	-	-	-	X
60	MG	1H	3297	-	-	-	X
60	MG	1H	3298	-	-	-	X
60	MG	29	302	-	-	-	X
60	MG	2L	101	-	-	-	X
60	MG	85	201	-	-	-	X
61	ZN	32	301	-	-	-	X

## 2 Entry composition [i](#)

There are 62 unique types of molecules in this entry. The entry contains 299951 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	119	Total	C	N	O	S	0	0	0
			884	549	168	164	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 type Z.

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	72	Total	C	N	O		0	0	0
			590	376	117	97				

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
19	AI	83	Total	C	N	O	S	0	0	0
			665	424	124	115	2			
19	AA	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	25	Total	C	N	O	0	0	0
			217	134	52	31			

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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	74	Total	C	N	O	P	S	0	0	0
			1595	719	286	514	74	2			
22	1L	74	Total	C	N	O	P	S	0	0	0
			1595	719	286	514	74	2			
22	3L	75	Total	C	N	O	P	S	0	0	0
			1615	728	288	522	75	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
			1645	734	298	535	77	1			
23	2L	77	Total	C	N	O	P	S	0	0	0
			1645	734	298	535	77	1			

There are 2 discrepancies between the modelled and reference sequences:

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

- Molecule 24 is a RNA chain called mRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
24	4K	15	Total	C	N	O	P	0	0	0
			325	147	68	95	15			
24	4L	16	Total	C	N	O	P	0	0	0
			347	157	73	101	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			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
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			

- 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			

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

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

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

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

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
39	B8	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	S	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	104	Total	C	N	O	S	0	0	0
			791	510	149	127	5			
44	C5	104	Total	C	N	O	S	0	0	0
			794	510	152	127	5			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
45	H8	175	Total	C	N	O	S	0	0	0
			1397	892	251	251	3			

- 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			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
46	E5	77	Total	C	N	O	S	0	0	0
			612	379	129	103	1			

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
48	K8	66	Total	C	N	O	S	0	0	0
			558	346	113	98	1			
48	G5	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	S	0	0	0
			468	298	90	80				
49	H5	59	Total	C	N	O	S	0	0	0
			468	298	90	80				

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
51	N8	59	Total	C	N	O	S	0	0	0
			458	288	90	75	5			
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 L33.

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
54	Q8	62	Total	C	N	O	S	0	0	0
			442	281	83	76	2			

- Molecule 55 is a RNA chain called 16S ribosomal RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
55	1G	1498	Total	C	N	O	P	0	0	0
			32204	14334	5973	10400	1497			

- Molecule 56 is a protein called 50S ribosomal protein L2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
56	19	273	Total	C	N	O	S	0	0	0
			2120	1338	421	358	3			

- Molecule 57 is a protein called 50S ribosomal protein L4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
57	39	208	Total	C	N	O	S	0	0	0
			1627	1037	304	283	3			

- Molecule 58 is a protein called 50S ribosomal protein L25.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
58	D5	179	Total	C	N	O	S	0	0	0
			1428	911	255	259	3			

- Molecule 59 is a protein called 50S ribosomal protein L35.

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

- Molecule 60 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
60	98	2	Total	Mg	0	0
			2	2		
60	45	3	Total	Mg	0	0
			3	3		
60	P8	1	Total	Mg	0	0
			1	1		
60	85	1	Total	Mg	0	0
			1	1		
60	C5	1	Total	Mg	0	0
			1	1		
60	13	140	Total	Mg	0	0
			140	140		
60	B8	1	Total	Mg	0	0
			1	1		
60	K8	1	Total	Mg	0	0
			1	1		
60	5I	1	Total	Mg	0	0
			1	1		
60	C8	1	Total	Mg	0	0
			1	1		
60	16	12	Total	Mg	0	0
			12	12		
60	25	1	Total	Mg	0	0
			1	1		
60	3K	1	Total	Mg	0	0
			1	1		
60	21	2	Total	Mg	0	0
			2	2		
60	2K	4	Total	Mg	0	0
			4	4		
60	4I	1	Total	Mg	0	0
			1	1		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
60	3I	1	Total 1	Mg 1	0	0
60	I8	2	Total 2	Mg 2	0	0
60	52	1	Total 1	Mg 1	0	0
60	68	1	Total 1	Mg 1	0	0
60	29	2	Total 2	Mg 2	0	0
60	78	3	Total 3	Mg 3	0	0
60	39	1	Total 1	Mg 1	0	0
60	1G	104	Total 104	Mg 104	0	0
60	11	2	Total 2	Mg 2	0	0
60	1H	438	Total 438	Mg 438	0	0
60	E5	1	Total 1	Mg 1	0	0
60	88	2	Total 2	Mg 2	0	0
60	49	1	Total 1	Mg 1	0	0
60	14	386	Total 386	Mg 386	0	0
60	19	1	Total 1	Mg 1	0	0
60	1J	7	Total 7	Mg 7	0	0
60	1K	1	Total 1	Mg 1	0	0
60	41	1	Total 1	Mg 1	0	0
60	2L	3	Total 3	Mg 3	0	0

- Molecule 61 is ZINC ION (three-letter code: ZN) (formula: Zn).



Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
61	32	1	Total 1	Zn 1	0	0
61	3E	1	Total 1	Zn 1	0	0
61	5I	1	Total 1	Zn 1	0	0
61	5A	1	Total 1	Zn 1	0	0
61	G8	1	Total 1	Zn 1	0	0
61	C5	1	Total 1	Zn 1	0	0

- Molecule 62 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
62	13	125	Total 125	O 125	0	0
62	3E	4	Total 4	O 4	0	0
62	3I	1	Total 1	O 1	0	0
62	5I	2	Total 2	O 2	0	0
62	7I	1	Total 1	O 1	0	0
62	1K	4	Total 4	O 4	0	0
62	3K	1	Total 1	O 1	0	0
62	4K	1	Total 1	O 1	0	0
62	1H	738	Total 738	O 738	0	0
62	16	15	Total 15	O 15	0	0
62	11	10	Total 10	O 10	0	0
62	21	4	Total 4	O 4	0	0
62	31	5	Total 5	O 5	0	0
62	78	3	Total 3	O 3	0	0

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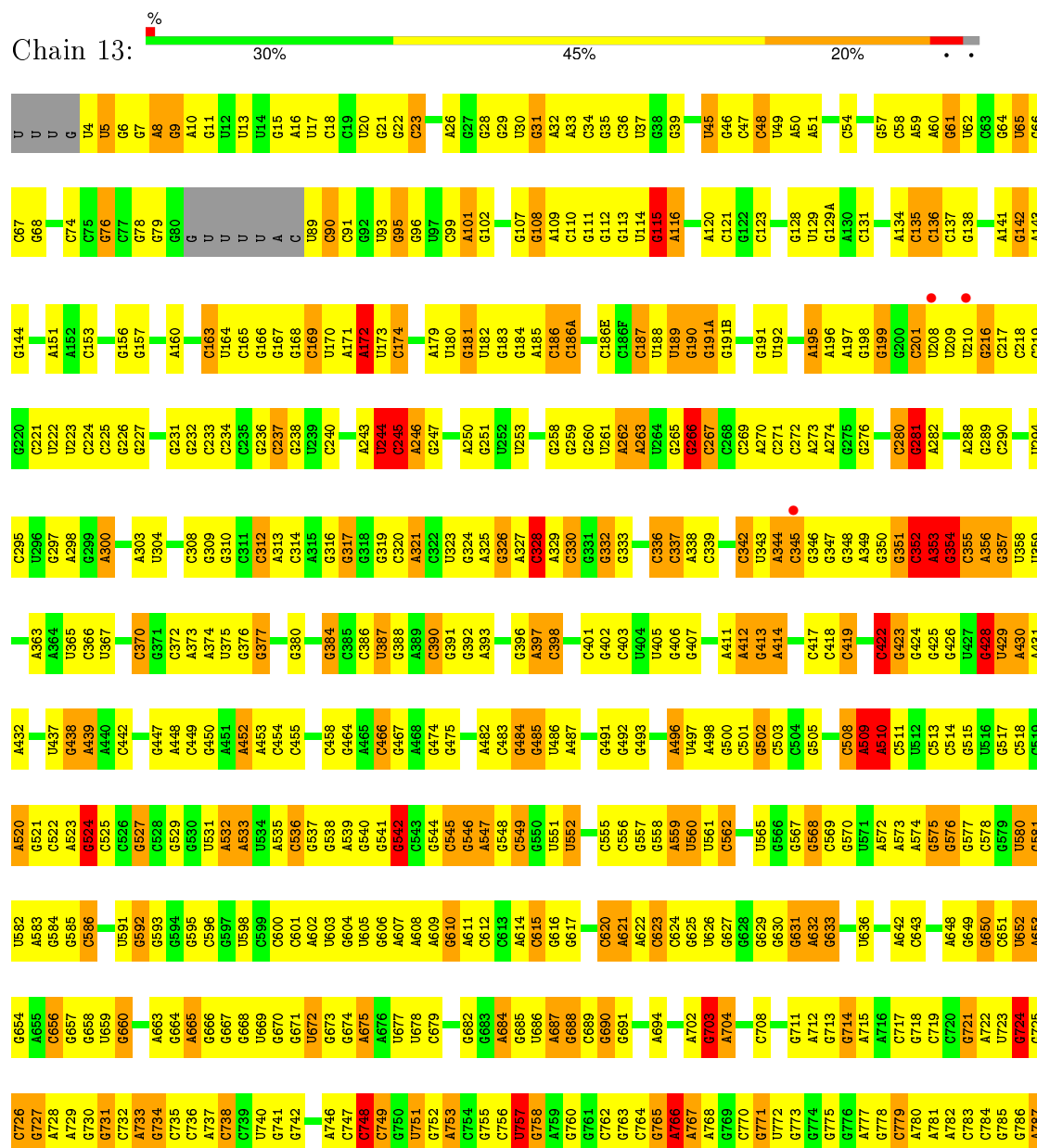
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
62	98	3	Total 3	O 3	0	0
62	B8	1	Total 1	O 1	0	0
62	C8	2	Total 2	O 2	0	0
62	D8	2	Total 2	O 2	0	0
62	G8	2	Total 2	O 2	0	0
62	L8	3	Total 3	O 3	0	0
62	Q8	1	Total 1	O 1	0	0
62	1G	74	Total 74	O 74	0	0
62	82	1	Total 1	O 1	0	0
62	BA	2	Total 2	O 2	0	0
62	4L	1	Total 1	O 1	0	0
62	14	446	Total 446	O 446	0	0
62	1J	12	Total 12	O 12	0	0
62	19	8	Total 8	O 8	0	0
62	39	1	Total 1	O 1	0	0
62	25	6	Total 6	O 6	0	0
62	85	2	Total 2	O 2	0	0
62	A5	1	Total 1	O 1	0	0
62	E5	1	Total 1	O 1	0	0
62	L5	1	Total 1	O 1	0	0
62	M5	2	Total 2	O 2	0	0

### 3 Residue-property plots

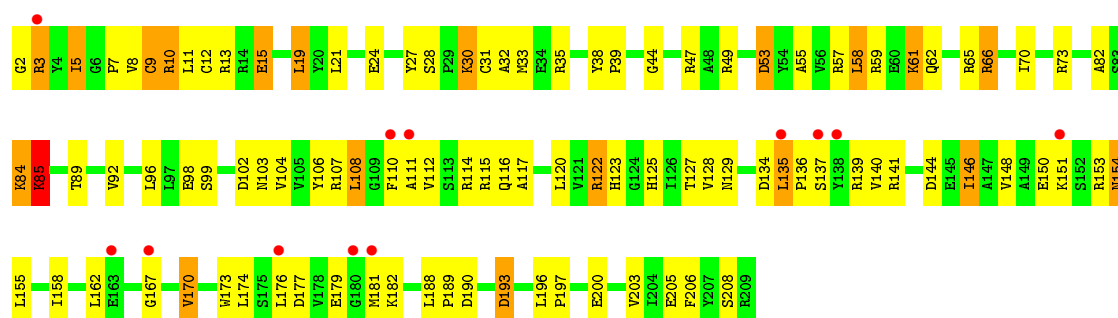
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according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

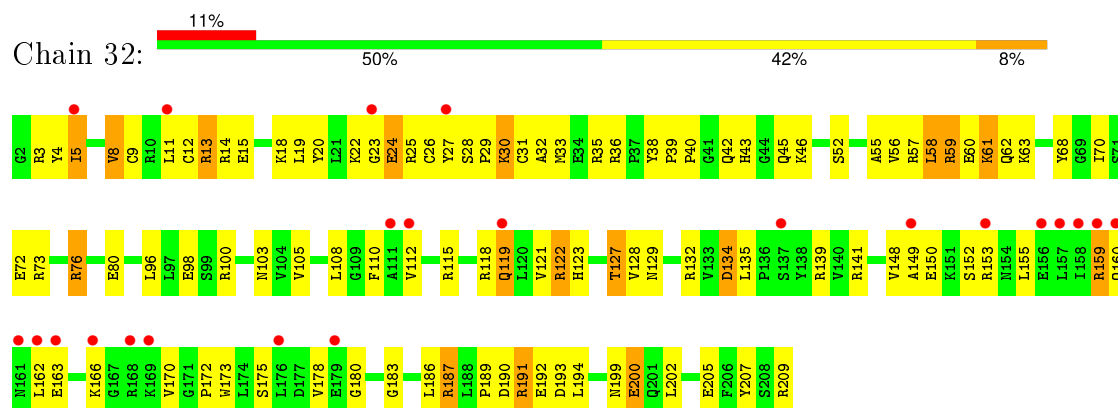




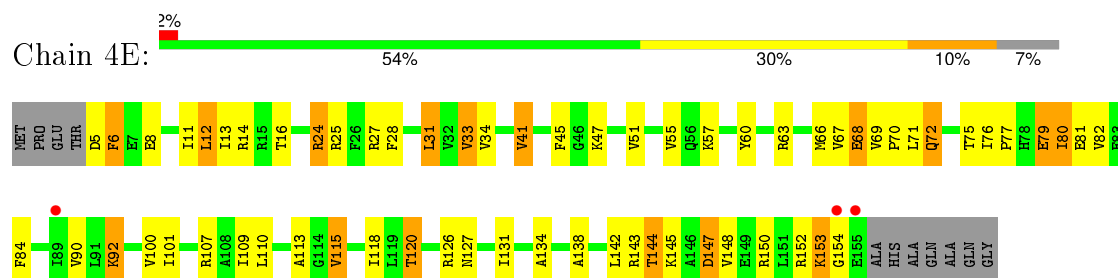




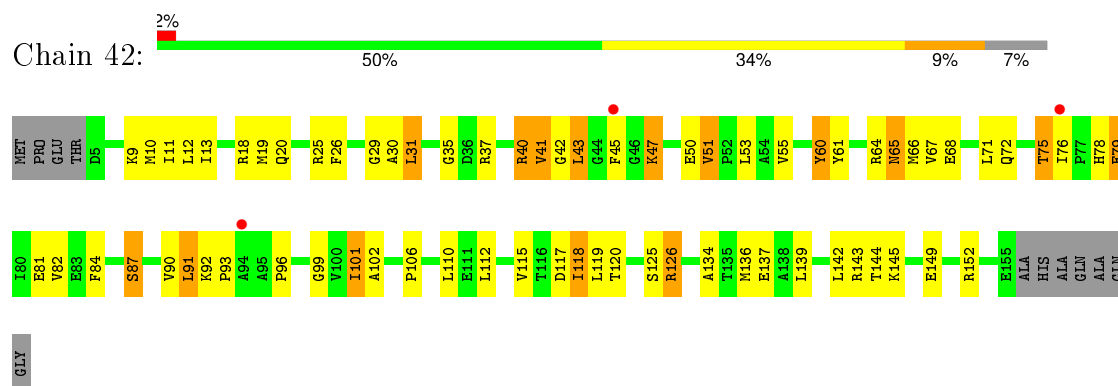
• Molecule 4: 30S ribosomal protein S4



• Molecule 5: 30S ribosomal protein S5



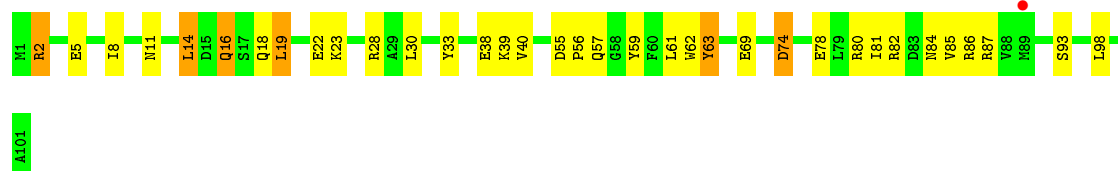
• Molecule 5: 30S ribosomal protein S5



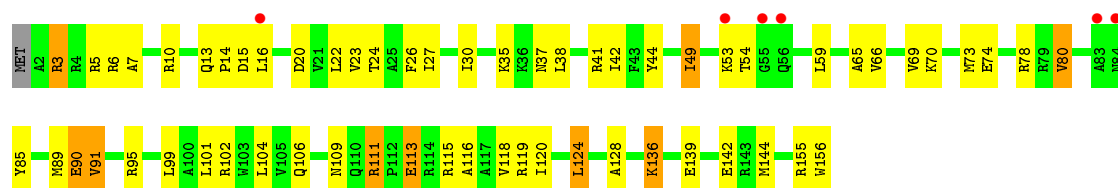
• Molecule 6: 30S ribosomal protein S6



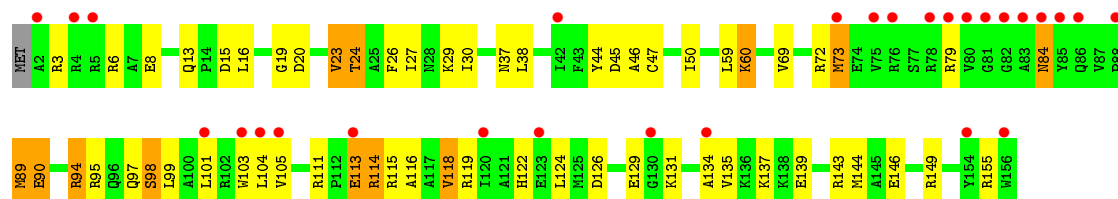
- Molecule 6: 30S ribosomal protein S6



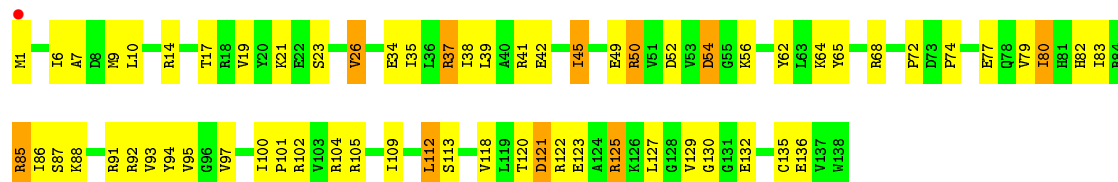
- Molecule 7: 30S ribosomal protein S7



- Molecule 7: 30S ribosomal protein S7



- Molecule 8: 30S ribosomal protein S8

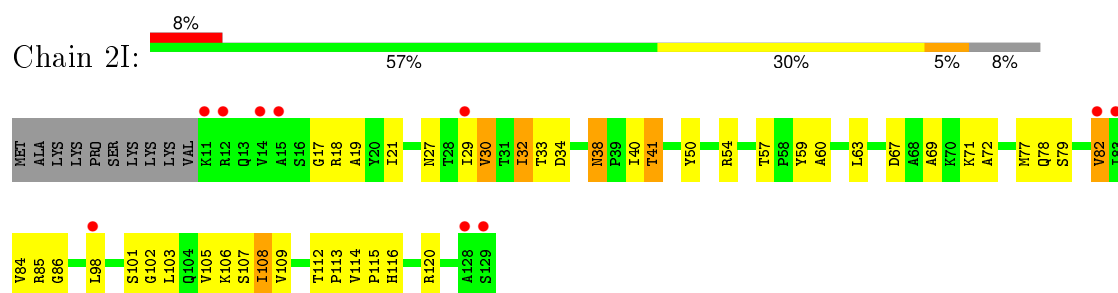


- Molecule 8: 30S ribosomal protein S8

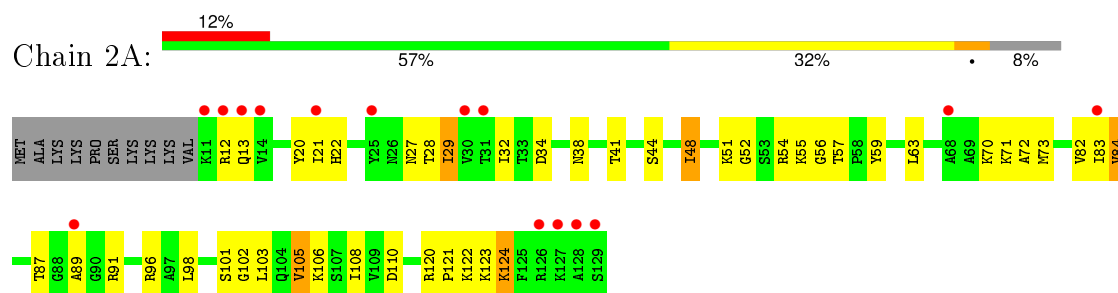




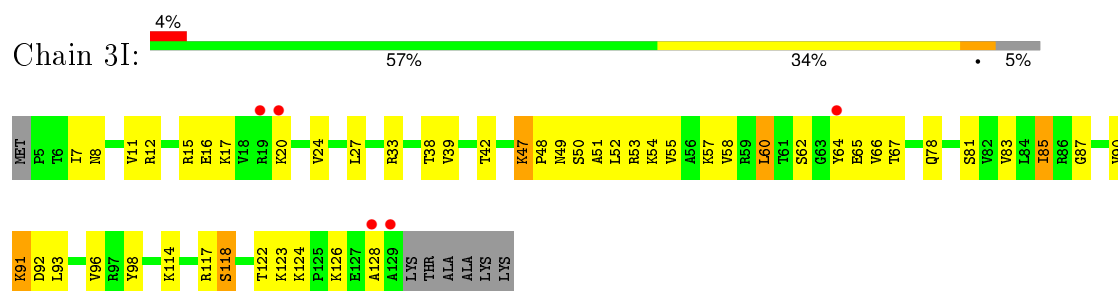




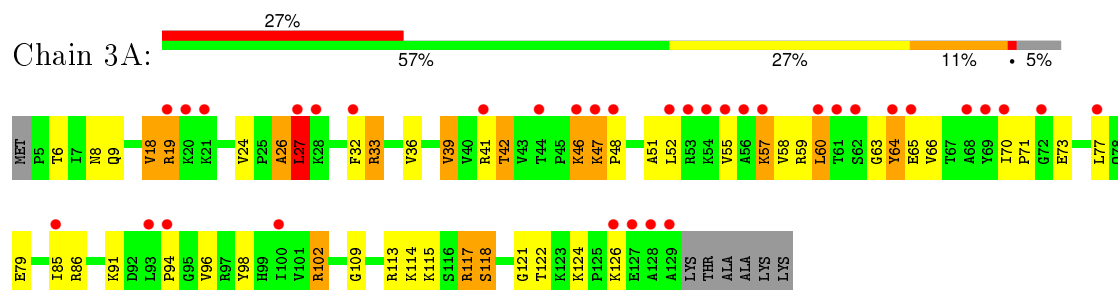
- Molecule 11: 30S ribosomal protein S11



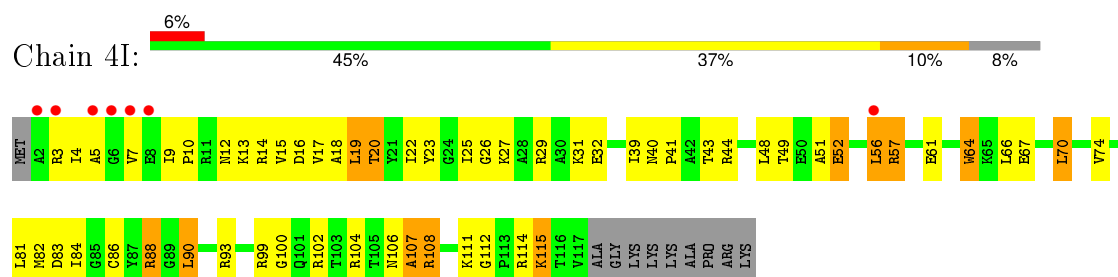
- Molecule 12: 30S ribosomal protein S12



- Molecule 12: 30S ribosomal protein S12



- Molecule 13: 30S ribosomal protein S13



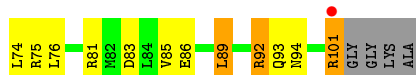
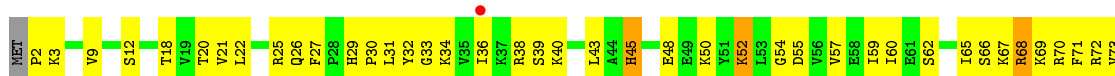
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- 
- | Category | Percentage |
|----------|------------|
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| V2       | 1.56%      |
| K3       | 1.56%      |
| I4       | 1.56%      |
| L5       | 1.56%      |
| L6       | 1.56%      |
| A7       | 1.56%      |
| R8       | 1.56%      |
| F9       | 1.56%      |
| G10      | 1.56%      |
| S11      | 1.56%      |
| K12      | 1.56%      |
| H13      | 1.56%      |
| M14      | 1.56%      |
| P15      | 1.56%      |
| H16      | 1.56%      |
| Y17      | 1.56%      |
| Y18      | 1.56%      |
| I19      | 1.56%      |
| V20      | 1.56%      |
| V21      | 1.56%      |
| T22      | 1.56%      |
| D23      | 1.56%      |
| A24      | 1.56%      |
| R25      | 1.56%      |
| R26      | 1.56%      |
| K27      | 1.56%      |
| R28      | 1.56%      |
| D29      | 1.56%      |
| G30      | 1.56%      |
| K31      | 1.56%      |
| Y32      | 1.56%      |
| I33      | 1.56%      |
| E34      | 1.56%      |
| K35      | 1.56%      |
| I36      | 1.56%      |
| G37      | 1.56%      |
| Y38      | 1.56%      |
| Y39      | 1.56%      |
| D40      | 1.56%      |
| P41      | 1.56%      |
| K42      | 1.56%      |
| K43      | 1.56%      |
| T44      | 1.56%      |
| T45      | 1.56%      |
| P46      | 1.56%      |
| D47      | 1.56%      |
| Y48      | 1.56%      |
| L49      | 1.56%      |
| K50      | 1.56%      |
| V51      | 1.56%      |
| D52      | 1.56%      |
| V53      | 1.56%      |
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| V55      | 1.56%      |
| R57      | 1.56%      |
| Y58      | 1.56%      |
| V59      | 1.56%      |
| V60      | 1.56%      |
| V61      | 1.56%      |
| V62      | 1.56%      |
| V63      | 1.56%      |
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| V66      | 1.56%      |



- Molecule 16: 30S ribosomal protein S16



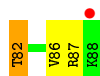
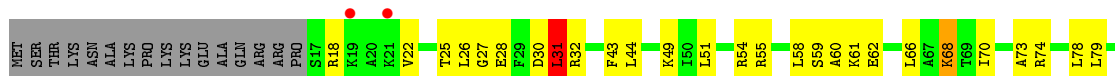
- Molecule 17: 30S ribosomal protein S17



- Molecule 17: 30S ribosomal protein S17



- Molecule 18: 30S ribosomal protein S18

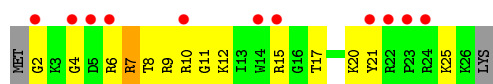


- Molecule 18: 30S ribosomal protein S18

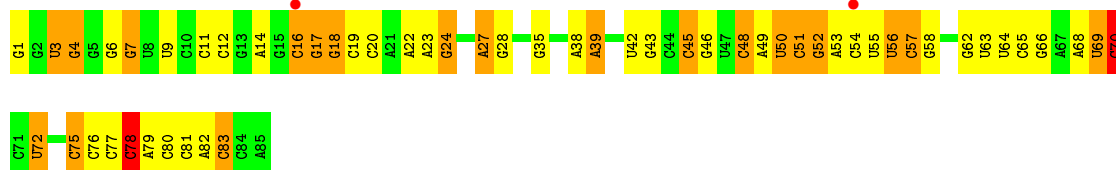


- Molecule 19: 30S ribosomal protein S19

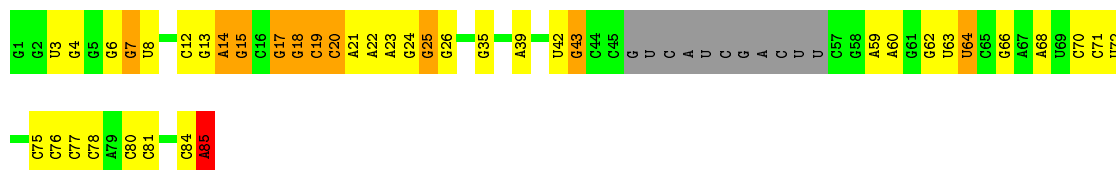




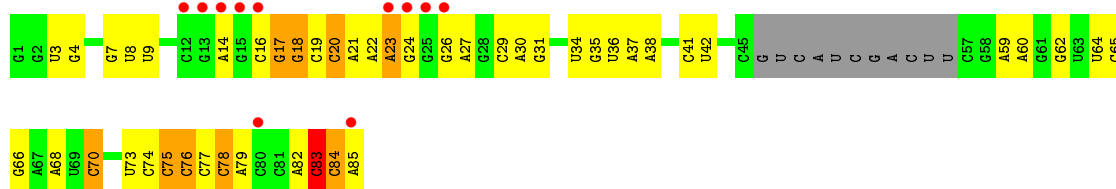
- Molecule 22: tRNA-Tyr



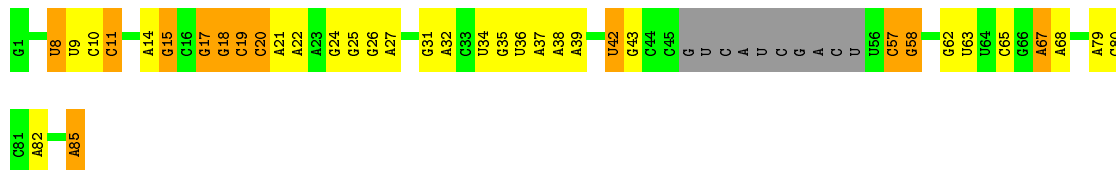
- Molecule 22: tRNA-Tyr



- Molecule 22: tRNA-Tyr



- Molecule 22: tRNA-Tyr



- Molecule 23: tRNA-fMET

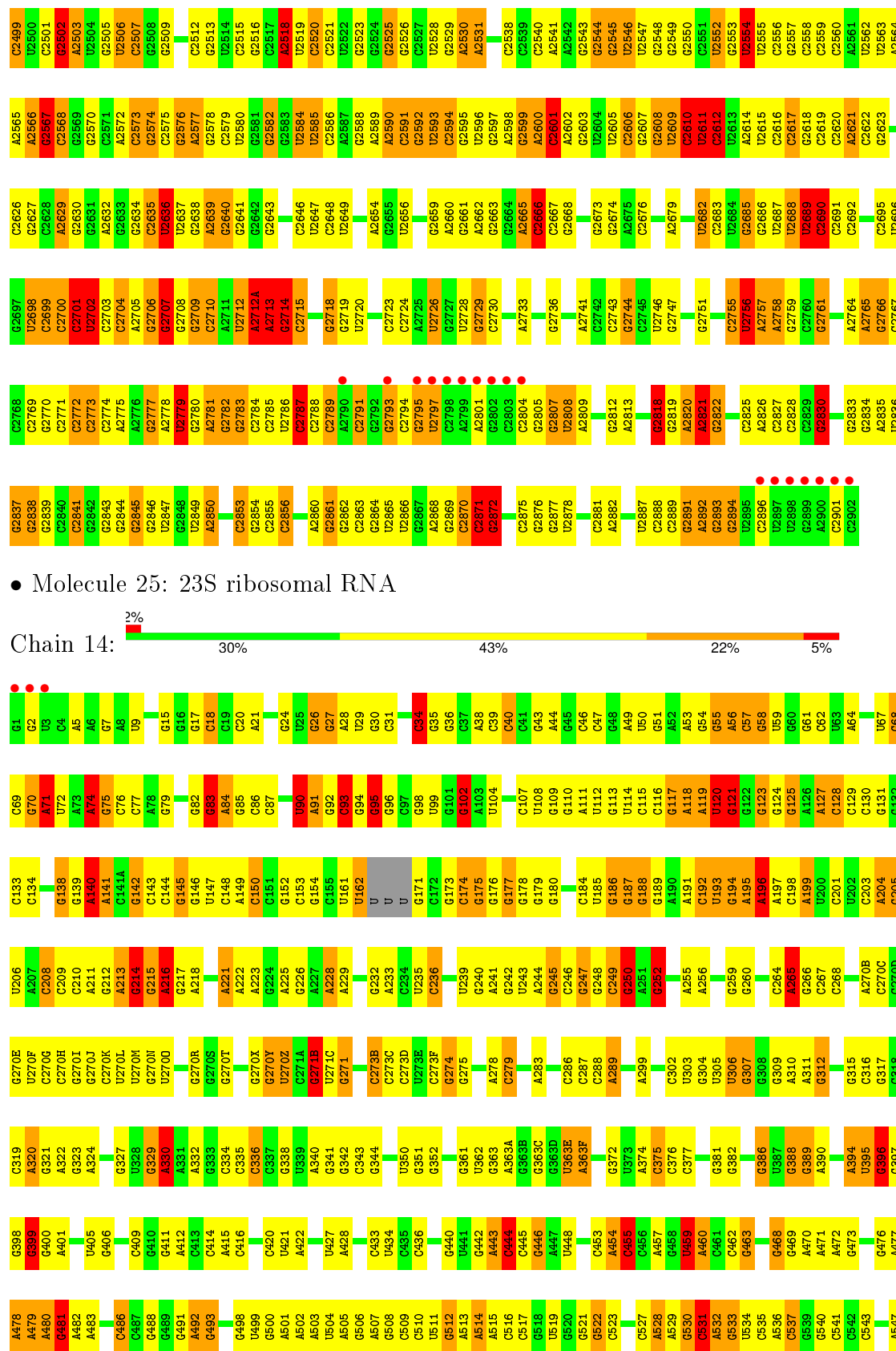




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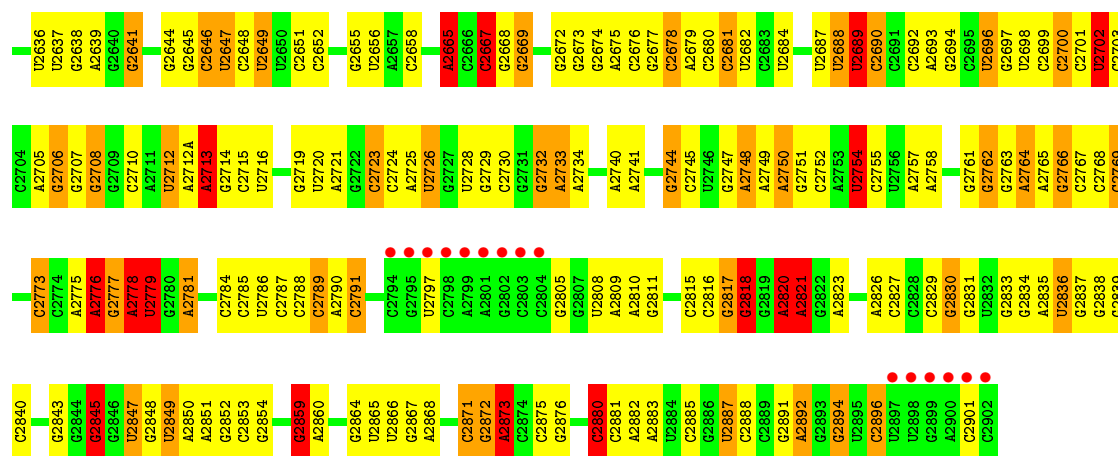
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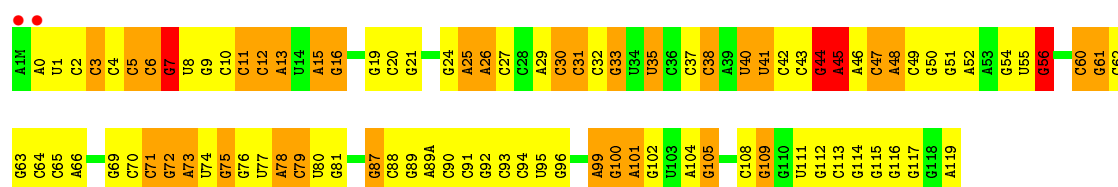


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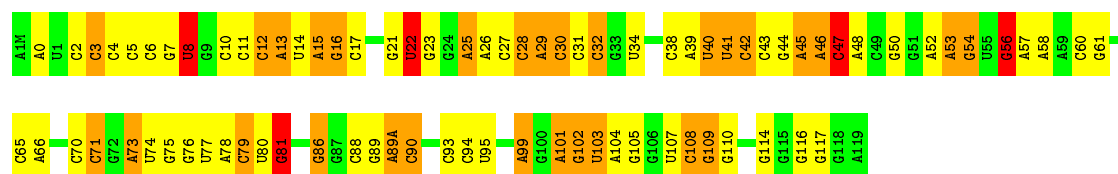
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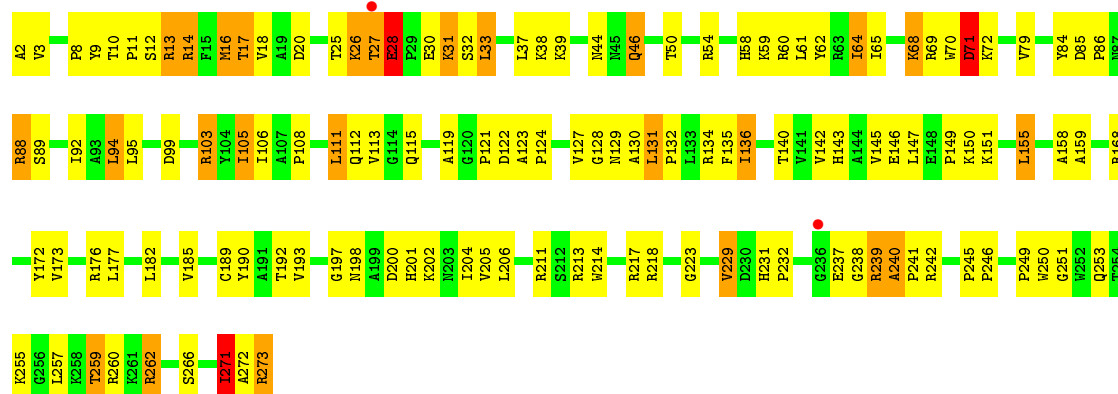
• Molecule 26: 5S ribosomal RNA



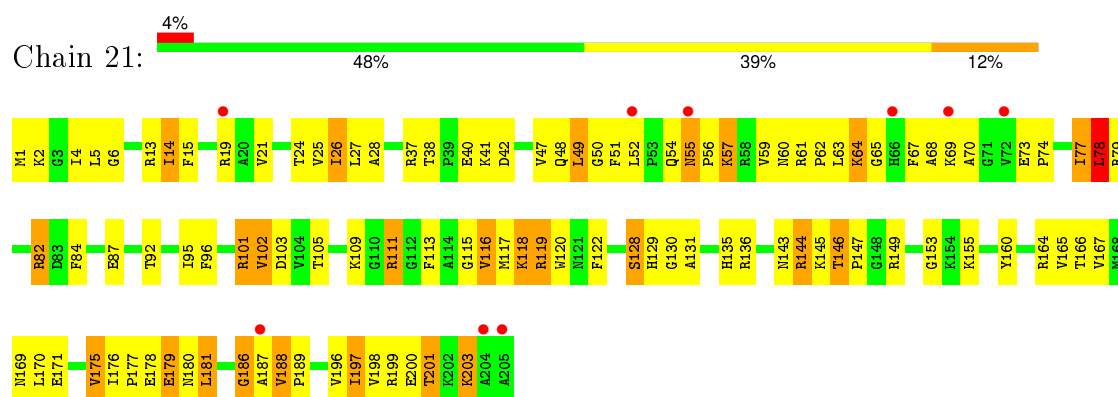
• Molecule 26: 5S ribosomal RNA



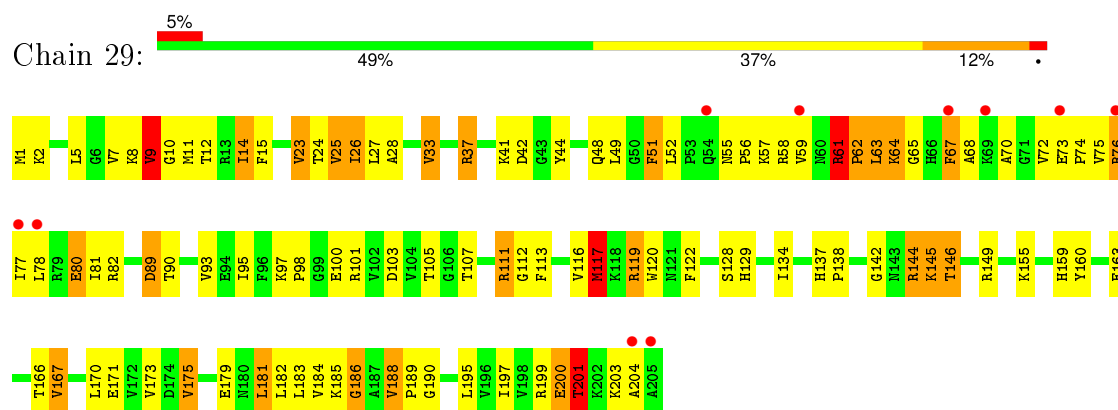
• Molecule 27: 50S ribosomal protein L2



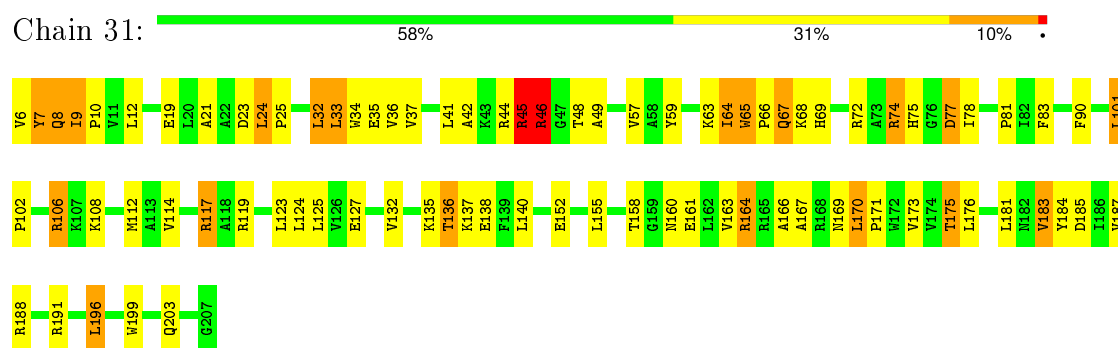
• Molecule 28: 50S ribosomal protein L3



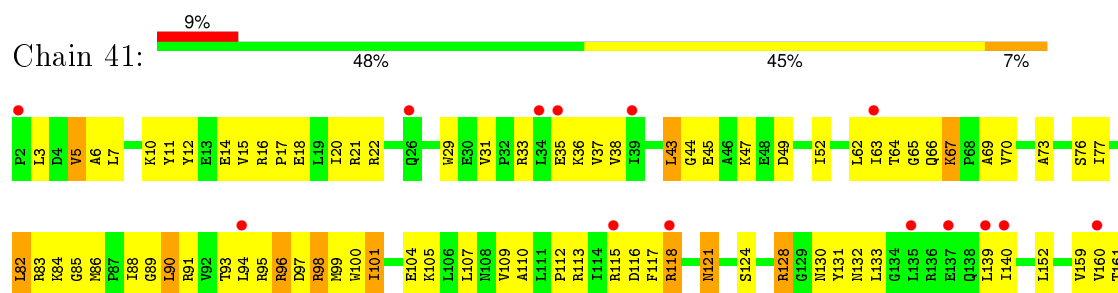
• Molecule 28: 50S ribosomal protein L3

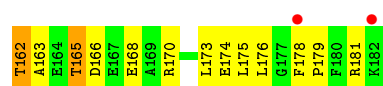


• Molecule 29: 50S ribosomal protein L4

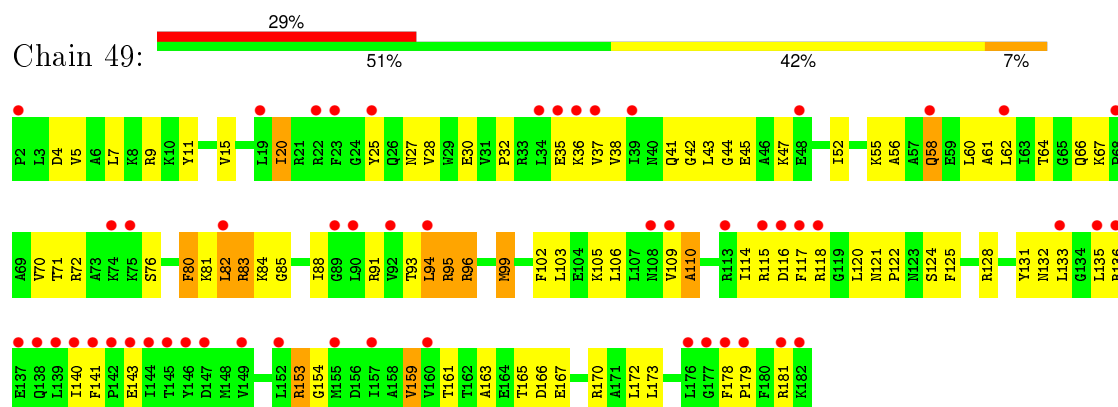


• Molecule 30: 50S ribosomal protein L5

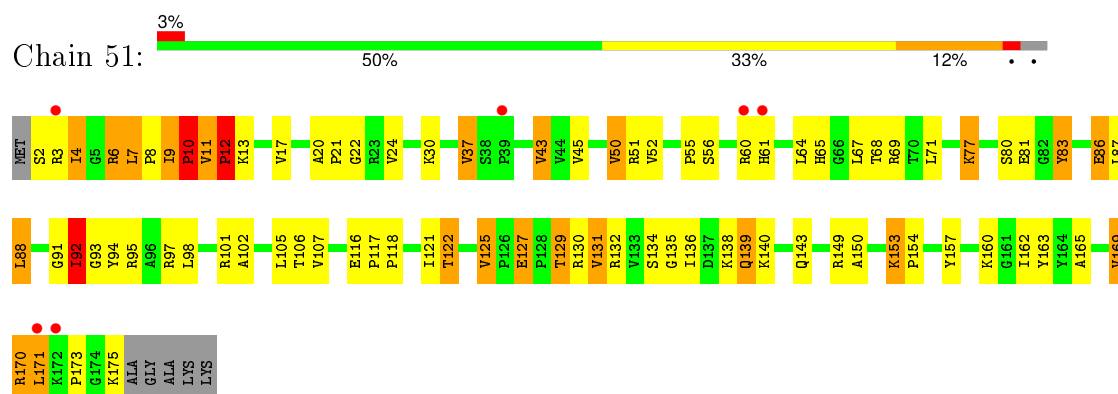




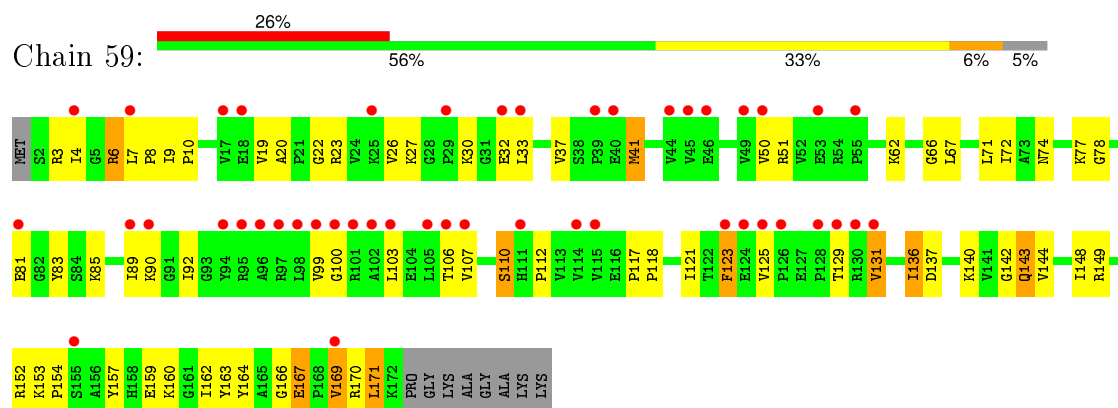
- Molecule 30: 50S ribosomal protein L5



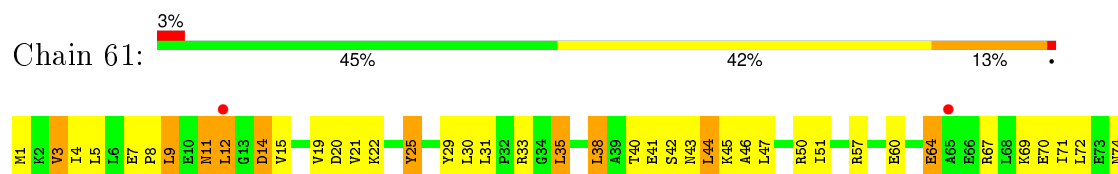
- Molecule 31: 50S ribosomal protein L6



- Molecule 31: 50S ribosomal protein L6



- Molecule 32: 50S ribosomal protein L9

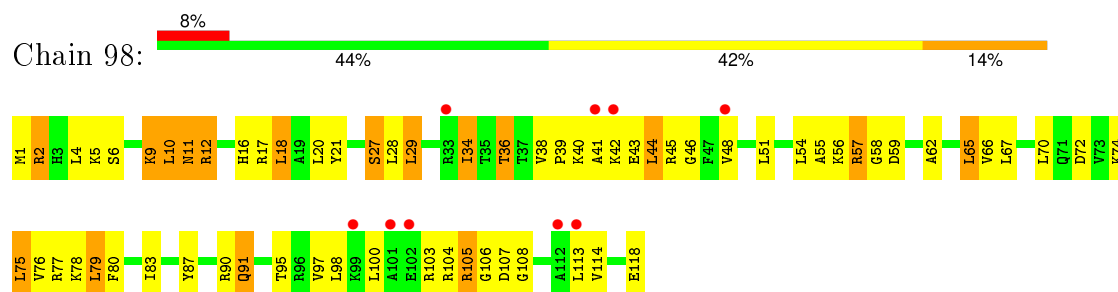




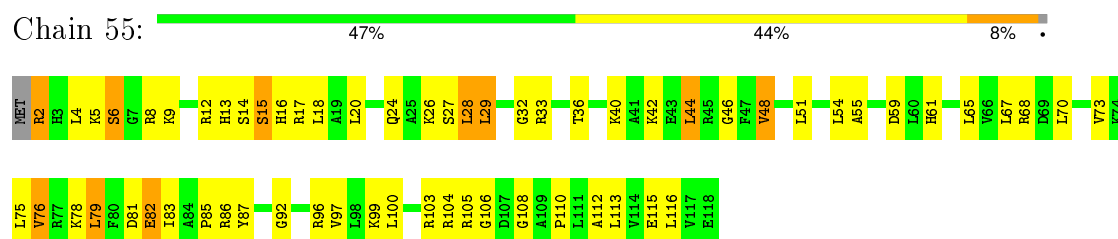




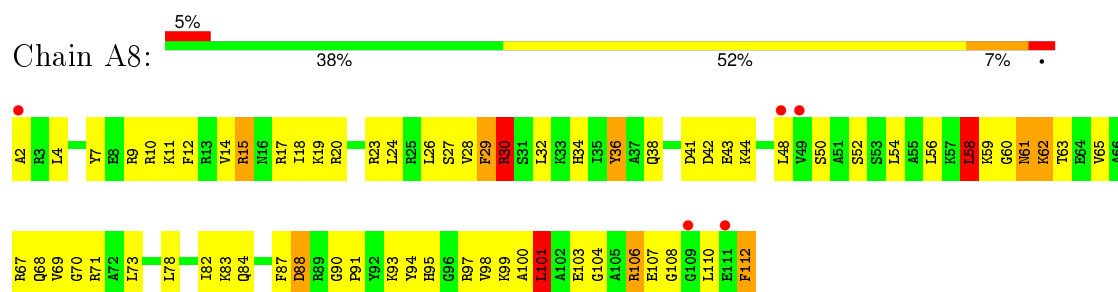
- Molecule 37: 50S ribosomal protein L17



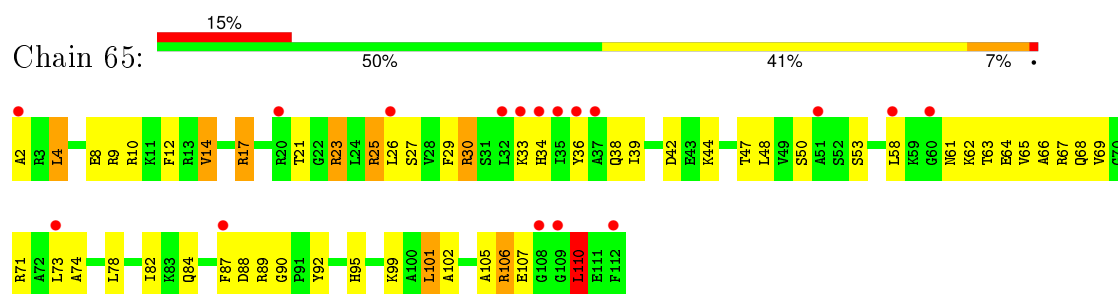
- Molecule 37: 50S ribosomal protein L17



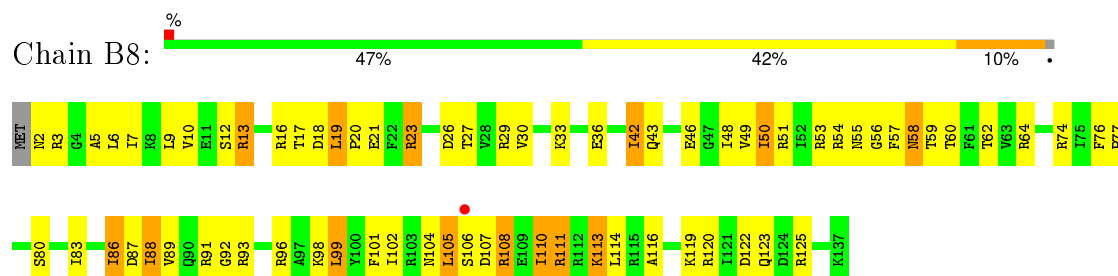
- Molecule 38: 50S ribosomal protein L18



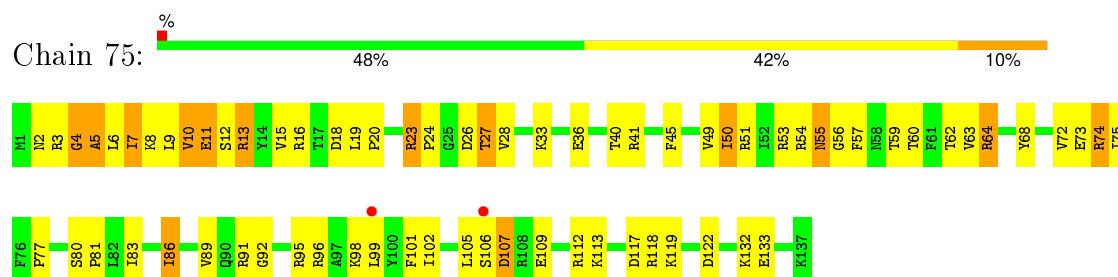
- Molecule 38: 50S ribosomal protein L18



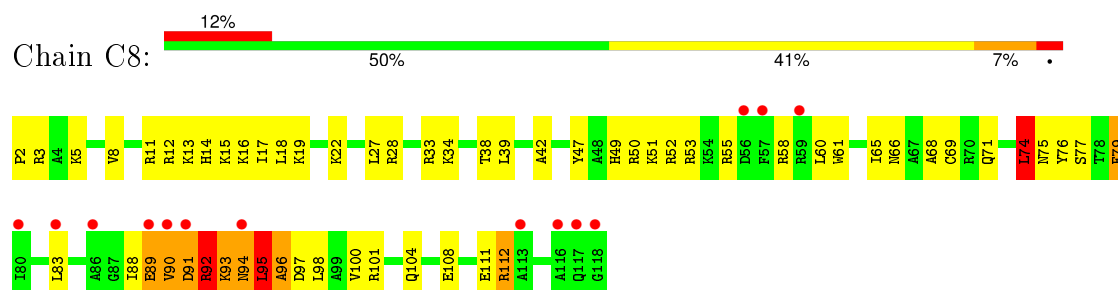
- Molecule 39: 50S ribosomal protein L19



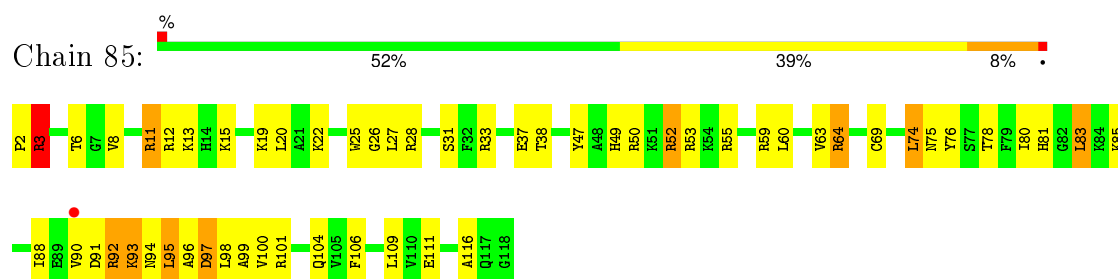
- Molecule 39: 50S ribosomal protein L19



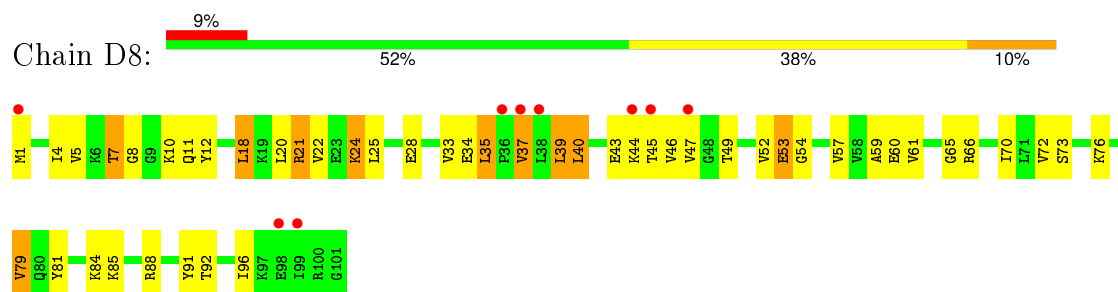
- Molecule 40: 50S ribosomal protein L20



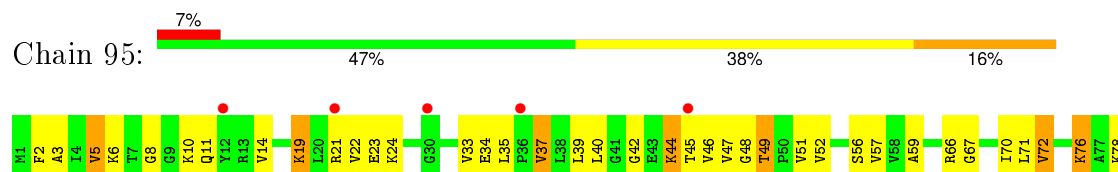
- Molecule 40: 50S ribosomal protein L20



- Molecule 41: 50S ribosomal protein L21

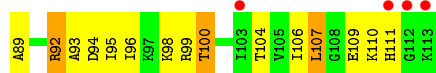


- Molecule 41: 50S ribosomal protein L21

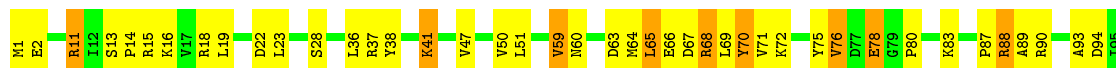




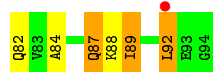
- Molecule 42: 50S ribosomal protein L22



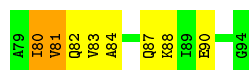
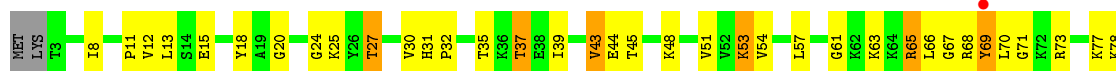
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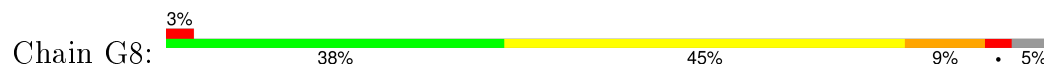
- Molecule 43: 50S ribosomal protein L23

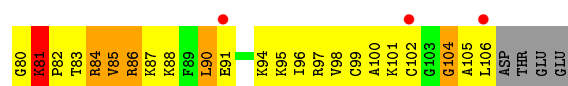


- Molecule 43: 50S ribosomal protein L23

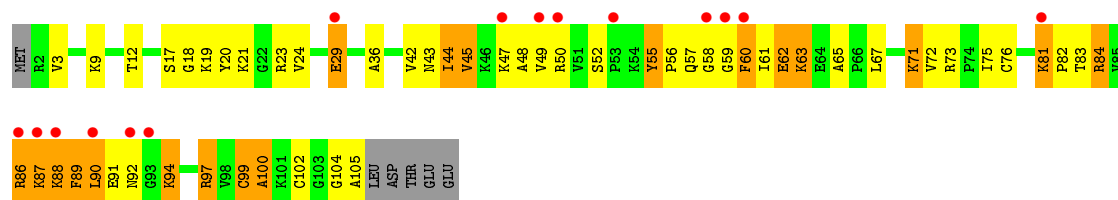


- Molecule 44: 50S ribosomal protein L24

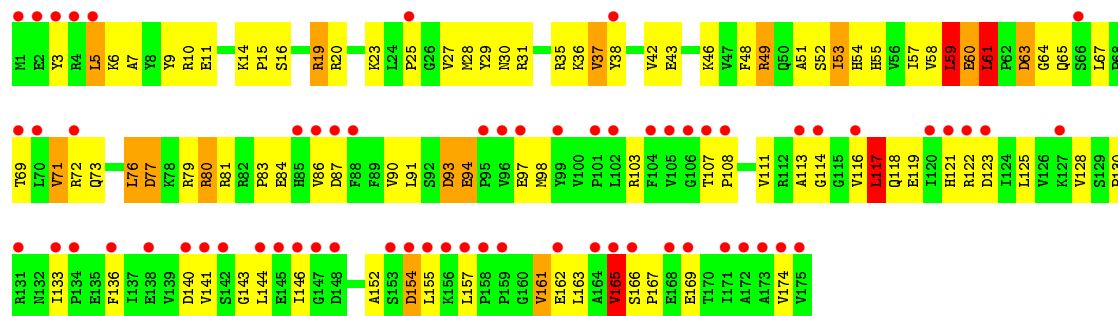




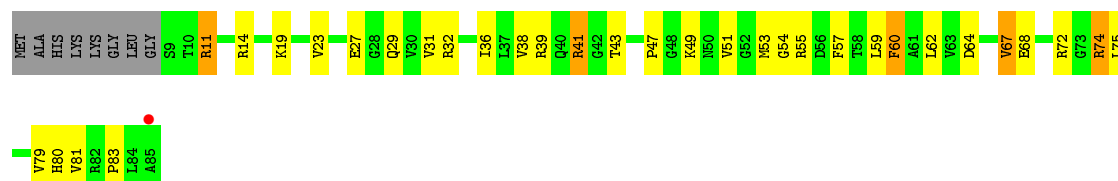
• Molecule 44: 50S ribosomal protein L24



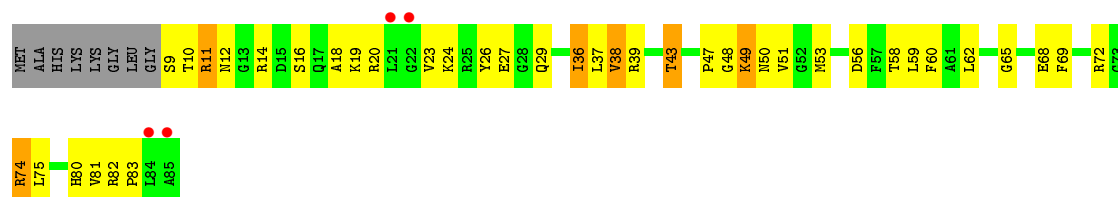
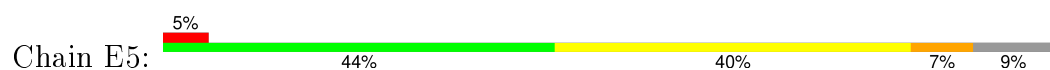
• Molecule 45: 50S ribosomal protein L25



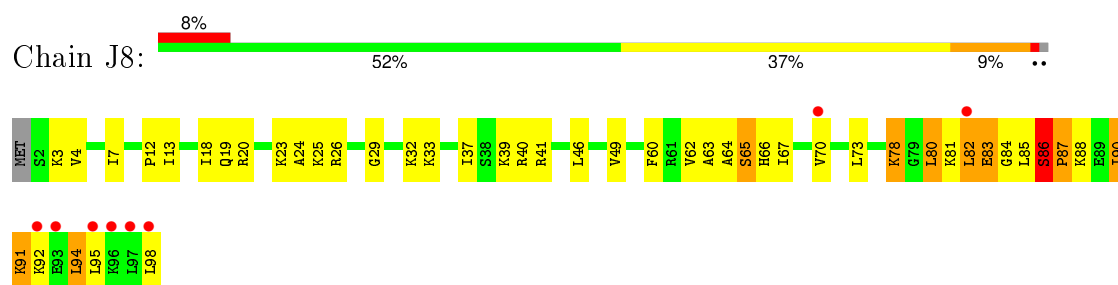
• Molecule 46: 50S ribosomal protein L27



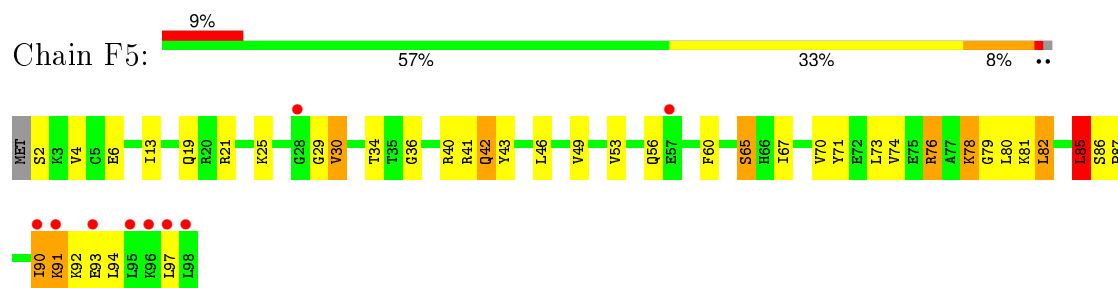
• Molecule 46: 50S ribosomal protein L27



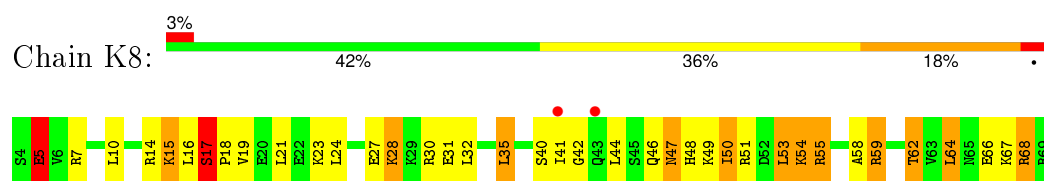
• Molecule 47: 50S ribosomal protein L28



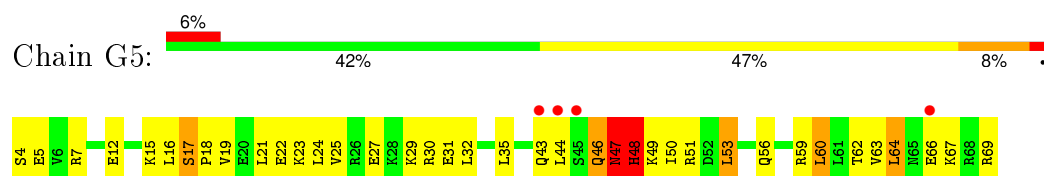
- Molecule 47: 50S ribosomal protein L28



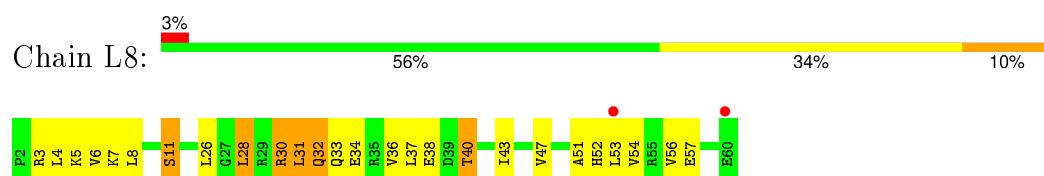
- Molecule 48: 50S ribosomal protein L29



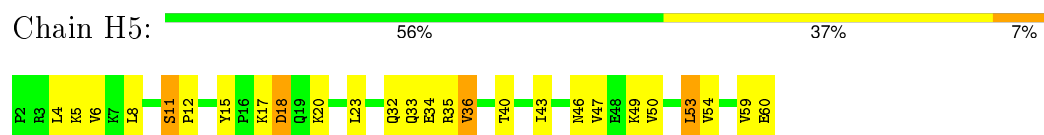
- Molecule 48: 50S ribosomal protein L29



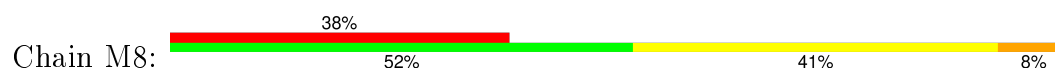
- Molecule 49: 50S ribosomal protein L30

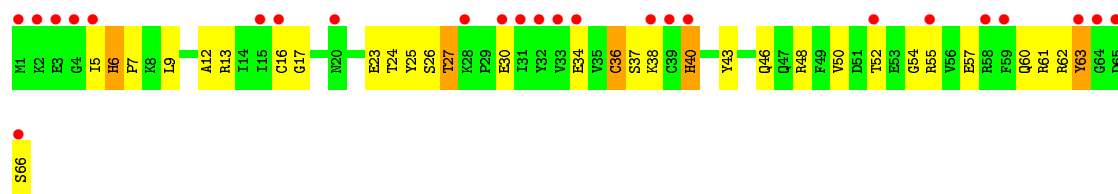


- Molecule 49: 50S ribosomal protein L30

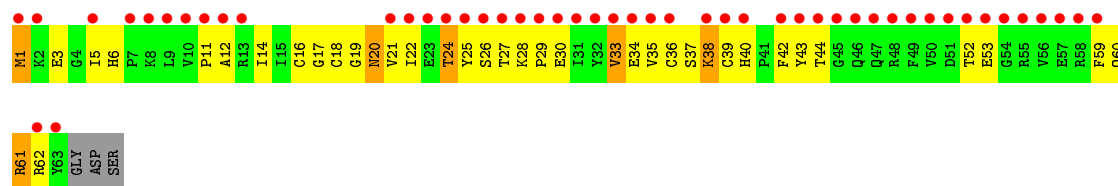
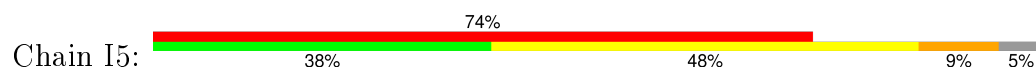


- Molecule 50: 50S ribosomal protein L31





- Molecule 50: 50S ribosomal protein L31



- Molecule 51: 50S ribosomal protein L32



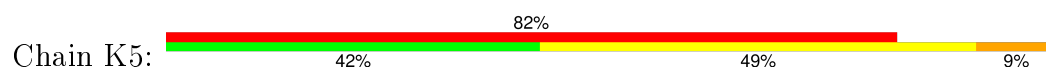
- Molecule 51: 50S ribosomal protein L32



- Molecule 52: 50S ribosomal protein L33



- Molecule 52: 50S ribosomal protein L33



- Molecule 53: 50S ribosomal protein L34

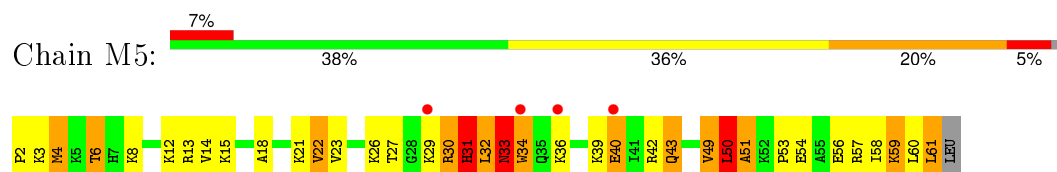
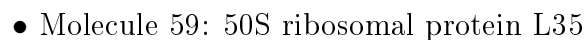
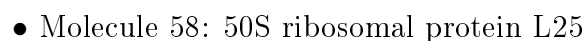






WORLDWIDE  
PDB  
PROTEIN DATA BANK





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	209.90Å 448.70Å 618.50Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	151.80 – 3.10 187.34 – 3.10	Depositor EDS
% Data completeness (in resolution range)	99.9 (151.80-3.10) 94.5 (187.34-3.10)	Depositor EDS
$R_{merge}$	0.41	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.80 (at 3.07Å)	Xtriage
Refinement program	PHENIX	Depositor
R, $R_{free}$	0.188 , 0.235 0.190 , 0.234	Depositor DCC
$R_{free}$ test set	2000 reflections (0.20%)	DCC
Wilson B-factor (Å <sup>2</sup> )	77.7	Xtriage
Anisotropy	0.262	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.28 , 77.2	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.43$ , $\langle L^2 \rangle = 0.26$	Xtriage
Outliers	0 of 1043636 reflections	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	299951	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	105.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.42% of the height of the origin peak. No significant pseudotranslation is detected.*

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

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.375 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, 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	0.83	25/36053 (0.1%)	1.49	573/56270 (1.0%)
2	12	0.34	0/1959	0.57	0/2642
2	1E	0.42	0/1959	0.65	4/2642 (0.2%)
3	22	0.37	0/1636	0.56	0/2205
3	2E	0.49	0/1629	0.68	1/2195 (0.0%)
4	32	0.46	0/1732	0.66	0/2318
4	3E	0.61	2/1732 (0.1%)	0.73	1/2318 (0.0%)
5	42	0.43	0/1171	0.67	0/1576
5	4E	0.58	0/1171	0.75	1/1576 (0.1%)
6	52	0.54	0/855	0.68	0/1154
6	5E	0.54	0/855	0.75	0/1154
7	62	0.41	0/1275	0.58	0/1709
7	6E	0.46	0/1275	0.59	0/1709
8	72	0.42	0/1135	0.59	0/1527
8	7E	0.52	0/1135	0.70	0/1527
9	82	0.38	0/1028	0.60	0/1379
9	8E	0.41	0/1028	0.66	0/1379
10	1A	0.35	0/814	0.59	0/1095
10	1I	0.43	0/814	0.61	0/1095
11	2A	0.47	0/899	0.67	0/1213
11	2I	0.54	0/899	0.76	1/1213 (0.1%)
12	3A	0.52	0/991	0.78	2/1327 (0.2%)
12	3I	0.73	0/991	0.88	0/1327
13	4A	0.38	0/943	0.59	0/1265
13	4I	0.48	0/938	0.73	0/1258
14	5A	0.42	0/484	0.73	0/643
14	5I	0.63	0/507	0.88	1/672 (0.1%)
15	6A	0.48	0/744	0.63	0/992
15	6I	0.57	0/744	0.75	1/992 (0.1%)
16	7A	0.51	0/721	0.69	0/970
16	7I	0.48	0/721	0.74	0/970
17	8A	0.49	0/847	0.63	0/1131

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
17	8I	0.53	0/847	0.75	0/1131
18	9A	0.49	0/595	0.71	0/790
18	9I	0.50	0/595	0.71	1/790 (0.1%)
19	AA	0.37	0/654	0.61	0/884
19	AI	0.48	0/680	0.75	0/915
20	BA	0.47	0/764	0.73	1/1007 (0.1%)
20	BI	0.40	0/764	0.69	1/1007 (0.1%)
21	1B	0.43	0/221	0.66	0/288
21	1F	0.40	0/221	0.58	0/288
22	1K	0.44	0/1851	1.06	7/2877 (0.2%)
22	1L	0.38	0/1594	0.92	3/2475 (0.1%)
22	3K	0.46	0/1594	0.98	1/2475 (0.0%)
22	3L	0.41	0/1616	0.92	1/2509 (0.0%)
23	2K	0.94	1/1725 (0.1%)	1.60	30/2689 (1.1%)
23	2L	0.76	1/1725 (0.1%)	1.35	10/2689 (0.4%)
24	4K	0.87	0/366	1.25	1/568 (0.2%)
24	4L	0.60	0/391	1.19	2/607 (0.3%)
25	14	0.97	94/70119 (0.1%)	1.69	1912/109464 (1.7%)
25	1H	1.16	199/70233 (0.3%)	1.94	3139/109643 (2.9%)
26	16	0.91	0/2928	1.65	54/4568 (1.2%)
26	1J	0.78	0/2928	1.48	38/4568 (0.8%)
27	11	0.87	1/2165 (0.0%)	1.03	6/2919 (0.2%)
28	21	0.68	0/1601	0.93	1/2160 (0.0%)
28	29	0.66	0/1601	0.89	1/2160 (0.0%)
29	31	0.79	3/1620 (0.2%)	0.93	6/2194 (0.3%)
30	41	0.52	0/1498	0.73	0/2016
30	49	0.40	0/1498	0.66	0/2016
31	51	0.58	0/1362	0.87	1/1841 (0.1%)
31	59	0.34	0/1341	0.59	0/1813
32	61	0.49	0/1151	0.75	2/1558 (0.1%)
32	69	0.47	0/1151	0.71	1/1558 (0.1%)
33	15	0.48	0/1131	0.67	0/1525
33	58	0.60	0/1131	0.82	0/1525
34	25	0.65	0/942	0.80	1/1269 (0.1%)
34	68	0.70	0/942	0.78	0/1269
35	35	0.64	0/1161	1.05	4/1544 (0.3%)
35	78	0.75	0/1161	1.10	6/1544 (0.4%)
36	45	0.65	1/1142 (0.1%)	0.88	2/1527 (0.1%)
36	88	0.84	1/1142 (0.1%)	1.03	3/1527 (0.2%)
37	55	0.65	0/973	0.84	0/1302
37	98	0.69	0/981	0.92	1/1312 (0.1%)
38	65	0.55	0/891	0.84	2/1187 (0.2%)
38	A8	0.62	0/891	0.93	4/1187 (0.3%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
39	75	0.61	0/1155	0.79	2/1542 (0.1%)
39	B8	0.65	0/1147	0.83	1/1532 (0.1%)
40	85	0.62	0/981	0.81	2/1306 (0.2%)
40	C8	0.72	0/981	0.96	3/1306 (0.2%)
41	95	0.58	0/789	0.81	0/1057
41	D8	0.64	0/789	0.82	1/1057 (0.1%)
42	A5	0.69	0/910	0.85	0/1220
42	E8	0.73	0/910	0.93	1/1220 (0.1%)
43	B5	0.75	0/739	0.81	0/993
43	F8	0.89	2/756 (0.3%)	0.96	1/1014 (0.1%)
44	C5	0.55	0/807	0.79	0/1076
44	G8	0.71	0/804	1.02	3/1073 (0.3%)
45	H8	0.48	0/1427	0.78	1/1935 (0.1%)
46	E5	0.68	0/620	0.90	0/827
46	I8	0.80	0/620	0.96	0/827
47	F5	0.64	0/769	0.93	1/1022 (0.1%)
47	J8	0.72	0/769	0.94	2/1022 (0.2%)
48	G5	0.58	0/560	0.81	1/741 (0.1%)
48	K8	0.82	2/560 (0.4%)	0.94	1/741 (0.1%)
49	H5	0.50	0/473	0.67	0/635
49	L8	0.64	0/473	0.78	0/635
50	I5	0.36	0/527	0.67	0/709
50	M8	0.38	0/545	0.62	0/733
51	J5	0.64	0/467	0.84	1/632 (0.2%)
51	N8	0.66	0/472	0.86	0/639
52	K5	0.46	0/396	0.78	0/529
52	O8	0.61	0/396	0.80	1/529 (0.2%)
53	L5	0.74	0/399	0.92	0/526
53	P8	0.99	0/399	1.07	2/526 (0.4%)
54	Q8	1.16	0/448	1.48	5/600 (0.8%)
55	1G	0.71	4/36049 (0.0%)	1.33	281/56262 (0.5%)
56	19	0.75	0/2170	0.96	5/2926 (0.2%)
57	39	0.63	1/1662 (0.1%)	0.87	2/2249 (0.1%)
58	D5	0.38	0/1460	0.62	0/1982
59	M5	0.74	0/486	1.13	2/638 (0.3%)
All	All	0.87	337/322487 (0.1%)	1.49	6146/482889 (1.3%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
4	3E	0	1
10	1A	0	1
12	3I	0	1
13	4I	0	1
14	5A	0	1
14	5I	0	1
19	AI	0	2
20	BA	0	1
27	11	0	3
28	21	0	4
28	29	0	5
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	3
35	78	0	6
36	45	0	3
36	88	0	2
37	98	0	1
39	75	0	1
39	B8	0	1
40	85	0	1
40	C8	0	2
41	95	0	1
43	B5	0	1
44	C5	0	2
44	G8	0	4
45	H8	0	3
47	F5	0	1
48	G5	0	3
48	K8	0	1
50	M8	0	1
52	K5	0	1
54	Q8	0	6
56	19	0	4
57	39	0	1
59	M5	0	3
All	All	0	82

The worst 5 of 337 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	1H	1614	A	N9-C4	-12.72	1.30	1.37
25	1H	2430	A	N9-C4	-12.06	1.30	1.37
1	13	792	A	N9-C4	-11.71	1.30	1.37
25	1H	774	A	N9-C4	-11.62	1.30	1.37
25	1H	71	A	N9-C4	-11.59	1.30	1.37

The worst 5 of 6146 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	1H	1899	G	N3-C4-N9	-25.74	110.56	126.00
25	1H	676	A	C2-N3-C4	-22.98	99.11	110.60
25	1H	1899	G	N3-C4-C5	22.06	139.63	128.60
25	14	1332	G	N3-C4-N9	-21.72	112.97	126.00
25	14	1332	G	N3-C4-C5	20.07	138.63	128.60

There are no chirality outliers.

5 of 82 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
4	3E	85	LYS	Peptide
12	3I	87	GLY	Peptide
13	4I	107	ALA	Peptide
14	5I	13	THR	Peptide
19	AI	4	SER	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	796	0
2	12	1924	0	1975	84	0
2	1E	1924	0	1975	77	0
3	22	1612	0	1677	69	0
3	2E	1605	0	1668	53	0
4	32	1702	0	1763	85	1
4	3E	1702	0	1763	84	0
5	42	1155	0	1213	42	0
5	4E	1155	0	1213	50	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	52	842	0	857	30	0
6	5E	842	0	857	33	1
7	62	1256	0	1296	53	0
7	6E	1256	0	1296	43	0
8	72	1115	0	1177	30	0
8	7E	1115	0	1177	46	0
9	82	1009	0	1037	66	0
9	8E	1009	0	1037	52	0
10	1A	801	0	849	53	0
10	1I	801	0	849	46	0
11	2A	884	0	904	39	0
11	2I	884	0	904	28	0
12	3A	975	0	1062	42	0
12	3I	975	0	1062	38	0
13	4A	933	0	992	49	0
13	4I	928	0	987	50	0
14	5A	475	0	511	27	0
14	5I	498	0	537	30	0
15	6A	733	0	771	27	0
15	6I	733	0	771	22	0
16	7A	705	0	725	21	0
16	7I	705	0	725	49	0
17	8A	834	0	904	27	0
17	8I	834	0	904	39	0
18	9A	590	0	662	13	0
18	9I	590	0	662	23	0
19	AA	640	0	633	38	0
19	AI	665	0	686	34	0
20	BA	762	0	861	35	0
20	BI	762	0	861	36	0
21	1B	217	0	234	11	0
21	1F	217	0	234	9	0
22	1K	1825	0	946	36	0
22	1L	1595	0	830	24	0
22	3K	1595	0	830	36	0
22	3L	1615	0	840	30	0
23	2K	1645	0	843	36	0
23	2L	1645	0	843	31	0
24	4K	325	0	165	6	0
24	4L	347	0	176	6	0
25	14	62605	0	31558	1370	0
25	1H	62707	0	31607	1469	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
26	16	2617	0	1328	79	0
26	1J	2617	0	1328	75	0
27	11	2115	0	2195	120	0
28	21	1568	0	1634	107	0
28	29	1568	0	1634	100	0
29	31	1585	0	1632	84	0
30	41	1473	0	1535	76	0
30	49	1473	0	1535	56	0
31	51	1336	0	1418	61	0
31	59	1316	0	1395	52	0
32	61	1136	0	1223	48	1
32	69	1136	0	1223	53	0
33	15	1104	0	1180	45	0
33	58	1104	0	1180	64	0
34	25	932	0	996	41	0
34	68	932	0	996	34	0
35	35	1144	0	1228	102	0
35	78	1144	0	1228	89	0
36	45	1121	0	1179	65	0
36	88	1121	0	1179	59	0
37	55	959	0	1021	47	0
37	98	967	0	1033	59	0
38	65	881	0	943	46	0
38	A8	881	0	943	53	0
39	75	1141	0	1202	47	0
39	B8	1133	0	1190	55	0
40	85	963	0	1022	46	0
40	C8	963	0	1022	60	0
41	95	778	0	852	56	0
41	D8	778	0	852	21	0
42	A5	899	0	964	32	0
42	E8	899	0	964	34	0
43	B5	725	0	778	29	0
43	F8	742	0	803	42	0
44	C5	794	0	883	47	0
44	G8	791	0	880	61	0
45	H8	1397	0	1430	71	0
46	E5	612	0	633	39	0
46	I8	612	0	633	28	0
47	F5	762	0	848	30	0
47	J8	762	0	848	29	0
48	G5	558	0	610	24	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
48	K8	558	0	610	31	0
49	H5	468	0	518	18	0
49	L8	468	0	518	15	0
50	I5	515	0	514	34	0
50	M8	533	0	526	22	0
51	J5	453	0	475	20	0
51	N8	458	0	480	25	0
52	K5	389	0	404	24	0
52	O8	389	0	404	23	0
53	L5	391	0	432	14	0
53	P8	391	0	432	15	0
54	Q8	442	0	452	59	0
55	1G	32204	0	16256	685	1
56	19	2120	0	2197	107	0
57	39	1627	0	1680	91	0
58	D5	1428	0	1454	51	0
59	M5	480	0	549	43	0
60	11	2	0	0	0	0
60	13	140	0	0	0	0
60	14	386	0	0	0	0
60	16	12	0	0	0	0
60	19	1	0	0	0	0
60	1G	104	0	0	0	0
60	1H	438	0	0	0	0
60	1J	7	0	0	0	0
60	1K	1	0	0	0	0
60	21	2	0	0	0	0
60	25	1	0	0	0	0
60	29	2	0	0	0	0
60	2K	4	0	0	0	0
60	2L	3	0	0	0	0
60	39	1	0	0	0	0
60	3I	1	0	0	0	0
60	3K	1	0	0	0	0
60	41	1	0	0	0	0
60	45	3	0	0	0	0
60	49	1	0	0	0	0
60	4I	1	0	0	0	0
60	52	1	0	0	0	0
60	5I	1	0	0	0	0
60	68	1	0	0	0	0
60	78	3	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
60	85	1	0	0	0	0
60	88	2	0	0	0	0
60	98	2	0	0	0	0
60	B8	1	0	0	0	0
60	C5	1	0	0	0	0
60	C8	1	0	0	0	0
60	E5	1	0	0	0	0
60	I8	2	0	0	0	0
60	K8	1	0	0	0	0
60	P8	1	0	0	0	0
61	32	1	0	0	0	0
61	3E	1	0	0	0	0
61	5A	1	0	0	0	0
61	5I	1	0	0	0	0
61	C5	1	0	0	0	0
61	G8	1	0	0	0	0
62	11	10	0	0	0	0
62	13	125	0	0	36	0
62	14	446	0	0	126	0
62	16	15	0	0	3	0
62	19	8	0	0	1	0
62	1G	74	0	0	23	0
62	1H	738	0	0	226	0
62	1J	12	0	0	5	0
62	1K	4	0	0	0	0
62	21	4	0	0	2	0
62	25	6	0	0	1	0
62	31	5	0	0	0	0
62	39	1	0	0	0	0
62	3E	4	0	0	0	0
62	3I	1	0	0	0	0
62	3K	1	0	0	0	0
62	4K	1	0	0	0	0
62	4L	1	0	0	0	0
62	5I	2	0	0	0	0
62	78	3	0	0	0	0
62	7I	1	0	0	0	0
62	82	1	0	0	0	0
62	85	2	0	0	1	0
62	98	3	0	0	1	0
62	A5	1	0	0	0	0
62	B8	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
62	BA	2	0	0	1	0
62	C8	2	0	0	0	0
62	D8	2	0	0	0	0
62	E5	1	0	0	0	0
62	G8	2	0	0	0	0
62	L5	1	0	0	0	0
62	L8	3	0	0	0	0
62	M5	2	0	0	0	0
62	Q8	1	0	0	0	0
All	All	299951	0	200664	8116	2

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 17.

The worst 5 of 8116 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)
22:1L:35:QUO:C4	22:1L:35:QUO:N3	1.71	1.53
22:1K:35:QUO:N3	22:1K:35:QUO:C4	1.69	1.53
22:3K:35:QUO:C4	22:3K:35:QUO:N3	1.71	1.52
22:3L:35:QUO:N3	22:3L:35:QUO:C4	1.72	1.49
25:1H:973:A:OP2	62:1H:3767:HOH:O	1.69	1.10

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

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:5E:15:ASP:OD2	4:32:27:TYR:OH[4_555]	2.10	0.10
32:61:91:SER:OG	55:1G:368:U:OP1[4_555]	2.18	0.02

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

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%)	207 (88%)	25 (11%)	3 (1%)	15	50
2	1E	235/256 (92%)	202 (86%)	32 (14%)	1 (0%)	39	75
3	22	204/239 (85%)	188 (92%)	16 (8%)	0	100	100
3	2E	203/239 (85%)	187 (92%)	16 (8%)	0	100	100
4	32	206/208 (99%)	184 (89%)	22 (11%)	0	100	100
4	3E	206/208 (99%)	193 (94%)	13 (6%)	0	100	100
5	42	149/162 (92%)	145 (97%)	4 (3%)	0	100	100
5	4E	149/162 (92%)	145 (97%)	3 (2%)	1 (1%)	26	65
6	52	99/101 (98%)	98 (99%)	1 (1%)	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	65
8	7E	136/138 (99%)	129 (95%)	7 (5%)	0	100	100
9	82	125/128 (98%)	115 (92%)	10 (8%)	0	100	100
9	8E	125/128 (98%)	109 (87%)	15 (12%)	1 (1%)	24	63
10	1A	97/105 (92%)	89 (92%)	8 (8%)	0	100	100
10	1I	97/105 (92%)	88 (91%)	9 (9%)	0	100	100
11	2A	117/129 (91%)	105 (90%)	12 (10%)	0	100	100
11	2I	117/129 (91%)	102 (87%)	13 (11%)	2 (2%)	11	43
12	3A	123/132 (93%)	105 (85%)	14 (11%)	4 (3%)	5	26
12	3I	123/132 (93%)	108 (88%)	15 (12%)	0	100	100
13	4A	115/126 (91%)	98 (85%)	16 (14%)	1 (1%)	21	61
13	4I	114/126 (90%)	97 (85%)	17 (15%)	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	43
15	6A	86/89 (97%)	81 (94%)	5 (6%)	0	100	100
15	6I	86/89 (97%)	76 (88%)	10 (12%)	0	100	100
16	7A	82/88 (93%)	78 (95%)	4 (5%)	0	100	100
16	7I	82/88 (93%)	78 (95%)	4 (5%)	0	100	100
17	8A	98/105 (93%)	90 (92%)	8 (8%)	0	100	100
17	8I	98/105 (93%)	94 (96%)	4 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
18	9A	70/88 (80%)	65 (93%)	5 (7%)	0	100	100
18	9I	70/88 (80%)	62 (89%)	7 (10%)	1 (1%)	14	48
19	AA	80/93 (86%)	65 (81%)	13 (16%)	2 (2%)	7	32
19	AI	81/93 (87%)	70 (86%)	9 (11%)	2 (2%)	7	32
20	BA	97/106 (92%)	88 (91%)	9 (9%)	0	100	100
20	BI	97/106 (92%)	89 (92%)	8 (8%)	0	100	100
21	1B	23/27 (85%)	19 (83%)	4 (17%)	0	100	100
21	1F	23/27 (85%)	21 (91%)	2 (9%)	0	100	100
27	11	270/272 (99%)	251 (93%)	15 (6%)	4 (2%)	13	46
28	21	203/205 (99%)	172 (85%)	28 (14%)	3 (2%)	13	46
28	29	203/205 (99%)	162 (80%)	33 (16%)	8 (4%)	4	22
29	31	200/202 (99%)	185 (92%)	14 (7%)	1 (0%)	34	72
30	41	179/181 (99%)	159 (89%)	17 (10%)	3 (2%)	11	43
30	49	179/181 (99%)	160 (89%)	16 (9%)	3 (2%)	11	43
31	51	172/180 (96%)	150 (87%)	17 (10%)	5 (3%)	6	29
31	59	169/180 (94%)	138 (82%)	27 (16%)	4 (2%)	7	33
32	61	144/146 (99%)	120 (83%)	20 (14%)	4 (3%)	6	30
32	69	144/146 (99%)	120 (83%)	21 (15%)	3 (2%)	9	37
33	15	136/138 (99%)	123 (90%)	12 (9%)	1 (1%)	26	65
33	58	136/138 (99%)	121 (89%)	10 (7%)	5 (4%)	4	23
34	25	120/122 (98%)	114 (95%)	6 (5%)	0	100	100
34	68	120/122 (98%)	114 (95%)	6 (5%)	0	100	100
35	35	148/150 (99%)	109 (74%)	31 (21%)	8 (5%)	2	14
35	78	148/150 (99%)	116 (78%)	28 (19%)	4 (3%)	6	31
36	45	139/141 (99%)	115 (83%)	23 (16%)	1 (1%)	26	65
36	88	139/141 (99%)	109 (78%)	26 (19%)	4 (3%)	6	29
37	55	115/118 (98%)	107 (93%)	8 (7%)	0	100	100
37	98	116/118 (98%)	105 (90%)	10 (9%)	1 (1%)	21	61
38	65	109/111 (98%)	89 (82%)	19 (17%)	1 (1%)	21	61
38	A8	109/111 (98%)	93 (85%)	15 (14%)	1 (1%)	21	61
39	75	135/137 (98%)	117 (87%)	15 (11%)	3 (2%)	8	36

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
39	B8	134/137 (98%)	123 (92%)	11 (8%)	0	100	100
40	85	115/117 (98%)	109 (95%)	5 (4%)	1 (1%)	21	61
40	C8	115/117 (98%)	104 (90%)	8 (7%)	3 (3%)	7	32
41	95	99/101 (98%)	78 (79%)	17 (17%)	4 (4%)	4	21
41	D8	99/101 (98%)	94 (95%)	3 (3%)	2 (2%)	9	38
42	A5	111/113 (98%)	105 (95%)	6 (5%)	0	100	100
42	E8	111/113 (98%)	106 (96%)	4 (4%)	1 (1%)	21	61
43	B5	90/94 (96%)	83 (92%)	6 (7%)	1 (1%)	17	55
43	F8	92/94 (98%)	86 (94%)	4 (4%)	2 (2%)	8	36
44	C5	102/110 (93%)	76 (74%)	24 (24%)	2 (2%)	9	38
44	G8	102/110 (93%)	78 (76%)	18 (18%)	6 (6%)	2	12
45	H8	173/175 (99%)	146 (84%)	18 (10%)	9 (5%)	2	15
46	E5	75/85 (88%)	72 (96%)	3 (4%)	0	100	100
46	I8	75/85 (88%)	66 (88%)	8 (11%)	1 (1%)	15	50
47	F5	95/98 (97%)	88 (93%)	5 (5%)	2 (2%)	9	37
47	J8	95/98 (97%)	86 (90%)	7 (7%)	2 (2%)	9	37
48	G5	64/66 (97%)	60 (94%)	2 (3%)	2 (3%)	5	27
48	K8	64/66 (97%)	60 (94%)	4 (6%)	0	100	100
49	H5	57/59 (97%)	53 (93%)	4 (7%)	0	100	100
49	L8	57/59 (97%)	55 (96%)	2 (4%)	0	100	100
50	I5	61/66 (92%)	36 (59%)	23 (38%)	2 (3%)	5	26
50	M8	64/66 (97%)	43 (67%)	19 (30%)	2 (3%)	5	27
51	J5	56/59 (95%)	50 (89%)	5 (9%)	1 (2%)	11	42
51	N8	57/59 (97%)	51 (90%)	6 (10%)	0	100	100
52	K5	43/45 (96%)	27 (63%)	16 (37%)	0	100	100
52	O8	43/45 (96%)	32 (74%)	11 (26%)	0	100	100
53	L5	43/49 (88%)	42 (98%)	1 (2%)	0	100	100
53	P8	43/49 (88%)	41 (95%)	2 (5%)	0	100	100
54	Q8	60/65 (92%)	39 (65%)	11 (18%)	10 (17%)	0	0
56	19	271/276 (98%)	258 (95%)	9 (3%)	4 (2%)	13	46
57	39	206/210 (98%)	175 (85%)	26 (13%)	5 (2%)	7	33

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
58	D5	177/206 (86%)	139 (78%)	30 (17%)	8 (4%)	3	17
59	M5	58/61 (95%)	46 (79%)	9 (16%)	3 (5%)	2	15
All	All	11344/11923 (95%)	10035 (88%)	1149 (10%)	160 (1%)	14	48

5 of 160 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
14	5I	25	VAL
18	9I	22	VAL
36	88	80	GLU
44	G8	53	PRO
44	G8	81	LYS

### 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%)	181 (88%)	24 (12%)	7	26
2	1E	205/220 (93%)	176 (86%)	29 (14%)	4	18
3	22	160/188 (85%)	140 (88%)	20 (12%)	6	22
3	2E	159/188 (85%)	140 (88%)	19 (12%)	6	25
4	32	180/180 (100%)	153 (85%)	27 (15%)	3	15
4	3E	180/180 (100%)	148 (82%)	32 (18%)	2	10
5	42	116/123 (94%)	94 (81%)	22 (19%)	2	8
5	4E	116/123 (94%)	98 (84%)	18 (16%)	3	14
6	52	90/90 (100%)	79 (88%)	11 (12%)	6	24
6	5E	90/90 (100%)	81 (90%)	9 (10%)	9	34
7	62	126/127 (99%)	105 (83%)	21 (17%)	3	11
7	6E	126/127 (99%)	107 (85%)	19 (15%)	3	15
8	72	119/119 (100%)	106 (89%)	13 (11%)	8	30
8	7E	119/119 (100%)	96 (81%)	23 (19%)	2	8

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
9	82	98/99 (99%)	85 (87%)	13 (13%)	5	20
9	8E	98/99 (99%)	77 (79%)	21 (21%)	1	5
10	1A	89/92 (97%)	81 (91%)	8 (9%)	12	41
10	1I	89/92 (97%)	78 (88%)	11 (12%)	6	23
11	2A	90/99 (91%)	82 (91%)	8 (9%)	12	42
11	2I	90/99 (91%)	81 (90%)	9 (10%)	9	34
12	3A	104/109 (95%)	91 (88%)	13 (12%)	6	22
12	3I	104/109 (95%)	92 (88%)	12 (12%)	7	27
13	4A	94/101 (93%)	77 (82%)	17 (18%)	2	9
13	4I	94/101 (93%)	76 (81%)	18 (19%)	2	8
14	5A	48/50 (96%)	43 (90%)	5 (10%)	9	32
14	5I	50/50 (100%)	39 (78%)	11 (22%)	1	5
15	6A	79/80 (99%)	71 (90%)	8 (10%)	9	33
15	6I	79/80 (99%)	67 (85%)	12 (15%)	3	14
16	7A	72/74 (97%)	63 (88%)	9 (12%)	6	22
16	7I	72/74 (97%)	58 (81%)	14 (19%)	2	7
17	8A	95/97 (98%)	88 (93%)	7 (7%)	17	51
17	8I	95/97 (98%)	79 (83%)	16 (17%)	2	11
18	9A	63/77 (82%)	49 (78%)	14 (22%)	1	5
18	9I	63/77 (82%)	55 (87%)	8 (13%)	5	22
19	AA	66/80 (82%)	55 (83%)	11 (17%)	3	11
19	AI	72/80 (90%)	58 (81%)	14 (19%)	2	7
20	BA	76/82 (93%)	57 (75%)	19 (25%)	1	2
20	BI	76/82 (93%)	67 (88%)	9 (12%)	6	25
21	1B	20/22 (91%)	19 (95%)	1 (5%)	30	67
21	1F	20/22 (91%)	17 (85%)	3 (15%)	3	15
27	11	214/214 (100%)	174 (81%)	40 (19%)	2	8
28	21	165/165 (100%)	131 (79%)	34 (21%)	1	6
28	29	165/165 (100%)	131 (79%)	34 (21%)	1	6
29	31	161/161 (100%)	133 (83%)	28 (17%)	2	11
30	41	155/155 (100%)	133 (86%)	22 (14%)	4	18

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
30	49	155/155 (100%)	132 (85%)	23 (15%)	4	16
31	51	145/148 (98%)	112 (77%)	33 (23%)	1	4
31	59	143/148 (97%)	128 (90%)	15 (10%)	8	31
32	61	122/122 (100%)	97 (80%)	25 (20%)	1	6
32	69	122/122 (100%)	102 (84%)	20 (16%)	3	12
33	15	117/117 (100%)	96 (82%)	21 (18%)	2	10
33	58	117/117 (100%)	92 (79%)	25 (21%)	1	5
34	25	100/100 (100%)	83 (83%)	17 (17%)	2	11
34	68	100/100 (100%)	87 (87%)	13 (13%)	5	21
35	35	116/116 (100%)	82 (71%)	34 (29%)	0	1
35	78	116/116 (100%)	84 (72%)	32 (28%)	0	1
36	45	111/111 (100%)	92 (83%)	19 (17%)	2	11
36	88	111/111 (100%)	90 (81%)	21 (19%)	2	8
37	55	100/101 (99%)	79 (79%)	21 (21%)	1	6
37	98	101/101 (100%)	81 (80%)	20 (20%)	1	7
38	65	87/87 (100%)	69 (79%)	18 (21%)	1	6
38	A8	87/87 (100%)	66 (76%)	21 (24%)	1	3
39	75	120/120 (100%)	95 (79%)	25 (21%)	1	6
39	B8	119/120 (99%)	91 (76%)	28 (24%)	1	4
40	85	93/93 (100%)	78 (84%)	15 (16%)	3	13
40	C8	93/93 (100%)	78 (84%)	15 (16%)	3	13
41	95	82/82 (100%)	63 (77%)	19 (23%)	1	4
41	D8	82/82 (100%)	57 (70%)	25 (30%)	0	1
42	A5	92/92 (100%)	70 (76%)	22 (24%)	1	3
42	E8	92/92 (100%)	74 (80%)	18 (20%)	1	7
43	B5	74/76 (97%)	56 (76%)	18 (24%)	1	3
43	F8	76/76 (100%)	62 (82%)	14 (18%)	2	9
44	C5	85/91 (93%)	64 (75%)	21 (25%)	1	3
44	G8	85/91 (93%)	69 (81%)	16 (19%)	2	8
45	H8	154/154 (100%)	129 (84%)	25 (16%)	3	12
46	E5	62/67 (92%)	54 (87%)	8 (13%)	5	21

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
46	I8	62/67 (92%)	54 (87%)	8 (13%)	5	21
47	F5	82/83 (99%)	68 (83%)	14 (17%)	2	11
47	J8	82/83 (99%)	67 (82%)	15 (18%)	2	9
48	G5	62/62 (100%)	46 (74%)	16 (26%)	0	2
48	K8	62/62 (100%)	44 (71%)	18 (29%)	0	1
49	H5	51/51 (100%)	41 (80%)	10 (20%)	1	7
49	L8	51/51 (100%)	41 (80%)	10 (20%)	1	7
50	I5	57/59 (97%)	47 (82%)	10 (18%)	2	10
50	M8	59/59 (100%)	50 (85%)	9 (15%)	3	14
51	J5	51/51 (100%)	42 (82%)	9 (18%)	2	10
51	N8	51/51 (100%)	41 (80%)	10 (20%)	1	7
52	K5	44/44 (100%)	38 (86%)	6 (14%)	5	19
52	O8	44/44 (100%)	32 (73%)	12 (27%)	0	1
53	L5	38/42 (90%)	31 (82%)	7 (18%)	2	9
53	P8	38/42 (90%)	31 (82%)	7 (18%)	2	9
54	Q8	41/55 (74%)	26 (63%)	15 (37%)	0	0
56	19	214/218 (98%)	165 (77%)	49 (23%)	1	4
57	39	165/166 (99%)	132 (80%)	33 (20%)	1	7
58	D5	158/179 (88%)	132 (84%)	26 (16%)	3	12
59	M5	50/51 (98%)	35 (70%)	15 (30%)	0	1
All	All	9568/9886 (97%)	7886 (82%)	1682 (18%)	2	10

5 of 1682 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
45	H8	154	ASP
5	42	41	VAL
44	C5	87	LYS
47	J8	94	LEU
54	Q8	11	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 19 such sidechains are listed below:

Mol	Chain	Res	Type
43	F8	31	HIS
18	9A	63	GLN
41	95	87	HIS
42	E8	60	ASN
42	A5	60	ASN

### 5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	13	1496/1522 (98%)	320 (21%)	31 (2%)
22	1K	82/85 (96%)	30 (36%)	8 (9%)
22	1L	70/85 (82%)	26 (37%)	3 (4%)
22	3K	70/85 (82%)	15 (21%)	2 (2%)
22	3L	71/85 (83%)	16 (22%)	3 (4%)
23	2K	76/77 (98%)	19 (25%)	2 (2%)
23	2L	76/77 (98%)	14 (18%)	2 (2%)
24	4K	14/30 (46%)	6 (42%)	0
24	4L	15/30 (50%)	6 (40%)	1 (6%)
25	14	2905/2912 (99%)	646 (22%)	39 (1%)
25	1H	2911/2912 (99%)	636 (21%)	55 (1%)
26	16	121/122 (99%)	22 (18%)	1 (0%)
26	1J	121/122 (99%)	35 (28%)	1 (0%)
55	1G	1496/1522 (98%)	322 (21%)	36 (2%)
All	All	9524/9666 (98%)	2113 (22%)	184 (1%)

5 of 2113 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	13	5	U
1	13	9	G
1	13	13	U
1	13	30	U
1	13	32	A

5 of 184 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
25	1H	1799	G
55	1G	197	A
25	14	2191	G
25	1H	1984	G
25	1H	2476	A

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

38 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	5.47	6 (33%)	21,38,41	5.89	6 (28%)
22	QUO	1K	35	24,22	27,35,36	5.68	9 (33%)	30,52,55	3.90	10 (33%)
22	MIA	1K	38	22	22,31,32	1.00	1 (4%)	26,44,47	2.49	6 (23%)
22	PSU	1K	40	22	15,21,22	0.90	1 (6%)	16,30,33	2.01	4 (25%)
22	5MU	1K	63	22	13,22,23	1.65	2 (15%)	16,32,35	1.50	1 (6%)
22	PSU	1K	64	22	15,21,22	1.16	2 (13%)	16,30,33	1.84	4 (25%)
22	4SU	1K	8	22	12,21,22	3.22	2 (16%)	15,30,33	1.02	1 (6%)
22	OMG	1L	17	22	18,26,27	5.60	6 (33%)	21,38,41	6.19	7 (33%)
22	QUO	1L	35	24,22	27,35,36	5.97	10 (37%)	30,52,55	4.08	9 (30%)
22	MIA	1L	38	22	22,31,32	1.08	1 (4%)	26,44,47	2.90	5 (19%)
22	PSU	1L	40	22	15,21,22	1.07	1 (6%)	16,30,33	2.04	4 (25%)
22	5MU	1L	63	22	13,22,23	1.70	2 (15%)	16,32,35	1.32	1 (6%)
22	PSU	1L	64	22	15,21,22	0.88	1 (6%)	16,30,33	2.20	4 (25%)
22	4SU	1L	8	22	12,21,22	3.18	2 (16%)	15,30,33	1.04	1 (6%)
23	H2U	2K	21	23	17,21,22	2.12	4 (23%)	23,30,33	2.66	5 (21%)
23	OMC	2K	33	23	15,22,23	2.18	4 (26%)	20,31,34	1.78	2 (10%)
23	5MU	2K	55	60,23	13,22,23	1.67	2 (15%)	16,32,35	1.61	1 (6%)
23	PSU	2K	56	23	15,21,22	1.15	2 (13%)	16,30,33	1.84	3 (18%)
23	4SU	2K	8	23	12,21,22	3.38	2 (16%)	15,30,33	0.73	0
23	H2U	2L	21	23	17,21,22	2.26	4 (23%)	23,30,33	2.82	5 (21%)
23	OMC	2L	33	23	15,22,23	2.18	4 (26%)	20,31,34	1.56	2 (10%)
23	5MU	2L	55	23	13,22,23	1.68	2 (15%)	16,32,35	1.13	1 (6%)
23	PSU	2L	56	23	15,21,22	1.05	1 (6%)	16,30,33	1.84	3 (18%)
23	4SU	2L	8	23	12,21,22	3.32	2 (16%)	15,30,33	0.66	0
22	OMG	3K	17	22	18,26,27	5.70	6 (33%)	21,38,41	6.39	6 (28%)
22	QUO	3K	35	22	27,35,36	5.93	9 (33%)	30,52,55	4.08	10 (33%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
22	MIA	3K	38	22	22,31,32	1.27	1 (4%)	26,44,47	1.29	4 (15%)
22	PSU	3K	40	22	15,21,22	0.98	1 (6%)	16,30,33	2.20	3 (18%)
22	5MU	3K	63	22	13,22,23	1.68	2 (15%)	16,32,35	1.22	1 (6%)
22	PSU	3K	64	22	15,21,22	1.17	3 (20%)	16,30,33	2.16	4 (25%)
22	4SU	3K	8	22	12,21,22	3.14	2 (16%)	15,30,33	1.06	1 (6%)
22	OMG	3L	17	22	18,26,27	5.75	6 (33%)	21,38,41	6.37	6 (28%)
22	QUO	3L	35	22	27,35,36	6.01	9 (33%)	30,52,55	4.34	12 (40%)
22	MIA	3L	38	22	22,31,32	1.00	2 (9%)	26,44,47	1.42	6 (23%)
22	PSU	3L	40	22	15,21,22	1.16	1 (6%)	16,30,33	2.16	4 (25%)
22	5MU	3L	63	22	13,22,23	1.68	2 (15%)	16,32,35	1.35	1 (6%)
22	PSU	3L	64	22	15,21,22	0.95	1 (6%)	16,30,33	1.98	4 (25%)
22	4SU	3L	8	22	12,21,22	3.34	2 (16%)	15,30,33	1.04	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
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
22	OMG	1L	17	22	-	0/5/27/28	0/3/3/3
22	QUO	1L	35	24,22	-	0/6/43/44	0/4/4/4
22	MIA	1L	38	22	-	2/11/33/34	0/3/3/3
22	PSU	1L	40	22	-	0/7/25/26	0/2/2/2
22	5MU	1L	63	22	-	0/3/25/26	0/2/2/2
22	PSU	1L	64	22	-	0/7/25/26	0/2/2/2
22	4SU	1L	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	5MU	2K	55	60,23	-	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
23	H2U	2L	21	23	-	0/7/38/39	0/2/2/2
23	OMC	2L	33	23	-	0/5/27/28	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
23	5MU	2L	55	23	-	0/3/25/26	0/2/2/2
23	PSU	2L	56	23	-	0/7/25/26	0/2/2/2
23	4SU	2L	8	23	-	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
22	OMG	3L	17	22	-	0/5/27/28	0/3/3/3
22	QUO	3L	35	22	-	0/6/43/44	0/4/4/4
22	MIA	3L	38	22	-	0/11/33/34	0/3/3/3
22	PSU	3L	40	22	-	0/7/25/26	0/2/2/2
22	5MU	3L	63	22	-	0/3/25/26	0/2/2/2
22	PSU	3L	64	22	-	0/7/25/26	0/2/2/2
22	4SU	3L	8	22	-	0/3/25/26	0/2/2/2

The worst 5 of 120 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	3L	17	OMG	C8-N7	-13.65	1.08	1.34
22	3K	17	OMG	C8-N7	-13.57	1.08	1.34
22	1K	17	OMG	C8-N7	-13.44	1.08	1.34
22	1L	17	OMG	C8-N7	-13.29	1.09	1.34
22	3K	35	QUO	C8-N9	-10.52	1.23	1.38

The worst 5 of 148 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	3L	35	QUO	C8-N9-C1'	-15.85	113.07	125.45
22	1L	35	QUO	C8-N9-C1'	-14.92	113.80	125.45
22	1K	17	OMG	C6-C5-C4	-12.42	106.66	120.86
22	3K	35	QUO	C8-N9-C1'	-12.39	115.77	125.45
22	3L	17	OMG	C6-C5-C4	-11.97	107.18	120.86

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
22	1L	38	MIA	N3-C2-S10-C11

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Mol	Chain	Res	Type	Atoms
22	1L	38	MIA	N1-C2-S10-C11

There are no ring outliers.

26 monomers are involved in 46 short contacts:

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

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 1137 ligands modelled in this entry, 1137 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
55	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	3.01

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	13	1498/1522 (98%)	-0.47	8 (0%) 91 83	52, 95, 191, 430	0
2	12	237/256 (92%)	0.24	12 (5%) 32 13	115, 168, 226, 251	0
2	1E	237/256 (92%)	-0.08	3 (1%) 79 62	104, 142, 195, 252	0
3	22	206/239 (86%)	0.83	28 (13%) 4 2	124, 151, 185, 240	0
3	2E	205/239 (85%)	0.29	10 (4%) 33 14	83, 109, 154, 191	0
4	32	208/208 (100%)	0.70	23 (11%) 7 2	90, 116, 161, 199	0
4	3E	208/208 (100%)	0.44	12 (5%) 26 11	75, 106, 145, 171	0
5	42	151/162 (93%)	0.32	3 (1%) 68 46	98, 124, 157, 188	0
5	4E	151/162 (93%)	0.09	3 (1%) 68 46	73, 98, 129, 175	0
6	52	101/101 (100%)	0.14	1 (0%) 84 69	78, 101, 133, 177	0
6	5E	101/101 (100%)	0.07	1 (0%) 84 69	75, 102, 131, 171	0
7	62	155/156 (99%)	1.02	28 (18%) 2 1	101, 128, 163, 204	0
7	6E	155/156 (99%)	0.28	6 (3%) 43 21	95, 117, 154, 199	0
8	72	138/138 (100%)	0.76	18 (13%) 5 2	93, 127, 152, 171	0
8	7E	138/138 (100%)	0.15	1 (0%) 89 78	81, 106, 133, 157	0
9	82	127/128 (99%)	0.77	14 (11%) 7 2	110, 159, 203, 214	0
9	8E	127/128 (99%)	0.12	6 (4%) 35 16	86, 139, 183, 217	0
10	1A	99/105 (94%)	0.64	10 (10%) 9 3	120, 162, 202, 221	0
10	1I	99/105 (94%)	0.06	3 (3%) 54 29	84, 134, 180, 197	0
11	2A	119/129 (92%)	1.16	15 (12%) 5 2	85, 111, 149, 259	0
11	2I	119/129 (92%)	0.45	10 (8%) 14 4	68, 101, 158, 186	0
12	3A	125/132 (94%)	1.43	35 (28%) 1 0	78, 103, 165, 208	0
12	3I	125/132 (94%)	0.13	5 (4%) 42 20	60, 72, 138, 239	0
13	4A	117/126 (92%)	1.75	43 (36%) 0 0	107, 146, 182, 217	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
13	4I	116/126 (92%)	0.36	7 (6%) 25 10	85, 122, 159, 196	0
14	5A	58/61 (95%)	1.91	27 (46%) 0 0	120, 150, 175, 199	0
14	5I	61/61 (100%)	0.04	0 100 100	83, 100, 131, 187	0
15	6A	88/89 (98%)	0.62	5 (5%) 27 11	78, 110, 141, 162	0
15	6I	88/89 (98%)	-0.23	0 100 100	75, 99, 133, 167	0
16	7A	84/88 (95%)	0.65	3 (3%) 46 23	87, 101, 148, 183	0
16	7I	84/88 (95%)	0.57	8 (9%) 10 4	95, 115, 160, 193	0
17	8A	100/105 (95%)	1.26	24 (24%) 1 0	88, 111, 142, 212	0
17	8I	100/105 (95%)	-0.08	2 (2%) 68 46	85, 108, 137, 174	0
18	9A	72/88 (81%)	0.93	8 (11%) 7 2	90, 117, 165, 216	0
18	9I	72/88 (81%)	0.24	3 (4%) 40 19	81, 106, 165, 192	0
19	AA	82/93 (88%)	2.10	44 (53%) 0 0	120, 163, 207, 254	0
19	AI	83/93 (89%)	0.23	6 (7%) 18 7	91, 122, 184, 229	0
20	BA	99/106 (93%)	0.55	6 (6%) 25 10	85, 110, 159, 210	0
20	BI	99/106 (93%)	0.51	9 (9%) 11 4	101, 123, 179, 208	0
21	1B	25/27 (92%)	1.85	11 (44%) 0 0	109, 131, 161, 194	0
21	1F	25/27 (92%)	0.46	1 (4%) 42 20	88, 106, 144, 196	0
22	1K	78/85 (91%)	-0.06	2 (2%) 59 35	78, 184, 302, 353	0
22	1L	67/85 (78%)	0.85	11 (16%) 2 1	118, 208, 263, 287	0
22	3K	67/85 (78%)	-0.51	0 100 100	64, 176, 247, 292	0
22	3L	68/85 (80%)	-0.27	0 100 100	72, 188, 243, 285	0
23	2K	72/77 (93%)	-0.53	0 100 100	61, 89, 126, 155	0
23	2L	72/77 (93%)	-0.39	0 100 100	72, 104, 146, 163	0
24	4K	15/30 (50%)	-0.33	0 100 100	64, 95, 185, 192	0
24	4L	16/30 (53%)	0.59	1 (6%) 23 9	84, 129, 213, 234	0
25	14	2907/2912 (99%)	-0.22	53 (1%) 71 50	48, 80, 246, 500	0
25	1H	2912/2912 (100%)	-0.13	35 (1%) 81 64	37, 68, 231, 416	0
26	16	122/122 (100%)	-0.33	2 (1%) 74 55	65, 88, 112, 273	0
26	1J	122/122 (100%)	-0.56	0 100 100	79, 111, 139, 235	0
27	11	272/272 (100%)	0.05	2 (0%) 89 78	39, 60, 90, 171	0
28	21	205/205 (100%)	0.52	9 (4%) 38 17	47, 86, 159, 217	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
28	29	205/205 (100%)	0.21	10 (4%) 33 14	55, 92, 186, 254	0
29	31	202/202 (100%)	-0.13	0 100 100	44, 75, 130, 195	0
30	41	181/181 (100%)	0.51	16 (8%) 12 4	80, 104, 155, 203	0
30	49	181/181 (100%)	1.51	53 (29%) 1 0	99, 133, 183, 213	0
31	51	174/180 (96%)	0.25	6 (3%) 49 24	74, 108, 142, 187	0
31	59	171/180 (95%)	1.28	46 (26%) 1 0	129, 194, 264, 306	0
32	61	146/146 (100%)	0.30	5 (3%) 49 24	71, 128, 164, 189	0
32	69	146/146 (100%)	0.43	9 (6%) 24 10	78, 126, 180, 217	0
33	15	138/138 (100%)	-0.30	0 100 100	73, 104, 157, 174	0
33	58	138/138 (100%)	0.80	12 (8%) 13 4	60, 90, 143, 192	0
34	25	122/122 (100%)	0.34	4 (3%) 50 26	64, 84, 113, 129	0
34	68	122/122 (100%)	0.40	1 (0%) 87 75	54, 72, 94, 105	0
35	35	150/150 (100%)	0.45	14 (9%) 11 4	55, 107, 169, 217	0
35	78	150/150 (100%)	-0.18	3 (2%) 68 46	45, 82, 117, 215	0
36	45	141/141 (100%)	0.35	9 (6%) 23 9	73, 107, 152, 190	0
36	88	141/141 (100%)	0.39	8 (5%) 27 11	55, 79, 127, 152	0
37	55	117/118 (99%)	-0.21	0 100 100	54, 77, 104, 141	0
37	98	118/118 (100%)	0.69	9 (7%) 17 6	55, 79, 105, 134	0
38	65	111/111 (100%)	0.97	17 (15%) 3 1	87, 113, 162, 235	0
38	A8	111/111 (100%)	0.35	5 (4%) 37 17	72, 90, 136, 206	0
39	75	137/137 (100%)	-0.14	2 (1%) 76 58	75, 95, 162, 229	0
39	B8	136/137 (99%)	0.08	1 (0%) 89 78	67, 90, 153, 191	0
40	85	117/117 (100%)	-0.07	1 (0%) 85 72	65, 89, 142, 206	0
40	C8	117/117 (100%)	0.67	14 (11%) 6 2	51, 79, 131, 184	0
41	95	101/101 (100%)	0.51	7 (6%) 20 7	61, 129, 158, 199	0
41	D8	101/101 (100%)	0.96	9 (8%) 12 4	53, 105, 180, 251	0
42	A5	113/113 (100%)	-0.02	1 (0%) 85 72	57, 72, 119, 205	0
42	E8	113/113 (100%)	0.83	6 (5%) 30 13	54, 69, 115, 197	0
43	B5	92/94 (97%)	0.02	1 (1%) 82 66	60, 80, 115, 161	0
43	F8	94/94 (100%)	0.50	3 (3%) 51 27	51, 66, 102, 137	0
44	C5	104/110 (94%)	0.83	15 (14%) 3 2	88, 130, 215, 257	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
44	G8	104/110 (94%)	0.22	3 (2%) 55 31	67, 98, 165, 204	0
45	H8	175/175 (100%)	1.85	65 (37%) 0 0	83, 136, 224, 250	0
46	E5	77/85 (90%)	0.45	4 (5%) 31 13	61, 85, 112, 202	0
46	I8	77/85 (90%)	0.30	1 (1%) 79 62	52, 69, 99, 223	0
47	F5	97/98 (98%)	0.75	9 (9%) 11 4	55, 80, 162, 236	0
47	J8	97/98 (98%)	0.39	8 (8%) 14 5	46, 69, 184, 208	0
48	G5	66/66 (100%)	0.38	4 (6%) 25 10	77, 102, 150, 231	0
48	K8	66/66 (100%)	0.24	2 (3%) 54 29	58, 77, 117, 208	0
49	H5	59/59 (100%)	0.09	0 100 100	76, 98, 151, 172	0
49	L8	59/59 (100%)	0.50	2 (3%) 49 24	59, 77, 114, 147	0
50	I5	63/66 (95%)	4.55	49 (77%) 0 0	165, 220, 260, 276	0
50	M8	66/66 (100%)	1.75	25 (37%) 0 0	114, 177, 241, 262	0
51	J5	58/59 (98%)	-0.07	2 (3%) 49 24	56, 81, 192, 229	0
51	N8	59/59 (100%)	1.43	9 (15%) 3 1	46, 82, 212, 227	0
52	K5	45/45 (100%)	4.29	37 (82%) 0 0	136, 199, 245, 278	0
52	O8	45/45 (100%)	2.50	25 (55%) 0 0	111, 162, 201, 227	0
53	L5	45/49 (91%)	-0.02	0 100 100	47, 56, 71, 90	0
53	P8	45/49 (91%)	-0.21	0 100 100	38, 46, 61, 76	0
54	Q8	62/65 (95%)	0.20	3 (4%) 34 15	56, 72, 111, 166	0
55	1G	1498/1522 (98%)	-0.28	5 (0%) 94 88	65, 110, 185, 415	0
56	19	273/276 (98%)	0.30	7 (2%) 59 35	47, 71, 97, 127	0
57	39	208/210 (99%)	0.31	9 (4%) 39 18	56, 99, 194, 251	0
58	D5	179/206 (86%)	0.89	31 (17%) 2 1	111, 162, 259, 295	0
59	M5	60/61 (98%)	0.44	4 (6%) 21 7	67, 81, 131, 191	0
All	All	21050/21589 (97%)	0.18	1168 (5%) 29 12	37, 98, 201, 500	0

The worst 5 of 1168 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
50	I5	31	ILE	17.4
51	N8	59	GLU	16.3
12	3I	129	ALA	14.0
28	29	205	ALA	13.7
25	1H	2799	A	13.7

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

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
22	QUO	3L	35	32/33	0.91	0.31	-	124,129,153,158	0
22	5MU	1L	63	21/22	0.89	0.16	-	179,192,198,199	0
22	PSU	3K	40	20/21	0.95	0.12	-	101,110,114,118	0
22	QUO	1L	35	32/33	0.90	0.32	-	107,128,151,155	0
22	PSU	1L	64	20/21	0.87	0.13	-	160,190,212,217	0
22	4SU	1L	8	20/21	0.86	0.28	-	196,199,202,204	0
22	4SU	3K	8	20/21	0.81	0.14	-	175,183,197,200	0
22	PSU	1L	40	20/21	0.91	0.17	-	106,139,158,159	0
22	PSU	1K	64	20/21	0.91	0.17	-	119,139,152,156	0
23	OMC	2L	33	21/22	0.98	0.16	-	90,96,100,103	0
22	5MU	1K	63	21/22	0.91	0.22	-	137,144,151,152	0
22	MIA	3K	38	29/30	0.95	0.14	-	100,113,136,140	0
22	OMG	1L	17	24/25	0.67	0.38	-	214,233,260,267	0
22	OMG	3K	17	24/25	0.88	0.18	-	198,221,226,229	0
23	5MU	2K	55	21/22	0.95	0.14	-	93,103,114,118	0
22	PSU	3L	40	20/21	0.94	0.16	-	112,122,127,128	0
22	QUO	3K	35	32/33	0.94	0.14	-	109,116,133,141	0
23	PSU	2K	56	20/21	0.95	0.09	-	92,99,106,110	0
23	H2U	2K	21	20/21	0.87	0.23	-	133,176,266,270	0
22	5MU	3L	63	21/22	0.88	0.20	-	184,193,204,205	0
22	PSU	3K	64	20/21	0.78	0.17	-	204,248,266,281	0
22	OMG	3L	17	24/25	0.74	0.22	-	197,218,241,244	0
23	H2U	2L	21	20/21	0.81	0.21	-	165,170,178,179	0
22	4SU	3L	8	20/21	0.74	0.13	-	189,200,212,215	0
22	PSU	1K	40	20/21	0.95	0.12	-	81,102,111,111	0
23	OMC	2K	33	21/22	0.97	0.17	-	72,75,81,86	0
23	4SU	2L	8	20/21	0.92	0.12	-	103,112,116,121	0
22	MIA	1K	38	29/30	0.95	0.18	-	64,83,97,102	0
22	5MU	3K	63	21/22	0.85	0.17	-	197,231,241,247	0
22	4SU	1K	8	20/21	0.79	0.16	-	149,171,199,201	0
23	4SU	2K	8	20/21	0.95	0.14	-	87,91,98,101	0
22	MIA	1L	38	29/30	0.93	0.29	-	102,126,149,151	0
23	5MU	2L	55	21/22	0.95	0.12	-	118,122,133,134	0
22	PSU	3L	64	20/21	0.71	0.22	-	190,201,215,215	0
22	MIA	3L	38	29/30	0.93	0.18	-	112,126,138,143	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
22	OMG	1K	17	24/25	0.86	0.16	-	148,195,234,241	0
22	QUO	1K	35	32/33	0.94	0.18	-	73,84,105,108	0
23	PSU	2L	56	20/21	0.94	0.08	-	107,113,120,121	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, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
60	MG	14	3286	1/1	0.86	0.93	69.20	60,60,60,60	0
60	MG	14	3232	1/1	0.83	0.66	46.70	92,92,92,92	0
60	MG	1H	3030	1/1	0.72	0.58	32.61	70,70,70,70	0
60	MG	1H	3107	1/1	0.94	0.47	29.07	63,63,63,63	0
60	MG	1H	3298	1/1	0.74	0.43	26.95	56,56,56,56	0
60	MG	14	3246	1/1	0.96	0.45	26.58	81,81,81,81	0
60	MG	1H	3012	1/1	0.95	0.52	25.73	49,49,49,49	0
60	MG	14	3066	1/1	0.94	0.43	25.44	47,47,47,47	0
60	MG	14	3094	1/1	0.98	0.40	25.02	58,58,58,58	0
60	MG	1G	1656	1/1	0.69	0.38	23.93	86,86,86,86	0
60	MG	14	3058	1/1	0.97	0.35	23.26	64,64,64,64	0
60	MG	14	3064	1/1	0.64	0.48	22.28	70,70,70,70	0
60	MG	13	1668	1/1	0.54	0.46	22.10	114,114,114,114	0
60	MG	1H	3050	1/1	0.92	0.32	20.80	54,54,54,54	0
60	MG	14	3284	1/1	0.90	0.43	20.53	75,75,75,75	0
60	MG	14	3258	1/1	0.86	0.32	20.33	65,65,65,65	0
60	MG	14	3100	1/1	0.97	0.46	20.14	49,49,49,49	0
60	MG	1H	3016	1/1	0.97	0.32	20.04	42,42,42,42	0
60	MG	14	3097	1/1	0.97	0.39	18.86	54,54,54,54	0
60	MG	1H	3202	1/1	0.95	0.46	18.61	43,43,43,43	0
60	MG	14	3036	1/1	0.96	0.37	18.49	66,66,66,66	0
60	MG	14	3305	1/1	0.83	0.28	18.38	94,94,94,94	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
60	MG	1H	3147	1/1	0.71	0.42	18.22	76,76,76,76	0
60	MG	14	3290	1/1	0.96	0.33	18.03	78,78,78,78	0
60	MG	13	1648	1/1	0.83	0.48	18.01	76,76,76,76	0
60	MG	14	3086	1/1	0.99	0.45	16.87	48,48,48,48	0
60	MG	1H	3270	1/1	0.88	0.42	16.51	58,58,58,58	0
60	MG	13	1710	1/1	0.65	0.34	16.49	104,104,104,104	0
60	MG	13	1660	1/1	0.94	0.37	16.27	70,70,70,70	0
60	MG	14	3082	1/1	0.95	0.44	15.72	65,65,65,65	0
60	MG	14	3115	1/1	0.97	0.34	15.53	39,39,39,39	0
60	MG	14	3061	1/1	0.93	0.34	15.39	49,49,49,49	0
60	MG	1H	3076	1/1	0.97	0.35	15.23	44,44,44,44	0
60	MG	14	3179	1/1	0.99	0.30	15.15	51,51,51,51	0
60	MG	1H	3010	1/1	0.98	0.38	15.03	50,50,50,50	0
60	MG	1H	3034	1/1	0.96	0.37	14.94	38,38,38,38	0
60	MG	14	3010	1/1	0.98	0.38	14.86	54,54,54,54	0
60	MG	1H	3256	1/1	0.77	0.42	14.71	93,93,93,93	0
60	MG	16	205	1/1	0.91	0.27	14.52	79,79,79,79	0
60	MG	14	3028	1/1	0.71	0.35	14.49	77,77,77,77	0
60	MG	1H	3115	1/1	0.92	0.41	13.88	52,52,52,52	0
60	MG	1H	3002	1/1	0.97	0.33	13.87	51,51,51,51	0
60	MG	1H	3287	1/1	0.93	0.28	13.52	54,54,54,54	0
60	MG	13	1621	1/1	0.98	0.43	13.48	62,62,62,62	0
60	MG	13	1642	1/1	0.81	0.29	13.22	63,63,63,63	0
60	MG	13	1664	1/1	0.93	0.27	13.13	68,68,68,68	0
60	MG	14	3079	1/1	0.97	0.35	13.00	68,68,68,68	0
60	MG	1H	3087	1/1	0.90	0.33	12.98	72,72,72,72	0
60	MG	85	201	1/1	0.83	0.42	12.87	71,71,71,71	0
60	MG	14	3068	1/1	0.98	0.37	12.85	53,53,53,53	0
60	MG	13	1627	1/1	0.97	0.39	12.72	50,50,50,50	0
60	MG	14	3306	1/1	0.89	0.31	12.57	67,67,67,67	0
60	MG	1H	3191	1/1	0.92	0.33	12.52	73,73,73,73	0
60	MG	14	3074	1/1	0.94	0.49	12.51	53,53,53,53	0
60	MG	1G	1631	1/1	0.96	0.32	11.79	83,83,83,83	0
60	MG	1H	3042	1/1	0.91	0.29	11.64	54,54,54,54	0
60	MG	1G	1673	1/1	0.82	0.33	11.50	186,186,186,186	0
60	MG	1H	3060	1/1	0.89	0.32	11.02	64,64,64,64	0
60	MG	1H	3142	1/1	0.94	0.26	11.01	57,57,57,57	0
60	MG	1H	3083	1/1	0.97	0.37	10.95	44,44,44,44	0
60	MG	1H	3014	1/1	0.97	0.33	10.72	52,52,52,52	0
60	MG	1H	3024	1/1	0.97	0.26	10.60	51,51,51,51	0
60	MG	1G	1632	1/1	0.88	0.41	10.60	89,89,89,89	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
60	MG	1H	3075	1/1	0.99	0.28	10.33	41,41,41,41	0
60	MG	1H	3184	1/1	0.84	0.25	10.25	58,58,58,58	0
60	MG	1H	3164	1/1	0.85	0.25	10.08	60,60,60,60	0
60	MG	14	3090	1/1	0.89	0.38	9.98	63,63,63,63	0
60	MG	14	3127	1/1	0.97	0.30	9.94	71,71,71,71	0
60	MG	14	3192	1/1	0.72	0.20	9.68	80,80,80,80	0
60	MG	14	3054	1/1	0.97	0.45	9.43	64,64,64,64	0
60	MG	14	3161	1/1	0.95	0.30	9.37	69,69,69,69	0
60	MG	14	3156	1/1	0.91	0.26	9.09	54,54,54,54	0
60	MG	14	3214	1/1	0.98	0.34	9.08	84,84,84,84	0
60	MG	14	3270	1/1	0.94	0.31	8.80	57,57,57,57	0
60	MG	14	3294	1/1	0.59	0.42	8.70	91,91,91,91	0
60	MG	14	3225	1/1	0.96	0.24	8.68	53,53,53,53	0
60	MG	14	3012	1/1	0.98	0.32	8.67	59,59,59,59	0
60	MG	14	3235	1/1	0.97	0.31	8.61	78,78,78,78	0
60	MG	14	3151	1/1	0.89	0.23	8.51	55,55,55,55	0
60	MG	1H	3051	1/1	0.96	0.36	8.36	61,61,61,61	0
60	MG	13	1650	1/1	0.89	0.28	8.28	77,77,77,77	0
60	MG	1H	3175	1/1	0.97	0.32	8.23	81,81,81,81	0
60	MG	13	1672	1/1	0.98	0.28	8.21	63,63,63,63	0
60	MG	14	3004	1/1	0.99	0.25	8.09	53,53,53,53	0
60	MG	14	3035	1/1	0.99	0.33	8.08	57,57,57,57	0
60	MG	14	3083	1/1	0.96	0.30	8.03	56,56,56,56	0
60	MG	14	3206	1/1	0.92	0.26	8.00	63,63,63,63	0
60	MG	1H	3268	1/1	0.96	0.47	7.99	58,58,58,58	0
60	MG	13	1651	1/1	0.97	0.30	7.98	54,54,54,54	0
60	MG	14	3177	1/1	0.86	0.28	7.88	61,61,61,61	0
60	MG	1H	3066	1/1	0.98	0.34	7.73	36,36,36,36	0
60	MG	1H	3048	1/1	0.87	0.26	7.65	51,51,51,51	0
60	MG	14	3245	1/1	0.67	0.27	7.33	82,82,82,82	0
60	MG	13	1605	1/1	0.96	0.22	7.29	71,71,71,71	0
60	MG	14	3153	1/1	0.71	0.35	7.07	61,61,61,61	0
60	MG	14	3102	1/1	0.95	0.30	7.06	46,46,46,46	0
60	MG	14	3157	1/1	0.96	0.34	7.03	69,69,69,69	0
60	MG	1H	3229	1/1	0.91	0.27	6.92	56,56,56,56	0
60	MG	1G	1601	1/1	0.96	0.35	6.79	59,59,59,59	0
60	MG	1H	3297	1/1	0.89	0.48	6.74	63,63,63,63	0
60	MG	14	3237	1/1	0.74	0.21	6.68	66,66,66,66	0
60	MG	14	3288	1/1	0.72	0.26	6.67	61,61,61,61	0
60	MG	14	3147	1/1	0.73	0.32	6.50	99,99,99,99	0
60	MG	1H	3265	1/1	0.92	0.25	6.37	75,75,75,75	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
60	MG	1G	1667	1/1	0.95	0.31	6.35	66,66,66,66	0
60	MG	1G	1625	1/1	0.86	0.27	6.24	72,72,72,72	0
60	MG	14	3112	1/1	0.96	0.38	6.07	72,72,72,72	0
60	MG	14	3134	1/1	0.95	0.20	5.79	84,84,84,84	0
60	MG	1H	3020	1/1	0.89	0.26	5.73	59,59,59,59	0
60	MG	1G	1678	1/1	0.94	0.24	5.55	79,79,79,79	0
60	MG	1H	3187	1/1	0.91	0.26	5.54	60,60,60,60	0
60	MG	1H	3207	1/1	0.75	0.24	5.44	63,63,63,63	0
60	MG	1H	3069	1/1	0.96	0.30	5.44	60,60,60,60	0
60	MG	1H	3033	1/1	0.99	0.31	5.38	61,61,61,61	0
60	MG	14	3203	1/1	0.95	0.31	5.30	66,66,66,66	0
60	MG	14	3281	1/1	0.83	0.22	5.29	63,63,63,63	0
60	MG	1G	1674	1/1	0.91	0.24	5.28	84,84,84,84	0
60	MG	13	1617	1/1	0.84	0.17	5.08	99,99,99,99	0
60	MG	14	3223	1/1	0.81	0.30	5.07	67,67,67,67	0
60	MG	16	201	1/1	0.80	0.20	4.99	78,78,78,78	0
60	MG	14	3095	1/1	0.92	0.21	4.98	66,66,66,66	0
60	MG	1H	3054	1/1	0.95	0.27	4.98	56,56,56,56	0
60	MG	1H	3259	1/1	0.91	0.18	4.80	59,59,59,59	0
60	MG	1H	3023	1/1	0.93	0.33	4.79	58,58,58,58	0
60	MG	14	3137	1/1	0.91	0.35	4.67	69,69,69,69	0
60	MG	14	3118	1/1	0.88	0.23	4.63	60,60,60,60	0
60	MG	14	3208	1/1	0.87	0.24	4.57	66,66,66,66	0
60	MG	14	3289	1/1	0.98	0.22	4.41	65,65,65,65	0
60	MG	14	3042	1/1	0.94	0.27	4.41	44,44,44,44	0
60	MG	1H	3021	1/1	0.85	0.19	4.33	59,59,59,59	0
60	MG	1H	3110	1/1	0.75	0.24	4.31	43,43,43,43	0
60	MG	1G	1688	1/1	0.93	0.34	4.25	105,105,105,105	0
60	MG	14	3023	1/1	0.97	0.26	4.19	74,74,74,74	0
60	MG	14	3279	1/1	0.88	0.15	4.17	76,76,76,76	0
60	MG	14	3176	1/1	0.97	0.28	4.04	67,67,67,67	0
60	MG	1H	3223	1/1	0.85	0.21	4.00	44,44,44,44	0
60	MG	1H	3099	1/1	0.84	0.20	3.98	49,49,49,49	0
60	MG	14	3233	1/1	0.93	0.27	3.97	69,69,69,69	0
60	MG	14	3098	1/1	0.93	0.47	3.96	59,59,59,59	0
60	MG	14	3130	1/1	0.96	0.25	3.73	53,53,53,53	0
60	MG	14	3119	1/1	0.98	0.22	3.71	65,65,65,65	0
60	MG	1H	3294	1/1	0.82	0.22	3.68	66,66,66,66	0
60	MG	14	3011	1/1	0.97	0.21	3.63	58,58,58,58	0
60	MG	1H	3067	1/1	0.97	0.26	3.55	46,46,46,46	0
60	MG	29	302	1/1	0.85	0.23	3.54	79,79,79,79	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
60	MG	1H	3199	1/1	0.93	0.27	3.51	74,74,74,74	0
60	MG	1H	3157	1/1	0.94	0.22	3.41	58,58,58,58	0
60	MG	14	3139	1/1	0.97	0.23	3.31	53,53,53,53	0
60	MG	14	3034	1/1	0.98	0.28	3.24	62,62,62,62	0
60	MG	13	1604	1/1	0.97	0.29	3.24	74,74,74,74	0
60	MG	1G	1657	1/1	0.75	0.30	3.23	102,102,102,102	0
60	MG	1G	1611	1/1	0.95	0.24	3.23	103,103,103,103	0
60	MG	1H	3239	1/1	0.63	0.25	3.19	48,48,48,48	0
61	ZN	32	301	1/1	0.98	0.35	3.13	108,108,108,108	0
60	MG	1G	1684	1/1	0.87	0.23	3.11	91,91,91,91	0
60	MG	2L	101	1/1	0.97	0.25	3.08	72,72,72,72	0
60	MG	14	3386	1/1	0.97	0.33	3.06	57,57,57,57	0
60	MG	1H	3242	1/1	0.86	0.21	3.06	74,74,74,74	0
60	MG	1H	3122	1/1	0.88	0.20	3.01	56,56,56,56	0
60	MG	14	3052	1/1	0.97	0.31	3.00	55,55,55,55	0
60	MG	16	204	1/1	0.71	0.18	2.98	83,83,83,83	0
60	MG	1H	3246	1/1	0.68	0.20	2.89	73,73,73,73	0
60	MG	1H	3096	1/1	0.95	0.32	2.89	53,53,53,53	0
60	MG	1G	1614	1/1	0.97	0.19	2.88	109,109,109,109	0
60	MG	14	3092	1/1	0.91	0.27	2.84	62,62,62,62	0
60	MG	1H	3169	1/1	0.88	0.21	2.83	63,63,63,63	0
60	MG	1H	3173	1/1	0.90	0.18	2.82	72,72,72,72	0
60	MG	13	1608	1/1	0.96	0.20	2.82	70,70,70,70	0
60	MG	1G	1644	1/1	0.98	0.24	2.80	85,85,85,85	0
60	MG	1H	3058	1/1	0.90	0.20	2.80	57,57,57,57	0
60	MG	14	3229	1/1	0.95	0.24	2.80	84,84,84,84	0
60	MG	14	3299	1/1	0.83	0.18	2.68	60,60,60,60	0
60	MG	14	3163	1/1	0.45	0.21	2.66	80,80,80,80	0
60	MG	13	1692	1/1	0.72	0.25	2.58	78,78,78,78	0
60	MG	1H	3221	1/1	0.96	0.37	2.46	58,58,58,58	0
60	MG	14	3219	1/1	0.97	0.20	2.45	48,48,48,48	0
60	MG	14	3238	1/1	0.95	0.20	2.37	56,56,56,56	0
60	MG	1H	3062	1/1	0.99	0.21	2.36	39,39,39,39	0
60	MG	14	3221	1/1	0.96	0.26	2.29	56,56,56,56	0
60	MG	14	3088	1/1	0.95	0.29	2.29	64,64,64,64	0
60	MG	14	3231	1/1	0.98	0.26	2.19	79,79,79,79	0
60	MG	1H	3037	1/1	0.97	0.24	2.17	53,53,53,53	0
60	MG	1H	3132	1/1	0.98	0.34	2.16	73,73,73,73	0
60	MG	1H	3044	1/1	0.97	0.21	2.16	73,73,73,73	0
60	MG	1H	3127	1/1	0.85	0.18	2.14	44,44,44,44	0
60	MG	1H	3143	1/1	0.89	0.27	2.03	50,50,50,50	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
60	MG	14	3217	1/1	0.93	0.20	1.85	71,71,71,71	0
60	MG	14	3045	1/1	0.97	0.34	1.84	45,45,45,45	0
60	MG	13	1698	1/1	0.91	0.19	1.84	86,86,86,86	0
60	MG	1G	1602	1/1	0.94	0.23	1.82	69,69,69,69	0
61	ZN	3E	301	1/1	0.97	0.39	1.76	90,90,90,90	0
60	MG	14	3273	1/1	0.83	0.21	1.76	65,65,65,65	0
60	MG	13	1700	1/1	0.88	0.16	1.75	102,102,102,102	0
60	MG	1H	3063	1/1	0.99	0.20	1.68	43,43,43,43	0
60	MG	13	1649	1/1	0.87	0.20	1.63	75,75,75,75	0
60	MG	13	1696	1/1	0.64	0.17	1.54	82,82,82,82	0
60	MG	16	203	1/1	0.80	0.24	1.52	77,77,77,77	0
60	MG	1H	3337	1/1	0.93	0.15	1.52	66,66,66,66	0
60	MG	2K	104	1/1	0.96	0.28	1.51	54,54,54,54	0
60	MG	1H	3092	1/1	0.99	0.22	1.51	44,44,44,44	0
60	MG	13	1713	1/1	0.82	0.25	1.51	96,96,96,96	0
60	MG	14	3152	1/1	0.69	0.14	1.48	96,96,96,96	0
60	MG	1H	3111	1/1	0.90	0.18	1.47	49,49,49,49	0
60	MG	14	3263	1/1	0.88	0.18	1.39	63,63,63,63	0
60	MG	1H	3176	1/1	0.94	0.21	1.39	73,73,73,73	0
60	MG	1H	3053	1/1	0.98	0.23	1.38	51,51,51,51	0
60	MG	14	3209	1/1	0.84	0.21	1.38	77,77,77,77	0
60	MG	13	1679	1/1	0.95	0.18	1.33	70,70,70,70	0
60	MG	1H	3005	1/1	0.98	0.23	1.23	47,47,47,47	0
60	MG	1H	3009	1/1	0.96	0.23	1.23	48,48,48,48	0
60	MG	14	3260	1/1	0.81	0.14	1.21	73,73,73,73	0
60	MG	1H	3282	1/1	0.93	0.17	1.19	56,56,56,56	0
60	MG	1H	3007	1/1	0.96	0.26	1.09	33,33,33,33	0
60	MG	14	3234	1/1	0.94	0.18	1.03	57,57,57,57	0
60	MG	13	1658	1/1	0.84	0.16	0.95	57,57,57,57	0
60	MG	1H	3436	1/1	0.99	0.22	0.93	63,63,63,63	0
60	MG	14	3213	1/1	0.97	0.29	0.90	69,69,69,69	0
60	MG	1H	3149	1/1	0.77	0.18	0.85	56,56,56,56	0
60	MG	14	3172	1/1	0.98	0.20	0.84	57,57,57,57	0
60	MG	1H	3086	1/1	0.86	0.18	0.84	53,53,53,53	0
60	MG	13	1662	1/1	0.89	0.17	0.71	89,89,89,89	0
60	MG	1H	3235	1/1	0.95	0.17	0.68	59,59,59,59	0
60	MG	1H	3095	1/1	0.98	0.21	0.67	49,49,49,49	0
60	MG	3I	201	1/1	0.95	0.16	0.67	59,59,59,59	0
60	MG	1H	3437	1/1	0.98	0.25	0.61	52,52,52,52	0
60	MG	13	1632	1/1	0.95	0.17	0.54	55,55,55,55	0
61	ZN	G8	201	1/1	0.74	0.30	0.50	209,209,209,209	0
60	MG	14	3026	1/1	0.94	0.17	0.49	77,77,77,77	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
60	MG	13	1678	1/1	0.78	0.24	0.45	163,163,163,163	0
60	MG	13	1681	1/1	0.79	0.19	0.33	88,88,88,88	0
60	MG	1G	1669	1/1	0.93	0.23	0.30	84,84,84,84	0
60	MG	1H	3088	1/1	0.96	0.25	0.28	66,66,66,66	0
60	MG	1H	3227	1/1	0.93	0.24	0.18	65,65,65,65	0
60	MG	13	1616	1/1	0.92	0.23	0.18	100,100,100,100	0
60	MG	45	201	1/1	0.93	0.20	0.12	81,81,81,81	0
60	MG	14	3030	1/1	0.88	0.13	0.12	71,71,71,71	0
60	MG	13	1674	1/1	0.93	0.23	0.10	184,184,184,184	0
60	MG	14	3049	1/1	0.97	0.17	0.04	53,53,53,53	0
60	MG	1H	3253	1/1	0.81	0.17	0.03	56,56,56,56	0
60	MG	1G	1671	1/1	0.88	0.18	0.01	77,77,77,77	0
60	MG	1H	3081	1/1	0.94	0.21	-0.04	34,34,34,34	0
60	MG	1H	3281	1/1	0.94	0.15	-0.14	69,69,69,69	0
60	MG	14	3169	1/1	0.93	0.18	-0.14	46,46,46,46	0
60	MG	13	1703	1/1	0.79	0.22	-0.14	111,111,111,111	0
60	MG	13	1646	1/1	0.95	0.13	-0.17	111,111,111,111	0
60	MG	14	3031	1/1	0.85	0.14	-0.22	75,75,75,75	0
60	MG	88	201	1/1	0.98	0.30	-0.23	81,81,81,81	0
60	MG	14	3044	1/1	0.97	0.19	-0.30	39,39,39,39	0
60	MG	1H	3192	1/1	0.88	0.16	-0.38	84,84,84,84	0
60	MG	1H	3361	1/1	0.94	0.16	-0.46	78,78,78,78	0
60	MG	14	3025	1/1	0.90	0.14	-0.53	81,81,81,81	0
60	MG	1H	3404	1/1	0.99	0.18	-0.53	79,79,79,79	0
60	MG	1G	1613	1/1	0.82	0.15	-0.57	116,116,116,116	0
60	MG	1G	1642	1/1	0.93	0.16	-0.57	87,87,87,87	0
60	MG	B8	201	1/1	0.95	0.19	-0.61	97,97,97,97	0
60	MG	1H	3025	1/1	0.95	0.18	-0.63	51,51,51,51	0
60	MG	1G	1629	1/1	0.93	0.15	-0.65	99,99,99,99	0
60	MG	14	3344	1/1	0.95	0.15	-0.71	54,54,54,54	0
60	MG	13	1680	1/1	0.86	0.16	-0.72	68,68,68,68	0
60	MG	16	209	1/1	0.99	0.12	-0.75	81,81,81,81	0
60	MG	1H	3271	1/1	0.95	0.15	-0.77	62,62,62,62	0
60	MG	14	3361	1/1	0.93	0.16	-0.79	60,60,60,60	0
60	MG	1G	1610	1/1	0.89	0.15	-0.81	78,78,78,78	0
61	ZN	5A	101	1/1	0.92	0.12	-0.91	129,129,129,129	0
60	MG	13	1739	1/1	0.94	0.13	-0.94	68,68,68,68	0
60	MG	1H	3390	1/1	0.77	0.14	-0.98	74,74,74,74	0
60	MG	1H	3438	1/1	0.91	0.12	-0.98	78,78,78,78	0
60	MG	1H	3379	1/1	0.89	0.18	-0.98	75,75,75,75	0
60	MG	1G	1704	1/1	0.94	0.15	-0.98	91,91,91,91	0
61	ZN	5I	102	1/1	0.99	0.14	-0.98	90,90,90,90	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
60	MG	5I	101	1/1	0.86	0.13	-1.01	83,83,83,83	0
60	MG	11	301	1/1	0.92	0.17	-1.01	42,42,42,42	0
60	MG	1H	3094	1/1	0.97	0.13	-1.02	35,35,35,35	0
60	MG	13	1677	1/1	0.79	0.12	-1.07	67,67,67,67	0
60	MG	1G	1616	1/1	0.89	0.14	-1.15	125,125,125,125	0
60	MG	14	3256	1/1	0.79	0.14	-1.17	64,64,64,64	0
60	MG	88	202	1/1	0.74	0.17	-1.19	78,78,78,78	0
60	MG	14	3313	1/1	0.94	0.17	-1.19	53,53,53,53	0
60	MG	13	1719	1/1	0.97	0.11	-1.20	74,74,74,74	0
60	MG	14	3293	1/1	0.98	0.11	-1.24	85,85,85,85	0
60	MG	19	301	1/1	0.95	0.15	-1.24	87,87,87,87	0
60	MG	1H	3156	1/1	0.89	0.15	-1.27	62,62,62,62	0
61	ZN	C5	202	1/1	0.65	0.18	-1.28	197,197,197,197	0
60	MG	14	3257	1/1	0.80	0.14	-1.36	69,69,69,69	0
60	MG	1H	3022	1/1	0.94	0.14	-1.37	51,51,51,51	0
60	MG	14	3268	1/1	0.95	0.13	-1.43	74,74,74,74	0
60	MG	13	1630	1/1	0.78	0.15	-1.46	51,51,51,51	0
60	MG	13	1740	1/1	0.93	0.12	-1.50	54,54,54,54	0
60	MG	1J	201	1/1	0.89	0.10	-1.54	105,105,105,105	0
60	MG	1G	1698	1/1	0.91	0.10	-1.56	113,113,113,113	0
60	MG	21	302	1/1	0.94	0.13	-1.57	64,64,64,64	0
60	MG	1G	1628	1/1	0.97	0.12	-1.59	78,78,78,78	0
60	MG	13	1671	1/1	0.93	0.13	-1.61	64,64,64,64	0
60	MG	45	202	1/1	0.95	0.06	-1.63	94,94,94,94	0
60	MG	1H	3266	1/1	0.98	0.15	-1.63	65,65,65,65	0
60	MG	14	3032	1/1	0.94	0.10	-1.65	103,103,103,103	0
60	MG	14	3347	1/1	0.92	0.15	-1.72	83,83,83,83	0
60	MG	1H	3355	1/1	0.91	0.11	-1.75	51,51,51,51	0
60	MG	41	201	1/1	0.84	0.10	-1.77	75,75,75,75	0
60	MG	14	3331	1/1	0.97	0.10	-1.78	51,51,51,51	0
60	MG	1H	3335	1/1	0.86	0.10	-1.88	74,74,74,74	0
60	MG	13	1691	1/1	0.93	0.13	-1.90	96,96,96,96	0
60	MG	14	3227	1/1	0.89	0.13	-1.91	69,69,69,69	0
60	MG	98	202	1/1	0.96	0.11	-1.93	69,69,69,69	0
60	MG	1H	3362	1/1	0.94	0.15	-1.93	47,47,47,47	0
60	MG	4I	201	1/1	0.85	0.07	-1.96	86,86,86,86	0
60	MG	1H	3344	1/1	0.97	0.17	-2.00	47,47,47,47	0
60	MG	1H	3406	1/1	0.95	0.11	-2.09	44,44,44,44	0
60	MG	1H	3261	1/1	0.97	0.14	-2.10	44,44,44,44	0
60	MG	49	201	1/1	0.78	0.12	-2.12	93,93,93,93	0
60	MG	39	301	1/1	0.88	0.13	-2.15	86,86,86,86	0
60	MG	1G	1691	1/1	0.97	0.11	-2.17	85,85,85,85	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
60	MG	1H	3325	1/1	0.98	0.11	-2.17	41,41,41,41	0
60	MG	1H	3331	1/1	0.93	0.09	-2.18	44,44,44,44	0
60	MG	14	3345	1/1	0.99	0.15	-2.25	69,69,69,69	0
60	MG	1H	3118	1/1	0.86	0.13	-2.25	56,56,56,56	0
60	MG	14	3015	1/1	0.91	0.11	-2.25	50,50,50,50	0
60	MG	1H	3084	1/1	0.98	0.14	-2.26	43,43,43,43	0
60	MG	14	3343	1/1	0.98	0.14	-2.36	46,46,46,46	0
60	MG	1G	1606	1/1	0.97	0.08	-2.37	85,85,85,85	0
60	MG	1J	206	1/1	0.83	0.10	-2.37	125,125,125,125	0
60	MG	1G	1620	1/1	0.95	0.14	-2.38	83,83,83,83	0
60	MG	13	1731	1/1	0.97	0.08	-2.39	63,63,63,63	0
60	MG	14	3311	1/1	0.95	0.12	-2.42	58,58,58,58	0
60	MG	14	3230	1/1	0.94	0.16	-2.47	51,51,51,51	0
60	MG	13	1639	1/1	0.96	0.12	-2.49	93,93,93,93	0
60	MG	16	207	1/1	0.80	0.09	-2.49	62,62,62,62	0
60	MG	14	3021	1/1	0.95	0.12	-2.51	68,68,68,68	0
60	MG	1H	3324	1/1	0.95	0.09	-2.52	45,45,45,45	0
60	MG	1G	1692	1/1	0.99	0.12	-2.56	67,67,67,67	0
60	MG	1H	3327	1/1	0.99	0.15	-2.60	45,45,45,45	0
60	MG	1H	3314	1/1	0.95	0.14	-2.62	38,38,38,38	0
60	MG	1H	3408	1/1	0.97	0.10	-2.68	50,50,50,50	0
60	MG	1H	3315	1/1	0.98	0.12	-2.69	59,59,59,59	0
60	MG	1H	3364	1/1	0.92	0.15	-2.70	51,51,51,51	0
60	MG	14	3287	1/1	0.99	0.15	-2.71	57,57,57,57	0
60	MG	14	3350	1/1	0.96	0.09	-2.76	65,65,65,65	0
60	MG	13	1673	1/1	0.79	0.09	-2.76	69,69,69,69	0
60	MG	1H	3377	1/1	0.89	0.12	-2.81	60,60,60,60	0
60	MG	1H	3139	1/1	0.99	0.14	-2.82	39,39,39,39	0
60	MG	13	1720	1/1	0.96	0.06	-2.85	96,96,96,96	0
60	MG	1G	1699	1/1	0.91	0.12	-2.87	108,108,108,108	0
60	MG	1H	3226	1/1	0.98	0.08	-3.04	41,41,41,41	0
60	MG	13	1721	1/1	0.98	0.10	-3.07	80,80,80,80	0
60	MG	1H	3347	1/1	0.99	0.10	-3.17	70,70,70,70	0
60	MG	1G	1679	1/1	0.95	0.11	-3.18	71,71,71,71	0
60	MG	1H	3369	1/1	0.96	0.16	-3.20	46,46,46,46	0
60	MG	1H	3380	1/1	0.98	0.13	-3.24	53,53,53,53	0
60	MG	1H	3308	1/1	0.97	0.11	-3.37	39,39,39,39	0
60	MG	14	3316	1/1	0.99	0.12	-3.43	58,58,58,58	0
60	MG	14	3335	1/1	0.96	0.15	-3.46	60,60,60,60	0
60	MG	1H	3257	1/1	0.96	0.08	-3.48	52,52,52,52	0
60	MG	13	1611	1/1	0.98	0.08	-3.52	84,84,84,84	0
60	MG	1H	3225	1/1	0.97	0.16	-3.53	38,38,38,38	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
60	MG	14	3325	1/1	0.81	0.10	-3.59	50,50,50,50	0
60	MG	1H	3392	1/1	0.94	0.14	-3.66	53,53,53,53	0
60	MG	13	1718	1/1	0.97	0.13	-3.67	54,54,54,54	0
60	MG	13	1730	1/1	0.93	0.08	-3.72	103,103,103,103	0
60	MG	14	3385	1/1	0.97	0.07	-3.76	44,44,44,44	0
60	MG	13	1717	1/1	0.95	0.10	-3.76	63,63,63,63	0
60	MG	14	3377	1/1	0.93	0.09	-3.79	71,71,71,71	0
60	MG	13	1643	1/1	0.93	0.06	-3.81	75,75,75,75	0
60	MG	1H	3329	1/1	0.90	0.08	-3.82	51,51,51,51	0
60	MG	14	3368	1/1	0.95	0.07	-3.88	83,83,83,83	0
60	MG	1H	3321	1/1	0.97	0.12	-3.89	57,57,57,57	0
60	MG	14	3339	1/1	0.92	0.13	-3.92	62,62,62,62	0
60	MG	14	3342	1/1	0.98	0.11	-3.98	48,48,48,48	0
60	MG	14	3340	1/1	0.97	0.10	-4.00	50,50,50,50	0
60	MG	1G	1695	1/1	0.89	0.10	-4.01	83,83,83,83	0
60	MG	1G	1626	1/1	0.90	0.10	-4.07	87,87,87,87	0
60	MG	1H	3312	1/1	0.90	0.12	-4.13	45,45,45,45	0
60	MG	1H	3435	1/1	0.98	0.09	-4.23	36,36,36,36	0
60	MG	14	3362	1/1	0.94	0.08	-4.27	74,74,74,74	0
60	MG	14	3320	1/1	0.95	0.10	-4.31	52,52,52,52	0
60	MG	14	3332	1/1	0.92	0.14	-4.39	71,71,71,71	0
60	MG	14	3321	1/1	0.96	0.10	-4.39	78,78,78,78	0
60	MG	13	1685	1/1	0.98	0.06	-4.47	80,80,80,80	0
60	MG	1H	3341	1/1	0.99	0.06	-4.59	77,77,77,77	0
60	MG	1G	1693	1/1	0.97	0.09	-4.71	76,76,76,76	0
60	MG	1H	3230	1/1	0.94	0.11	-4.72	39,39,39,39	0
60	MG	14	3280	1/1	0.80	0.13	-4.72	55,55,55,55	0
60	MG	1H	3264	1/1	0.93	0.13	-4.76	66,66,66,66	0
60	MG	13	1727	1/1	0.93	0.07	-4.79	86,86,86,86	0
60	MG	14	3103	1/1	0.98	0.13	-4.82	55,55,55,55	0
60	MG	1H	3396	1/1	0.94	0.10	-4.84	56,56,56,56	0
60	MG	1H	3363	1/1	0.96	0.11	-4.88	52,52,52,52	0
60	MG	14	3326	1/1	0.95	0.11	-4.97	54,54,54,54	0
60	MG	14	3329	1/1	0.92	0.12	-5.07	65,65,65,65	0
60	MG	13	1738	1/1	0.86	0.08	-5.19	81,81,81,81	0
60	MG	1H	3422	1/1	0.97	0.04	-5.23	87,87,87,87	0
60	MG	14	3349	1/1	0.97	0.07	-5.26	61,61,61,61	0
60	MG	1H	3353	1/1	0.96	0.12	-5.38	51,51,51,51	0
60	MG	14	3324	1/1	0.94	0.08	-5.41	63,63,63,63	0
60	MG	1H	3416	1/1	0.96	0.07	-5.41	55,55,55,55	0
60	MG	1H	3342	1/1	0.94	0.10	-5.47	59,59,59,59	0
60	MG	1H	3370	1/1	0.97	0.12	-5.49	45,45,45,45	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
60	MG	1H	3318	1/1	0.93	0.08	-5.51	45,45,45,45	0
60	MG	1H	3309	1/1	0.89	0.10	-5.51	56,56,56,56	0
60	MG	1H	3343	1/1	0.99	0.11	-5.52	44,44,44,44	0
60	MG	14	3019	1/1	0.97	0.07	-5.57	44,44,44,44	0
60	MG	1H	3332	1/1	0.88	0.10	-5.62	49,49,49,49	0
60	MG	1H	3368	1/1	0.99	0.08	-5.66	46,46,46,46	0
60	MG	1H	3372	1/1	0.97	0.10	-5.81	61,61,61,61	0
60	MG	14	3357	1/1	0.86	0.06	-5.86	96,96,96,96	0
60	MG	14	3355	1/1	0.90	0.08	-5.90	68,68,68,68	0
60	MG	1H	3311	1/1	0.95	0.11	-6.06	42,42,42,42	0
60	MG	14	3356	1/1	0.77	0.08	-6.20	66,66,66,66	0
60	MG	1G	1621	1/1	0.93	0.09	-6.20	68,68,68,68	0
60	MG	1H	3397	1/1	0.99	0.10	-6.30	50,50,50,50	0
60	MG	1H	3429	1/1	0.95	0.11	-6.36	61,61,61,61	0
60	MG	1H	3065	1/1	0.96	0.11	-6.49	39,39,39,39	0
60	MG	1H	3394	1/1	0.99	0.10	-6.54	43,43,43,43	0
60	MG	1H	3399	1/1	0.96	0.11	-6.67	60,60,60,60	0
60	MG	14	3315	1/1	0.98	0.10	-6.71	52,52,52,52	0
60	MG	14	3314	1/1	0.96	0.12	-6.71	63,63,63,63	0
60	MG	1H	3405	1/1	0.92	0.06	-6.94	73,73,73,73	0
60	MG	1H	3367	1/1	0.95	0.06	-7.24	56,56,56,56	0
60	MG	1H	3381	1/1	0.96	0.12	-7.25	41,41,41,41	0
60	MG	1H	3401	1/1	0.94	0.11	-7.61	61,61,61,61	0
60	MG	14	3360	1/1	0.94	0.10	-7.97	103,103,103,103	0
60	MG	1H	3105	1/1	0.94	0.09	-8.36	59,59,59,59	0
60	MG	1H	3349	1/1	0.91	0.09	-8.64	58,58,58,58	0
60	MG	14	3337	1/1	0.97	0.08	-8.85	59,59,59,59	0
60	MG	14	3318	1/1	0.86	0.11	-9.69	76,76,76,76	0
60	MG	13	1724	1/1	0.94	0.05	-10.78	82,82,82,82	0
60	MG	14	3373	1/1	0.98	0.10	-11.72	65,65,65,65	0
60	MG	14	3367	1/1	0.94	0.08	-11.74	90,90,90,90	0
60	MG	13	1723	1/1	0.96	0.06	-12.28	85,85,85,85	0
60	MG	1H	3354	1/1	0.99	0.07	-14.01	39,39,39,39	0
60	MG	1H	3319	1/1	0.98	0.11	-15.25	46,46,46,46	0
60	MG	14	3382	1/1	0.95	0.11	-16.16	100,100,100,100	0
60	MG	14	3376	1/1	0.96	0.04	-	91,91,91,91	0
60	MG	1H	3154	1/1	0.77	0.30	-	89,89,89,89	0
60	MG	1H	3102	1/1	0.94	0.32	-	61,61,61,61	0
60	MG	14	3300	1/1	0.90	0.44	-	76,76,76,76	0
60	MG	14	3363	1/1	0.81	0.07	-	73,73,73,73	0
60	MG	14	3144	1/1	0.76	0.45	-	80,80,80,80	0
60	MG	14	3307	1/1	0.84	0.43	-	82,82,82,82	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
60	MG	13	1683	1/1	0.86	0.32	-	89,89,89,89	0
60	MG	1H	3409	1/1	0.84	0.17	-	99,99,99,99	0
60	MG	1H	3350	1/1	0.93	0.14	-	47,47,47,47	0
60	MG	1H	3004	1/1	0.97	0.35	-	45,45,45,45	0
60	MG	14	3166	1/1	0.92	0.38	-	73,73,73,73	0
60	MG	1H	3357	1/1	0.92	0.10	-	69,69,69,69	0
60	MG	E5	101	1/1	0.58	0.20	-	80,80,80,80	0
60	MG	1H	3190	1/1	0.95	0.42	-	61,61,61,61	0
60	MG	13	1709	1/1	0.49	0.23	-	81,81,81,81	0
60	MG	1G	1694	1/1	0.92	0.09	-	110,110,110,110	0
60	MG	14	3336	1/1	0.94	0.06	-	80,80,80,80	0
60	MG	1H	3241	1/1	0.89	0.31	-	61,61,61,61	0
60	MG	78	203	1/1	0.83	0.39	-	87,87,87,87	0
60	MG	1G	1681	1/1	0.81	0.73	-	107,107,107,107	0
60	MG	1G	1630	1/1	0.93	0.26	-	80,80,80,80	0
60	MG	1H	3293	1/1	0.64	0.39	-	80,80,80,80	0
60	MG	1H	3304	1/1	0.89	0.18	-	69,69,69,69	0
60	MG	13	1689	1/1	0.74	0.14	-	83,83,83,83	0
60	MG	14	3013	1/1	0.96	0.33	-	61,61,61,61	0
60	MG	1H	3236	1/1	0.95	0.19	-	55,55,55,55	0
60	MG	14	3309	1/1	0.80	0.34	-	72,72,72,72	0
60	MG	13	1619	1/1	0.92	0.30	-	70,70,70,70	0
60	MG	14	3080	1/1	0.97	0.27	-	78,78,78,78	0
60	MG	1H	3402	1/1	0.96	0.11	-	109,109,109,109	0
60	MG	14	3071	1/1	0.98	0.48	-	68,68,68,68	0
60	MG	1H	3064	1/1	0.96	0.20	-	51,51,51,51	0
60	MG	1G	1619	1/1	0.91	0.25	-	82,82,82,82	0
60	MG	1H	3136	1/1	0.61	0.26	-	72,72,72,72	0
60	MG	1H	3032	1/1	0.98	0.38	-	41,41,41,41	0
60	MG	1H	3348	1/1	0.94	0.07	-	82,82,82,82	0
60	MG	1H	3204	1/1	0.80	0.30	-	62,62,62,62	0
60	MG	1G	1685	1/1	0.89	0.27	-	136,136,136,136	0
60	MG	13	1705	1/1	0.72	0.20	-	83,83,83,83	0
60	MG	14	3101	1/1	0.89	0.52	-	65,65,65,65	0
60	MG	14	3312	1/1	0.94	0.16	-	57,57,57,57	0
60	MG	14	3029	1/1	0.95	0.20	-	75,75,75,75	0
60	MG	1H	3254	1/1	0.81	0.41	-	57,57,57,57	0
60	MG	1H	3300	1/1	0.95	0.28	-	52,52,52,52	0
60	MG	1H	3431	1/1	0.95	0.07	-	73,73,73,73	0
60	MG	1H	3276	1/1	0.82	0.57	-	76,76,76,76	0
60	MG	14	3039	1/1	0.58	0.23	-	75,75,75,75	0
60	MG	1H	3112	1/1	0.95	0.14	-	62,62,62,62	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
60	MG	13	1704	1/1	0.92	0.20	-	71,71,71,71	0
60	MG	1H	3289	1/1	0.96	0.48	-	71,71,71,71	0
60	MG	1G	1634	1/1	0.95	0.19	-	112,112,112,112	0
60	MG	14	3359	1/1	0.97	0.11	-	69,69,69,69	0
60	MG	1H	3424	1/1	0.83	0.08	-	115,115,115,115	0
60	MG	1H	3046	1/1	0.97	0.17	-	90,90,90,90	0
60	MG	1H	3365	1/1	0.82	0.12	-	88,88,88,88	0
60	MG	14	3274	1/1	0.84	0.33	-	79,79,79,79	0
60	MG	1H	3307	1/1	0.93	0.33	-	74,74,74,74	0
60	MG	1H	3427	1/1	0.77	0.11	-	92,92,92,92	0
60	MG	1G	1660	1/1	0.89	0.36	-	78,78,78,78	0
60	MG	13	1736	1/1	0.54	0.08	-	141,141,141,141	0
60	MG	1H	3378	1/1	0.86	0.13	-	67,67,67,67	0
60	MG	14	3366	1/1	0.92	0.06	-	102,102,102,102	0
60	MG	1G	1624	1/1	0.98	0.38	-	70,70,70,70	0
60	MG	1H	3232	1/1	0.94	0.20	-	71,71,71,71	0
60	MG	1G	1677	1/1	0.97	0.22	-	88,88,88,88	0
60	MG	14	3236	1/1	0.97	0.30	-	66,66,66,66	0
60	MG	14	3009	1/1	0.98	0.23	-	50,50,50,50	0
60	MG	1H	3302	1/1	0.82	0.27	-	67,67,67,67	0
60	MG	1H	3305	1/1	0.91	0.31	-	99,99,99,99	0
60	MG	1H	3278	1/1	0.84	0.30	-	64,64,64,64	0
60	MG	13	1601	1/1	0.97	0.26	-	66,66,66,66	0
60	MG	13	1676	1/1	0.92	0.23	-	63,63,63,63	0
60	MG	1G	1703	1/1	0.43	0.12	-	128,128,128,128	0
60	MG	1H	3205	1/1	0.86	0.37	-	60,60,60,60	0
60	MG	1H	3162	1/1	0.81	0.14	-	67,67,67,67	0
60	MG	14	3087	1/1	0.95	0.30	-	78,78,78,78	0
60	MG	1H	3194	1/1	0.72	0.31	-	71,71,71,71	0
60	MG	1G	1639	1/1	0.75	0.34	-	82,82,82,82	0
60	MG	14	3283	1/1	0.89	0.60	-	79,79,79,79	0
60	MG	14	3148	1/1	0.81	0.32	-	86,86,86,86	0
60	MG	1H	3072	1/1	0.91	0.45	-	70,70,70,70	0
60	MG	14	3024	1/1	0.98	0.33	-	81,81,81,81	0
60	MG	1H	3269	1/1	0.98	0.34	-	58,58,58,58	0
60	MG	1H	3426	1/1	0.87	0.08	-	112,112,112,112	0
60	MG	1H	3326	1/1	0.91	0.16	-	57,57,57,57	0
60	MG	14	3218	1/1	0.94	0.27	-	67,67,67,67	0
60	MG	13	1607	1/1	0.98	0.09	-	75,75,75,75	0
60	MG	14	3250	1/1	0.90	0.33	-	65,65,65,65	0
60	MG	14	3171	1/1	0.92	0.38	-	78,78,78,78	0
60	MG	98	201	1/1	0.98	0.26	-	62,62,62,62	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
60	MG	13	1722	1/1	0.89	0.18	-	82,82,82,82	0
60	MG	14	3164	1/1	0.90	0.44	-	75,75,75,75	0
60	MG	1H	3129	1/1	0.89	0.61	-	72,72,72,72	0
60	MG	1G	1680	1/1	0.83	0.37	-	162,162,162,162	0
60	MG	1H	3277	1/1	0.95	0.20	-	59,59,59,59	0
60	MG	1H	3077	1/1	0.89	0.39	-	70,70,70,70	0
60	MG	14	3059	1/1	0.86	0.38	-	72,72,72,72	0
60	MG	1H	3043	1/1	0.97	0.22	-	70,70,70,70	0
60	MG	1K	101	1/1	0.97	0.04	-	93,93,93,93	0
60	MG	1H	3218	1/1	0.84	0.39	-	84,84,84,84	0
60	MG	1H	3210	1/1	0.97	0.29	-	72,72,72,72	0
60	MG	1H	3090	1/1	0.85	0.30	-	67,67,67,67	0
60	MG	1H	3200	1/1	0.98	0.44	-	69,69,69,69	0
60	MG	1H	3356	1/1	0.90	0.16	-	54,54,54,54	0
60	MG	1H	3070	1/1	0.96	0.47	-	45,45,45,45	0
60	MG	1G	1687	1/1	0.85	0.15	-	83,83,83,83	0
60	MG	1H	3283	1/1	0.95	0.30	-	64,64,64,64	0
60	MG	14	3055	1/1	0.99	0.40	-	60,60,60,60	0
60	MG	1H	3049	1/1	0.93	0.29	-	66,66,66,66	0
60	MG	14	3187	1/1	0.83	0.58	-	84,84,84,84	0
60	MG	16	212	1/1	0.94	0.10	-	71,71,71,71	0
60	MG	1G	1658	1/1	0.91	0.33	-	71,71,71,71	0
60	MG	1G	1627	1/1	0.80	0.31	-	66,66,66,66	0
60	MG	1H	3216	1/1	0.86	0.24	-	73,73,73,73	0
60	MG	14	3073	1/1	0.99	0.43	-	40,40,40,40	0
60	MG	1H	3038	1/1	0.94	0.61	-	59,59,59,59	0
60	MG	1H	3240	1/1	0.91	0.28	-	109,109,109,109	0
60	MG	14	3063	1/1	0.90	0.51	-	70,70,70,70	0
60	MG	14	3338	1/1	0.91	0.16	-	52,52,52,52	0
60	MG	1H	3393	1/1	0.97	0.08	-	68,68,68,68	0
60	MG	1H	3414	1/1	0.96	0.06	-	75,75,75,75	0
60	MG	1H	3359	1/1	0.94	0.09	-	83,83,83,83	0
60	MG	14	3244	1/1	0.84	0.29	-	75,75,75,75	0
60	MG	1H	3267	1/1	0.65	0.26	-	83,83,83,83	0
60	MG	14	3253	1/1	0.59	0.58	-	71,71,71,71	0
60	MG	1H	3415	1/1	0.88	0.10	-	75,75,75,75	0
60	MG	1H	3040	1/1	0.96	0.12	-	58,58,58,58	0
60	MG	13	1635	1/1	0.95	0.34	-	63,63,63,63	0
60	MG	1H	3163	1/1	0.95	0.48	-	64,64,64,64	0
60	MG	14	3351	1/1	0.93	0.14	-	93,93,93,93	0
60	MG	13	1609	1/1	0.85	0.41	-	64,64,64,64	0
60	MG	14	3372	1/1	0.93	0.05	-	79,79,79,79	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
60	MG	14	3155	1/1	0.98	0.12	-	63,63,63,63	0
60	MG	13	1641	1/1	0.75	0.24	-	74,74,74,74	0
60	MG	13	1625	1/1	0.94	0.49	-	75,75,75,75	0
60	MG	13	1633	1/1	0.98	0.21	-	46,46,46,46	0
60	MG	1H	3179	1/1	0.94	0.33	-	57,57,57,57	0
60	MG	14	3264	1/1	0.87	0.39	-	91,91,91,91	0
60	MG	14	3183	1/1	0.97	0.24	-	84,84,84,84	0
60	MG	13	1708	1/1	0.86	0.36	-	167,167,167,167	0
60	MG	14	3141	1/1	0.74	0.30	-	85,85,85,85	0
60	MG	14	3210	1/1	0.86	0.44	-	79,79,79,79	0
60	MG	13	1734	1/1	0.96	0.10	-	108,108,108,108	0
60	MG	14	3211	1/1	0.77	0.47	-	108,108,108,108	0
60	MG	14	3303	1/1	0.87	0.59	-	93,93,93,93	0
60	MG	1G	1645	1/1	0.83	0.17	-	78,78,78,78	0
60	MG	1H	3336	1/1	0.97	0.11	-	88,88,88,88	0
60	MG	1H	3243	1/1	0.95	0.22	-	60,60,60,60	0
60	MG	1H	3093	1/1	0.81	0.20	-	64,64,64,64	0
60	MG	14	3008	1/1	0.98	0.45	-	53,53,53,53	0
60	MG	14	3165	1/1	0.82	0.24	-	84,84,84,84	0
60	MG	13	1622	1/1	0.95	0.48	-	86,86,86,86	0
60	MG	14	3259	1/1	0.86	0.20	-	76,76,76,76	0
60	MG	13	1603	1/1	0.93	0.25	-	57,57,57,57	0
60	MG	1H	3151	1/1	0.94	0.43	-	77,77,77,77	0
60	MG	1H	3383	1/1	0.98	0.13	-	64,64,64,64	0
60	MG	1H	3385	1/1	0.97	0.10	-	66,66,66,66	0
60	MG	14	3051	1/1	0.98	0.26	-	61,61,61,61	0
60	MG	1H	3376	1/1	0.97	0.10	-	43,43,43,43	0
60	MG	1H	3417	1/1	0.95	0.08	-	98,98,98,98	0
60	MG	13	1654	1/1	0.91	0.30	-	69,69,69,69	0
60	MG	P8	101	1/1	0.81	0.55	-	70,70,70,70	0
60	MG	14	3358	1/1	0.73	0.27	-	86,86,86,86	0
60	MG	1H	3137	1/1	0.92	0.26	-	72,72,72,72	0
60	MG	1H	3073	1/1	0.98	0.35	-	53,53,53,53	0
60	MG	13	1693	1/1	0.86	0.17	-	89,89,89,89	0
60	MG	14	3174	1/1	0.89	0.45	-	77,77,77,77	0
60	MG	14	3330	1/1	0.94	0.13	-	58,58,58,58	0
60	MG	1H	3109	1/1	0.96	0.31	-	50,50,50,50	0
60	MG	14	3379	1/1	0.89	0.09	-	104,104,104,104	0
60	MG	1H	3172	1/1	0.80	0.18	-	71,71,71,71	0
60	MG	1H	3209	1/1	0.85	0.44	-	81,81,81,81	0
60	MG	14	3380	1/1	0.87	0.09	-	92,92,92,92	0
60	MG	14	3180	1/1	0.88	0.30	-	85,85,85,85	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
60	MG	13	1712	1/1	0.98	0.13	-	112,112,112,112	0
60	MG	1H	3250	1/1	0.86	0.41	-	68,68,68,68	0
60	MG	1H	3185	1/1	0.82	0.30	-	65,65,65,65	0
60	MG	14	3005	1/1	0.95	0.34	-	46,46,46,46	0
60	MG	14	3091	1/1	0.74	0.39	-	67,67,67,67	0
60	MG	13	1653	1/1	0.51	0.32	-	83,83,83,83	0
60	MG	1H	3145	1/1	0.85	0.33	-	63,63,63,63	0
60	MG	16	202	1/1	0.89	0.51	-	82,82,82,82	0
60	MG	16	206	1/1	0.95	0.32	-	70,70,70,70	0
60	MG	14	3348	1/1	0.93	0.10	-	83,83,83,83	0
60	MG	14	3222	1/1	0.97	0.30	-	43,43,43,43	0
60	MG	1H	3133	1/1	0.94	0.52	-	83,83,83,83	0
60	MG	1G	1617	1/1	0.89	0.08	-	83,83,83,83	0
60	MG	1H	3352	1/1	0.95	0.09	-	46,46,46,46	0
60	MG	1H	3252	1/1	0.81	0.43	-	66,66,66,66	0
60	MG	1G	1659	1/1	0.54	0.26	-	118,118,118,118	0
60	MG	13	1656	1/1	0.64	0.32	-	84,84,84,84	0
60	MG	1H	3101	1/1	0.93	0.45	-	77,77,77,77	0
60	MG	14	3189	1/1	0.78	0.73	-	73,73,73,73	0
60	MG	1H	3303	1/1	0.94	0.66	-	90,90,90,90	0
60	MG	13	1728	1/1	0.76	0.08	-	88,88,88,88	0
60	MG	14	3037	1/1	0.84	0.42	-	79,79,79,79	0
60	MG	1H	3126	1/1	0.94	0.12	-	79,79,79,79	0
60	MG	14	3160	1/1	0.96	0.34	-	56,56,56,56	0
60	MG	13	1690	1/1	0.77	0.32	-	86,86,86,86	0
60	MG	1H	3421	1/1	0.74	0.14	-	138,138,138,138	0
60	MG	14	3128	1/1	0.67	0.31	-	86,86,86,86	0
60	MG	1G	1661	1/1	0.87	0.32	-	69,69,69,69	0
60	MG	13	1624	1/1	0.97	0.41	-	77,77,77,77	0
60	MG	1H	3419	1/1	0.90	0.09	-	99,99,99,99	0
60	MG	14	3191	1/1	0.92	0.33	-	69,69,69,69	0
60	MG	25	201	1/1	0.81	0.04	-	125,125,125,125	0
60	MG	14	3093	1/1	0.73	0.46	-	70,70,70,70	0
60	MG	78	201	1/1	0.92	0.21	-	66,66,66,66	0
60	MG	1H	3388	1/1	0.98	0.10	-	57,57,57,57	0
60	MG	1H	3288	1/1	0.78	0.44	-	92,92,92,92	0
60	MG	1H	3333	1/1	0.97	0.10	-	55,55,55,55	0
60	MG	1H	3374	1/1	0.90	0.11	-	86,86,86,86	0
60	MG	13	1699	1/1	0.47	0.25	-	89,89,89,89	0
60	MG	1H	3384	1/1	0.94	0.08	-	85,85,85,85	0
60	MG	14	3215	1/1	0.82	0.48	-	69,69,69,69	0
60	MG	13	1602	1/1	0.99	0.21	-	65,65,65,65	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
60	MG	14	3168	1/1	0.96	0.49	-	77,77,77,77	0
60	MG	1H	3340	1/1	0.98	0.14	-	65,65,65,65	0
60	MG	1H	3279	1/1	0.80	0.38	-	71,71,71,71	0
60	MG	1G	1668	1/1	0.83	0.49	-	95,95,95,95	0
60	MG	1H	3338	1/1	0.90	0.06	-	83,83,83,83	0
60	MG	13	1629	1/1	0.89	0.34	-	62,62,62,62	0
60	MG	13	1634	1/1	0.91	0.39	-	67,67,67,67	0
60	MG	14	3072	1/1	0.96	0.34	-	66,66,66,66	0
60	MG	1H	3231	1/1	0.89	0.30	-	91,91,91,91	0
60	MG	1H	3003	1/1	0.91	0.33	-	45,45,45,45	0
60	MG	13	1682	1/1	0.85	0.33	-	85,85,85,85	0
60	MG	1H	3217	1/1	0.95	0.39	-	75,75,75,75	0
60	MG	1H	3222	1/1	0.69	0.44	-	77,77,77,77	0
60	MG	14	3167	1/1	0.71	0.22	-	93,93,93,93	0
60	MG	14	3266	1/1	0.95	0.46	-	81,81,81,81	0
60	MG	1H	3113	1/1	0.91	0.35	-	53,53,53,53	0
60	MG	1H	3296	1/1	0.83	0.17	-	69,69,69,69	0
60	MG	1G	1676	1/1	0.82	0.30	-	90,90,90,90	0
60	MG	14	3200	1/1	0.86	0.80	-	91,91,91,91	0
60	MG	14	3085	1/1	0.90	0.23	-	52,52,52,52	0
60	MG	1G	1663	1/1	0.84	0.14	-	93,93,93,93	0
60	MG	1H	3195	1/1	0.93	0.52	-	75,75,75,75	0
60	MG	14	3135	1/1	0.80	0.36	-	78,78,78,78	0
60	MG	1H	3262	1/1	0.83	0.39	-	80,80,80,80	0
60	MG	14	3184	1/1	0.84	0.57	-	75,75,75,75	0
60	MG	1G	1641	1/1	0.59	0.14	-	130,130,130,130	0
60	MG	1H	3211	1/1	0.93	0.26	-	84,84,84,84	0
60	MG	14	3084	1/1	0.96	0.27	-	60,60,60,60	0
60	MG	13	1638	1/1	0.88	0.35	-	80,80,80,80	0
60	MG	1J	203	1/1	0.78	0.26	-	91,91,91,91	0
60	MG	11	302	1/1	0.87	0.21	-	54,54,54,54	0
60	MG	14	3375	1/1	0.86	0.04	-	90,90,90,90	0
60	MG	1H	3104	1/1	0.97	0.40	-	63,63,63,63	0
60	MG	1G	1654	1/1	0.91	0.27	-	66,66,66,66	0
60	MG	1G	1651	1/1	0.85	0.43	-	87,87,87,87	0
60	MG	13	1675	1/1	0.90	0.29	-	67,67,67,67	0
60	MG	1H	3119	1/1	0.97	0.46	-	67,67,67,67	0
60	MG	13	1714	1/1	0.88	0.22	-	89,89,89,89	0
60	MG	1H	3418	1/1	0.91	0.08	-	81,81,81,81	0
60	MG	14	3327	1/1	0.94	0.15	-	58,58,58,58	0
60	MG	14	3370	1/1	0.89	0.07	-	116,116,116,116	0
60	MG	1H	3238	1/1	0.97	0.35	-	50,50,50,50	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
60	MG	1H	3423	1/1	0.91	0.08	-	60,60,60,60	0
60	MG	13	1702	1/1	0.83	0.21	-	80,80,80,80	0
60	MG	1H	3295	1/1	0.50	0.32	-	87,87,87,87	0
60	MG	1G	1683	1/1	0.91	0.25	-	109,109,109,109	0
60	MG	1H	3248	1/1	0.89	0.25	-	97,97,97,97	0
60	MG	14	3014	1/1	0.95	0.31	-	79,79,79,79	0
60	MG	1H	3019	1/1	0.97	0.23	-	33,33,33,33	0
60	MG	1H	3100	1/1	0.91	0.58	-	74,74,74,74	0
60	MG	14	3003	1/1	0.94	0.34	-	45,45,45,45	0
60	MG	1H	3159	1/1	0.82	0.35	-	77,77,77,77	0
60	MG	14	3251	1/1	0.98	0.31	-	69,69,69,69	0
60	MG	1H	3258	1/1	0.92	0.43	-	64,64,64,64	0
60	MG	14	3104	1/1	0.81	0.33	-	70,70,70,70	0
60	MG	1H	3103	1/1	0.54	0.36	-	88,88,88,88	0
60	MG	K8	101	1/1	0.96	0.34	-	69,69,69,69	0
60	MG	13	1729	1/1	0.96	0.04	-	76,76,76,76	0
60	MG	1G	1603	1/1	0.96	0.11	-	79,79,79,79	0
60	MG	1H	3186	1/1	0.79	0.32	-	79,79,79,79	0
60	MG	1H	3360	1/1	0.92	0.14	-	99,99,99,99	0
60	MG	14	3188	1/1	0.83	0.22	-	93,93,93,93	0
60	MG	14	3304	1/1	0.91	0.44	-	66,66,66,66	0
60	MG	1H	3150	1/1	0.88	0.29	-	63,63,63,63	0
60	MG	1H	3290	1/1	0.94	0.15	-	76,76,76,76	0
60	MG	1G	1648	1/1	0.89	0.29	-	78,78,78,78	0
60	MG	14	3076	1/1	0.96	0.34	-	44,44,44,44	0
60	MG	14	3323	1/1	0.98	0.09	-	57,57,57,57	0
60	MG	1H	3011	1/1	0.99	0.20	-	37,37,37,37	0
60	MG	1H	3214	1/1	0.85	0.26	-	62,62,62,62	0
60	MG	14	3109	1/1	0.90	0.51	-	82,82,82,82	0
60	MG	14	3150	1/1	0.85	0.23	-	92,92,92,92	0
60	MG	1J	204	1/1	0.93	0.33	-	92,92,92,92	0
60	MG	1G	1653	1/1	0.74	0.25	-	73,73,73,73	0
60	MG	1H	3301	1/1	0.95	0.29	-	70,70,70,70	0
60	MG	1H	3196	1/1	0.81	0.70	-	91,91,91,91	0
60	MG	14	3220	1/1	0.94	0.12	-	44,44,44,44	0
60	MG	1H	3346	1/1	0.98	0.05	-	67,67,67,67	0
60	MG	14	3048	1/1	0.88	0.27	-	59,59,59,59	0
60	MG	14	3297	1/1	0.84	0.41	-	100,100,100,100	0
60	MG	1H	3171	1/1	0.92	0.49	-	69,69,69,69	0
60	MG	13	1640	1/1	0.88	0.32	-	76,76,76,76	0
60	MG	1H	3387	1/1	0.95	0.11	-	53,53,53,53	0
60	MG	1G	1664	1/1	0.94	0.20	-	74,74,74,74	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
60	MG	14	3114	1/1	0.92	0.68	-	91,91,91,91	0
60	MG	C8	201	1/1	0.96	0.23	-	89,89,89,89	0
60	MG	14	3075	1/1	0.94	0.40	-	49,49,49,49	0
60	MG	45	203	1/1	0.88	0.17	-	66,66,66,66	0
60	MG	1H	3310	1/1	0.94	0.15	-	50,50,50,50	0
60	MG	1G	1607	1/1	0.97	0.20	-	98,98,98,98	0
60	MG	1G	1615	1/1	0.94	0.30	-	87,87,87,87	0
60	MG	1H	3373	1/1	0.98	0.09	-	70,70,70,70	0
60	MG	13	1687	1/1	0.97	0.12	-	73,73,73,73	0
60	MG	1G	1633	1/1	0.87	0.41	-	95,95,95,95	0
60	MG	1H	3108	1/1	0.64	0.49	-	77,77,77,77	0
60	MG	14	3271	1/1	0.99	0.15	-	67,67,67,67	0
60	MG	1G	1604	1/1	0.91	0.17	-	78,78,78,78	0
60	MG	1G	1605	1/1	0.94	0.21	-	81,81,81,81	0
60	MG	14	3106	1/1	0.90	0.47	-	62,62,62,62	0
60	MG	1G	1689	1/1	0.83	0.38	-	86,86,86,86	0
60	MG	1H	3018	1/1	0.97	0.28	-	53,53,53,53	0
60	MG	1H	3140	1/1	0.87	0.28	-	59,59,59,59	0
60	MG	14	3277	1/1	0.76	0.14	-	81,81,81,81	0
60	MG	52	201	1/1	0.89	0.12	-	77,77,77,77	0
60	MG	14	3158	1/1	0.90	0.19	-	54,54,54,54	0
60	MG	1G	1636	1/1	0.98	0.24	-	89,89,89,89	0
60	MG	14	3269	1/1	0.83	0.23	-	60,60,60,60	0
60	MG	2K	101	1/1	0.86	0.15	-	81,81,81,81	0
60	MG	14	3053	1/1	0.92	0.61	-	66,66,66,66	0
60	MG	1G	1701	1/1	0.76	0.08	-	106,106,106,106	0
60	MG	1H	3183	1/1	0.96	0.30	-	61,61,61,61	0
60	MG	14	3275	1/1	0.89	0.53	-	76,76,76,76	0
60	MG	14	3067	1/1	0.96	0.51	-	48,48,48,48	0
60	MG	14	3132	1/1	0.94	0.37	-	84,84,84,84	0
60	MG	1G	1637	1/1	0.97	0.22	-	67,67,67,67	0
60	MG	14	3081	1/1	0.78	0.40	-	86,86,86,86	0
60	MG	14	3122	1/1	0.95	0.39	-	66,66,66,66	0
60	MG	14	3131	1/1	0.95	0.39	-	39,39,39,39	0
60	MG	14	3296	1/1	0.98	0.23	-	135,135,135,135	0
60	MG	14	3204	1/1	0.92	0.29	-	105,105,105,105	0
60	MG	1H	3339	1/1	0.89	0.15	-	75,75,75,75	0
60	MG	14	3105	1/1	0.82	0.23	-	82,82,82,82	0
60	MG	1H	3158	1/1	0.96	0.49	-	65,65,65,65	0
60	MG	1H	3079	1/1	0.97	0.37	-	39,39,39,39	0
60	MG	13	1707	1/1	0.85	0.46	-	114,114,114,114	0
60	MG	1H	3161	1/1	0.97	0.23	-	50,50,50,50	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
60	MG	14	3124	1/1	0.92	0.32	-	82,82,82,82	0
60	MG	1H	3116	1/1	0.63	0.20	-	69,69,69,69	0
60	MG	1H	3323	1/1	0.97	0.10	-	58,58,58,58	0
60	MG	2L	102	1/1	0.38	0.36	-	95,95,95,95	0
60	MG	1H	3028	1/1	0.88	0.32	-	51,51,51,51	0
60	MG	14	3267	1/1	0.98	0.26	-	71,71,71,71	0
60	MG	13	1670	1/1	0.97	0.07	-	66,66,66,66	0
60	MG	14	3060	1/1	0.96	0.29	-	63,63,63,63	0
60	MG	14	3352	1/1	0.98	0.12	-	77,77,77,77	0
60	MG	1H	3074	1/1	0.95	0.40	-	57,57,57,57	0
60	MG	14	3282	1/1	0.89	0.17	-	73,73,73,73	0
60	MG	13	1725	1/1	0.96	0.05	-	96,96,96,96	0
60	MG	14	3116	1/1	0.97	0.40	-	53,53,53,53	0
60	MG	1J	205	1/1	0.94	0.10	-	119,119,119,119	0
60	MG	14	3261	1/1	0.23	0.28	-	136,136,136,136	0
60	MG	14	3136	1/1	0.86	0.34	-	90,90,90,90	0
60	MG	13	1666	1/1	0.87	0.26	-	94,94,94,94	0
60	MG	14	3226	1/1	0.81	0.44	-	68,68,68,68	0
60	MG	1H	3284	1/1	0.87	0.15	-	66,66,66,66	0
60	MG	1H	3375	1/1	0.80	0.11	-	48,48,48,48	0
60	MG	1H	3035	1/1	0.94	0.26	-	63,63,63,63	0
60	MG	14	3149	1/1	0.92	0.36	-	73,73,73,73	0
60	MG	1H	3106	1/1	0.92	0.18	-	66,66,66,66	0
60	MG	1H	3071	1/1	0.88	0.31	-	57,57,57,57	0
60	MG	13	1711	1/1	0.64	0.41	-	83,83,83,83	0
60	MG	1H	3057	1/1	0.98	0.40	-	47,47,47,47	0
60	MG	14	3240	1/1	0.94	0.30	-	50,50,50,50	0
60	MG	14	3046	1/1	0.97	0.37	-	80,80,80,80	0
60	MG	14	3295	1/1	0.91	0.17	-	77,77,77,77	0
60	MG	14	3243	1/1	0.95	0.48	-	61,61,61,61	0
60	MG	14	3002	1/1	0.95	0.35	-	50,50,50,50	0
60	MG	1H	3244	1/1	0.96	0.28	-	56,56,56,56	0
60	MG	13	1686	1/1	0.91	0.19	-	76,76,76,76	0
60	MG	1H	3174	1/1	0.96	0.60	-	53,53,53,53	0
60	MG	I8	101	1/1	0.69	0.22	-	70,70,70,70	0
60	MG	1G	1618	1/1	0.94	0.49	-	86,86,86,86	0
60	MG	14	3333	1/1	0.95	0.11	-	55,55,55,55	0
60	MG	14	3242	1/1	0.96	0.34	-	53,53,53,53	0
60	MG	14	3018	1/1	0.24	0.31	-	103,103,103,103	0
60	MG	1H	3328	1/1	0.95	0.13	-	50,50,50,50	0
60	MG	13	1637	1/1	0.89	0.48	-	76,76,76,76	0
60	MG	1H	3316	1/1	0.95	0.16	-	42,42,42,42	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
60	MG	1H	3167	1/1	0.62	0.38	-	83,83,83,83	0
60	MG	14	3173	1/1	0.93	0.43	-	61,61,61,61	0
60	MG	1G	1638	1/1	0.91	0.43	-	88,88,88,88	0
60	MG	14	3185	1/1	0.86	0.42	-	76,76,76,76	0
60	MG	16	208	1/1	0.92	0.13	-	84,84,84,84	0
60	MG	1H	3121	1/1	0.98	0.17	-	43,43,43,43	0
60	MG	2K	102	1/1	0.93	0.21	-	84,84,84,84	0
60	MG	13	1631	1/1	0.88	0.28	-	74,74,74,74	0
60	MG	1G	1702	1/1	0.79	0.08	-	124,124,124,124	0
60	MG	1H	3389	1/1	0.92	0.11	-	47,47,47,47	0
60	MG	14	3113	1/1	0.98	0.34	-	58,58,58,58	0
60	MG	14	3317	1/1	0.88	0.10	-	54,54,54,54	0
60	MG	1H	3047	1/1	0.86	0.33	-	73,73,73,73	0
60	MG	13	1733	1/1	0.94	0.08	-	75,75,75,75	0
60	MG	14	3248	1/1	0.85	0.26	-	80,80,80,80	0
60	MG	14	3249	1/1	0.94	0.29	-	61,61,61,61	0
60	MG	1H	3306	1/1	0.85	0.48	-	77,77,77,77	0
60	MG	1G	1608	1/1	0.92	0.27	-	95,95,95,95	0
60	MG	14	3145	1/1	0.70	0.64	-	82,82,82,82	0
60	MG	14	3328	1/1	0.95	0.16	-	72,72,72,72	0
60	MG	14	3371	1/1	0.69	0.07	-	106,106,106,106	0
60	MG	1G	1665	1/1	0.77	0.39	-	75,75,75,75	0
60	MG	14	3308	1/1	0.85	0.57	-	66,66,66,66	0
60	MG	14	3069	1/1	0.79	0.61	-	78,78,78,78	0
60	MG	14	3365	1/1	0.92	0.07	-	90,90,90,90	0
60	MG	13	1645	1/1	0.98	0.39	-	57,57,57,57	0
60	MG	14	3384	1/1	0.86	0.04	-	122,122,122,122	0
60	MG	1H	3182	1/1	0.89	0.62	-	91,91,91,91	0
60	MG	1G	1666	1/1	0.94	0.39	-	113,113,113,113	0
60	MG	1G	1697	1/1	0.94	0.08	-	111,111,111,111	0
60	MG	13	1618	1/1	0.58	0.24	-	77,77,77,77	0
60	MG	1H	3134	1/1	0.94	0.51	-	64,64,64,64	0
60	MG	1H	3059	1/1	0.97	0.46	-	41,41,41,41	0
60	MG	1G	1662	1/1	0.83	0.44	-	84,84,84,84	0
60	MG	1H	3433	1/1	0.79	0.10	-	91,91,91,91	0
60	MG	1H	3153	1/1	0.80	0.36	-	59,59,59,59	0
60	MG	1H	3114	1/1	0.93	0.38	-	61,61,61,61	0
60	MG	1H	3272	1/1	0.91	0.30	-	72,72,72,72	0
60	MG	14	3123	1/1	0.77	0.34	-	81,81,81,81	0
60	MG	13	1644	1/1	0.94	0.32	-	55,55,55,55	0
60	MG	14	3089	1/1	0.97	0.34	-	52,52,52,52	0
60	MG	21	301	1/1	0.98	0.28	-	49,49,49,49	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
60	MG	1H	3234	1/1	0.93	0.45	-	53,53,53,53	0
60	MG	1H	3237	1/1	0.94	0.12	-	63,63,63,63	0
60	MG	13	1688	1/1	0.82	0.34	-	66,66,66,66	0
60	MG	1H	3224	1/1	0.95	0.13	-	37,37,37,37	0
60	MG	1H	3219	1/1	0.97	0.25	-	123,123,123,123	0
60	MG	14	3125	1/1	0.90	0.17	-	63,63,63,63	0
60	MG	14	3195	1/1	0.70	0.38	-	90,90,90,90	0
60	MG	1H	3045	1/1	0.85	0.48	-	65,65,65,65	0
60	MG	1H	3395	1/1	0.93	0.09	-	69,69,69,69	0
60	MG	14	3181	1/1	0.95	0.18	-	73,73,73,73	0
60	MG	14	3194	1/1	0.96	0.33	-	63,63,63,63	0
60	MG	1J	202	1/1	0.67	0.30	-	85,85,85,85	0
60	MG	1G	1682	1/1	0.90	0.24	-	115,115,115,115	0
60	MG	1H	3061	1/1	0.90	0.27	-	56,56,56,56	0
60	MG	14	3202	1/1	0.96	0.43	-	72,72,72,72	0
60	MG	14	3285	1/1	0.77	0.14	-	62,62,62,62	0
60	MG	1H	3247	1/1	0.99	0.20	-	60,60,60,60	0
60	MG	1H	3041	1/1	0.91	0.48	-	58,58,58,58	0
60	MG	14	3062	1/1	0.92	0.48	-	66,66,66,66	0
60	MG	1H	3097	1/1	0.98	0.43	-	60,60,60,60	0
60	MG	14	3143	1/1	0.73	0.58	-	76,76,76,76	0
60	MG	C5	201	1/1	0.86	0.74	-	107,107,107,107	0
60	MG	14	3341	1/1	0.92	0.10	-	66,66,66,66	0
60	MG	14	3381	1/1	0.95	0.10	-	79,79,79,79	0
60	MG	13	1661	1/1	0.91	0.42	-	70,70,70,70	0
60	MG	14	3254	1/1	0.94	0.19	-	78,78,78,78	0
60	MG	1H	3371	1/1	0.77	0.07	-	91,91,91,91	0
60	MG	13	1665	1/1	0.84	0.32	-	91,91,91,91	0
60	MG	1H	3144	1/1	0.89	0.23	-	78,78,78,78	0
60	MG	1G	1652	1/1	0.90	0.37	-	72,72,72,72	0
60	MG	13	1626	1/1	0.95	0.34	-	50,50,50,50	0
60	MG	13	1694	1/1	0.98	0.09	-	115,115,115,115	0
60	MG	1H	3026	1/1	0.94	0.31	-	80,80,80,80	0
60	MG	1H	3420	1/1	0.94	0.12	-	111,111,111,111	0
60	MG	1H	3068	1/1	0.96	0.40	-	52,52,52,52	0
60	MG	14	3047	1/1	0.96	0.29	-	72,72,72,72	0
60	MG	1H	3017	1/1	0.96	0.18	-	54,54,54,54	0
60	MG	1H	3407	1/1	0.81	0.10	-	76,76,76,76	0
60	MG	13	1735	1/1	0.89	0.12	-	153,153,153,153	0
60	MG	14	3133	1/1	0.88	0.37	-	80,80,80,80	0
60	MG	14	3126	1/1	0.95	0.20	-	82,82,82,82	0
60	MG	14	3041	1/1	0.96	0.29	-	72,72,72,72	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
60	MG	1H	3228	1/1	0.96	0.12	-	42,42,42,42	0
60	MG	14	3193	1/1	0.80	0.35	-	76,76,76,76	0
60	MG	1H	3260	1/1	0.97	0.15	-	62,62,62,62	0
60	MG	14	3056	1/1	0.95	0.32	-	65,65,65,65	0
60	MG	13	1623	1/1	0.95	0.45	-	76,76,76,76	0
60	MG	14	3043	1/1	0.96	0.33	-	64,64,64,64	0
60	MG	1H	3152	1/1	0.90	0.28	-	76,76,76,76	0
60	MG	1H	3285	1/1	0.88	0.17	-	61,61,61,61	0
60	MG	1G	1609	1/1	0.96	0.21	-	74,74,74,74	0
60	MG	1H	3181	1/1	0.73	0.36	-	81,81,81,81	0
60	MG	14	3369	1/1	0.96	0.11	-	79,79,79,79	0
60	MG	14	3186	1/1	0.88	0.53	-	62,62,62,62	0
60	MG	1H	3201	1/1	0.94	0.52	-	65,65,65,65	0
60	MG	1H	3203	1/1	0.89	0.38	-	91,91,91,91	0
60	MG	14	3190	1/1	0.96	0.28	-	68,68,68,68	0
60	MG	14	3197	1/1	0.90	0.28	-	79,79,79,79	0
60	MG	14	3196	1/1	0.93	0.82	-	82,82,82,82	0
60	MG	14	3022	1/1	0.92	0.24	-	48,48,48,48	0
60	MG	1G	1700	1/1	0.88	0.09	-	152,152,152,152	0
60	MG	1H	3006	1/1	0.95	0.27	-	42,42,42,42	0
60	MG	13	1706	1/1	0.89	0.35	-	85,85,85,85	0
60	MG	1H	3135	1/1	0.89	0.28	-	50,50,50,50	0
60	MG	14	3291	1/1	0.80	0.18	-	80,80,80,80	0
60	MG	13	1701	1/1	0.73	0.27	-	85,85,85,85	0
60	MG	14	3334	1/1	0.93	0.07	-	80,80,80,80	0
60	MG	1H	3039	1/1	0.95	0.33	-	46,46,46,46	0
60	MG	1H	3212	1/1	0.80	0.52	-	89,89,89,89	0
60	MG	1G	1622	1/1	0.96	0.43	-	52,52,52,52	0
60	MG	1H	3124	1/1	0.93	0.29	-	68,68,68,68	0
60	MG	1H	3131	1/1	0.92	0.46	-	76,76,76,76	0
60	MG	1H	3177	1/1	0.97	0.32	-	62,62,62,62	0
60	MG	14	3110	1/1	0.98	0.54	-	56,56,56,56	0
60	MG	14	3346	1/1	0.82	0.07	-	108,108,108,108	0
60	MG	1J	207	1/1	0.81	0.10	-	92,92,92,92	0
60	MG	1H	3056	1/1	0.92	0.21	-	67,67,67,67	0
60	MG	1H	3117	1/1	0.96	0.31	-	57,57,57,57	0
60	MG	14	3162	1/1	0.91	0.30	-	83,83,83,83	0
60	MG	1H	3188	1/1	0.94	0.22	-	63,63,63,63	0
60	MG	14	3374	1/1	0.94	0.05	-	107,107,107,107	0
60	MG	14	3301	1/1	0.87	0.21	-	75,75,75,75	0
60	MG	14	3040	1/1	0.93	0.29	-	66,66,66,66	0
60	MG	1H	3197	1/1	0.89	0.30	-	70,70,70,70	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
60	MG	1H	3286	1/1	0.90	0.29	-	72,72,72,72	0
60	MG	1H	3130	1/1	0.93	0.38	-	73,73,73,73	0
60	MG	13	1726	1/1	0.94	0.09	-	97,97,97,97	0
60	MG	1H	3138	1/1	0.96	0.52	-	81,81,81,81	0
60	MG	14	3298	1/1	0.95	0.33	-	64,64,64,64	0
60	MG	14	3170	1/1	0.97	0.37	-	81,81,81,81	0
60	MG	14	3159	1/1	0.94	0.37	-	64,64,64,64	0
60	MG	13	1716	1/1	0.88	0.19	-	77,77,77,77	0
60	MG	13	1606	1/1	0.97	0.30	-	78,78,78,78	0
60	MG	14	3383	1/1	0.79	0.08	-	101,101,101,101	0
60	MG	78	202	1/1	0.89	0.20	-	46,46,46,46	0
60	MG	14	3378	1/1	0.74	0.10	-	75,75,75,75	0
60	MG	13	1613	1/1	0.94	0.28	-	66,66,66,66	0
60	MG	14	3111	1/1	0.95	0.49	-	72,72,72,72	0
60	MG	14	3077	1/1	0.97	0.30	-	49,49,49,49	0
60	MG	14	3252	1/1	0.79	0.38	-	76,76,76,76	0
60	MG	1H	3403	1/1	0.91	0.18	-	83,83,83,83	0
60	MG	1H	3233	1/1	0.86	0.38	-	69,69,69,69	0
60	MG	14	3146	1/1	0.97	0.25	-	74,74,74,74	0
60	MG	13	1636	1/1	0.95	0.24	-	66,66,66,66	0
60	MG	1H	3358	1/1	0.98	0.09	-	55,55,55,55	0
60	MG	14	3107	1/1	0.94	0.46	-	69,69,69,69	0
60	MG	14	3364	1/1	0.94	0.12	-	89,89,89,89	0
60	MG	1H	3430	1/1	0.83	0.05	-	95,95,95,95	0
60	MG	1H	3351	1/1	0.96	0.06	-	68,68,68,68	0
60	MG	14	3016	1/1	0.98	0.33	-	52,52,52,52	0
60	MG	14	3140	1/1	0.94	0.17	-	46,46,46,46	0
60	MG	1G	1670	1/1	0.93	0.08	-	93,93,93,93	0
60	MG	1H	3413	1/1	0.88	0.11	-	103,103,103,103	0
60	MG	2L	103	1/1	0.90	0.27	-	67,67,67,67	0
60	MG	1H	3170	1/1	0.95	0.33	-	76,76,76,76	0
60	MG	1H	3160	1/1	0.89	0.53	-	76,76,76,76	0
60	MG	1H	3251	1/1	0.41	0.28	-	73,73,73,73	0
60	MG	14	3262	1/1	0.84	0.23	-	63,63,63,63	0
60	MG	13	1663	1/1	0.81	0.34	-	93,93,93,93	0
60	MG	2K	103	1/1	0.85	0.34	-	76,76,76,76	0
60	MG	14	3292	1/1	0.97	0.14	-	77,77,77,77	0
60	MG	1H	3273	1/1	0.91	0.27	-	55,55,55,55	0
60	MG	14	3310	1/1	0.98	0.14	-	46,46,46,46	0
60	MG	13	1659	1/1	0.92	0.33	-	79,79,79,79	0
60	MG	1H	3398	1/1	0.88	0.04	-	71,71,71,71	0
60	MG	14	3027	1/1	0.96	0.25	-	65,65,65,65	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
60	MG	14	3001	1/1	0.95	0.11	-	44,44,44,44	0
60	MG	14	3117	1/1	0.88	0.32	-	74,74,74,74	0
60	MG	16	210	1/1	0.89	0.08	-	64,64,64,64	0
60	MG	1H	3434	1/1	0.94	0.08	-	44,44,44,44	0
60	MG	14	3129	1/1	0.93	0.28	-	56,56,56,56	0
60	MG	1H	3320	1/1	0.99	0.11	-	41,41,41,41	0
60	MG	13	1657	1/1	0.94	0.47	-	73,73,73,73	0
60	MG	1H	3029	1/1	0.91	0.39	-	65,65,65,65	0
60	MG	13	1697	1/1	0.92	0.07	-	95,95,95,95	0
60	MG	68	201	1/1	0.73	0.46	-	83,83,83,83	0
60	MG	1H	3085	1/1	0.95	0.26	-	47,47,47,47	0
60	MG	13	1669	1/1	0.98	0.40	-	84,84,84,84	0
60	MG	13	1684	1/1	0.96	0.34	-	66,66,66,66	0
60	MG	1G	1690	1/1	0.92	0.43	-	75,75,75,75	0
60	MG	13	1620	1/1	0.89	0.33	-	64,64,64,64	0
60	MG	1H	3078	1/1	0.95	0.16	-	46,46,46,46	0
60	MG	13	1667	1/1	0.35	0.41	-	102,102,102,102	0
60	MG	1G	1672	1/1	0.96	0.20	-	84,84,84,84	0
60	MG	1G	1646	1/1	0.84	0.27	-	77,77,77,77	0
60	MG	1H	3189	1/1	0.96	0.24	-	62,62,62,62	0
60	MG	13	1628	1/1	0.90	0.47	-	72,72,72,72	0
60	MG	14	3017	1/1	0.94	0.28	-	68,68,68,68	0
60	MG	14	3354	1/1	0.93	0.09	-	74,74,74,74	0
60	MG	14	3006	1/1	0.99	0.30	-	49,49,49,49	0
60	MG	1H	3098	1/1	0.96	0.37	-	69,69,69,69	0
60	MG	1H	3386	1/1	0.99	0.10	-	53,53,53,53	0
60	MG	1G	1686	1/1	0.97	0.18	-	115,115,115,115	0
60	MG	1G	1649	1/1	0.88	0.34	-	76,76,76,76	0
60	MG	1H	3317	1/1	0.93	0.16	-	74,74,74,74	0
60	MG	14	3070	1/1	0.95	0.42	-	61,61,61,61	0
60	MG	1H	3082	1/1	0.89	0.32	-	39,39,39,39	0
60	MG	14	3198	1/1	0.86	0.34	-	63,63,63,63	0
60	MG	1H	3146	1/1	0.92	0.35	-	84,84,84,84	0
60	MG	1H	3215	1/1	0.92	0.41	-	80,80,80,80	0
60	MG	14	3038	1/1	0.96	0.52	-	60,60,60,60	0
60	MG	14	3120	1/1	0.97	0.28	-	53,53,53,53	0
60	MG	1H	3036	1/1	0.98	0.34	-	52,52,52,52	0
60	MG	1H	3411	1/1	0.95	0.10	-	68,68,68,68	0
60	MG	14	3247	1/1	0.96	0.24	-	73,73,73,73	0
60	MG	1H	3425	1/1	0.96	0.10	-	60,60,60,60	0
60	MG	1H	3208	1/1	0.95	0.11	-	56,56,56,56	0
60	MG	14	3278	1/1	0.90	0.29	-	71,71,71,71	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
60	MG	1G	1655	1/1	0.90	0.26	-	96,96,96,96	0
60	MG	1G	1647	1/1	0.96	0.53	-	76,76,76,76	0
60	MG	3K	101	1/1	0.98	0.20	-	83,83,83,83	0
60	MG	1H	3412	1/1	0.87	0.08	-	93,93,93,93	0
60	MG	1H	3391	1/1	0.98	0.06	-	58,58,58,58	0
60	MG	14	3099	1/1	0.97	0.34	-	58,58,58,58	0
60	MG	1H	3128	1/1	0.96	0.42	-	49,49,49,49	0
60	MG	1H	3280	1/1	0.84	0.22	-	70,70,70,70	0
60	MG	13	1615	1/1	0.94	0.31	-	75,75,75,75	0
60	MG	1H	3330	1/1	0.94	0.11	-	51,51,51,51	0
60	MG	14	3138	1/1	0.95	0.50	-	50,50,50,50	0
60	MG	1H	3052	1/1	0.97	0.11	-	44,44,44,44	0
60	MG	13	1715	1/1	0.91	0.36	-	82,82,82,82	0
60	MG	14	3255	1/1	0.93	0.37	-	75,75,75,75	0
60	MG	1H	3245	1/1	0.91	0.17	-	50,50,50,50	0
60	MG	1G	1650	1/1	0.93	0.46	-	88,88,88,88	0
60	MG	13	1732	1/1	0.97	0.07	-	86,86,86,86	0
60	MG	14	3276	1/1	0.78	0.21	-	66,66,66,66	0
60	MG	14	3302	1/1	0.87	0.34	-	87,87,87,87	0
60	MG	1H	3055	1/1	0.97	0.20	-	45,45,45,45	0
60	MG	13	1614	1/1	0.94	0.27	-	82,82,82,82	0
60	MG	14	3212	1/1	0.93	0.47	-	106,106,106,106	0
60	MG	1H	3198	1/1	0.88	0.27	-	64,64,64,64	0
60	MG	1H	3274	1/1	0.98	0.18	-	71,71,71,71	0
60	MG	1H	3220	1/1	0.90	0.38	-	78,78,78,78	0
60	MG	1H	3166	1/1	0.93	0.36	-	83,83,83,83	0
60	MG	1H	3013	1/1	0.97	0.30	-	48,48,48,48	0
60	MG	1G	1640	1/1	0.96	0.59	-	105,105,105,105	0
60	MG	13	1647	1/1	0.93	0.42	-	83,83,83,83	0
60	MG	1H	3165	1/1	0.84	0.27	-	77,77,77,77	0
60	MG	14	3272	1/1	0.81	0.25	-	55,55,55,55	0
60	MG	14	3142	1/1	0.95	0.29	-	68,68,68,68	0
60	MG	14	3353	1/1	0.98	0.07	-	72,72,72,72	0
60	MG	1H	3089	1/1	0.86	0.24	-	69,69,69,69	0
60	MG	1H	3125	1/1	0.88	0.14	-	34,34,34,34	0
60	MG	1H	3292	1/1	0.95	0.38	-	89,89,89,89	0
60	MG	1H	3123	1/1	0.95	0.23	-	65,65,65,65	0
60	MG	1G	1643	1/1	0.88	0.21	-	80,80,80,80	0
60	MG	14	3078	1/1	0.94	0.27	-	59,59,59,59	0
60	MG	1H	3031	1/1	0.65	0.40	-	78,78,78,78	0
60	MG	13	1652	1/1	0.95	0.38	-	61,61,61,61	0
60	MG	14	3216	1/1	0.60	0.51	-	80,80,80,80	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
60	MG	1G	1635	1/1	0.64	0.38	-	104,104,104,104	0
60	MG	14	3108	1/1	0.90	0.58	-	71,71,71,71	0
60	MG	14	3224	1/1	0.94	0.56	-	51,51,51,51	0
60	MG	14	3241	1/1	0.95	0.20	-	65,65,65,65	0
60	MG	1H	3334	1/1	0.95	0.14	-	59,59,59,59	0
60	MG	1H	3255	1/1	0.69	0.38	-	71,71,71,71	0
60	MG	14	3033	1/1	0.98	0.27	-	58,58,58,58	0
60	MG	1H	3080	1/1	0.95	0.29	-	59,59,59,59	0
60	MG	1H	3263	1/1	0.97	0.42	-	72,72,72,72	0
60	MG	14	3319	1/1	0.95	0.06	-	98,98,98,98	0
60	MG	1G	1696	1/1	0.97	0.07	-	108,108,108,108	0
60	MG	14	3201	1/1	0.89	0.58	-	81,81,81,81	0
60	MG	14	3175	1/1	0.90	0.38	-	80,80,80,80	0
60	MG	1H	3249	1/1	0.94	0.40	-	72,72,72,72	0
60	MG	1H	3206	1/1	0.94	0.22	-	58,58,58,58	0
60	MG	13	1610	1/1	0.95	0.16	-	67,67,67,67	0
60	MG	14	3020	1/1	0.98	0.25	-	57,57,57,57	0
60	MG	1H	3410	1/1	0.84	0.07	-	87,87,87,87	0
60	MG	14	3205	1/1	0.90	0.35	-	72,72,72,72	0
60	MG	13	1655	1/1	0.95	0.27	-	97,97,97,97	0
60	MG	1G	1612	1/1	0.91	0.31	-	84,84,84,84	0
60	MG	14	3096	1/1	0.69	0.22	-	60,60,60,60	0
60	MG	14	3182	1/1	0.93	0.52	-	81,81,81,81	0
60	MG	1H	3193	1/1	0.88	0.34	-	67,67,67,67	0
60	MG	1H	3015	1/1	0.96	0.22	-	56,56,56,56	0
60	MG	1H	3432	1/1	0.92	0.07	-	107,107,107,107	0
60	MG	29	301	1/1	0.98	0.30	-	48,48,48,48	0
60	MG	14	3199	1/1	0.92	0.59	-	66,66,66,66	0
60	MG	1H	3141	1/1	0.85	0.54	-	70,70,70,70	0
60	MG	14	3154	1/1	0.92	0.24	-	64,64,64,64	0
60	MG	1H	3213	1/1	0.83	0.38	-	95,95,95,95	0
60	MG	14	3007	1/1	0.96	0.41	-	54,54,54,54	0
60	MG	14	3057	1/1	0.94	0.41	-	62,62,62,62	0
60	MG	1H	3168	1/1	0.95	0.38	-	72,72,72,72	0
60	MG	1H	3180	1/1	0.86	0.26	-	87,87,87,87	0
60	MG	1G	1623	1/1	0.94	0.49	-	82,82,82,82	0
60	MG	14	3178	1/1	0.86	0.38	-	66,66,66,66	0
60	MG	14	3322	1/1	0.96	0.12	-	42,42,42,42	0
60	MG	14	3265	1/1	0.97	0.40	-	78,78,78,78	0
60	MG	1H	3400	1/1	0.83	0.07	-	82,82,82,82	0
60	MG	14	3065	1/1	0.87	0.57	-	71,71,71,71	0
60	MG	1H	3091	1/1	0.95	0.18	-	60,60,60,60	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
60	MG	13	1737	1/1	0.95	0.10	-	91,91,91,91	0
60	MG	1H	3313	1/1	0.97	0.09	-	36,36,36,36	0
60	MG	14	3228	1/1	0.97	0.36	-	76,76,76,76	0
60	MG	1H	3001	1/1	0.95	0.31	-	36,36,36,36	0
60	MG	1H	3382	1/1	0.93	0.06	-	68,68,68,68	0
60	MG	1H	3027	1/1	0.95	0.40	-	79,79,79,79	0
60	MG	1H	3345	1/1	0.95	0.09	-	65,65,65,65	0
60	MG	1H	3299	1/1	0.83	0.24	-	72,72,72,72	0
60	MG	1H	3428	1/1	0.82	0.06	-	102,102,102,102	0
60	MG	14	3050	1/1	0.97	0.15	-	54,54,54,54	0
60	MG	1H	3322	1/1	0.90	0.15	-	48,48,48,48	0
60	MG	1H	3178	1/1	0.89	0.31	-	80,80,80,80	0
60	MG	1H	3148	1/1	0.92	0.65	-	67,67,67,67	0
60	MG	1H	3008	1/1	0.99	0.27	-	47,47,47,47	0
60	MG	1H	3155	1/1	0.69	0.50	-	60,60,60,60	0
60	MG	14	3207	1/1	0.84	0.25	-	74,74,74,74	0
60	MG	14	3121	1/1	0.83	0.43	-	64,64,64,64	0
60	MG	18	102	1/1	0.78	0.23	-	56,56,56,56	0
60	MG	14	3239	1/1	0.97	0.37	-	83,83,83,83	0
60	MG	13	1695	1/1	0.91	0.21	-	90,90,90,90	0
60	MG	16	211	1/1	0.88	0.08	-	87,87,87,87	0
60	MG	1G	1675	1/1	0.80	0.19	-	86,86,86,86	0
60	MG	1H	3366	1/1	0.92	0.16	-	53,53,53,53	0
60	MG	1H	3275	1/1	0.93	0.26	-	58,58,58,58	0
60	MG	13	1612	1/1	0.98	0.18	-	67,67,67,67	0
60	MG	1H	3120	1/1	0.91	0.36	-	63,63,63,63	0
60	MG	1H	3291	1/1	0.80	0.28	-	71,71,71,71	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.