



# wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 15, 2017 – 09:03 am GMT

PDB ID : 4WRO  
Title : Complex of 70S ribosome with tRNA-Phe and mRNA with C-A mismatch in the second position in the A-site  
Authors : Rozov, A.; Demeshkina, N.; Yusupov, M.; Yusupova, G.  
Deposited on : 2014-10-24  
Resolution : 3.05 Å(reported)

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

We welcome your comments at [validation@mail.wwpdb.org](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 : 1.7.2 (RC1), CSD as538be (2017)  
Xtriage (Phenix) : 1.9-1692  
EDS : trunk28620  
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : recalc28972

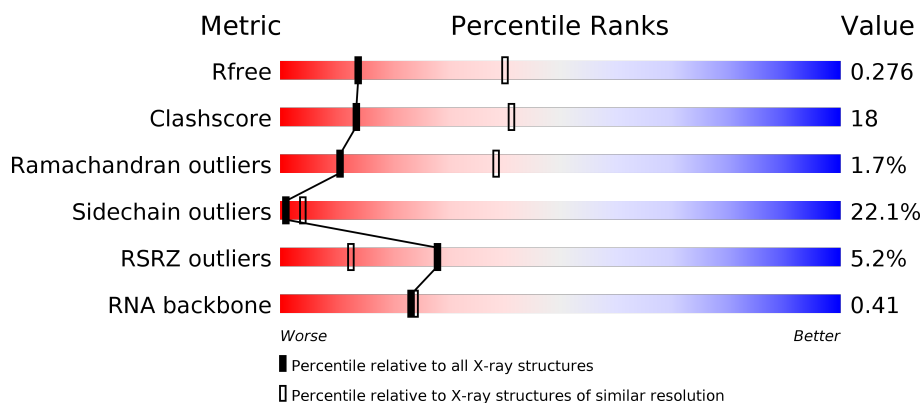
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.05 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	100719	1348 (3.10-3.02)
Clashscore	112137	1462 (3.10-3.02)
Ramachandran outliers	110173	1410 (3.10-3.02)
Sidechain outliers	110143	1410 (3.10-3.02)
RSRZ outliers	101464	1355 (3.10-3.02)
RNA backbone	2435	1037 (3.42-2.70)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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>27%</div> <div>44%</div> <div>23%</div> <div>• •</div> </div>
1	1G	1522	<div> <div>29%</div> <div>46%</div> <div>20%</div> <div>• •</div> </div>
2	1L	76	<div> <div>9%</div> <div>29%</div> <div>45%</div> <div>26%</div> </div>
2	3K	76	<div> <div>9%</div> <div>20%</div> <div>47%</div> <div>33%</div> </div>

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Mol	Chain	Length	Quality of chain
2	3L	76	
3	2K	77	
3	2L	77	
4	4K	30	
4	4L	30	
5	14	2917	
5	1H	2917	
6	12	256	
6	1E	256	
7	22	239	
7	2E	239	
8	32	209	
8	3E	209	
9	4E	162	
10	5E	101	
11	6E	156	
12	7E	138	
13	8E	128	
14	1I	105	
15	2I	129	
16	3I	132	
17	4I	126	
18	5I	61	
19	6I	89	
20	7I	88	

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Mol	Chain	Length	Quality of chain
21	8I	105	
22	9I	88	
23	AI	93	
24	BI	106	
25	1F	27	
26	1K	76	
27	16	122	
27	1J	122	
28	11	276	
29	21	206	
30	31	210	
31	41	182	
32	51	180	
33	61	148	
34	58	140	
35	68	122	
36	78	150	
37	88	141	
38	98	118	
39	A8	112	
40	B8	146	
41	C8	118	
42	D8	101	
43	E8	113	
44	F8	96	

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Mol	Chain	Length	Quality of chain
45	G8	110	
46	H8	206	
47	I8	85	
48	J8	98	
49	K8	72	
50	L8	60	
51	M8	71	
52	N8	60	
53	O8	54	
54	P8	49	
55	Q8	65	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
56	MG	13	1601	-	-	-	X
56	MG	13	1606	-	-	-	X
56	MG	13	1608	-	-	-	X
56	MG	13	1611	-	-	-	X
56	MG	13	1613	-	-	-	X
56	MG	13	1615	-	-	-	X
56	MG	13	1621	-	-	-	X
56	MG	13	1626	-	-	-	X
56	MG	13	1630	-	-	-	X
56	MG	13	1631	-	-	-	X
56	MG	13	1641	-	-	-	X
56	MG	13	1643	-	-	-	X
56	MG	13	1648	-	-	-	X
56	MG	13	1659	-	-	-	X
56	MG	13	1664	-	-	-	X
56	MG	13	1670	-	-	-	X
56	MG	13	1671	-	-	-	X
56	MG	13	1673	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
56	MG	13	1676	-	-	-	X
56	MG	13	1682	-	-	-	X
56	MG	13	1691	-	-	-	X
56	MG	13	1707	-	-	-	X
56	MG	13	1722	-	-	-	X
56	MG	14	3011	-	-	-	X
56	MG	14	3021	-	-	-	X
56	MG	14	3022	-	-	-	X
56	MG	14	3023	-	-	-	X
56	MG	14	3027	-	-	-	X
56	MG	14	3031	-	-	-	X
56	MG	14	3035	-	-	-	X
56	MG	14	3036	-	-	-	X
56	MG	14	3037	-	-	-	X
56	MG	14	3040	-	-	-	X
56	MG	14	3041	-	-	-	X
56	MG	14	3042	-	-	-	X
56	MG	14	3052	-	-	-	X
56	MG	14	3056	-	-	-	X
56	MG	14	3068	-	-	-	X
56	MG	14	3073	-	-	-	X
56	MG	14	3076	-	-	-	X
56	MG	14	3095	-	-	-	X
56	MG	14	3096	-	-	-	X
56	MG	14	3107	-	-	-	X
56	MG	14	3121	-	-	-	X
56	MG	14	3122	-	-	-	X
56	MG	14	3125	-	-	-	X
56	MG	14	3156	-	-	-	X
56	MG	14	3160	-	-	-	X
56	MG	14	3175	-	-	-	X
56	MG	14	3182	-	-	-	X
56	MG	14	3191	-	-	-	X
56	MG	14	3198	-	-	-	X
56	MG	14	3227	-	-	-	X
56	MG	14	3230	-	-	-	X
56	MG	14	3240	-	-	-	X
56	MG	16	201	-	-	-	X
56	MG	16	206	-	-	-	X
56	MG	1G	1601	-	-	-	X
56	MG	1G	1602	-	-	-	X
56	MG	1G	1609	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
56	MG	1G	1617	-	-	-	X
56	MG	1G	1620	-	-	-	X
56	MG	1G	1640	-	-	-	X
56	MG	1G	1663	-	-	-	X
56	MG	1G	1669	-	-	-	X
56	MG	1G	1675	-	-	-	X
56	MG	1H	3001	-	-	-	X
56	MG	1H	3004	-	-	-	X
56	MG	1H	3010	-	-	-	X
56	MG	1H	3011	-	-	-	X
56	MG	1H	3015	-	-	-	X
56	MG	1H	3020	-	-	-	X
56	MG	1H	3021	-	-	-	X
56	MG	1H	3023	-	-	-	X
56	MG	1H	3025	-	-	-	X
56	MG	1H	3026	-	-	-	X
56	MG	1H	3027	-	-	-	X
56	MG	1H	3032	-	-	-	X
56	MG	1H	3033	-	-	-	X
56	MG	1H	3036	-	-	-	X
56	MG	1H	3037	-	-	-	X
56	MG	1H	3041	-	-	-	X
56	MG	1H	3045	-	-	-	X
56	MG	1H	3047	-	-	-	X
56	MG	1H	3048	-	-	-	X
56	MG	1H	3052	-	-	-	X
56	MG	1H	3054	-	-	-	X
56	MG	1H	3057	-	-	-	X
56	MG	1H	3058	-	-	-	X
56	MG	1H	3065	-	-	-	X
56	MG	1H	3066	-	-	-	X
56	MG	1H	3072	-	-	-	X
56	MG	1H	3078	-	-	-	X
56	MG	1H	3081	-	-	-	X
56	MG	1H	3082	-	-	-	X
56	MG	1H	3085	-	-	-	X
56	MG	1H	3089	-	-	-	X
56	MG	1H	3092	-	-	-	X
56	MG	1H	3095	-	-	-	X
56	MG	1H	3098	-	-	-	X
56	MG	1H	3103	-	-	-	X
56	MG	1H	3108	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
56	MG	1H	3109	-	-	-	X
56	MG	1H	3111	-	-	-	X
56	MG	1H	3118	-	-	-	X
56	MG	1H	3124	-	-	-	X
56	MG	1H	3128	-	-	-	X
56	MG	1H	3132	-	-	-	X
56	MG	1H	3133	-	-	-	X
56	MG	1H	3136	-	-	-	X
56	MG	1H	3138	-	-	-	X
56	MG	1H	3142	-	-	-	X
56	MG	1H	3145	-	-	-	X
56	MG	1H	3146	-	-	-	X
56	MG	1H	3149	-	-	-	X
56	MG	1H	3151	-	-	-	X
56	MG	1H	3152	-	-	-	X
56	MG	1H	3164	-	-	-	X
56	MG	1H	3167	-	-	-	X
56	MG	1H	3176	-	-	-	X
56	MG	1H	3185	-	-	-	X
56	MG	1H	3186	-	-	-	X
56	MG	1H	3189	-	-	-	X
56	MG	1H	3199	-	-	-	X
56	MG	1H	3203	-	-	-	X
56	MG	1H	3204	-	-	-	X
56	MG	1H	3221	-	-	-	X
56	MG	1H	3230	-	-	-	X
56	MG	1H	3232	-	-	-	X
56	MG	1H	3240	-	-	-	X
56	MG	1H	3258	-	-	-	X
56	MG	1H	3263	-	-	-	X
56	MG	1H	3278	-	-	-	X
56	MG	1H	3305	-	-	-	X
56	MG	1H	3312	-	-	-	X
56	MG	1H	3323	-	-	-	X
56	MG	1H	3358	-	-	-	X
56	MG	1H	3366	-	-	-	X
56	MG	1H	3389	-	-	-	X
56	MG	1H	3392	-	-	-	X
56	MG	1H	3399	-	-	-	X
56	MG	1H	3416	-	-	-	X
56	MG	1H	3482	-	-	-	X
56	MG	1H	3532	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
56	MG	1J	204	-	-	-	X
56	MG	2I	302	-	-	-	X
56	MG	2K	101	-	-	-	X
56	MG	2K	103	-	-	-	X
56	MG	3I	201	-	-	-	X
56	MG	J8	101	-	-	-	X
57	ZN	3E	303	-	-	-	X

## 2 Entry composition

There are 58 unique types of molecules in this entry. The entry contains 260090 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	1497	Total	C	N	O	P	0	0	0
			32185	14324	5968	10396	1497			
1	1G	1497	Total	C	N	O	P	0	0	0
			32182	14324	5968	10394	1496			

- Molecule 2 is a RNA chain called tRNA-Phe.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	1L	76	Total	C	N	O	P	S	0	0	0
			1627	730	290	530	75	2			
2	3L	76	Total	C	N	O	P	S	0	0	0
			1627	730	290	530	75	2			
2	3K	76	Total	C	N	O	P	S	0	0	0
			1627	730	290	530	75	2			

- Molecule 3 is a RNA chain called tRNA-fMet.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
3	2L	77	Total	C	N	O	P	S	0	0	0
			1645	734	298	535	77	1			
3	2K	77	Total	C	N	O	P	S	0	0	0
			1645	734	298	535	77	1			

- Molecule 4 is a RNA chain called RNA (30-MER).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	4L	9	Total	C	N	O	P	0	0	0
			191	86	35	61	9			
4	4K	13	Total	C	N	O	P	0	0	0
			279	126	55	85	13			

- Molecule 5 is a RNA chain called 23S ribosomal RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	14	2909	Total	C	N	O	P	0	0	0
			62647	27884	11716	20139	2908			
5	1H	2912	Total	C	N	O	P	0	0	0
			62707	27911	11722	20163	2911			

There are 6 discrepancies between the modelled and reference sequences:

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

- Molecule 6 is a protein called 30S ribosomal protein S2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	1E	237	Total	C	N	O	S	0	0	0
			1924	1228	344	347	5			
6	12	237	Total	C	N	O	S	0	0	0
			1924	1228	344	347	5			

- Molecule 7 is a protein called 30S ribosomal protein S3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	2E	205	Total	C	N	O	S	0	0	0
			1605	1011	313	280	1			
7	22	206	Total	C	N	O	S	0	0	0
			1612	1016	314	281	1			

- Molecule 8 is a protein called 30S ribosomal protein S4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	3E	208	Total	C	N	O	S	0	0	0
			1702	1066	339	290	7			
8	32	208	Total	C	N	O	S	0	0	0
			1702	1066	339	290	7			

- Molecule 9 is a protein called 30S ribosomal protein S5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	4E	151	Total	C	N	O	S	0	0	0
			1155	729	218	204	4			

- Molecule 10 is a protein called 30S ribosomal protein S6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	5E	101	Total	C	N	O	S	0	0	0
			842	531	155	153	3			

- Molecule 11 is a protein called 30S ribosomal protein S7.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	6E	155	Total	C	N	O	S	0	0	0
			1256	781	252	217	6			

- Molecule 12 is a protein called 30S ribosomal protein S8.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	7E	138	Total	C	N	O	S	0	0	0
			1115	705	215	192	3			

- Molecule 13 is a protein called 30S ribosomal protein S9.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
13	8E	127	Total	C	N	O	0	0	0
			1009	639	197	173			

- Molecule 14 is a protein called 30S ribosomal protein S10.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
14	1I	99	Total	C	N	O	S	0	0	0
			801	504	157	139	1			

- Molecule 15 is a protein called 30S ribosomal protein S11.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
15	2I	119	Total	C	N	O	S	0	0	0
			884	549	168	164	3			

- Molecule 16 is a protein called 30S ribosomal protein S12.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
16	3I	125	Total	C	N	O	S	0	0	0
			975	614	196	164	1			

- Molecule 17 is a protein called 30S ribosomal protein S13.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
17	4I	118	Total	C	N	O	S	0	0	0
			938	580	193	163	2			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
4I	119	ALA	GLY	conflict	UNP P80377

- Molecule 18 is a protein called 30S ribosomal protein S14 type Z.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
18	5I	60	Total	C	N	O	S	0	0	0
			491	312	104	71	4			

- Molecule 19 is a protein called 30S ribosomal protein S15.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
19	6I	88	Total	C	N	O	S	0	0	0
			733	459	147	125	2			

- Molecule 20 is a protein called 30S ribosomal protein S16.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
20	7I	84	Total	C	N	O	S	0	0	0
			705	446	140	118	1			

- Molecule 21 is a protein called 30S ribosomal protein S17.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
21	8I	100	Total	C	N	O	S	0	0	0
			834	534	155	143	2			

- Molecule 22 is a protein called 30S ribosomal protein S18.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
22	9I	72	Total	C	N	O	0	0	0
			590	376	117	97			

- Molecule 23 is a protein called 30S ribosomal protein S19.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
23	AI	81	Total	C	N	O	S	0	0	0
			647	413	119	113	2			

- Molecule 24 is a protein called 30S ribosomal protein S20.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
24	BI	99	Total	C	N	O	S	0	0	0
			762	470	162	128	2			

- Molecule 25 is a protein called 30S ribosomal protein Thx.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
25	1F	25	Total	C	N	O	0	0	0
			217	134	52	31			

- Molecule 26 is a RNA chain called tRNA-Phe.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
26	1K	74	Total	C	N	O	P	S	0	0	0
			1587	712	286	514	73	2			

- Molecule 27 is a RNA chain called 5S ribosomal RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
27	1J	122	Total	C	N	O	P	0	0	0
			2617	1166	486	844	121			
27	16	122	Total	C	N	O	P	0	0	0
			2617	1166	486	844	121			

- Molecule 28 is a protein called 50S ribosomal protein L2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
28	11	272	Total	C	N	O	S	0	0	0
			2115	1335	420	357	3			

- Molecule 29 is a protein called 50S ribosomal protein L3.

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

- Molecule 30 is a protein called 50S ribosomal protein L4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
30	31	202	Total	C	N	O	S	0	0	0
			1585	1011	297	275	2			

- Molecule 31 is a protein called 50S ribosomal protein L5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
31	41	181	Total	C	N	O	S	0	0	0
			1473	942	268	259	4			

- Molecule 32 is a protein called 50S ribosomal protein L6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
32	51	174	Total	C	N	O	S	0	0	0
			1336	848	251	236	1			

- Molecule 33 is a protein called 50S ribosomal protein L9.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
33	61	146	Total	C	N	O	S	0	0	0
			1136	726	201	208	1			

- Molecule 34 is a protein called 50S ribosomal protein L13.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
34	58	138	Total	C	N	O	S	0	0	0
			1104	712	206	182	4			

- Molecule 35 is a protein called 50S ribosomal protein L14.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
35	68	122	Total	C	N	O	S	0	0	0
			932	588	171	169	4			

- Molecule 36 is a protein called 50S ribosomal protein L15.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
36	78	150	Total	C	N	O	S	0	0	0
			1144	712	232	197	3			

- Molecule 37 is a protein called 50S ribosomal protein L16.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
37	88	138	Total	C	N	O	S	0	0	0
			1086	693	208	179	6			

- Molecule 38 is a protein called 50S ribosomal protein L17.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
38	98	118	Total	C	N	O	S	0	0	0
			967	604	203	159	1			

- Molecule 39 is a protein called 50S ribosomal protein L18.

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

- Molecule 40 is a protein called 50S ribosomal protein L19.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
40	B8	137	Total	C	N	O	S	0	0	0
			1141	710	234	196	1			

- Molecule 41 is a protein called 50S ribosomal protein L20.

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

- Molecule 42 is a protein called 50S ribosomal protein L21.

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

- Molecule 43 is a protein called 50S ribosomal protein L22.



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

- Molecule 44 is a protein called 50S ribosomal protein L23.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
44	F8	94	Total	C	N	O	S	0	0	0
			742	482	134	125	1			

- Molecule 45 is a protein called 50S ribosomal protein L24.

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

- Molecule 46 is a protein called 50S ribosomal protein L25.

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

- Molecule 47 is a protein called 50S ribosomal protein L27.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
47	I8	80	Total	C	N	O	S	0	0	0
			626	388	132	105	1			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
I8	6	ALA	GLY	conflict	UNP P60493
I8	8	ALA	GLY	conflict	UNP P60493

- Molecule 48 is a protein called 50S ribosomal protein L28.

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

- Molecule 49 is a protein called 50S ribosomal protein L29.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
49	K8	67	Total	C	N	O	S	0	0	0
			563	349	114	99	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
50	L8	57	Total	C	N	O		0	0	0
			452	288	88	76				

- Molecule 51 is a protein called 50S ribosomal protein L31.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
51	M8	66	Total	C	N	O	S	0	0	0
			533	335	96	97	5			

- Molecule 52 is a protein called 50S ribosomal protein L32.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
52	N8	58	Total	C	N	O	S	0	0	0
			453	285	89	74	5			

- Molecule 53 is a protein called 50S ribosomal protein L33.

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

- Molecule 54 is a protein called 50S ribosomal protein L34.

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

- Molecule 55 is a protein called 50S ribosomal protein L35.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
55	Q8	60	Total	C	N	O	S	0	0	0
			480	306	98	74	2			

- Molecule 56 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
56	P8	1	Total 1 Mg 1	0	0
56	13	149	Total 149 Mg 149	0	0
56	1J	7	Total 7 Mg 7	0	0
56	5I	1	Total 1 Mg 1	0	0
56	16	13	Total 13 Mg 13	0	0
56	21	2	Total 2 Mg 2	0	0
56	2K	8	Total 8 Mg 8	0	0
56	L8	1	Total 1 Mg 1	0	0
56	3I	1	Total 1 Mg 1	0	0
56	I8	1	Total 1 Mg 1	0	0
56	5E	1	Total 1 Mg 1	0	0
56	78	1	Total 1 Mg 1	0	0
56	J8	1	Total 1 Mg 1	0	0
56	1L	1	Total 1 Mg 1	0	0
56	1G	96	Total 96 Mg 96	0	0
56	11	2	Total 2 Mg 2	0	0
56	1H	537	Total 537 Mg 537	0	0
56	88	2	Total 2 Mg 2	0	0
56	14	421	Total 421 Mg 421	0	0
56	3E	2	Total 2 Mg 2	0	0
56	3L	3	Total 3 Mg 3	0	0
56	1K	2	Total 2 Mg 2	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
56	4I	2	Total	Mg	0	0
			2	2		
56	2L	4	Total	Mg	0	0
			4	4		

- Molecule 57 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
57	14	1	Total	Zn	0	0
			1	1		
57	32	1	Total	Zn	0	0
			1	1		
57	3E	1	Total	Zn	0	0
			1	1		
57	1G	1	Total	Zn	0	0
			1	1		
57	G8	1	Total	Zn	0	0
			1	1		
57	5I	1	Total	Zn	0	0
			1	1		

- Molecule 58 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
58	13	230	Total	O	0	0
			230	230		
58	2L	1	Total	O	0	0
			1	1		
58	4L	2	Total	O	0	0
			2	2		
58	14	863	Total	O	0	0
			863	863		
58	3E	1	Total	O	0	0
			1	1		
58	4E	3	Total	O	0	0
			3	3		
58	8E	2	Total	O	0	0
			2	2		
58	1I	1	Total	O	0	0
			1	1		
58	3I	1	Total	O	0	0
			1	1		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
58	5I	1	Total 1	O 1	0	0
58	6I	1	Total 1	O 1	0	0
58	7I	1	Total 1	O 1	0	0
58	BI	1	Total 1	O 1	0	0
58	1K	6	Total 6	O 6	0	0
58	2K	8	Total 8	O 8	0	0
58	3K	1	Total 1	O 1	0	0
58	4K	4	Total 4	O 4	0	0
58	1H	1212	Total 1212	O 1212	0	0
58	1J	12	Total 12	O 12	0	0
58	16	21	Total 21	O 21	0	0
58	11	9	Total 9	O 9	0	0
58	21	3	Total 3	O 3	0	0
58	31	8	Total 8	O 8	0	0
58	58	3	Total 3	O 3	0	0
58	78	6	Total 6	O 6	0	0
58	98	1	Total 1	O 1	0	0
58	B8	1	Total 1	O 1	0	0
58	C8	3	Total 3	O 3	0	0
58	D8	1	Total 1	O 1	0	0
58	E8	2	Total 2	O 2	0	0

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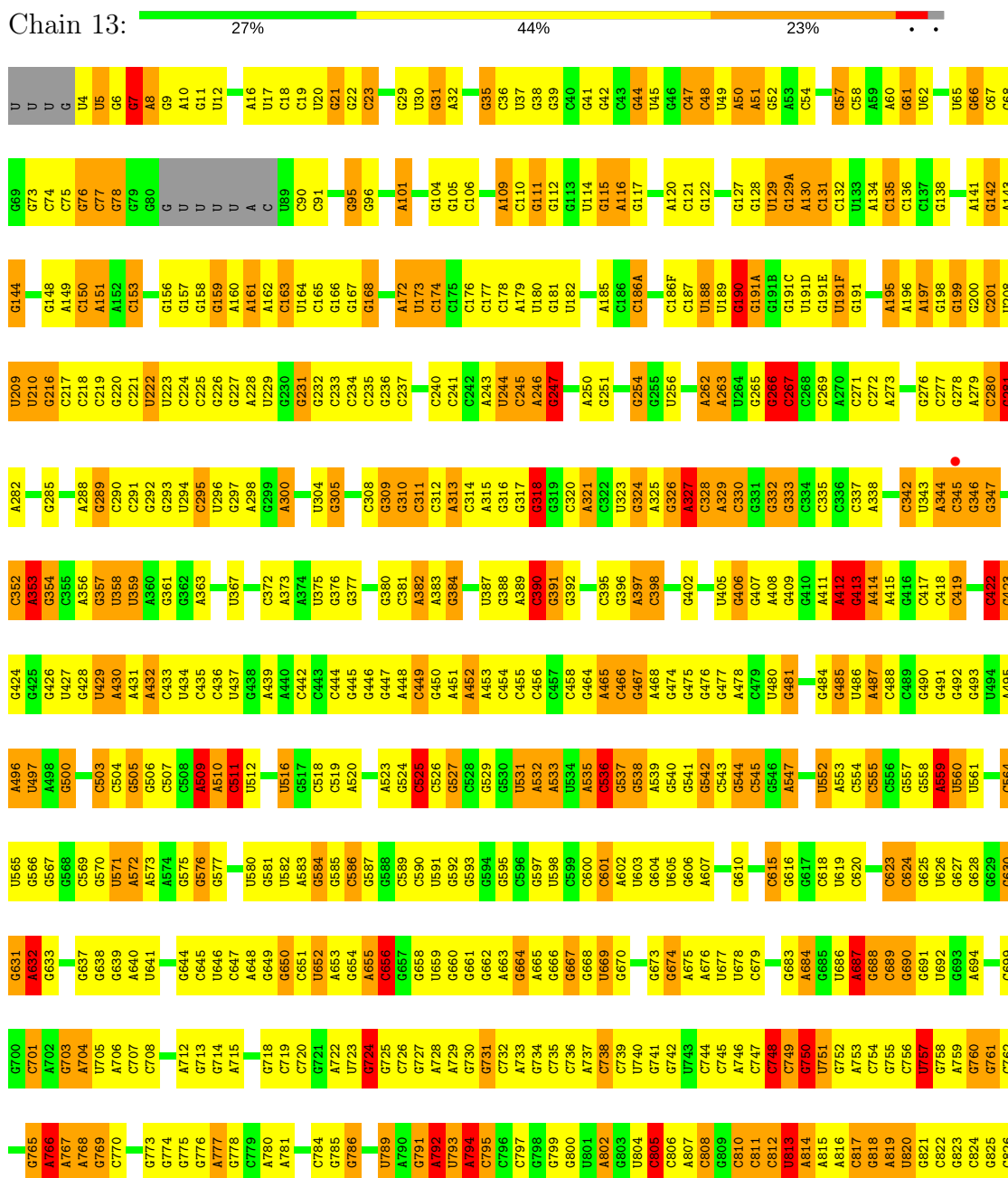
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
58	F8	2	Total	O	0	0
			2	2		
58	G8	3	Total	O	0	0
			3	3		
58	I8	5	Total	O	0	0
			5	5		
58	J8	1	Total	O	0	0
			1	1		
58	L8	1	Total	O	0	0
			1	1		
58	P8	4	Total	O	0	0
			4	4		
58	Q8	1	Total	O	0	0
			1	1		
58	1G	106	Total	O	0	0
			106	106		

### 3 Residue-property plots

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

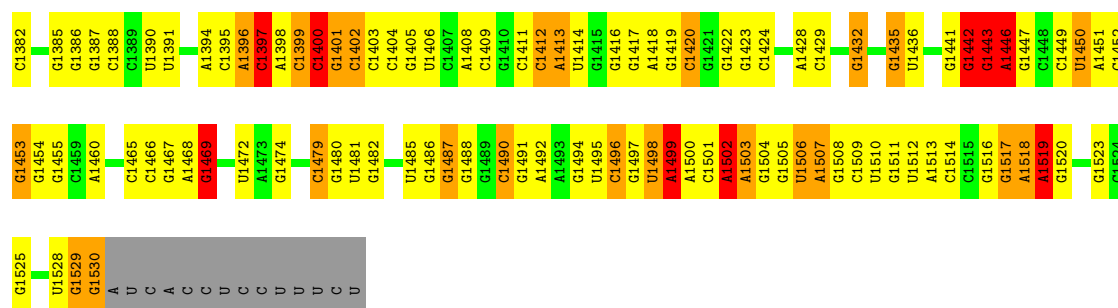
#### • Molecule 1: 16S ribosomal RNA



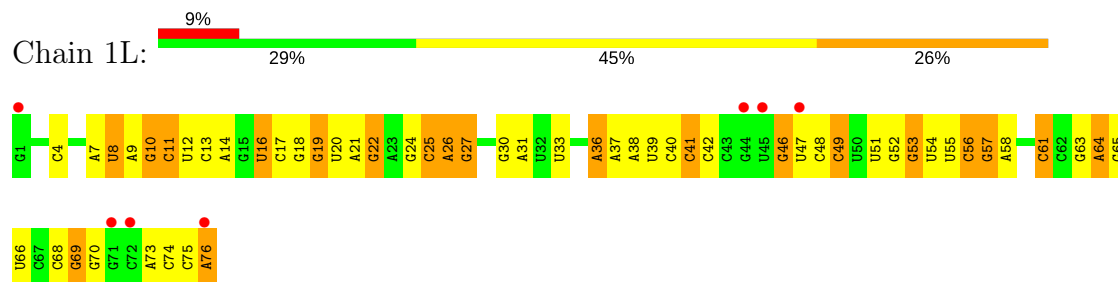




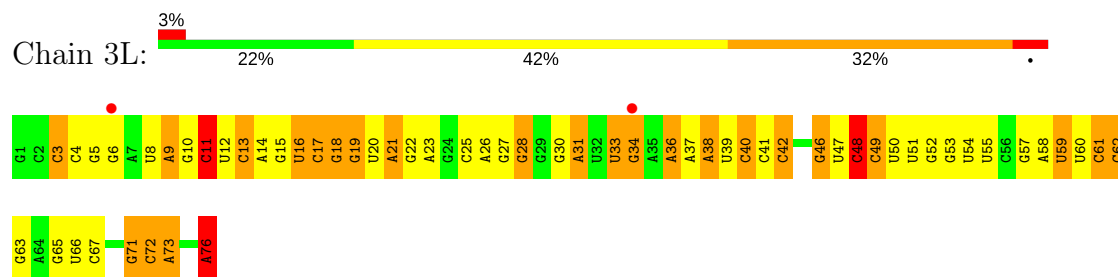
C1321	C1322	G1257	G1190	U1125	C1054	A994	G983	A864	U789	C719	A640	G575	C511	G361	C1321
G1258	G1259	C1260	A1191	U1126	A1055	C995	C994	A865	A790	C720	U641	G576	U512	G362	G289
C1261	C1262	C1263	G1192	G1127	G1057	G998	A935	C866	G791	G721	A642	C577	C513	A363	C290
C1264	C1265	C1266	C1193	C1128	G1057	C998A	C936	G867	A792	A722	C645	C578	G517	C366	C291
C1267	C1268	C1269	G1194	G1129	C1058	U999	A938	C868	A793	G723	U646	U580	G518	U367	G297
C1270	C1271	C1272	C1195	A1130	C1059	G999	C939	G869	A794	G724	C647	U581	C519	U368	A298
C1273	C1274	C1275	G1196	G1131	C1060	A1000	C940	A872	G800	G725	C648	U582	A520	U369	A299
C1276	C1277	C1278	G1197	C1132	G1061	G1001	G941	A873	U801	G726	A648	U583	A521	U370	A300
C1279	C1280	C1281	G1198	G1133	U1062	G1002	G942	A874	A802	G727	G649	U584	A522	C370	G301
C1282	C1283	C1284	G1199	G1134	C1063	G1003	G943	C875	G803	A728	G650	U585	A523	C371	G302
C1285	C1286	C1287	C1200	U1135	C1064	A1004	U944	C876	U804	G730	U652	U586	A524	C372	G303
C1288	C1289	C1290	G1201	U1136	U1065	A1005	G945	C879	C805	G731	A653	U587	A525	A373	A303
C1291	C1292	C1293	G1202	G1137	C1066	C1006	A946	C880	C806	C732	G654	U588	C526	A374	U304
C1294	C1295	C1296	C1203	G1138	A1067	G1009	G947	C881	A807	A733	A655	C589	G527	U375	G305
C1297	C1298	C1299	A1204	C1140	C1068	G1010	G948	C882	G807	A734	G660	C590	G528	G376	G306
C1300	C1301	C1302	G1205	U1141	C1069	G1011	C949	C883	C810	C735	G661	C591	G529	G377	G307
C1303	C1304	C1305	C1142	G1070	U1071	G1012	A950	C884	C811	C736	G662	C592	G530	A382	G308
C1306	C1307	C1308	G1143	C1071	U1072	A1014	U951	C885	C812	C737	G663	C593	G531	A383	G309
C1309	C1310	C1311	G1144	U1073	U1073	A1015	U952	C886	U813	C738	A683	C594	U531	A384	G310
C1312	C1313	C1314	C1145	U1074	C1075	A1016	G953	G887	A814	C739	G684	C595	A532	C385	G311
C1315	C1316	C1317	U1146	C1076	U1076	G1017	U954	G888	A815	C740	A665	U598	A533	C386	G312
C1318	C1319	C1320	G1077	U1077	G1077	U1020	U955	G889	A816	C741	G666	C599	C536	U387	G313
C1321	C1322	C1323	G1081	U1081	G1081	G1023	U956	C890	C817	C742	G667	C600	G537	C380	G314
C1324	C1325	C1326	G1082	U1082	G1082	U1024	U957	C891	C818	C743	G668	C601	G538	C381	G315
C1327	C1328	C1329	U1085	U1085	U1085	U1025	A958	C892	A819	C744	G673	A602	A539	C391	G316
C1330	C1331	C1332	U1086	U1086	U1086	U1026	A959	C893	U820	C745	G674	A603	G540	C392	G317
C1333	C1334	C1335	U1087	U1087	U1087	U1027	A960	C894	U821	C746	G675	A604	G541	C393	G318
C1336	C1337	C1338	U1088	U1088	U1088	U1028	A961	C895	A822	C747	G676	A605	G542	C394	G319
C1339	C1340	C1341	U1089	U1089	U1089	U1029	A962	C896	G829	C748	G677	A606	G543	C395	G320
C1342	C1343	C1344	U1090	U1090	U1090	U1030	C967	C897	A830	C749	G678	A607	C544	C396	G321
C1345	C1346	C1347	U1091	U1091	U1091	U1031	A968	C898	U831	C750	G679	A608	C545	C397	G322
C1348	C1349	C1350	U1092	U1092	U1092	U1032	A969	C899	G825	C751	G680	A609	C546	C398	G323
C1351	C1352	C1353	U1093	U1093	U1093	U1033	C970	C904	G826	C752	G681	A610	C547	C401	G324
C1354	C1355	C1356	U1094	U1094	U1094	U1034	C971	U905	G827	C753	G682	A611	C548	C402	G325
C1357	C1358	C1359	U1095	U1095	U1095	U1035	C972	G906	G828	C754	G683	A612	C549	C403	G326
C1360	C1361	C1362	U1096	U1096	U1096	U1036	C973	A909	G829	C755	G684	A613	C550	C404	G327
C1363	C1364	C1365	U1097	U1097	U1097	U1037	A974	C910	A841	C756	G685	A614	C551	C405	G328
C1366	C1367	C1368	U1098	U1098	U1098	U1038	A975	U911	C842	C757	G686	A615	C552	C406	G329
C1369	C1370	C1371	U1099	U1099	U1099	U1039	C976	C912	U843	C758	G687	A616	C553	C407	G330
C1372	C1373	C1374	U1100	U1100	U1100	U1040	A977	A913	C848	C759	G688	A617	C554	C408	G331
C1375	C1376	C1377	U1101	U1101	U1101	U1041	A978	A914	C849	C760	G689	A618	C555	C409	G332
C1378	C1379	C1380	U1102	U1102	U1102	U1042	C979	A915	U850	C761	G690	A619	C556	C410	G333
C1381	C1382	C1383	U1103	U1103	U1103	U1043	C980	A916	U851	C762	G691	A620	C557	C411	G334
C1384	C1385	C1386	U1104	U1104	U1104	U1044	U981	C917	C852	C763	G692	A621	C558	C412	G335
C1387	C1388	C1389	U1105	U1105	U1105	U1045	U982	A918	C853	C764	G693	A622	C559	C413	G336
C1390	C1391	C1392	U1106	U1106	U1106	U1046	A983	A919	C854	C765	G694	A623	C560	C414	G337
C1393	C1394	C1395	U1107	U1107	U1107	U1047	C984	U920	G855	C766	G695	A624	C561	C415	G338
C1396	C1397	C1398	U1108	U1108	U1108	U1048	C985	U921	C856	C767	G696	A625	C562	C416	G339
C1399	C1400	C1401	U1109	U1109	U1109	U1049	A986	U922	C857	C768	G697	A626	C563	C417	G340
C1402	C1403	C1404	U1110	U1110	U1110	U1050	U987	C924	C858	C769	G698	A627	C564	C418	G341
C1405	C1406	C1407	U1111	U1111	U1111	U1051	G988	C925	C859	C770	G699	A628	C565	C419	G342
C1408	C1409	C1410	U1112	U1112	U1112	U1052	U991	C926	A860	C771	G700	A629	C566	C420	G343
C1411	C1412	C1413	U1113	U1113	U1113	U1053	U992	C927	C861	C772	G701	A630	C567	C421	G344
C1414	C1415	C1416	U1114	U1114	U1114	U1054	G993	C928	C862	C773	G702	A631	C568	C422	G345
C1417	C1418	C1419	U1115	U1115	U1115	U1055	U994	C929	C863	C774	G703	A632	C569	C423	G346
C1420	C1421	C1422	U1116	U1116	U1116	U1056	U995	C930	C864	C775	G704	A633	C570	C424	G347
C1423	C1424	C1425	U1117	U1117	U1117	U1057	G996	C931	C865	C776	G705	A634	C571	C425	G348
C1426	C1427	C1428	U1118	U1118	U1118	U1058	U997	C932	C866	C777	G706	A635	C572	C426	G349
C1429	C1430	C1431	U1119	U1119	U1119	U1059	U998	C933	C867	C778	G707	A636	C573	C427	G350
C1432	C1433	C1434	U1120	U1120	U1120	U1060	U999	C934	C868	C779	G708	A637	C574	C428	G351
C1435	C1436	C1437	U1121	U1121	U1121	U1061	G999	C935	C869	C780	G709	A638	C575	C429	G352
C1438	C1439	C1440	U1122	U1122	U1122	U1062	U999	C936	C870	C781	G710	A639	C576	C430	G353
C1441	C1442	C1443	U1123	U1123	U1123	U1063	U999	C937	C871	C782	G711	A640	C577	C431	G354
C1444	C1445	C1446	U1124	U1124	U1124	U1064	U999	C938	C872	C783	G712	A641	C578	C432	G355
C1447	C1448	C1449	U1125	U1125	U1125	U1065	U999	C939	C873	C784	G713	A642	C579	C433	G356
C1450	C1451	C1452	U1126	U1126	U1126	U1066	U999	C940	C874	C785	G714	A643	C580	C434	G357
C1453	C1454	C1455	U1127	U1127	U1127	U1067	U999	C941	C875	C786	G715	A644	C581	C435	G358
C1456	C1457	C1458	U1128	U1128	U1128	U1068	U999	C942	C876	C787	G716	A645	C582	C436	G359
C1459	C1460	C1461	U1129	U1129	U1129	U1069	U999	C943	C877	C788	G717	A646	C583	C437	G360
C1462	C1463	C1464	U1130	U1130	U1130	U1070	U999	C944	C878	C789	G718	A647	C584	C438	G361
C1465	C1466	C1467	U1131	U1131	U1131	U1071	U999	C945	C879	C790	G719	A648	C585	C439	G362
C1468	C1469	C1470	U1132	U1132	U1132	U1072	U999	C946	C880	C791	G720	A649	C586	C440	G363
C1471	C1472	C1473	U1133	U1133	U1133	U1073	U999	C947	C881	C792	G721	A650	C587	C441	G364
C1474	C1475	C1476	U1134	U1134	U1134	U1074	U999	C948	C882	C793	G722	A651	C588	C442	G365
C1477	C1478	C1479	U1135	U1135	U1135	U1075	U999	C949	C883	C794	G723	A652	C589	C443	G366
C1480	C1481	C1482	U1136	U1136	U1136	U1076	U999	C950	C884	C795	G724	A653	C590	C444	G367
C1483	C1484	C1485	U1137	U1137	U1137	U1077	U999	C951	C885	C796	G725	A654	C591	C445	G368
C1486	C1487	C1488	U1138	U1138	U1138	U1078	U999	C952	C886	C797	G726	A655	C592	C446	G369
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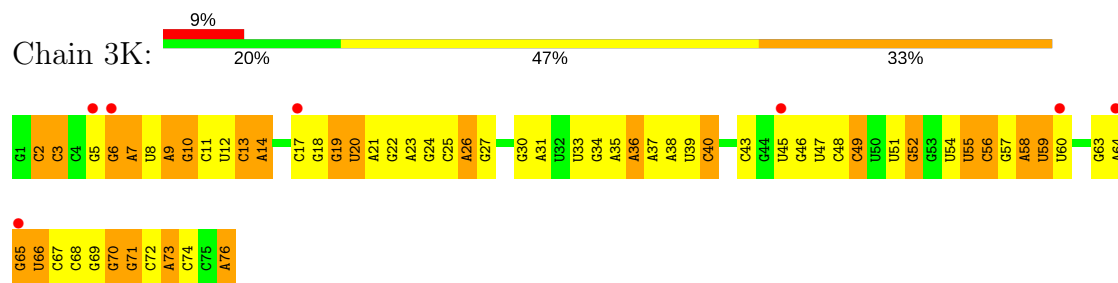
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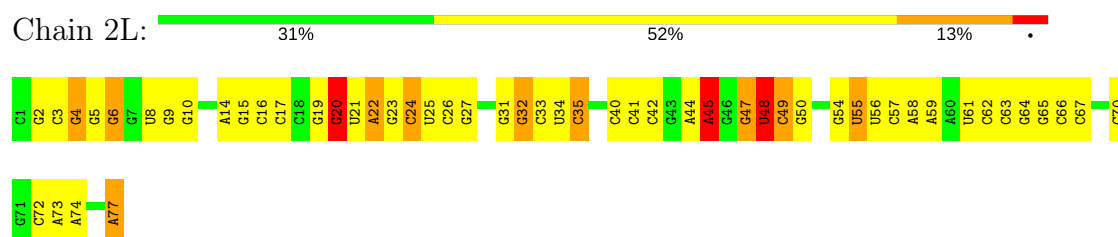
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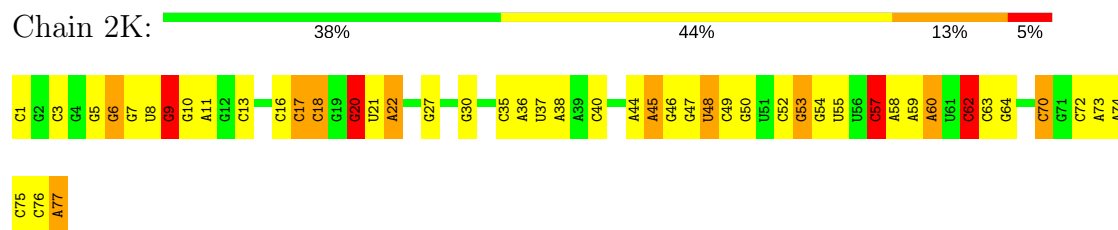
- Molecule 2: tRNA-Phe



- Molecule 3: tRNA-fMet



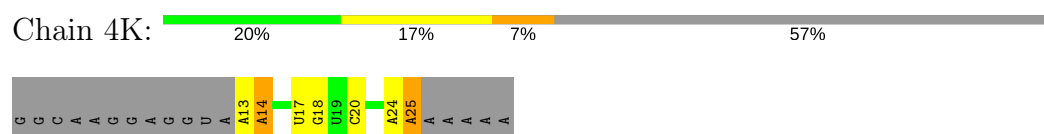
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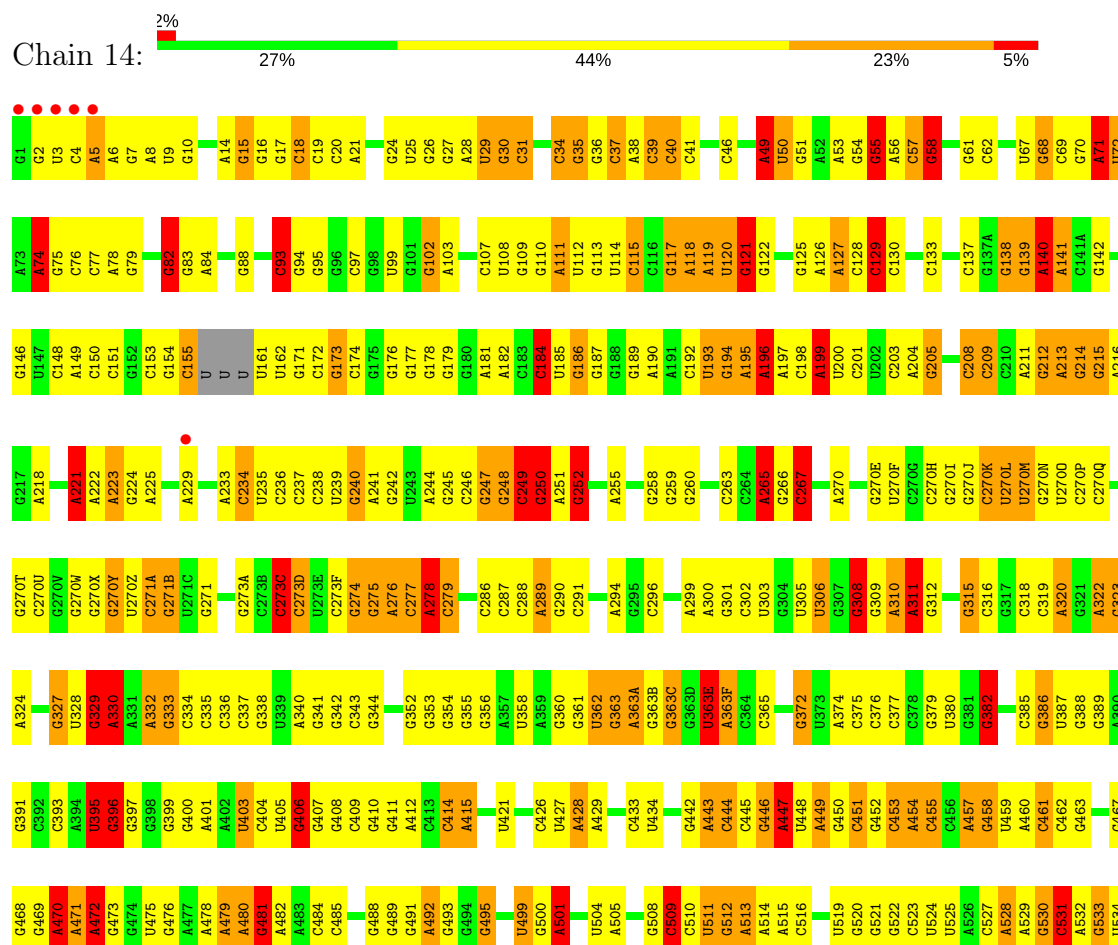
• Molecule 4: RNA (30-MER)



• Molecule 4: RNA (30-MER)

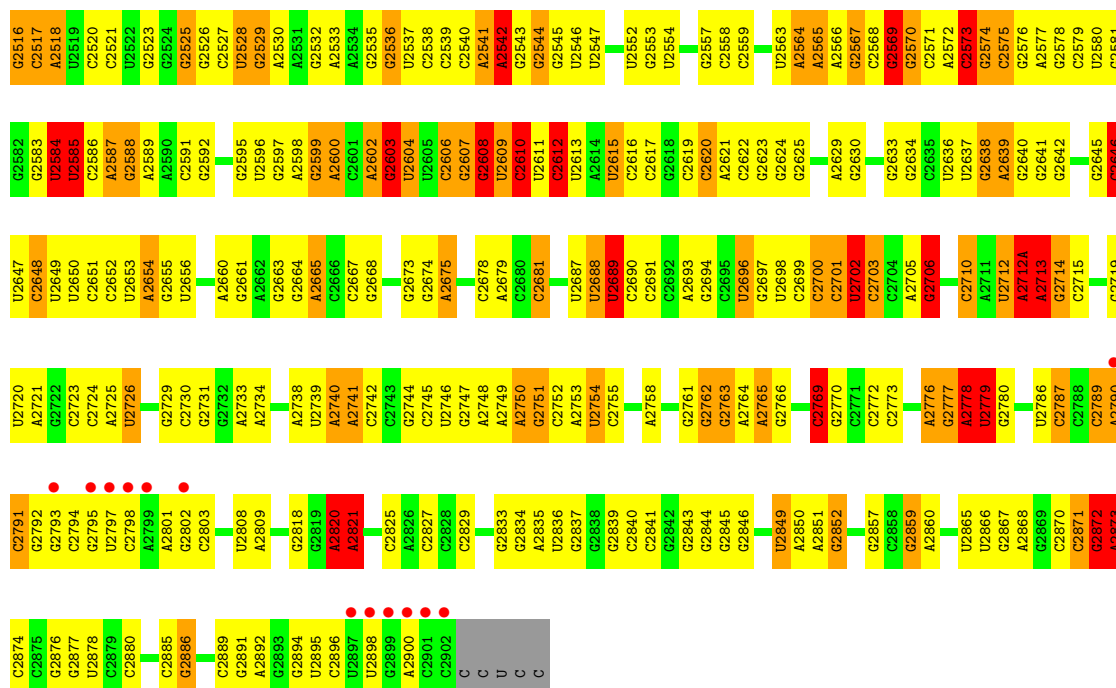


• Molecule 5: 23S ribosomal RNA

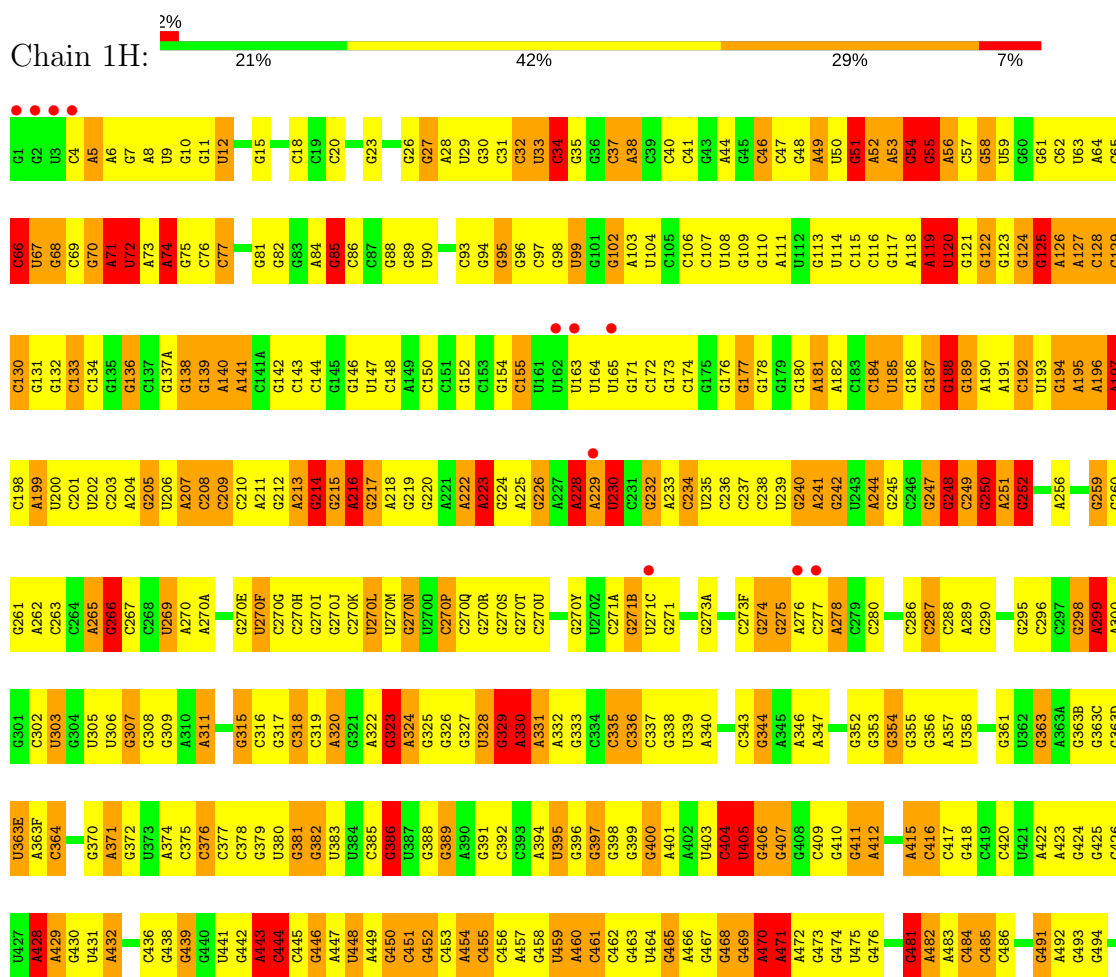


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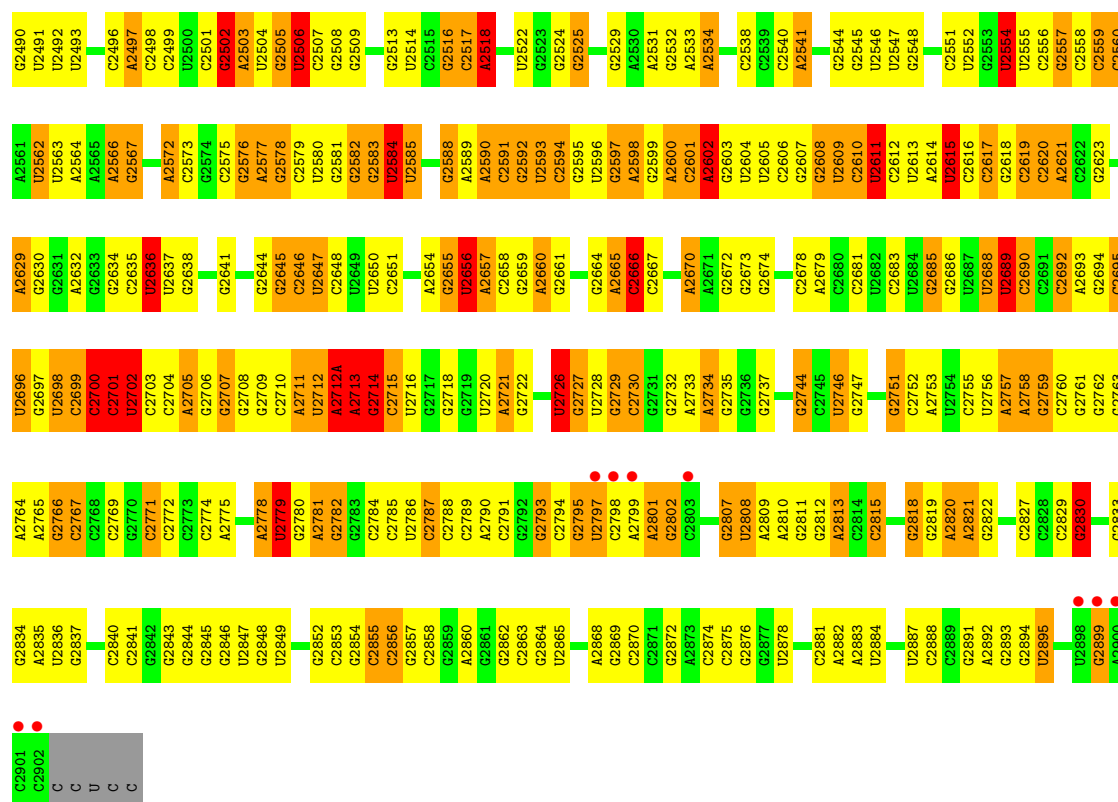
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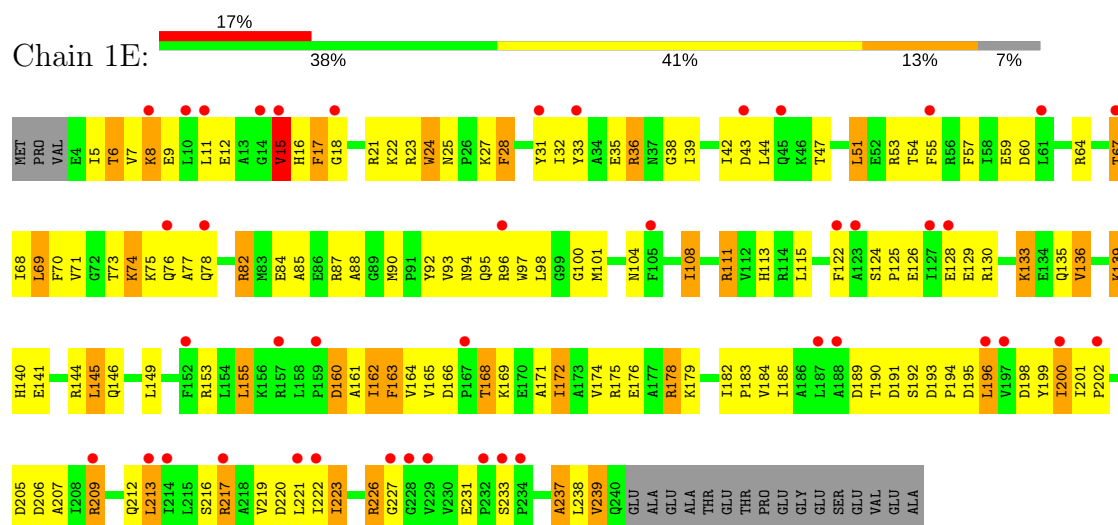


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G1984	C1985	U1986	C1987	U1988	U1989	A1990	U1991	U1992	U1993	U1994	U1995	U1996	U1997	U1998	U1999	U2000	U2001	U2002	U2003	U2004	U2005	U2006	U2007	U2008	U2009	U2010	U2011	U2012	U2013	U2014	U2015	U2016	U2017	U2018	U2019	U2020	U2021	U2022	U2023	U2024	U2025	U2026	U2027	U2028	U2029	U2030	U2031	U2032	U2033	U2034	U2035	U2036	U2037	U2038	U2039	U2040	U2041	U2042	U2043	U2044	U2045	U2046	U2047	U2048	U2049	U2050	U2051	U2052	U2053	U2054	U2055	U2056	U2057	U2058	U2059	U2060	U2061	U2062	U2063	U2064	U2065	U2066	U2067	U2068	U2069	U2070	U2071	U2072	U2073	U2074	U2075	U2076	U2077	U2078	U2079	U2080	U2081	U2082	U2083	U2084	U2085	U2086	U2087	U2088	U2089	U2090	U2091	U2092	U2093	U2094	U2095	U2096	U2097	U2098	U2099	U2100	U2101	U2102	U2103	U2104	U2105	U2106	U2107	U2108	U2109	U2110	U2111	U2112	U2113	U2114	U2115	U2116	U2117	U2118	U2119	U2120	U2121	U2122	U2123	U2124	U2125	U2126	U2127	U2128	U2129	U2130	U2131	U2132	U2133	U2134	U2135	U2136	U2137	U2138	U2139	U2140	U2141	U2142	U2143	U2144	U2145	U2146	U2147	U2148	U2149	U2150	U2151	U2152	U2153	U2154	U2155	U2156	U2157	U2158	U2159	U2160	U2161
C2095	U2096	G2100	G2101	G2102	G2103	G2104	C2105	G2106	C2107	G2108	U2109	G2110	C2111	G2112	U2113	U2114	G2115	U2116	U2117	U2118	U2119	U2120	U2121	U2122	U2123	U2124	U2125	U2126	U2127	U2128	U2129	U2130	U2131	U2132	U2133	U2134	U2135	U2136	U2137	U2138	U2139	U2140	U2141	U2142	U2143	U2144	U2145	U2146	U2147	U2148	U2149	U2150	U2151	U2152	U2153	U2154	U2155	U2156	U2157	U2158	U2159	U2160	U2161																																																																																																																		
G2162	C2163	C2164	G2165	G2166	U2167	G2168	A2169	A2170	A2171	U2172	G2173	A2174	C2175	A2176	C2177	G2178	G2179	U2180	G2181	G2182	G2183	G2184	C2185	G2186	G2190	G2191	G2192	G2193	G2194	A2195	A2196	G2197	G2198	G2199	G2200	G2201	G2202	G2203	G2204	G2205	G2206	G2207	G2208	G2209	G2210	G2211	A2212	U2213	G2214	G2215	G2216	G2217	G2220	A2221	A2222	A2223	A2224	A2225	A2226	A2227	A2228	A2229	G2230	G2231	U2232	U2233	G2234	G2235	G2236	G2237	G2238	G2239	G2240																																																																																																								
A2241	G2242	U2243	U2244	A2245	G2246	A2247	A2248	U2249	G2250	G2251	G2252	G2253	C2254	G2255	G2256	U2257	G2258	G2259	G2260	G2261	U2262	G2263	G2264	U2265	A2266	A2267	A2268	A2269	G2270	G2271	U2272	A2273	A2274	C2275	G2276	G2277	A2278	G2279	G2280	G2281	G2282	C2283	G2284	G2285	A2286	A2287	A2288	G2289	G2290	U2291	G2292	G2293	G2294	G2295	G2296	G2297	A2298	G2299	G2300	G2301																																																																																																																					
G2302	G2303	A2304	A2305	G2306	G2307	G2308	A2309	A2310	A2311	U2312	G2313	C2314	G2315	G2316	G2317	G2318	G2319	A2320	G2321	G2322	G2323	G2324	G2325	G2326	A2327	A2328	G2329	G2330	G2331	A2332	A2333	G2334	A2335	G2336	G2337	G2338	G2339	G2340	G2341	G2342	G2343	U2344	G2345	A2346	G2347	U2348	G2349	C2350	G2351	A2352	G2353	G2354	G2355	G2356	U2357	G2358	G2359	A2360																																																																																																																							

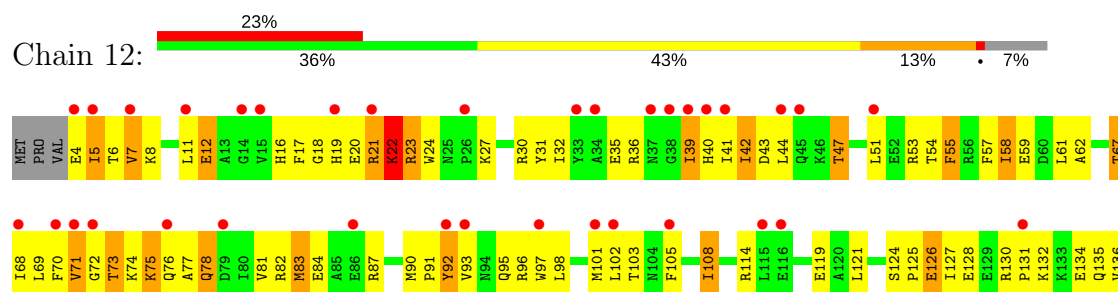


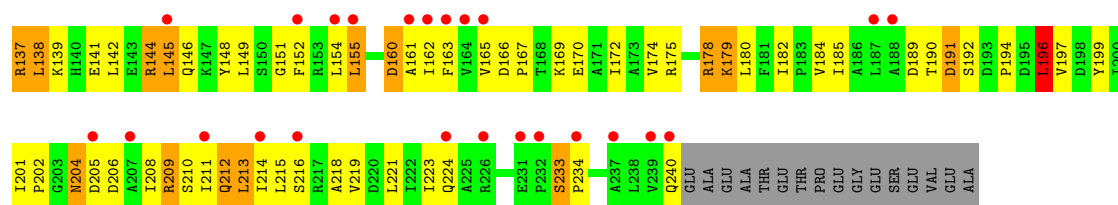


### • Molecule 6: 30S ribosomal protein S2



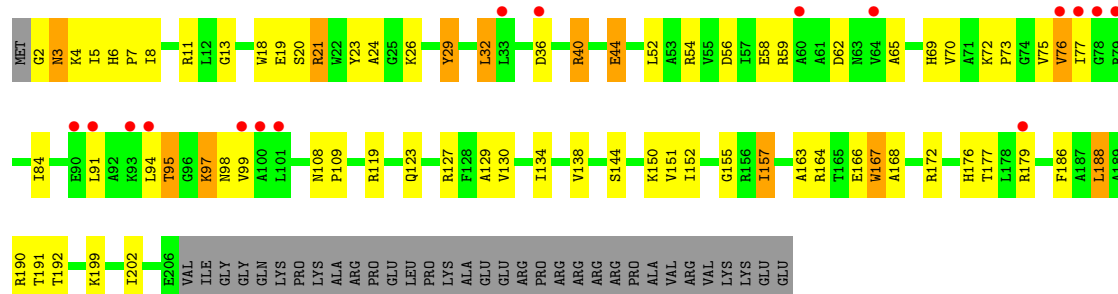
### • Molecule 6: 30S ribosomal protein S2





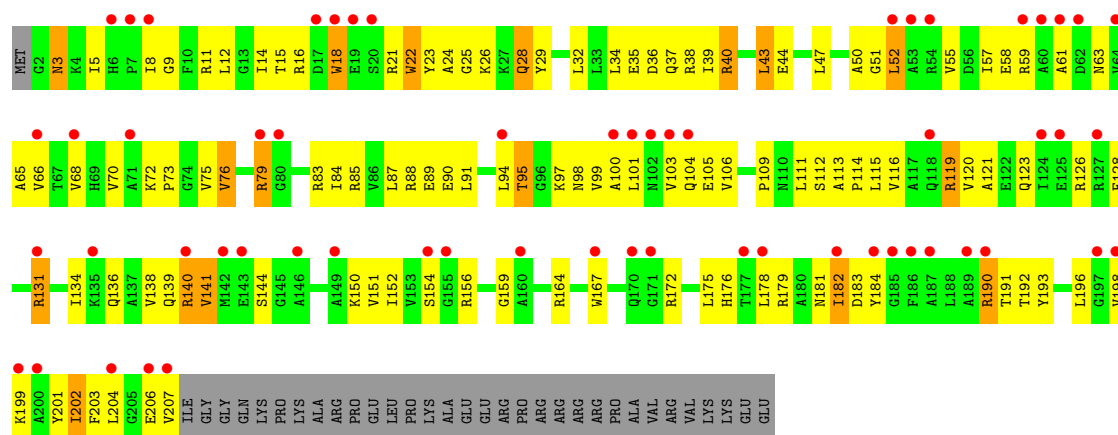
• Molecule 7: 30S ribosomal protein S3

Chain 2E:



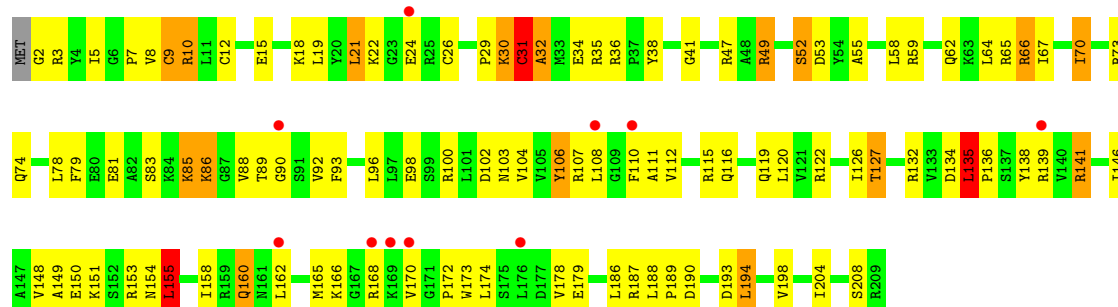
• Molecule 7: 30S ribosomal protein S3

Chain 22:

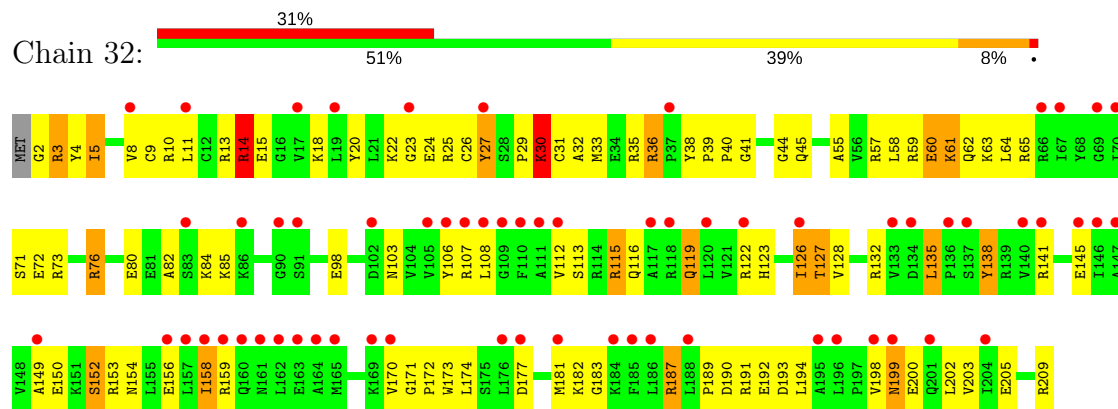


• Molecule 8: 30S ribosomal protein S4

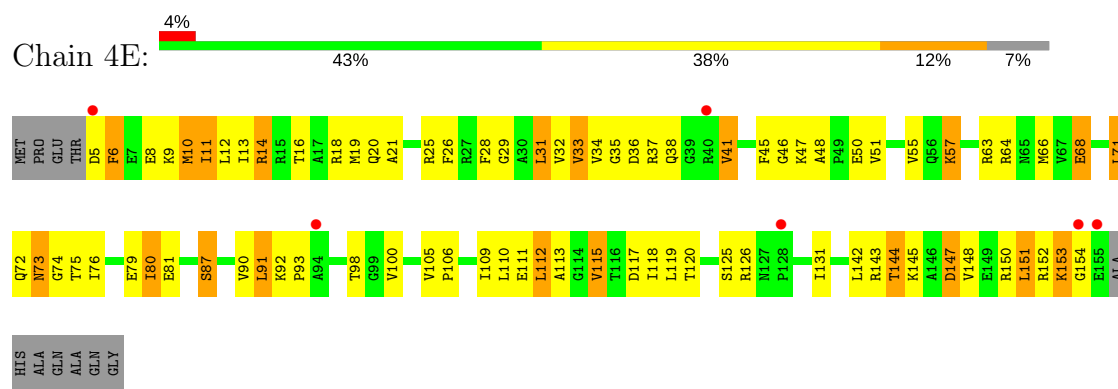
Chain 3E:



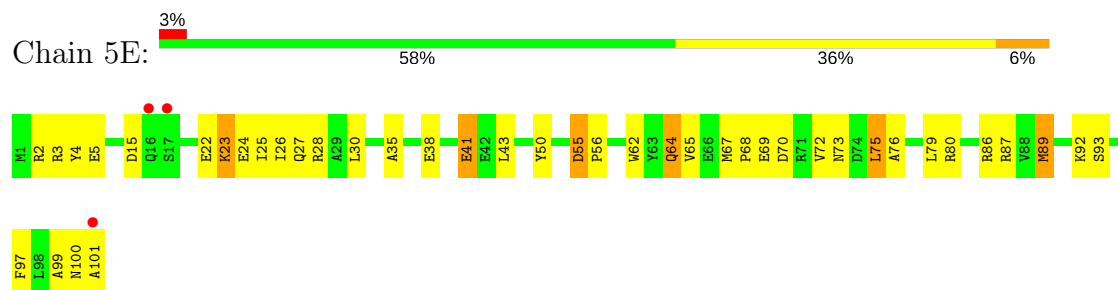
- Molecule 8: 30S ribosomal protein S4



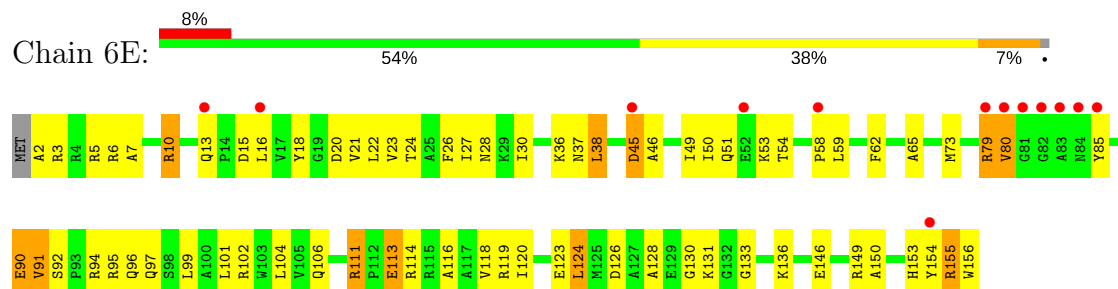
- Molecule 9: 30S ribosomal protein S5



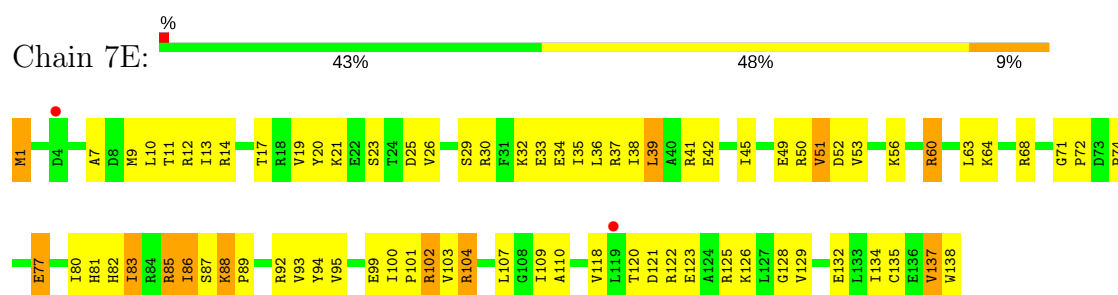
- Molecule 10: 30S ribosomal protein S6



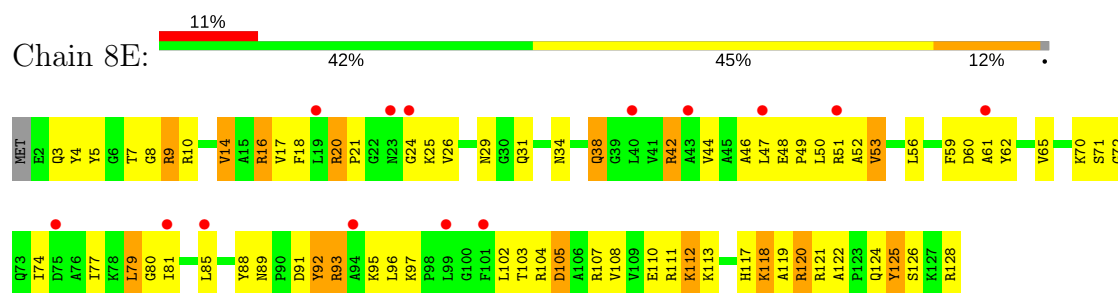
- Molecule 11: 30S ribosomal protein S7



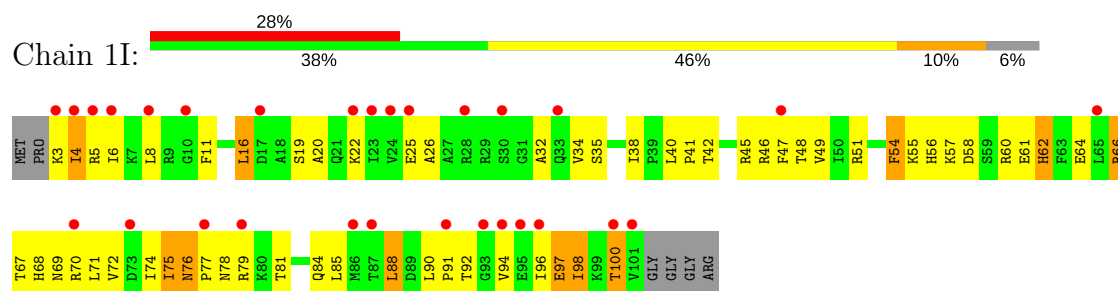
- Molecule 12: 30S ribosomal protein S8



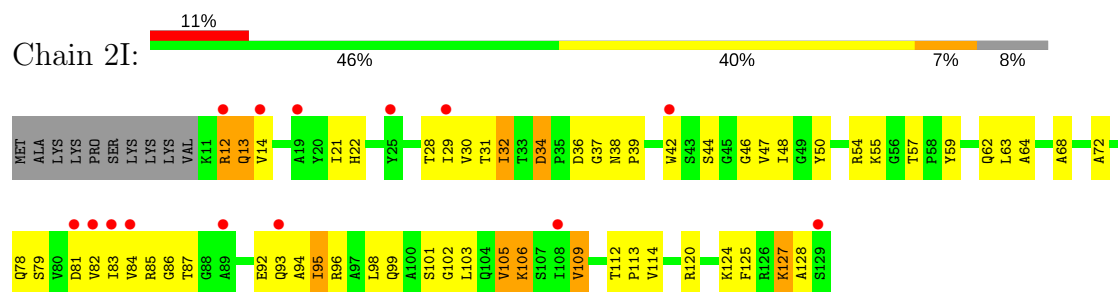
• Molecule 13: 30S ribosomal protein S9



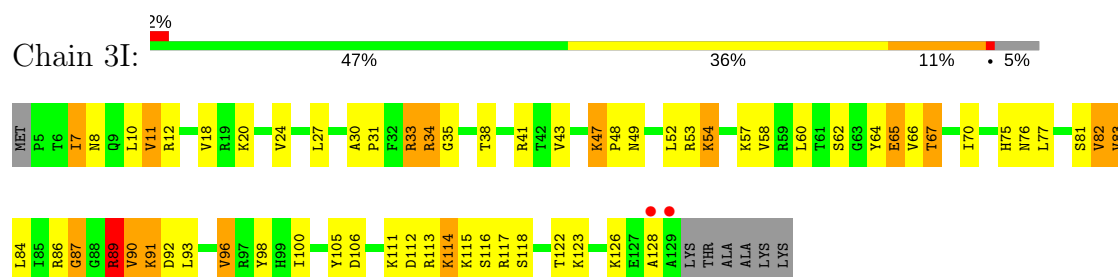
• Molecule 14: 30S ribosomal protein S10



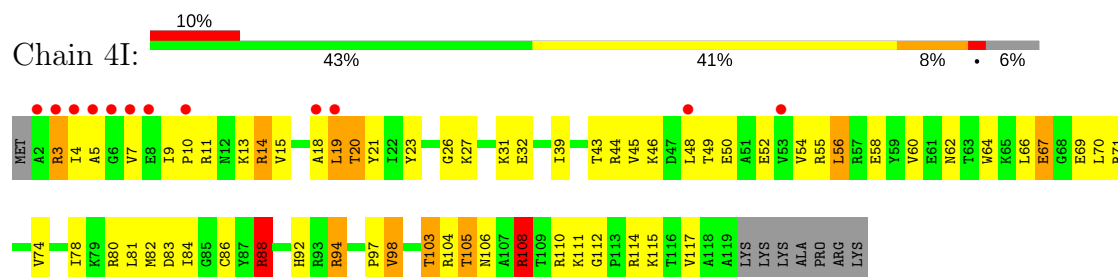
• Molecule 15: 30S ribosomal protein S11



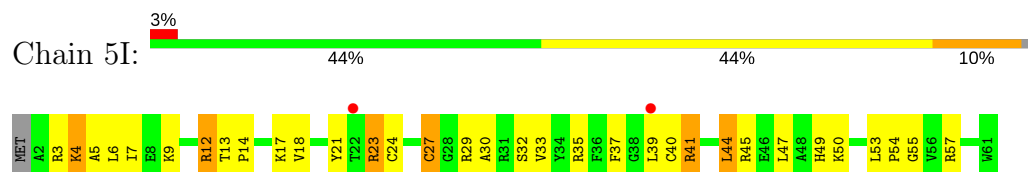
• Molecule 16: 30S ribosomal protein S12



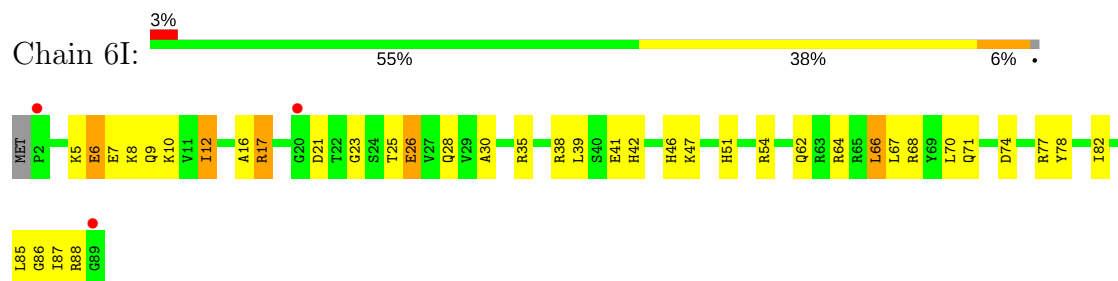
- Molecule 17: 30S ribosomal protein S13



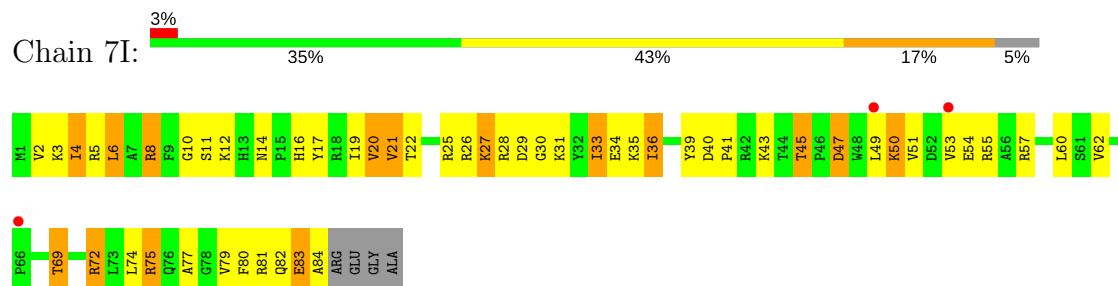
- Molecule 18: 30S ribosomal protein S14 type Z



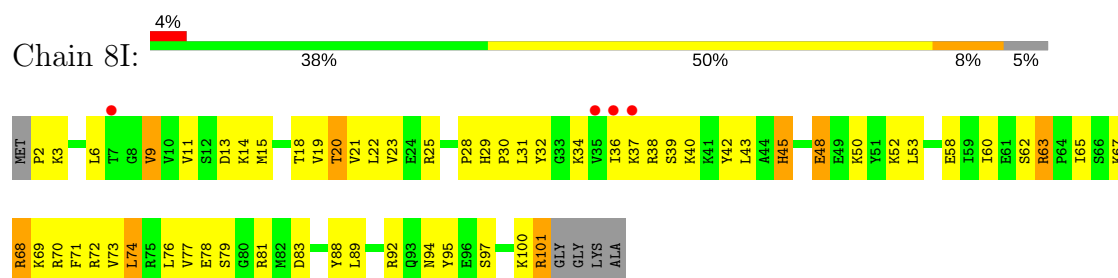
- Molecule 19: 30S ribosomal protein S15



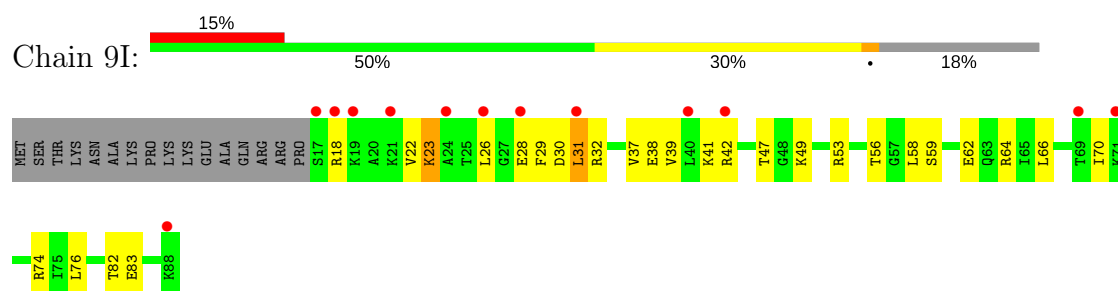
- Molecule 20: 30S ribosomal protein S16



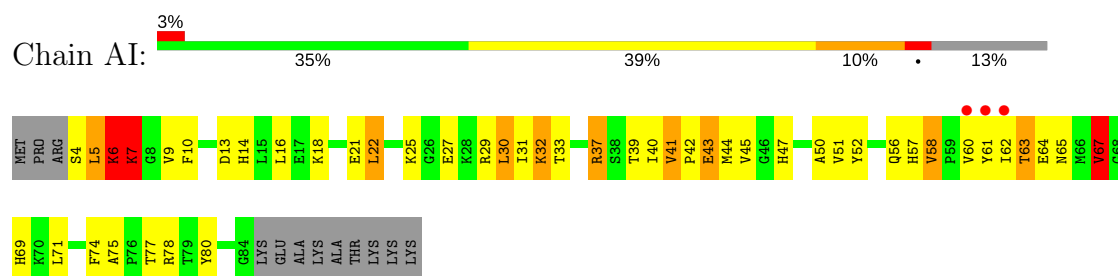
- Molecule 21: 30S ribosomal protein S17



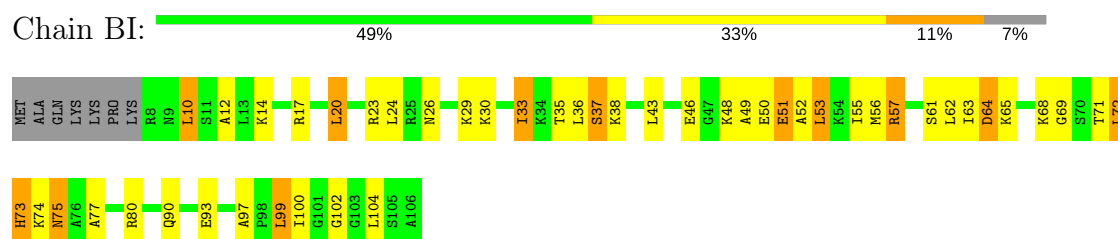
- Molecule 22: 30S ribosomal protein S18



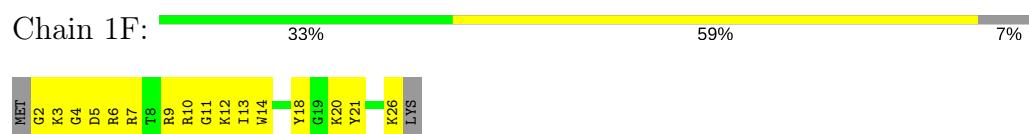
- Molecule 23: 30S ribosomal protein S19



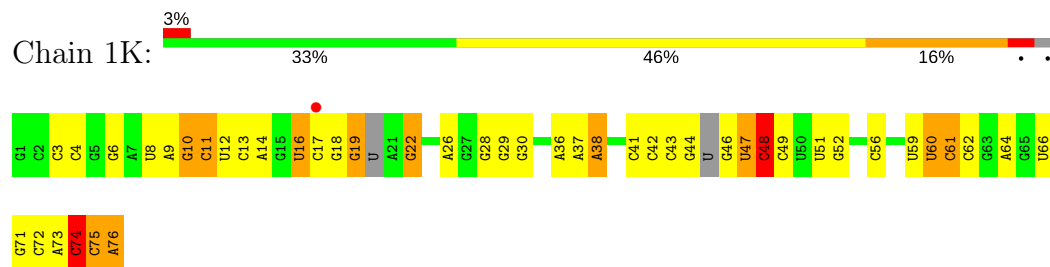
- Molecule 24: 30S ribosomal protein S20



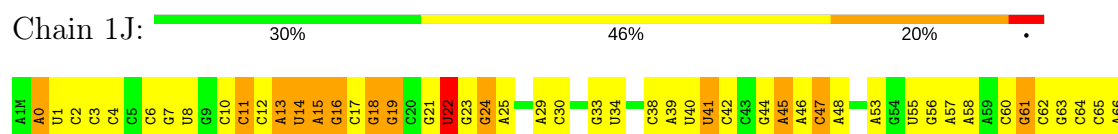
- Molecule 25: 30S ribosomal protein Thx

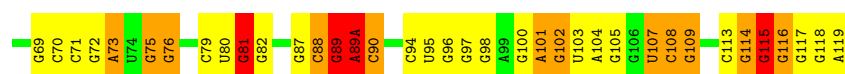


- Molecule 26: tRNA-Phe

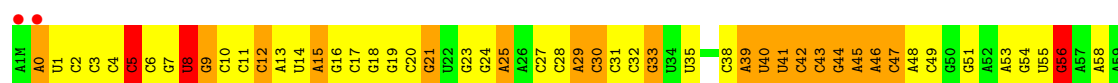


- Molecule 27: 5S ribosomal RNA

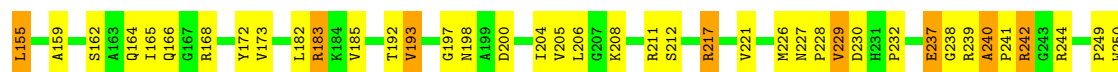
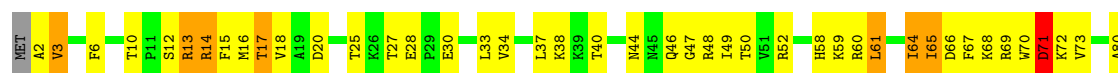




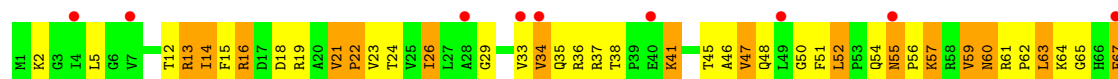
• Molecule 27: 5S ribosomal RNA



• Molecule 28: 50S ribosomal protein L2

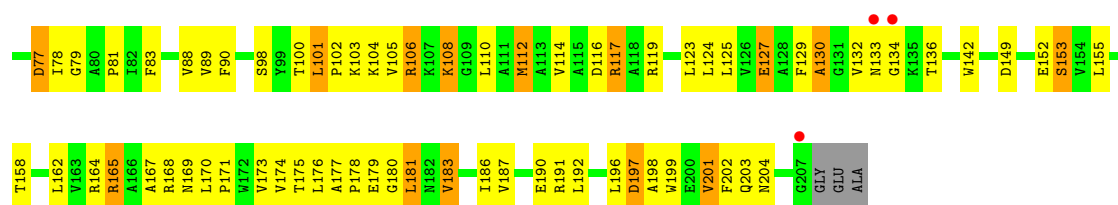


• Molecule 29: 50S ribosomal protein L3

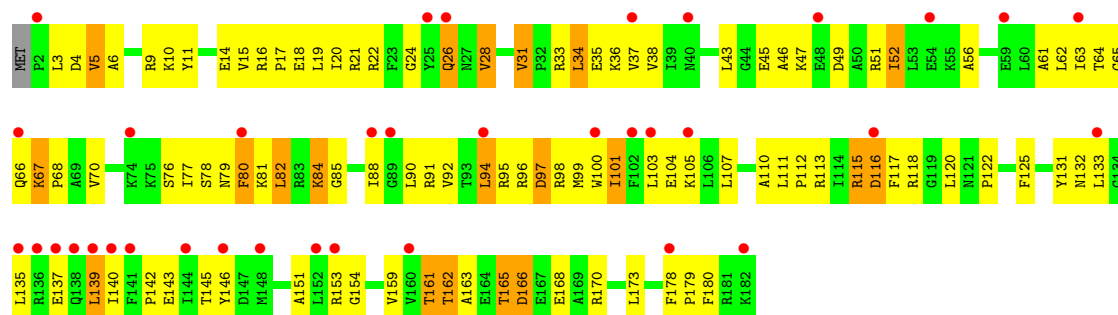
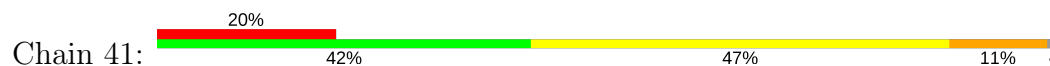


• Molecule 30: 50S ribosomal protein L4

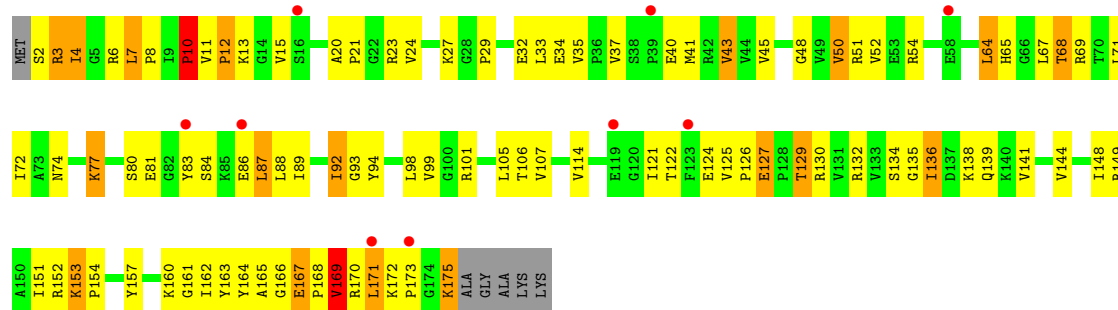




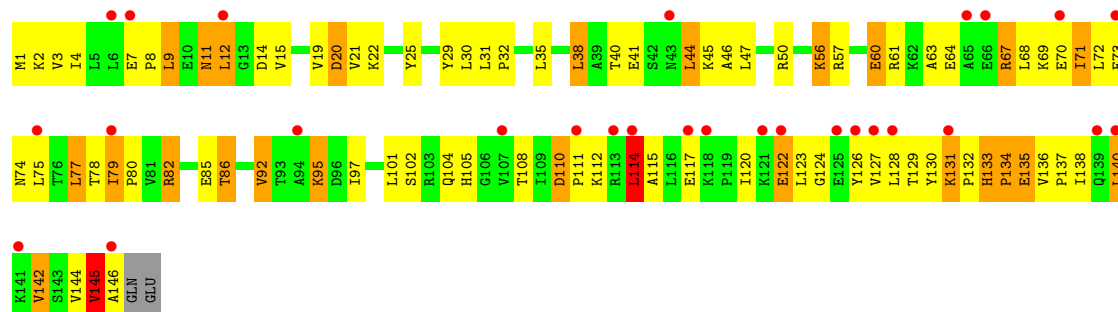
• Molecule 31: 50S ribosomal protein L5



• Molecule 32: 50S ribosomal protein L6

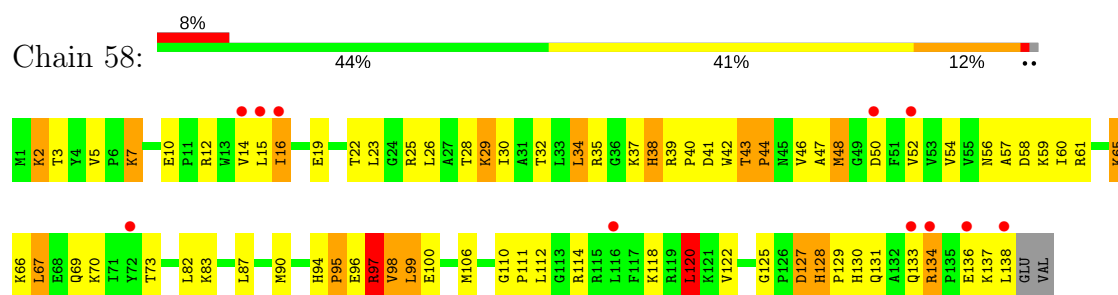


• Molecule 33: 50S ribosomal protein L9

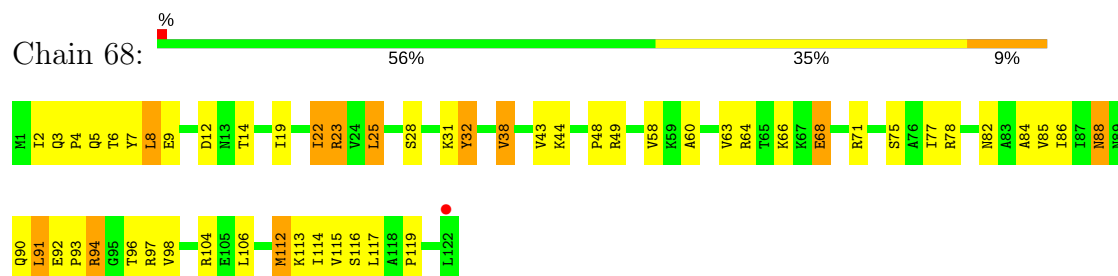


• Molecule 34: 50S ribosomal protein L13

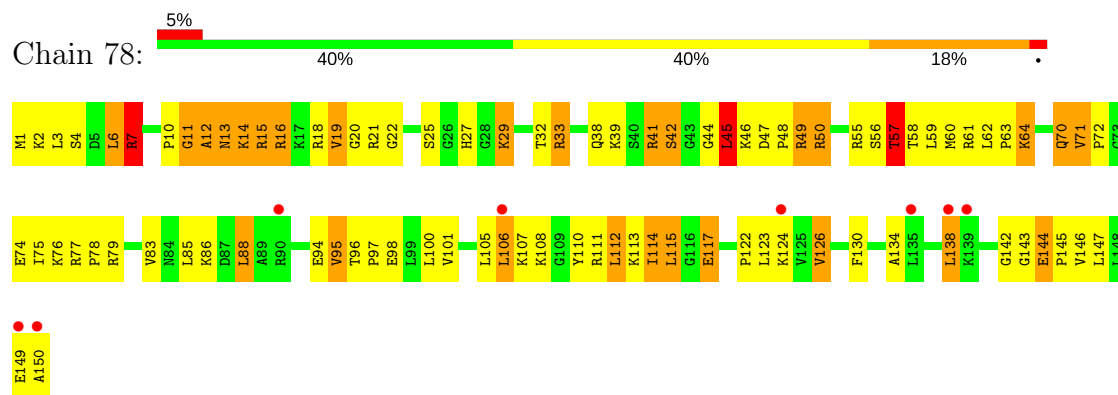




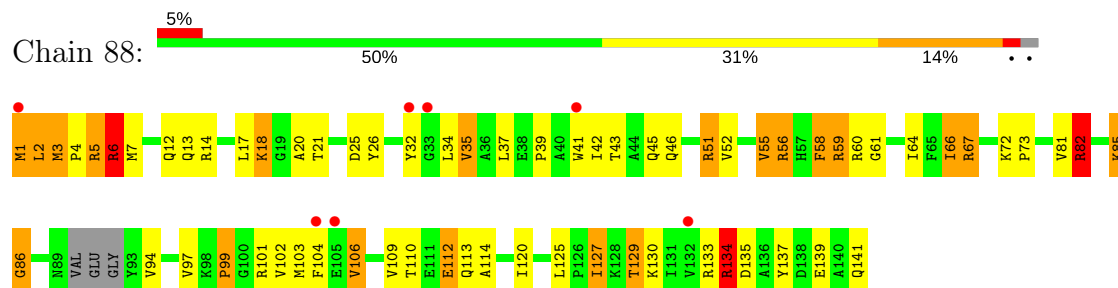
• Molecule 35: 50S ribosomal protein L14



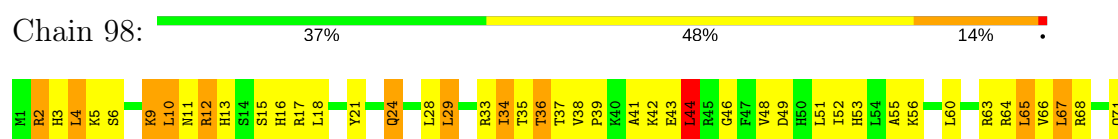
• Molecule 36: 50S ribosomal protein L15



• Molecule 37: 50S ribosomal protein L16



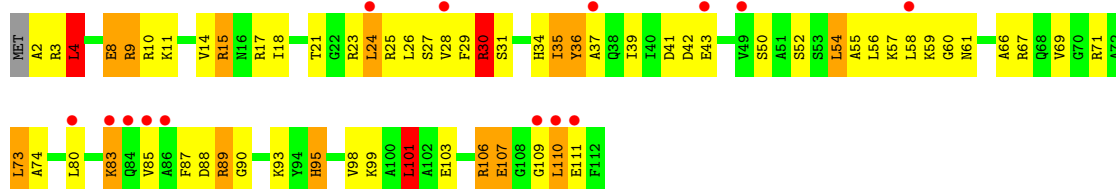
• Molecule 38: 50S ribosomal protein L17





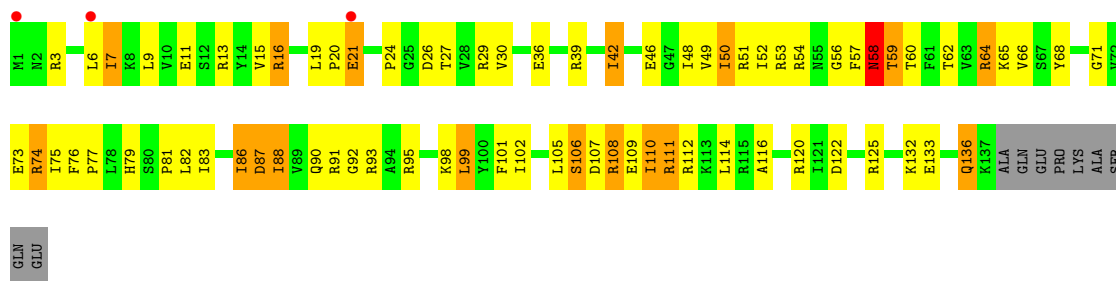
• Molecule 39: 50S ribosomal protein L18

Chain A8: 13% 43% 41% 13%



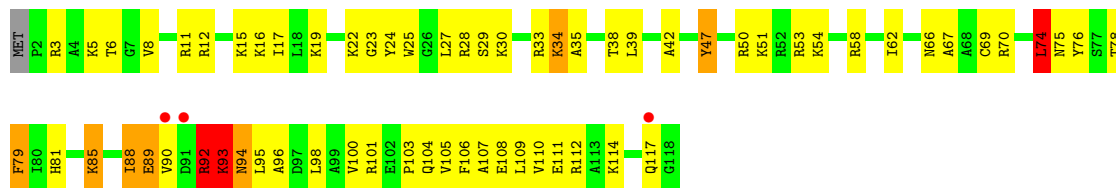
• Molecule 40: 50S ribosomal protein L19

Chain B8: 2% 42% 39% 12% 6%



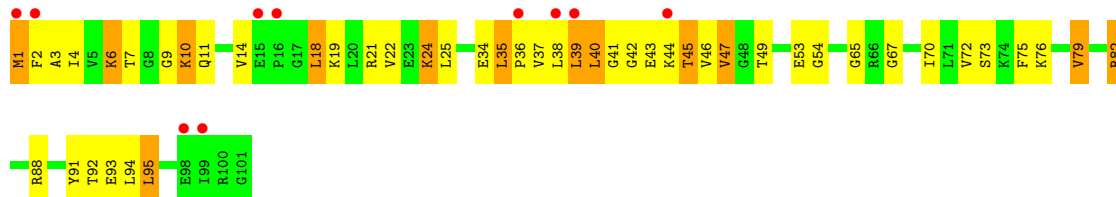
• Molecule 41: 50S ribosomal protein L20

Chain C8: 3% 44% 47% 6%



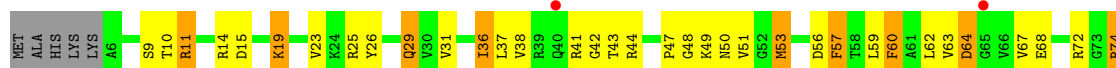
• Molecule 42: 50S ribosomal protein L21

Chain D8: 10% 52% 35% 13%



• Molecule 43: 50S ribosomal protein L22

Chain E8: 4% 58% 33% 10%

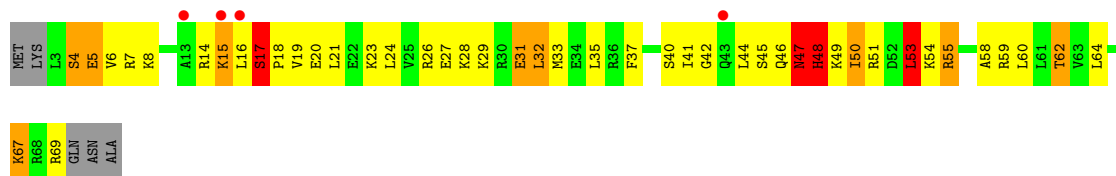




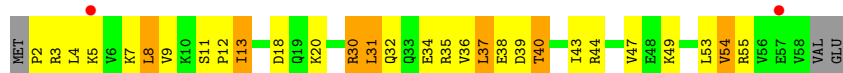
- Molecule 48: 50S ribosomal protein L28



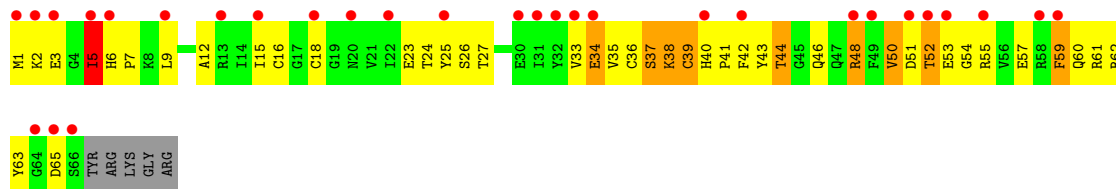
- Molecule 49: 50S ribosomal protein L29



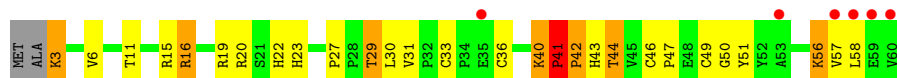
- Molecule 50: 50S ribosomal protein L30



- Molecule 51: 50S ribosomal protein L31



- Molecule 52: 50S ribosomal protein L32



- Molecule 53: 50S ribosomal protein L33



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	209.40Å 447.70Å 619.40Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	151.96 – 3.05 254.70 – 3.05	Depositor EDS
% Data completeness (in resolution range)	99.9 (151.96-3.05) 92.8 (254.70-3.05)	Depositor EDS
$R_{merge}$	0.33	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.58 (at 3.07Å)	Xtriage
Refinement program	PHENIX	Depositor
R, $R_{free}$	0.193 , 0.231 0.250 , 0.276	Depositor DCC
$R_{free}$ test set	2000 reflections (0.20%)	DCC
Wilson B-factor (Å <sup>2</sup> )	88.3	Xtriage
Anisotropy	0.232	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.28 , 77.2	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.44$ , $\langle L^2 \rangle = 0.26$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.92	EDS
Total number of atoms	260090	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	113.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.45% 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, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

## 5 Model quality ⓘ

### 5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: OMC, ZN, MIA, MG, H2U, 4SU, 7MG, 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	0.87	14/36028 (0.0%)	1.59	679/56231 (1.2%)
1	1G	0.75	2/36025 (0.0%)	1.44	481/56227 (0.9%)
2	1L	0.51	1/1625 (0.1%)	1.02	1/2531 (0.0%)
2	3K	0.57	0/1625	1.17	11/2531 (0.4%)
2	3L	0.63	0/1625	1.20	16/2531 (0.6%)
3	2K	1.02	2/1721 (0.1%)	1.69	42/2682 (1.6%)
3	2L	0.78	1/1721 (0.1%)	1.49	23/2682 (0.9%)
4	4K	1.03	0/313	1.37	4/485 (0.8%)
4	4L	1.26	0/213	1.79	4/329 (1.2%)
5	14	0.99	84/70167 (0.1%)	1.74	2119/109541 (1.9%)
5	1H	1.24	280/70233 (0.4%)	2.01	3566/109643 (3.3%)
6	12	0.40	0/1959	0.68	2/2642 (0.1%)
6	1E	0.48	0/1959	0.74	0/2642
7	22	0.45	0/1636	0.67	1/2205 (0.0%)
7	2E	0.58	0/1629	0.74	0/2195
8	32	0.53	0/1732	0.76	1/2318 (0.0%)
8	3E	0.65	2/1732 (0.1%)	0.80	3/2318 (0.1%)
9	4E	0.62	0/1171	0.81	0/1576
10	5E	0.61	0/855	0.78	0/1154
11	6E	0.56	0/1275	0.70	0/1709
12	7E	0.59	0/1135	0.79	0/1527
13	8E	0.52	0/1028	0.75	1/1379 (0.1%)
14	1I	0.54	0/814	0.75	0/1095
15	2I	0.64	0/899	0.85	1/1213 (0.1%)
16	3I	0.79	0/991	1.03	4/1327 (0.3%)
17	4I	0.59	0/948	0.84	2/1272 (0.2%)
18	5I	0.83	1/500 (0.2%)	0.85	1/664 (0.2%)
19	6I	0.62	0/744	0.84	0/992
20	7I	0.56	0/721	0.77	0/970
21	8I	0.60	0/847	0.77	0/1131
22	9I	0.58	0/595	0.79	0/790
23	AI	0.60	0/661	0.84	0/890

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
24	BI	0.47	0/764	0.73	1/1007 (0.1%)
25	1F	0.52	0/221	0.81	0/288
26	1K	0.56	0/1602	1.16	9/2493 (0.4%)
27	16	0.97	2/2928 (0.1%)	1.87	95/4568 (2.1%)
27	1J	0.80	1/2928 (0.0%)	1.48	31/4568 (0.7%)
28	11	0.96	3/2165 (0.1%)	1.09	6/2919 (0.2%)
29	21	0.78	0/1601	0.99	3/2160 (0.1%)
30	31	0.88	1/1620 (0.1%)	1.02	6/2194 (0.3%)
31	41	0.65	0/1498	0.86	1/2016 (0.0%)
32	51	0.68	0/1362	0.92	3/1841 (0.2%)
33	61	0.59	0/1151	0.83	0/1558
34	58	0.69	0/1131	0.88	1/1525 (0.1%)
35	68	0.75	0/942	0.85	1/1269 (0.1%)
36	78	0.82	0/1161	1.14	3/1544 (0.2%)
37	88	0.94	0/1106	1.13	4/1478 (0.3%)
38	98	0.66	0/981	1.00	1/1312 (0.1%)
39	A8	0.74	0/891	1.05	6/1187 (0.5%)
40	B8	0.77	0/1155	0.92	0/1542
41	C8	0.82	0/981	0.93	1/1306 (0.1%)
42	D8	0.69	0/789	0.93	2/1057 (0.2%)
43	E8	0.77	0/910	0.98	2/1220 (0.2%)
44	F8	1.00	2/756 (0.3%)	1.04	4/1014 (0.4%)
45	G8	0.83	0/804	1.11	6/1073 (0.6%)
46	H8	0.54	0/1427	0.84	1/1935 (0.1%)
47	I8	0.86	0/634	1.01	0/847
48	J8	0.84	0/769	1.03	4/1022 (0.4%)
49	K8	0.99	2/565 (0.4%)	1.16	4/748 (0.5%)
50	L8	0.70	0/457	0.99	1/613 (0.2%)
51	M8	0.58	0/545	0.84	0/733
52	N8	0.69	0/467	0.98	1/632 (0.2%)
53	O8	0.81	1/396 (0.3%)	0.97	0/529
54	P8	0.98	0/399	1.12	1/526 (0.2%)
55	Q8	1.30	3/486 (0.6%)	1.71	9/638 (1.4%)
All	All	0.96	402/280719 (0.1%)	1.64	7169/426784 (1.7%)

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
6	12	0	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
6	1E	0	3
8	32	0	2
8	3E	0	1
13	8E	0	1
16	3I	0	1
17	4I	0	1
20	7I	0	1
23	AI	0	2
28	11	0	1
29	21	0	3
30	31	0	2
31	41	0	2
33	61	0	4
36	78	0	3
37	88	0	1
38	98	0	1
39	A8	0	1
40	B8	0	1
41	C8	0	1
45	G8	0	4
46	H8	0	2
47	I8	0	2
48	J8	0	1
49	K8	0	2
51	M8	0	1
52	N8	0	2
53	O8	0	3
55	Q8	0	8
All	All	0	58

The worst 5 of 402 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	1H	2430	A	N9-C4	-15.74	1.28	1.37
5	1H	774	A	N9-C4	-13.11	1.29	1.37
5	1H	1786	A	N9-C4	-13.10	1.29	1.37
18	5I	27	CYS	CB-SG	-12.07	1.61	1.82
5	14	783	A	N9-C4	-11.82	1.30	1.37

The worst 5 of 7169 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	1H	1899	G	N3-C4-N9	-27.85	109.29	126.00
5	1H	1786	A	C2-N3-C4	-22.12	99.54	110.60
5	1H	917	A	N1-C2-N3	21.20	139.90	129.30
5	1H	1332	G	N3-C4-N9	-21.08	113.35	126.00
5	1H	1899	G	N3-C4-C5	21.00	139.10	128.60

There are no chirality outliers.

5 of 58 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
6	1E	15	VAL	Peptide
6	1E	169	LYS	Peptide
6	1E	237	ALA	Peptide
8	3E	31	CYS	Peptide
13	8E	110	GLU	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	32185	0	16244	835	0
1	1G	32182	0	16243	773	1
2	1L	1627	0	842	40	0
2	3K	1627	0	842	51	0
2	3L	1627	0	842	53	0
3	2K	1645	0	845	23	0
3	2L	1645	0	845	38	0
4	4K	279	0	142	6	0
4	4L	191	0	98	8	0
5	14	62647	0	31582	1217	0
5	1H	62707	0	31606	1584	1
6	12	1924	0	1975	116	0
6	1E	1924	0	1975	112	0
7	22	1612	0	1677	87	0
7	2E	1605	0	1668	48	0
8	32	1702	0	1763	87	0
8	3E	1702	0	1763	82	0
9	4E	1155	0	1213	67	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
10	5E	842	0	857	29	0
11	6E	1256	0	1296	51	0
12	7E	1115	0	1177	61	0
13	8E	1009	0	1037	60	0
14	1I	801	0	849	56	0
15	2I	884	0	904	39	0
16	3I	975	0	1062	47	0
17	4I	938	0	997	54	0
18	5I	491	0	529	28	0
19	6I	733	0	771	32	0
20	7I	705	0	725	50	0
21	8I	834	0	904	58	0
22	9I	590	0	662	25	0
23	AI	647	0	665	50	0
24	BI	762	0	861	35	0
25	1F	217	0	234	19	0
26	1K	1587	0	822	25	0
27	16	2617	0	1328	74	0
27	1J	2617	0	1328	81	0
28	11	2115	0	2195	102	0
29	21	1568	0	1634	92	0
30	31	1585	0	1632	93	0
31	41	1473	0	1535	99	0
32	51	1336	0	1418	73	0
33	61	1136	0	1223	66	0
34	58	1104	0	1180	60	0
35	68	932	0	996	42	0
36	78	1144	0	1228	96	0
37	88	1086	0	1129	57	0
38	98	967	0	1033	61	0
39	A8	881	0	943	61	0
40	B8	1141	0	1202	70	0
41	C8	963	0	1022	68	0
42	D8	778	0	852	39	0
43	E8	899	0	964	30	0
44	F8	742	0	803	46	0
45	G8	791	0	881	61	0
46	H8	1397	0	1430	78	0
47	I8	626	0	642	38	0
48	J8	762	0	848	37	0
49	K8	563	0	612	30	0
50	L8	452	0	503	23	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
51	M8	533	0	526	38	0
52	N8	453	0	475	29	0
53	O8	389	0	404	35	0
54	P8	391	0	432	17	0
55	Q8	480	0	549	106	0
56	11	2	0	0	0	0
56	13	149	0	0	0	0
56	14	421	0	0	0	0
56	16	13	0	0	0	0
56	1G	96	0	0	0	0
56	1H	537	0	0	0	0
56	1J	7	0	0	0	0
56	1K	2	0	0	0	0
56	1L	1	0	0	0	0
56	21	2	0	0	0	0
56	2K	8	0	0	0	0
56	2L	4	0	0	0	0
56	3E	2	0	0	0	0
56	3I	1	0	0	0	0
56	3L	3	0	0	0	0
56	41	2	0	0	0	0
56	5E	1	0	0	0	0
56	5I	1	0	0	0	0
56	78	1	0	0	0	0
56	88	2	0	0	0	0
56	I8	1	0	0	0	0
56	J8	1	0	0	0	0
56	L8	1	0	0	0	0
56	P8	1	0	0	0	0
57	14	1	0	0	0	0
57	1G	1	0	0	0	0
57	32	1	0	0	0	0
57	3E	1	0	0	0	0
57	5I	1	0	0	0	0
57	G8	1	0	0	0	0
58	11	9	0	0	3	0
58	13	230	0	0	36	0
58	14	863	0	0	119	0
58	16	21	0	0	3	0
58	1G	106	0	0	22	0
58	1H	1212	0	0	257	0
58	1I	1	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
58	1J	12	0	0	4	0
58	1K	6	0	0	0	0
58	2I	3	0	0	2	0
58	2K	8	0	0	1	0
58	2L	1	0	0	0	0
58	3I	8	0	0	0	0
58	3E	1	0	0	0	0
58	3I	1	0	0	0	0
58	3K	1	0	0	0	0
58	4E	3	0	0	0	0
58	4K	4	0	0	0	0
58	4L	2	0	0	0	0
58	58	3	0	0	0	0
58	5I	1	0	0	0	0
58	6I	1	0	0	0	0
58	78	6	0	0	0	0
58	7I	1	0	0	0	0
58	8E	2	0	0	0	0
58	98	1	0	0	1	0
58	B8	1	0	0	0	0
58	BI	1	0	0	0	0
58	C8	3	0	0	2	0
58	D8	1	0	0	0	0
58	E8	2	0	0	0	0
58	F8	2	0	0	0	0
58	G8	3	0	0	0	0
58	I8	5	0	0	1	0
58	J8	1	0	0	0	0
58	L8	1	0	0	1	0
58	P8	4	0	0	0	0
58	Q8	1	0	0	0	0
All	All	260090	0	157464	7103	1

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

The worst 5 of 7103 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)
5:1H:567:A:OP1	58:1H:3610:HOH:O	1.72	1.07
5:1H:2714:G:OP2	58:1H:3679:HOH:O	1.74	1.03

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:1H:987:G:OP2	58:1H:4091:HOH:O	1.74	1.03
36:78:19:VAL:HG12	36:78:21:ARG:H	1.24	1.02
5:1H:945:A:OP1	58:1H:4240:HOH:O	1.80	1.00

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

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:1H:2137:C:OP1	1:1G:999:U:O2'[4_555]	2.11	0.09

## 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	
6	12	235/256 (92%)	196 (83%)	35 (15%)	4 (2%)	11	38
6	1E	235/256 (92%)	199 (85%)	33 (14%)	3 (1%)	14	45
7	22	204/239 (85%)	185 (91%)	19 (9%)	0	100	100
7	2E	203/239 (85%)	182 (90%)	21 (10%)	0	100	100
8	32	206/209 (99%)	181 (88%)	23 (11%)	2 (1%)	18	52
8	3E	206/209 (99%)	186 (90%)	18 (9%)	2 (1%)	18	52
9	4E	149/162 (92%)	138 (93%)	10 (7%)	1 (1%)	25	61
10	5E	99/101 (98%)	93 (94%)	6 (6%)	0	100	100
11	6E	153/156 (98%)	145 (95%)	8 (5%)	0	100	100
12	7E	136/138 (99%)	125 (92%)	10 (7%)	1 (1%)	25	61
13	8E	125/128 (98%)	105 (84%)	20 (16%)	0	100	100
14	1I	97/105 (92%)	89 (92%)	8 (8%)	0	100	100
15	2I	117/129 (91%)	102 (87%)	14 (12%)	1 (1%)	20	55

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
16	3I	123/132 (93%)	103 (84%)	20 (16%)	0	100	100
17	4I	116/126 (92%)	97 (84%)	18 (16%)	1 (1%)	20	55
18	5I	58/61 (95%)	47 (81%)	9 (16%)	2 (3%)	4	21
19	6I	86/89 (97%)	79 (92%)	7 (8%)	0	100	100
20	7I	82/88 (93%)	76 (93%)	6 (7%)	0	100	100
21	8I	98/105 (93%)	94 (96%)	4 (4%)	0	100	100
22	9I	70/88 (80%)	60 (86%)	8 (11%)	2 (3%)	5	25
23	AI	79/93 (85%)	66 (84%)	9 (11%)	4 (5%)	2	13
24	BI	97/106 (92%)	80 (82%)	17 (18%)	0	100	100
25	1F	23/27 (85%)	21 (91%)	2 (9%)	0	100	100
28	11	270/276 (98%)	252 (93%)	15 (6%)	3 (1%)	17	50
29	21	203/206 (98%)	164 (81%)	29 (14%)	10 (5%)	2	14
30	31	200/210 (95%)	182 (91%)	16 (8%)	2 (1%)	18	52
31	41	179/182 (98%)	156 (87%)	20 (11%)	3 (2%)	11	38
32	51	172/180 (96%)	143 (83%)	22 (13%)	7 (4%)	3	17
33	61	144/148 (97%)	117 (81%)	24 (17%)	3 (2%)	8	32
34	58	136/140 (97%)	117 (86%)	15 (11%)	4 (3%)	5	25
35	68	120/122 (98%)	112 (93%)	8 (7%)	0	100	100
36	78	148/150 (99%)	116 (78%)	27 (18%)	5 (3%)	4	21
37	88	134/141 (95%)	110 (82%)	20 (15%)	4 (3%)	5	24
38	98	116/118 (98%)	100 (86%)	15 (13%)	1 (1%)	20	55
39	A8	109/112 (97%)	89 (82%)	19 (17%)	1 (1%)	20	55
40	B8	135/146 (92%)	120 (89%)	14 (10%)	1 (1%)	25	61
41	C8	115/118 (98%)	107 (93%)	5 (4%)	3 (3%)	6	27
42	D8	99/101 (98%)	92 (93%)	6 (6%)	1 (1%)	18	52
43	E8	111/113 (98%)	101 (91%)	10 (9%)	0	100	100
44	F8	92/96 (96%)	83 (90%)	7 (8%)	2 (2%)	8	31
45	G8	102/110 (93%)	80 (78%)	16 (16%)	6 (6%)	2	10
46	H8	173/206 (84%)	141 (82%)	24 (14%)	8 (5%)	3	15
47	I8	78/85 (92%)	66 (85%)	11 (14%)	1 (1%)	14	45
48	J8	95/98 (97%)	85 (90%)	8 (8%)	2 (2%)	8	32

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
49	K8	65/72 (90%)	57 (88%)	6 (9%)	2 (3%)	5	23
50	L8	55/60 (92%)	50 (91%)	4 (7%)	1 (2%)	10	36
51	M8	64/71 (90%)	40 (62%)	22 (34%)	2 (3%)	5	23
52	N8	56/60 (93%)	46 (82%)	8 (14%)	2 (4%)	4	20
53	O8	43/54 (80%)	28 (65%)	13 (30%)	2 (5%)	3	14
54	P8	43/49 (88%)	41 (95%)	2 (5%)	0	100	100
55	Q8	58/65 (89%)	33 (57%)	19 (33%)	6 (10%)	0	3
All	All	6312/6731 (94%)	5477 (87%)	730 (12%)	105 (2%)	11	38

5 of 105 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
29	21	83	ASP
32	51	169	VAL
36	78	57	THR
45	G8	54	LYS
49	K8	48	HIS

### 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	
6	12	205/220 (93%)	155 (76%)	50 (24%)	1	2
6	1E	205/220 (93%)	157 (77%)	48 (23%)	1	3
7	22	160/188 (85%)	130 (81%)	30 (19%)	2	7
7	2E	159/188 (85%)	131 (82%)	28 (18%)	2	9
8	32	180/181 (99%)	149 (83%)	31 (17%)	2	9
8	3E	180/181 (99%)	143 (79%)	37 (21%)	1	5
9	4E	116/123 (94%)	87 (75%)	29 (25%)	1	2
10	5E	90/90 (100%)	79 (88%)	11 (12%)	6	21
11	6E	126/127 (99%)	101 (80%)	25 (20%)	1	6

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
12	7E	119/119 (100%)	98 (82%)	21 (18%)	2	9
13	8E	98/99 (99%)	74 (76%)	24 (24%)	1	2
14	1I	89/92 (97%)	71 (80%)	18 (20%)	1	5
15	2I	90/99 (91%)	76 (84%)	14 (16%)	3	12
16	3I	104/109 (95%)	83 (80%)	21 (20%)	1	5
17	4I	94/101 (93%)	70 (74%)	24 (26%)	0	2
18	5I	49/50 (98%)	41 (84%)	8 (16%)	3	11
19	6I	79/80 (99%)	67 (85%)	12 (15%)	3	13
20	7I	72/74 (97%)	54 (75%)	18 (25%)	1	2
21	8I	95/97 (98%)	79 (83%)	16 (17%)	2	10
22	9I	63/77 (82%)	58 (92%)	5 (8%)	14	44
23	AI	70/80 (88%)	50 (71%)	20 (29%)	0	1
24	BI	76/82 (93%)	60 (79%)	16 (21%)	1	5
25	1F	20/22 (91%)	19 (95%)	1 (5%)	28	63
28	11	214/218 (98%)	169 (79%)	45 (21%)	1	5
29	21	165/166 (99%)	125 (76%)	40 (24%)	1	2
30	31	161/166 (97%)	127 (79%)	34 (21%)	1	5
31	41	155/156 (99%)	125 (81%)	30 (19%)	1	6
32	51	145/148 (98%)	110 (76%)	35 (24%)	1	2
33	61	122/124 (98%)	87 (71%)	35 (29%)	0	1
34	58	117/119 (98%)	92 (79%)	25 (21%)	1	4
35	68	100/100 (100%)	85 (85%)	15 (15%)	3	13
36	78	116/116 (100%)	82 (71%)	34 (29%)	0	1
37	88	104/111 (94%)	75 (72%)	29 (28%)	0	1
38	98	101/101 (100%)	72 (71%)	29 (29%)	0	1
39	A8	87/88 (99%)	68 (78%)	19 (22%)	1	4
40	B8	120/127 (94%)	93 (78%)	27 (22%)	1	3
41	C8	93/94 (99%)	76 (82%)	17 (18%)	2	8
42	D8	82/82 (100%)	63 (77%)	19 (23%)	1	3
43	E8	92/92 (100%)	71 (77%)	21 (23%)	1	3
44	F8	76/78 (97%)	61 (80%)	15 (20%)	1	6

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
45	G8	85/91 (93%)	56 (66%)	29 (34%)	0	0
46	H8	154/179 (86%)	114 (74%)	40 (26%)	0	1
47	I8	61/67 (91%)	47 (77%)	14 (23%)	1	3
48	J8	82/83 (99%)	65 (79%)	17 (21%)	1	5
49	K8	62/67 (92%)	39 (63%)	23 (37%)	0	0
50	L8	49/52 (94%)	40 (82%)	9 (18%)	2	7
51	M8	59/63 (94%)	42 (71%)	17 (29%)	0	1
52	N8	51/52 (98%)	37 (72%)	14 (28%)	0	1
53	O8	44/52 (85%)	31 (70%)	13 (30%)	0	1
54	P8	38/42 (90%)	32 (84%)	6 (16%)	3	11
55	Q8	50/55 (91%)	31 (62%)	19 (38%)	0	0
All	All	5324/5588 (95%)	4147 (78%)	1177 (22%)	1	4

5 of 1177 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
31	41	84	LYS
36	78	13	ASN
6	12	76	GLN
32	51	10	PRO
33	61	82	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 15 such sidechains are listed below:

Mol	Chain	Res	Type
23	AI	56	GLN
29	21	135	HIS
47	I8	29	GLN
15	2I	93	GLN
44	F8	31	HIS

### 5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	13	1495/1522 (98%)	353 (23%)	0
1	1G	1495/1522 (98%)	374 (25%)	0

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Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
2	1L	74/76 (97%)	32 (43%)	0
2	3K	74/76 (97%)	36 (48%)	0
2	3L	74/76 (97%)	32 (43%)	0
26	1K	70/76 (92%)	32 (45%)	0
27	16	121/122 (99%)	26 (21%)	0
27	1J	121/122 (99%)	31 (25%)	0
3	2K	76/77 (98%)	15 (19%)	0
3	2L	76/77 (98%)	17 (22%)	0
4	4K	12/30 (40%)	2 (16%)	0
4	4L	8/30 (26%)	4 (50%)	0
5	14	2908/2917 (99%)	754 (25%)	0
5	1H	2911/2917 (99%)	685 (23%)	0
All	All	9515/9640 (98%)	2393 (25%)	0

5 of 2393 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	13	5	U
1	13	6	G
1	13	7	G
1	13	8	A
1	13	9	G

There are no RNA pucker outliers to report.

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

41 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
26	H2U	1K	16	26	17,21,22	2.61	4 (23%)	21,30,33	3.03	5 (23%)
26	PSU	1K	32	26,56	16,21,22	1.16	2 (12%)	20,30,33	3.61	5 (25%)
26	MIA	1K	37	26	23,31,32	1.01	1 (4%)	25,44,47	1.57	5 (20%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
26	PSU	1K	39	26	16,21,22	0.97	1 (6%)	20,30,33	3.61	7 (35%)
26	7MG	1K	46	26	20,26,27	3.44	6 (30%)	22,39,42	2.00	7 (31%)
26	PSU	1K	55	26	16,21,22	1.16	1 (6%)	20,30,33	3.93	6 (30%)
26	4SU	1K	8	26	14,21,22	3.00	2 (14%)	15,30,33	1.29	2 (13%)
2	H2U	1L	16	2	17,21,22	2.39	4 (23%)	21,30,33	3.12	5 (23%)
2	H2U	1L	20	2	17,21,22	2.30	4 (23%)	21,30,33	2.96	5 (23%)
2	PSU	1L	32	2	16,21,22	1.28	2 (12%)	20,30,33	4.29	7 (35%)
2	MIA	1L	37	2	23,31,32	1.34	2 (8%)	25,44,47	1.60	5 (20%)
2	PSU	1L	39	2	16,21,22	1.13	1 (6%)	20,30,33	3.82	6 (30%)
2	7MG	1L	46	2	20,26,27	3.43	5 (25%)	22,39,42	1.92	7 (31%)
2	PSU	1L	55	2	16,21,22	1.38	3 (18%)	20,30,33	4.17	5 (25%)
2	4SU	1L	8	2	14,21,22	3.01	2 (14%)	15,30,33	1.58	2 (13%)
3	H2U	2K	21	3	17,21,22	2.90	3 (17%)	21,30,33	2.96	4 (19%)
3	OMC	2K	33	3	15,22,23	2.24	4 (26%)	19,31,34	1.03	2 (10%)
3	7MG	2K	47	3	20,26,27	3.36	6 (30%)	22,39,42	1.77	5 (22%)
3	PSU	2K	56	3	16,21,22	1.33	3 (18%)	20,30,33	3.62	5 (25%)
3	4SU	2K	8	3	14,21,22	3.21	2 (14%)	15,30,33	1.14	2 (13%)
3	H2U	2L	21	3	17,21,22	2.27	4 (23%)	21,30,33	2.78	4 (19%)
3	OMC	2L	33	3	15,22,23	2.11	4 (26%)	19,31,34	1.08	1 (5%)
3	7MG	2L	47	3	20,26,27	3.28	6 (30%)	22,39,42	1.89	5 (22%)
3	PSU	2L	56	3	16,21,22	1.36	2 (12%)	20,30,33	3.66	5 (25%)
3	4SU	2L	8	3	14,21,22	3.39	2 (14%)	15,30,33	1.05	2 (13%)
2	H2U	3K	16	2	17,21,22	2.32	4 (23%)	21,30,33	3.06	5 (23%)
2	H2U	3K	20	2	17,21,22	2.34	4 (23%)	21,30,33	3.15	5 (23%)
2	PSU	3K	32	2	16,21,22	1.13	1 (6%)	20,30,33	3.63	7 (35%)
2	MIA	3K	37	2	23,31,32	1.54	2 (8%)	25,44,47	3.31	5 (20%)
2	PSU	3K	39	2	16,21,22	1.18	1 (6%)	20,30,33	3.88	6 (30%)
2	7MG	3K	46	2	20,26,27	3.43	5 (25%)	22,39,42	1.94	7 (31%)
2	PSU	3K	55	2	16,21,22	1.15	3 (18%)	20,30,33	3.55	7 (35%)
2	4SU	3K	8	2	14,21,22	3.18	2 (14%)	15,30,33	1.18	2 (13%)
2	H2U	3L	16	2	17,21,22	2.30	4 (23%)	21,30,33	2.97	4 (19%)
2	H2U	3L	20	2	17,21,22	2.37	4 (23%)	21,30,33	3.13	5 (23%)
2	PSU	3L	32	2	16,21,22	1.22	1 (6%)	20,30,33	3.86	7 (35%)
2	MIA	3L	37	2	23,31,32	1.81	2 (8%)	25,44,47	3.21	5 (20%)
2	PSU	3L	39	2	16,21,22	1.16	1 (6%)	20,30,33	3.80	4 (20%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	7MG	3L	46	2	20,26,27	3.54	5 (25%)	22,39,42	1.93	5 (22%)
2	PSU	3L	55	2	16,21,22	1.00	1 (6%)	20,30,33	3.59	5 (25%)
2	4SU	3L	8	2	14,21,22	3.17	2 (14%)	15,30,33	1.59	2 (13%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
26	H2U	1K	16	26	-	0/7/38/39	0/2/2/2
26	PSU	1K	32	26,56	-	0/7/25/26	0/2/2/2
26	MIA	1K	37	26	-	0/11/33/34	0/3/3/3
26	PSU	1K	39	26	-	0/7/25/26	0/2/2/2
26	7MG	1K	46	26	-	0/7/37/38	0/3/3/3
26	PSU	1K	55	26	-	0/7/25/26	0/2/2/2
26	4SU	1K	8	26	-	0/3/25/26	0/2/2/2
2	H2U	1L	16	2	-	0/7/38/39	0/2/2/2
2	H2U	1L	20	2	-	0/7/38/39	0/2/2/2
2	PSU	1L	32	2	-	1/7/25/26	0/2/2/2
2	MIA	1L	37	2	-	2/11/33/34	0/3/3/3
2	PSU	1L	39	2	-	0/7/25/26	0/2/2/2
2	7MG	1L	46	2	-	0/7/37/38	0/3/3/3
2	PSU	1L	55	2	-	0/7/25/26	0/2/2/2
2	4SU	1L	8	2	-	0/3/25/26	0/2/2/2
3	H2U	2K	21	3	-	0/7/38/39	0/2/2/2
3	OMC	2K	33	3	-	0/5/27/28	0/2/2/2
3	7MG	2K	47	3	-	0/7/37/38	0/3/3/3
3	PSU	2K	56	3	-	0/7/25/26	0/2/2/2
3	4SU	2K	8	3	-	0/3/25/26	0/2/2/2
3	H2U	2L	21	3	-	0/7/38/39	0/2/2/2
3	OMC	2L	33	3	-	0/5/27/28	0/2/2/2
3	7MG	2L	47	3	-	0/7/37/38	0/3/3/3
3	PSU	2L	56	3	-	0/7/25/26	0/2/2/2
3	4SU	2L	8	3	-	0/3/25/26	0/2/2/2
2	H2U	3K	16	2	-	0/7/38/39	0/2/2/2
2	H2U	3K	20	2	-	0/7/38/39	0/2/2/2
2	PSU	3K	32	2	-	0/7/25/26	0/2/2/2
2	MIA	3K	37	2	-	0/11/33/34	0/3/3/3
2	PSU	3K	39	2	-	0/7/25/26	0/2/2/2
2	7MG	3K	46	2	-	0/7/37/38	0/3/3/3
2	PSU	3K	55	2	-	0/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	4SU	3K	8	2	-	0/3/25/26	0/2/2/2
2	H2U	3L	16	2	-	0/7/38/39	0/2/2/2
2	H2U	3L	20	2	-	0/7/38/39	0/2/2/2
2	PSU	3L	32	2	-	0/7/25/26	0/2/2/2
2	MIA	3L	37	2	-	0/11/33/34	0/3/3/3
2	PSU	3L	39	2	-	0/7/25/26	0/2/2/2
2	7MG	3L	46	2	-	0/7/37/38	0/3/3/3
2	PSU	3L	55	2	-	0/7/25/26	0/2/2/2
2	4SU	3L	8	2	-	0/3/25/26	0/2/2/2

The worst 5 of 118 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	1K	46	7MG	C5-C4	-5.59	1.24	1.39
2	3L	46	7MG	C5-C4	-5.54	1.24	1.39
2	1L	46	7MG	C5-C4	-5.52	1.24	1.39
3	2K	47	7MG	C5-C4	-5.40	1.24	1.39
2	3K	46	7MG	C5-C4	-5.33	1.24	1.39

The worst 5 of 195 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	1L	32	PSU	N1-C2-N3	-13.89	118.41	128.40
2	1L	55	PSU	N1-C2-N3	-13.45	118.73	128.40
2	3L	32	PSU	N1-C2-N3	-13.31	118.83	128.40
2	1L	39	PSU	N1-C2-N3	-13.27	118.86	128.40
2	3K	39	PSU	N1-C2-N3	-13.25	118.87	128.40

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	1L	37	MIA	N1-C2-S10-C11
2	1L	37	MIA	N3-C2-S10-C11
2	1L	32	PSU	O4'-C1'-C5-C4

There are no ring outliers.

26 monomers are involved in 52 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
26	1K	16	H2U	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
26	1K	37	MIA	1	0
26	1K	46	7MG	1	0
26	1K	8	4SU	1	0
2	1L	16	H2U	1	0
2	1L	37	MIA	1	0
2	1L	39	PSU	3	0
2	1L	46	7MG	2	0
2	1L	55	PSU	1	0
2	1L	8	4SU	4	0
3	2K	47	7MG	5	0
3	2K	8	4SU	1	0
3	2L	33	OMC	3	0
3	2L	47	7MG	2	0
3	2L	56	PSU	2	0
3	2L	8	4SU	2	0
2	3K	20	H2U	1	0
2	3K	37	MIA	4	0
2	3K	39	PSU	1	0
2	3K	55	PSU	3	0
2	3L	16	H2U	1	0
2	3L	20	H2U	4	0
2	3L	37	MIA	2	0
2	3L	46	7MG	2	0
2	3L	55	PSU	1	0
2	3L	8	4SU	2	0

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 1265 ligands modelled in this entry, 1265 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.



## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	1497/1522 (98%)	-0.47	1 (0%) 95 90	62, 106, 190, 319	0
1	1G	1497/1522 (98%)	-0.38	20 (1%) 77 57	78, 126, 199, 313	0
2	1L	68/76 (89%)	0.30	7 (10%) 7 2	144, 237, 271, 321	0
2	3K	68/76 (89%)	0.35	7 (10%) 7 2	76, 227, 273, 285	0
2	3L	68/76 (89%)	-0.22	2 (2%) 52 27	95, 217, 254, 268	0
3	2K	72/77 (93%)	-0.42	0 100 100	74, 96, 125, 136	0
3	2L	72/77 (93%)	-0.76	0 100 100	87, 122, 154, 170	0
4	4K	13/30 (43%)	-0.40	0 100 100	74, 92, 138, 142	0
4	4L	9/30 (30%)	-0.28	0 100 100	104, 111, 123, 125	0
5	14	2909/2917 (99%)	-0.33	57 (1%) 65 42	59, 96, 254, 399	0
5	1H	2912/2917 (99%)	-0.09	53 (1%) 69 45	45, 78, 243, 371	0
6	12	237/256 (92%)	1.33	59 (24%) 1 0	143, 177, 205, 218	0
6	1E	237/256 (92%)	0.75	43 (18%) 1 0	114, 148, 178, 191	0
7	22	206/239 (86%)	1.52	59 (28%) 1 0	139, 159, 187, 204	0
7	2E	205/239 (85%)	0.42	16 (7%) 14 5	92, 114, 150, 155	0
8	32	208/209 (99%)	1.44	64 (30%) 0 0	103, 127, 150, 155	0
8	3E	208/209 (99%)	0.03	10 (4%) 31 14	87, 115, 142, 155	0
9	4E	151/162 (93%)	0.22	6 (3%) 39 19	82, 104, 128, 177	0
10	5E	101/101 (100%)	0.53	3 (2%) 51 26	85, 108, 131, 146	0
11	6E	155/156 (99%)	0.53	13 (8%) 12 4	104, 120, 156, 189	0
12	7E	138/138 (100%)	0.23	2 (1%) 75 54	98, 116, 128, 138	0
13	8E	127/128 (99%)	0.68	14 (11%) 6 2	91, 137, 163, 179	0
14	1I	99/105 (94%)	1.16	29 (29%) 1 0	86, 134, 171, 177	0
15	2I	119/129 (92%)	0.77	14 (11%) 5 2	79, 110, 145, 183	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
16	3I	125/132 (94%)	-0.17	2 (1%) 72 49	73, 84, 121, 204	0
17	4I	118/126 (93%)	0.51	12 (10%) 7 2	85, 123, 147, 162	0
18	5I	60/61 (98%)	0.31	2 (3%) 47 23	91, 103, 123, 133	0
19	6I	88/89 (98%)	0.22	3 (3%) 46 23	85, 109, 123, 143	0
20	7I	84/88 (95%)	0.01	3 (3%) 43 21	108, 119, 153, 170	0
21	8I	100/105 (95%)	-0.12	4 (4%) 39 19	96, 114, 125, 129	0
22	9I	72/88 (81%)	1.21	13 (18%) 1 0	93, 111, 145, 177	0
23	AI	81/93 (87%)	0.33	3 (3%) 42 21	99, 123, 149, 161	0
24	BI	99/106 (93%)	-0.03	0 100 100	113, 127, 166, 172	0
25	1F	25/27 (92%)	-0.05	0 100 100	99, 111, 125, 154	0
26	1K	67/76 (88%)	-0.01	2 (2%) 51 26	92, 192, 262, 271	0
27	16	122/122 (100%)	-0.27	2 (1%) 72 49	73, 96, 118, 204	0
27	1J	122/122 (100%)	-0.43	0 100 100	94, 140, 168, 212	0
28	11	272/276 (98%)	0.11	1 (0%) 92 81	46, 70, 87, 96	0
29	21	205/206 (99%)	0.53	22 (10%) 7 2	56, 97, 145, 164	0
30	31	202/210 (96%)	0.31	11 (5%) 26 12	52, 80, 120, 139	0
31	41	181/182 (99%)	1.02	36 (19%) 1 0	84, 107, 142, 155	0
32	51	174/180 (96%)	0.39	9 (5%) 28 12	86, 110, 126, 154	0
33	61	146/148 (98%)	1.04	28 (19%) 1 0	81, 136, 154, 161	0
34	58	138/140 (98%)	0.52	11 (7%) 13 5	71, 96, 137, 154	0
35	68	122/122 (100%)	0.17	1 (0%) 86 69	64, 83, 101, 116	0
36	78	150/150 (100%)	0.32	8 (5%) 27 12	51, 84, 109, 169	0
37	88	138/141 (97%)	0.29	7 (5%) 29 13	58, 84, 104, 139	0
38	98	118/118 (100%)	0.06	0 100 100	70, 90, 114, 121	0
39	A8	111/112 (99%)	0.77	14 (12%) 4 1	78, 94, 125, 141	0
40	B8	137/146 (93%)	0.04	3 (2%) 62 39	79, 99, 157, 179	0
41	C8	117/118 (99%)	0.16	3 (2%) 56 31	60, 83, 118, 150	0
42	D8	101/101 (100%)	0.70	10 (9%) 8 3	63, 106, 143, 159	0
43	E8	113/113 (100%)	0.41	4 (3%) 44 22	64, 80, 116, 169	0
44	F8	94/96 (97%)	0.34	3 (3%) 48 24	59, 75, 98, 115	0
45	G8	104/110 (94%)	0.36	1 (0%) 82 64	76, 98, 138, 169	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
46	H8	175/206 (84%)	0.83	24 (13%) 3 1	88, 128, 212, 220	0
47	I8	80/85 (94%)	0.36	4 (5%) 30 13	61, 76, 110, 122	0
48	J8	97/98 (98%)	0.77	15 (15%) 2 1	57, 77, 129, 175	0
49	K8	67/72 (93%)	0.29	4 (5%) 23 9	66, 84, 101, 143	0
50	L8	57/60 (95%)	0.35	2 (3%) 44 22	66, 85, 111, 117	0
51	M8	66/71 (92%)	2.18	30 (45%) 0 0	119, 163, 218, 238	0
52	N8	58/60 (96%)	0.87	6 (10%) 7 2	57, 104, 195, 203	0
53	O8	45/54 (83%)	5.46	38 (84%) 0 0	115, 146, 171, 183	0
54	P8	45/49 (91%)	-0.24	0 100 100	46, 55, 70, 82	0
55	Q8	60/65 (92%)	0.52	4 (6%) 19 7	62, 77, 102, 118	0
All	All	15912/16371 (97%)	0.07	824 (5%) 28 12	45, 103, 202, 399	0

The worst 5 of 824 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
52	N8	59	GLU	15.7
5	14	654(J)	A	15.0
5	1H	2901	C	14.1
5	14	654(I)	C	13.7
5	1H	2902	C	13.1

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

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 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
2	PSU	3L	55	20/21	0.74	0.12	-	180,202,212,213	0
26	PSU	1K	32	20/21	0.91	0.13	-	107,112,124,131	0
2	7MG	3K	46	24/25	0.58	0.20	-	193,206,217,221	0
3	H2U	2K	21	20/21	0.81	0.23	-	114,124,134,134	0
2	H2U	3L	16	20/21	0.62	0.19	-	181,194,205,211	0
26	H2U	1K	16	20/21	0.77	0.26	-	122,160,190,196	0
2	7MG	3L	46	24/25	0.70	0.14	-	190,197,206,218	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
2	H2U	3K	16	20/21	0.75	0.27	-	165,195,210,211	0
2	H2U	3L	20	20/21	0.59	0.20	-	180,188,201,202	0
2	7MG	1L	46	24/25	0.78	0.16	-	172,200,218,231	0
26	MIA	1K	37	29/30	0.95	0.18	-	84,92,107,113	0
2	MIA	3L	37	29/30	0.74	0.25	-	148,168,178,187	0
3	4SU	2L	8	20/21	0.90	0.11	-	115,120,123,126	0
2	MIA	1L	37	29/30	0.88	0.22	-	131,147,155,157	0
3	PSU	2L	56	20/21	0.90	0.10	-	123,130,136,139	0
3	7MG	2K	47	24/25	0.93	0.13	-	97,106,114,116	0
2	4SU	1L	8	20/21	0.74	0.12	-	185,201,207,213	0
3	OMC	2K	33	21/22	0.96	0.17	-	75,80,86,87	0
2	MIA	3K	37	29/30	0.91	0.21	-	123,142,147,157	0
2	H2U	1L	16	20/21	0.58	0.32	-	157,192,217,227	0
2	PSU	3K	55	20/21	0.62	0.15	-	190,210,228,233	0
3	4SU	2K	8	20/21	0.94	0.17	-	89,95,103,105	0
3	H2U	2L	21	20/21	0.79	0.18	-	135,143,147,157	0
2	4SU	3K	8	20/21	0.50	0.18	-	200,207,220,233	0
2	PSU	3K	39	20/21	0.90	0.15	-	117,127,130,138	0
2	PSU	3L	39	20/21	0.73	0.21	-	134,144,154,160	0
26	4SU	1K	8	20/21	0.73	0.12	-	164,174,189,190	0
3	7MG	2L	47	24/25	0.92	0.12	-	126,134,139,140	0
2	H2U	1L	20	20/21	0.54	0.36	-	141,165,187,195	0
3	OMC	2L	33	21/22	0.96	0.14	-	104,109,112,118	0
2	4SU	3L	8	20/21	0.69	0.12	-	191,196,208,218	0
3	PSU	2K	56	20/21	0.92	0.17	-	101,106,113,119	0
2	PSU	1L	39	20/21	0.89	0.10	-	140,150,158,160	0
26	7MG	1K	46	24/25	0.84	0.12	-	149,160,172,176	0
2	PSU	1L	55	20/21	0.56	0.21	-	165,197,211,225	0
2	PSU	3L	32	20/21	0.71	0.16	-	133,144,152,153	0
2	PSU	3K	32	20/21	0.83	0.17	-	127,135,142,151	0
26	PSU	1K	55	20/21	0.81	0.21	-	133,151,166,168	0
2	PSU	1L	32	20/21	0.71	0.20	-	149,152,163,169	0
26	PSU	1K	39	20/21	0.96	0.13	-	86,100,107,110	0
2	H2U	3K	20	20/21	0.66	0.44	-	140,167,205,206	0

### 6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 6.4 Ligands ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. 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
56	MG	1H	3204	1/1	0.92	0.47	40.22	70,70,70,70	0
56	MG	1H	3078	1/1	0.90	0.45	35.82	80,80,80,80	0
56	MG	1H	3176	1/1	0.96	0.47	34.11	76,76,76,76	0
56	MG	1H	3258	1/1	0.71	0.46	33.01	63,63,63,63	0
56	MG	1H	3263	1/1	0.56	0.51	30.87	87,87,87,87	0
56	MG	2K	103	1/1	0.41	0.32	26.84	88,88,88,88	0
56	MG	13	1707	1/1	0.89	0.38	26.68	98,98,98,98	0
56	MG	1H	3138	1/1	0.51	0.36	26.63	72,72,72,72	0
56	MG	13	1664	1/1	0.96	0.37	25.28	88,88,88,88	0
56	MG	1H	3149	1/1	0.90	0.40	21.49	60,60,60,60	0
56	MG	1H	3054	1/1	0.76	0.40	20.35	67,67,67,67	0
56	MG	1H	3085	1/1	0.83	0.29	20.22	64,64,64,64	0
56	MG	1H	3203	1/1	0.87	0.48	20.15	101,101,101,101	0
56	MG	1H	3045	1/1	0.79	0.39	19.08	66,66,66,66	0
56	MG	13	1641	1/1	0.97	0.31	18.84	80,80,80,80	0
56	MG	1H	3047	1/1	0.98	0.33	17.76	62,62,62,62	0
56	MG	1H	3136	1/1	0.89	0.33	16.53	69,69,69,69	0
56	MG	13	1626	1/1	0.86	0.32	16.23	56,56,56,56	0
56	MG	1H	3133	1/1	0.90	0.38	16.01	69,69,69,69	0
56	MG	13	1648	1/1	0.86	0.36	15.98	91,91,91,91	0
56	MG	1H	3145	1/1	0.94	0.27	15.50	70,70,70,70	0
56	MG	14	3056	1/1	0.89	0.28	15.24	69,69,69,69	0
56	MG	1H	3108	1/1	0.93	0.38	15.22	44,44,44,44	0
56	MG	1H	3072	1/1	0.95	0.39	15.11	52,52,52,52	0
56	MG	16	201	1/1	0.93	0.33	14.91	91,91,91,91	0
56	MG	14	3036	1/1	0.94	0.32	14.82	80,80,80,80	0
56	MG	13	1643	1/1	0.64	0.32	14.69	96,96,96,96	0
56	MG	13	1621	1/1	0.96	0.47	14.66	64,64,64,64	0
56	MG	14	3073	1/1	0.90	0.27	14.63	64,64,64,64	0
56	MG	1G	1617	1/1	0.90	0.27	13.50	90,90,90,90	0
56	MG	1H	3011	1/1	0.98	0.33	13.42	51,51,51,51	0
56	MG	1H	3312	1/1	0.57	0.29	13.37	83,83,83,83	0
56	MG	14	3076	1/1	0.99	0.28	12.77	60,60,60,60	0
56	MG	1H	3048	1/1	0.95	0.35	12.71	52,52,52,52	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	13	1613	1/1	0.94	0.31	12.60	79,79,79,79	0
56	MG	1H	3015	1/1	0.98	0.36	11.93	54,54,54,54	0
56	MG	1H	3103	1/1	0.92	0.31	11.86	60,60,60,60	0
56	MG	1H	3023	1/1	0.84	0.28	11.70	85,85,85,85	0
56	MG	1H	3001	1/1	0.98	0.37	11.66	49,49,49,49	0
56	MG	1G	1640	1/1	0.89	0.23	11.37	107,107,107,107	0
56	MG	2K	101	1/1	0.98	0.28	11.22	74,74,74,74	0
56	MG	1G	1669	1/1	0.81	0.34	11.03	105,105,105,105	0
56	MG	1H	3041	1/1	0.95	0.43	10.90	75,75,75,75	0
56	MG	1H	3109	1/1	0.78	0.35	10.77	79,79,79,79	0
56	MG	1H	3323	1/1	0.87	0.30	10.64	100,100,100,100	0
56	MG	13	1691	1/1	0.72	0.30	10.47	87,87,87,87	0
56	MG	14	3095	1/1	0.94	0.21	10.14	87,87,87,87	0
56	MG	1G	1675	1/1	0.88	0.23	10.13	93,93,93,93	0
56	MG	16	206	1/1	0.86	0.20	10.09	88,88,88,88	0
56	MG	14	3040	1/1	0.94	0.32	9.97	86,86,86,86	0
56	MG	14	3156	1/1	0.69	0.34	9.82	92,92,92,92	0
56	MG	13	1608	1/1	0.95	0.34	9.82	79,79,79,79	0
56	MG	1H	3189	1/1	0.78	0.32	9.49	67,67,67,67	0
56	MG	1H	3058	1/1	0.83	0.33	9.48	80,80,80,80	0
56	MG	1H	3124	1/1	0.79	0.26	9.32	72,72,72,72	0
56	MG	13	1631	1/1	0.96	0.30	9.20	62,62,62,62	0
56	MG	1H	3004	1/1	0.96	0.32	9.16	63,63,63,63	0
56	MG	1H	3033	1/1	0.96	0.33	9.07	72,72,72,72	0
56	MG	14	3042	1/1	0.91	0.21	8.98	69,69,69,69	0
56	MG	1H	3146	1/1	0.93	0.34	8.70	81,81,81,81	0
56	MG	1H	3199	1/1	0.91	0.47	8.58	101,101,101,101	0
56	MG	1H	3164	1/1	0.86	0.27	8.45	56,56,56,56	0
56	MG	1H	3186	1/1	0.43	0.26	8.36	74,74,74,74	0
56	MG	13	1671	1/1	0.94	0.20	8.35	92,92,92,92	0
56	MG	1H	3089	1/1	0.79	0.25	8.25	56,56,56,56	0
56	MG	1H	3032	1/1	0.81	0.33	8.23	79,79,79,79	0
56	MG	1H	3240	1/1	0.89	0.32	8.16	82,82,82,82	0
56	MG	1H	3128	1/1	0.81	0.27	7.83	69,69,69,69	0
56	MG	13	1659	1/1	0.97	0.30	7.39	94,94,94,94	0
56	MG	1H	3027	1/1	0.96	0.24	7.17	58,58,58,58	0
56	MG	1H	3230	1/1	0.94	0.28	7.03	73,73,73,73	0
56	MG	1H	3052	1/1	0.98	0.31	6.89	77,77,77,77	0
56	MG	1J	204	1/1	0.72	0.26	6.77	108,108,108,108	0
56	MG	21	302	1/1	0.91	0.35	6.69	84,84,84,84	0
56	MG	14	3052	1/1	0.95	0.31	6.58	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
56	MG	14	3021	1/1	0.85	0.26	6.34	81,81,81,81	0
56	MG	14	3041	1/1	0.88	0.28	6.32	59,59,59,59	0
56	MG	1H	3036	1/1	0.95	0.24	6.31	59,59,59,59	0
56	MG	1H	3151	1/1	0.70	0.23	6.13	60,60,60,60	0
56	MG	1H	3118	1/1	0.88	0.25	6.05	87,87,87,87	0
56	MG	1H	3167	1/1	0.78	0.27	5.98	59,59,59,59	0
56	MG	1H	3232	1/1	0.96	0.30	5.98	46,46,46,46	0
56	MG	1H	3081	1/1	0.99	0.26	5.88	54,54,54,54	0
56	MG	14	3027	1/1	0.93	0.25	5.79	89,89,89,89	0
56	MG	1G	1620	1/1	0.98	0.27	5.58	93,93,93,93	0
56	MG	1H	3305	1/1	0.92	0.26	5.42	76,76,76,76	0
56	MG	14	3096	1/1	0.89	0.22	5.38	64,64,64,64	0
56	MG	1H	3221	1/1	0.86	0.45	5.29	88,88,88,88	0
56	MG	1H	3152	1/1	0.61	0.24	5.25	75,75,75,75	0
56	MG	1G	1663	1/1	0.81	0.33	5.05	120,120,120,120	0
56	MG	14	3107	1/1	0.79	0.19	5.02	74,74,74,74	0
56	MG	13	1611	1/1	0.76	0.21	5.01	79,79,79,79	0
56	MG	14	3011	1/1	0.97	0.23	4.99	65,65,65,65	0
56	MG	14	3122	1/1	0.91	0.21	4.94	77,77,77,77	0
56	MG	14	3037	1/1	0.66	0.23	4.78	62,62,62,62	0
56	MG	1G	1602	1/1	0.91	0.26	4.76	76,76,76,76	0
56	MG	14	3068	1/1	0.98	0.23	4.74	64,64,64,64	0
56	MG	13	1630	1/1	0.90	0.20	4.65	80,80,80,80	0
56	MG	1H	3278	1/1	0.68	0.38	4.64	74,74,74,74	0
56	MG	13	1676	1/1	0.68	0.20	4.59	89,89,89,89	0
56	MG	1H	3185	1/1	0.71	0.20	4.55	70,70,70,70	0
56	MG	13	1606	1/1	0.86	0.27	4.44	83,83,83,83	0
56	MG	1H	3532	1/1	0.85	0.37	4.38	116,116,116,116	0
56	MG	1H	3066	1/1	0.94	0.23	4.34	48,48,48,48	0
56	MG	13	1601	1/1	0.95	0.27	4.14	71,71,71,71	0
56	MG	1H	3021	1/1	0.99	0.26	4.09	84,84,84,84	0
56	MG	13	1682	1/1	0.95	0.19	4.07	135,135,135,135	0
56	MG	1H	3358	1/1	0.94	0.25	4.04	65,65,65,65	0
56	MG	14	3198	1/1	0.86	0.19	3.89	90,90,90,90	0
56	MG	14	3035	1/1	0.99	0.23	3.84	68,68,68,68	0
56	MG	1G	1601	1/1	0.98	0.21	3.69	90,90,90,90	0
56	MG	1H	3020	1/1	0.96	0.22	3.68	67,67,67,67	0
56	MG	14	3022	1/1	0.96	0.19	3.68	83,83,83,83	0
56	MG	1H	3095	1/1	0.90	0.26	3.63	87,87,87,87	0
56	MG	13	1722	1/1	0.96	0.19	3.62	87,87,87,87	0
56	MG	13	1670	1/1	0.95	0.20	3.60	95,95,95,95	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	1H	3111	1/1	0.89	0.23	3.59	67,67,67,67	0
56	MG	3I	201	1/1	0.69	0.26	3.56	68,68,68,68	0
56	MG	1H	3082	1/1	0.91	0.23	3.43	40,40,40,40	0
56	MG	1H	3010	1/1	0.94	0.32	3.37	46,46,46,46	0
56	MG	1H	3037	1/1	0.93	0.29	3.29	51,51,51,51	0
56	MG	14	3227	1/1	0.87	0.16	3.18	106,106,106,106	0
56	MG	14	3125	1/1	0.55	0.16	3.16	77,77,77,77	0
56	MG	1H	3132	1/1	0.85	0.22	3.15	71,71,71,71	0
56	MG	1H	3026	1/1	0.84	0.22	3.14	61,61,61,61	0
56	MG	14	3160	1/1	0.86	0.20	3.01	81,81,81,81	0
56	MG	1H	3057	1/1	0.97	0.21	2.94	64,64,64,64	0
56	MG	13	1673	1/1	0.97	0.21	2.90	84,84,84,84	0
57	ZN	3E	303	1/1	0.96	0.41	2.82	127,127,127,127	0
56	MG	14	3182	1/1	0.94	0.19	2.81	66,66,66,66	0
56	MG	1H	3065	1/1	0.97	0.25	2.80	51,51,51,51	0
56	MG	14	3023	1/1	0.92	0.22	2.78	67,67,67,67	0
56	MG	14	3230	1/1	0.69	0.16	2.77	86,86,86,86	0
56	MG	1H	3416	1/1	0.97	0.21	2.77	48,48,48,48	0
56	MG	14	3191	1/1	0.96	0.20	2.75	90,90,90,90	0
56	MG	1H	3389	1/1	0.88	0.21	2.71	98,98,98,98	0
56	MG	1H	3142	1/1	0.95	0.24	2.66	82,82,82,82	0
56	MG	1H	3392	1/1	0.96	0.23	2.59	67,67,67,67	0
56	MG	14	3175	1/1	0.74	0.17	2.57	83,83,83,83	0
56	MG	1H	3092	1/1	0.69	0.19	2.53	66,66,66,66	0
56	MG	13	1615	1/1	0.93	0.27	2.42	100,100,100,100	0
56	MG	1H	3366	1/1	0.65	0.21	2.38	74,74,74,74	0
56	MG	J8	101	1/1	0.95	0.37	2.36	67,67,67,67	0
56	MG	1H	3098	1/1	0.99	0.27	2.34	63,63,63,63	0
56	MG	14	3240	1/1	0.62	0.23	2.31	90,90,90,90	0
56	MG	14	3121	1/1	0.81	0.15	2.23	91,91,91,91	0
56	MG	1H	3025	1/1	0.87	0.18	2.22	67,67,67,67	0
56	MG	1G	1609	1/1	0.98	0.17	2.18	96,96,96,96	0
56	MG	1H	3482	1/1	0.97	0.19	2.08	81,81,81,81	0
56	MG	14	3031	1/1	0.92	0.16	2.04	83,83,83,83	0
56	MG	1H	3399	1/1	0.98	0.20	2.03	50,50,50,50	0
56	MG	1H	3101	1/1	0.92	0.20	1.95	57,57,57,57	0
56	MG	1H	3188	1/1	0.75	0.18	1.88	67,67,67,67	0
56	MG	14	3029	1/1	0.85	0.15	1.88	86,86,86,86	0
56	MG	1G	1665	1/1	0.74	0.17	1.85	99,99,99,99	0
56	MG	1H	3028	1/1	0.94	0.23	1.82	59,59,59,59	0
56	MG	14	3412	1/1	0.84	0.20	1.75	93,93,93,93	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	1H	3038	1/1	0.97	0.25	1.73	78,78,78,78	0
56	MG	88	201	1/1	0.96	0.34	1.66	73,73,73,73	0
56	MG	1H	3042	1/1	0.77	0.22	1.62	62,62,62,62	0
56	MG	14	3162	1/1	0.83	0.21	1.57	107,107,107,107	0
56	MG	14	3187	1/1	0.95	0.16	1.48	63,63,63,63	0
56	MG	1H	3107	1/1	0.81	0.18	1.41	84,84,84,84	0
56	MG	14	3189	1/1	0.93	0.16	1.33	72,72,72,72	0
56	MG	1H	3174	1/1	0.84	0.16	1.26	63,63,63,63	0
56	MG	1J	205	1/1	0.66	0.26	1.24	113,113,113,113	0
56	MG	14	3169	1/1	0.95	0.16	1.22	65,65,65,65	0
56	MG	14	3034	1/1	0.94	0.19	1.16	78,78,78,78	0
56	MG	14	3090	1/1	0.98	0.16	1.10	87,87,87,87	0
56	MG	1H	3202	1/1	0.94	0.29	1.08	87,87,87,87	0
56	MG	13	1706	1/1	0.52	0.23	1.04	93,93,93,93	0
56	MG	14	3114	1/1	0.62	0.15	1.04	69,69,69,69	0
56	MG	1H	3219	1/1	0.96	0.18	0.96	73,73,73,73	0
56	MG	13	1680	1/1	0.74	0.18	0.95	107,107,107,107	0
56	MG	1H	3008	1/1	0.96	0.26	0.90	41,41,41,41	0
56	MG	14	3183	1/1	0.60	0.19	0.84	74,74,74,74	0
56	MG	1G	1621	1/1	0.75	0.16	0.82	122,122,122,122	0
56	MG	13	1715	1/1	0.96	0.17	0.81	85,85,85,85	0
56	MG	1H	3365	1/1	0.93	0.19	0.75	71,71,71,71	0
56	MG	2L	101	1/1	0.96	0.17	0.70	86,86,86,86	0
56	MG	78	201	1/1	0.88	0.17	0.68	79,79,79,79	0
56	MG	13	1632	1/1	0.98	0.17	0.67	74,74,74,74	0
56	MG	1G	1644	1/1	0.87	0.21	0.66	102,102,102,102	0
56	MG	1H	3147	1/1	0.86	0.20	0.64	69,69,69,69	0
56	MG	1H	3061	1/1	0.95	0.20	0.64	52,52,52,52	0
56	MG	14	3320	1/1	0.98	0.16	0.62	84,84,84,84	0
56	MG	14	3014	1/1	0.93	0.17	0.61	73,73,73,73	0
56	MG	1H	3398	1/1	0.94	0.19	0.59	58,58,58,58	0
56	MG	14	3246	1/1	0.63	0.14	0.56	97,97,97,97	0
56	MG	14	3004	1/1	0.98	0.15	0.54	61,61,61,61	0
56	MG	1H	3239	1/1	0.72	0.16	0.48	88,88,88,88	0
56	MG	14	3127	1/1	0.86	0.15	0.48	88,88,88,88	0
56	MG	14	3013	1/1	0.81	0.17	0.46	65,65,65,65	0
56	MG	14	3084	1/1	0.92	0.16	0.39	70,70,70,70	0
56	MG	14	3351	1/1	0.94	0.15	0.33	70,70,70,70	0
56	MG	1G	1670	1/1	0.89	0.14	0.33	96,96,96,96	0
56	MG	13	1654	1/1	0.88	0.22	0.31	125,125,125,125	0
56	MG	13	1605	1/1	0.97	0.17	0.27	82,82,82,82	0
56	MG	1H	3252	1/1	0.93	0.16	0.24	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
57	ZN	32	301	1/1	0.98	0.32	0.17	119,119,119,119	0
56	MG	13	1724	1/1	0.91	0.16	0.15	116,116,116,116	0
56	MG	1H	3076	1/1	0.90	0.17	0.11	64,64,64,64	0
56	MG	16	205	1/1	0.88	0.15	0.09	87,87,87,87	0
56	MG	13	1663	1/1	0.81	0.13	0.07	107,107,107,107	0
56	MG	13	1616	1/1	0.88	0.17	-0.01	95,95,95,95	0
56	MG	14	3190	1/1	0.70	0.15	-0.01	90,90,90,90	0
57	ZN	G8	201	1/1	0.63	0.24	-0.04	176,176,176,176	0
56	MG	13	1609	1/1	0.93	0.15	-0.07	83,83,83,83	0
56	MG	41	202	1/1	0.86	0.20	-0.09	85,85,85,85	0
56	MG	14	3097	1/1	0.83	0.15	-0.18	71,71,71,71	0
56	MG	13	1667	1/1	0.87	0.15	-0.20	91,91,91,91	0
57	ZN	5I	102	1/1	0.99	0.20	-0.25	96,96,96,96	0
56	MG	1G	1603	1/1	0.97	0.17	-0.28	77,77,77,77	0
56	MG	13	1627	1/1	0.97	0.16	-0.39	64,64,64,64	0
56	MG	11	302	1/1	0.96	0.20	-0.39	42,42,42,42	0
56	MG	16	210	1/1	0.88	0.15	-0.42	105,105,105,105	0
56	MG	1G	1618	1/1	0.83	0.15	-0.42	102,102,102,102	0
56	MG	14	3055	1/1	0.98	0.14	-0.45	59,59,59,59	0
56	MG	13	1604	1/1	0.92	0.14	-0.46	80,80,80,80	0
56	MG	1H	3235	1/1	0.94	0.17	-0.47	61,61,61,61	0
56	MG	14	3252	1/1	0.87	0.12	-0.48	74,74,74,74	0
56	MG	14	3032	1/1	0.95	0.13	-0.53	87,87,87,87	0
56	MG	1H	3063	1/1	0.89	0.17	-0.66	54,54,54,54	0
56	MG	1H	3383	1/1	0.96	0.15	-0.72	59,59,59,59	0
56	MG	14	3171	1/1	0.96	0.12	-0.79	84,84,84,84	0
56	MG	5I	101	1/1	0.78	0.15	-0.80	82,82,82,82	0
56	MG	1H	3345	1/1	0.86	0.15	-0.87	66,66,66,66	0
56	MG	13	1637	1/1	0.79	0.14	-0.92	71,71,71,71	0
56	MG	14	3110	1/1	0.90	0.16	-0.93	61,61,61,61	0
56	MG	14	3217	1/1	0.81	0.15	-0.94	159,159,159,159	0
56	MG	1G	1615	1/1	0.80	0.13	-1.00	86,86,86,86	0
56	MG	1H	3162	1/1	0.89	0.17	-1.02	69,69,69,69	0
56	MG	13	1709	1/1	0.94	0.14	-1.04	72,72,72,72	0
56	MG	3E	301	1/1	0.96	0.14	-1.13	116,116,116,116	0
56	MG	1H	3330	1/1	0.97	0.17	-1.13	53,53,53,53	0
56	MG	14	3193	1/1	0.81	0.14	-1.13	78,78,78,78	0
56	MG	1G	1642	1/1	0.95	0.15	-1.14	130,130,130,130	0
56	MG	1H	3327	1/1	0.97	0.17	-1.15	61,61,61,61	0
56	MG	1H	3447	1/1	0.97	0.12	-1.19	74,74,74,74	0
56	MG	1H	3528	1/1	0.97	0.13	-1.20	61,61,61,61	0
56	MG	1H	3064	1/1	0.98	0.16	-1.21	52,52,52,52	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	1H	3412	1/1	0.93	0.13	-1.22	70,70,70,70	0
56	MG	14	3019	1/1	0.96	0.14	-1.23	73,73,73,73	0
56	MG	1H	3452	1/1	0.95	0.16	-1.24	50,50,50,50	0
56	MG	14	3277	1/1	0.96	0.13	-1.24	54,54,54,54	0
56	MG	1H	3166	1/1	0.95	0.17	-1.27	53,53,53,53	0
56	MG	1H	3208	1/1	0.81	0.17	-1.29	53,53,53,53	0
56	MG	14	3116	1/1	0.88	0.12	-1.33	75,75,75,75	0
56	MG	14	3173	1/1	0.92	0.12	-1.42	66,66,66,66	0
56	MG	1H	3071	1/1	0.84	0.16	-1.44	38,38,38,38	0
56	MG	1H	3343	1/1	0.98	0.17	-1.46	52,52,52,52	0
56	MG	1H	3537	1/1	0.89	0.14	-1.49	55,55,55,55	0
56	MG	13	1686	1/1	0.94	0.15	-1.53	84,84,84,84	0
56	MG	1H	3116	1/1	0.98	0.15	-1.57	66,66,66,66	0
56	MG	14	3167	1/1	0.93	0.12	-1.58	67,67,67,67	0
56	MG	1H	3404	1/1	0.96	0.15	-1.62	74,74,74,74	0
56	MG	14	3159	1/1	0.94	0.13	-1.65	64,64,64,64	0
56	MG	1H	3337	1/1	0.93	0.16	-1.66	65,65,65,65	0
56	MG	1H	3341	1/1	0.99	0.16	-1.66	43,43,43,43	0
56	MG	1H	3395	1/1	0.91	0.16	-1.67	59,59,59,59	0
56	MG	41	201	1/1	0.85	0.19	-1.69	85,85,85,85	0
56	MG	13	1739	1/1	0.94	0.12	-1.70	103,103,103,103	0
56	MG	1G	1652	1/1	0.96	0.12	-1.70	81,81,81,81	0
56	MG	1H	3117	1/1	0.71	0.15	-1.71	57,57,57,57	0
56	MG	1H	3129	1/1	0.80	0.15	-1.71	57,57,57,57	0
56	MG	1H	3414	1/1	0.96	0.17	-1.71	67,67,67,67	0
56	MG	14	3153	1/1	0.69	0.12	-1.76	82,82,82,82	0
56	MG	5E	201	1/1	0.93	0.17	-1.81	93,93,93,93	0
56	MG	1H	3408	1/1	0.90	0.16	-1.83	60,60,60,60	0
56	MG	13	1701	1/1	0.49	0.14	-1.83	71,71,71,71	0
56	MG	13	1735	1/1	0.91	0.09	-1.83	78,78,78,78	0
56	MG	14	3150	1/1	0.89	0.12	-1.84	57,57,57,57	0
56	MG	14	3202	1/1	0.94	0.11	-1.85	106,106,106,106	0
56	MG	1H	3153	1/1	0.98	0.15	-1.86	77,77,77,77	0
56	MG	13	1713	1/1	0.96	0.09	-1.87	99,99,99,99	0
56	MG	13	1647	1/1	0.86	0.06	-1.87	83,83,83,83	0
56	MG	1H	3468	1/1	0.70	0.12	-1.88	115,115,115,115	0
56	MG	13	1675	1/1	0.73	0.10	-1.88	131,131,131,131	0
56	MG	14	3300	1/1	0.96	0.12	-1.91	69,69,69,69	0
56	MG	14	3007	1/1	0.95	0.15	-1.92	69,69,69,69	0
56	MG	13	1746	1/1	0.93	0.07	-1.92	102,102,102,102	0
56	MG	14	3264	1/1	0.93	0.09	-1.95	78,78,78,78	0
56	MG	1H	3448	1/1	0.96	0.14	-1.96	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
56	MG	1H	3264	1/1	0.86	0.14	-1.96	68,68,68,68	0
56	MG	1H	3396	1/1	0.96	0.14	-1.96	61,61,61,61	0
56	MG	1H	3355	1/1	0.95	0.14	-1.97	72,72,72,72	0
56	MG	1H	3083	1/1	0.97	0.15	-1.99	51,51,51,51	0
56	MG	1H	3536	1/1	0.93	0.07	-2.05	43,43,43,43	0
56	MG	14	3286	1/1	0.95	0.12	-2.05	62,62,62,62	0
56	MG	1G	1688	1/1	0.71	0.10	-2.07	122,122,122,122	0
56	MG	1H	3405	1/1	0.89	0.12	-2.11	78,78,78,78	0
56	MG	14	3328	1/1	0.93	0.11	-2.12	73,73,73,73	0
56	MG	1H	3456	1/1	0.92	0.14	-2.17	69,69,69,69	0
56	MG	16	204	1/1	0.84	0.11	-2.17	68,68,68,68	0
56	MG	1G	1637	1/1	0.96	0.11	-2.18	89,89,89,89	0
56	MG	1H	3432	1/1	0.95	0.15	-2.24	69,69,69,69	0
56	MG	13	1721	1/1	0.96	0.14	-2.24	99,99,99,99	0
56	MG	1H	3093	1/1	0.95	0.12	-2.25	56,56,56,56	0
56	MG	14	3360	1/1	0.88	0.08	-2.30	104,104,104,104	0
56	MG	1H	3331	1/1	0.97	0.16	-2.35	49,49,49,49	0
56	MG	1H	3339	1/1	1.00	0.11	-2.38	60,60,60,60	0
56	MG	1J	201	1/1	0.96	0.10	-2.42	123,123,123,123	0
56	MG	13	1710	1/1	0.90	0.13	-2.48	61,61,61,61	0
56	MG	1H	3437	1/1	0.96	0.14	-2.50	70,70,70,70	0
56	MG	14	3047	1/1	0.96	0.09	-2.54	68,68,68,68	0
56	MG	14	3357	1/1	0.94	0.10	-2.65	82,82,82,82	0
56	MG	14	3275	1/1	0.98	0.12	-2.72	58,58,58,58	0
56	MG	1H	3391	1/1	0.95	0.10	-2.76	58,58,58,58	0
56	MG	1H	3397	1/1	0.93	0.12	-2.80	52,52,52,52	0
56	MG	1H	3351	1/1	0.96	0.12	-2.81	65,65,65,65	0
56	MG	14	3323	1/1	0.96	0.14	-2.83	59,59,59,59	0
56	MG	13	1633	1/1	0.96	0.12	-2.83	84,84,84,84	0
56	MG	1H	3342	1/1	0.96	0.12	-2.83	60,60,60,60	0
56	MG	1H	3442	1/1	0.91	0.11	-2.88	74,74,74,74	0
56	MG	14	3283	1/1	0.91	0.07	-2.94	78,78,78,78	0
56	MG	1H	3380	1/1	0.91	0.11	-2.99	44,44,44,44	0
56	MG	14	3308	1/1	0.95	0.10	-3.00	69,69,69,69	0
56	MG	14	3314	1/1	0.86	0.10	-3.05	59,59,59,59	0
56	MG	14	3420	1/1	0.59	0.12	-3.13	91,91,91,91	0
56	MG	1G	1605	1/1	0.94	0.10	-3.24	95,95,95,95	0
56	MG	14	3074	1/1	0.85	0.10	-3.29	89,89,89,89	0
56	MG	14	3371	1/1	0.92	0.10	-3.30	102,102,102,102	0
56	MG	1G	1683	1/1	0.89	0.11	-3.33	97,97,97,97	0
56	MG	1H	3378	1/1	0.88	0.14	-3.34	77,77,77,77	0
56	MG	13	1620	1/1	0.85	0.10	-3.38	81,81,81,81	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	1H	3102	1/1	0.94	0.15	-3.42	45,45,45,45	0
56	MG	1H	3430	1/1	0.95	0.09	-3.42	50,50,50,50	0
56	MG	1H	3155	1/1	0.93	0.11	-3.43	65,65,65,65	0
56	MG	14	3092	1/1	0.85	0.09	-3.45	61,61,61,61	0
56	MG	14	3378	1/1	0.42	0.07	-3.49	126,126,126,126	0
56	MG	1H	3286	1/1	0.71	0.13	-3.55	88,88,88,88	0
56	MG	14	3177	1/1	0.75	0.11	-3.56	81,81,81,81	0
56	MG	14	3318	1/1	0.97	0.09	-3.57	69,69,69,69	0
56	MG	1G	1685	1/1	0.90	0.10	-3.59	91,91,91,91	0
56	MG	1H	3350	1/1	0.96	0.12	-3.80	52,52,52,52	0
56	MG	14	3322	1/1	0.89	0.08	-3.83	80,80,80,80	0
56	MG	14	3394	1/1	0.80	0.10	-3.85	102,102,102,102	0
56	MG	14	3025	1/1	0.95	0.09	-3.88	87,87,87,87	0
56	MG	14	3285	1/1	0.92	0.09	-3.91	68,68,68,68	0
56	MG	14	3393	1/1	0.81	0.08	-3.98	111,111,111,111	0
56	MG	1H	3521	1/1	0.45	0.12	-4.13	89,89,89,89	0
56	MG	14	3324	1/1	0.93	0.08	-4.14	63,63,63,63	0
56	MG	1H	3367	1/1	0.92	0.13	-4.25	50,50,50,50	0
56	MG	13	1726	1/1	0.74	0.08	-4.26	96,96,96,96	0
56	MG	14	3392	1/1	0.93	0.10	-4.32	77,77,77,77	0
56	MG	14	3294	1/1	0.94	0.07	-4.36	59,59,59,59	0
56	MG	1H	3326	1/1	0.95	0.13	-4.44	54,54,54,54	0
56	MG	1H	3087	1/1	0.98	0.12	-4.49	69,69,69,69	0
56	MG	16	213	1/1	0.77	0.09	-4.61	102,102,102,102	0
56	MG	13	1678	1/1	0.93	0.10	-4.63	85,85,85,85	0
56	MG	1H	3435	1/1	0.95	0.13	-4.64	52,52,52,52	0
56	MG	14	3321	1/1	0.96	0.07	-4.68	62,62,62,62	0
56	MG	1H	3332	1/1	0.95	0.15	-4.69	64,64,64,64	0
56	MG	14	3289	1/1	0.87	0.10	-4.72	77,77,77,77	0
56	MG	14	3411	1/1	0.93	0.07	-4.78	106,106,106,106	0
56	MG	14	3184	1/1	0.89	0.08	-4.79	79,79,79,79	0
56	MG	1H	3348	1/1	0.98	0.12	-4.82	60,60,60,60	0
56	MG	1H	3334	1/1	0.97	0.07	-4.86	56,56,56,56	0
56	MG	1H	3390	1/1	0.95	0.11	-4.94	61,61,61,61	0
56	MG	14	3319	1/1	0.90	0.08	-5.02	86,86,86,86	0
56	MG	1H	3074	1/1	0.97	0.15	-5.06	46,46,46,46	0
56	MG	14	3388	1/1	0.87	0.06	-5.13	90,90,90,90	0
56	MG	14	3210	1/1	0.92	0.09	-5.16	100,100,100,100	0
56	MG	1G	1657	1/1	0.80	0.08	-5.20	112,112,112,112	0
56	MG	1H	3329	1/1	0.95	0.12	-5.21	52,52,52,52	0
56	MG	14	3306	1/1	0.96	0.08	-5.24	66,66,66,66	0
56	MG	14	3333	1/1	0.97	0.06	-5.28	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
56	MG	14	3354	1/1	0.92	0.05	-5.31	90,90,90,90	0
56	MG	1H	3024	1/1	0.95	0.08	-5.39	61,61,61,61	0
56	MG	1H	3493	1/1	0.97	0.11	-5.53	68,68,68,68	0
56	MG	14	3379	1/1	0.75	0.06	-5.58	126,126,126,126	0
56	MG	14	3089	1/1	0.93	0.06	-5.65	54,54,54,54	0
56	MG	14	3276	1/1	0.95	0.09	-5.78	85,85,85,85	0
56	MG	1H	3169	1/1	0.94	0.10	-5.79	49,49,49,49	0
56	MG	14	3389	1/1	0.87	0.09	-5.87	72,72,72,72	0
56	MG	1H	3359	1/1	0.90	0.10	-6.45	93,93,93,93	0
56	MG	1H	3484	1/1	0.83	0.08	-6.62	105,105,105,105	0
56	MG	1H	3451	1/1	0.93	0.07	-6.73	88,88,88,88	0
56	MG	1H	3450	1/1	0.90	0.12	-6.74	88,88,88,88	0
56	MG	1H	3385	1/1	0.96	0.11	-6.77	62,62,62,62	0
56	MG	14	3292	1/1	0.98	0.09	-7.25	73,73,73,73	0
56	MG	1H	3357	1/1	0.90	0.08	-7.25	72,72,72,72	0
56	MG	2K	108	1/1	0.88	0.07	-7.31	92,92,92,92	0
56	MG	1H	3518	1/1	0.86	0.06	-7.39	89,89,89,89	0
56	MG	13	1717	1/1	0.97	0.06	-7.49	64,64,64,64	0
56	MG	13	1728	1/1	0.95	0.07	-7.52	80,80,80,80	0
56	MG	1H	3533	1/1	0.92	0.05	-7.87	106,106,106,106	0
56	MG	14	3149	1/1	0.97	0.09	-8.38	58,58,58,58	0
56	MG	1H	3511	1/1	0.94	0.11	-8.46	84,84,84,84	0
56	MG	1H	3407	1/1	0.92	0.06	-8.55	59,59,59,59	0
56	MG	1H	3441	1/1	0.89	0.05	-10.55	73,73,73,73	0
56	MG	1H	3349	1/1	0.99	0.06	-10.56	68,68,68,68	0
56	MG	1H	3384	1/1	0.97	0.10	-11.57	50,50,50,50	0
56	MG	1H	3379	1/1	0.88	0.07	-12.34	90,90,90,90	0
56	MG	1H	3363	1/1	0.62	0.06	-13.08	83,83,83,83	0
56	MG	14	3365	1/1	0.82	0.07	-13.13	89,89,89,89	0
56	MG	1H	3513	1/1	0.91	0.06	-15.43	104,104,104,104	0
56	MG	1H	3182	1/1	0.73	0.40	-	69,69,69,69	0
56	MG	14	3259	1/1	0.65	0.39	-	104,104,104,104	0
56	MG	13	1700	1/1	0.85	0.36	-	103,103,103,103	0
56	MG	1H	3340	1/1	0.95	0.12	-	76,76,76,76	0
56	MG	1H	3259	1/1	0.82	0.29	-	79,79,79,79	0
56	MG	1H	3055	1/1	0.89	0.27	-	77,77,77,77	0
56	MG	14	3251	1/1	0.80	0.32	-	83,83,83,83	0
56	MG	1H	3419	1/1	0.83	0.09	-	86,86,86,86	0
56	MG	1H	3449	1/1	0.97	0.08	-	91,91,91,91	0
56	MG	14	3020	1/1	0.95	0.20	-	62,62,62,62	0
56	MG	1H	3243	1/1	0.86	0.57	-	85,85,85,85	0
56	MG	13	1692	1/1	0.65	0.29	-	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
56	MG	1H	3292	1/1	0.91	0.10	-	80,80,80,80	0
56	MG	14	3267	1/1	0.83	0.27	-	79,79,79,79	0
56	MG	1H	3049	1/1	0.98	0.28	-	59,59,59,59	0
56	MG	1H	3455	1/1	0.82	0.05	-	101,101,101,101	0
56	MG	14	3146	1/1	0.89	0.35	-	91,91,91,91	0
56	MG	14	3287	1/1	0.94	0.07	-	70,70,70,70	0
56	MG	1H	3295	1/1	0.85	0.32	-	72,72,72,72	0
56	MG	14	3272	1/1	0.34	0.25	-	100,100,100,100	0
56	MG	1H	3516	1/1	0.86	0.13	-	114,114,114,114	0
56	MG	14	3248	1/1	0.86	0.29	-	91,91,91,91	0
56	MG	1G	1616	1/1	0.81	0.21	-	97,97,97,97	0
56	MG	13	1662	1/1	0.89	0.35	-	94,94,94,94	0
56	MG	14	3406	1/1	0.88	0.21	-	84,84,84,84	0
56	MG	1H	3135	1/1	0.95	0.40	-	74,74,74,74	0
56	MG	14	3060	1/1	0.95	0.24	-	84,84,84,84	0
56	MG	1H	3200	1/1	0.96	0.25	-	77,77,77,77	0
56	MG	1H	3311	1/1	0.62	0.39	-	93,93,93,93	0
56	MG	1H	3313	1/1	0.96	0.17	-	86,86,86,86	0
56	MG	1H	3062	1/1	0.86	0.27	-	61,61,61,61	0
56	MG	1H	3526	1/1	0.93	0.06	-	78,78,78,78	0
56	MG	13	1628	1/1	0.92	0.20	-	51,51,51,51	0
56	MG	1H	3178	1/1	0.84	0.26	-	61,61,61,61	0
56	MG	1H	3144	1/1	0.96	0.17	-	63,63,63,63	0
56	MG	1G	1672	1/1	0.70	0.20	-	98,98,98,98	0
56	MG	1H	3502	1/1	0.87	0.08	-	109,109,109,109	0
56	MG	1H	3271	1/1	0.46	0.43	-	100,100,100,100	0
56	MG	1H	3175	1/1	0.82	0.41	-	69,69,69,69	0
56	MG	1K	102	1/1	0.90	0.10	-	107,107,107,107	0
56	MG	14	3224	1/1	0.95	0.12	-	66,66,66,66	0
56	MG	1H	3280	1/1	0.58	0.40	-	101,101,101,101	0
56	MG	1H	3470	1/1	0.90	0.08	-	81,81,81,81	0
56	MG	13	1640	1/1	0.87	0.26	-	81,81,81,81	0
56	MG	1H	3104	1/1	0.96	0.31	-	57,57,57,57	0
56	MG	1G	1658	1/1	0.88	0.32	-	91,91,91,91	0
56	MG	14	3049	1/1	0.97	0.16	-	60,60,60,60	0
56	MG	14	3303	1/1	0.90	0.04	-	92,92,92,92	0
56	MG	1H	3333	1/1	0.91	0.14	-	64,64,64,64	0
56	MG	14	3071	1/1	0.75	0.20	-	63,63,63,63	0
56	MG	3L	103	1/1	0.89	0.26	-	99,99,99,99	0
56	MG	14	3219	1/1	0.61	0.31	-	100,100,100,100	0
56	MG	14	3088	1/1	0.94	0.24	-	88,88,88,88	0
56	MG	1H	3262	1/1	0.89	0.23	-	86,86,86,86	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	1H	3388	1/1	0.90	0.09	-	90,90,90,90	0
56	MG	1H	3483	1/1	0.81	0.17	-	116,116,116,116	0
56	MG	14	3305	1/1	0.91	0.07	-	89,89,89,89	0
56	MG	1H	3209	1/1	0.96	0.15	-	68,68,68,68	0
56	MG	13	1694	1/1	0.89	0.12	-	94,94,94,94	0
56	MG	14	3353	1/1	0.87	0.19	-	94,94,94,94	0
56	MG	1H	3039	1/1	0.97	0.23	-	87,87,87,87	0
56	MG	14	3083	1/1	0.69	0.22	-	86,86,86,86	0
56	MG	1G	1667	1/1	0.80	0.32	-	124,124,124,124	0
56	MG	1H	3019	1/1	0.96	0.17	-	48,48,48,48	0
56	MG	1H	3479	1/1	0.96	0.10	-	72,72,72,72	0
56	MG	1H	3043	1/1	0.78	0.41	-	62,62,62,62	0
56	MG	14	3002	1/1	0.98	0.18	-	62,62,62,62	0
56	MG	1H	3425	1/1	0.96	0.08	-	77,77,77,77	0
56	MG	14	3263	1/1	0.82	0.16	-	97,97,97,97	0
56	MG	14	3235	1/1	0.80	0.27	-	92,92,92,92	0
56	MG	14	3315	1/1	0.71	0.11	-	76,76,76,76	0
56	MG	14	3336	1/1	0.86	0.46	-	114,114,114,114	0
56	MG	1H	3328	1/1	0.94	0.12	-	75,75,75,75	0
56	MG	13	1603	1/1	0.96	0.27	-	67,67,67,67	0
56	MG	14	3062	1/1	0.97	0.10	-	70,70,70,70	0
56	MG	14	3048	1/1	0.93	0.11	-	63,63,63,63	0
56	MG	1H	3266	1/1	0.75	0.33	-	94,94,94,94	0
56	MG	1H	3233	1/1	0.94	0.16	-	65,65,65,65	0
56	MG	14	3128	1/1	0.52	0.31	-	91,91,91,91	0
56	MG	1H	3106	1/1	0.86	0.34	-	70,70,70,70	0
56	MG	14	3194	1/1	0.86	0.13	-	73,73,73,73	0
56	MG	1H	3179	1/1	0.86	0.23	-	75,75,75,75	0
56	MG	14	3383	1/1	0.86	0.14	-	114,114,114,114	0
56	MG	14	3069	1/1	0.97	0.34	-	73,73,73,73	0
56	MG	14	3257	1/1	0.39	0.17	-	93,93,93,93	0
56	MG	13	1651	1/1	0.86	0.28	-	76,76,76,76	0
56	MG	14	3390	1/1	0.91	0.07	-	111,111,111,111	0
56	MG	14	3221	1/1	0.82	0.35	-	99,99,99,99	0
56	MG	1H	3009	1/1	0.97	0.41	-	58,58,58,58	0
56	MG	14	3174	1/1	0.68	0.23	-	82,82,82,82	0
56	MG	16	209	1/1	0.90	0.22	-	74,74,74,74	0
56	MG	14	3102	1/1	0.82	0.47	-	73,73,73,73	0
56	MG	1G	1682	1/1	0.94	0.08	-	86,86,86,86	0
56	MG	1H	3307	1/1	0.75	0.31	-	86,86,86,86	0
56	MG	14	3377	1/1	0.96	0.04	-	88,88,88,88	0
56	MG	13	1704	1/1	0.70	0.26	-	113,113,113,113	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	13	1736	1/1	0.96	0.14	-	95,95,95,95	0
56	MG	1H	3035	1/1	0.96	0.24	-	76,76,76,76	0
56	MG	3L	102	1/1	0.86	0.09	-	146,146,146,146	0
56	MG	14	3199	1/1	0.56	0.23	-	83,83,83,83	0
56	MG	14	3250	1/1	0.72	0.28	-	98,98,98,98	0
56	MG	1G	1607	1/1	0.15	0.26	-	96,96,96,96	0
56	MG	13	1696	1/1	0.81	0.22	-	91,91,91,91	0
56	MG	1H	3509	1/1	0.88	0.06	-	91,91,91,91	0
56	MG	14	3307	1/1	0.90	0.07	-	81,81,81,81	0
56	MG	14	3242	1/1	0.51	0.29	-	89,89,89,89	0
56	MG	14	3278	1/1	0.97	0.07	-	62,62,62,62	0
56	MG	1G	1686	1/1	0.97	0.09	-	117,117,117,117	0
56	MG	14	3268	1/1	0.55	0.20	-	96,96,96,96	0
56	MG	14	3381	1/1	0.91	0.05	-	110,110,110,110	0
56	MG	14	3204	1/1	0.91	0.19	-	87,87,87,87	0
56	MG	14	3295	1/1	0.88	0.03	-	90,90,90,90	0
56	MG	13	1684	1/1	0.54	0.23	-	108,108,108,108	0
56	MG	1H	3091	1/1	0.94	0.35	-	65,65,65,65	0
56	MG	1H	3249	1/1	0.97	0.13	-	75,75,75,75	0
56	MG	1H	3315	1/1	0.90	0.39	-	93,93,93,93	0
56	MG	1H	3068	1/1	0.62	0.45	-	68,68,68,68	0
56	MG	2L	103	1/1	0.87	0.14	-	85,85,85,85	0
56	MG	13	1712	1/1	0.93	0.08	-	84,84,84,84	0
56	MG	14	3385	1/1	0.95	0.07	-	83,83,83,83	0
56	MG	1H	3368	1/1	0.93	0.14	-	58,58,58,58	0
56	MG	1G	1664	1/1	0.83	0.29	-	90,90,90,90	0
56	MG	14	3407	1/1	0.78	0.10	-	110,110,110,110	0
56	MG	1H	3122	1/1	0.53	0.27	-	77,77,77,77	0
56	MG	1H	3504	1/1	0.74	0.12	-	117,117,117,117	0
56	MG	13	1666	1/1	0.98	0.06	-	86,86,86,86	0
56	MG	1H	3050	1/1	0.96	0.30	-	62,62,62,62	0
56	MG	1H	3226	1/1	0.96	0.29	-	87,87,87,87	0
56	MG	1H	3302	1/1	0.53	0.37	-	88,88,88,88	0
56	MG	1H	3299	1/1	0.86	0.40	-	83,83,83,83	0
56	MG	14	3245	1/1	0.70	0.17	-	83,83,83,83	0
56	MG	1H	3268	1/1	0.81	0.33	-	84,84,84,84	0
56	MG	1H	3498	1/1	0.93	0.09	-	74,74,74,74	0
56	MG	1H	3284	1/1	0.91	0.38	-	81,81,81,81	0
56	MG	13	1725	1/1	0.75	0.10	-	114,114,114,114	0
56	MG	14	3126	1/1	0.96	0.32	-	80,80,80,80	0
56	MG	14	3343	1/1	0.94	0.05	-	81,81,81,81	0
56	MG	13	1638	1/1	0.88	0.33	-	68,68,68,68	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	14	3147	1/1	0.75	0.29	-	93,93,93,93	0
56	MG	13	1639	1/1	0.96	0.19	-	87,87,87,87	0
56	MG	1H	3228	1/1	0.96	0.21	-	67,67,67,67	0
56	MG	13	1644	1/1	0.96	0.39	-	87,87,87,87	0
56	MG	14	3262	1/1	0.55	0.13	-	101,101,101,101	0
56	MG	1H	3207	1/1	0.76	0.34	-	76,76,76,76	0
56	MG	1H	3422	1/1	0.62	0.14	-	99,99,99,99	0
56	MG	1G	1634	1/1	0.84	0.44	-	114,114,114,114	0
56	MG	14	3395	1/1	0.80	0.09	-	105,105,105,105	0
56	MG	1H	3127	1/1	0.92	0.37	-	64,64,64,64	0
56	MG	1H	3191	1/1	0.90	0.23	-	83,83,83,83	0
56	MG	14	3386	1/1	0.83	0.06	-	96,96,96,96	0
56	MG	1G	1692	1/1	0.79	0.06	-	106,106,106,106	0
56	MG	14	3139	1/1	0.93	0.30	-	97,97,97,97	0
56	MG	13	1618	1/1	0.94	0.35	-	67,67,67,67	0
56	MG	14	3358	1/1	0.72	0.16	-	98,98,98,98	0
56	MG	14	3387	1/1	0.97	0.06	-	90,90,90,90	0
56	MG	14	3170	1/1	0.91	0.11	-	77,77,77,77	0
56	MG	14	3130	1/1	0.73	0.26	-	98,98,98,98	0
56	MG	1H	3294	1/1	0.46	0.54	-	88,88,88,88	0
56	MG	14	3065	1/1	0.96	0.15	-	71,71,71,71	0
56	MG	1H	3059	1/1	0.96	0.28	-	70,70,70,70	0
56	MG	1H	3317	1/1	0.93	0.19	-	75,75,75,75	0
56	MG	1H	3376	1/1	0.90	0.09	-	88,88,88,88	0
56	MG	1J	202	1/1	0.82	0.18	-	93,93,93,93	0
56	MG	1G	1648	1/1	0.84	0.32	-	85,85,85,85	0
56	MG	13	1677	1/1	0.54	0.36	-	96,96,96,96	0
56	MG	14	3195	1/1	0.91	0.13	-	51,51,51,51	0
56	MG	1G	1626	1/1	0.96	0.24	-	99,99,99,99	0
56	MG	13	1740	1/1	0.97	0.07	-	83,83,83,83	0
56	MG	14	3409	1/1	0.85	0.09	-	109,109,109,109	0
56	MG	1H	3040	1/1	0.84	0.36	-	72,72,72,72	0
56	MG	1H	3413	1/1	0.95	0.15	-	82,82,82,82	0
56	MG	1H	3387	1/1	0.98	0.11	-	63,63,63,63	0
56	MG	14	3067	1/1	0.94	0.17	-	76,76,76,76	0
56	MG	1H	3494	1/1	0.84	0.07	-	107,107,107,107	0
56	MG	1G	1651	1/1	0.81	0.19	-	95,95,95,95	0
56	MG	1H	3377	1/1	0.95	0.10	-	90,90,90,90	0
56	MG	13	1741	1/1	0.59	0.08	-	99,99,99,99	0
56	MG	1H	3369	1/1	0.86	0.15	-	58,58,58,58	0
56	MG	14	3327	1/1	0.95	0.09	-	70,70,70,70	0
56	MG	14	3342	1/1	0.86	0.08	-	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
56	MG	1H	3251	1/1	0.94	0.15	-	115,115,115,115	0
56	MG	1H	3110	1/1	0.76	0.36	-	75,75,75,75	0
56	MG	1H	3140	1/1	0.64	0.43	-	87,87,87,87	0
56	MG	14	3082	1/1	0.98	0.23	-	75,75,75,75	0
56	MG	14	3239	1/1	0.79	0.24	-	92,92,92,92	0
56	MG	1H	3097	1/1	0.79	0.18	-	76,76,76,76	0
56	MG	14	3172	1/1	0.91	0.18	-	87,87,87,87	0
56	MG	14	3157	1/1	0.61	0.19	-	68,68,68,68	0
56	MG	14	3290	1/1	0.86	0.13	-	68,68,68,68	0
56	MG	13	1625	1/1	0.92	0.32	-	74,74,74,74	0
56	MG	14	3112	1/1	0.86	0.23	-	85,85,85,85	0
56	MG	1H	3067	1/1	0.92	0.28	-	75,75,75,75	0
56	MG	13	1749	1/1	0.92	0.10	-	107,107,107,107	0
56	MG	1H	3236	1/1	0.89	0.12	-	72,72,72,72	0
56	MG	1H	3044	1/1	0.86	0.26	-	76,76,76,76	0
56	MG	13	1720	1/1	0.94	0.10	-	105,105,105,105	0
56	MG	13	1653	1/1	0.85	0.28	-	91,91,91,91	0
56	MG	1H	3474	1/1	0.88	0.09	-	103,103,103,103	0
56	MG	1H	3206	1/1	0.82	0.38	-	76,76,76,76	0
56	MG	14	3249	1/1	0.96	0.13	-	89,89,89,89	0
56	MG	1H	3297	1/1	0.69	0.29	-	79,79,79,79	0
56	MG	14	3030	1/1	0.86	0.18	-	84,84,84,84	0
56	MG	14	3326	1/1	0.91	0.08	-	58,58,58,58	0
56	MG	1H	3170	1/1	0.78	0.15	-	71,71,71,71	0
56	MG	14	3359	1/1	0.92	0.07	-	117,117,117,117	0
56	MG	1G	1646	1/1	0.93	0.43	-	108,108,108,108	0
56	MG	1H	3510	1/1	0.85	0.07	-	99,99,99,99	0
56	MG	13	1727	1/1	0.97	0.11	-	111,111,111,111	0
56	MG	1G	1610	1/1	0.94	0.09	-	103,103,103,103	0
56	MG	13	1711	1/1	0.70	0.08	-	106,106,106,106	0
56	MG	1H	3177	1/1	0.91	0.43	-	72,72,72,72	0
56	MG	1H	3272	1/1	0.85	0.34	-	92,92,92,92	0
56	MG	14	3368	1/1	0.81	0.07	-	105,105,105,105	0
56	MG	14	3115	1/1	0.79	0.28	-	82,82,82,82	0
56	MG	1H	3356	1/1	0.90	0.14	-	81,81,81,81	0
56	MG	1H	3112	1/1	0.84	0.23	-	72,72,72,72	0
56	MG	14	3093	1/1	0.97	0.23	-	58,58,58,58	0
56	MG	1H	3190	1/1	0.84	0.43	-	85,85,85,85	0
56	MG	14	3135	1/1	0.66	0.17	-	84,84,84,84	0
56	MG	1H	3245	1/1	0.93	0.15	-	73,73,73,73	0
56	MG	1H	3181	1/1	0.96	0.34	-	84,84,84,84	0
56	MG	14	3253	1/1	0.73	0.13	-	73,73,73,73	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	14	3243	1/1	0.60	0.18	-	93,93,93,93	0
56	MG	1H	3381	1/1	0.87	0.10	-	78,78,78,78	0
56	MG	1H	3496	1/1	0.92	0.08	-	103,103,103,103	0
56	MG	1H	3347	1/1	0.91	0.12	-	54,54,54,54	0
56	MG	14	3179	1/1	0.87	0.09	-	71,71,71,71	0
56	MG	1H	3354	1/1	0.86	0.11	-	106,106,106,106	0
56	MG	11	301	1/1	0.87	0.30	-	78,78,78,78	0
56	MG	14	3028	1/1	0.92	0.23	-	101,101,101,101	0
56	MG	1H	3370	1/1	0.98	0.16	-	67,67,67,67	0
56	MG	14	3044	1/1	0.90	0.25	-	52,52,52,52	0
56	MG	14	3231	1/1	0.79	0.13	-	79,79,79,79	0
56	MG	1H	3157	1/1	0.95	0.29	-	57,57,57,57	0
56	MG	13	1645	1/1	0.86	0.27	-	94,94,94,94	0
56	MG	1H	3495	1/1	0.93	0.15	-	75,75,75,75	0
56	MG	1H	3120	1/1	0.70	0.30	-	89,89,89,89	0
56	MG	14	3310	1/1	0.92	0.10	-	65,65,65,65	0
56	MG	14	3218	1/1	0.69	0.23	-	95,95,95,95	0
56	MG	1H	3512	1/1	0.93	0.13	-	80,80,80,80	0
56	MG	14	3091	1/1	0.95	0.19	-	64,64,64,64	0
56	MG	1H	3508	1/1	0.84	0.10	-	117,117,117,117	0
56	MG	1H	3088	1/1	0.88	0.09	-	71,71,71,71	0
56	MG	1H	3353	1/1	0.81	0.08	-	100,100,100,100	0
56	MG	14	3270	1/1	0.69	0.29	-	98,98,98,98	0
56	MG	1H	3523	1/1	0.79	0.09	-	115,115,115,115	0
56	MG	2K	107	1/1	0.89	0.10	-	86,86,86,86	0
56	MG	1H	3276	1/1	0.71	0.19	-	87,87,87,87	0
56	MG	1H	3321	1/1	0.74	0.30	-	93,93,93,93	0
56	MG	14	3273	1/1	0.91	0.13	-	106,106,106,106	0
56	MG	1H	3029	1/1	0.82	0.22	-	91,91,91,91	0
56	MG	14	3192	1/1	0.94	0.35	-	102,102,102,102	0
56	MG	14	3238	1/1	0.92	0.14	-	94,94,94,94	0
56	MG	1H	3006	1/1	0.97	0.40	-	48,48,48,48	0
56	MG	14	3001	1/1	0.96	0.24	-	62,62,62,62	0
56	MG	1H	3436	1/1	0.85	0.16	-	73,73,73,73	0
56	MG	14	3154	1/1	0.57	0.34	-	59,59,59,59	0
56	MG	1H	3374	1/1	0.95	0.08	-	70,70,70,70	0
56	MG	14	3180	1/1	0.85	0.18	-	104,104,104,104	0
56	MG	14	3364	1/1	0.80	0.09	-	132,132,132,132	0
56	MG	1H	3431	1/1	0.91	0.12	-	71,71,71,71	0
56	MG	14	3332	1/1	0.93	0.05	-	94,94,94,94	0
56	MG	1H	3217	1/1	0.76	0.39	-	96,96,96,96	0
56	MG	1H	3417	1/1	0.86	0.12	-	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
56	MG	14	3142	1/1	0.81	0.13	-	89,89,89,89	0
56	MG	1H	3241	1/1	0.93	0.20	-	87,87,87,87	0
56	MG	14	3057	1/1	0.98	0.32	-	74,74,74,74	0
56	MG	1G	1633	1/1	0.83	0.34	-	101,101,101,101	0
56	MG	16	207	1/1	0.49	0.34	-	96,96,96,96	0
56	MG	13	1719	1/1	0.93	0.17	-	100,100,100,100	0
56	MG	13	1634	1/1	0.87	0.17	-	76,76,76,76	0
56	MG	14	3018	1/1	0.95	0.15	-	96,96,96,96	0
56	MG	1H	3080	1/1	0.94	0.38	-	76,76,76,76	0
56	MG	1H	3163	1/1	0.71	0.31	-	82,82,82,82	0
56	MG	13	1657	1/1	0.77	0.50	-	84,84,84,84	0
56	MG	1H	3352	1/1	0.83	0.14	-	106,106,106,106	0
56	MG	14	3113	1/1	0.86	0.26	-	57,57,57,57	0
56	MG	1H	3316	1/1	0.34	0.27	-	102,102,102,102	0
56	MG	1H	3090	1/1	0.97	0.30	-	65,65,65,65	0
56	MG	1H	3051	1/1	0.89	0.19	-	71,71,71,71	0
56	MG	13	1668	1/1	0.86	0.09	-	98,98,98,98	0
56	MG	14	3064	1/1	0.91	0.21	-	60,60,60,60	0
56	MG	14	3015	1/1	0.94	0.25	-	83,83,83,83	0
56	MG	1H	3250	1/1	0.91	0.32	-	78,78,78,78	0
56	MG	13	1705	1/1	0.58	0.22	-	82,82,82,82	0
56	MG	1G	1645	1/1	0.91	0.19	-	102,102,102,102	0
56	MG	13	1655	1/1	0.78	0.29	-	68,68,68,68	0
56	MG	1H	3503	1/1	0.95	0.10	-	64,64,64,64	0
56	MG	1H	3319	1/1	0.82	0.30	-	87,87,87,87	0
56	MG	1H	3325	1/1	0.82	0.28	-	96,96,96,96	0
56	MG	1H	3222	1/1	0.76	0.66	-	97,97,97,97	0
56	MG	13	1619	1/1	0.97	0.36	-	71,71,71,71	0
56	MG	1H	3073	1/1	0.92	0.39	-	55,55,55,55	0
56	MG	14	3265	1/1	0.60	0.17	-	96,96,96,96	0
56	MG	14	3355	1/1	0.80	0.09	-	78,78,78,78	0
56	MG	14	3101	1/1	0.53	0.24	-	99,99,99,99	0
56	MG	1H	3099	1/1	0.90	0.30	-	74,74,74,74	0
56	MG	1H	3514	1/1	0.99	0.09	-	96,96,96,96	0
56	MG	13	1695	1/1	0.74	0.40	-	100,100,100,100	0
56	MG	1H	3394	1/1	0.93	0.18	-	58,58,58,58	0
56	MG	1H	3462	1/1	0.96	0.17	-	106,106,106,106	0
56	MG	14	3117	1/1	0.91	0.24	-	69,69,69,69	0
56	MG	14	3356	1/1	0.96	0.03	-	85,85,85,85	0
56	MG	13	1661	1/1	0.89	0.12	-	75,75,75,75	0
56	MG	1H	3304	1/1	0.62	0.38	-	94,94,94,94	0
56	MG	2L	104	1/1	0.76	0.10	-	95,95,95,95	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	13	1652	1/1	0.91	0.42	-	83,83,83,83	0
56	MG	14	3188	1/1	0.96	0.10	-	83,83,83,83	0
56	MG	14	3072	1/1	0.86	0.17	-	82,82,82,82	0
56	MG	3L	101	1/1	0.90	0.24	-	116,116,116,116	0
56	MG	1H	3192	1/1	0.92	0.34	-	81,81,81,81	0
56	MG	14	3225	1/1	0.74	0.23	-	103,103,103,103	0
56	MG	1H	3193	1/1	0.98	0.30	-	89,89,89,89	0
56	MG	14	3075	1/1	0.93	0.31	-	83,83,83,83	0
56	MG	1G	1689	1/1	0.94	0.08	-	114,114,114,114	0
56	MG	14	3280	1/1	0.95	0.10	-	64,64,64,64	0
56	MG	13	1737	1/1	0.86	0.12	-	116,116,116,116	0
56	MG	2K	106	1/1	0.92	0.07	-	94,94,94,94	0
56	MG	14	3086	1/1	0.97	0.25	-	72,72,72,72	0
56	MG	1H	3290	1/1	0.83	0.37	-	82,82,82,82	0
56	MG	13	1636	1/1	0.95	0.41	-	74,74,74,74	0
56	MG	1H	3310	1/1	0.49	0.38	-	84,84,84,84	0
56	MG	14	3241	1/1	0.43	0.18	-	139,139,139,139	0
56	MG	14	3369	1/1	0.94	0.06	-	73,73,73,73	0
56	MG	14	3206	1/1	0.89	0.17	-	86,86,86,86	0
56	MG	13	1730	1/1	0.82	0.08	-	111,111,111,111	0
56	MG	1H	3402	1/1	0.92	0.04	-	102,102,102,102	0
56	MG	1H	3126	1/1	0.90	0.49	-	96,96,96,96	0
56	MG	14	3053	1/1	0.68	0.36	-	78,78,78,78	0
56	MG	14	3124	1/1	0.79	0.35	-	80,80,80,80	0
56	MG	1G	1612	1/1	0.67	0.14	-	109,109,109,109	0
56	MG	1H	3361	1/1	0.95	0.09	-	103,103,103,103	0
56	MG	1H	3143	1/1	0.92	0.31	-	81,81,81,81	0
56	MG	1H	3506	1/1	0.98	0.15	-	57,57,57,57	0
56	MG	1G	1629	1/1	0.85	0.19	-	75,75,75,75	0
56	MG	16	202	1/1	0.90	0.24	-	68,68,68,68	0
56	MG	13	1729	1/1	0.96	0.10	-	73,73,73,73	0
56	MG	I8	101	1/1	0.90	0.08	-	89,89,89,89	0
56	MG	14	3132	1/1	0.79	0.12	-	84,84,84,84	0
56	MG	1H	3214	1/1	0.93	0.23	-	101,101,101,101	0
56	MG	14	3309	1/1	0.88	0.09	-	53,53,53,53	0
56	MG	21	301	1/1	0.95	0.34	-	56,56,56,56	0
56	MG	13	1681	1/1	0.80	0.50	-	116,116,116,116	0
56	MG	14	3108	1/1	0.96	0.12	-	68,68,68,68	0
56	MG	1H	3246	1/1	0.80	0.28	-	81,81,81,81	0
56	MG	1H	3515	1/1	0.76	0.24	-	107,107,107,107	0
56	MG	14	3024	1/1	0.85	0.20	-	64,64,64,64	0
56	MG	1G	1604	1/1	0.94	0.14	-	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
56	MG	13	1734	1/1	0.91	0.14	-	79,79,79,79	0
56	MG	1G	1654	1/1	0.94	0.13	-	115,115,115,115	0
56	MG	14	3299	1/1	0.85	0.15	-	68,68,68,68	0
56	MG	1H	3212	1/1	0.62	0.33	-	79,79,79,79	0
56	MG	14	3161	1/1	0.84	0.14	-	100,100,100,100	0
56	MG	1H	3409	1/1	0.95	0.13	-	50,50,50,50	0
56	MG	14	3152	1/1	0.85	0.10	-	67,67,67,67	0
56	MG	1G	1636	1/1	0.89	0.21	-	89,89,89,89	0
56	MG	14	3080	1/1	0.74	0.21	-	96,96,96,96	0
56	MG	14	3373	1/1	0.66	0.04	-	138,138,138,138	0
56	MG	14	3418	1/1	0.73	0.07	-	128,128,128,128	0
56	MG	14	3012	1/1	0.96	0.26	-	54,54,54,54	0
56	MG	14	3338	1/1	0.97	0.10	-	62,62,62,62	0
56	MG	14	3244	1/1	0.36	0.22	-	82,82,82,82	0
56	MG	1H	3224	1/1	0.88	0.26	-	67,67,67,67	0
56	MG	14	3155	1/1	0.85	0.11	-	68,68,68,68	0
56	MG	1H	3270	1/1	0.77	0.26	-	75,75,75,75	0
56	MG	1G	1608	1/1	0.93	0.19	-	86,86,86,86	0
56	MG	1H	3234	1/1	0.86	0.37	-	96,96,96,96	0
56	MG	P8	101	1/1	0.74	0.32	-	76,76,76,76	0
56	MG	1G	1639	1/1	0.89	0.21	-	104,104,104,104	0
56	MG	1G	1632	1/1	0.96	0.34	-	92,92,92,92	0
56	MG	14	3010	1/1	0.99	0.16	-	65,65,65,65	0
56	MG	14	3405	1/1	0.89	0.12	-	93,93,93,93	0
56	MG	14	3070	1/1	0.70	0.43	-	92,92,92,92	0
56	MG	1H	3443	1/1	0.94	0.11	-	111,111,111,111	0
56	MG	14	3226	1/1	0.83	0.21	-	83,83,83,83	0
56	MG	1H	3360	1/1	0.92	0.09	-	94,94,94,94	0
56	MG	1H	3242	1/1	0.57	0.40	-	82,82,82,82	0
56	MG	14	3203	1/1	0.87	0.30	-	103,103,103,103	0
56	MG	1H	3499	1/1	0.96	0.07	-	66,66,66,66	0
56	MG	14	3214	1/1	0.55	0.30	-	88,88,88,88	0
56	MG	1H	3318	1/1	0.66	0.31	-	101,101,101,101	0
56	MG	1J	206	1/1	0.80	0.11	-	106,106,106,106	0
56	MG	1G	1635	1/1	0.52	0.28	-	82,82,82,82	0
56	MG	14	3331	1/1	0.90	0.07	-	73,73,73,73	0
56	MG	1G	1693	1/1	0.93	0.06	-	109,109,109,109	0
56	MG	13	1679	1/1	0.21	0.31	-	94,94,94,94	0
56	MG	1H	3524	1/1	0.70	0.06	-	104,104,104,104	0
56	MG	1G	1650	1/1	0.85	0.20	-	91,91,91,91	0
56	MG	1H	3475	1/1	0.82	0.19	-	114,114,114,114	0
56	MG	1H	3439	1/1	0.73	0.11	-	77,77,77,77	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	1H	3487	1/1	0.83	0.12	-	101,101,101,101	0
56	MG	1H	3172	1/1	0.96	0.26	-	60,60,60,60	0
56	MG	14	3254	1/1	0.80	0.18	-	91,91,91,91	0
56	MG	1H	3486	1/1	0.85	0.09	-	97,97,97,97	0
56	MG	13	1716	1/1	0.97	0.13	-	58,58,58,58	0
56	MG	1H	3225	1/1	0.75	0.42	-	87,87,87,87	0
56	MG	14	3404	1/1	0.74	0.05	-	97,97,97,97	0
56	MG	1G	1630	1/1	0.86	0.37	-	92,92,92,92	0
56	MG	1H	3100	1/1	0.97	0.17	-	48,48,48,48	0
56	MG	13	1702	1/1	0.66	0.41	-	109,109,109,109	0
56	MG	14	3026	1/1	0.87	0.13	-	55,55,55,55	0
56	MG	14	3178	1/1	0.97	0.12	-	86,86,86,86	0
56	MG	1H	3531	1/1	0.60	0.09	-	109,109,109,109	0
56	MG	1H	3156	1/1	0.95	0.40	-	85,85,85,85	0
56	MG	14	3344	1/1	0.89	0.12	-	100,100,100,100	0
56	MG	1H	3018	1/1	0.98	0.26	-	67,67,67,67	0
56	MG	14	3311	1/1	0.93	0.11	-	62,62,62,62	0
56	MG	13	1610	1/1	0.88	0.32	-	86,86,86,86	0
56	MG	1H	3415	1/1	0.75	0.06	-	94,94,94,94	0
56	MG	13	1732	1/1	0.92	0.13	-	99,99,99,99	0
56	MG	1H	3053	1/1	0.92	0.31	-	56,56,56,56	0
56	MG	1G	1614	1/1	0.91	0.18	-	92,92,92,92	0
56	MG	14	3284	1/1	0.75	0.08	-	104,104,104,104	0
56	MG	14	3220	1/1	0.72	0.53	-	108,108,108,108	0
56	MG	1H	3158	1/1	0.94	0.27	-	64,64,64,64	0
56	MG	14	3059	1/1	0.94	0.35	-	83,83,83,83	0
56	MG	1H	3386	1/1	0.88	0.12	-	58,58,58,58	0
56	MG	14	3346	1/1	0.96	0.07	-	88,88,88,88	0
56	MG	14	3006	1/1	0.98	0.33	-	68,68,68,68	0
56	MG	88	202	1/1	0.69	0.32	-	60,60,60,60	0
56	MG	14	3281	1/1	0.96	0.10	-	74,74,74,74	0
56	MG	14	3087	1/1	0.90	0.31	-	89,89,89,89	0
56	MG	1G	1627	1/1	0.90	0.24	-	83,83,83,83	0
56	MG	1H	3220	1/1	0.53	0.37	-	82,82,82,82	0
56	MG	1H	3293	1/1	0.76	0.36	-	95,95,95,95	0
56	MG	14	3391	1/1	0.94	0.05	-	96,96,96,96	0
56	MG	14	3061	1/1	0.94	0.27	-	49,49,49,49	0
56	MG	1H	3084	1/1	0.97	0.36	-	64,64,64,64	0
56	MG	14	3337	1/1	0.91	0.05	-	90,90,90,90	0
56	MG	14	3145	1/1	0.72	0.20	-	57,57,57,57	0
56	MG	1H	3472	1/1	0.86	0.11	-	95,95,95,95	0
56	MG	14	3301	1/1	0.95	0.09	-	87,87,87,87	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	14	3400	1/1	0.92	0.11	-	112,112,112,112	0
56	MG	1H	3480	1/1	0.89	0.10	-	100,100,100,100	0
56	MG	1G	1628	1/1	0.78	0.46	-	83,83,83,83	0
56	MG	1H	3287	1/1	0.82	0.27	-	88,88,88,88	0
56	MG	14	3016	1/1	0.80	0.32	-	65,65,65,65	0
56	MG	14	3376	1/1	0.77	0.24	-	122,122,122,122	0
56	MG	1H	3497	1/1	0.96	0.08	-	64,64,64,64	0
56	MG	1G	1696	1/1	0.52	0.12	-	113,113,113,113	0
56	MG	1H	3364	1/1	0.93	0.07	-	71,71,71,71	0
56	MG	14	3133	1/1	0.81	0.36	-	82,82,82,82	0
56	MG	13	1685	1/1	0.64	0.34	-	91,91,91,91	0
56	MG	13	1699	1/1	0.44	0.19	-	146,146,146,146	0
56	MG	14	3186	1/1	0.89	0.30	-	84,84,84,84	0
56	MG	1H	3420	1/1	0.79	0.09	-	114,114,114,114	0
56	MG	14	3296	1/1	0.85	0.07	-	97,97,97,97	0
56	MG	13	1714	1/1	0.98	0.08	-	79,79,79,79	0
56	MG	1H	3168	1/1	0.77	0.39	-	77,77,77,77	0
56	MG	1G	1671	1/1	0.86	0.11	-	92,92,92,92	0
56	MG	1H	3371	1/1	0.97	0.09	-	73,73,73,73	0
56	MG	14	3234	1/1	0.94	0.28	-	81,81,81,81	0
56	MG	1H	3119	1/1	0.89	0.48	-	70,70,70,70	0
56	MG	13	1660	1/1	0.92	0.40	-	76,76,76,76	0
56	MG	14	3176	1/1	0.96	0.17	-	88,88,88,88	0
56	MG	1H	3507	1/1	0.85	0.08	-	101,101,101,101	0
56	MG	14	3003	1/1	0.99	0.21	-	49,49,49,49	0
56	MG	1H	3253	1/1	0.76	0.49	-	87,87,87,87	0
56	MG	14	3098	1/1	0.82	0.13	-	53,53,53,53	0
56	MG	1H	3322	1/1	0.94	0.23	-	77,77,77,77	0
56	MG	13	1742	1/1	0.70	0.09	-	124,124,124,124	0
56	MG	1H	3005	1/1	0.89	0.28	-	51,51,51,51	0
56	MG	1H	3125	1/1	0.56	0.19	-	97,97,97,97	0
56	MG	1G	1690	1/1	0.88	0.14	-	120,120,120,120	0
56	MG	1H	3400	1/1	0.96	0.11	-	72,72,72,72	0
56	MG	14	3403	1/1	0.91	0.11	-	70,70,70,70	0
56	MG	1H	3257	1/1	0.59	0.27	-	85,85,85,85	0
56	MG	1H	3429	1/1	0.91	0.12	-	64,64,64,64	0
56	MG	13	1629	1/1	0.89	0.34	-	84,84,84,84	0
56	MG	1H	3461	1/1	0.95	0.06	-	89,89,89,89	0
56	MG	13	1623	1/1	0.87	0.38	-	98,98,98,98	0
56	MG	1G	1681	1/1	0.95	0.10	-	93,93,93,93	0
56	MG	1G	1676	1/1	0.60	0.24	-	113,113,113,113	0
56	MG	14	3417	1/1	0.94	0.07	-	118,118,118,118	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	1H	3406	1/1	0.95	0.12	-	76,76,76,76	0
56	MG	1H	3215	1/1	0.79	0.32	-	88,88,88,88	0
56	MG	14	3348	1/1	0.84	0.07	-	111,111,111,111	0
56	MG	1H	3375	1/1	0.82	0.08	-	103,103,103,103	0
56	MG	1H	3423	1/1	0.93	0.13	-	77,77,77,77	0
56	MG	1H	3161	1/1	0.53	0.29	-	101,101,101,101	0
56	MG	14	3164	1/1	0.52	0.12	-	76,76,76,76	0
56	MG	14	3103	1/1	0.74	0.28	-	84,84,84,84	0
56	MG	1H	3282	1/1	0.85	0.23	-	60,60,60,60	0
56	MG	14	3106	1/1	0.67	0.28	-	93,93,93,93	0
56	MG	1H	3121	1/1	0.92	0.26	-	59,59,59,59	0
56	MG	14	3312	1/1	0.96	0.04	-	93,93,93,93	0
56	MG	1H	3130	1/1	0.67	0.21	-	83,83,83,83	0
56	MG	14	3362	1/1	0.91	0.10	-	101,101,101,101	0
56	MG	14	3063	1/1	0.96	0.31	-	70,70,70,70	0
56	MG	1H	3060	1/1	0.95	0.12	-	56,56,56,56	0
56	MG	13	1718	1/1	0.79	0.07	-	108,108,108,108	0
56	MG	1H	3077	1/1	0.82	0.48	-	81,81,81,81	0
56	MG	1H	3256	1/1	0.81	0.14	-	83,83,83,83	0
56	MG	14	3077	1/1	0.97	0.11	-	68,68,68,68	0
56	MG	1H	3211	1/1	0.88	0.38	-	69,69,69,69	0
56	MG	14	3288	1/1	0.93	0.06	-	78,78,78,78	0
56	MG	14	3143	1/1	0.86	0.35	-	88,88,88,88	0
56	MG	1H	3522	1/1	0.92	0.25	-	74,74,74,74	0
56	MG	1H	3231	1/1	0.86	0.33	-	92,92,92,92	0
56	MG	14	3399	1/1	0.86	0.09	-	116,116,116,116	0
56	MG	1H	3440	1/1	0.94	0.06	-	98,98,98,98	0
56	MG	1H	3288	1/1	0.67	0.45	-	73,73,73,73	0
56	MG	1H	3492	1/1	0.97	0.06	-	90,90,90,90	0
56	MG	1H	3277	1/1	0.73	0.60	-	98,98,98,98	0
56	MG	1H	3007	1/1	0.82	0.29	-	58,58,58,58	0
56	MG	1H	3469	1/1	0.94	0.06	-	95,95,95,95	0
57	ZN	1G	1697	1/1	0.90	0.35	-	149,149,149,149	0
56	MG	13	1733	1/1	0.84	0.06	-	102,102,102,102	0
56	MG	1G	1622	1/1	0.85	0.17	-	128,128,128,128	0
56	MG	14	3419	1/1	0.85	0.14	-	135,135,135,135	0
56	MG	1L	101	1/1	0.94	0.08	-	94,94,94,94	0
56	MG	1H	3227	1/1	0.65	0.33	-	77,77,77,77	0
56	MG	1H	3139	1/1	0.54	0.23	-	70,70,70,70	0
56	MG	1H	3490	1/1	0.74	0.07	-	147,147,147,147	0
56	MG	1G	1679	1/1	0.98	0.08	-	109,109,109,109	0
56	MG	14	3104	1/1	0.76	0.12	-	78,78,78,78	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	14	3298	1/1	0.82	0.07	-	79,79,79,79	0
56	MG	14	3370	1/1	0.86	0.08	-	90,90,90,90	0
56	MG	13	1748	1/1	0.95	0.03	-	96,96,96,96	0
56	MG	1H	3446	1/1	0.92	0.17	-	87,87,87,87	0
56	MG	14	3081	1/1	0.94	0.32	-	90,90,90,90	0
56	MG	14	3045	1/1	0.85	0.20	-	82,82,82,82	0
56	MG	14	3111	1/1	0.69	0.39	-	98,98,98,98	0
56	MG	14	3382	1/1	0.78	0.19	-	94,94,94,94	0
56	MG	1G	1660	1/1	0.97	0.27	-	105,105,105,105	0
56	MG	1H	3303	1/1	0.91	0.25	-	84,84,84,84	0
56	MG	1G	1694	1/1	0.75	0.13	-	105,105,105,105	0
56	MG	13	1672	1/1	0.88	0.26	-	103,103,103,103	0
56	MG	14	3384	1/1	0.96	0.10	-	98,98,98,98	0
56	MG	14	3341	1/1	0.96	0.12	-	65,65,65,65	0
56	MG	1H	3141	1/1	0.88	0.42	-	78,78,78,78	0
56	MG	13	1731	1/1	0.62	0.11	-	115,115,115,115	0
56	MG	1H	3183	1/1	0.78	0.15	-	61,61,61,61	0
56	MG	1H	3216	1/1	0.81	0.32	-	87,87,87,87	0
56	MG	14	3402	1/1	0.65	0.08	-	105,105,105,105	0
56	MG	1G	1659	1/1	0.92	0.07	-	150,150,150,150	0
56	MG	14	3038	1/1	0.89	0.20	-	96,96,96,96	0
56	MG	1G	1655	1/1	0.96	0.12	-	127,127,127,127	0
56	MG	1H	3296	1/1	0.88	0.22	-	71,71,71,71	0
56	MG	14	3258	1/1	0.63	0.23	-	80,80,80,80	0
56	MG	14	3413	1/1	0.84	0.07	-	100,100,100,100	0
56	MG	1H	3520	1/1	0.97	0.22	-	91,91,91,91	0
56	MG	2L	102	1/1	0.74	0.38	-	85,85,85,85	0
56	MG	1H	3344	1/1	0.95	0.14	-	69,69,69,69	0
56	MG	14	3008	1/1	0.97	0.36	-	61,61,61,61	0
56	MG	14	3350	1/1	0.98	0.07	-	64,64,64,64	0
56	MG	1H	3306	1/1	0.61	0.28	-	81,81,81,81	0
56	MG	14	3141	1/1	0.86	0.30	-	72,72,72,72	0
56	MG	13	1745	1/1	0.97	0.05	-	104,104,104,104	0
56	MG	1H	3458	1/1	0.56	0.23	-	126,126,126,126	0
56	MG	1G	1684	1/1	0.94	0.07	-	121,121,121,121	0
56	MG	1H	3301	1/1	0.89	0.50	-	110,110,110,110	0
56	MG	14	3266	1/1	0.76	0.23	-	107,107,107,107	0
56	MG	14	3237	1/1	0.90	0.28	-	85,85,85,85	0
56	MG	1H	3094	1/1	0.97	0.14	-	65,65,65,65	0
56	MG	1H	3500	1/1	0.96	0.07	-	82,82,82,82	0
56	MG	1H	3115	1/1	0.75	0.25	-	78,78,78,78	0
56	MG	1H	3478	1/1	0.94	0.11	-	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
56	MG	14	3138	1/1	0.93	0.14	-	71,71,71,71	0
56	MG	1G	1641	1/1	0.90	0.28	-	92,92,92,92	0
56	MG	1H	3433	1/1	0.79	0.21	-	92,92,92,92	0
56	MG	1H	3279	1/1	0.84	0.19	-	80,80,80,80	0
56	MG	1G	1643	1/1	0.95	0.14	-	147,147,147,147	0
56	MG	14	3410	1/1	0.73	0.23	-	112,112,112,112	0
56	MG	1G	1673	1/1	0.60	0.18	-	93,93,93,93	0
56	MG	1H	3314	1/1	0.90	0.09	-	81,81,81,81	0
56	MG	14	3119	1/1	0.47	0.23	-	97,97,97,97	0
56	MG	14	3005	1/1	0.96	0.20	-	59,59,59,59	0
56	MG	14	3228	1/1	0.87	0.30	-	109,109,109,109	0
56	MG	14	3313	1/1	0.95	0.12	-	65,65,65,65	0
56	MG	13	1687	1/1	0.65	0.36	-	94,94,94,94	0
56	MG	1H	3459	1/1	0.89	0.10	-	101,101,101,101	0
56	MG	1H	3105	1/1	0.91	0.42	-	89,89,89,89	0
56	MG	1H	3335	1/1	0.97	0.10	-	45,45,45,45	0
56	MG	14	3339	1/1	0.93	0.11	-	56,56,56,56	0
56	MG	1H	3505	1/1	0.98	0.10	-	78,78,78,78	0
56	MG	1H	3285	1/1	0.96	0.23	-	82,82,82,82	0
56	MG	1G	1691	1/1	0.95	0.08	-	98,98,98,98	0
56	MG	14	3058	1/1	0.96	0.25	-	89,89,89,89	0
56	MG	14	3302	1/1	0.88	0.14	-	76,76,76,76	0
56	MG	13	1674	1/1	0.74	0.24	-	83,83,83,83	0
56	MG	1H	3070	1/1	0.96	0.41	-	61,61,61,61	0
56	MG	1H	3298	1/1	0.81	0.18	-	71,71,71,71	0
56	MG	1H	3273	1/1	0.48	0.52	-	101,101,101,101	0
56	MG	14	3223	1/1	0.91	0.23	-	60,60,60,60	0
56	MG	14	3166	1/1	0.94	0.29	-	85,85,85,85	0
56	MG	1H	3002	1/1	0.89	0.34	-	43,43,43,43	0
56	MG	1G	1611	1/1	0.93	0.10	-	89,89,89,89	0
56	MG	1H	3445	1/1	0.85	0.12	-	81,81,81,81	0
56	MG	14	3380	1/1	0.96	0.07	-	87,87,87,87	0
56	MG	14	3421	1/1	0.90	0.09	-	136,136,136,136	0
56	MG	14	3401	1/1	0.93	0.07	-	90,90,90,90	0
56	MG	14	3255	1/1	0.02	0.27	-	102,102,102,102	0
56	MG	1H	3086	1/1	0.81	0.17	-	75,75,75,75	0
56	MG	1H	3460	1/1	0.95	0.09	-	81,81,81,81	0
56	MG	14	3291	1/1	0.97	0.11	-	52,52,52,52	0
56	MG	1H	3261	1/1	0.58	0.32	-	98,98,98,98	0
56	MG	1H	3424	1/1	0.97	0.13	-	92,92,92,92	0
56	MG	1G	1662	1/1	0.91	0.14	-	81,81,81,81	0
56	MG	1G	1619	1/1	0.97	0.27	-	87,87,87,87	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	14	3165	1/1	0.88	0.13	-	69,69,69,69	0
56	MG	1H	3463	1/1	0.83	0.10	-	81,81,81,81	0
56	MG	14	3347	1/1	0.94	0.09	-	88,88,88,88	0
56	MG	1H	3137	1/1	0.75	0.37	-	87,87,87,87	0
56	MG	1H	3467	1/1	0.95	0.09	-	57,57,57,57	0
56	MG	14	3330	1/1	0.98	0.11	-	50,50,50,50	0
56	MG	1G	1624	1/1	0.95	0.16	-	88,88,88,88	0
56	MG	1H	3013	1/1	0.97	0.35	-	59,59,59,59	0
56	MG	1H	3444	1/1	0.71	0.15	-	119,119,119,119	0
56	MG	14	3229	1/1	0.85	0.25	-	107,107,107,107	0
56	MG	1H	3254	1/1	0.58	0.37	-	90,90,90,90	0
56	MG	14	3232	1/1	0.93	0.10	-	100,100,100,100	0
56	MG	1G	1666	1/1	0.76	0.12	-	101,101,101,101	0
56	MG	1H	3373	1/1	0.84	0.07	-	75,75,75,75	0
56	MG	13	1697	1/1	0.52	0.17	-	92,92,92,92	0
56	MG	1H	3131	1/1	0.94	0.13	-	71,71,71,71	0
56	MG	1G	1661	1/1	0.77	0.16	-	104,104,104,104	0
56	MG	1H	3471	1/1	0.87	0.11	-	91,91,91,91	0
56	MG	1H	3180	1/1	0.88	0.20	-	63,63,63,63	0
56	MG	1H	3427	1/1	0.98	0.16	-	56,56,56,56	0
56	MG	13	1723	1/1	0.88	0.12	-	85,85,85,85	0
56	MG	14	3123	1/1	0.65	0.28	-	93,93,93,93	0
56	MG	13	1622	1/1	0.95	0.26	-	99,99,99,99	0
56	MG	1H	3046	1/1	0.93	0.21	-	46,46,46,46	0
56	MG	14	3349	1/1	0.93	0.26	-	82,82,82,82	0
56	MG	14	3211	1/1	0.95	0.10	-	94,94,94,94	0
56	MG	13	1635	1/1	0.60	0.32	-	85,85,85,85	0
56	MG	1H	3034	1/1	0.95	0.30	-	46,46,46,46	0
56	MG	16	212	1/1	0.95	0.07	-	84,84,84,84	0
56	MG	13	1743	1/1	0.87	0.09	-	125,125,125,125	0
56	MG	14	3256	1/1	0.81	0.18	-	86,86,86,86	0
56	MG	1H	3160	1/1	0.65	0.27	-	81,81,81,81	0
56	MG	14	3051	1/1	0.84	0.31	-	83,83,83,83	0
56	MG	1H	3274	1/1	0.69	0.37	-	87,87,87,87	0
56	MG	1H	3075	1/1	0.96	0.35	-	52,52,52,52	0
56	MG	14	3366	1/1	0.83	0.11	-	90,90,90,90	0
56	MG	14	3197	1/1	0.70	0.19	-	83,83,83,83	0
56	MG	13	1683	1/1	0.93	0.40	-	101,101,101,101	0
56	MG	14	3216	1/1	0.68	0.24	-	106,106,106,106	0
56	MG	14	3144	1/1	0.94	0.21	-	83,83,83,83	0
56	MG	1H	3338	1/1	0.98	0.11	-	64,64,64,64	0
56	MG	1H	3275	1/1	0.71	0.26	-	83,83,83,83	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	1G	1638	1/1	0.96	0.14	-	89,89,89,89	0
56	MG	1H	3229	1/1	0.90	0.33	-	82,82,82,82	0
56	MG	1H	3362	1/1	0.98	0.05	-	68,68,68,68	0
56	MG	14	3334	1/1	0.97	0.06	-	111,111,111,111	0
56	MG	14	3109	1/1	0.64	0.17	-	67,67,67,67	0
56	MG	1H	3154	1/1	0.97	0.36	-	77,77,77,77	0
56	MG	16	203	1/1	0.72	0.33	-	82,82,82,82	0
56	MG	1H	3012	1/1	0.99	0.20	-	52,52,52,52	0
56	MG	1H	3477	1/1	0.93	0.10	-	114,114,114,114	0
56	MG	14	3398	1/1	0.95	0.08	-	76,76,76,76	0
56	MG	14	3207	1/1	0.95	0.10	-	72,72,72,72	0
56	MG	1H	3530	1/1	0.69	0.06	-	111,111,111,111	0
56	MG	14	3079	1/1	0.95	0.26	-	83,83,83,83	0
56	MG	1H	3184	1/1	0.92	0.51	-	73,73,73,73	0
56	MG	13	1617	1/1	0.72	0.29	-	85,85,85,85	0
56	MG	1H	3454	1/1	0.97	0.15	-	87,87,87,87	0
56	MG	1G	1678	1/1	0.76	0.12	-	98,98,98,98	0
56	MG	13	1607	1/1	0.94	0.40	-	88,88,88,88	0
56	MG	14	3316	1/1	0.97	0.09	-	57,57,57,57	0
56	MG	14	3099	1/1	0.96	0.34	-	82,82,82,82	0
56	MG	1H	3283	1/1	0.64	0.27	-	103,103,103,103	0
56	MG	14	3205	1/1	0.98	0.22	-	99,99,99,99	0
56	MG	1J	203	1/1	0.92	0.14	-	96,96,96,96	0
56	MG	14	3201	1/1	0.82	0.17	-	86,86,86,86	0
56	MG	1H	3382	1/1	0.97	0.08	-	55,55,55,55	0
56	MG	14	3140	1/1	-0.06	0.39	-	113,113,113,113	0
56	MG	2K	104	1/1	0.92	0.25	-	88,88,88,88	0
56	MG	13	1642	1/1	0.82	0.41	-	76,76,76,76	0
56	MG	1H	3213	1/1	0.96	0.28	-	78,78,78,78	0
56	MG	14	3340	1/1	0.90	0.08	-	104,104,104,104	0
56	MG	1H	3401	1/1	0.91	0.07	-	87,87,87,87	0
56	MG	1H	3534	1/1	0.86	0.17	-	101,101,101,101	0
56	MG	13	1698	1/1	0.50	0.28	-	91,91,91,91	0
56	MG	1G	1606	1/1	0.89	0.15	-	102,102,102,102	0
56	MG	1H	3079	1/1	0.98	0.18	-	46,46,46,46	0
56	MG	1H	3150	1/1	0.94	0.44	-	86,86,86,86	0
56	MG	14	3131	1/1	0.84	0.35	-	89,89,89,89	0
56	MG	14	3196	1/1	0.83	0.12	-	69,69,69,69	0
56	MG	16	208	1/1	0.84	0.48	-	88,88,88,88	0
56	MG	14	3361	1/1	0.88	0.07	-	119,119,119,119	0
56	MG	14	3352	1/1	0.89	0.07	-	91,91,91,91	0
56	MG	1H	3372	1/1	0.90	0.10	-	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
56	MG	1H	3198	1/1	0.86	0.39	-	82,82,82,82	0
56	MG	1H	3003	1/1	0.94	0.25	-	60,60,60,60	0
56	MG	1H	3464	1/1	0.84	0.13	-	90,90,90,90	0
56	MG	1H	3022	1/1	0.89	0.33	-	89,89,89,89	0
56	MG	1G	1647	1/1	0.91	0.31	-	102,102,102,102	0
56	MG	13	1665	1/1	0.86	0.18	-	90,90,90,90	0
56	MG	1H	3030	1/1	0.63	0.31	-	87,87,87,87	0
56	MG	1H	3260	1/1	0.87	0.27	-	93,93,93,93	0
56	MG	14	3151	1/1	0.96	0.09	-	56,56,56,56	0
56	MG	14	3017	1/1	0.98	0.24	-	70,70,70,70	0
56	MG	1H	3393	1/1	0.92	0.13	-	51,51,51,51	0
56	MG	2K	102	1/1	0.91	0.16	-	92,92,92,92	0
56	MG	1J	207	1/1	0.77	0.05	-	100,100,100,100	0
56	MG	1H	3201	1/1	0.90	0.20	-	68,68,68,68	0
56	MG	1H	3438	1/1	0.97	0.09	-	63,63,63,63	0
56	MG	14	3415	1/1	0.91	0.05	-	121,121,121,121	0
56	MG	1H	3096	1/1	0.89	0.32	-	66,66,66,66	0
56	MG	1H	3489	1/1	0.97	0.05	-	89,89,89,89	0
56	MG	2K	105	1/1	0.55	0.29	-	102,102,102,102	0
56	MG	14	3105	1/1	0.76	0.35	-	60,60,60,60	0
56	MG	14	3050	1/1	0.73	0.24	-	74,74,74,74	0
56	MG	1G	1649	1/1	0.63	0.25	-	84,84,84,84	0
56	MG	14	3304	1/1	0.97	0.06	-	89,89,89,89	0
56	MG	1H	3481	1/1	0.84	0.07	-	76,76,76,76	0
56	MG	1H	3289	1/1	0.81	0.20	-	79,79,79,79	0
56	MG	1H	3346	1/1	0.96	0.12	-	58,58,58,58	0
56	MG	14	3282	1/1	0.91	0.08	-	76,76,76,76	0
56	MG	1H	3300	1/1	0.36	0.53	-	102,102,102,102	0
56	MG	13	1689	1/1	0.90	0.50	-	92,92,92,92	0
56	MG	1H	3017	1/1	0.95	0.13	-	63,63,63,63	0
56	MG	1G	1625	1/1	0.42	0.31	-	108,108,108,108	0
56	MG	14	3269	1/1	0.73	0.14	-	84,84,84,84	0
56	MG	1H	3173	1/1	0.70	0.22	-	73,73,73,73	0
56	MG	14	3367	1/1	0.79	0.05	-	115,115,115,115	0
56	MG	1H	3525	1/1	0.89	0.13	-	113,113,113,113	0
56	MG	14	3185	1/1	0.77	0.28	-	80,80,80,80	0
56	MG	14	3397	1/1	0.79	0.10	-	94,94,94,94	0
56	MG	14	3416	1/1	0.61	0.15	-	116,116,116,116	0
56	MG	14	3200	1/1	0.48	0.30	-	94,94,94,94	0
56	MG	1H	3476	1/1	0.73	0.06	-	95,95,95,95	0
56	MG	1H	3491	1/1	0.81	0.05	-	99,99,99,99	0
56	MG	1H	3237	1/1	0.78	0.30	-	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
56	MG	1G	1674	1/1	0.70	0.20	-	92,92,92,92	0
56	MG	1G	1677	1/1	0.77	0.27	-	96,96,96,96	0
56	MG	14	3066	1/1	0.94	0.12	-	62,62,62,62	0
56	MG	1H	3426	1/1	0.96	0.15	-	59,59,59,59	0
56	MG	3E	302	1/1	0.79	0.24	-	121,121,121,121	0
56	MG	1H	3517	1/1	0.76	0.10	-	105,105,105,105	0
56	MG	1G	1653	1/1	0.93	0.12	-	99,99,99,99	0
56	MG	1H	3197	1/1	0.82	0.50	-	101,101,101,101	0
56	MG	1H	3194	1/1	0.85	0.14	-	83,83,83,83	0
56	MG	1H	3269	1/1	0.68	0.33	-	78,78,78,78	0
56	MG	14	3236	1/1	0.89	0.42	-	92,92,92,92	0
56	MG	1H	3324	1/1	0.91	0.09	-	81,81,81,81	0
56	MG	13	1614	1/1	0.88	0.21	-	98,98,98,98	0
56	MG	L8	101	1/1	0.70	0.40	-	81,81,81,81	0
56	MG	14	3279	1/1	0.91	0.03	-	115,115,115,115	0
56	MG	1H	3056	1/1	0.82	0.26	-	74,74,74,74	0
56	MG	14	3134	1/1	0.96	0.23	-	82,82,82,82	0
56	MG	1H	3411	1/1	0.76	0.12	-	80,80,80,80	0
56	MG	13	1658	1/1	0.93	0.42	-	79,79,79,79	0
56	MG	1H	3527	1/1	0.58	0.11	-	103,103,103,103	0
56	MG	1H	3195	1/1	0.87	0.20	-	91,91,91,91	0
56	MG	14	3039	1/1	0.89	0.19	-	81,81,81,81	0
56	MG	1H	3031	1/1	0.93	0.30	-	58,58,58,58	0
56	MG	14	3222	1/1	0.97	0.12	-	62,62,62,62	0
56	MG	14	3043	1/1	0.95	0.23	-	52,52,52,52	0
56	MG	14	3233	1/1	0.40	0.19	-	77,77,77,77	0
56	MG	14	3335	1/1	0.99	0.12	-	89,89,89,89	0
56	MG	1H	3473	1/1	0.93	0.08	-	109,109,109,109	0
56	MG	1H	3016	1/1	0.94	0.30	-	61,61,61,61	0
56	MG	1H	3159	1/1	0.96	0.15	-	53,53,53,53	0
56	MG	1H	3114	1/1	0.92	0.29	-	75,75,75,75	0
56	MG	14	3414	1/1	0.74	0.06	-	99,99,99,99	0
56	MG	1H	3519	1/1	0.79	0.10	-	93,93,93,93	0
56	MG	14	3396	1/1	0.90	0.26	-	101,101,101,101	0
56	MG	1H	3210	1/1	0.82	0.17	-	71,71,71,71	0
56	MG	1H	3291	1/1	0.84	0.15	-	93,93,93,93	0
56	MG	14	3274	1/1	0.94	0.14	-	69,69,69,69	0
56	MG	14	3261	1/1	0.63	0.21	-	91,91,91,91	0
56	MG	1H	3014	1/1	0.97	0.37	-	62,62,62,62	0
56	MG	14	3271	1/1	0.90	0.15	-	99,99,99,99	0
56	MG	1H	3457	1/1	0.94	0.08	-	81,81,81,81	0
56	MG	13	1747	1/1	0.60	0.08	-	107,107,107,107	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	14	3363	1/1	0.71	0.06	-	120,120,120,120	0
56	MG	13	1650	1/1	0.83	0.22	-	105,105,105,105	0
56	MG	1H	3308	1/1	0.93	0.20	-	85,85,85,85	0
56	MG	1H	3248	1/1	0.74	0.37	-	82,82,82,82	0
56	MG	1H	3529	1/1	0.60	0.09	-	113,113,113,113	0
56	MG	1H	3255	1/1	0.49	0.33	-	110,110,110,110	0
56	MG	1H	3069	1/1	0.97	0.34	-	53,53,53,53	0
56	MG	1H	3134	1/1	0.82	0.29	-	90,90,90,90	0
56	MG	14	3137	1/1	0.86	0.15	-	96,96,96,96	0
56	MG	14	3213	1/1	0.76	0.27	-	76,76,76,76	0
56	MG	1H	3403	1/1	0.80	0.12	-	78,78,78,78	0
56	MG	1H	3113	1/1	0.94	0.32	-	84,84,84,84	0
56	MG	14	3129	1/1	0.57	0.17	-	89,89,89,89	0
56	MG	14	3085	1/1	0.97	0.17	-	70,70,70,70	0
56	MG	13	1693	1/1	0.41	0.24	-	86,86,86,86	0
56	MG	14	3163	1/1	0.81	0.15	-	109,109,109,109	0
56	MG	13	1688	1/1	0.77	0.56	-	106,106,106,106	0
56	MG	14	3293	1/1	0.95	0.11	-	73,73,73,73	0
56	MG	1G	1695	1/1	0.85	0.07	-	94,94,94,94	0
56	MG	1H	3453	1/1	0.91	0.06	-	83,83,83,83	0
56	MG	14	3209	1/1	0.92	0.13	-	71,71,71,71	0
56	MG	14	3100	1/1	0.83	0.31	-	69,69,69,69	0
56	MG	1H	3238	1/1	0.82	0.15	-	98,98,98,98	0
56	MG	13	1656	1/1	0.88	0.23	-	84,84,84,84	0
56	MG	1H	3320	1/1	0.82	0.16	-	95,95,95,95	0
56	MG	14	3148	1/1	0.34	0.19	-	96,96,96,96	0
56	MG	14	3345	1/1	0.96	0.05	-	82,82,82,82	0
56	MG	1H	3410	1/1	0.96	0.05	-	66,66,66,66	0
56	MG	14	3181	1/1	0.85	0.14	-	84,84,84,84	0
56	MG	14	3168	1/1	0.93	0.20	-	58,58,58,58	0
56	MG	14	3375	1/1	0.88	0.09	-	92,92,92,92	0
56	MG	1H	3218	1/1	0.82	0.20	-	91,91,91,91	0
56	MG	1G	1687	1/1	0.91	0.10	-	134,134,134,134	0
56	MG	1H	3418	1/1	0.96	0.10	-	77,77,77,77	0
56	MG	13	1744	1/1	0.80	0.09	-	112,112,112,112	0
56	MG	1H	3465	1/1	0.89	0.07	-	85,85,85,85	0
56	MG	1H	3336	1/1	0.92	0.11	-	53,53,53,53	0
56	MG	13	1624	1/1	0.83	0.37	-	89,89,89,89	0
56	MG	14	3120	1/1	0.89	0.12	-	82,82,82,82	0
56	MG	1H	3171	1/1	0.83	0.27	-	65,65,65,65	0
56	MG	14	3158	1/1	0.86	0.41	-	83,83,83,83	0
56	MG	14	3078	1/1	0.90	0.21	-	67,67,67,67	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	14	3372	1/1	0.29	0.21	-	114,114,114,114	0
56	MG	13	1708	1/1	0.07	0.42	-	112,112,112,112	0
56	MG	13	1669	1/1	0.75	0.36	-	78,78,78,78	0
56	MG	13	1612	1/1	0.93	0.32	-	68,68,68,68	0
56	MG	1H	3123	1/1	0.94	0.34	-	90,90,90,90	0
56	MG	1H	3267	1/1	0.96	0.18	-	96,96,96,96	0
56	MG	1G	1613	1/1	0.92	0.18	-	98,98,98,98	0
56	MG	13	1602	1/1	0.98	0.25	-	70,70,70,70	0
56	MG	1H	3485	1/1	0.93	0.10	-	105,105,105,105	0
56	MG	14	3118	1/1	0.67	0.36	-	110,110,110,110	0
56	MG	14	3009	1/1	0.97	0.17	-	73,73,73,73	0
56	MG	14	3408	1/1	0.90	0.07	-	96,96,96,96	0
56	MG	1H	3535	1/1	0.59	0.08	-	115,115,115,115	0
56	MG	16	211	1/1	0.96	0.13	-	80,80,80,80	0
56	MG	14	3260	1/1	0.90	0.12	-	112,112,112,112	0
56	MG	1H	3421	1/1	0.95	0.08	-	74,74,74,74	0
56	MG	14	3297	1/1	0.95	0.06	-	80,80,80,80	0
56	MG	14	3329	1/1	0.82	0.06	-	88,88,88,88	0
56	MG	1H	3165	1/1	0.85	0.18	-	45,45,45,45	0
56	MG	14	3247	1/1	0.71	0.20	-	89,89,89,89	0
56	MG	1H	3223	1/1	0.88	0.12	-	88,88,88,88	0
56	MG	1G	1680	1/1	0.84	0.05	-	126,126,126,126	0
56	MG	1K	101	1/1	0.98	0.22	-	91,91,91,91	0
56	MG	1G	1656	1/1	0.78	0.16	-	112,112,112,112	0
56	MG	14	3208	1/1	0.89	0.09	-	69,69,69,69	0
56	MG	1H	3309	1/1	0.79	0.38	-	94,94,94,94	0
56	MG	14	3215	1/1	0.87	0.18	-	91,91,91,91	0
56	MG	1G	1623	1/1	0.87	0.45	-	108,108,108,108	0
56	MG	1H	3247	1/1	0.65	0.39	-	105,105,105,105	0
56	MG	1H	3196	1/1	0.94	0.21	-	56,56,56,56	0
56	MG	1H	3281	1/1	0.97	0.38	-	85,85,85,85	0
56	MG	1H	3205	1/1	0.71	0.38	-	78,78,78,78	0
56	MG	1H	3244	1/1	0.72	0.35	-	85,85,85,85	0
56	MG	13	1690	1/1	0.53	0.48	-	109,109,109,109	0
56	MG	14	3325	1/1	0.86	0.08	-	110,110,110,110	0
56	MG	13	1649	1/1	0.81	0.32	-	102,102,102,102	0
56	MG	1H	3501	1/1	0.83	0.14	-	81,81,81,81	0
56	MG	14	3212	1/1	0.77	0.17	-	85,85,85,85	0
56	MG	13	1738	1/1	0.87	0.10	-	109,109,109,109	0
56	MG	1H	3265	1/1	0.68	0.37	-	94,94,94,94	0
56	MG	1H	3488	1/1	0.51	0.12	-	134,134,134,134	0
56	MG	14	3317	1/1	0.98	0.12	-	98,98,98,98	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	14	3054	1/1	0.79	0.26	-	70,70,70,70	0
56	MG	14	3094	1/1	0.84	0.19	-	89,89,89,89	0
56	MG	1H	3187	1/1	0.92	0.42	-	72,72,72,72	0
56	MG	14	3136	1/1	0.89	0.13	-	92,92,92,92	0
56	MG	1H	3434	1/1	0.94	0.06	-	107,107,107,107	0
56	MG	1G	1668	1/1	0.98	0.26	-	90,90,90,90	0
56	MG	1H	3466	1/1	0.79	0.08	-	105,105,105,105	0
56	MG	1H	3428	1/1	0.96	0.15	-	56,56,56,56	0
56	MG	14	3046	1/1	0.96	0.17	-	70,70,70,70	0
56	MG	14	3374	1/1	0.80	0.12	-	131,131,131,131	0
56	MG	14	3033	1/1	0.96	0.18	-	63,63,63,63	0
56	MG	13	1646	1/1	0.78	0.23	-	80,80,80,80	0
56	MG	1H	3148	1/1	0.82	0.30	-	65,65,65,65	0
56	MG	13	1703	1/1	0.45	0.41	-	105,105,105,105	0
56	MG	1G	1631	1/1	0.86	0.22	-	88,88,88,88	0
57	ZN	14	3422	1/1	0.41	0.19	-	181,181,181,181	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.