



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 26, 2026 – 03:27 PM UTC

PDB ID : 6N9F / pdb_00006n9f
Title : Crystal structure of the *Thermus thermophilus* 70S ribosome in complex with a short substrate mimic ACCA-DPhe and bound to mRNA and P-site tRNA at 3.7Å resolution
Authors : Melnikov, S.V.; Khabibullina, N.F.; Mairhofer, E.; Vargas-Rodriguez, O.; Reynolds, N.M.; Micura, R.; Soll, D.; Polikanov, Y.S.
Deposited on : 2018-12-03
Resolution : 3.70 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

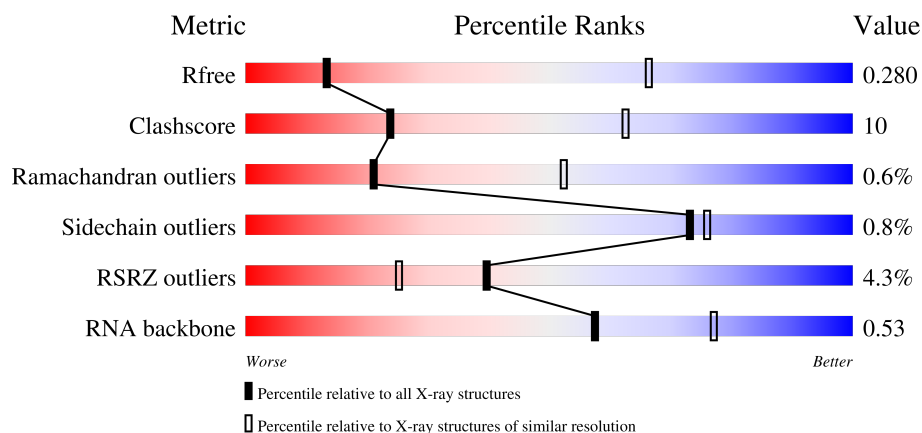
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.70 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.



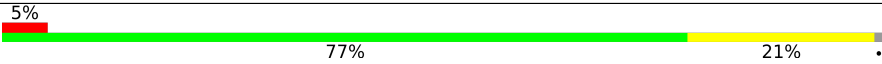
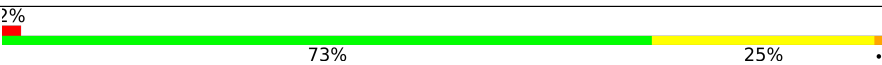
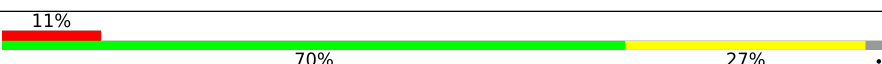
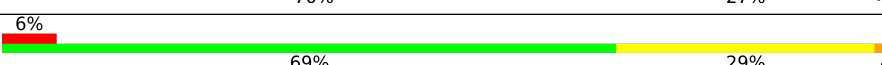
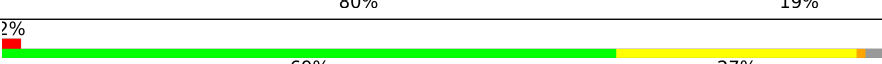
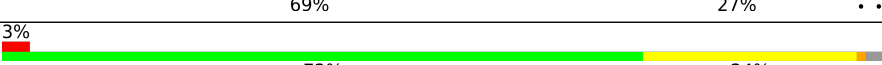
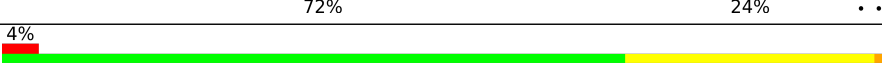
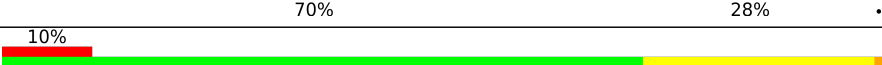
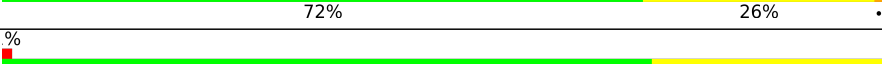
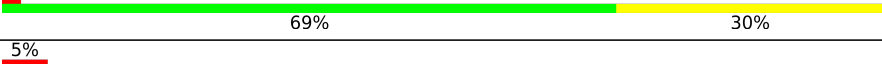
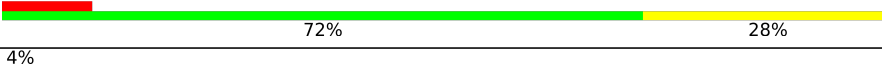
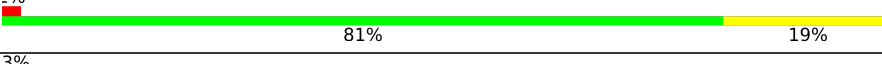
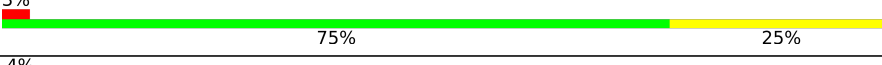
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1131 (3.80-3.60)
Clashscore	190562	1171 (3.80-3.60)
Ramachandran outliers	187476	1129 (3.80-3.60)
Sidechain outliers	187428	1126 (3.80-3.60)
RSRZ outliers	180081	1130 (3.80-3.60)
RNA backbone	3983	1007 (4.30-3.08)

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

Mol	Chain	Length	Quality of chain
1	1A	2915	4% 54% 38% 7%
1	2A	2915	3% 53% 37% 6%
2	1B	121	59% 38%

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Mol	Chain	Length	Quality of chain
2	2B	121	
3	1D	276	
3	2D	276	
4	1E	206	
4	2E	206	
5	1F	210	
5	2F	210	
6	1G	182	
6	2G	182	
7	1H	180	
7	2H	180	
8	1I	148	
8	2I	148	
9	1N	140	
9	2N	140	
10	1O	122	
10	2O	122	
11	1P	150	
11	2P	150	
12	1Q	141	
12	2Q	141	
13	1R	118	
13	2R	118	
14	1S	112	
14	2S	112	

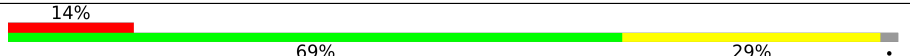
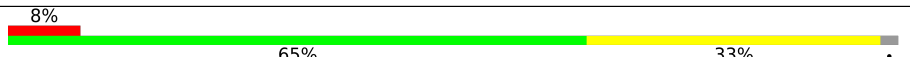
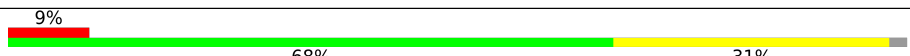
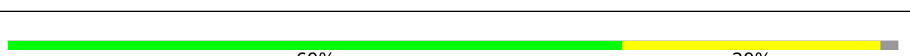
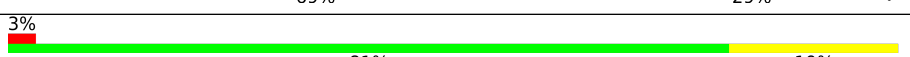
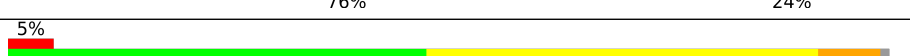
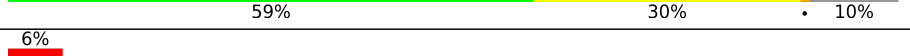
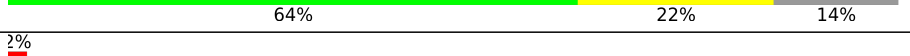
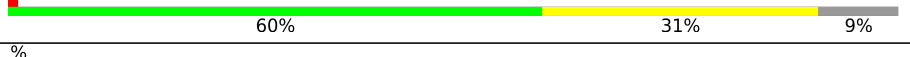
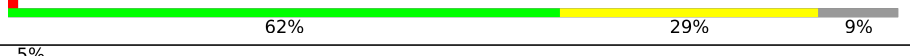
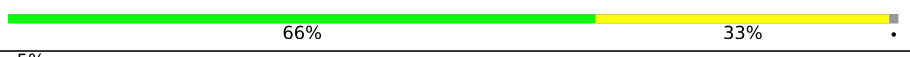
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Mol	Chain	Length	Quality of chain
15	1T	146	
15	2T	146	
16	1U	118	
16	2U	118	
17	1V	101	
17	2V	101	
18	1W	113	
18	2W	113	
19	1X	96	
19	2X	96	
20	1Y	110	
20	2Y	110	
21	1Z	206	
21	2Z	206	
22	10	85	
22	20	85	
23	11	98	
23	21	98	
24	12	72	
24	22	72	
25	13	60	
25	23	60	
26	14	71	
26	24	71	
27	15	60	

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Mol	Chain	Length	Quality of chain
27	25	60	
28	16	54	
28	26	54	
29	17	49	
29	27	49	
30	18	65	
30	28	65	
31	19	37	
31	29	37	
32	1a	1521	
32	2a	1521	
33	1b	256	
33	2b	256	
34	1c	239	
34	2c	239	
35	1d	209	
35	2d	209	
36	1e	162	
36	2e	162	
37	1f	101	
37	2f	101	
38	1g	156	
38	2g	156	
39	1h	138	
39	2h	138	

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Mol	Chain	Length	Quality of chain
40	1i	128	
40	2i	128	
41	1j	105	
41	2j	105	
42	1k	129	
42	2k	129	
43	1l	132	
43	2l	132	
44	1m	126	
44	2m	126	
45	1n	61	
45	2n	61	
46	1o	89	
46	2o	89	
47	1p	88	
47	2p	88	
48	1q	105	
48	2q	105	
49	1r	88	
49	2r	88	
50	1s	93	
50	2s	93	
51	1t	106	
51	2t	106	
52	1u	27	

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Mol	Chain	Length	Quality of chain
52	2u	27	
53	1v	24	
53	2v	24	
54	1w	4	
54	2w	4	
55	1x	77	
55	2x	77	

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	1A	3214	-	-	-	X
56	MG	1A	3246	-	-	-	X
56	MG	1A	3375	-	-	-	X
56	MG	1A	3394	-	-	-	X
56	MG	1A	3487	-	-	-	X
56	MG	1A	3492	-	-	-	X
56	MG	1B	211	-	-	-	X
56	MG	1a	1663	-	-	-	X
56	MG	2A	3156	-	-	-	X
56	MG	2A	3415	-	-	-	X
56	MG	2A	3421	-	-	-	X
56	MG	2a	1672	-	-	-	X
58	SF4	1d	302	-	-	X	-
58	SF4	2d	302	-	-	X	-

2 Entry composition

There are 59 unique types of molecules in this entry. The entry contains 288175 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 23S Ribosomal RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	1A	2871	Total	C	N	O	P	0	0	0
			61852	27531	11572	19878	2871			
1	2A	2800	Total	C	N	O	P	0	0	0
			60322	26848	11284	19390	2800			

- Molecule 2 is a RNA chain called 5S Ribosomal RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	1B	120	Total	C	N	O	P	0	0	0
			2577	1146	476	835	120			
2	2B	120	Total	C	N	O	P	0	0	0
			2575	1146	476	833	120			

- Molecule 3 is a protein called 50S Ribosomal Protein L2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	1D	275	Total	C	N	O	S	0	0	0
			2136	1349	423	361	3			
3	2D	275	Total	C	N	O	S	0	0	0
			2136	1349	423	361	3			

- Molecule 4 is a protein called 50S Ribosomal Protein L3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	1E	204	Total	C	N	O	S	0	0	0
			1559	985	298	270	6			
4	2E	204	Total	C	N	O	S	0	0	0
			1559	985	298	270	6			

- Molecule 5 is a protein called 50S Ribosomal Protein L4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	1F	203	Total	C	N	O	S	0	0	1
			1584	1009	298	275	2			
5	2F	203	Total	C	N	O	S	0	0	1
			1580	1007	297	274	2			

- Molecule 6 is a protein called 50S Ribosomal Protein L5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	1G	181	Total	C	N	O	S	0	0	0
			1423	913	253	253	4			
6	2G	181	Total	C	N	O	S	0	0	0
			1428	913	258	253	4			

- Molecule 7 is a protein called 50S Ribosomal Protein L6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	1H	174	Total	C	N	O	S	0	0	0
			1330	845	248	236	1			
7	2H	174	Total	C	N	O	S	0	0	0
			1330	845	248	236	1			

- Molecule 8 is a protein called 50S Ribosomal Protein L9.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	1I	146	Total	C	N	O	S	0	0	0
			1097	701	191	204	1			
8	2I	146	Total	C	N	O	S	0	0	0
			1064	681	186	196	1			

- Molecule 9 is a protein called 50S Ribosomal Protein L13.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	1N	140	Total	C	N	O	S	0	0	0
			1117	719	207	187	4			
9	2N	140	Total	C	N	O	S	0	0	0
			1117	719	207	187	4			

- Molecule 10 is a protein called 50S Ribosomal Protein L14.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	1O	122	Total	C	N	O	S	0	0	0
			933	588	171	170	4			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	2O	122	Total	C	N	O	S	0	0	0
			933	588	171	170	4			

- Molecule 11 is a protein called 50S Ribosomal Protein L15.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	1P	149	Total	C	N	O	S	0	0	0
			1135	706	230	196	3			
11	2P	149	Total	C	N	O	S	0	0	0
			1135	706	230	196	3			

- Molecule 12 is a protein called 50S Ribosomal Protein L16.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	1Q	141	Total	C	N	O	S	0	0	0
			1122	715	212	188	7			
12	2Q	141	Total	C	N	O	S	0	0	0
			1122	715	212	188	7			

- Molecule 13 is a protein called 50S Ribosomal Protein L17.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	1R	118	Total	C	N	O	S	0	0	0
			968	604	203	160	1			
13	2R	118	Total	C	N	O	S	0	0	0
			968	604	203	160	1			

- Molecule 14 is a protein called 50S Ribosomal Protein L18.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
14	1S	110	Total	C	N	O	0	0	0
			873	550	174	149			
14	2S	110	Total	C	N	O	0	0	0
			870	549	173	148			

- Molecule 15 is a protein called 50S Ribosomal Protein L19.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
15	1T	131	Total	C	N	O	S	0	0	0
			1091	680	225	185	1			
15	2T	131	Total	C	N	O	S	0	0	0
			1083	675	224	183	1			

- Molecule 16 is a protein called 50S Ribosomal Protein L20.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
16	1U	116	Total	C	N	O	S	0	0	0
			959	608	201	149	1			
16	2U	116	Total	C	N	O	S	0	0	0
			959	608	201	149	1			

- Molecule 17 is a protein called 50S Ribosomal Protein L21.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
17	1V	101	Total	C	N	O	S	0	0	0
			771	495	140	135	1			
17	2V	101	Total	C	N	O	S	0	0	0
			771	495	140	135	1			

- Molecule 18 is a protein called 50S Ribosomal Protein L22.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
18	1W	112	Total	C	N	O	S	0	0	0
			886	557	174	153	2			
18	2W	112	Total	C	N	O	S	0	0	0
			886	557	174	153	2			

- Molecule 19 is a protein called 50S Ribosomal Protein L23.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
19	1X	95	Total	C	N	O	S	0	0	0
			750	488	135	126	1			
19	2X	95	Total	C	N	O	S	0	0	0
			750	488	135	126	1			

- Molecule 20 is a protein called 50S ribosomal protein L24.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
20	1Y	107	Total	C	N	O	S	0	0	0
			806	517	152	131	6			
20	2Y	107	Total	C	N	O	S	0	0	0
			806	517	152	131	6			

- Molecule 21 is a protein called 50S ribosomal protein L25.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
21	1Z	154	Total	C	N	O	S	0	0	0
			1240	795	222	220	3			
21	2Z	160	Total	C	N	O	S	0	0	0
			1271	814	228	227	2			

- Molecule 22 is a protein called 50S ribosomal protein L27.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
22	10	83	Total	C	N	O	S	0	0	0
			653	404	139	109	1			
22	20	83	Total	C	N	O	S	0	0	0
			653	404	139	109	1			

- Molecule 23 is a protein called 50S ribosomal protein L28.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
23	11	97	Total	C	N	O	S	0	0	0
			755	475	148	131	1			
23	21	97	Total	C	N	O	S	0	0	0
			755	475	148	131	1			

- Molecule 24 is a protein called 50S ribosomal protein L29.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
24	12	70	Total	C	N	O	S	0	0	0
			588	365	118	103	2			
24	22	70	Total	C	N	O	S	0	0	0
			588	365	118	103	2			

- Molecule 25 is a protein called 50S ribosomal protein L30.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
25	13	59	Total	C	N	O	0	0	0
			469	298	90	81			
25	23	59	Total	C	N	O	0	0	0
			464	296	90	78			

- Molecule 26 is a protein called 50S ribosomal protein L31.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
26	14	69	Total	C	N	O	S	0	0	0
			552	349	99	99	5			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
26	24	69	Total	C	N	O	S	0	0	0
			532	339	97	91	5			

- Molecule 27 is a protein called 50S ribosomal protein L32.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
27	15	59	Total	C	N	O	S	0	0	0
			455	285	89	76	5			
27	25	59	Total	C	N	O	S	0	0	0
			455	285	89	76	5			

- Molecule 28 is a protein called 50S ribosomal protein L33.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
28	16	53	Total	C	N	O	S	0	0	0
			453	281	91	77	4			
28	26	53	Total	C	N	O	S	0	0	0
			449	279	91	75	4			

- Molecule 29 is a protein called 50S ribosomal protein L34.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
29	17	48	Total	C	N	O	S	0	0	0
			418	257	104	55	2			
29	27	48	Total	C	N	O	S	0	0	0
			418	257	104	55	2			

- Molecule 30 is a protein called 50S Ribosomal Protein L35.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
30	18	64	Total	C	N	O	S	0	0	0
			517	331	102	82	2			
30	28	64	Total	C	N	O	S	0	0	0
			517	331	102	82	2			

- Molecule 31 is a protein called 50S Ribosomal Protein L36.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
31	19	37	Total	C	N	O	S	0	0	0
			307	188	68	47	4			
31	29	37	Total	C	N	O	S	0	0	0
			307	188	68	47	4			

- Molecule 32 is a RNA chain called 16S Ribosomal RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
32	1a	1500	Total	C	N	O	P	0	0	0
			32246	14358	5975	10413	1500			
32	2a	1503	Total	C	N	O	P	0	0	0
			32327	14396	5990	10438	1503			

- Molecule 33 is a protein called 30S Ribosomal Protein S2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
33	1b	231	Total	C	N	O	S	0	0	0
			1846	1179	331	331	5			
33	2b	231	Total	C	N	O	S	0	0	0
			1825	1167	326	327	5			

- Molecule 34 is a protein called 30S Ribosomal Protein S3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
34	1c	206	Total	C	N	O	S	0	0	0
			1548	973	301	273	1			
34	2c	206	Total	C	N	O	S	0	0	0
			1542	968	300	273	1			

- Molecule 35 is a protein called 30S Ribosomal Protein S4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
35	1d	208	Total	C	N	O	S	0	0	0
			1655	1038	326	284	7			
35	2d	208	Total	C	N	O	S	0	0	0
			1674	1050	333	284	7			

- Molecule 36 is a protein called 30S Ribosomal Protein S5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
36	1e	148	Total	C	N	O	S	0	0	0
			1129	714	213	198	4			
36	2e	148	Total	C	N	O	S	0	0	0
			1133	716	214	199	4			

- Molecule 37 is a protein called 30S Ribosomal Protein S6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
37	1f	100	Total	C	N	O	S	0	0	0
			810	514	144	149	3			
37	2f	100	Total	C	N	O	S	0	0	0
			816	516	146	151	3			

- Molecule 38 is a protein called 30S Ribosomal Protein S7.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
38	1g	155	Total	C	N	O	S	0	0	0
			1231	766	243	216	6			
38	2g	155	Total	C	N	O	S	0	0	0
			1235	769	244	216	6			

- Molecule 39 is a protein called 30S Ribosomal Protein S8.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
39	1h	137	Total	C	N	O	S	0	0	0
			1088	689	206	191	2			
39	2h	137	Total	C	N	O	S	0	0	0
			1088	689	206	191	2			

- Molecule 40 is a protein called 30S ribosomal protein S9.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
40	1i	127	Total	C	N	O	0	0	0
			983	623	193	167			
40	2i	127	Total	C	N	O	0	0	0
			978	619	190	169			

- Molecule 41 is a protein called 30S ribosomal protein S10.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
41	1j	97	Total	C	N	O	0	0	0
			709	440	138	131			
41	2j	96	Total	C	N	O	0	0	0
			714	445	138	131			

- Molecule 42 is a protein called 30S ribosomal protein S11.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
42	1k	114	Total	C	N	O	S	0	0	0
			829	516	155	155	3			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
42	2k	114	Total	C	N	O	S	0	0	0
			833	519	156	155	3			

- Molecule 43 is a protein called 30S ribosomal protein S12.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
43	1l	122	Total	C	N	O	S	0	0	0
			932	586	185	159	2			
43	2l	122	Total	C	N	O	S	0	0	0
			932	586	185	159	2			

- Molecule 44 is a protein called 30S ribosomal protein S13.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
44	1m	123	Total	C	N	O	S	0	0	0
			958	592	198	166	2			
44	2m	122	Total	C	N	O	S	0	0	0
			950	586	197	165	2			

- Molecule 45 is a protein called 30S ribosomal protein S14 type Z.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
45	1n	60	Total	C	N	O	S	0	0	0
			492	312	104	72	4			
45	2n	60	Total	C	N	O	S	0	0	0
			492	312	104	72	4			

- Molecule 46 is a protein called 30S ribosomal protein S15.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
46	1o	88	Total	C	N	O	S	0	0	0
			728	456	144	126	2			
46	2o	88	Total	C	N	O	S	0	0	0
			728	456	144	126	2			

- Molecule 47 is a protein called 30S ribosomal protein S16.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
47	1p	82	Total	C	N	O	S	0	0	0
			681	433	134	113	1			
47	2p	82	Total	C	N	O	S	0	0	0
			677	430	133	113	1			

- Molecule 48 is a protein called 30S ribosomal protein S17.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
48	1q	99	Total	C	N	O	S	0	0	0
			823	528	151	142	2			
48	2q	99	Total	C	N	O	S	0	0	0
			823	528	151	142	2			

- Molecule 49 is a protein called 30S ribosomal protein S18.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
49	1r	68	Total	C	N	O		0	0	0
			555	355	108	92				
49	2r	68	Total	C	N	O		0	0	0
			555	355	108	92				

- Molecule 50 is a protein called 30S Ribosomal Protein S19.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
50	1s	83	Total	C	N	O	S	0	0	0
			652	417	120	113	2			
50	2s	83	Total	C	N	O	S	0	0	0
			646	412	119	113	2			

- Molecule 51 is a protein called 30S Ribosomal Protein S20.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
51	1t	96	Total	C	N	O	S	0	0	0
			728	446	156	124	2			
51	2t	96	Total	C	N	O	S	0	0	0
			727	446	155	124	2			

- Molecule 52 is a protein called 30S ribosomal protein Thx.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
52	1u	23	Total	C	N	O	0	0	0
			199	122	48	29			
52	2u	23	Total	C	N	O	0	0	0
			199	122	48	29			

- Molecule 53 is a RNA chain called mRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
53	1v	7	Total	C	N	O	P	0	0	0
			153	69	32	45	7			
53	2v	6	Total	C	N	O	P	0	0	0
			113	49	22	36	6			

- Molecule 54 is a RNA chain called ACCA-DPhe.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
54	1w	4	Total	C	N	O	P	0	0	1
			75	38	13	21	3			
54	2w	4	Total	C	N	O	P	0	0	1
			75	38	13	21	3			

- Molecule 55 is a RNA chain called P-site tRNA, Deacylated Initiator Methionyl-tRNA.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
55	1x	76	Total	C	N	O	P	S	0	0	0
			1625	725	294	529	76	1			
55	2x	76	Total	C	N	O	P	S	0	0	0
			1625	725	294	529	76	1			

- Molecule 56 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
56	1A	548	Total	Mg	0	0
			548	548		
56	1B	19	Total	Mg	0	0
			19	19		
56	1D	4	Total	Mg	0	0
			4	4		
56	1E	4	Total	Mg	0	0
			4	4		
56	1F	2	Total	Mg	0	0
			2	2		
56	1G	1	Total	Mg	0	0
			1	1		
56	1H	1	Total	Mg	0	0
			1	1		
56	1P	2	Total	Mg	0	0
			2	2		
56	1Q	2	Total	Mg	0	0
			2	2		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
56	1R	2	Total 2	Mg 2	0	0
56	1T	3	Total 3	Mg 3	0	0
56	1V	3	Total 3	Mg 3	0	0
56	1W	1	Total 1	Mg 1	0	0
56	1X	1	Total 1	Mg 1	0	0
56	1Y	1	Total 1	Mg 1	0	0
56	1Z	1	Total 1	Mg 1	0	0
56	10	4	Total 4	Mg 4	0	0
56	15	1	Total 1	Mg 1	0	0
56	16	1	Total 1	Mg 1	0	0
56	17	2	Total 2	Mg 2	0	0
56	18	2	Total 2	Mg 2	0	0
56	19	1	Total 1	Mg 1	0	0
56	1a	89	Total 89	Mg 89	0	0
56	1d	1	Total 1	Mg 1	0	0
56	1e	1	Total 1	Mg 1	0	0
56	1l	1	Total 1	Mg 1	0	0
56	1r	1	Total 1	Mg 1	0	0
56	1t	1	Total 1	Mg 1	0	0
56	1v	1	Total 1	Mg 1	0	0
56	1x	9	Total 9	Mg 9	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
56	2A	474	Total 474	Mg 474	0	0
56	2B	10	Total 10	Mg 10	0	0
56	2D	3	Total 3	Mg 3	0	0
56	2E	5	Total 5	Mg 5	0	0
56	2F	1	Total 1	Mg 1	0	0
56	2O	1	Total 1	Mg 1	0	0
56	2Q	1	Total 1	Mg 1	0	0
56	2R	2	Total 2	Mg 2	0	0
56	2W	1	Total 1	Mg 1	0	0
56	2Z	1	Total 1	Mg 1	0	0
56	20	1	Total 1	Mg 1	0	0
56	21	1	Total 1	Mg 1	0	0
56	23	1	Total 1	Mg 1	0	0
56	25	1	Total 1	Mg 1	0	0
56	27	1	Total 1	Mg 1	0	0
56	28	2	Total 2	Mg 2	0	0
56	2a	113	Total 113	Mg 113	0	0
56	2c	1	Total 1	Mg 1	0	0
56	2d	1	Total 1	Mg 1	0	0
56	2f	2	Total 2	Mg 2	0	0
56	2l	2	Total 2	Mg 2	0	0

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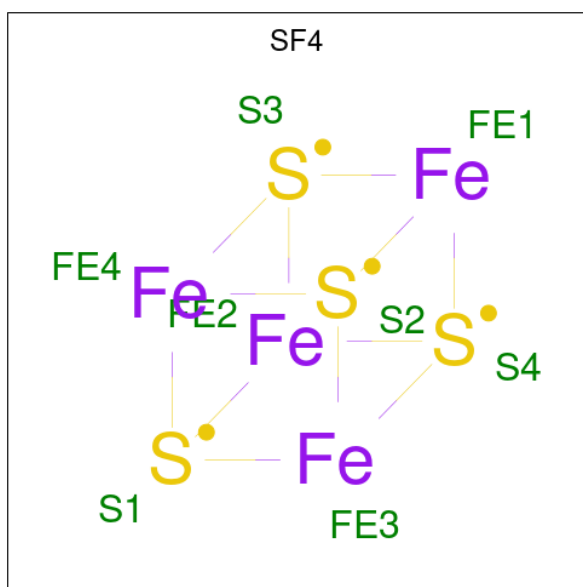
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
56	2n	1	Total 1	Mg 1	0	0
56	2q	1	Total 1	Mg 1	0	0
56	2r	1	Total 1	Mg 1	0	0
56	2x	1	Total 1	Mg 1	0	0

- Molecule 57 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
57	1Y	1	Total 1	Zn 1	0	0
57	14	1	Total 1	Zn 1	0	0
57	15	1	Total 1	Zn 1	0	0
57	16	1	Total 1	Zn 1	0	0
57	19	1	Total 1	Zn 1	0	0
57	1n	1	Total 1	Zn 1	0	0
57	2Y	1	Total 1	Zn 1	0	0
57	24	1	Total 1	Zn 1	0	0
57	25	1	Total 1	Zn 1	0	0
57	26	1	Total 1	Zn 1	0	0
57	29	1	Total 1	Zn 1	0	0
57	2n	1	Total 1	Zn 1	0	0

- Molecule 58 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe₄S₄).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
58	1d	1	Total	Fe	S	0	0
			8	4	4		
58	2d	1	Total	Fe	S	0	0
			8	4	4		

- Molecule 59 is water.

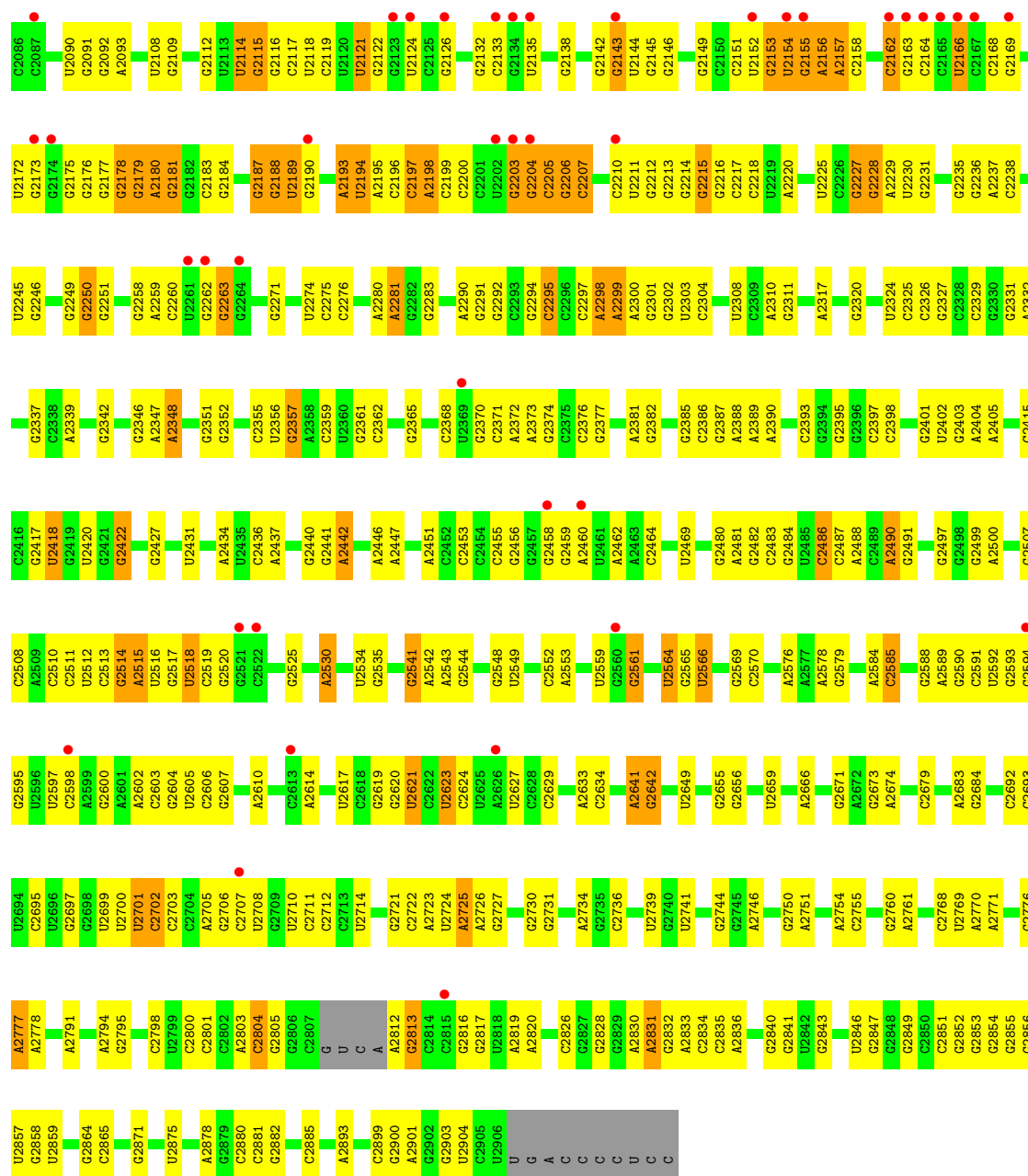
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
59	1A	145	Total	O	0	0
			145	145		
59	1B	6	Total	O	0	0
			6	6		
59	1D	4	Total	O	0	0
			4	4		
59	1F	2	Total	O	0	0
			2	2		
59	1O	1	Total	O	0	0
			1	1		
59	1X	1	Total	O	0	0
			1	1		
59	10	1	Total	O	0	0
			1	1		
59	1a	12	Total	O	0	0
			12	12		
59	2A	44	Total	O	0	0
			44	44		
59	2E	1	Total	O	0	0
			1	1		

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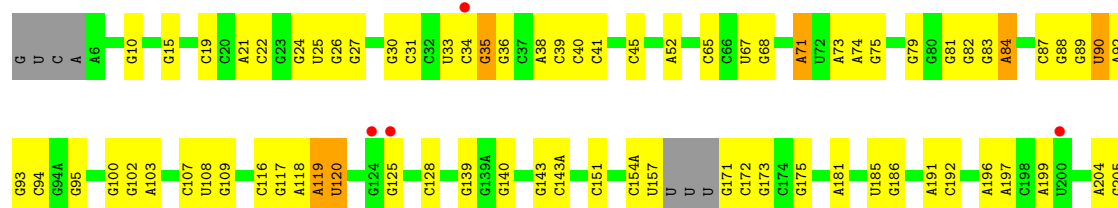
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
59	2a	30	Total	O	0	0
			30	30		

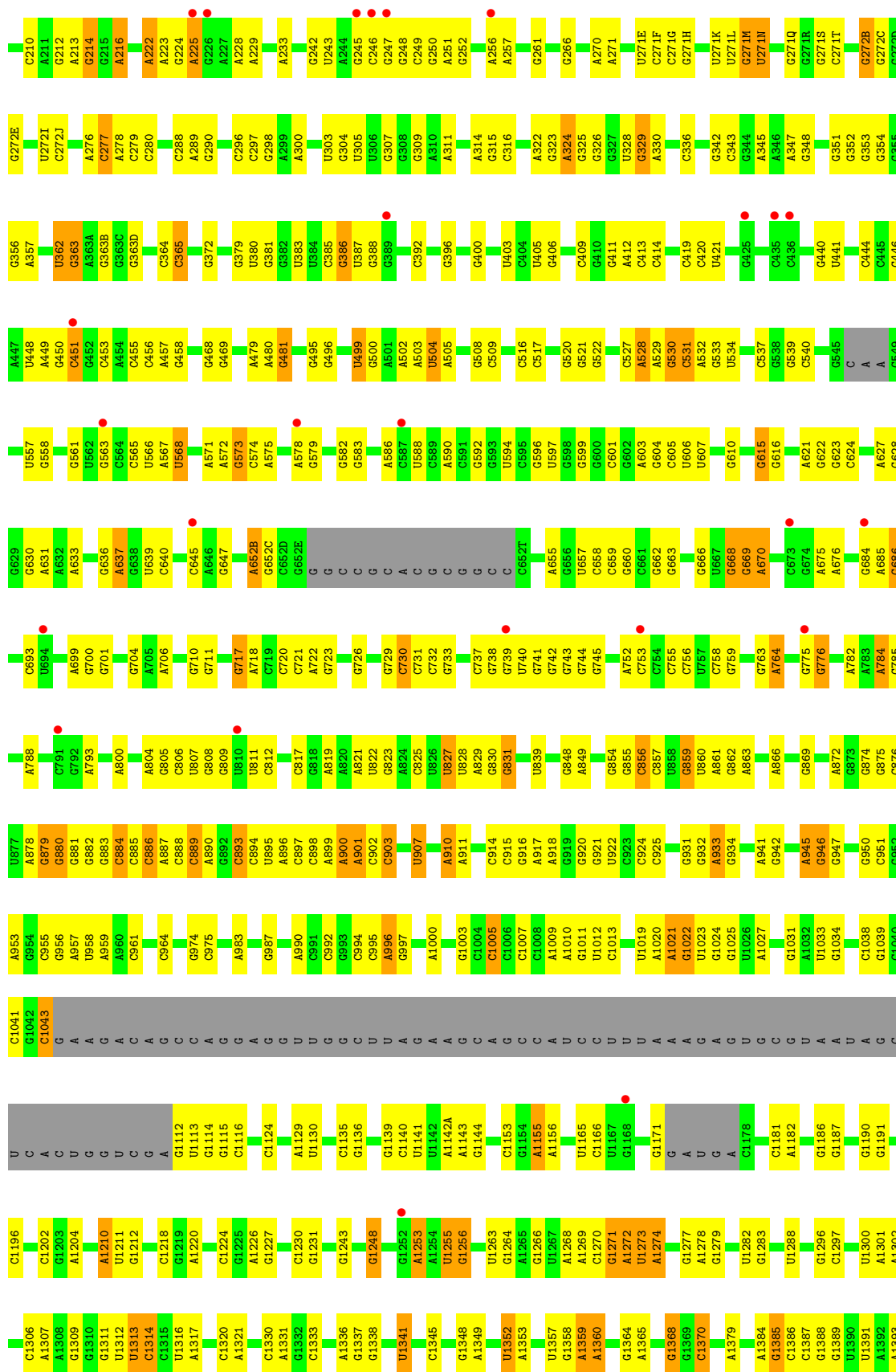
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• Molecule 1: 23S Ribosomal RNA

Chain 2A: 3% 53% 37% 6%



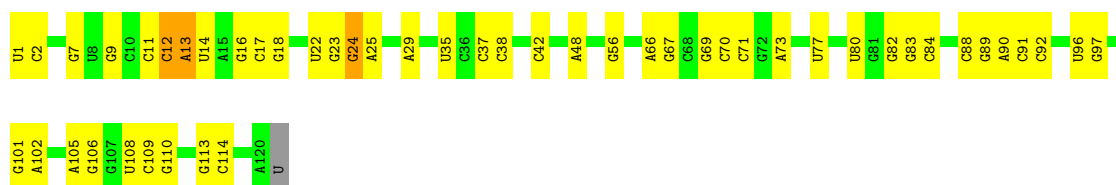


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U1394	A1395	U1396	G1410	C1411	A1412	G1413	G1416	C1417	G1418	U1419	A1420	G1421	C1422	G1423	G1424	G1425	G1426	C1427	C1428	A1434	G1435	C1436	C1437	G1442	A1445	G1448	A1449	G1450	C1450A	C1451	G1455	A1459	A1460	G1461	C1462	C1463	C1464	A1465	G1466	C1467	C1468	A1469	G1470	A1471	G1478	G1479	G1480	U1481	C1482	G1484						



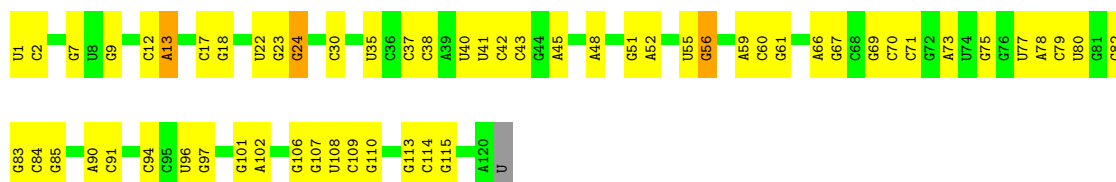
• Molecule 2: 5S Ribosomal RNA

Chain 1B: 59% 38%



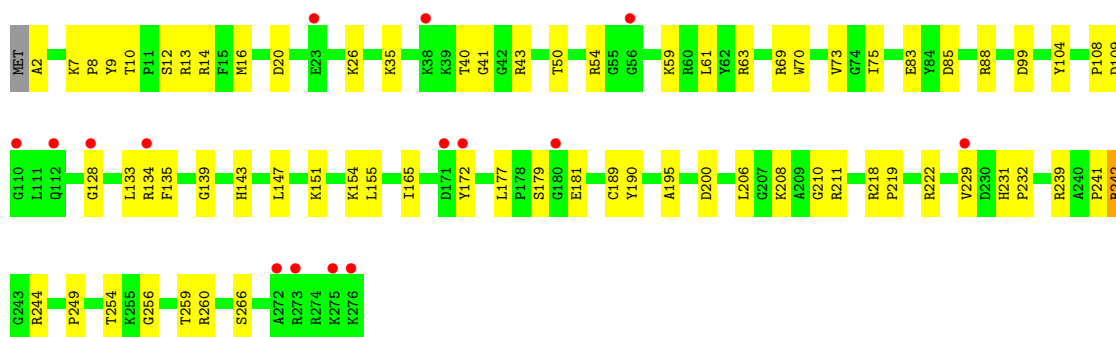
• Molecule 2: 5S Ribosomal RNA

Chain 2B: 51% 45%



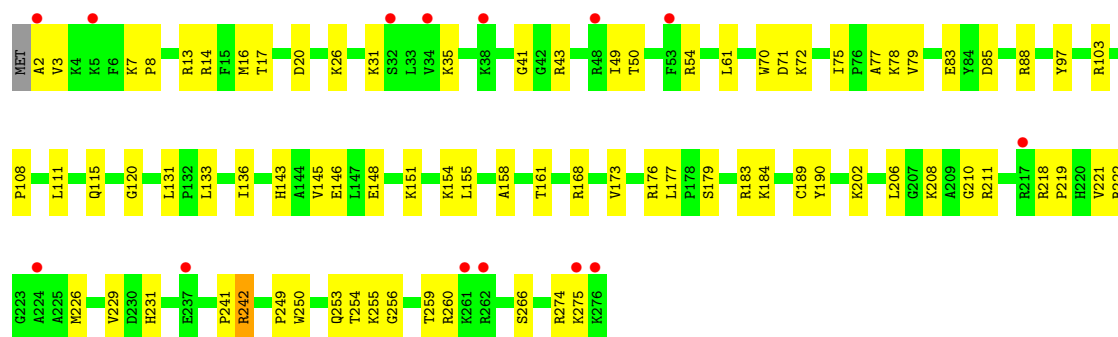
• Molecule 3: 50S Ribosomal Protein L2

Chain 1D: 5% 74% 25%

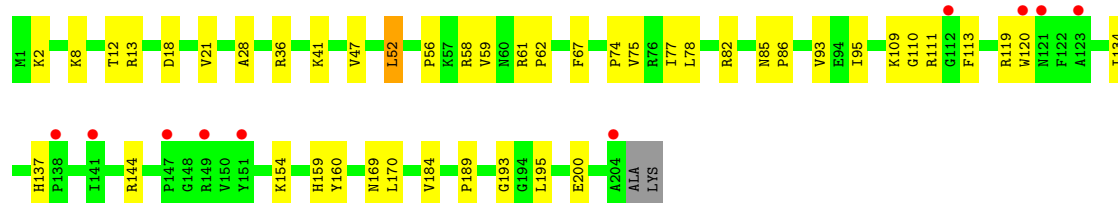
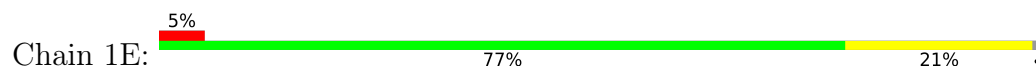


• Molecule 3: 50S Ribosomal Protein L2

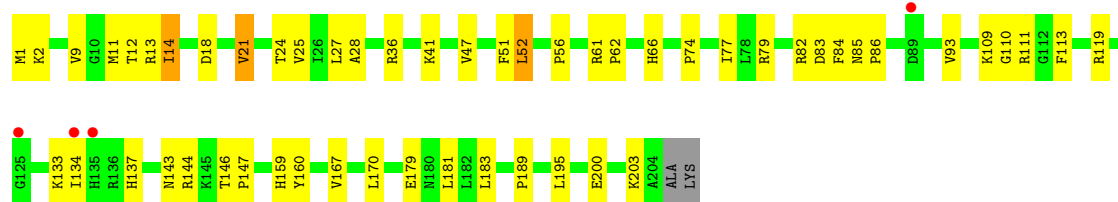
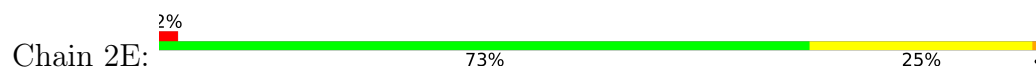
Chain 2D: 5% 71% 29%



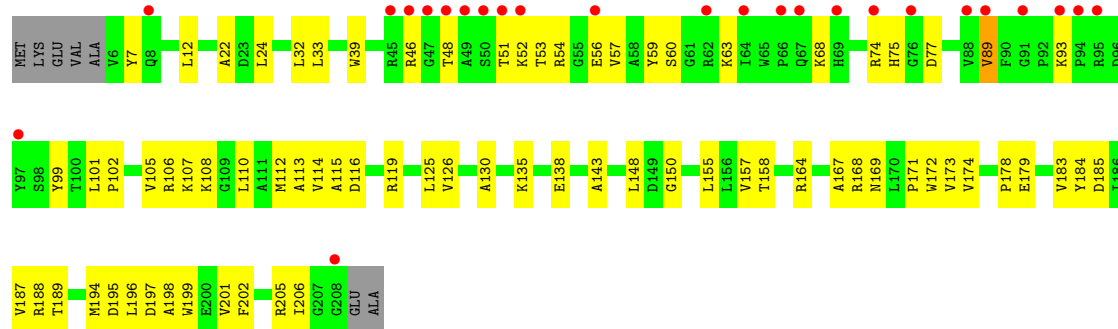
• Molecule 4: 50S Ribosomal Protein L3



• Molecule 4: 50S Ribosomal Protein L3

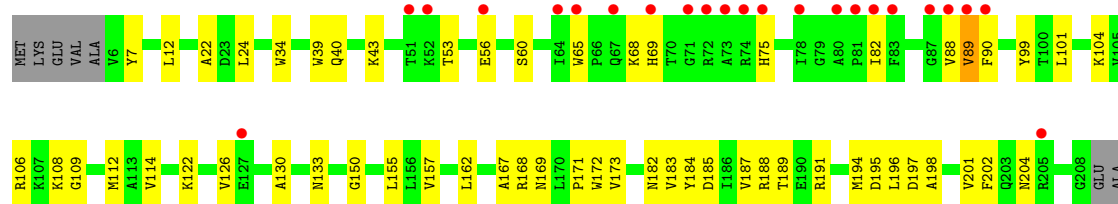


• Molecule 5: 50S Ribosomal Protein L4

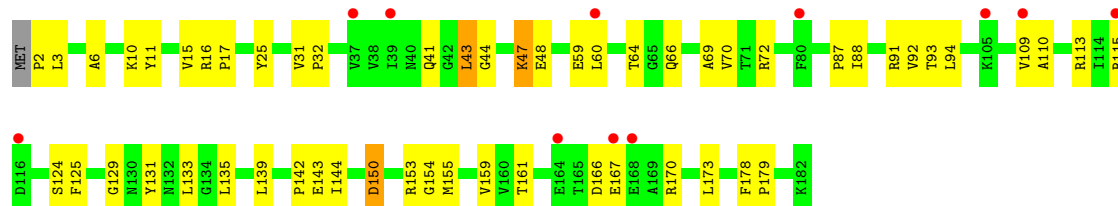


• Molecule 5: 50S Ribosomal Protein L4

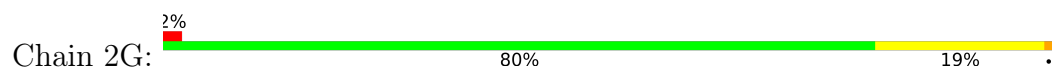




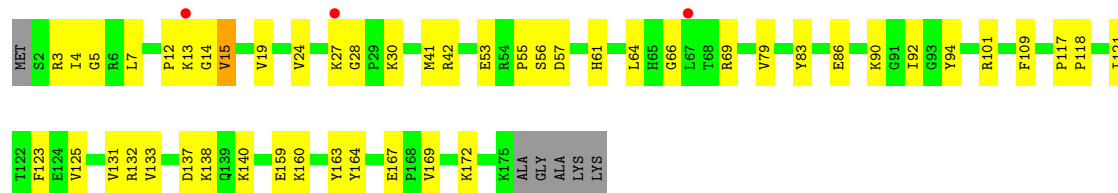
• Molecule 6: 50S Ribosomal Protein L5



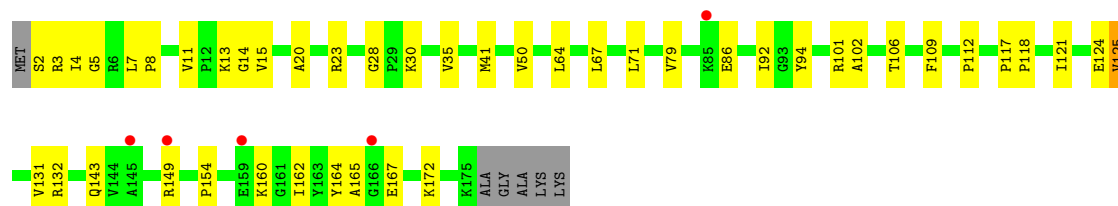
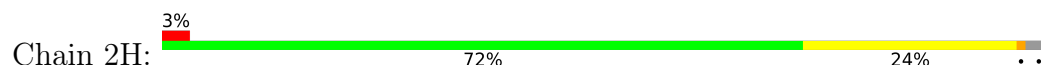
• Molecule 6: 50S Ribosomal Protein L5



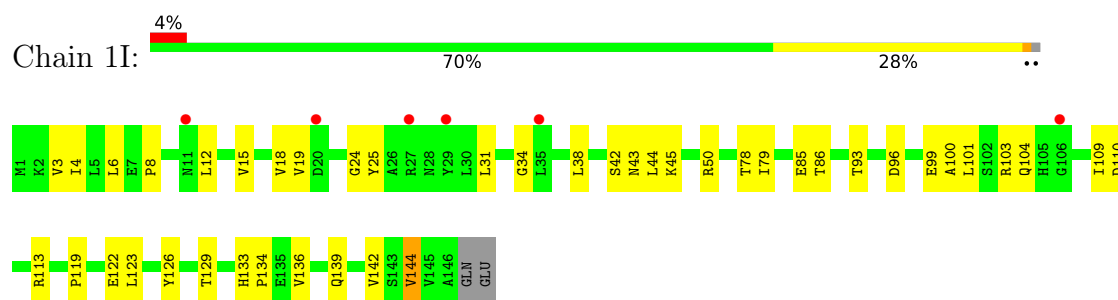
• Molecule 7: 50S Ribosomal Protein L6



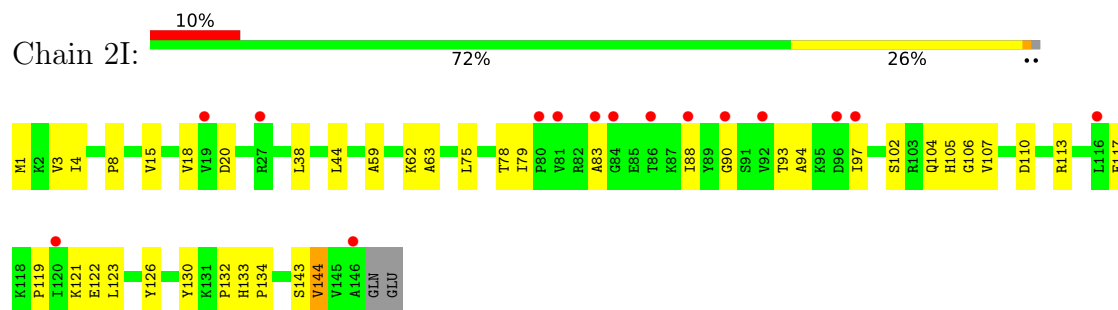
• Molecule 7: 50S Ribosomal Protein L6



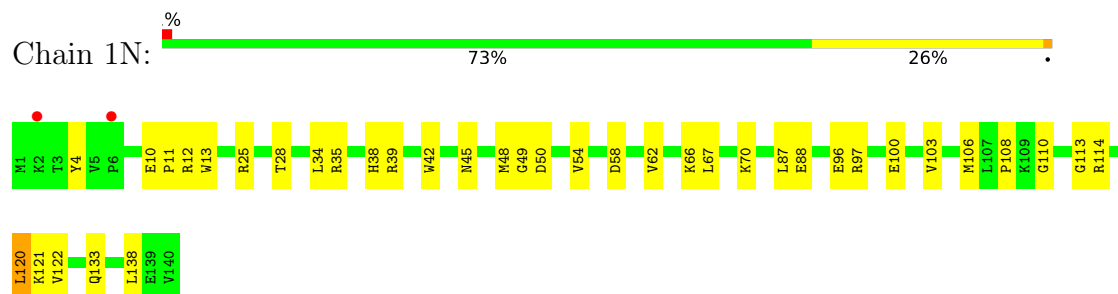
• Molecule 8: 50S Ribosomal Protein L9



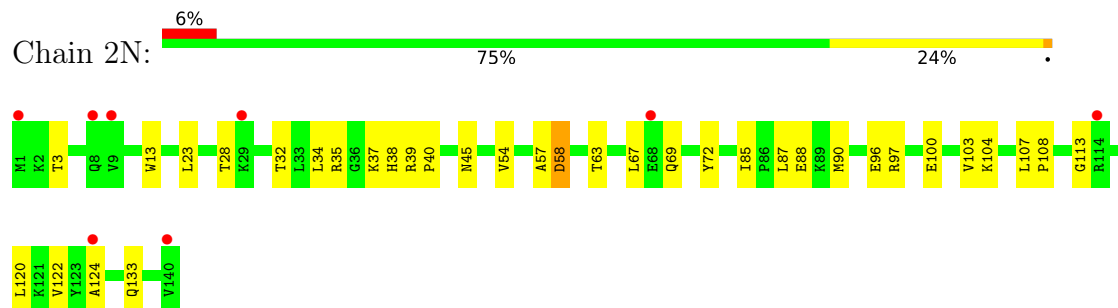
• Molecule 8: 50S Ribosomal Protein L9



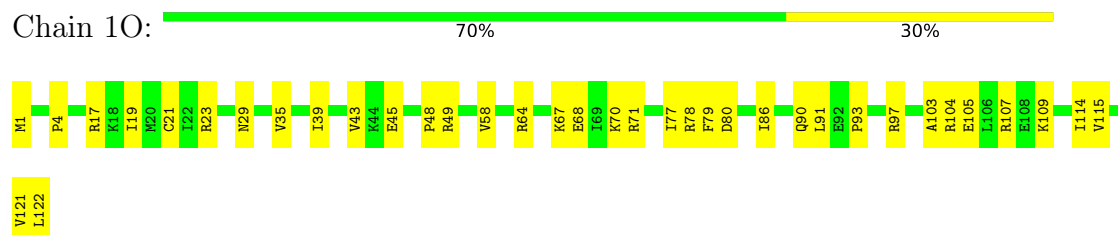
• Molecule 9: 50S Ribosomal Protein L13



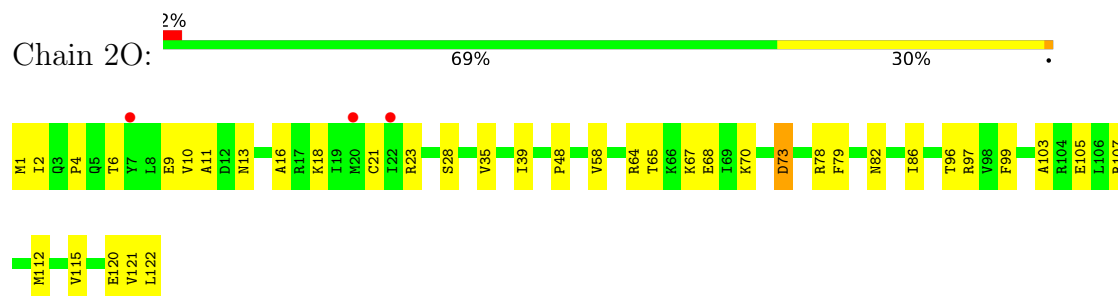
• Molecule 9: 50S Ribosomal Protein L13



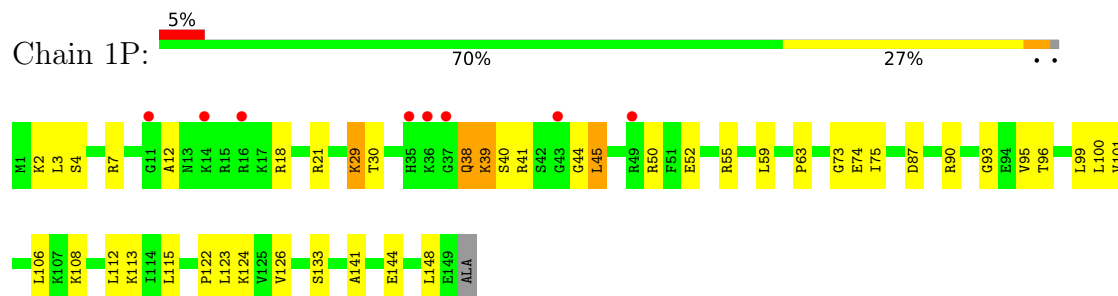
• Molecule 10: 50S Ribosomal Protein L14



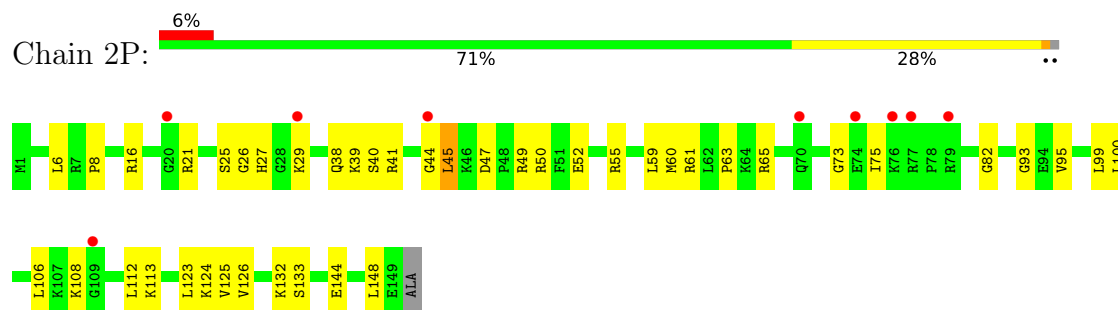
- Molecule 10: 50S Ribosomal Protein L14



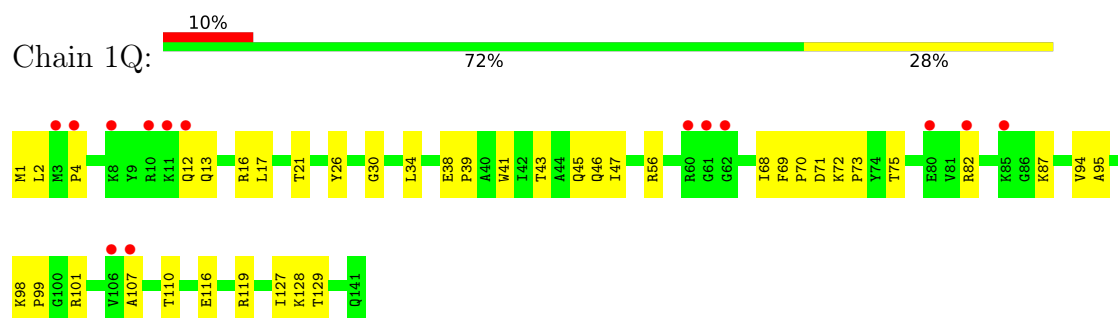
- Molecule 11: 50S Ribosomal Protein L15



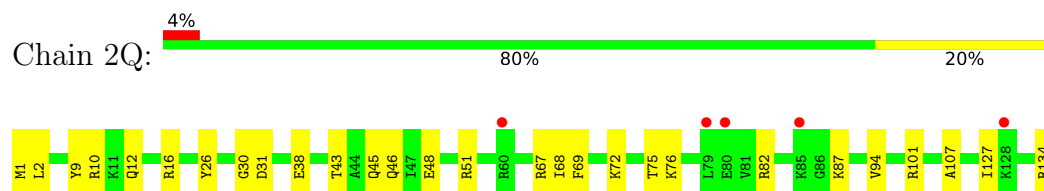
- Molecule 11: 50S Ribosomal Protein L15



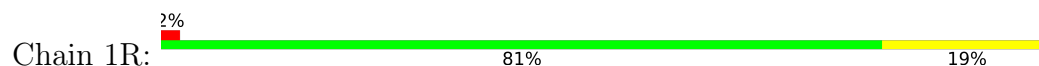
- Molecule 12: 50S Ribosomal Protein L16



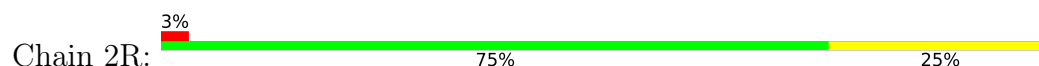
- Molecule 12: 50S Ribosomal Protein L16



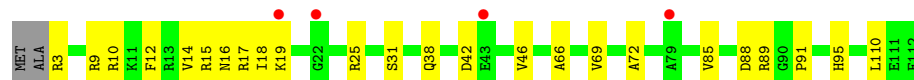
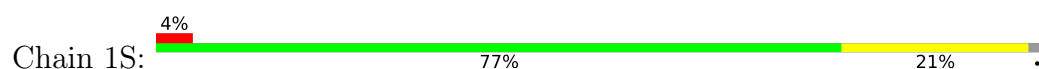
● Molecule 13: 50S Ribosomal Protein L17



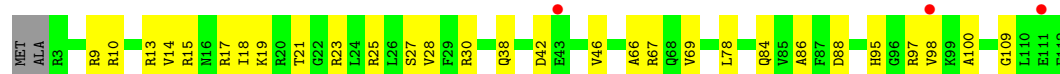
● Molecule 13: 50S Ribosomal Protein L17



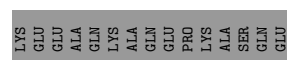
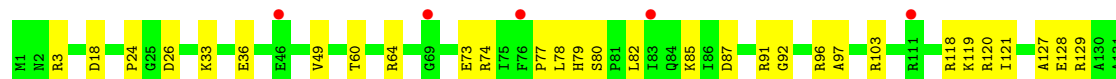
● Molecule 14: 50S Ribosomal Protein L18



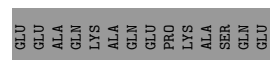
● Molecule 14: 50S Ribosomal Protein L18



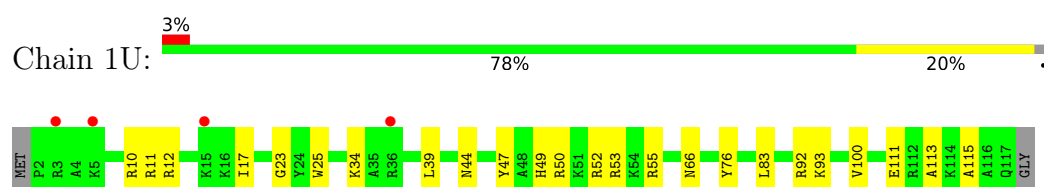
● Molecule 15: 50S Ribosomal Protein L19



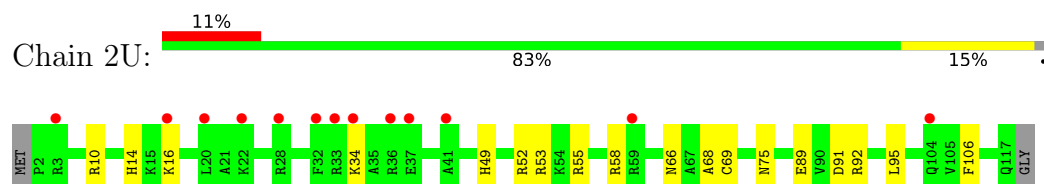
● Molecule 15: 50S Ribosomal Protein L19



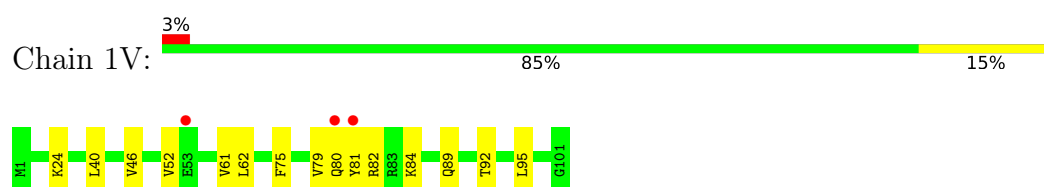
● Molecule 16: 50S Ribosomal Protein L20



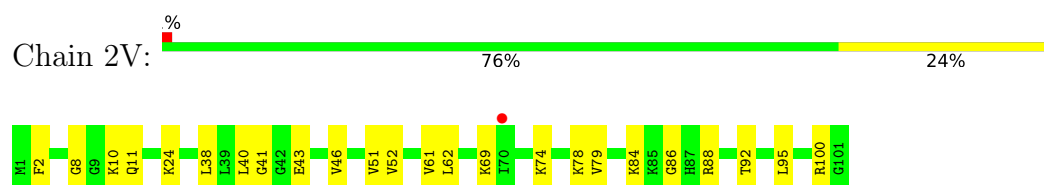
- Molecule 16: 50S Ribosomal Protein L20



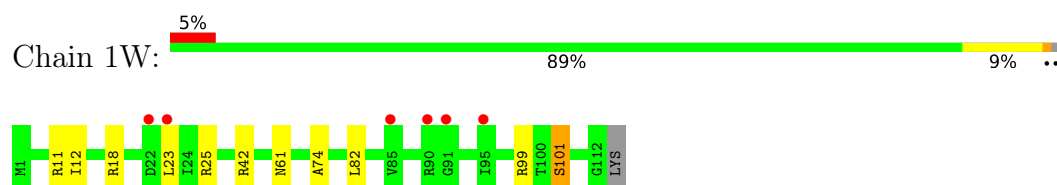
- Molecule 17: 50S Ribosomal Protein L21



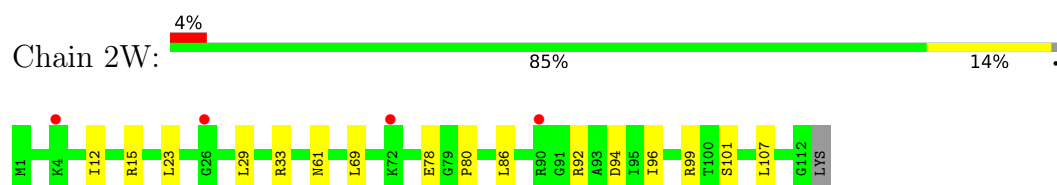
- Molecule 17: 50S Ribosomal Protein L21



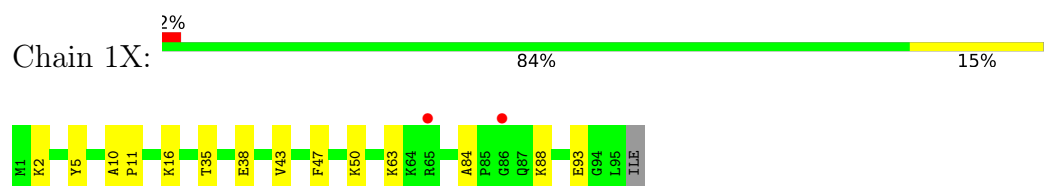
- Molecule 18: 50S Ribosomal Protein L22



- Molecule 18: 50S Ribosomal Protein L22



- Molecule 19: 50S Ribosomal Protein L23



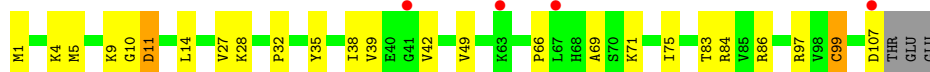
- Molecule 19: 50S Ribosomal Protein L23

Chain 2X: 



- Molecule 20: 50S ribosomal protein L24

Chain 1Y: 



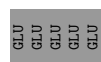
- Molecule 20: 50S ribosomal protein L24

Chain 2Y: 



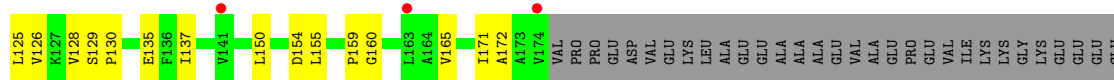
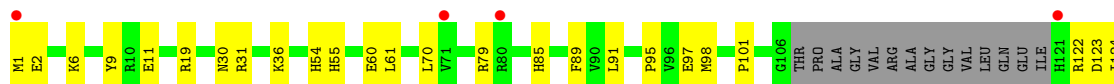
- Molecule 21: 50S ribosomal protein L25

Chain 1Z: 



- Molecule 21: 50S ribosomal protein L25

Chain 2Z: 

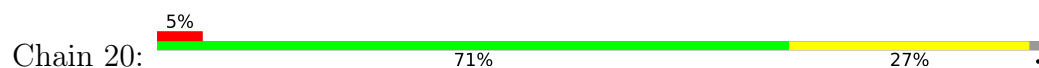


- Molecule 22: 50S ribosomal protein L27

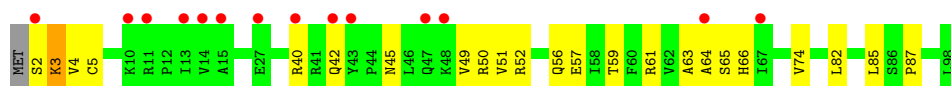
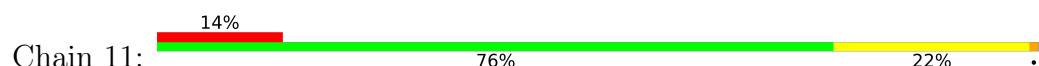
Chain 10: 



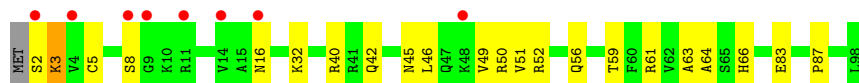
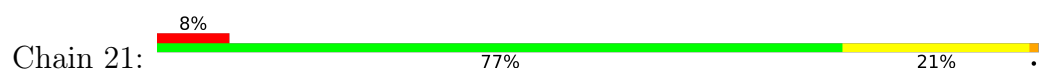
- Molecule 22: 50S ribosomal protein L27



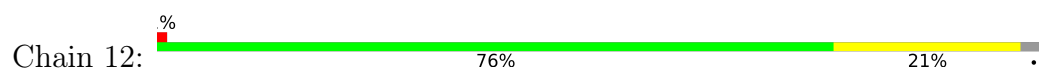
- Molecule 23: 50S ribosomal protein L28



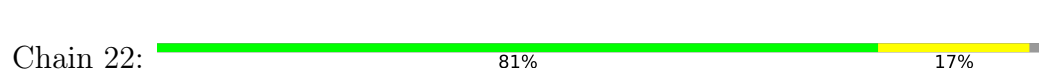
- Molecule 23: 50S ribosomal protein L28



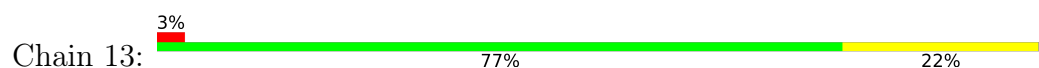
- Molecule 24: 50S ribosomal protein L29



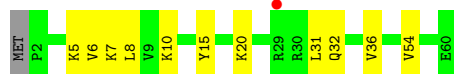
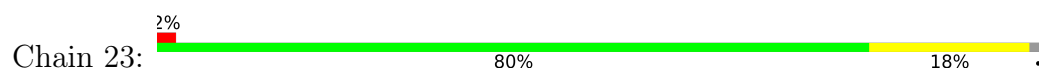
- Molecule 24: 50S ribosomal protein L29



- Molecule 25: 50S ribosomal protein L30



- Molecule 25: 50S ribosomal protein L30



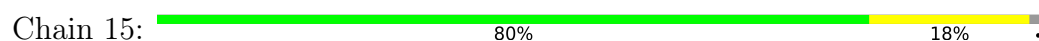
- Molecule 26: 50S ribosomal protein L31



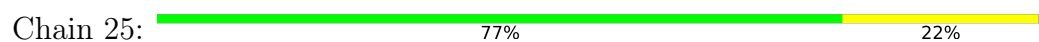
- Molecule 26: 50S ribosomal protein L31



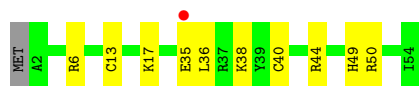
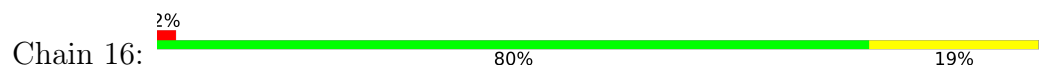
- Molecule 27: 50S ribosomal protein L32



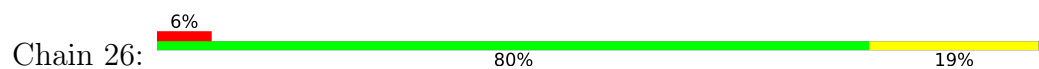
- Molecule 27: 50S ribosomal protein L32



- Molecule 28: 50S ribosomal protein L33



- Molecule 28: 50S ribosomal protein L33



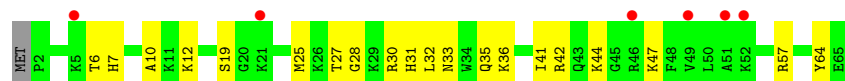
- Molecule 29: 50S ribosomal protein L34



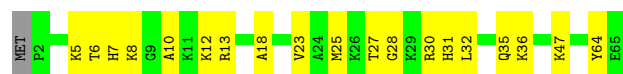
- Molecule 29: 50S ribosomal protein L34



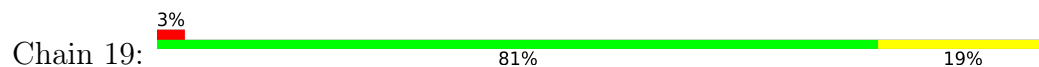
- Molecule 30: 50S Ribosomal Protein L35



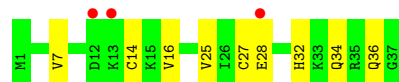
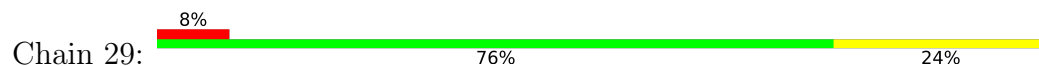
- Molecule 30: 50S Ribosomal Protein L35



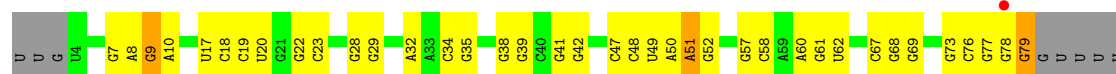
- Molecule 31: 50S Ribosomal Protein L36



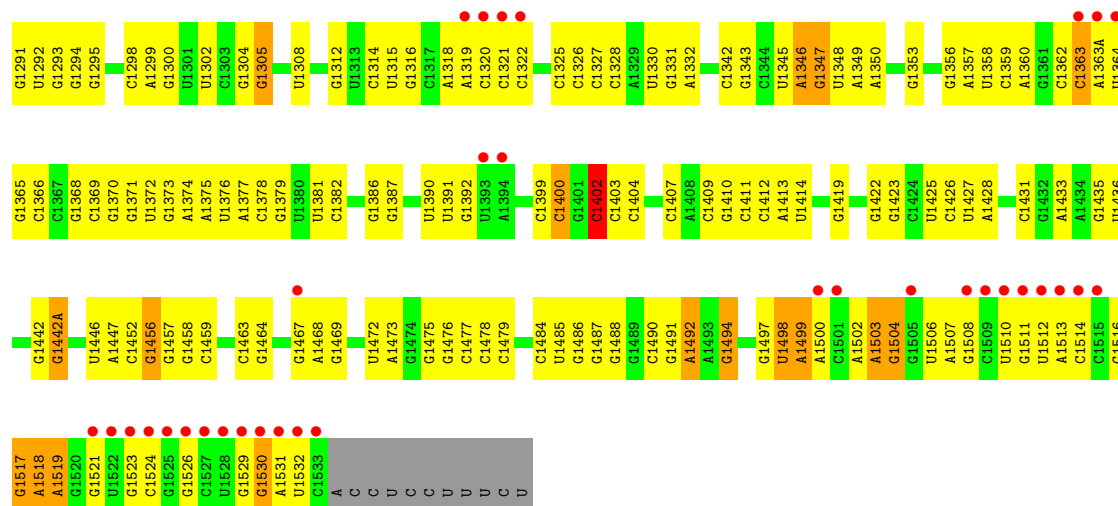
- Molecule 31: 50S Ribosomal Protein L36



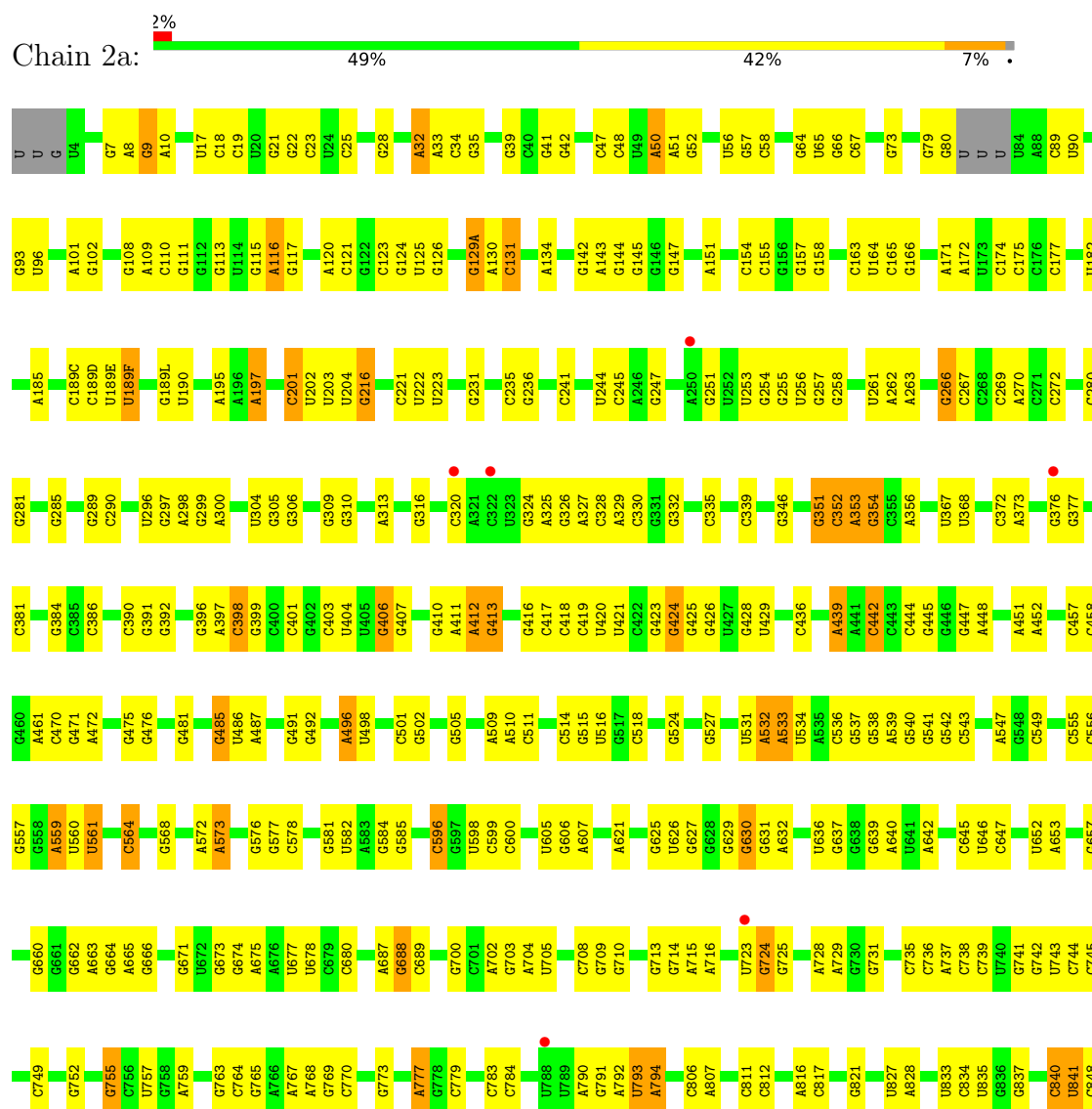
- Molecule 32: 16S Ribosomal RNA



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G1225	C1158	C1158	G1079	G1023	A949	G838	C746	G541	G450	A360	C278	A179	C
C1226	U1159	U1159	A1080	G1024	U950	U839	C749	C542	A451	G360	G279	U180	U90
A1227	C1162	C1162	G1081	U1025	G951	C840	C750	C543	A452	G361	C280	U182	C91
C1228	C1163	C1163	G1084	G1026	U952	U841	C754	G544	C455	G362	C281	U183	C92
U1232	C1164	C1164	U1085	C1027	G953	C842	C755	C545	C456	U367	G282	A185	G93
U1233	C1165	C1165	U1086	C1028	G954	C843	C756	G546	C457	U368	G283	C186	U96
U1235	A1166	A1166	G1089	C1030	U955	U850	C757	A547	A461	C372	U296	U189	U99
A1236	A1167	A1167	U1090	G1030A	A958	G851	C758	C548	C470	A373	G297	C189	C100
C1237	A1168	A1168	U1091	C1030B	A959	G852	C759	C549	G475	G376	A298	G189D	A101
A1238	C1171	C1171	U1092	G1030C	U960	G853	C760	C550	G476	U300	G301	U189F	G102
C1241	C1172	C1172	U1093	G1030D	U961	G854	C761	A553	U480	G384	G302	C189D	G105
G1242	G1173	G1173	U1094	A1030E	C962	G855	C762	C556	G481	C385	G303	U189E	C106
C1243	C1174	C1174	U1095	G1031	A963	U856	C763	A559	U482	C386	G304	U189F	G107
C1244	G1175	G1175	U1096	G1032	A964	U857	C764	U560	U483	C387	U304	U189G	G108
A1248	A1176	A1176	U1097	A1033	A965	U858	C765	U561	G484	U387	G305	U189H	G109
C1249	C1177	C1177	U1098	G1034	G966	U859	C766	C562	U485	G396	G306	U189I	A109
A1250	C1178	C1178	U1099	A1034	G967	U860	C767	A563	U486	A397	U306	U189J	C110
A1251	A1179	A1179	U1100	G1035	A968	U861	C768	U564	G487	C398	G307	G189L	G111
A1252	C1180	C1180	U1101	A1035	A969	U862	C769	U565	U488	C399	U308	U192	G112
G1253	A1181	A1181	U1102	G1036	C970	A663	C770	U566	G490	G300	C314	C193	C121
C1254	C1182	C1182	U1103	A1036	G971	U664	C771	U567	G491	G301	A315	C194	G122
G1255	A1183	A1183	U1104	G1037	G972	A665	C772	U568	G502	C501	G316	U202	G123
A1256	C1184	C1184	U1105	A1038	G973	U666	C773	C569	G503	G402	G317	A196	A116
G1257	G1185	G1185	U1106	G1039	A974	U667	C774	U569	U498	C403	G318	A197	G117
U1258	G1186	G1186	U1107	A1040	A975	U668	C775	U570	U499	U404	G319	G200	C121
C1259	C1187	C1187	U1108	G1041	A976	U669	C776	U571	G500	G405	C320	C201	G126
G1260	A1188	A1188	U1109	A1042	A977	U670	C777	U572	G501	C406	A321	G216	C131
C1261	G1189	G1189	U1110	G1043	A978	U671	C778	U573	G502	G407	C322	U203	G127
G1262	C1190	C1190	U1111	A1044	G979	U672	C779	U574	G503	C408	U323	U204	G128
A1263	A1191	A1191	U1112	G1045	G980	U673	C780	U575	G504	G409	G324	G217	C132
G1264	C1192	C1192	U1113	A1046	A981	U674	C781	U576	G505	A411	A325	G218	G133
G1265	G1193	G1193	U1114	G1047	U982	U675	C782	U577	G506	G412	A326	C219	C134
C1266	A1194	A1194	U1115	A1048	U983	U676	C783	U578	G507	C413	C327	C220	A134
G1267	C1195	C1195	U1116	G1049	C984	U677	C784	U579	C508	C414	A328	U222	A143
A1268	U1196	U1196	U1117	A1050	C985	U678	C785	U580	A509	C415	A329	G227	G144
C1269	C1197	C1197	U1118	A1051	A986	U679	C786	U581	A510	C416	A330	A228	G145
G1270	G1200	G1200	U1119	U1052	G987	U680	C787	U582	C511	C417	G332	G238	A149
G1271	A1201	A1201	U1120	G1053	U992	U681	C788	U583	C512	U421	C333	G239	A150
G1272	C1202	C1202	U1121	A1054	G993	U682	C789	U584	G524	G422	C334	G240	A151
G1273	G1206	G1206	U1122	G1055	U994	U683	C790	U585	G525	G423	C335	C245	C150
A1275	C1207	C1207	U1123	A1056	U995	U684	C791	U586	G526	G424	C336	G246	A151
G1276	C1208	C1208	U1124	G1057	U996	U685	C792	U587	G527	G425	C337	A246	G159
C1277	U1209	U1209	U1125	U1058	U997	U686	C793	U588	G528	G426	A338	G247	A160
U1278	C1210	C1210	U1126	G1059	U1000	U687	C794	U589	G529	U427	U340	A250	A161
A1279	U1211	U1211	U1127	A1060	U1001	U688	C795	U590	G530	U428	C342	G251	A162
U1280	C1212	C1212	U1128	G1061	U1002	U689	C796	U591	G531	U429	C343	G252	C163
C1281	A1213	A1213	U1129	A1062	G1003	U690	C797	U592	G532	U430	U344	G253	U164
U1282	C1214	C1214	U1130	U1063	U1004	U691	C798	U593	G533	G431	A345	G254	C165
G1283	G1215	G1215	U1131	G1064	A1005	U692	C799	U594	G534	G432	G346	A262	G166
C1284	U1216	U1216	U1132	A1065	U1006	U693	C800	U595	G535	G433	G347	A263	G167
A1285	C1217	C1217	U1133	U1066	C1007	U694	C801	U596	G536	G434	G348	G266	A171
U1286	U1218	U1218	U1134	A1067	U1008	U695	C802	U597	G537	G435	A349	C267	A172
A1287	C1219	C1219	U1135	U1068	U1009	U696	C803	U598	G538	G436	G350	C268	U173
U1288	U1220	U1220	U1136	G1069	A1010	U697	C804	U599	G539	G437	U341	C269	C174
G1290	C1221	C1221	U1137	A1070	U1011	U698	C805	U600	G540	G438	C342	G354	



• Molecule 32: 16S Ribosomal RNA





Q212	Q215	Q216	Q217	A218	V219	I222	A225	S235	Y236	A237	LEU	VAL	GLN	GLU	GLU	THR	GLU	THR	PRO	GLU	GLY	GLY	SER	GLU	VAL	ALA																				
MI01	LI02	LI08	SI09	RI10	RI11	V112	RI14	LI15	SI24	PI25	EI26	LI27	RI30	PI31	RI44	LI49	RI53	LI54	LI55	LI62	FI63	PI67	VI74	RI75	EI76	LI77	RI78	KI79	PI83	VI84	LI85	DI89	SI92	DI93	PI94	DI98	YI99	D206	A207	I208	R209	Q95	H97	I210	I211	
MET	PRO	VAL	GLU	ILE	THR	V7	K8	E9	LI2	VI5	H16	F17	E20	H21	K22	R23	W24	T47	L51	E52	R56	D60	L61	A62	M63	R64	G65	G66	V71	G72	T73	Q76	A77	Q78	D79	I80	E84	R87	A88	P91	Y92	V93	O94	R96	H97	I98

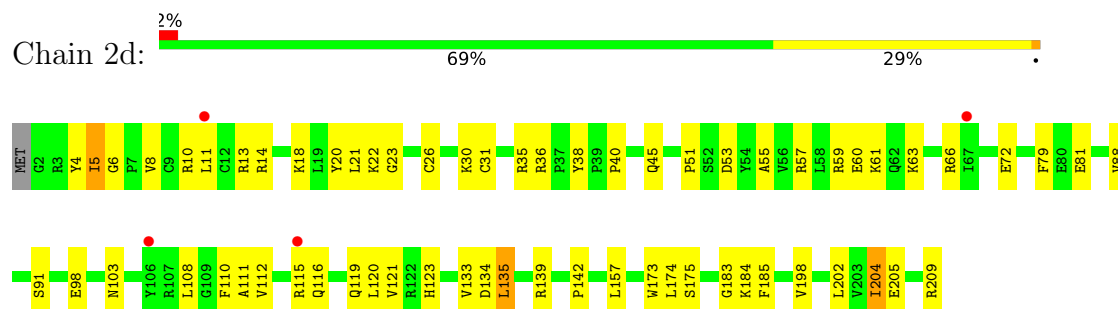
[illegible]

PRO	LYS	ALA	GLU	GLY	ARG	PRO	ARG	ARG	ARG	ARG	ARG	ARG	PRO	ALA	VAL	ARG	VAL	LYS	LYS	GLU	GLU	GLU	PRO	ARG	PRO	GLY	GLN	LYS	PRO	ALA	ARG	PRO	GLY	GLU	VAL																							
V103	G2	N3			H6	P7	I8	G9	F10	R11	L12		T15	R16	D17	V18	E19	S20	R21		A24		Y29		D36	Q37	R38	I39	R40	G41	L42	L43	E44	K45	E46	L47		A53	R54	D56	I57	E58	R59	A60		N63	V64	A65		V68		A71	K72	P73		G78		R83

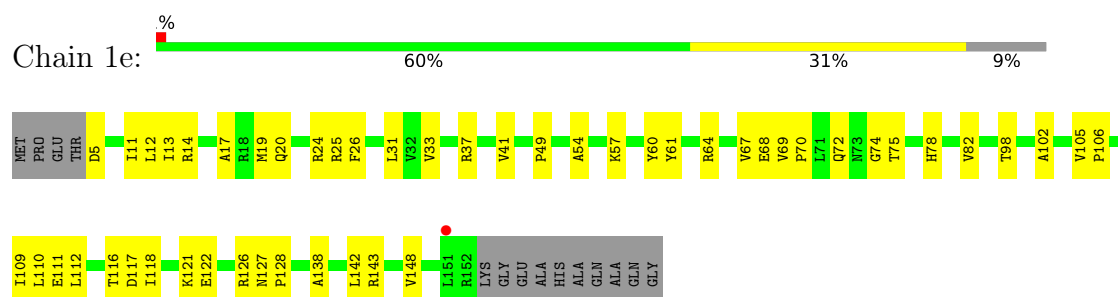
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	Y104	10
	V105	10
	L108	10
	G109	10
	F110	10
	A111	10
	V112	10
MET	R115	10
	L118	10
	Q119	10
	L120	10
	V121	10
	R122	10
	H123	10
	G124	10
	H125	10
	V133	10
D134	10	
MET	L135	10
	Y138	10
	R139	10
	A147	10
	L158	10
	L162	10
	K166	10
	V170	10
	F172	10
	V173	10
L174	10	
MET	S175	10
	K182	10
	G183	10
	K184	10
	L187	10
	L188	10
	P189	10
	D193	10
	L194	10
	A195	10
MET	L196	10
	P197	10
	F198	10
	G199	10
	R200	10
	K201	10
	G202	10
	E203	10
	R204	10
	C205	10
P206	10	
MET	K209	10
	R210	10
	G211	10
	F212	10
	A213	10
	V214	10
	L215	10
	R216	10
	G217	10
	F218	10
A219	10	
MET	V220	10
	L221	10
	R222	10
	G223	10
	E224	10
	R225	10
	C226	10
	P229	10
	K230	10
	C31	10
A32	10	
K33	10	
E34	10	
R35	10	
MET	Y38	10
	P39	10
	P40	10
	Q45	10
	S52	10
	V56	10
	R57	10
	K61	10
	Q62	10
	B66	10
E72	10	
F79	10	
V83	10	
MET	S91	10
	L94	10
	L96	10
	P197	10
	F198	10
	G199	10
	R200	10
	K201	10
	G202	10
	E203	10
R204	10	
C205	10	
P206	10	
MET	K209	10
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	R216	10
	G217	10
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P39	10	
P40	10	
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S52	10	
V56	10	
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Q62	10	
B66	10	
E72	10	
F79	10	
V83	10	
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C205	10	
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K209	10	
R210	10	
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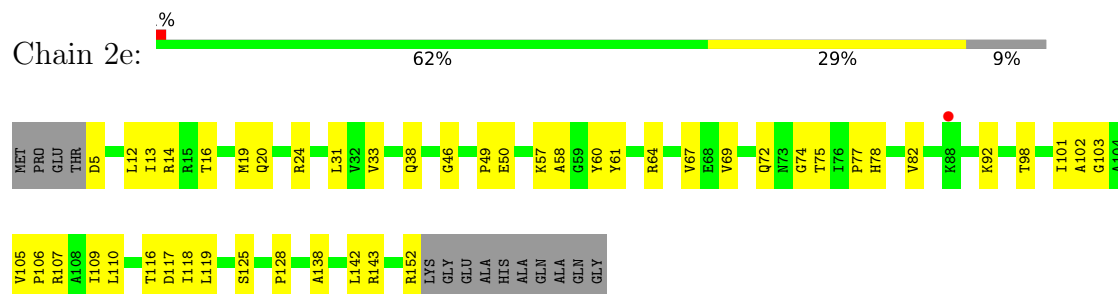
- Molecule 35: 30S Ribosomal Protein S4



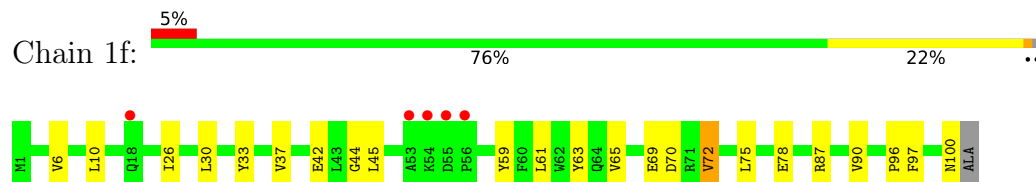
- Molecule 36: 30S Ribosomal Protein S5



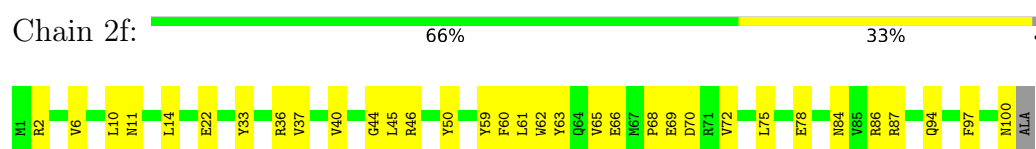
- Molecule 36: 30S Ribosomal Protein S5



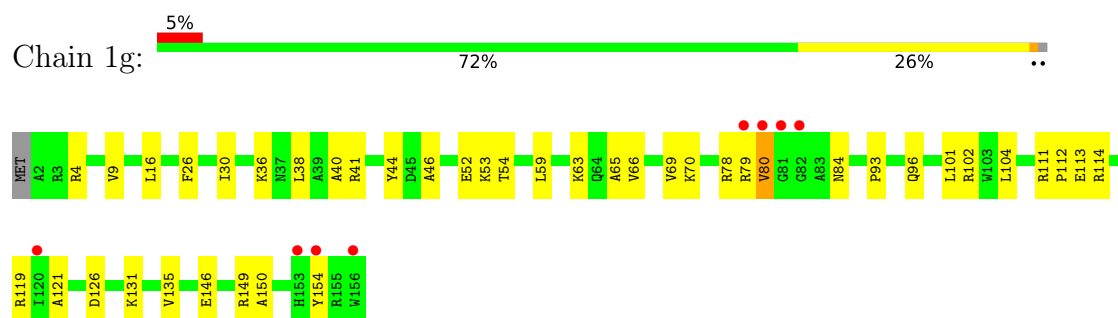
- Molecule 37: 30S Ribosomal Protein S6



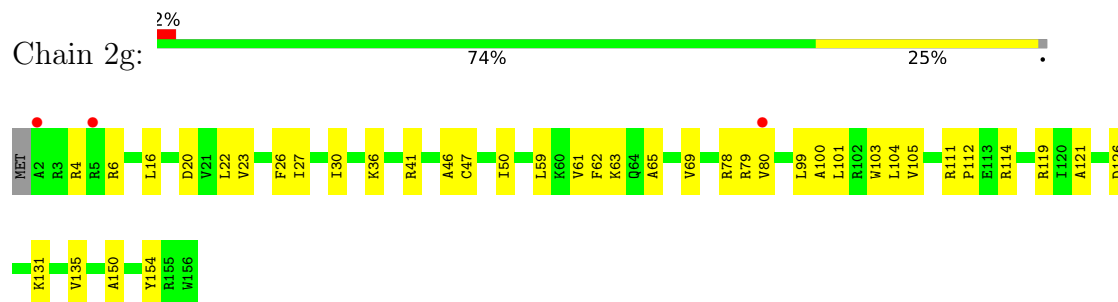
- Molecule 37: 30S Ribosomal Protein S6



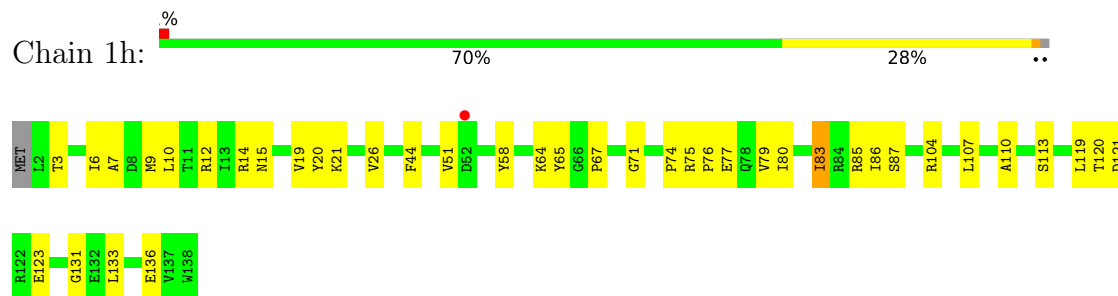
- Molecule 38: 30S Ribosomal Protein S7



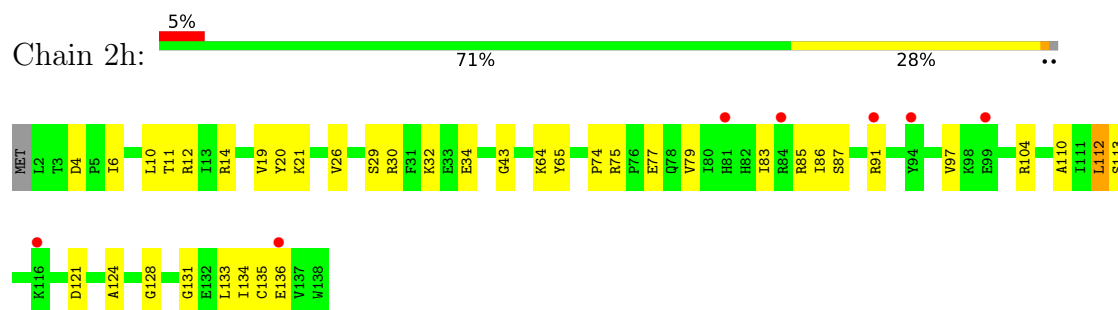
- Molecule 38: 30S Ribosomal Protein S7



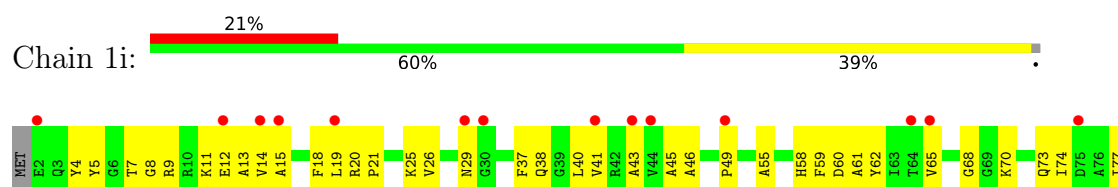
- Molecule 39: 30S Ribosomal Protein S8



- Molecule 39: 30S Ribosomal Protein S8

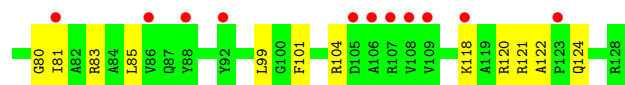
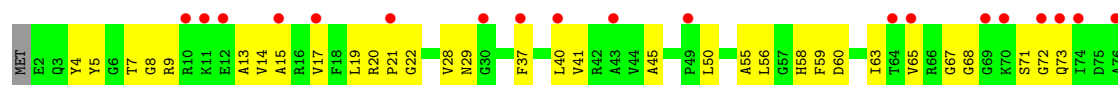


- Molecule 40: 30S ribosomal protein S9

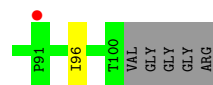
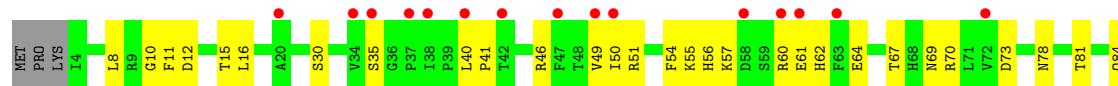




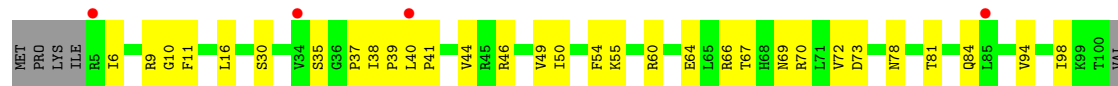
- Molecule 40: 30S ribosomal protein S9



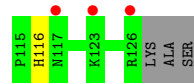
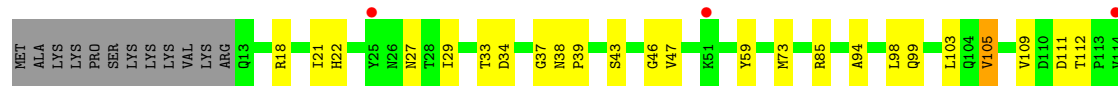
- Molecule 41: 30S ribosomal protein S10



- Molecule 41: 30S ribosomal protein S10

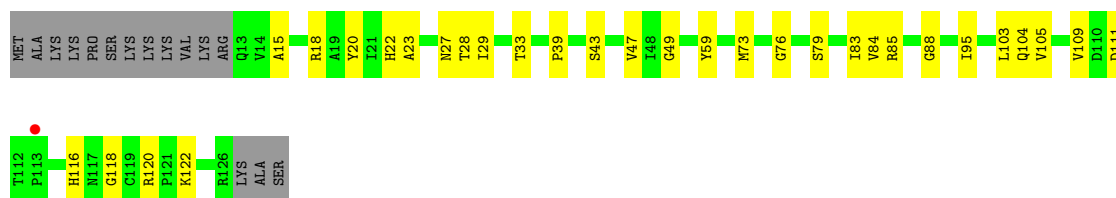


- Molecule 42: 30S ribosomal protein S11

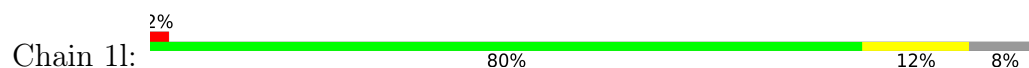


- Molecule 42: 30S ribosomal protein S11

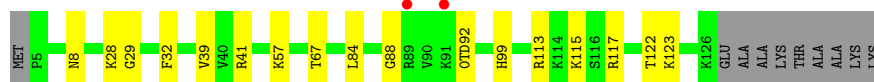
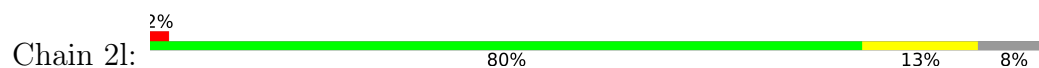




- Molecule 43: 30S ribosomal protein S12



- Molecule 43: 30S ribosomal protein S12



- Molecule 44: 30S ribosomal protein S13



- Molecule 44: 30S ribosomal protein S13



- Molecule 45: 30S ribosomal protein S14 type Z

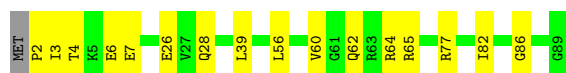
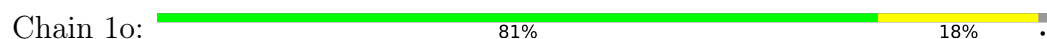




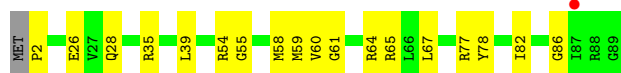
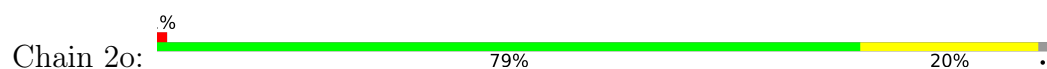
- Molecule 45: 30S ribosomal protein S14 type Z



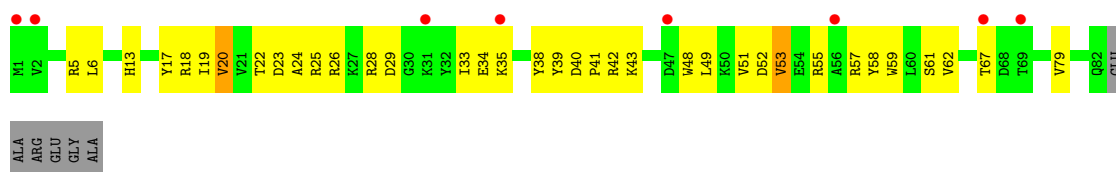
- Molecule 46: 30S ribosomal protein S15



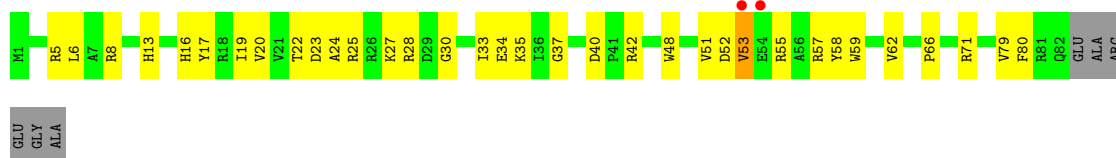
- Molecule 46: 30S ribosomal protein S15



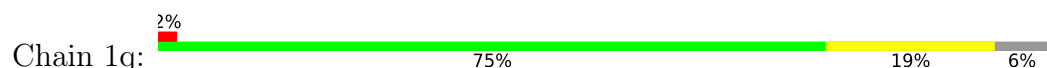
- Molecule 47: 30S ribosomal protein S16

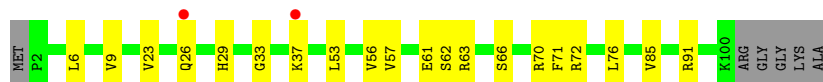


- Molecule 47: 30S ribosomal protein S16

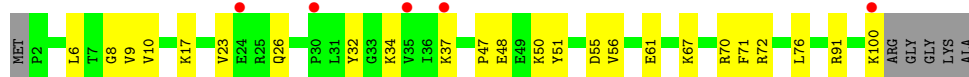
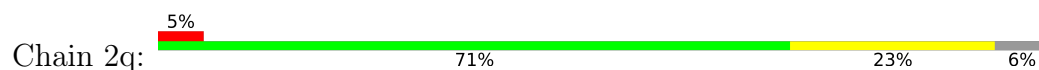


- Molecule 48: 30S ribosomal protein S17





- Molecule 48: 30S ribosomal protein S17



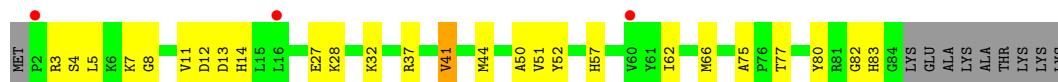
- Molecule 49: 30S ribosomal protein S18



- Molecule 49: 30S ribosomal protein S18



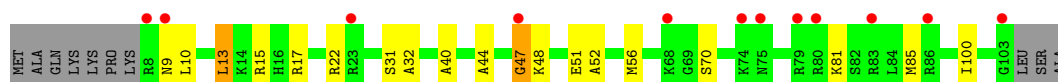
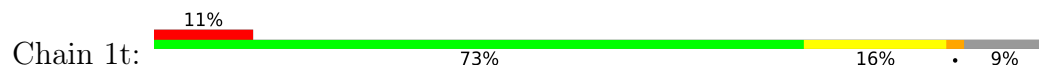
- Molecule 50: 30S Ribosomal Protein S19



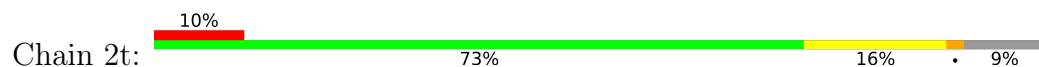
- Molecule 50: 30S Ribosomal Protein S19



- Molecule 51: 30S Ribosomal Protein S20

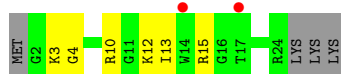


- Molecule 51: 30S Ribosomal Protein S20





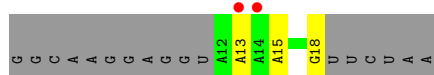
- Molecule 52: 30S ribosomal protein Thx



- Molecule 52: 30S ribosomal protein Thx



- Molecule 53: mRNA



- Molecule 53: mRNA



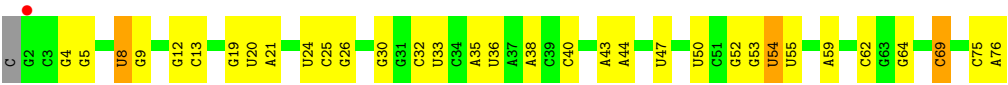
- Molecule 54: ACCA-DPhe



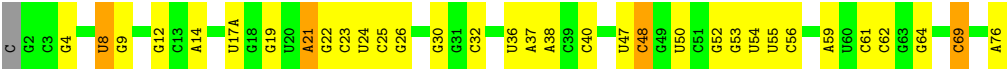
- Molecule 54: ACCA-DPhe



- Molecule 55: P-site tRNA, Deacylated Initiator Methionyl-tRNA



● Molecule 55: P-site tRNA, Deacylated Initiator Methionyl-tRNA



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	211.39Å 452.15Å 617.64Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	255.01 – 3.70 255.01 – 3.70	Depositor EDS
% Data completeness (in resolution range)	98.5 (255.01-3.70) 98.5 (255.01-3.70)	Depositor EDS
R_{merge}	0.18	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.26 (at 3.68Å)	Xtriage
Refinement program	PHENIX 1.8.2	Depositor
R, R_{free}	0.236 , 0.279 0.237 , 0.280	Depositor DCC
R_{free} test set	30953 reflections (4.96%)	wwPDB-VP
Wilson B-factor (Å ²)	123.6	Xtriage
Anisotropy	0.051	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 114.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.43$, $\langle L^2 \rangle = 0.25$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.86	EDS
Total number of atoms	288175	wwPDB-VP
Average B, all atoms (Å ²)	103.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.69% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: 7MG, SF4, 0TD, PSU, 2MU, UR3, KGV, OMG, MG, 4SU, 2MG, MA6, 4OC, 5MC, 5MU, ZN, 2MA, M2G

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	1A	0.21	0/69009	0.33	0/107712
1	2A	0.18	0/67293	0.32	0/105034
2	1B	0.15	0/2882	0.28	0/4494
2	2B	0.15	0/2879	0.27	0/4487
3	1D	0.25	1/2186 (0.0%)	0.41	0/2944
3	2D	0.25	1/2186 (0.0%)	0.41	0/2944
4	1E	0.18	0/1592	0.41	0/2149
4	2E	0.20	0/1592	0.40	0/2149
5	1F	0.20	0/1619	0.39	0/2193
5	2F	0.18	0/1615	0.38	0/2188
6	1G	0.18	0/1448	0.39	0/1957
6	2G	0.18	0/1453	0.39	0/1963
7	1H	0.21	0/1356	0.37	0/1834
7	2H	0.19	0/1356	0.36	0/1834
8	1I	0.18	0/1112	0.38	0/1514
8	2I	0.19	0/1079	0.34	0/1475
9	1N	0.18	0/1144	0.38	0/1543
9	2N	0.16	0/1144	0.35	0/1543
10	1O	0.20	0/943	0.37	0/1269
10	2O	0.24	0/943	0.43	1/1269 (0.1%)
11	1P	0.21	0/1152	0.44	0/1533
11	2P	0.20	0/1152	0.51	1/1533 (0.1%)
12	1Q	0.19	0/1143	0.38	0/1527
12	2Q	0.17	0/1143	0.37	0/1527
13	1R	0.18	0/982	0.42	0/1312
13	2R	0.21	0/982	0.40	0/1312
14	1S	0.18	0/883	0.39	0/1176
14	2S	0.17	0/880	0.37	0/1172
15	1T	0.17	0/1105	0.39	0/1477
15	2T	0.19	0/1097	0.40	0/1468
16	1U	0.20	0/977	0.38	0/1301

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
16	2U	0.18	0/977	0.35	0/1301
17	1V	0.18	0/782	0.36	0/1049
17	2V	0.17	0/782	0.36	0/1049
18	1W	0.20	0/897	0.38	0/1205
18	2W	0.20	0/897	0.40	0/1205
19	1X	0.20	0/764	0.42	0/1025
19	2X	0.18	0/764	0.37	0/1025
20	1Y	0.20	0/819	0.38	0/1095
20	2Y	0.18	0/819	0.35	0/1095
21	1Z	0.17	0/1267	0.41	0/1717
21	2Z	0.18	0/1299	0.39	0/1763
22	10	0.19	0/662	0.40	0/881
22	20	0.17	0/662	0.38	0/881
23	11	0.21	0/762	0.39	0/1014
23	21	0.19	0/762	0.37	0/1014
24	12	0.25	0/590	0.40	0/781
24	22	0.18	0/590	0.36	0/781
25	13	0.25	0/474	0.47	0/635
25	23	0.21	0/469	0.43	0/630
26	14	0.30	0/565	0.63	0/761
26	24	0.24	0/545	0.51	0/737
27	15	0.21	0/469	0.41	0/635
27	25	0.19	0/469	0.38	0/635
28	16	0.20	0/460	0.40	0/613
28	26	0.16	0/456	0.39	0/608
29	17	0.26	0/426	0.46	0/561
29	27	0.21	0/426	0.44	0/561
30	18	0.20	0/525	0.37	0/691
30	28	0.18	0/525	0.36	0/691
31	19	0.21	0/310	0.45	0/407
31	29	0.19	0/310	0.41	0/407
32	1a	0.17	0/35795	0.31	0/55864
32	2a	0.17	0/35886	0.31	0/56005
33	1b	0.20	0/1881	0.41	0/2542
33	2b	0.21	0/1860	0.40	0/2518
34	1c	0.18	0/1572	0.35	0/2126
34	2c	0.18	0/1566	0.36	0/2119
35	1d	0.18	0/1685	0.40	0/2262
35	2d	0.18	0/1704	0.39	0/2284
36	1e	0.18	0/1145	0.41	0/1543
36	2e	0.18	0/1149	0.41	0/1548
37	1f	0.16	0/823	0.37	0/1115
37	2f	0.17	0/829	0.36	0/1123

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
38	1g	0.23	0/1250	0.38	0/1679
38	2g	0.22	0/1254	0.37	0/1683
39	1h	0.18	0/1108	0.38	0/1494
39	2h	0.16	0/1108	0.37	0/1494
40	1i	0.21	0/1002	0.46	0/1346
40	2i	0.25	0/997	0.44	0/1343
41	1j	0.19	0/722	0.40	0/982
41	2j	0.19	0/727	0.40	0/988
42	1k	0.16	0/844	0.34	0/1145
42	2k	0.18	0/848	0.34	0/1149
43	1l	0.17	0/937	0.38	0/1260
43	2l	0.18	0/937	0.41	0/1260
44	1m	0.18	0/969	0.39	0/1302
44	2m	0.18	0/961	0.39	0/1291
45	1n	0.17	0/501	0.40	0/664
45	2n	0.18	0/501	0.39	0/664
46	1o	0.16	0/739	0.35	0/985
46	2o	0.17	0/739	0.34	0/985
47	1p	0.17	0/697	0.38	0/939
47	2p	0.18	0/693	0.40	0/935
48	1q	0.17	0/836	0.36	0/1117
48	2q	0.16	0/836	0.35	0/1117
49	1r	0.16	0/560	0.33	0/746
49	2r	0.20	0/560	0.35	0/746
50	1s	0.21	0/667	0.40	0/900
50	2s	0.19	0/661	0.43	0/893
51	1t	0.23	0/730	0.42	0/965
51	2t	0.25	0/729	0.42	0/965
52	1u	0.19	0/203	0.39	0/266
52	2u	0.21	0/203	0.41	0/266
53	1v	0.22	0/172	0.25	0/266
53	2v	0.15	0/126	0.29	0/195
54	1w	0.24	0/45	0.38	0/68
54	2w	0.20	0/45	0.41	0/68
55	1x	0.22	0/1725	0.33	0/2689
55	2x	0.22	1/1725 (0.1%)	0.31	0/2689
All	All	0.19	3/310103 (0.0%)	0.34	2/463879 (0.0%)

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
21	1Z	0	1
21	2Z	0	1
33	2b	0	1
All	All	0	3

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	2D	7	LYS	C-N	-7.89	1.15	1.33
3	1D	7	LYS	C-N	-5.15	1.21	1.33
55	2x	8	4SU	O3'-P	5.05	1.61	1.56

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	2O	73	ASP	N-CA-C	-5.84	106.13	113.20
11	2P	26	GLY	N-CA-C	-5.67	107.92	115.40

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
21	1Z	159	PRO	Peptide
21	2Z	159	PRO	Peptide
33	2b	8	LYS	Peptide

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	1A	61852	0	31192	879	0
1	2A	60322	0	30424	817	0
2	1B	2577	0	1305	35	0
2	2B	2575	0	1303	46	0
3	1D	2136	0	2218	62	0
3	2D	2136	0	2218	77	0
4	1E	1559	0	1618	36	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	2E	1559	0	1618	46	0
5	1F	1584	0	1625	52	0
5	2F	1580	0	1619	40	0
6	1G	1423	0	1436	38	0
6	2G	1428	0	1438	25	0
7	1H	1330	0	1407	32	0
7	2H	1330	0	1407	28	0
8	1I	1097	0	1140	30	0
8	2I	1064	0	1082	23	0
9	1N	1117	0	1184	29	0
9	2N	1117	0	1184	28	0
10	1O	933	0	996	30	0
10	2O	933	0	996	29	0
11	1P	1135	0	1212	42	0
11	2P	1135	0	1212	39	0
12	1Q	1122	0	1179	30	0
12	2Q	1122	0	1179	25	0
13	1R	968	0	1033	15	0
13	2R	968	0	1033	24	0
14	1S	873	0	927	21	0
14	2S	870	0	923	22	0
15	1T	1091	0	1150	25	0
15	2T	1083	0	1136	23	0
16	1U	959	0	1019	24	0
16	2U	959	0	1019	23	0
17	1V	771	0	830	9	0
17	2V	771	0	830	15	0
18	1W	886	0	940	9	0
18	2W	886	0	940	13	0
19	1X	750	0	814	11	0
19	2X	750	0	814	11	0
20	1Y	806	0	881	19	0
20	2Y	806	0	881	21	0
21	1Z	1240	0	1240	26	0
21	2Z	1271	0	1273	25	0
22	10	653	0	674	20	0
22	20	653	0	674	20	0
23	11	755	0	826	16	0
23	21	755	0	826	19	0
24	12	588	0	643	12	0
24	22	588	0	643	7	0
25	13	469	0	518	10	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
25	23	464	0	514	7	0
26	14	552	0	533	25	0
26	24	532	0	503	22	0
27	15	455	0	465	10	0
27	25	455	0	465	10	0
28	16	453	0	473	7	0
28	26	449	0	469	7	0
29	17	418	0	467	11	0
29	27	418	0	467	13	0
30	18	517	0	582	19	0
30	28	517	0	582	19	0
31	19	307	0	335	5	0
31	29	307	0	335	7	0
32	1a	32246	0	16296	595	0
32	2a	32327	0	16339	558	0
33	1b	1846	0	1867	61	0
33	2b	1825	0	1828	61	0
34	1c	1548	0	1535	33	0
34	2c	1542	0	1517	40	0
35	1d	1655	0	1672	60	0
35	2d	1674	0	1714	53	0
36	1e	1129	0	1185	35	0
36	2e	1133	0	1191	38	0
37	1f	810	0	804	18	0
37	2f	816	0	808	28	0
38	1g	1231	0	1238	28	0
38	2g	1235	0	1249	26	0
39	1h	1088	0	1126	36	0
39	2h	1088	0	1126	32	0
40	1i	983	0	986	41	0
40	2i	978	0	966	36	0
41	1j	709	0	650	24	0
41	2j	714	0	672	25	0
42	1k	829	0	825	19	0
42	2k	833	0	836	18	0
43	1l	932	0	981	12	0
43	2l	932	0	981	12	0
44	1m	958	0	1002	35	0
44	2m	950	0	988	32	0
45	1n	492	0	529	22	0
45	2n	492	0	529	20	0
46	1o	728	0	760	12	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
46	2o	728	0	760	14	0
47	1p	681	0	697	24	0
47	2p	677	0	686	22	0
48	1q	823	0	891	12	0
48	2q	823	0	891	16	0
49	1r	555	0	618	12	0
49	2r	555	0	618	17	0
50	1s	652	0	662	20	0
50	2s	646	0	644	21	0
51	1t	728	0	798	17	0
51	2t	727	0	796	13	0
52	1u	199	0	208	5	0
52	2u	199	0	208	10	0
53	1v	153	0	77	2	0
53	2v	113	0	54	0	0
54	1w	75	0	22	4	0
54	2w	75	0	22	2	0
55	1x	1625	0	829	23	0
55	2x	1625	0	829	24	0
56	10	4	0	0	0	0
56	15	1	0	0	0	0
56	16	1	0	0	0	0
56	17	2	0	0	0	0
56	18	2	0	0	0	0
56	19	1	0	0	0	0
56	1A	548	0	0	0	0
56	1B	19	0	0	0	0
56	1D	4	0	0	0	0
56	1E	4	0	0	0	0
56	1F	2	0	0	0	0
56	1G	1	0	0	0	0
56	1H	1	0	0	0	0
56	1P	2	0	0	0	0
56	1Q	2	0	0	0	0
56	1R	2	0	0	0	0
56	1T	3	0	0	0	0
56	1V	3	0	0	0	0
56	1W	1	0	0	0	0
56	1X	1	0	0	0	0
56	1Y	1	0	0	0	0
56	1Z	1	0	0	0	0
56	1a	89	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
56	1d	1	0	0	0	0
56	1e	1	0	0	0	0
56	1l	1	0	0	0	0
56	1r	1	0	0	0	0
56	1t	1	0	0	0	0
56	1v	1	0	0	0	0
56	1x	9	0	0	0	0
56	20	1	0	0	0	0
56	21	1	0	0	0	0
56	23	1	0	0	0	0
56	25	1	0	0	0	0
56	27	1	0	0	0	0
56	28	2	0	0	0	0
56	2A	474	0	0	0	0
56	2B	10	0	0	0	0
56	2D	3	0	0	0	0
56	2E	5	0	0	0	0
56	2F	1	0	0	0	0
56	2O	1	0	0	0	0
56	2Q	1	0	0	0	0
56	2R	2	0	0	0	0
56	2W	1	0	0	0	0
56	2Z	1	0	0	0	0
56	2a	113	0	0	0	0
56	2c	1	0	0	0	0
56	2d	1	0	0	0	0
56	2f	2	0	0	0	0
56	2l	2	0	0	0	0
56	2n	1	0	0	0	0
56	2q	1	0	0	0	0
56	2r	1	0	0	0	0
56	2x	1	0	0	0	0
57	14	1	0	0	0	0
57	15	1	0	0	0	0
57	16	1	0	0	0	0
57	19	1	0	0	0	0
57	1Y	1	0	0	0	0
57	1n	1	0	0	0	0
57	24	1	0	0	0	0
57	25	1	0	0	0	0
57	26	1	0	0	0	0
57	29	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
57	2Y	1	0	0	0	0
57	2n	1	0	0	0	0
58	1d	8	0	0	3	0
58	2d	8	0	0	2	0
59	10	1	0	0	0	0
59	1A	145	0	0	12	0
59	1B	6	0	0	0	0
59	1D	4	0	0	2	0
59	1F	2	0	0	0	0
59	1O	1	0	0	0	0
59	1X	1	0	0	0	0
59	1a	12	0	0	1	0
59	2A	44	0	0	5	0
59	2E	1	0	0	0	0
59	2a	30	0	0	2	0
All	All	288175	0	193379	4547	0

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 10.

The worst 5 of 4547 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)
1:1A:1100:A:N6	1:1A:1151:U:H3	1.51	1.06
32:1a:931:C:N4	32:1a:1386:G:H1	1.54	1.03
55:1x:4:G:H1	55:1x:69:C:H42	1.01	1.01
32:1a:1162:C:H42	32:1a:1174:G:H1	0.99	0.98
32:1a:927:G:H1	32:1a:1390:U:H3	1.11	0.98

There are no symmetry-related clashes.

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	
3	1D	273/276 (99%)	262 (96%)	11 (4%)	0	100	100
3	2D	273/276 (99%)	265 (97%)	8 (3%)	0	100	100
4	1E	202/206 (98%)	194 (96%)	7 (4%)	1 (0%)	24	56
4	2E	202/206 (98%)	190 (94%)	11 (5%)	1 (0%)	24	56
5	1F	201/210 (96%)	194 (96%)	5 (2%)	2 (1%)	12	43
5	2F	201/210 (96%)	194 (96%)	5 (2%)	2 (1%)	12	43
6	1G	179/182 (98%)	165 (92%)	13 (7%)	1 (1%)	21	52
6	2G	179/182 (98%)	170 (95%)	6 (3%)	3 (2%)	7	34
7	1H	172/180 (96%)	162 (94%)	9 (5%)	1 (1%)	21	52
7	2H	172/180 (96%)	168 (98%)	3 (2%)	1 (1%)	21	52
8	1I	144/148 (97%)	130 (90%)	13 (9%)	1 (1%)	18	50
8	2I	144/148 (97%)	130 (90%)	13 (9%)	1 (1%)	18	50
9	1N	138/140 (99%)	132 (96%)	6 (4%)	0	100	100
9	2N	138/140 (99%)	132 (96%)	5 (4%)	1 (1%)	18	50
10	1O	120/122 (98%)	113 (94%)	7 (6%)	0	100	100
10	2O	120/122 (98%)	112 (93%)	8 (7%)	0	100	100
11	1P	147/150 (98%)	137 (93%)	6 (4%)	4 (3%)	4	27
11	2P	147/150 (98%)	137 (93%)	8 (5%)	2 (1%)	9	37
12	1Q	139/141 (99%)	133 (96%)	6 (4%)	0	100	100
12	2Q	139/141 (99%)	132 (95%)	7 (5%)	0	100	100
13	1R	116/118 (98%)	110 (95%)	5 (4%)	1 (1%)	14	45
13	2R	116/118 (98%)	111 (96%)	5 (4%)	0	100	100
14	1S	108/112 (96%)	103 (95%)	5 (5%)	0	100	100
14	2S	108/112 (96%)	104 (96%)	3 (3%)	1 (1%)	14	45
15	1T	129/146 (88%)	125 (97%)	4 (3%)	0	100	100
15	2T	129/146 (88%)	122 (95%)	7 (5%)	0	100	100
16	1U	114/118 (97%)	112 (98%)	2 (2%)	0	100	100
16	2U	114/118 (97%)	114 (100%)	0	0	100	100
17	1V	99/101 (98%)	91 (92%)	7 (7%)	1 (1%)	12	43
17	2V	99/101 (98%)	94 (95%)	3 (3%)	2 (2%)	6	32
18	1W	110/113 (97%)	107 (97%)	3 (3%)	0	100	100
18	2W	110/113 (97%)	107 (97%)	3 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
19	1X	93/96 (97%)	90 (97%)	3 (3%)	0	100	100
19	2X	93/96 (97%)	89 (96%)	4 (4%)	0	100	100
20	1Y	105/110 (96%)	100 (95%)	5 (5%)	0	100	100
20	2Y	105/110 (96%)	99 (94%)	6 (6%)	0	100	100
21	1Z	148/206 (72%)	134 (90%)	13 (9%)	1 (1%)	18	50
21	2Z	156/206 (76%)	142 (91%)	12 (8%)	2 (1%)	9	38
22	10	81/85 (95%)	77 (95%)	3 (4%)	1 (1%)	10	40
22	20	81/85 (95%)	76 (94%)	5 (6%)	0	100	100
23	11	95/98 (97%)	93 (98%)	1 (1%)	1 (1%)	11	42
23	21	95/98 (97%)	93 (98%)	1 (1%)	1 (1%)	11	42
24	12	68/72 (94%)	68 (100%)	0	0	100	100
24	22	68/72 (94%)	68 (100%)	0	0	100	100
25	13	57/60 (95%)	54 (95%)	3 (5%)	0	100	100
25	23	57/60 (95%)	55 (96%)	2 (4%)	0	100	100
26	14	67/71 (94%)	51 (76%)	12 (18%)	4 (6%)	1	15
26	24	67/71 (94%)	51 (76%)	10 (15%)	6 (9%)	0	8
27	15	57/60 (95%)	53 (93%)	4 (7%)	0	100	100
27	25	57/60 (95%)	52 (91%)	5 (9%)	0	100	100
28	16	51/54 (94%)	46 (90%)	5 (10%)	0	100	100
28	26	51/54 (94%)	50 (98%)	1 (2%)	0	100	100
29	17	46/49 (94%)	46 (100%)	0	0	100	100
29	27	46/49 (94%)	46 (100%)	0	0	100	100
30	18	62/65 (95%)	60 (97%)	2 (3%)	0	100	100
30	28	62/65 (95%)	62 (100%)	0	0	100	100
31	19	35/37 (95%)	34 (97%)	1 (3%)	0	100	100
31	29	35/37 (95%)	34 (97%)	1 (3%)	0	100	100
33	1b	229/256 (90%)	204 (89%)	21 (9%)	4 (2%)	7	34
33	2b	229/256 (90%)	207 (90%)	18 (8%)	4 (2%)	7	34
34	1c	204/239 (85%)	190 (93%)	14 (7%)	0	100	100
34	2c	204/239 (85%)	189 (93%)	15 (7%)	0	100	100
35	1d	206/209 (99%)	200 (97%)	5 (2%)	1 (0%)	24	56

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
35	2d	206/209 (99%)	200 (97%)	5 (2%)	1 (0%)	24	56
36	1e	146/162 (90%)	138 (94%)	8 (6%)	0	100	100
36	2e	146/162 (90%)	139 (95%)	7 (5%)	0	100	100
37	1f	98/101 (97%)	95 (97%)	3 (3%)	0	100	100
37	2f	98/101 (97%)	94 (96%)	4 (4%)	0	100	100
38	1g	153/156 (98%)	142 (93%)	8 (5%)	3 (2%)	6	32
38	2g	153/156 (98%)	141 (92%)	10 (6%)	2 (1%)	9	38
39	1h	135/138 (98%)	129 (96%)	6 (4%)	0	100	100
39	2h	135/138 (98%)	131 (97%)	4 (3%)	0	100	100
40	1i	125/128 (98%)	117 (94%)	7 (6%)	1 (1%)	16	48
40	2i	125/128 (98%)	116 (93%)	9 (7%)	0	100	100
41	1j	95/105 (90%)	87 (92%)	7 (7%)	1 (1%)	11	42
41	2j	94/105 (90%)	85 (90%)	8 (8%)	1 (1%)	11	42
42	1k	112/129 (87%)	104 (93%)	7 (6%)	1 (1%)	14	45
42	2k	112/129 (87%)	104 (93%)	6 (5%)	2 (2%)	6	34
43	1l	119/132 (90%)	112 (94%)	7 (6%)	0	100	100
43	2l	119/132 (90%)	112 (94%)	7 (6%)	0	100	100
44	1m	121/126 (96%)	114 (94%)	6 (5%)	1 (1%)	16	48
44	2m	120/126 (95%)	114 (95%)	6 (5%)	0	100	100
45	1n	58/61 (95%)	56 (97%)	2 (3%)	0	100	100
45	2n	58/61 (95%)	58 (100%)	0	0	100	100
46	1o	86/89 (97%)	81 (94%)	4 (5%)	1 (1%)	10	40
46	2o	86/89 (97%)	83 (96%)	3 (4%)	0	100	100
47	1p	80/88 (91%)	72 (90%)	7 (9%)	1 (1%)	9	38
47	2p	80/88 (91%)	74 (92%)	5 (6%)	1 (1%)	9	38
48	1q	97/105 (92%)	94 (97%)	3 (3%)	0	100	100
48	2q	97/105 (92%)	90 (93%)	7 (7%)	0	100	100
49	1r	66/88 (75%)	65 (98%)	1 (2%)	0	100	100
49	2r	66/88 (75%)	65 (98%)	1 (2%)	0	100	100
50	1s	81/93 (87%)	74 (91%)	7 (9%)	0	100	100
50	2s	81/93 (87%)	75 (93%)	5 (6%)	1 (1%)	10	40

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
51	1t	94/106 (89%)	86 (92%)	6 (6%)	2 (2%)	5	31
51	2t	94/106 (89%)	83 (88%)	8 (8%)	3 (3%)	3	25
52	1u	21/27 (78%)	21 (100%)	0	0	100	100
52	2u	21/27 (78%)	20 (95%)	1 (5%)	0	100	100
All	All	11370/12128 (94%)	10736 (94%)	561 (5%)	73 (1%)	21	52

5 of 73 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
6	1G	47	LYS
21	1Z	2	GLU
23	11	3	LYS
26	14	46	GLN
26	14	57	GLU

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	
3	1D	215/218 (99%)	214 (100%)	1 (0%)	81	80
3	2D	215/218 (99%)	214 (100%)	1 (0%)	81	80
4	1E	164/166 (99%)	163 (99%)	1 (1%)	78	79
4	2E	164/166 (99%)	162 (99%)	2 (1%)	63	72
5	1F	160/166 (96%)	160 (100%)	0	100	100
5	2F	159/166 (96%)	158 (99%)	1 (1%)	78	79
6	1G	143/156 (92%)	138 (96%)	5 (4%)	32	54
6	2G	143/156 (92%)	141 (99%)	2 (1%)	59	70
7	1H	144/148 (97%)	143 (99%)	1 (1%)	76	77
7	2H	144/148 (97%)	142 (99%)	2 (1%)	59	70
8	1I	113/124 (91%)	112 (99%)	1 (1%)	70	75
8	2I	105/124 (85%)	103 (98%)	2 (2%)	50	65

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
9	1N	118/119 (99%)	117 (99%)	1 (1%)	73	76
9	2N	118/119 (99%)	117 (99%)	1 (1%)	73	76
10	1O	100/100 (100%)	100 (100%)	0	100	100
10	2O	100/100 (100%)	100 (100%)	0	100	100
11	1P	115/116 (99%)	114 (99%)	1 (1%)	70	75
11	2P	115/116 (99%)	114 (99%)	1 (1%)	70	75
12	1Q	111/111 (100%)	110 (99%)	1 (1%)	70	75
12	2Q	111/111 (100%)	111 (100%)	0	100	100
13	1R	101/101 (100%)	100 (99%)	1 (1%)	68	74
13	2R	101/101 (100%)	100 (99%)	1 (1%)	68	74
14	1S	86/88 (98%)	86 (100%)	0	100	100
14	2S	85/88 (97%)	85 (100%)	0	100	100
15	1T	115/127 (91%)	115 (100%)	0	100	100
15	2T	113/127 (89%)	113 (100%)	0	100	100
16	1U	93/94 (99%)	93 (100%)	0	100	100
16	2U	93/94 (99%)	92 (99%)	1 (1%)	65	73
17	1V	80/82 (98%)	78 (98%)	2 (2%)	42	61
17	2V	80/82 (98%)	78 (98%)	2 (2%)	42	61
18	1W	90/92 (98%)	89 (99%)	1 (1%)	65	73
18	2W	90/92 (98%)	90 (100%)	0	100	100
19	1X	77/78 (99%)	77 (100%)	0	100	100
19	2X	77/78 (99%)	77 (100%)	0	100	100
20	1Y	85/91 (93%)	83 (98%)	2 (2%)	43	61
20	2Y	85/91 (93%)	84 (99%)	1 (1%)	63	72
21	1Z	135/179 (75%)	135 (100%)	0	100	100
21	2Z	137/179 (76%)	137 (100%)	0	100	100
22	10	65/67 (97%)	65 (100%)	0	100	100
22	20	65/67 (97%)	65 (100%)	0	100	100
23	11	80/83 (96%)	79 (99%)	1 (1%)	61	71
23	21	80/83 (96%)	80 (100%)	0	100	100
24	12	65/67 (97%)	65 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
24	22	65/67 (97%)	65 (100%)	0	100	100
25	13	51/52 (98%)	51 (100%)	0	100	100
25	23	50/52 (96%)	50 (100%)	0	100	100
26	14	59/63 (94%)	57 (97%)	2 (3%)	32	55
26	24	53/63 (84%)	52 (98%)	1 (2%)	50	65
27	15	50/52 (96%)	49 (98%)	1 (2%)	48	64
27	25	50/52 (96%)	49 (98%)	1 (2%)	48	64
28	16	51/52 (98%)	51 (100%)	0	100	100
28	26	50/52 (96%)	50 (100%)	0	100	100
29	17	41/42 (98%)	41 (100%)	0	100	100
29	27	41/42 (98%)	41 (100%)	0	100	100
30	18	54/55 (98%)	54 (100%)	0	100	100
30	28	54/55 (98%)	54 (100%)	0	100	100
31	19	34/34 (100%)	34 (100%)	0	100	100
31	29	34/34 (100%)	34 (100%)	0	100	100
33	1b	192/220 (87%)	191 (100%)	1 (0%)	81	80
33	2b	187/220 (85%)	183 (98%)	4 (2%)	47	64
34	1c	142/188 (76%)	139 (98%)	3 (2%)	47	64
34	2c	140/188 (74%)	138 (99%)	2 (1%)	59	70
35	1d	169/181 (93%)	166 (98%)	3 (2%)	51	67
35	2d	173/181 (96%)	170 (98%)	3 (2%)	53	67
36	1e	113/123 (92%)	112 (99%)	1 (1%)	70	75
36	2e	114/123 (93%)	113 (99%)	1 (1%)	70	75
37	1f	84/90 (93%)	83 (99%)	1 (1%)	63	72
37	2f	85/90 (94%)	85 (100%)	0	100	100
38	1g	119/127 (94%)	118 (99%)	1 (1%)	73	76
38	2g	120/127 (94%)	120 (100%)	0	100	100
39	1h	114/119 (96%)	113 (99%)	1 (1%)	70	75
39	2h	114/119 (96%)	113 (99%)	1 (1%)	70	75
40	1i	90/99 (91%)	90 (100%)	0	100	100
40	2i	89/99 (90%)	89 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
41	1j	66/92 (72%)	66 (100%)	0	100	100
41	2j	69/92 (75%)	68 (99%)	1 (1%)	59	70
42	1k	82/99 (83%)	82 (100%)	0	100	100
42	2k	83/99 (84%)	83 (100%)	0	100	100
43	1l	96/108 (89%)	96 (100%)	0	100	100
43	2l	96/108 (89%)	96 (100%)	0	100	100
44	1m	93/101 (92%)	93 (100%)	0	100	100
44	2m	92/101 (91%)	91 (99%)	1 (1%)	65	73
45	1n	49/50 (98%)	48 (98%)	1 (2%)	48	64
45	2n	49/50 (98%)	48 (98%)	1 (2%)	48	64
46	1o	78/80 (98%)	78 (100%)	0	100	100
46	2o	78/80 (98%)	78 (100%)	0	100	100
47	1p	69/74 (93%)	68 (99%)	1 (1%)	59	70
47	2p	68/74 (92%)	68 (100%)	0	100	100
48	1q	94/97 (97%)	94 (100%)	0	100	100
48	2q	94/97 (97%)	94 (100%)	0	100	100
49	1r	59/77 (77%)	58 (98%)	1 (2%)	53	67
49	2r	59/77 (77%)	59 (100%)	0	100	100
50	1s	69/80 (86%)	67 (97%)	2 (3%)	37	57
50	2s	67/80 (84%)	66 (98%)	1 (2%)	57	68
51	1t	70/82 (85%)	69 (99%)	1 (1%)	59	70
51	2t	70/82 (85%)	69 (99%)	1 (1%)	59	70
52	1u	18/22 (82%)	18 (100%)	0	100	100
52	2u	18/22 (82%)	18 (100%)	0	100	100
All	All	9303/10064 (92%)	9229 (99%)	74 (1%)	73	76

5 of 74 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
27	25	6	VAL
45	2n	33	VAL
33	2b	124	SER
35	2d	135	LEU
34	1c	49	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 99 such sidechains are listed below:

Mol	Chain	Res	Type
6	2G	58	GLN
24	22	46	GLN
10	2O	3	GLN
17	2V	64	HIS
33	2b	78	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	1A	2865/2915 (98%)	421 (14%)	24 (0%)
1	2A	2791/2915 (95%)	440 (15%)	19 (0%)
2	1B	120/121 (99%)	10 (8%)	1 (0%)
2	2B	119/121 (98%)	12 (10%)	1 (0%)
32	1a	1497/1521 (98%)	240 (16%)	0
32	2a	1501/1521 (98%)	244 (16%)	0
53	1v	6/24 (25%)	1 (16%)	0
53	2v	4/24 (16%)	0	0
54	1w	1/4 (25%)	1 (100%)	0
54	2w	1/4 (25%)	1 (100%)	0
55	1x	75/77 (97%)	6 (8%)	0
55	2x	75/77 (97%)	9 (12%)	0
All	All	9055/9324 (97%)	1385 (15%)	45 (0%)

5 of 1385 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	1A	12	U
1	1A	14	A
1	1A	15	G
1	1A	34	C
1	1A	45	C

5 of 45 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	2A	277	C
1	2A	1442	G
1	2A	528	A
1	2A	900	A
1	2A	1653	G

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

58 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
1	5MU	2A	1939	1	19,22,23	1.36	4 (21%)	27,32,35	2.12	6 (22%)
32	7MG	2a	527	32	23,26,27	1.35	3 (13%)	27,39,42	2.63	7 (25%)
32	5MC	2a	1400	32	19,22,23	1.74	3 (15%)	26,32,35	1.12	2 (7%)
1	5MC	1A	1984	1	19,22,23	1.62	3 (15%)	26,32,35	1.22	3 (11%)
43	0TD	1l	92	43	8,9,10	4.40	1 (12%)	6,11,13	8.02	2 (33%)
32	5MC	1a	1400	32	19,22,23	1.73	3 (15%)	26,32,35	1.12	2 (7%)
32	UR3	1a	1498	32	19,22,23	1.03	1 (5%)	26,32,35	1.73	3 (11%)
1	PSU	1A	1933	1	18,21,22	1.39	2 (11%)	21,30,33	1.97	4 (19%)
55	4SU	1x	8	55	18,21,22	1.98	5 (27%)	25,30,33	1.85	8 (32%)
32	4OC	1a	1402	32	20,23,24	0.76	0	25,32,35	0.86	1 (4%)
1	5MU	2A	1915	1	19,22,23	1.42	5 (26%)	27,32,35	2.02	6 (22%)
32	5MC	1a	967	32	19,22,23	1.67	2 (10%)	26,32,35	1.19	3 (11%)
1	5MC	2A	1942	1	19,22,23	1.74	3 (15%)	26,32,35	1.19	3 (11%)
1	4OC	2A	1920	1	19,22,24	0.79	0	25,31,35	0.82	0
55	5MC	1x	32	55	19,22,23	1.61	3 (15%)	26,32,35	1.20	3 (11%)
1	PSU	1A	1939	1	18,21,22	1.38	2 (11%)	21,30,33	2.03	3 (14%)
32	PSU	2a	516	32	18,21,22	1.35	2 (11%)	21,30,33	1.91	4 (19%)
55	PSU	2x	55	55	18,21,22	1.35	2 (11%)	21,30,33	2.05	4 (19%)
55	5MC	2x	32	55	19,22,23	1.66	3 (15%)	26,32,35	1.18	3 (11%)
32	7MG	1a	527	32	23,26,27	1.34	3 (13%)	27,39,42	2.60	6 (22%)
1	OMG	1A	2263	55,1	23,26,27	1.21	3 (13%)	32,38,41	2.10	8 (25%)
1	OMG	2A	2251	55,1	23,26,27	1.24	3 (13%)	32,38,41	2.12	7 (21%)
32	2MG	1a	1207	32	23,26,27	1.25	3 (13%)	33,38,41	2.11	6 (18%)
32	2MG	2a	1207	32	23,26,27	1.21	3 (13%)	33,38,41	2.26	10 (30%)
43	0TD	2l	92	43	8,9,10	4.44	1 (12%)	6,11,13	6.20	2 (33%)
32	M2G	1a	966	32	24,27,28	1.32	4 (16%)	33,40,43	1.90	6 (18%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
32	MA6	2a	1519	32	23,26,27	1.56	4 (17%)	33,38,41	2.38	13 (39%)
1	5MU	1A	1961	1	19,22,23	1.41	5 (26%)	27,32,35	2.26	6 (22%)
1	4OC	1A	1942	1	19,22,24	0.82	0	25,31,35	1.01	1 (4%)
32	5MC	2a	1407	32	19,22,23	1.67	2 (10%)	26,32,35	1.15	3 (11%)
32	4OC	2a	1402	32	20,23,24	0.80	0	25,32,35	0.92	0
32	MA6	1a	1519	32	23,26,27	1.52	4 (17%)	33,38,41	2.33	11 (33%)
1	5MC	2A	1962	1	19,22,23	1.58	3 (15%)	26,32,35	1.22	2 (7%)
32	UR3	2a	1498	32	19,22,23	1.05	2 (10%)	26,32,35	1.67	3 (11%)
55	4SU	2x	8	55	18,21,22	1.99	5 (27%)	25,30,33	1.62	7 (28%)
32	5MC	1a	1407	32	19,22,23	1.66	2 (10%)	26,32,35	1.16	3 (11%)
1	PSU	2A	1917	1	18,21,22	1.40	2 (11%)	21,30,33	2.01	3 (14%)
55	5MU	1x	54	55	19,22,23	1.44	6 (31%)	27,32,35	1.89	8 (29%)
32	5MC	2a	967	32	19,22,23	1.75	2 (10%)	26,32,35	1.07	2 (7%)
1	2MU	2A	2552	1	19,22,24	1.26	3 (15%)	25,31,36	1.97	6 (24%)
32	5MC	2a	1404	32	19,22,23	1.63	3 (15%)	26,32,35	1.14	3 (11%)
32	MA6	1a	1518	32	23,26,27	1.51	5 (21%)	33,38,41	2.30	13 (39%)
1	PSU	2A	2605	1	18,21,22	1.35	3 (16%)	21,30,33	1.94	4 (19%)
1	2MA	1A	2515	56,1	22,25,26	1.44	5 (22%)	32,37,40	2.31	7 (21%)
1	5MC	1A	1964	1	19,22,23	1.73	3 (15%)	26,32,35	1.13	3 (11%)
1	PSU	1A	2617	1	18,21,22	1.38	2 (11%)	21,30,33	1.99	4 (19%)
55	PSU	1x	55	55	18,21,22	1.36	2 (11%)	21,30,33	2.06	4 (19%)
54	KGV	1w	76	54	33,36,37	1.33	6 (18%)	41,51,54	1.74	8 (19%)
1	2MA	2A	2503	1	22,25,26	1.49	5 (22%)	32,37,40	2.35	7 (21%)
55	5MU	2x	54	55	19,22,23	1.44	6 (31%)	27,32,35	2.07	8 (29%)
1	5MU	1A	1937	1	19,22,23	1.46	4 (21%)	27,32,35	2.19	7 (25%)
32	5MC	1a	1404	32	19,22,23	1.65	3 (15%)	26,32,35	1.14	2 (7%)
54	KGV	2w	76	54,56	33,36,37	1.33	5 (15%)	41,51,54	1.87	9 (21%)
32	M2G	2a	966	32	24,27,28	1.31	4 (16%)	33,40,43	1.86	6 (18%)
32	MA6	2a	1518	32	23,26,27	1.54	5 (21%)	33,38,41	2.27	14 (42%)
32	PSU	1a	516	32	18,21,22	1.41	2 (11%)	21,30,33	1.92	4 (19%)
1	PSU	2A	1911	1	18,21,22	1.40	2 (11%)	21,30,33	2.08	3 (14%)
1	2MU	1A	2564	1	19,22,24	1.30	3 (15%)	25,31,36	1.79	5 (20%)

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
1	5MU	2A	1939	1	-	0/7/25/26	0/2/2/2
32	7MG	2a	527	32	-	0/7/37/38	0/3/3/3
32	5MC	2a	1400	32	-	2/7/25/26	0/2/2/2
1	5MC	1A	1984	1	-	0/7/25/26	0/2/2/2
43	0TD	1l	92	43	-	2/7/12/14	-
32	5MC	1a	1400	32	-	2/7/25/26	0/2/2/2
32	UR3	1a	1498	32	-	0/7/25/26	0/2/2/2
1	PSU	1A	1933	1	-	0/7/25/26	0/2/2/2
55	4SU	1x	8	55	-	0/7/25/26	0/2/2/2
32	4OC	1a	1402	32	-	2/9/29/30	0/2/2/2
1	5MU	2A	1915	1	-	0/7/25/26	0/2/2/2
32	5MC	1a	967	32	-	2/7/25/26	0/2/2/2
1	5MC	2A	1942	1	-	0/7/25/26	0/2/2/2
1	4OC	2A	1920	1	-	0/9/27/30	0/2/2/2
55	5MC	1x	32	55	-	0/7/25/26	0/2/2/2
1	PSU	1A	1939	1	-	0/7/25/26	0/2/2/2
32	PSU	2a	516	32	-	0/7/25/26	0/2/2/2
55	PSU	2x	55	55	-	0/7/25/26	0/2/2/2
55	5MC	2x	32	55	-	0/7/25/26	0/2/2/2
32	7MG	1a	527	32	-	2/7/37/38	0/3/3/3
1	OMG	1A	2263	55,1	-	0/9/27/28	0/3/3/3
1	OMG	2A	2251	55,1	-	0/9/27/28	0/3/3/3
32	2MG	1a	1207	32	-	0/9/27/28	0/3/3/3
32	2MG	2a	1207	32	-	0/9/27/28	0/3/3/3
43	0TD	2l	92	43	-	1/7/12/14	-
32	M2G	1a	966	32	-	0/11/29/30	0/3/3/3
32	MA6	2a	1519	32	-	4/11/29/30	0/3/3/3
1	5MU	1A	1961	1	-	0/7/25/26	0/2/2/2
1	4OC	1A	1942	1	-	0/9/27/30	0/2/2/2
32	5MC	2a	1407	32	-	0/7/25/26	0/2/2/2
32	4OC	2a	1402	32	-	2/9/29/30	0/2/2/2
32	MA6	1a	1519	32	-	4/11/29/30	0/3/3/3
1	5MC	2A	1962	1	-	0/7/25/26	0/2/2/2
32	UR3	2a	1498	32	-	0/7/25/26	0/2/2/2
55	4SU	2x	8	55	-	0/7/25/26	0/2/2/2
32	5MC	1a	1407	32	-	0/7/25/26	0/2/2/2
1	PSU	2A	1917	1	-	0/7/25/26	0/2/2/2
55	5MU	1x	54	55	-	0/7/25/26	0/2/2/2
32	5MC	2a	967	32	-	0/7/25/26	0/2/2/2
1	2MU	2A	2552	1	-	0/9/27/28	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
32	5MC	2a	1404	32	-	0/7/25/26	0/2/2/2
32	MA6	1a	1518	32	-	2/11/29/30	0/3/3/3
1	PSU	2A	2605	1	-	0/7/25/26	0/2/2/2
1	2MA	1A	2515	56,1	-	0/7/25/26	0/3/3/3
1	5MC	1A	1964	1	-	0/7/25/26	0/2/2/2
1	PSU	1A	2617	1	-	0/7/25/26	0/2/2/2
55	PSU	1x	55	55	-	0/7/25/26	0/2/2/2
54	KGV	1w	76	54	-	6/19/37/38	0/4/4/4
1	2MA	2A	2503	1	-	1/7/25/26	0/3/3/3
55	5MU	2x	54	55	-	0/7/25/26	0/2/2/2
1	5MU	1A	1937	1	-	0/7/25/26	0/2/2/2
32	5MC	1a	1404	32	-	0/7/25/26	0/2/2/2
54	KGV	2w	76	54,56	-	6/19/37/38	0/4/4/4
32	M2G	2a	966	32	-	3/11/29/30	0/3/3/3
32	MA6	2a	1518	32	-	1/11/29/30	0/3/3/3
32	PSU	1a	516	32	-	2/7/25/26	0/2/2/2
1	PSU	2A	1911	1	-	0/7/25/26	0/2/2/2
1	2MU	1A	2564	1	-	0/9/27/28	0/2/2/2

The worst 5 of 175 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
43	2l	92	0TD	CB-SB	-12.18	1.70	1.82
43	1l	92	0TD	CB-SB	-12.13	1.70	1.82
32	2a	1400	5MC	C5-C4	6.47	1.49	1.44
32	2a	967	5MC	C5-C4	6.43	1.49	1.44
32	1a	1400	5MC	C5-C4	6.38	1.48	1.44

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
43	1l	92	0TD	CSB-SB-CB	-19.35	67.58	102.36
43	2l	92	0TD	CSB-SB-CB	-14.82	75.73	102.36
32	2a	527	7MG	N9-C4-N3	9.01	138.67	125.46
32	1a	527	7MG	N9-C4-N3	8.98	138.62	125.46
1	2A	2503	2MA	C5-C4-N3	-8.41	118.33	127.18

There are no chirality outliers.

5 of 44 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
32	1a	516	PSU	C2'-C1'-C5-C4
32	1a	516	PSU	C2'-C1'-C5-C6
32	2a	1400	5MC	O4'-C4'-C5'-O5'
32	1a	1402	4OC	O4'-C4'-C5'-O5'
32	2a	1402	4OC	O4'-C4'-C5'-O5'

There are no ring outliers.

29 monomers are involved in 38 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	2A	1939	5MU	1	0
32	2a	1400	5MC	1	0
32	1a	1498	UR3	2	0
55	1x	8	4SU	1	0
32	1a	1402	4OC	1	0
32	1a	967	5MC	1	0
1	1A	2263	OMG	1	0
1	2A	2251	OMG	2	0
32	1a	1207	2MG	1	0
32	2a	1207	2MG	3	0
32	1a	966	M2G	1	0
32	2a	1519	MA6	1	0
32	2a	1402	4OC	2	0
32	1a	1519	MA6	2	0
1	2A	1962	5MC	1	0
55	2x	8	4SU	3	0
55	1x	54	5MU	2	0
32	2a	967	5MC	1	0
1	2A	2552	2MU	1	0
32	2a	1404	5MC	1	0
32	1a	1518	MA6	2	0
1	2A	2605	PSU	1	0
1	1A	2515	2MA	2	0
54	1w	76	KGV	1	0
1	1A	1937	5MU	1	0
32	2a	966	M2G	1	0
32	2a	1518	MA6	2	0
1	2A	1911	PSU	1	0
1	1A	2564	2MU	2	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 1353 ligands modelled in this entry, 1351 are monoatomic - leaving 2 for Mogul analysis.

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	$\# Z > 2$
58	SF4	1d	302	35	0,12,12	-	-	-		
58	SF4	2d	302	35	0,12,12	-	-	-		

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
58	SF4	1d	302	35	-	-	0/6/5/5
58	SF4	2d	302	35	-	-	0/6/5/5

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.

2 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
58	1d	302	SF4	3	0
58	2d	302	SF4	2	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
3	2D	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	2D	7:LYS	C	8:PRO	N	1.15

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	1A	2860/2915 (98%)	0.22	115 (4%) 42 27	74, 93, 132, 148	0
1	2A	2789/2915 (95%)	0.13	95 (3%) 48 30	81, 97, 127, 148	0
2	1B	120/121 (99%)	0.03	0 100 100	93, 111, 121, 125	0
2	2B	120/121 (99%)	0.02	0 100 100	102, 115, 123, 137	0
3	1D	275/276 (99%)	0.62	15 (5%) 30 20	76, 86, 97, 117	0
3	2D	275/276 (99%)	0.52	14 (5%) 33 22	79, 93, 105, 120	0
4	1E	204/206 (99%)	0.32	10 (4%) 35 23	78, 97, 111, 119	0
4	2E	204/206 (99%)	0.15	4 (1%) 65 41	80, 96, 107, 115	0
5	1F	203/210 (96%)	0.58	25 (12%) 8 10	72, 92, 109, 120	0
5	2F	203/210 (96%)	0.45	23 (11%) 10 11	85, 99, 114, 123	0
6	1G	181/182 (99%)	0.56	11 (6%) 27 18	100, 112, 122, 126	0
6	2G	181/182 (99%)	0.50	3 (1%) 69 43	102, 115, 125, 135	0
7	1H	174/180 (96%)	0.18	3 (1%) 69 43	91, 103, 113, 124	0
7	2H	174/180 (96%)	0.49	5 (2%) 53 33	97, 114, 123, 132	0
8	1I	146/148 (98%)	0.06	6 (4%) 41 26	89, 105, 115, 125	0
8	2I	146/148 (98%)	0.70	15 (10%) 12 12	97, 118, 130, 135	0
9	1N	140/140 (100%)	0.36	2 (1%) 73 48	85, 96, 109, 118	0
9	2N	140/140 (100%)	0.45	8 (5%) 29 20	91, 102, 115, 122	0
10	1O	122/122 (100%)	0.45	0 100 100	83, 96, 109, 117	0
10	2O	122/122 (100%)	0.35	3 (2%) 58 36	82, 93, 101, 112	0
11	1P	149/150 (99%)	0.45	8 (5%) 31 21	80, 98, 116, 126	0
11	2P	149/150 (99%)	0.27	9 (6%) 27 19	86, 103, 115, 124	0
12	1Q	141/141 (100%)	0.80	14 (9%) 13 13	82, 98, 110, 117	0
12	2Q	141/141 (100%)	0.26	5 (3%) 47 30	88, 101, 113, 125	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
13	1R	118/118 (100%)	0.28	2 (1%) 69 43	86, 95, 107, 114	0
13	2R	118/118 (100%)	0.36	3 (2%) 58 36	83, 94, 102, 110	0
14	1S	110/112 (98%)	0.29	4 (3%) 46 29	94, 109, 118, 123	0
14	2S	110/112 (98%)	0.41	3 (2%) 56 35	98, 111, 118, 126	0
15	1T	131/146 (89%)	0.50	5 (3%) 44 28	88, 101, 116, 125	0
15	2T	131/146 (89%)	0.44	4 (3%) 51 32	85, 96, 110, 121	0
16	1U	116/118 (98%)	0.39	4 (3%) 48 30	76, 95, 107, 114	0
16	2U	116/118 (98%)	0.66	13 (11%) 10 11	88, 100, 109, 118	0
17	1V	101/101 (100%)	0.28	3 (2%) 52 32	79, 97, 110, 115	0
17	2V	101/101 (100%)	0.03	1 (0%) 79 55	87, 103, 116, 122	0
18	1W	112/113 (99%)	0.58	6 (5%) 31 21	81, 91, 109, 124	0
18	2W	112/113 (99%)	0.34	4 (3%) 46 29	81, 93, 107, 119	0
19	1X	95/96 (98%)	0.19	2 (2%) 63 40	82, 91, 106, 117	0
19	2X	95/96 (98%)	0.26	2 (2%) 63 40	86, 98, 113, 121	0
20	1Y	107/110 (97%)	0.40	4 (3%) 45 28	83, 96, 109, 114	0
20	2Y	107/110 (97%)	0.60	9 (8%) 17 14	90, 105, 118, 124	0
21	1Z	154/206 (74%)	0.45	7 (4%) 38 24	96, 111, 120, 128	0
21	2Z	160/206 (77%)	0.48	7 (4%) 39 25	101, 113, 123, 130	0
22	10	83/85 (97%)	0.33	5 (6%) 27 19	90, 101, 110, 116	0
22	20	83/85 (97%)	0.35	4 (4%) 35 23	92, 104, 111, 113	0
23	11	97/98 (98%)	0.79	14 (14%) 6 8	82, 92, 107, 114	0
23	21	97/98 (98%)	0.54	8 (8%) 17 14	86, 98, 110, 119	0
24	12	70/72 (97%)	0.15	1 (1%) 73 48	81, 92, 103, 122	0
24	22	70/72 (97%)	0.14	0 100 100	93, 106, 116, 121	0
25	13	59/60 (98%)	0.22	2 (3%) 48 30	78, 97, 116, 134	0
25	23	59/60 (98%)	0.14	1 (1%) 69 43	88, 99, 118, 130	0
26	14	69/71 (97%)	0.68	3 (4%) 40 25	107, 122, 134, 137	0
26	24	69/71 (97%)	0.37	3 (4%) 40 25	106, 118, 131, 135	0
27	15	59/60 (98%)	0.28	0 100 100	82, 93, 107, 111	0
27	25	59/60 (98%)	0.08	0 100 100	84, 92, 109, 112	0
28	16	53/54 (98%)	0.03	1 (1%) 66 42	86, 98, 110, 122	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
28	26	53/54 (98%)	0.35	3 (5%) 29 20	94, 104, 115, 123	0
29	17	48/49 (97%)	1.16	7 (14%) 6 8	72, 82, 99, 113	0
29	27	48/49 (97%)	0.66	4 (8%) 17 14	83, 91, 105, 117	0
30	18	64/65 (98%)	0.90	6 (9%) 14 13	82, 90, 99, 112	0
30	28	64/65 (98%)	0.38	0 100 100	89, 97, 106, 112	0
31	19	37/37 (100%)	0.40	1 (2%) 56 35	91, 98, 106, 107	0
31	29	37/37 (100%)	0.68	3 (8%) 18 14	97, 106, 115, 118	0
32	1a	1488/1521 (97%)	0.36	69 (4%) 37 24	85, 114, 131, 153	0
32	2a	1491/1521 (98%)	0.08	27 (1%) 67 42	87, 108, 129, 149	0
33	1b	231/256 (90%)	0.23	4 (1%) 69 43	104, 117, 126, 132	0
33	2b	231/256 (90%)	0.29	0 100 100	101, 117, 127, 136	0
34	1c	206/239 (86%)	0.70	14 (6%) 23 17	104, 119, 128, 133	0
34	2c	206/239 (86%)	0.23	5 (2%) 59 37	104, 116, 124, 131	0
35	1d	208/209 (99%)	0.45	5 (2%) 59 37	97, 112, 122, 130	0
35	2d	208/209 (99%)	0.17	4 (1%) 66 42	91, 105, 114, 121	0
36	1e	148/162 (91%)	0.17	1 (0%) 84 63	96, 110, 119, 124	0
36	2e	148/162 (91%)	0.10	1 (0%) 84 63	93, 107, 118, 126	0
37	1f	100/101 (99%)	0.27	5 (5%) 34 22	86, 105, 115, 117	0
37	2f	100/101 (99%)	0.10	0 100 100	95, 108, 117, 123	0
38	1g	155/156 (99%)	0.53	8 (5%) 33 22	101, 115, 126, 132	0
38	2g	155/156 (99%)	0.27	3 (1%) 66 42	102, 114, 124, 129	0
39	1h	137/138 (99%)	0.15	1 (0%) 84 63	100, 110, 119, 129	0
39	2h	137/138 (99%)	0.43	7 (5%) 33 22	94, 106, 116, 126	0
40	1i	127/128 (99%)	1.18	27 (21%) 2 3	109, 120, 126, 130	0
40	2i	127/128 (99%)	1.30	30 (23%) 2 2	103, 118, 126, 129	0
41	1j	97/105 (92%)	1.11	16 (16%) 4 6	111, 122, 130, 135	0
41	2j	96/105 (91%)	0.55	4 (4%) 40 25	111, 122, 129, 137	0
42	1k	114/129 (88%)	0.31	6 (5%) 32 21	94, 105, 115, 122	0
42	2k	114/129 (88%)	0.25	1 (0%) 81 58	96, 110, 119, 122	0
43	1l	121/132 (91%)	0.16	2 (1%) 69 43	92, 105, 114, 116	0
43	2l	121/132 (91%)	0.06	2 (1%) 69 43	89, 102, 112, 116	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
44	1m	123/126 (97%)	0.59	7 (5%) 29 20	104, 116, 125, 136	0
44	2m	122/126 (96%)	0.90	16 (13%) 7 9	106, 117, 124, 130	0
45	1n	60/61 (98%)	1.17	15 (25%) 2 2	105, 117, 126, 134	0
45	2n	60/61 (98%)	0.52	3 (5%) 34 22	107, 117, 125, 128	0
46	1o	88/89 (98%)	0.10	0 100 100	93, 105, 114, 118	0
46	2o	88/89 (98%)	0.12	1 (1%) 78 53	89, 106, 115, 123	0
47	1p	82/88 (93%)	1.06	8 (9%) 13 13	106, 114, 122, 129	0
47	2p	82/88 (93%)	0.48	2 (2%) 59 37	85, 100, 109, 114	0
48	1q	99/105 (94%)	0.31	2 (2%) 65 41	92, 107, 116, 122	0
48	2q	99/105 (94%)	0.31	5 (5%) 33 22	92, 104, 113, 120	0
49	1r	68/88 (77%)	0.08	0 100 100	94, 105, 113, 124	0
49	2r	68/88 (77%)	0.11	1 (1%) 72 46	97, 107, 119, 122	0
50	1s	83/93 (89%)	0.72	3 (3%) 46 29	108, 119, 128, 133	0
50	2s	83/93 (89%)	0.70	4 (4%) 35 23	103, 118, 125, 128	0
51	1t	96/106 (90%)	0.85	12 (12%) 8 10	103, 111, 120, 122	0
51	2t	96/106 (90%)	0.61	11 (11%) 9 11	92, 104, 115, 121	0
52	1u	23/27 (85%)	1.20	2 (8%) 16 14	112, 118, 121, 125	0
52	2u	23/27 (85%)	0.59	1 (4%) 40 25	112, 118, 123, 127	0
53	1v	7/24 (29%)	1.57	2 (28%) 1 2	105, 107, 133, 138	0
53	2v	6/24 (25%)	0.20	0 100 100	106, 113, 119, 134	0
54	1w	3/4 (75%)	3.26	1 (33%) 1 1	88, 88, 101, 110	0
54	2w	3/4 (75%)	3.04	1 (33%) 1 1	93, 93, 104, 105	0
55	1x	72/77 (93%)	0.10	1 (1%) 73 48	85, 111, 123, 134	0
55	2x	72/77 (93%)	-0.11	0 100 100	92, 113, 121, 132	0
All	All	20603/21452 (96%)	0.32	882 (4%) 40 25	72, 104, 125, 153	0

The worst 5 of 882 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
54	1w	73	A	9.7
54	2w	73	A	8.8
1	2A	2179	C	7.5
8	2I	84	GLY	7.1
38	2g	80	VAL	6.7

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

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
55	PSU	2x	55	20/21	0.69	0.10	105,119,134,136	0
55	4SU	2x	8	20/21	0.76	0.09	106,121,131,139	0
32	PSU	1a	516	20/21	0.78	0.08	105,119,129,131	0
55	5MU	1x	54	21/22	0.79	0.10	108,113,121,124	0
55	4SU	1x	8	20/21	0.81	0.09	106,116,122,129	0
55	PSU	1x	55	20/21	0.82	0.09	99,110,130,130	0
1	5MU	1A	1937	21/22	0.83	0.09	102,113,123,145	0
32	2MG	2a	1207	24/25	0.84	0.09	102,116,123,129	0
1	PSU	1A	1933	20/21	0.85	0.09	84,98,106,107	0
55	5MC	1x	32	21/22	0.87	0.11	98,107,111,124	0
1	5MU	2A	1939	21/22	0.87	0.17	77,88,97,102	0
1	5MU	2A	1915	21/22	0.87	0.07	103,108,119,134	0
32	5MC	2a	967	21/22	0.87	0.09	93,101,111,116	0
55	5MC	2x	32	21/22	0.88	0.08	106,110,114,119	0
32	2MG	1a	1207	24/25	0.88	0.09	105,114,134,137	0
1	5MC	1A	1964	21/22	0.89	0.09	81,91,96,98	0
32	M2G	2a	966	25/26	0.89	0.10	94,103,117,121	0
43	0TD	2l	92	10/11	0.90	0.16	101,110,117,134	0
32	PSU	2a	516	20/21	0.90	0.06	93,110,115,116	0
1	PSU	2A	1917	20/21	0.90	0.07	96,99,107,111	0
32	5MC	1a	1400	21/22	0.90	0.12	96,105,118,123	0
55	5MU	2x	54	21/22	0.90	0.09	104,110,120,126	0
32	5MC	1a	1407	21/22	0.90	0.10	96,103,114,123	0
32	5MC	1a	967	21/22	0.90	0.12	108,116,125,130	0
32	4OC	2a	1402	22/23	0.91	0.12	94,104,112,115	0
1	PSU	2A	1911	20/21	0.91	0.07	89,100,112,117	0
1	4OC	1A	1942	21/23	0.91	0.10	86,99,108,110	0
32	7MG	2a	527	24/25	0.91	0.09	97,107,113,115	0
32	5MC	2a	1400	21/22	0.91	0.10	99,109,117,118	0
32	M2G	1a	966	25/26	0.92	0.11	102,108,121,122	0
1	5MU	1A	1961	21/22	0.92	0.12	66,83,90,94	0
32	7MG	1a	527	24/25	0.93	0.09	100,108,119,126	0
1	PSU	1A	1939	20/21	0.93	0.06	86,100,107,115	0
32	UR3	1a	1498	21/22	0.94	0.12	86,95,101,105	0
32	UR3	2a	1498	21/22	0.94	0.15	92,102,109,111	0
54	KGV	1w	76	33/34	0.94	0.13	80,87,97,101	0
1	PSU	2A	2605	20/21	0.94	0.10	70,86,90,91	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
1	4OC	2A	1920	21/23	0.94	0.09	93,100,108,109	0
1	5MC	2A	1962	21/22	0.94	0.12	66,90,94,99	0
32	4OC	1a	1402	22/23	0.94	0.13	87,102,109,116	0
1	OMG	2A	2251	24/25	0.94	0.10	77,93,100,104	0
32	5MC	1a	1404	21/22	0.94	0.13	89,96,99,110	0
32	5MC	2a	1404	21/22	0.94	0.09	91,98,104,109	0
1	2MA	2A	2503	23/24	0.94	0.12	80,86,93,105	0
1	2MU	2A	2552	21/23	0.95	0.09	77,85,90,96	0
32	MA6	2a	1518	24/25	0.95	0.10	90,100,106,108	0
32	MA6	2a	1519	24/25	0.95	0.12	80,100,106,109	0
1	2MA	1A	2515	23/24	0.95	0.13	69,78,88,94	0
1	5MC	2A	1942	21/22	0.95	0.08	78,92,102,106	0
1	2MU	1A	2564	21/23	0.95	0.14	83,90,99,103	0
43	0TD	1l	92	10/11	0.96	0.09	102,110,112,117	0
1	PSU	1A	2617	20/21	0.96	0.12	71,82,92,95	0
32	MA6	1a	1518	24/25	0.96	0.09	87,93,98,101	0
1	OMG	1A	2263	24/25	0.96	0.16	70,82,95,97	0
32	MA6	1a	1519	24/25	0.96	0.12	82,94,101,105	0
1	5MC	1A	1984	21/22	0.96	0.10	80,89,92,99	0
32	5MC	2a	1407	21/22	0.96	0.10	81,93,102,104	0
54	KGV	2w	76	33/34	0.96	0.12	75,89,98,102	0

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	1a	1663	1/1	0.30	0.43	97,97,97,97	0
56	MG	2A	3087	1/1	0.32	0.11	96,96,96,96	0
56	MG	2A	3115	1/1	0.32	0.26	90,90,90,90	0
56	MG	2c	301	1/1	0.39	0.20	94,94,94,94	0
56	MG	2A	3013	1/1	0.41	0.21	97,97,97,97	0
56	MG	2A	3426	1/1	0.43	0.33	88,88,88,88	0
56	MG	2A	3226	1/1	0.43	0.25	82,82,82,82	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	1A	3237	1/1	0.44	0.24	90,90,90,90	0
56	MG	2a	1611	1/1	0.47	0.22	97,97,97,97	0
56	MG	2A	3140	1/1	0.47	0.29	81,81,81,81	0
56	MG	1A	3395	1/1	0.48	0.21	96,96,96,96	0
56	MG	2A	3168	1/1	0.48	0.21	82,82,82,82	0
56	MG	1A	3182	1/1	0.50	0.22	100,100,100,100	0
56	MG	1a	1604	1/1	0.51	0.28	88,88,88,88	0
56	MG	1B	212	1/1	0.52	0.30	79,79,79,79	0
56	MG	1B	202	1/1	0.52	0.16	114,114,114,114	0
56	MG	2n	101	1/1	0.52	0.36	77,77,77,77	0
56	MG	2a	1672	1/1	0.53	0.43	89,89,89,89	0
56	MG	2A	3371	1/1	0.54	0.29	86,86,86,86	0
56	MG	2A	3003	1/1	0.55	0.20	72,72,72,72	0
56	MG	2A	3301	1/1	0.55	0.23	83,83,83,83	0
56	MG	1A	3368	1/1	0.55	0.28	76,76,76,76	0
56	MG	1A	3529	1/1	0.55	0.35	73,73,73,73	0
56	MG	1B	211	1/1	0.56	0.43	74,74,74,74	0
56	MG	1A	3360	1/1	0.56	0.31	84,84,84,84	0
56	MG	2A	3034	1/1	0.56	0.26	102,102,102,102	0
56	MG	2A	3079	1/1	0.56	0.27	86,86,86,86	0
56	MG	1a	1662	1/1	0.57	0.34	89,89,89,89	0
56	MG	1A	3054	1/1	0.57	0.35	71,71,71,71	0
56	MG	1B	218	1/1	0.58	0.29	78,78,78,78	0
56	MG	1a	1609	1/1	0.58	0.28	106,106,106,106	0
56	MG	1a	1614	1/1	0.59	0.29	74,74,74,74	0
56	MG	1A	3492	1/1	0.59	0.40	66,66,66,66	0
56	MG	2A	3421	1/1	0.59	0.59	83,83,83,83	0
56	MG	1A	3098	1/1	0.59	0.30	77,77,77,77	0
56	MG	1A	3283	1/1	0.60	0.17	76,76,76,76	0
56	MG	2B	208	1/1	0.60	0.32	83,83,83,83	0
56	MG	28	102	1/1	0.60	0.19	74,74,74,74	0
56	MG	1A	3232	1/1	0.60	0.23	59,59,59,59	0
56	MG	2A	3370	1/1	0.60	0.28	89,89,89,89	0
56	MG	1A	3245	1/1	0.60	0.28	74,74,74,74	0
56	MG	1A	3376	1/1	0.60	0.26	92,92,92,92	0
56	MG	1A	3217	1/1	0.61	0.21	98,98,98,98	0
56	MG	1A	3145	1/1	0.61	0.21	84,84,84,84	0
56	MG	1r	101	1/1	0.61	0.27	74,74,74,74	0
56	MG	2A	3393	1/1	0.61	0.34	84,84,84,84	0
56	MG	2A	3176	1/1	0.62	0.30	75,75,75,75	0
56	MG	2A	3186	1/1	0.62	0.25	64,64,64,64	0
56	MG	2A	3218	1/1	0.62	0.13	77,77,77,77	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	1a	1683	1/1	0.62	0.23	84,84,84,84	0
56	MG	2A	3150	1/1	0.62	0.21	79,79,79,79	0
56	MG	2a	1632	1/1	0.62	0.28	82,82,82,82	0
56	MG	2A	3153	1/1	0.62	0.20	81,81,81,81	0
56	MG	2a	1702	1/1	0.62	0.20	74,74,74,74	0
56	MG	1A	3189	1/1	0.62	0.20	83,83,83,83	0
56	MG	2A	3171	1/1	0.62	0.16	77,77,77,77	0
56	MG	2A	3314	1/1	0.63	0.32	75,75,75,75	0
56	MG	2A	3107	1/1	0.63	0.21	91,91,91,91	0
56	MG	1A	3467	1/1	0.63	0.29	82,82,82,82	0
56	MG	2a	1646	1/1	0.63	0.20	79,79,79,79	0
56	MG	1A	3101	1/1	0.63	0.21	95,95,95,95	0
56	MG	2a	1689	1/1	0.63	0.20	91,91,91,91	0
56	MG	1A	3296	1/1	0.63	0.23	80,80,80,80	0
56	MG	1A	3430	1/1	0.63	0.11	108,108,108,108	0
56	MG	1B	208	1/1	0.63	0.30	73,73,73,73	0
56	MG	1B	217	1/1	0.64	0.18	92,92,92,92	0
56	MG	2A	3354	1/1	0.64	0.30	82,82,82,82	0
56	MG	25	101	1/1	0.64	0.36	65,65,65,65	0
56	MG	1A	3353	1/1	0.65	0.34	72,72,72,72	0
56	MG	2A	3038	1/1	0.65	0.18	87,87,87,87	0
56	MG	1x	103	1/1	0.65	0.14	95,95,95,95	0
56	MG	1A	3008	1/1	0.65	0.17	100,100,100,100	0
56	MG	2A	3163	1/1	0.65	0.21	66,66,66,66	0
56	MG	1A	3148	1/1	0.65	0.20	51,51,51,51	0
56	MG	2A	3161	1/1	0.66	0.30	66,66,66,66	0
56	MG	2A	3428	1/1	0.66	0.23	85,85,85,85	0
56	MG	1A	3055	1/1	0.66	0.23	86,86,86,86	0
56	MG	1A	3121	1/1	0.66	0.16	75,75,75,75	0
56	MG	1A	3320	1/1	0.66	0.33	71,71,71,71	0
56	MG	1a	1616	1/1	0.66	0.29	75,75,75,75	0
56	MG	2a	1616	1/1	0.66	0.14	87,87,87,87	0
56	MG	1A	3294	1/1	0.67	0.30	75,75,75,75	0
56	MG	1A	3385	1/1	0.67	0.17	79,79,79,79	0
56	MG	2a	1613	1/1	0.67	0.21	90,90,90,90	0
56	MG	2A	3372	1/1	0.67	0.11	73,73,73,73	0
56	MG	2A	3146	1/1	0.67	0.24	79,79,79,79	0
56	MG	2A	3062	1/1	0.67	0.30	72,72,72,72	0
56	MG	1A	3194	1/1	0.67	0.40	71,71,71,71	0
56	MG	1A	3429	1/1	0.67	0.24	80,80,80,80	0
56	MG	2A	3431	1/1	0.67	0.35	65,65,65,65	0
56	MG	2A	3090	1/1	0.67	0.09	82,82,82,82	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	1A	3096	1/1	0.67	0.13	95,95,95,95	0
56	MG	1A	3179	1/1	0.68	0.32	69,69,69,69	0
56	MG	1A	3394	1/1	0.68	0.41	50,50,50,50	0
56	MG	1x	108	1/1	0.68	0.18	103,103,103,103	0
56	MG	1A	3020	1/1	0.68	0.24	69,69,69,69	0
56	MG	2A	3075	1/1	0.68	0.20	75,75,75,75	0
56	MG	2a	1639	1/1	0.68	0.14	64,64,64,64	0
56	MG	2a	1619	1/1	0.69	0.09	62,62,62,62	0
56	MG	2A	3469	1/1	0.69	0.19	78,78,78,78	0
56	MG	2B	207	1/1	0.69	0.14	91,91,91,91	0
56	MG	1A	3110	1/1	0.69	0.34	75,75,75,75	0
56	MG	2a	1664	1/1	0.69	0.14	77,77,77,77	0
56	MG	1P	201	1/1	0.69	0.17	80,80,80,80	0
56	MG	2A	3330	1/1	0.69	0.20	80,80,80,80	0
56	MG	1A	3028	1/1	0.69	0.24	63,63,63,63	0
56	MG	1A	3128	1/1	0.69	0.14	70,70,70,70	0
56	MG	1B	203	1/1	0.69	0.09	75,75,75,75	0
56	MG	1A	3428	1/1	0.70	0.27	75,75,75,75	0
56	MG	2A	3251	1/1	0.70	0.14	85,85,85,85	0
56	MG	2A	3296	1/1	0.70	0.24	89,89,89,89	0
56	MG	1A	3029	1/1	0.70	0.26	94,94,94,94	0
56	MG	1A	3114	1/1	0.70	0.19	72,72,72,72	0
56	MG	1A	3442	1/1	0.70	0.34	56,56,56,56	0
56	MG	1A	3322	1/1	0.70	0.19	71,71,71,71	0
56	MG	1A	3223	1/1	0.70	0.25	84,84,84,84	0
56	MG	1A	3515	1/1	0.70	0.10	60,60,60,60	0
56	MG	2A	3204	1/1	0.70	0.16	68,68,68,68	0
56	MG	1A	3013	1/1	0.70	0.25	70,70,70,70	0
56	MG	2A	3019	1/1	0.71	0.29	102,102,102,102	0
56	MG	1a	1617	1/1	0.71	0.22	87,87,87,87	0
56	MG	2A	3155	1/1	0.71	0.20	93,93,93,93	0
56	MG	2a	1604	1/1	0.71	0.16	83,83,83,83	0
56	MG	1A	3400	1/1	0.71	0.23	75,75,75,75	0
56	MG	1A	3412	1/1	0.71	0.26	75,75,75,75	0
56	MG	2a	1615	1/1	0.71	0.15	71,71,71,71	0
56	MG	1A	3413	1/1	0.71	0.11	79,79,79,79	0
56	MG	1a	1685	1/1	0.71	0.23	73,73,73,73	0
56	MG	1A	3216	1/1	0.71	0.21	69,69,69,69	0
56	MG	2a	1634	1/1	0.71	0.23	81,81,81,81	0
56	MG	2a	1635	1/1	0.71	0.36	90,90,90,90	0
56	MG	2A	3404	1/1	0.71	0.30	74,74,74,74	0
56	MG	1A	3005	1/1	0.71	0.25	91,91,91,91	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	2A	3100	1/1	0.71	0.13	68,68,68,68	0
56	MG	2a	1667	1/1	0.71	0.20	83,83,83,83	0
56	MG	1A	3171	1/1	0.71	0.24	71,71,71,71	0
56	MG	1A	3437	1/1	0.71	0.31	83,83,83,83	0
56	MG	2A	3434	1/1	0.71	0.14	79,79,79,79	0
56	MG	2A	3010	1/1	0.71	0.34	72,72,72,72	0
56	MG	1A	3259	1/1	0.71	0.23	73,73,73,73	0
56	MG	2A	3232	1/1	0.72	0.15	81,81,81,81	0
56	MG	1A	3435	1/1	0.72	0.24	75,75,75,75	0
56	MG	1A	3414	1/1	0.72	0.23	77,77,77,77	0
56	MG	1A	3426	1/1	0.72	0.17	90,90,90,90	0
56	MG	2a	1661	1/1	0.72	0.21	67,67,67,67	0
56	MG	2A	3307	1/1	0.72	0.38	73,73,73,73	0
56	MG	1A	3455	1/1	0.72	0.11	78,78,78,78	0
56	MG	2A	3202	1/1	0.72	0.25	86,86,86,86	0
56	MG	2a	1677	1/1	0.72	0.22	81,81,81,81	0
56	MG	1A	3070	1/1	0.72	0.19	72,72,72,72	0
56	MG	1A	3120	1/1	0.72	0.19	88,88,88,88	0
56	MG	2a	1630	1/1	0.72	0.31	65,65,65,65	0
56	MG	1A	3088	1/1	0.72	0.13	96,96,96,96	0
56	MG	2A	3006	1/1	0.73	0.25	86,86,86,86	0
56	MG	2A	3368	1/1	0.73	0.24	93,93,93,93	0
56	MG	1A	3036	1/1	0.73	0.17	96,96,96,96	0
56	MG	1a	1613	1/1	0.73	0.20	72,72,72,72	0
56	MG	2A	3249	1/1	0.73	0.27	75,75,75,75	0
56	MG	1A	3019	1/1	0.73	0.14	81,81,81,81	0
56	MG	2A	3397	1/1	0.73	0.29	73,73,73,73	0
56	MG	2A	3284	1/1	0.73	0.29	58,58,58,58	0
56	MG	1A	3485	1/1	0.73	0.38	50,50,50,50	0
56	MG	1A	3003	1/1	0.73	0.17	95,95,95,95	0
56	MG	1x	105	1/1	0.73	0.18	109,109,109,109	0
56	MG	1a	1643	1/1	0.73	0.25	87,87,87,87	0
56	MG	1A	3317	1/1	0.73	0.24	89,89,89,89	0
56	MG	1a	1623	1/1	0.74	0.21	87,87,87,87	0
56	MG	1a	1633	1/1	0.74	0.10	73,73,73,73	0
56	MG	1A	3188	1/1	0.74	0.31	86,86,86,86	0
56	MG	1a	1652	1/1	0.74	0.21	68,68,68,68	0
56	MG	2A	3225	1/1	0.74	0.16	83,83,83,83	0
56	MG	1A	3214	1/1	0.74	0.40	74,74,74,74	0
56	MG	1A	3445	1/1	0.74	0.09	70,70,70,70	0
56	MG	2A	3406	1/1	0.74	0.16	72,72,72,72	0
56	MG	2A	3023	1/1	0.74	0.22	74,74,74,74	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
56	MG	2A	3032	1/1	0.74	0.20	75,75,75,75	0
56	MG	2A	3427	1/1	0.74	0.10	102,102,102,102	0
56	MG	1A	3362	1/1	0.74	0.22	82,82,82,82	0
56	MG	1A	3363	1/1	0.74	0.26	51,51,51,51	0
56	MG	2a	1666	1/1	0.74	0.28	73,73,73,73	0
56	MG	1A	3473	1/1	0.74	0.38	68,68,68,68	0
56	MG	2A	3304	1/1	0.74	0.17	73,73,73,73	0
56	MG	1x	102	1/1	0.74	0.13	71,71,71,71	0
56	MG	1A	3215	1/1	0.74	0.31	65,65,65,65	0
56	MG	2a	1693	1/1	0.74	0.11	67,67,67,67	0
56	MG	2A	3175	1/1	0.74	0.12	71,71,71,71	0
56	MG	2A	3332	1/1	0.74	0.34	50,50,50,50	0
56	MG	1A	3030	1/1	0.74	0.26	84,84,84,84	0
56	MG	1a	1644	1/1	0.75	0.21	89,89,89,89	0
56	MG	1A	3184	1/1	0.75	0.27	54,54,54,54	0
56	MG	2A	3272	1/1	0.75	0.21	78,78,78,78	0
56	MG	2A	3415	1/1	0.75	0.42	74,74,74,74	0
56	MG	2A	3039	1/1	0.75	0.24	88,88,88,88	0
56	MG	2a	1633	1/1	0.75	0.29	74,74,74,74	0
56	MG	2A	3046	1/1	0.75	0.20	74,74,74,74	0
56	MG	1B	205	1/1	0.75	0.21	73,73,73,73	0
56	MG	2a	1637	1/1	0.75	0.16	75,75,75,75	0
56	MG	1A	3031	1/1	0.75	0.16	81,81,81,81	0
56	MG	10	103	1/1	0.75	0.16	69,69,69,69	0
56	MG	1a	1684	1/1	0.75	0.19	82,82,82,82	0
56	MG	2A	3438	1/1	0.75	0.27	64,64,64,64	0
56	MG	2A	3011	1/1	0.75	0.33	84,84,84,84	0
56	MG	1a	1603	1/1	0.75	0.09	110,110,110,110	0
56	MG	2a	1668	1/1	0.75	0.16	79,79,79,79	0
56	MG	2A	3203	1/1	0.75	0.17	66,66,66,66	0
56	MG	2a	1676	1/1	0.75	0.09	82,82,82,82	0
56	MG	2A	3016	1/1	0.75	0.18	70,70,70,70	0
56	MG	1d	301	1/1	0.75	0.15	96,96,96,96	0
56	MG	2a	1601	1/1	0.75	0.13	63,63,63,63	0
56	MG	2a	1699	1/1	0.75	0.20	61,61,61,61	0
56	MG	2A	3022	1/1	0.75	0.14	87,87,87,87	0
56	MG	1A	3108	1/1	0.75	0.18	76,76,76,76	0
56	MG	2f	202	1/1	0.75	0.11	84,84,84,84	0
56	MG	1A	3007	1/1	0.75	0.29	65,65,65,65	0
56	MG	10	102	1/1	0.76	0.26	84,84,84,84	0
56	MG	2A	3474	1/1	0.76	0.13	84,84,84,84	0
56	MG	2A	3235	1/1	0.76	0.20	66,66,66,66	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	1A	3392	1/1	0.76	0.34	54,54,54,54	0
56	MG	2A	3377	1/1	0.76	0.24	71,71,71,71	0
56	MG	1A	3100	1/1	0.76	0.20	74,74,74,74	0
56	MG	2A	3033	1/1	0.76	0.20	63,63,63,63	0
56	MG	1A	3308	1/1	0.76	0.30	82,82,82,82	0
56	MG	1A	3139	1/1	0.76	0.28	50,50,50,50	0
56	MG	2A	3112	1/1	0.76	0.18	84,84,84,84	0
56	MG	1A	3449	1/1	0.76	0.24	66,66,66,66	0
56	MG	2A	3118	1/1	0.76	0.16	66,66,66,66	0
56	MG	2A	3043	1/1	0.76	0.29	78,78,78,78	0
56	MG	1A	3409	1/1	0.76	0.12	71,71,71,71	0
56	MG	2A	3430	1/1	0.76	0.30	59,59,59,59	0
56	MG	2A	3056	1/1	0.76	0.20	88,88,88,88	0
56	MG	2A	3152	1/1	0.76	0.22	74,74,74,74	0
56	MG	1A	3390	1/1	0.76	0.27	67,67,67,67	0
56	MG	2A	3160	1/1	0.77	0.22	78,78,78,78	0
56	MG	1A	3084	1/1	0.77	0.18	77,77,77,77	0
56	MG	1a	1624	1/1	0.77	0.34	68,68,68,68	0
56	MG	2A	3398	1/1	0.77	0.35	66,66,66,66	0
56	MG	2A	3254	1/1	0.77	0.12	66,66,66,66	0
56	MG	1A	3427	1/1	0.77	0.18	56,56,56,56	0
56	MG	1a	1642	1/1	0.77	0.20	70,70,70,70	0
56	MG	2A	3285	1/1	0.77	0.26	55,55,55,55	0
56	MG	2A	3290	1/1	0.77	0.27	67,67,67,67	0
56	MG	1a	1602	1/1	0.77	0.13	70,70,70,70	0
56	MG	1A	3487	1/1	0.77	0.40	69,69,69,69	0
56	MG	1A	3053	1/1	0.77	0.38	80,80,80,80	0
56	MG	1A	3011	1/1	0.77	0.21	84,84,84,84	0
56	MG	2A	3313	1/1	0.77	0.34	75,75,75,75	0
56	MG	1A	3522	1/1	0.77	0.16	86,86,86,86	0
56	MG	2A	3447	1/1	0.77	0.37	53,53,53,53	0
56	MG	2A	3327	1/1	0.77	0.36	73,73,73,73	0
56	MG	2a	1675	1/1	0.77	0.21	85,85,85,85	0
56	MG	2A	3148	1/1	0.77	0.11	70,70,70,70	0
56	MG	2A	3206	1/1	0.77	0.27	78,78,78,78	0
56	MG	2A	3337	1/1	0.77	0.21	59,59,59,59	0
56	MG	2A	3351	1/1	0.77	0.33	73,73,73,73	0
56	MG	1a	1668	1/1	0.77	0.26	63,63,63,63	0
56	MG	1A	3375	1/1	0.77	0.41	58,58,58,58	0
56	MG	1G	201	1/1	0.77	0.13	90,90,90,90	0
56	MG	2d	301	1/1	0.77	0.22	68,68,68,68	0
56	MG	1A	3134	1/1	0.77	0.34	76,76,76,76	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	2A	3233	1/1	0.77	0.34	54,54,54,54	0
56	MG	1a	1629	1/1	0.78	0.13	85,85,85,85	0
56	MG	1A	3356	1/1	0.78	0.33	79,79,79,79	0
56	MG	2A	3317	1/1	0.78	0.28	57,57,57,57	0
56	MG	2A	3321	1/1	0.78	0.26	67,67,67,67	0
56	MG	1A	3282	1/1	0.78	0.16	94,94,94,94	0
56	MG	1A	3058	1/1	0.78	0.15	71,71,71,71	0
56	MG	1A	3405	1/1	0.78	0.20	74,74,74,74	0
56	MG	1A	3129	1/1	0.78	0.14	85,85,85,85	0
56	MG	2A	3345	1/1	0.78	0.30	58,58,58,58	0
56	MG	1A	3410	1/1	0.78	0.23	82,82,82,82	0
56	MG	2A	3352	1/1	0.78	0.20	67,67,67,67	0
56	MG	2A	3450	1/1	0.78	0.18	64,64,64,64	0
56	MG	2A	3455	1/1	0.78	0.39	61,61,61,61	0
56	MG	2A	3459	1/1	0.78	0.20	69,69,69,69	0
56	MG	1a	1606	1/1	0.78	0.07	81,81,81,81	0
56	MG	2A	3355	1/1	0.78	0.29	69,69,69,69	0
56	MG	2B	203	1/1	0.78	0.21	79,79,79,79	0
56	MG	1A	3012	1/1	0.78	0.28	70,70,70,70	0
56	MG	2A	3095	1/1	0.78	0.07	70,70,70,70	0
56	MG	1a	1679	1/1	0.78	0.31	76,76,76,76	0
56	MG	1A	3094	1/1	0.78	0.25	67,67,67,67	0
56	MG	1A	3246	1/1	0.78	0.61	50,50,50,50	0
56	MG	1A	3471	1/1	0.78	0.25	98,98,98,98	0
56	MG	2a	1610	1/1	0.78	0.21	82,82,82,82	0
56	MG	1A	3252	1/1	0.78	0.15	71,71,71,71	0
56	MG	1A	3192	1/1	0.78	0.14	64,64,64,64	0
56	MG	1A	3279	1/1	0.78	0.12	83,83,83,83	0
56	MG	2B	210	1/1	0.79	0.33	80,80,80,80	0
56	MG	2A	3088	1/1	0.79	0.08	61,61,61,61	0
56	MG	1A	3346	1/1	0.79	0.17	73,73,73,73	0
56	MG	2A	3091	1/1	0.79	0.15	82,82,82,82	0
56	MG	2A	3092	1/1	0.79	0.25	76,76,76,76	0
56	MG	2A	3224	1/1	0.79	0.12	74,74,74,74	0
56	MG	1A	3048	1/1	0.79	0.15	65,65,65,65	0
56	MG	1A	3060	1/1	0.79	0.17	55,55,55,55	0
56	MG	2A	3230	1/1	0.79	0.20	56,56,56,56	0
56	MG	1a	1661	1/1	0.79	0.29	74,74,74,74	0
56	MG	1A	3051	1/1	0.79	0.26	73,73,73,73	0
56	MG	1a	1608	1/1	0.79	0.19	78,78,78,78	0
56	MG	1a	1667	1/1	0.79	0.11	97,97,97,97	0
56	MG	2A	3401	1/1	0.79	0.16	87,87,87,87	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	2A	3403	1/1	0.79	0.29	81,81,81,81	0
56	MG	1A	3285	1/1	0.79	0.19	76,76,76,76	0
56	MG	1a	1671	1/1	0.79	0.13	71,71,71,71	0
56	MG	2A	3410	1/1	0.79	0.23	78,78,78,78	0
56	MG	1A	3238	1/1	0.79	0.12	80,80,80,80	0
56	MG	2a	1648	1/1	0.79	0.31	69,69,69,69	0
56	MG	2a	1658	1/1	0.79	0.29	60,60,60,60	0
56	MG	1a	1681	1/1	0.79	0.08	69,69,69,69	0
56	MG	1A	3461	1/1	0.79	0.20	71,71,71,71	0
56	MG	1A	3024	1/1	0.79	0.11	75,75,75,75	0
56	MG	1A	3105	1/1	0.79	0.23	65,65,65,65	0
56	MG	2A	3156	1/1	0.79	0.40	75,75,75,75	0
56	MG	1A	3315	1/1	0.79	0.24	50,50,50,50	0
56	MG	1A	3041	1/1	0.79	0.14	66,66,66,66	0
56	MG	2A	3047	1/1	0.79	0.10	63,63,63,63	0
56	MG	1a	1628	1/1	0.79	0.14	82,82,82,82	0
56	MG	2a	1686	1/1	0.79	0.26	70,70,70,70	0
56	MG	2a	1687	1/1	0.79	0.23	65,65,65,65	0
56	MG	1A	3042	1/1	0.79	0.18	80,80,80,80	0
56	MG	2A	3319	1/1	0.79	0.25	61,61,61,61	0
56	MG	2A	3172	1/1	0.79	0.24	72,72,72,72	0
56	MG	1x	104	1/1	0.79	0.07	107,107,107,107	0
56	MG	2a	1703	1/1	0.79	0.22	88,88,88,88	0
56	MG	2A	3078	1/1	0.79	0.23	82,82,82,82	0
56	MG	2A	3180	1/1	0.79	0.27	79,79,79,79	0
56	MG	1A	3268	1/1	0.79	0.22	50,50,50,50	0
56	MG	1A	3333	1/1	0.79	0.12	73,73,73,73	0
56	MG	1a	1638	1/1	0.80	0.12	67,67,67,67	0
56	MG	2A	3018	1/1	0.80	0.14	60,60,60,60	0
56	MG	1a	1639	1/1	0.80	0.12	92,92,92,92	0
56	MG	1A	3305	1/1	0.80	0.39	50,50,50,50	0
56	MG	1a	1687	1/1	0.80	0.21	90,90,90,90	0
56	MG	2A	3423	1/1	0.80	0.16	88,88,88,88	0
56	MG	2A	3200	1/1	0.80	0.19	81,81,81,81	0
56	MG	2A	3201	1/1	0.80	0.20	81,81,81,81	0
56	MG	2A	3031	1/1	0.80	0.15	89,89,89,89	0
56	MG	1A	3270	1/1	0.80	0.31	53,53,53,53	0
56	MG	1A	3091	1/1	0.80	0.16	58,58,58,58	0
56	MG	1t	201	1/1	0.80	0.29	89,89,89,89	0
56	MG	1A	3118	1/1	0.80	0.26	63,63,63,63	0
56	MG	1a	1657	1/1	0.80	0.29	72,72,72,72	0
56	MG	2A	3338	1/1	0.80	0.32	68,68,68,68	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	2A	3143	1/1	0.80	0.26	60,60,60,60	0
56	MG	1A	3433	1/1	0.80	0.21	67,67,67,67	0
56	MG	1A	3150	1/1	0.80	0.13	93,93,93,93	0
56	MG	1A	3130	1/1	0.80	0.12	73,73,73,73	0
56	MG	2A	3048	1/1	0.80	0.15	85,85,85,85	0
56	MG	2B	204	1/1	0.80	0.31	91,91,91,91	0
56	MG	1A	3329	1/1	0.80	0.23	52,52,52,52	0
56	MG	1A	3004	1/1	0.80	0.29	75,75,75,75	0
56	MG	2a	1688	1/1	0.80	0.13	59,59,59,59	0
56	MG	2A	3066	1/1	0.80	0.21	76,76,76,76	0
56	MG	2A	3072	1/1	0.80	0.26	77,77,77,77	0
56	MG	2A	3264	1/1	0.80	0.18	76,76,76,76	0
56	MG	2A	3009	1/1	0.80	0.10	67,67,67,67	0
56	MG	1A	3079	1/1	0.80	0.28	73,73,73,73	0
56	MG	1A	3388	1/1	0.80	0.27	50,50,50,50	0
56	MG	2A	3288	1/1	0.80	0.25	55,55,55,55	0
56	MG	2A	3402	1/1	0.80	0.15	73,73,73,73	0
56	MG	1A	3352	1/1	0.80	0.32	50,50,50,50	0
56	MG	2E	302	1/1	0.81	0.32	69,69,69,69	0
56	MG	1a	1673	1/1	0.81	0.07	75,75,75,75	0
56	MG	2A	3210	1/1	0.81	0.19	71,71,71,71	0
56	MG	1A	3336	1/1	0.81	0.29	50,50,50,50	0
56	MG	1A	3298	1/1	0.81	0.11	71,71,71,71	0
56	MG	2a	1606	1/1	0.81	0.16	65,65,65,65	0
56	MG	1a	1682	1/1	0.81	0.16	69,69,69,69	0
56	MG	2A	3028	1/1	0.81	0.12	86,86,86,86	0
56	MG	2A	3029	1/1	0.81	0.15	73,73,73,73	0
56	MG	1B	206	1/1	0.81	0.28	73,73,73,73	0
56	MG	2A	3388	1/1	0.81	0.33	50,50,50,50	0
56	MG	1A	3073	1/1	0.81	0.29	60,60,60,60	0
56	MG	2A	3394	1/1	0.81	0.33	67,67,67,67	0
56	MG	2a	1631	1/1	0.81	0.21	81,81,81,81	0
56	MG	1A	3465	1/1	0.81	0.34	63,63,63,63	0
56	MG	1A	3466	1/1	0.81	0.21	79,79,79,79	0
56	MG	2A	3250	1/1	0.81	0.14	88,88,88,88	0
56	MG	1A	3151	1/1	0.81	0.19	84,84,84,84	0
56	MG	1a	1635	1/1	0.81	0.20	76,76,76,76	0
56	MG	2a	1638	1/1	0.81	0.15	68,68,68,68	0
56	MG	1A	3309	1/1	0.81	0.27	62,62,62,62	0
56	MG	2A	3267	1/1	0.81	0.21	53,53,53,53	0
56	MG	2A	3409	1/1	0.81	0.19	69,69,69,69	0
56	MG	1A	3472	1/1	0.81	0.15	70,70,70,70	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	1A	3075	1/1	0.81	0.09	83,83,83,83	0
56	MG	1A	3206	1/1	0.81	0.16	59,59,59,59	0
56	MG	2A	3159	1/1	0.81	0.23	76,76,76,76	0
56	MG	2A	3053	1/1	0.81	0.13	59,59,59,59	0
56	MG	1A	3404	1/1	0.81	0.38	50,50,50,50	0
56	MG	1A	3489	1/1	0.81	0.17	85,85,85,85	0
56	MG	1A	3138	1/1	0.81	0.25	68,68,68,68	0
56	MG	2A	3068	1/1	0.81	0.19	79,79,79,79	0
56	MG	2A	3308	1/1	0.81	0.18	63,63,63,63	0
56	MG	2A	3069	1/1	0.81	0.10	82,82,82,82	0
56	MG	1A	3511	1/1	0.81	0.18	76,76,76,76	0
56	MG	1A	3127	1/1	0.81	0.20	73,73,73,73	0
56	MG	2A	3177	1/1	0.81	0.39	71,71,71,71	0
56	MG	2A	3076	1/1	0.81	0.18	67,67,67,67	0
56	MG	2A	3182	1/1	0.81	0.14	66,66,66,66	0
56	MG	1A	3068	1/1	0.81	0.11	67,67,67,67	0
56	MG	1A	3444	1/1	0.81	0.36	51,51,51,51	0
56	MG	1A	3533	1/1	0.81	0.17	104,104,104,104	0
56	MG	2A	3014	1/1	0.81	0.13	107,107,107,107	0
56	MG	1A	3016	1/1	0.81	0.22	79,79,79,79	0
56	MG	2A	3017	1/1	0.81	0.13	80,80,80,80	0
56	MG	2q	201	1/1	0.81	0.11	96,96,96,96	0
56	MG	1A	3454	1/1	0.82	0.26	50,50,50,50	0
56	MG	1v	101	1/1	0.82	0.15	67,67,67,67	0
56	MG	2A	3196	1/1	0.82	0.23	50,50,50,50	0
56	MG	1A	3173	1/1	0.82	0.20	66,66,66,66	0
56	MG	2a	1628	1/1	0.82	0.28	75,75,75,75	0
56	MG	1A	3243	1/1	0.82	0.34	50,50,50,50	0
56	MG	1A	3357	1/1	0.82	0.16	112,112,112,112	0
56	MG	1A	3326	1/1	0.82	0.51	54,54,54,54	0
56	MG	2A	3123	1/1	0.82	0.22	83,83,83,83	0
56	MG	2A	3133	1/1	0.82	0.20	76,76,76,76	0
56	MG	1A	3328	1/1	0.82	0.19	81,81,81,81	0
56	MG	2A	3001	1/1	0.82	0.43	61,61,61,61	0
56	MG	1A	3397	1/1	0.82	0.18	67,67,67,67	0
56	MG	2A	3051	1/1	0.82	0.15	73,73,73,73	0
56	MG	1a	1666	1/1	0.82	0.15	83,83,83,83	0
56	MG	1A	3166	1/1	0.82	0.15	66,66,66,66	0
56	MG	2a	1649	1/1	0.82	0.32	66,66,66,66	0
56	MG	1B	210	1/1	0.82	0.28	69,69,69,69	0
56	MG	1a	1670	1/1	0.82	0.13	73,73,73,73	0
56	MG	2A	3452	1/1	0.82	0.25	103,103,103,103	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	1A	3365	1/1	0.82	0.11	70,70,70,70	0
56	MG	2A	3246	1/1	0.82	0.23	69,69,69,69	0
56	MG	1A	3477	1/1	0.82	0.32	61,61,61,61	0
56	MG	1B	213	1/1	0.82	0.12	74,74,74,74	0
56	MG	2A	3369	1/1	0.82	0.14	78,78,78,78	0
56	MG	1a	1626	1/1	0.82	0.18	82,82,82,82	0
56	MG	1A	3366	1/1	0.82	0.10	57,57,57,57	0
56	MG	2a	1684	1/1	0.82	0.12	61,61,61,61	0
56	MG	2A	3257	1/1	0.82	0.25	50,50,50,50	0
56	MG	2A	3376	1/1	0.82	0.28	70,70,70,70	0
56	MG	1A	3225	1/1	0.82	0.17	80,80,80,80	0
56	MG	2F	301	1/1	0.82	0.25	79,79,79,79	0
56	MG	2a	1690	1/1	0.82	0.22	84,84,84,84	0
56	MG	2O	201	1/1	0.82	0.13	73,73,73,73	0
56	MG	23	101	1/1	0.82	0.23	65,65,65,65	0
56	MG	2A	3021	1/1	0.82	0.41	87,87,87,87	0
56	MG	1A	3443	1/1	0.82	0.23	65,65,65,65	0
56	MG	2a	1705	1/1	0.82	0.32	70,70,70,70	0
56	MG	2A	3280	1/1	0.82	0.44	50,50,50,50	0
56	MG	1A	3168	1/1	0.82	0.09	81,81,81,81	0
56	MG	1A	3254	1/1	0.82	0.30	69,69,69,69	0
56	MG	1A	3043	1/1	0.82	0.23	79,79,79,79	0
56	MG	16	101	1/1	0.82	0.32	83,83,83,83	0
56	MG	1A	3343	1/1	0.83	0.27	68,68,68,68	0
56	MG	1A	3432	1/1	0.83	0.23	61,61,61,61	0
56	MG	2A	3446	1/1	0.83	0.27	59,59,59,59	0
56	MG	1A	3221	1/1	0.83	0.57	50,50,50,50	0
56	MG	1A	3174	1/1	0.83	0.30	77,77,77,77	0
56	MG	1A	3263	1/1	0.83	0.23	64,64,64,64	0
56	MG	1A	3311	1/1	0.83	0.22	77,77,77,77	0
56	MG	2a	1640	1/1	0.83	0.29	67,67,67,67	0
56	MG	1a	1646	1/1	0.83	0.12	72,72,72,72	0
56	MG	2A	3097	1/1	0.83	0.20	77,77,77,77	0
56	MG	1A	3064	1/1	0.83	0.14	77,77,77,77	0
56	MG	1A	3195	1/1	0.83	0.27	50,50,50,50	0
56	MG	2A	3108	1/1	0.83	0.14	107,107,107,107	0
56	MG	1a	1659	1/1	0.83	0.23	68,68,68,68	0
56	MG	2A	3295	1/1	0.83	0.33	50,50,50,50	0
56	MG	2A	3113	1/1	0.83	0.12	70,70,70,70	0
56	MG	2D	303	1/1	0.83	0.15	61,61,61,61	0
56	MG	2A	3114	1/1	0.83	0.11	77,77,77,77	0
56	MG	2E	305	1/1	0.83	0.06	71,71,71,71	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	1A	3149	1/1	0.83	0.12	78,78,78,78	0
56	MG	1x	109	1/1	0.83	0.27	88,88,88,88	0
56	MG	1A	3213	1/1	0.83	0.31	71,71,71,71	0
56	MG	1A	3239	1/1	0.83	0.24	65,65,65,65	0
56	MG	1A	3411	1/1	0.83	0.24	57,57,57,57	0
56	MG	2A	3408	1/1	0.83	0.10	65,65,65,65	0
56	MG	1A	3170	1/1	0.83	0.14	73,73,73,73	0
56	MG	1A	3462	1/1	0.83	0.34	50,50,50,50	0
56	MG	2a	1692	1/1	0.83	0.14	59,59,59,59	0
56	MG	1A	3186	1/1	0.83	0.34	50,50,50,50	0
56	MG	1a	1620	1/1	0.83	0.13	95,95,95,95	0
56	MG	1A	3330	1/1	0.83	0.20	65,65,65,65	0
56	MG	1A	3035	1/1	0.83	0.07	55,55,55,55	0
56	MG	1A	3137	1/1	0.83	0.23	71,71,71,71	0
56	MG	2a	1706	1/1	0.83	0.27	62,62,62,62	0
56	MG	2a	1710	1/1	0.83	0.15	114,114,114,114	0
56	MG	1A	3341	1/1	0.83	0.32	50,50,50,50	0
56	MG	2a	1621	1/1	0.83	0.11	89,89,89,89	0
56	MG	1A	3389	1/1	0.83	0.26	60,60,60,60	0
56	MG	1A	3475	1/1	0.83	0.10	60,60,60,60	0
56	MG	2A	3433	1/1	0.83	0.21	66,66,66,66	0
56	MG	2A	3025	1/1	0.84	0.16	92,92,92,92	0
56	MG	2A	3026	1/1	0.84	0.27	69,69,69,69	0
56	MG	1A	3367	1/1	0.84	0.21	65,65,65,65	0
56	MG	1a	1634	1/1	0.84	0.14	86,86,86,86	0
56	MG	2A	3205	1/1	0.84	0.20	68,68,68,68	0
56	MG	2A	3362	1/1	0.84	0.15	77,77,77,77	0
56	MG	2A	3102	1/1	0.84	0.20	90,90,90,90	0
56	MG	1A	3408	1/1	0.84	0.14	72,72,72,72	0
56	MG	1A	3103	1/1	0.84	0.15	73,73,73,73	0
56	MG	2a	1607	1/1	0.84	0.17	70,70,70,70	0
56	MG	2a	1609	1/1	0.84	0.10	74,74,74,74	0
56	MG	2A	3223	1/1	0.84	0.22	55,55,55,55	0
56	MG	1A	3077	1/1	0.84	0.21	72,72,72,72	0
56	MG	2a	1612	1/1	0.84	0.10	74,74,74,74	0
56	MG	1a	1640	1/1	0.84	0.09	84,84,84,84	0
56	MG	2A	3035	1/1	0.84	0.15	92,92,92,92	0
56	MG	2A	3036	1/1	0.84	0.15	92,92,92,92	0
56	MG	1A	3348	1/1	0.84	0.32	74,74,74,74	0
56	MG	1A	3380	1/1	0.84	0.18	55,55,55,55	0
56	MG	2A	3124	1/1	0.84	0.12	77,77,77,77	0
56	MG	2A	3127	1/1	0.84	0.13	68,68,68,68	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	2A	3248	1/1	0.84	0.21	71,71,71,71	0
56	MG	2A	3129	1/1	0.84	0.16	67,67,67,67	0
56	MG	1A	3351	1/1	0.84	0.20	50,50,50,50	0
56	MG	1A	3123	1/1	0.84	0.27	72,72,72,72	0
56	MG	2A	3252	1/1	0.84	0.14	79,79,79,79	0
56	MG	2a	1636	1/1	0.84	0.24	79,79,79,79	0
56	MG	2A	3141	1/1	0.84	0.17	57,57,57,57	0
56	MG	1A	3420	1/1	0.84	0.17	58,58,58,58	0
56	MG	2A	3260	1/1	0.84	0.30	62,62,62,62	0
56	MG	2A	3411	1/1	0.84	0.26	62,62,62,62	0
56	MG	2a	1641	1/1	0.84	0.23	63,63,63,63	0
56	MG	2A	3144	1/1	0.84	0.17	88,88,88,88	0
56	MG	1a	1654	1/1	0.84	0.24	82,82,82,82	0
56	MG	2A	3269	1/1	0.84	0.18	73,73,73,73	0
56	MG	2A	3425	1/1	0.84	0.22	72,72,72,72	0
56	MG	2A	3050	1/1	0.84	0.14	87,87,87,87	0
56	MG	1a	1607	1/1	0.84	0.11	81,81,81,81	0
56	MG	1A	3106	1/1	0.84	0.19	90,90,90,90	0
56	MG	1A	3069	1/1	0.84	0.08	65,65,65,65	0
56	MG	1A	3017	1/1	0.84	0.28	77,77,77,77	0
56	MG	2A	3065	1/1	0.84	0.08	101,101,101,101	0
56	MG	2a	1674	1/1	0.84	0.23	67,67,67,67	0
56	MG	1A	3257	1/1	0.84	0.16	51,51,51,51	0
56	MG	2A	3437	1/1	0.84	0.24	51,51,51,51	0
56	MG	2A	3067	1/1	0.84	0.11	84,84,84,84	0
56	MG	2a	1680	1/1	0.84	0.28	53,53,53,53	0
56	MG	2A	3443	1/1	0.84	0.27	50,50,50,50	0
56	MG	2a	1685	1/1	0.84	0.26	67,67,67,67	0
56	MG	2A	3299	1/1	0.84	0.27	75,75,75,75	0
56	MG	1a	1615	1/1	0.84	0.14	80,80,80,80	0
56	MG	1A	3468	1/1	0.84	0.18	69,69,69,69	0
56	MG	2A	3451	1/1	0.84	0.20	62,62,62,62	0
56	MG	2A	3070	1/1	0.84	0.10	64,64,64,64	0
56	MG	1A	3056	1/1	0.84	0.17	82,82,82,82	0
56	MG	1a	1618	1/1	0.84	0.21	70,70,70,70	0
56	MG	2a	1694	1/1	0.84	0.19	73,73,73,73	0
56	MG	2a	1697	1/1	0.84	0.09	83,83,83,83	0
56	MG	2A	3467	1/1	0.84	0.09	86,86,86,86	0
56	MG	1A	3196	1/1	0.84	0.17	70,70,70,70	0
56	MG	1A	3023	1/1	0.84	0.14	57,57,57,57	0
56	MG	1a	1677	1/1	0.84	0.10	108,108,108,108	0
56	MG	2A	3082	1/1	0.84	0.19	71,71,71,71	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	1A	3183	1/1	0.84	0.15	59,59,59,59	0
56	MG	2A	3183	1/1	0.84	0.15	53,53,53,53	0
56	MG	2B	209	1/1	0.84	0.36	75,75,75,75	0
56	MG	1A	3476	1/1	0.84	0.24	54,54,54,54	0
56	MG	1A	3436	1/1	0.84	0.16	75,75,75,75	0
56	MG	1D	302	1/1	0.84	0.17	78,78,78,78	0
56	MG	2A	3294	1/1	0.85	0.21	67,67,67,67	0
56	MG	1A	3299	1/1	0.85	0.21	71,71,71,71	0
56	MG	2a	1620	1/1	0.85	0.17	72,72,72,72	0
56	MG	2A	3420	1/1	0.85	0.21	50,50,50,50	0
56	MG	2a	1627	1/1	0.85	0.18	82,82,82,82	0
56	MG	1Q	201	1/1	0.85	0.16	78,78,78,78	0
56	MG	2A	3185	1/1	0.85	0.13	72,72,72,72	0
56	MG	1X	101	1/1	0.85	0.25	85,85,85,85	0
56	MG	2A	3111	1/1	0.85	0.22	77,77,77,77	0
56	MG	2A	3197	1/1	0.85	0.11	87,87,87,87	0
56	MG	2A	3040	1/1	0.85	0.22	56,56,56,56	0
56	MG	1A	3300	1/1	0.85	0.13	70,70,70,70	0
56	MG	1A	3163	1/1	0.85	0.18	65,65,65,65	0
56	MG	1A	3256	1/1	0.85	0.35	50,50,50,50	0
56	MG	2A	3117	1/1	0.85	0.12	64,64,64,64	0
56	MG	17	102	1/1	0.85	0.08	54,54,54,54	0
56	MG	1A	3113	1/1	0.85	0.15	75,75,75,75	0
56	MG	2A	3439	1/1	0.85	0.22	56,56,56,56	0
56	MG	2A	3442	1/1	0.85	0.17	76,76,76,76	0
56	MG	1A	3258	1/1	0.85	0.26	68,68,68,68	0
56	MG	2A	3214	1/1	0.85	0.22	77,77,77,77	0
56	MG	1A	3440	1/1	0.85	0.27	81,81,81,81	0
56	MG	1A	3312	1/1	0.85	0.38	62,62,62,62	0
56	MG	2A	3342	1/1	0.85	0.24	61,61,61,61	0
56	MG	1A	3083	1/1	0.85	0.14	55,55,55,55	0
56	MG	1A	3229	1/1	0.85	0.20	62,62,62,62	0
56	MG	1A	3407	1/1	0.85	0.24	61,61,61,61	0
56	MG	1A	3125	1/1	0.85	0.20	51,51,51,51	0
56	MG	1A	3209	1/1	0.85	0.18	71,71,71,71	0
56	MG	2A	3360	1/1	0.85	0.16	76,76,76,76	0
56	MG	1A	3275	1/1	0.85	0.19	54,54,54,54	0
56	MG	1A	3460	1/1	0.85	0.13	64,64,64,64	0
56	MG	2a	1678	1/1	0.85	0.31	59,59,59,59	0
56	MG	2A	3236	1/1	0.85	0.18	55,55,55,55	0
56	MG	1A	3135	1/1	0.85	0.08	100,100,100,100	0
56	MG	1A	3187	1/1	0.85	0.21	80,80,80,80	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	1a	1674	1/1	0.85	0.07	89,89,89,89	0
56	MG	1A	3463	1/1	0.85	0.34	60,60,60,60	0
56	MG	1A	3369	1/1	0.85	0.23	51,51,51,51	0
56	MG	2A	3381	1/1	0.85	0.09	58,58,58,58	0
56	MG	2A	3386	1/1	0.85	0.05	66,66,66,66	0
56	MG	1A	3373	1/1	0.85	0.10	71,71,71,71	0
56	MG	2A	3084	1/1	0.85	0.14	56,56,56,56	0
56	MG	1A	3240	1/1	0.85	0.17	60,60,60,60	0
56	MG	2a	1695	1/1	0.85	0.11	53,53,53,53	0
56	MG	1a	1627	1/1	0.85	0.21	67,67,67,67	0
56	MG	2A	3164	1/1	0.85	0.15	78,78,78,78	0
56	MG	2A	3399	1/1	0.85	0.12	80,80,80,80	0
56	MG	1A	3109	1/1	0.85	0.19	52,52,52,52	0
56	MG	1A	3074	1/1	0.85	0.16	71,71,71,71	0
56	MG	1a	1686	1/1	0.85	0.33	50,50,50,50	0
56	MG	2A	3173	1/1	0.85	0.19	70,70,70,70	0
56	MG	2A	3093	1/1	0.85	0.19	71,71,71,71	0
56	MG	1A	3176	1/1	0.85	0.10	63,63,63,63	0
56	MG	1E	303	1/1	0.85	0.21	77,77,77,77	0
56	MG	2a	1614	1/1	0.85	0.08	76,76,76,76	0
56	MG	1A	3218	1/1	0.85	0.27	73,73,73,73	0
56	MG	2A	3190	1/1	0.86	0.16	53,53,53,53	0
56	MG	1A	3448	1/1	0.86	0.22	63,63,63,63	0
56	MG	1A	3306	1/1	0.86	0.19	50,50,50,50	0
56	MG	2a	1624	1/1	0.86	0.10	74,74,74,74	0
56	MG	2A	3198	1/1	0.86	0.12	75,75,75,75	0
56	MG	1A	3266	1/1	0.86	0.22	59,59,59,59	0
56	MG	1A	3531	1/1	0.86	0.16	71,71,71,71	0
56	MG	2A	3058	1/1	0.86	0.14	77,77,77,77	0
56	MG	1A	3190	1/1	0.86	0.24	78,78,78,78	0
56	MG	1A	3419	1/1	0.86	0.20	62,62,62,62	0
56	MG	1a	1611	1/1	0.86	0.15	78,78,78,78	0
56	MG	2A	3137	1/1	0.86	0.13	64,64,64,64	0
56	MG	2A	3138	1/1	0.86	0.15	90,90,90,90	0
56	MG	1A	3349	1/1	0.86	0.20	65,65,65,65	0
56	MG	1A	3350	1/1	0.86	0.21	72,72,72,72	0
56	MG	1A	3062	1/1	0.86	0.18	56,56,56,56	0
56	MG	2A	3445	1/1	0.86	0.40	51,51,51,51	0
56	MG	1A	3092	1/1	0.86	0.20	66,66,66,66	0
56	MG	2a	1643	1/1	0.86	0.15	77,77,77,77	0
56	MG	2A	3145	1/1	0.86	0.20	82,82,82,82	0
56	MG	1A	3072	1/1	0.86	0.17	73,73,73,73	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	1A	3037	1/1	0.86	0.15	53,53,53,53	0
56	MG	2A	3353	1/1	0.86	0.33	65,65,65,65	0
56	MG	2a	1660	1/1	0.86	0.32	72,72,72,72	0
56	MG	2A	3453	1/1	0.86	0.23	52,52,52,52	0
56	MG	2a	1663	1/1	0.86	0.14	50,50,50,50	0
56	MG	1A	3205	1/1	0.86	0.18	69,69,69,69	0
56	MG	1a	1621	1/1	0.86	0.18	83,83,83,83	0
56	MG	1A	3321	1/1	0.86	0.15	87,87,87,87	0
56	MG	2A	3154	1/1	0.86	0.14	76,76,76,76	0
56	MG	2a	1669	1/1	0.86	0.18	74,74,74,74	0
56	MG	2A	3473	1/1	0.86	0.17	95,95,95,95	0
56	MG	2A	3245	1/1	0.86	0.23	50,50,50,50	0
56	MG	1A	3044	1/1	0.86	0.12	59,59,59,59	0
56	MG	1A	3226	1/1	0.86	0.18	68,68,68,68	0
56	MG	2A	3158	1/1	0.86	0.17	68,68,68,68	0
56	MG	2A	3086	1/1	0.86	0.33	79,79,79,79	0
56	MG	1A	3208	1/1	0.86	0.22	50,50,50,50	0
56	MG	1A	3438	1/1	0.86	0.16	50,50,50,50	0
56	MG	2A	3162	1/1	0.86	0.18	64,64,64,64	0
56	MG	2E	301	1/1	0.86	0.10	69,69,69,69	0
56	MG	2A	3255	1/1	0.86	0.34	62,62,62,62	0
56	MG	2A	3387	1/1	0.86	0.25	50,50,50,50	0
56	MG	1A	3087	1/1	0.86	0.08	56,56,56,56	0
56	MG	1a	1631	1/1	0.86	0.19	70,70,70,70	0
56	MG	2A	3262	1/1	0.86	0.36	50,50,50,50	0
56	MG	1A	3484	1/1	0.86	0.22	63,63,63,63	0
56	MG	1A	3061	1/1	0.86	0.32	57,57,57,57	0
56	MG	1V	202	1/1	0.86	0.28	68,68,68,68	0
56	MG	2a	1603	1/1	0.86	0.25	70,70,70,70	0
56	MG	1A	3177	1/1	0.86	0.17	61,61,61,61	0
56	MG	2A	3278	1/1	0.86	0.28	50,50,50,50	0
56	MG	2A	3037	1/1	0.86	0.15	79,79,79,79	0
56	MG	1A	3488	1/1	0.86	0.23	50,50,50,50	0
56	MG	1A	3303	1/1	0.86	0.27	53,53,53,53	0
56	MG	1A	3265	1/1	0.86	0.17	53,53,53,53	0
56	MG	2A	3289	1/1	0.86	0.25	51,51,51,51	0
56	MG	1A	3495	1/1	0.86	0.27	50,50,50,50	0
56	MG	18	101	1/1	0.86	0.24	68,68,68,68	0
56	MG	1x	107	1/1	0.86	0.15	80,80,80,80	0
56	MG	1A	3447	1/1	0.86	0.15	72,72,72,72	0
56	MG	2r	101	1/1	0.86	0.12	84,84,84,84	0
56	MG	2A	3126	1/1	0.87	0.21	80,80,80,80	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	1A	3193	1/1	0.87	0.18	64,64,64,64	0
56	MG	1B	214	1/1	0.87	0.16	85,85,85,85	0
56	MG	2A	3131	1/1	0.87	0.29	51,51,51,51	0
56	MG	2A	3286	1/1	0.87	0.21	51,51,51,51	0
56	MG	2A	3027	1/1	0.87	0.11	82,82,82,82	0
56	MG	1A	3078	1/1	0.87	0.34	64,64,64,64	0
56	MG	2A	3199	1/1	0.87	0.33	72,72,72,72	0
56	MG	2A	3293	1/1	0.87	0.28	51,51,51,51	0
56	MG	2a	1623	1/1	0.87	0.12	84,84,84,84	0
56	MG	1a	1645	1/1	0.87	0.11	75,75,75,75	0
56	MG	2a	1626	1/1	0.87	0.21	67,67,67,67	0
56	MG	2A	3030	1/1	0.87	0.11	92,92,92,92	0
56	MG	2A	3419	1/1	0.87	0.15	72,72,72,72	0
56	MG	1a	1612	1/1	0.87	0.20	91,91,91,91	0
56	MG	1a	1649	1/1	0.87	0.11	66,66,66,66	0
56	MG	1A	3045	1/1	0.87	0.11	74,74,74,74	0
56	MG	2A	3303	1/1	0.87	0.22	69,69,69,69	0
56	MG	1D	301	1/1	0.87	0.24	72,72,72,72	0
56	MG	2A	3306	1/1	0.87	0.26	56,56,56,56	0
56	MG	1A	3093	1/1	0.87	0.13	82,82,82,82	0
56	MG	2A	3208	1/1	0.87	0.13	95,95,95,95	0
56	MG	2A	3312	1/1	0.87	0.30	72,72,72,72	0
56	MG	1A	3502	1/1	0.87	0.13	79,79,79,79	0
56	MG	2A	3089	1/1	0.87	0.19	78,78,78,78	0
56	MG	1A	3464	1/1	0.87	0.10	55,55,55,55	0
56	MG	2A	3220	1/1	0.87	0.17	78,78,78,78	0
56	MG	2A	3320	1/1	0.87	0.15	76,76,76,76	0
56	MG	1H	201	1/1	0.87	0.19	68,68,68,68	0
56	MG	2A	3324	1/1	0.87	0.25	73,73,73,73	0
56	MG	2a	1650	1/1	0.87	0.17	66,66,66,66	0
56	MG	2a	1657	1/1	0.87	0.25	50,50,50,50	0
56	MG	2A	3444	1/1	0.87	0.21	50,50,50,50	0
56	MG	1A	3415	1/1	0.87	0.23	71,71,71,71	0
56	MG	1A	3441	1/1	0.87	0.20	57,57,57,57	0
56	MG	2A	3094	1/1	0.87	0.07	74,74,74,74	0
56	MG	2A	3448	1/1	0.87	0.26	59,59,59,59	0
56	MG	2A	3449	1/1	0.87	0.46	50,50,50,50	0
56	MG	2A	3335	1/1	0.87	0.14	70,70,70,70	0
56	MG	2A	3227	1/1	0.87	0.25	54,54,54,54	0
56	MG	2A	3041	1/1	0.87	0.09	76,76,76,76	0
56	MG	1A	3278	1/1	0.87	0.24	66,66,66,66	0
56	MG	1A	3009	1/1	0.87	0.09	85,85,85,85	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	1A	3403	1/1	0.87	0.21	50,50,50,50	0
56	MG	2A	3103	1/1	0.87	0.10	61,61,61,61	0
56	MG	2A	3239	1/1	0.87	0.23	64,64,64,64	0
56	MG	2A	3106	1/1	0.87	0.10	70,70,70,70	0
56	MG	1A	3260	1/1	0.87	0.26	50,50,50,50	0
56	MG	2a	1681	1/1	0.87	0.13	71,71,71,71	0
56	MG	2B	201	1/1	0.87	0.15	70,70,70,70	0
56	MG	2A	3356	1/1	0.87	0.20	77,77,77,77	0
56	MG	2A	3357	1/1	0.87	0.35	67,67,67,67	0
56	MG	2A	3166	1/1	0.87	0.21	58,58,58,58	0
56	MG	15	101	1/1	0.87	0.20	53,53,53,53	0
56	MG	2A	3365	1/1	0.87	0.13	58,58,58,58	0
56	MG	2A	3170	1/1	0.87	0.12	58,58,58,58	0
56	MG	1A	3262	1/1	0.87	0.24	59,59,59,59	0
56	MG	1A	3152	1/1	0.87	0.10	100,100,100,100	0
56	MG	1A	3293	1/1	0.87	0.17	71,71,71,71	0
56	MG	2E	303	1/1	0.87	0.17	50,50,50,50	0
56	MG	2A	3174	1/1	0.87	0.13	52,52,52,52	0
56	MG	1a	1680	1/1	0.87	0.17	62,62,62,62	0
56	MG	1B	207	1/1	0.87	0.11	77,77,77,77	0
56	MG	2A	3379	1/1	0.87	0.19	78,78,78,78	0
56	MG	1A	3451	1/1	0.87	0.06	52,52,52,52	0
56	MG	1A	3453	1/1	0.87	0.28	60,60,60,60	0
56	MG	2A	3265	1/1	0.87	0.11	51,51,51,51	0
56	MG	2A	3181	1/1	0.87	0.20	65,65,65,65	0
56	MG	2A	3389	1/1	0.87	0.18	71,71,71,71	0
56	MG	1A	3116	1/1	0.87	0.12	65,65,65,65	0
56	MG	1A	3295	1/1	0.87	0.07	59,59,59,59	0
56	MG	2A	3275	1/1	0.87	0.12	61,61,61,61	0
56	MG	2A	3277	1/1	0.87	0.11	72,72,72,72	0
56	MG	2A	3273	1/1	0.88	0.12	56,56,56,56	0
56	MG	2A	3359	1/1	0.88	0.12	59,59,59,59	0
56	MG	1A	3425	1/1	0.88	0.26	73,73,73,73	0
56	MG	1A	3136	1/1	0.88	0.19	63,63,63,63	0
56	MG	1A	3310	1/1	0.88	0.29	54,54,54,54	0
56	MG	1A	3219	1/1	0.88	0.21	64,64,64,64	0
56	MG	1A	3141	1/1	0.88	0.08	89,89,89,89	0
56	MG	1A	3313	1/1	0.88	0.22	68,68,68,68	0
56	MG	1A	3199	1/1	0.88	0.24	61,61,61,61	0
56	MG	2A	3207	1/1	0.88	0.34	63,63,63,63	0
56	MG	2A	3375	1/1	0.88	0.22	62,62,62,62	0
56	MG	1A	3202	1/1	0.88	0.15	52,52,52,52	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	2A	3458	1/1	0.88	0.18	67,67,67,67	0
56	MG	1A	3434	1/1	0.88	0.15	54,54,54,54	0
56	MG	2a	1647	1/1	0.88	0.08	81,81,81,81	0
56	MG	2A	3211	1/1	0.88	0.22	60,60,60,60	0
56	MG	1A	3319	1/1	0.88	0.36	50,50,50,50	0
56	MG	1A	3143	1/1	0.88	0.22	76,76,76,76	0
56	MG	2a	1656	1/1	0.88	0.19	81,81,81,81	0
56	MG	1A	3052	1/1	0.88	0.18	71,71,71,71	0
56	MG	1x	106	1/1	0.88	0.11	79,79,79,79	0
56	MG	2A	3300	1/1	0.88	0.07	60,60,60,60	0
56	MG	1a	1610	1/1	0.88	0.13	68,68,68,68	0
56	MG	2A	3101	1/1	0.88	0.12	75,75,75,75	0
56	MG	1A	3153	1/1	0.88	0.34	61,61,61,61	0
56	MG	1A	3439	1/1	0.88	0.27	70,70,70,70	0
56	MG	1A	3406	1/1	0.88	0.18	59,59,59,59	0
56	MG	2D	302	1/1	0.88	0.09	62,62,62,62	0
56	MG	1A	3157	1/1	0.88	0.15	77,77,77,77	0
56	MG	2a	1670	1/1	0.88	0.16	62,62,62,62	0
56	MG	2A	3004	1/1	0.88	0.11	67,67,67,67	0
56	MG	2A	3005	1/1	0.88	0.29	68,68,68,68	0
56	MG	1A	3327	1/1	0.88	0.19	56,56,56,56	0
56	MG	2A	3405	1/1	0.88	0.06	71,71,71,71	0
56	MG	2A	3008	1/1	0.88	0.11	71,71,71,71	0
56	MG	1A	3158	1/1	0.88	0.33	69,69,69,69	0
56	MG	2a	1679	1/1	0.88	0.21	67,67,67,67	0
56	MG	2Z	301	1/1	0.88	0.16	54,54,54,54	0
56	MG	1A	3191	1/1	0.88	0.24	51,51,51,51	0
56	MG	2A	3247	1/1	0.88	0.27	50,50,50,50	0
56	MG	2A	3059	1/1	0.88	0.27	62,62,62,62	0
56	MG	2A	3414	1/1	0.88	0.19	76,76,76,76	0
56	MG	2A	3326	1/1	0.88	0.19	76,76,76,76	0
56	MG	1D	303	1/1	0.88	0.27	70,70,70,70	0
56	MG	2A	3329	1/1	0.88	0.16	61,61,61,61	0
56	MG	2A	3120	1/1	0.88	0.24	66,66,66,66	0
56	MG	2a	1691	1/1	0.88	0.19	62,62,62,62	0
56	MG	2a	1608	1/1	0.88	0.17	58,58,58,58	0
56	MG	1A	3178	1/1	0.88	0.18	57,57,57,57	0
56	MG	1A	3267	1/1	0.88	0.18	54,54,54,54	0
56	MG	1a	1622	1/1	0.88	0.07	99,99,99,99	0
56	MG	1A	3374	1/1	0.88	0.07	68,68,68,68	0
56	MG	2A	3339	1/1	0.88	0.34	52,52,52,52	0
56	MG	2a	1700	1/1	0.88	0.25	50,50,50,50	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	2A	3429	1/1	0.88	0.22	60,60,60,60	0
56	MG	1A	3146	1/1	0.88	0.23	65,65,65,65	0
56	MG	1P	202	1/1	0.88	0.35	84,84,84,84	0
56	MG	2A	3432	1/1	0.88	0.23	74,74,74,74	0
56	MG	1A	3131	1/1	0.88	0.43	53,53,53,53	0
56	MG	2A	3195	1/1	0.88	0.10	65,65,65,65	0
56	MG	2A	3435	1/1	0.88	0.21	71,71,71,71	0
56	MG	1A	3505	1/1	0.88	0.42	54,54,54,54	0
56	MG	1A	3272	1/1	0.88	0.31	50,50,50,50	0
56	MG	1a	1630	1/1	0.88	0.14	73,73,73,73	0
56	MG	1A	3274	1/1	0.88	0.16	55,55,55,55	0
56	MG	1A	3547	1/1	0.89	0.16	78,78,78,78	0
56	MG	2a	1625	1/1	0.89	0.08	74,74,74,74	0
56	MG	2A	3057	1/1	0.89	0.11	90,90,90,90	0
56	MG	1A	3469	1/1	0.89	0.23	61,61,61,61	0
56	MG	1A	3342	1/1	0.89	0.20	58,58,58,58	0
56	MG	2A	3060	1/1	0.89	0.17	71,71,71,71	0
56	MG	2A	3347	1/1	0.89	0.19	75,75,75,75	0
56	MG	2A	3350	1/1	0.89	0.35	69,69,69,69	0
56	MG	2A	3179	1/1	0.89	0.17	75,75,75,75	0
56	MG	17	101	1/1	0.89	0.11	77,77,77,77	0
56	MG	1a	1676	1/1	0.89	0.26	67,67,67,67	0
56	MG	2A	3122	1/1	0.89	0.12	66,66,66,66	0
56	MG	1A	3161	1/1	0.89	0.13	69,69,69,69	0
56	MG	2A	3266	1/1	0.89	0.12	59,59,59,59	0
56	MG	1A	3424	1/1	0.89	0.19	58,58,58,58	0
56	MG	1a	1632	1/1	0.89	0.13	68,68,68,68	0
56	MG	1A	3304	1/1	0.89	0.20	63,63,63,63	0
56	MG	2A	3128	1/1	0.89	0.14	88,88,88,88	0
56	MG	2A	3364	1/1	0.89	0.15	65,65,65,65	0
56	MG	1A	3399	1/1	0.89	0.09	62,62,62,62	0
56	MG	2A	3130	1/1	0.89	0.19	76,76,76,76	0
56	MG	2A	3071	1/1	0.89	0.12	72,72,72,72	0
56	MG	2A	3457	1/1	0.89	0.21	51,51,51,51	0
56	MG	2a	1652	1/1	0.89	0.12	69,69,69,69	0
56	MG	1A	3040	1/1	0.89	0.18	68,68,68,68	0
56	MG	2A	3281	1/1	0.89	0.20	57,57,57,57	0
56	MG	2A	3134	1/1	0.89	0.17	58,58,58,58	0
56	MG	2A	3373	1/1	0.89	0.21	73,73,73,73	0
56	MG	2A	3374	1/1	0.89	0.24	50,50,50,50	0
56	MG	2A	3073	1/1	0.89	0.14	50,50,50,50	0
56	MG	1a	1637	1/1	0.89	0.09	71,71,71,71	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	2a	1665	1/1	0.89	0.23	54,54,54,54	0
56	MG	2B	202	1/1	0.89	0.07	89,89,89,89	0
56	MG	2A	3287	1/1	0.89	0.23	51,51,51,51	0
56	MG	1A	3480	1/1	0.89	0.17	61,61,61,61	0
56	MG	2B	205	1/1	0.89	0.26	50,50,50,50	0
56	MG	1A	3090	1/1	0.89	0.46	75,75,75,75	0
56	MG	2A	3382	1/1	0.89	0.13	70,70,70,70	0
56	MG	1A	3142	1/1	0.89	0.29	67,67,67,67	0
56	MG	1A	3097	1/1	0.89	0.06	61,61,61,61	0
56	MG	2A	3083	1/1	0.89	0.09	57,57,57,57	0
56	MG	1e	201	1/1	0.89	0.06	80,80,80,80	0
56	MG	1A	3431	1/1	0.89	0.28	61,61,61,61	0
56	MG	2A	3149	1/1	0.89	0.35	64,64,64,64	0
56	MG	1A	3071	1/1	0.89	0.15	54,54,54,54	0
56	MG	2A	3217	1/1	0.89	0.12	71,71,71,71	0
56	MG	2A	3302	1/1	0.89	0.20	81,81,81,81	0
56	MG	1A	3457	1/1	0.89	0.20	58,58,58,58	0
56	MG	1A	3273	1/1	0.89	0.14	53,53,53,53	0
56	MG	20	101	1/1	0.89	0.28	64,64,64,64	0
56	MG	2A	3305	1/1	0.89	0.32	85,85,85,85	0
56	MG	1A	3501	1/1	0.89	0.17	66,66,66,66	0
56	MG	1A	3355	1/1	0.89	0.24	53,53,53,53	0
56	MG	1A	3085	1/1	0.89	0.28	77,77,77,77	0
56	MG	2a	1602	1/1	0.89	0.11	78,78,78,78	0
56	MG	1a	1655	1/1	0.89	0.12	84,84,84,84	0
56	MG	1A	3387	1/1	0.89	0.27	65,65,65,65	0
56	MG	2A	3228	1/1	0.89	0.15	78,78,78,78	0
56	MG	1A	3185	1/1	0.89	0.20	51,51,51,51	0
56	MG	1A	3277	1/1	0.89	0.10	83,83,83,83	0
56	MG	1A	3523	1/1	0.89	0.14	89,89,89,89	0
56	MG	2A	3418	1/1	0.89	0.15	77,77,77,77	0
56	MG	1A	3337	1/1	0.89	0.20	58,58,58,58	0
56	MG	1a	1664	1/1	0.89	0.17	92,92,92,92	0
56	MG	1a	1665	1/1	0.89	0.15	93,93,93,93	0
56	MG	2A	3049	1/1	0.89	0.13	90,90,90,90	0
56	MG	2A	3169	1/1	0.89	0.11	56,56,56,56	0
56	MG	1A	3021	1/1	0.89	0.14	81,81,81,81	0
56	MG	2A	3331	1/1	0.89	0.21	54,54,54,54	0
56	MG	1A	3393	1/1	0.89	0.21	50,50,50,50	0
56	MG	2A	3334	1/1	0.89	0.10	71,71,71,71	0
56	MG	1a	1625	1/1	0.89	0.05	87,87,87,87	0
56	MG	1A	3095	1/1	0.90	0.20	54,54,54,54	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	1A	3386	1/1	0.90	0.27	55,55,55,55	0
56	MG	1A	3197	1/1	0.90	0.12	53,53,53,53	0
56	MG	1A	3416	1/1	0.90	0.23	75,75,75,75	0
56	MG	1A	3446	1/1	0.90	0.15	75,75,75,75	0
56	MG	1A	3486	1/1	0.90	0.16	66,66,66,66	0
56	MG	2A	3366	1/1	0.90	0.19	68,68,68,68	0
56	MG	1A	3001	1/1	0.90	0.12	79,79,79,79	0
56	MG	1A	3224	1/1	0.90	0.13	81,81,81,81	0
56	MG	27	101	1/1	0.90	0.23	60,60,60,60	0
56	MG	2A	3080	1/1	0.90	0.18	87,87,87,87	0
56	MG	1A	3421	1/1	0.90	0.14	67,67,67,67	0
56	MG	1a	1660	1/1	0.90	0.19	62,62,62,62	0
56	MG	1A	3422	1/1	0.90	0.30	70,70,70,70	0
56	MG	1A	3022	1/1	0.90	0.10	82,82,82,82	0
56	MG	2a	1605	1/1	0.90	0.28	86,86,86,86	0
56	MG	1A	3496	1/1	0.90	0.28	51,51,51,51	0
56	MG	1A	3287	1/1	0.90	0.06	51,51,51,51	0
56	MG	2a	1673	1/1	0.90	0.16	53,53,53,53	0
56	MG	1A	3133	1/1	0.90	0.14	74,74,74,74	0
56	MG	2A	3378	1/1	0.90	0.11	63,63,63,63	0
56	MG	2A	3042	1/1	0.90	0.18	72,72,72,72	0
56	MG	1A	3002	1/1	0.90	0.09	67,67,67,67	0
56	MG	1A	3172	1/1	0.90	0.10	51,51,51,51	0
56	MG	2A	3384	1/1	0.90	0.17	77,77,77,77	0
56	MG	1A	3234	1/1	0.90	0.19	52,52,52,52	0
56	MG	2A	3323	1/1	0.90	0.22	64,64,64,64	0
56	MG	1A	3047	1/1	0.90	0.09	79,79,79,79	0
56	MG	2A	3147	1/1	0.90	0.16	61,61,61,61	0
56	MG	1Z	301	1/1	0.90	0.22	69,69,69,69	0
56	MG	1A	3210	1/1	0.90	0.16	54,54,54,54	0
56	MG	2a	1622	1/1	0.90	0.12	79,79,79,79	0
56	MG	2A	3098	1/1	0.90	0.14	81,81,81,81	0
56	MG	2A	3151	1/1	0.90	0.26	77,77,77,77	0
56	MG	1A	3018	1/1	0.90	0.20	50,50,50,50	0
56	MG	2A	3012	1/1	0.90	0.19	72,72,72,72	0
56	MG	1A	3301	1/1	0.90	0.19	57,57,57,57	0
56	MG	2A	3468	1/1	0.90	0.18	75,75,75,75	0
56	MG	1A	3025	1/1	0.90	0.20	70,70,70,70	0
56	MG	2a	1696	1/1	0.90	0.18	52,52,52,52	0
56	MG	2A	3105	1/1	0.90	0.30	75,75,75,75	0
56	MG	1A	3027	1/1	0.90	0.07	81,81,81,81	0
56	MG	1A	3010	1/1	0.90	0.12	88,88,88,88	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	2a	1701	1/1	0.90	0.26	65,65,65,65	0
56	MG	1A	3339	1/1	0.90	0.15	66,66,66,66	0
56	MG	1B	204	1/1	0.90	0.10	70,70,70,70	0
56	MG	2a	1704	1/1	0.90	0.15	65,65,65,65	0
56	MG	1A	3014	1/1	0.90	0.27	52,52,52,52	0
56	MG	2A	3219	1/1	0.90	0.15	90,90,90,90	0
56	MG	2A	3413	1/1	0.90	0.41	50,50,50,50	0
56	MG	1A	3249	1/1	0.90	0.22	50,50,50,50	0
56	MG	2A	3221	1/1	0.90	0.15	73,73,73,73	0
56	MG	2A	3417	1/1	0.90	0.20	52,52,52,52	0
56	MG	1A	3276	1/1	0.90	0.14	51,51,51,51	0
56	MG	1A	3080	1/1	0.90	0.07	76,76,76,76	0
56	MG	1B	209	1/1	0.90	0.10	57,57,57,57	0
56	MG	1A	3359	1/1	0.91	0.22	57,57,57,57	0
56	MG	2D	301	1/1	0.91	0.10	63,63,63,63	0
56	MG	1A	3015	1/1	0.91	0.12	54,54,54,54	0
56	MG	1A	3493	1/1	0.91	0.17	50,50,50,50	0
56	MG	2A	3007	1/1	0.91	0.08	82,82,82,82	0
56	MG	1A	3361	1/1	0.91	0.19	70,70,70,70	0
56	MG	1A	3288	1/1	0.91	0.10	56,56,56,56	0
56	MG	1A	3498	1/1	0.91	0.38	50,50,50,50	0
56	MG	2A	3424	1/1	0.91	0.59	81,81,81,81	0
56	MG	2A	3132	1/1	0.91	0.13	80,80,80,80	0
56	MG	2a	1662	1/1	0.91	0.25	52,52,52,52	0
56	MG	2A	3231	1/1	0.91	0.26	75,75,75,75	0
56	MG	2A	3298	1/1	0.91	0.31	56,56,56,56	0
56	MG	1B	215	1/1	0.91	0.12	87,87,87,87	0
56	MG	2A	3178	1/1	0.91	0.27	76,76,76,76	0
56	MG	1A	3049	1/1	0.91	0.14	60,60,60,60	0
56	MG	1A	3198	1/1	0.91	0.17	50,50,50,50	0
56	MG	1A	3347	1/1	0.91	0.19	57,57,57,57	0
56	MG	1A	3508	1/1	0.91	0.26	72,72,72,72	0
56	MG	1A	3509	1/1	0.91	0.14	56,56,56,56	0
56	MG	1A	3250	1/1	0.91	0.19	68,68,68,68	0
56	MG	2A	3436	1/1	0.91	0.24	76,76,76,76	0
56	MG	2A	3096	1/1	0.91	0.08	63,63,63,63	0
56	MG	1E	304	1/1	0.91	0.19	69,69,69,69	0
56	MG	2A	3311	1/1	0.91	0.35	50,50,50,50	0
56	MG	2A	3194	1/1	0.91	0.14	71,71,71,71	0
56	MG	1A	3396	1/1	0.91	0.16	64,64,64,64	0
56	MG	1A	3063	1/1	0.91	0.21	71,71,71,71	0
56	MG	2A	3316	1/1	0.91	0.17	50,50,50,50	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	1a	1653	1/1	0.91	0.14	61,61,61,61	0
56	MG	2A	3024	1/1	0.91	0.10	84,84,84,84	0
56	MG	2A	3063	1/1	0.91	0.17	61,61,61,61	0
56	MG	1A	3297	1/1	0.91	0.08	62,62,62,62	0
56	MG	1a	1619	1/1	0.91	0.08	63,63,63,63	0
56	MG	1A	3371	1/1	0.91	0.26	55,55,55,55	0
56	MG	2A	3325	1/1	0.91	0.21	73,73,73,73	0
56	MG	1A	3401	1/1	0.91	0.15	79,79,79,79	0
56	MG	2A	3110	1/1	0.91	0.10	70,70,70,70	0
56	MG	2A	3456	1/1	0.91	0.33	52,52,52,52	0
56	MG	1A	3099	1/1	0.91	0.12	64,64,64,64	0
56	MG	2A	3157	1/1	0.91	0.18	65,65,65,65	0
56	MG	2A	3270	1/1	0.91	0.22	66,66,66,66	0
56	MG	2A	3461	1/1	0.91	0.14	67,67,67,67	0
56	MG	2a	1698	1/1	0.91	0.18	57,57,57,57	0
56	MG	2A	3400	1/1	0.91	0.19	55,55,55,55	0
56	MG	2A	3271	1/1	0.91	0.16	58,58,58,58	0
56	MG	1A	3332	1/1	0.91	0.23	55,55,55,55	0
56	MG	2A	3470	1/1	0.91	0.09	83,83,83,83	0
56	MG	1A	3255	1/1	0.91	0.31	50,50,50,50	0
56	MG	2A	3336	1/1	0.91	0.23	55,55,55,55	0
56	MG	1A	3482	1/1	0.91	0.21	55,55,55,55	0
56	MG	1A	3354	1/1	0.91	0.12	51,51,51,51	0
56	MG	1A	3379	1/1	0.91	0.14	59,59,59,59	0
56	MG	2A	3341	1/1	0.91	0.26	51,51,51,51	0
56	MG	1A	3228	1/1	0.91	0.26	54,54,54,54	0
56	MG	2A	3077	1/1	0.91	0.07	58,58,58,58	0
56	MG	1A	3242	1/1	0.91	0.17	64,64,64,64	0
56	MG	2a	1645	1/1	0.91	0.21	66,66,66,66	0
56	MG	1A	3204	1/1	0.91	0.26	50,50,50,50	0
56	MG	1A	3115	1/1	0.92	0.29	51,51,51,51	0
56	MG	1a	1669	1/1	0.92	0.12	69,69,69,69	0
56	MG	1A	3200	1/1	0.92	0.26	51,51,51,51	0
56	MG	2A	3422	1/1	0.92	0.20	51,51,51,51	0
56	MG	2A	3238	1/1	0.92	0.12	77,77,77,77	0
56	MG	2a	1654	1/1	0.92	0.07	53,53,53,53	0
56	MG	18	102	1/1	0.92	0.36	56,56,56,56	0
56	MG	2A	3240	1/1	0.92	0.20	75,75,75,75	0
56	MG	1A	3280	1/1	0.92	0.09	53,53,53,53	0
56	MG	1A	3026	1/1	0.92	0.08	73,73,73,73	0
56	MG	1a	1675	1/1	0.92	0.15	60,60,60,60	0
56	MG	2Q	201	1/1	0.92	0.06	50,50,50,50	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	1A	3203	1/1	0.92	0.34	50,50,50,50	0
56	MG	1A	3086	1/1	0.92	0.08	63,63,63,63	0
56	MG	2A	3015	1/1	0.92	0.08	63,63,63,63	0
56	MG	1a	1678	1/1	0.92	0.15	109,109,109,109	0
56	MG	1A	3059	1/1	0.92	0.09	69,69,69,69	0
56	MG	28	101	1/1	0.92	0.27	53,53,53,53	0
56	MG	2A	3253	1/1	0.92	0.26	54,54,54,54	0
56	MG	2A	3104	1/1	0.92	0.21	64,64,64,64	0
56	MG	2a	1671	1/1	0.92	0.06	64,64,64,64	0
56	MG	1A	3500	1/1	0.92	0.26	50,50,50,50	0
56	MG	2A	3256	1/1	0.92	0.16	52,52,52,52	0
56	MG	1A	3164	1/1	0.92	0.21	74,74,74,74	0
56	MG	2A	3258	1/1	0.92	0.14	52,52,52,52	0
56	MG	1a	1641	1/1	0.92	0.08	67,67,67,67	0
56	MG	1A	3291	1/1	0.92	0.14	50,50,50,50	0
56	MG	2A	3109	1/1	0.92	0.09	76,76,76,76	0
56	MG	2A	3385	1/1	0.92	0.15	51,51,51,51	0
56	MG	1A	3504	1/1	0.92	0.15	54,54,54,54	0
56	MG	1A	3111	1/1	0.92	0.14	51,51,51,51	0
56	MG	2a	1683	1/1	0.92	0.31	53,53,53,53	0
56	MG	1A	3132	1/1	0.92	0.15	59,59,59,59	0
56	MG	1A	3314	1/1	0.92	0.22	59,59,59,59	0
56	MG	2A	3391	1/1	0.92	0.20	70,70,70,70	0
56	MG	1a	1647	1/1	0.92	0.21	58,58,58,58	0
56	MG	1a	1648	1/1	0.92	0.15	54,54,54,54	0
56	MG	2A	3396	1/1	0.92	0.09	96,96,96,96	0
56	MG	2A	3454	1/1	0.92	0.31	62,62,62,62	0
56	MG	2A	3213	1/1	0.92	0.16	83,83,83,83	0
56	MG	1A	3006	1/1	0.92	0.13	80,80,80,80	0
56	MG	1A	3398	1/1	0.92	0.15	57,57,57,57	0
56	MG	1A	3344	1/1	0.92	0.18	57,57,57,57	0
56	MG	1A	3212	1/1	0.92	0.20	50,50,50,50	0
56	MG	2A	3279	1/1	0.92	0.17	63,63,63,63	0
56	MG	2A	3462	1/1	0.92	0.22	66,66,66,66	0
56	MG	2A	3465	1/1	0.92	0.08	81,81,81,81	0
56	MG	1A	3478	1/1	0.92	0.22	50,50,50,50	0
56	MG	1A	3479	1/1	0.92	0.11	62,62,62,62	0
56	MG	2A	3282	1/1	0.92	0.15	71,71,71,71	0
56	MG	1A	3230	1/1	0.92	0.10	73,73,73,73	0
56	MG	2A	3407	1/1	0.92	0.11	75,75,75,75	0
56	MG	1A	3481	1/1	0.92	0.25	50,50,50,50	0
56	MG	2A	3346	1/1	0.92	0.21	50,50,50,50	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	1A	3548	1/1	0.92	0.13	60,60,60,60	0
56	MG	1B	201	1/1	0.92	0.16	67,67,67,67	0
56	MG	1A	3089	1/1	0.92	0.17	53,53,53,53	0
56	MG	1A	3154	1/1	0.92	0.15	58,58,58,58	0
56	MG	2f	201	1/1	0.92	0.14	75,75,75,75	0
56	MG	2B	206	1/1	0.92	0.13	71,71,71,71	0
56	MG	1A	3155	1/1	0.92	0.18	66,66,66,66	0
56	MG	1A	3323	1/1	0.92	0.25	54,54,54,54	0
56	MG	1A	3324	1/1	0.92	0.18	54,54,54,54	0
56	MG	2A	3348	1/1	0.93	0.28	53,53,53,53	0
56	MG	1A	3494	1/1	0.93	0.30	50,50,50,50	0
56	MG	1A	3292	1/1	0.93	0.07	53,53,53,53	0
56	MG	2A	3222	1/1	0.93	0.40	72,72,72,72	0
56	MG	2A	3165	1/1	0.93	0.08	65,65,65,65	0
56	MG	1A	3119	1/1	0.93	0.14	78,78,78,78	0
56	MG	1A	3497	1/1	0.93	0.17	58,58,58,58	0
56	MG	1A	3033	1/1	0.93	0.08	84,84,84,84	0
56	MG	1A	3231	1/1	0.93	0.20	65,65,65,65	0
56	MG	2A	3291	1/1	0.93	0.29	50,50,50,50	0
56	MG	2A	3292	1/1	0.93	0.17	52,52,52,52	0
56	MG	19	101	1/1	0.93	0.23	72,72,72,72	0
56	MG	2A	3363	1/1	0.93	0.20	66,66,66,66	0
56	MG	2W	201	1/1	0.93	0.08	64,64,64,64	0
56	MG	2A	3121	1/1	0.93	0.16	54,54,54,54	0
56	MG	2A	3074	1/1	0.93	0.14	63,63,63,63	0
56	MG	1A	3201	1/1	0.93	0.21	50,50,50,50	0
56	MG	1A	3402	1/1	0.93	0.17	53,53,53,53	0
56	MG	2A	3234	1/1	0.93	0.14	60,60,60,60	0
56	MG	1A	3378	1/1	0.93	0.09	71,71,71,71	0
56	MG	1A	3211	1/1	0.93	0.26	50,50,50,50	0
56	MG	1A	3507	1/1	0.93	0.20	64,64,64,64	0
56	MG	1l	201	1/1	0.93	0.20	64,64,64,64	0
56	MG	2A	3081	1/1	0.93	0.12	54,54,54,54	0
56	MG	2A	3241	1/1	0.93	0.20	68,68,68,68	0
56	MG	2A	3441	1/1	0.93	0.14	57,57,57,57	0
56	MG	2A	3242	1/1	0.93	0.10	63,63,63,63	0
56	MG	1A	3251	1/1	0.93	0.22	53,53,53,53	0
56	MG	1B	216	1/1	0.93	0.10	81,81,81,81	0
56	MG	2A	3310	1/1	0.93	0.25	50,50,50,50	0
56	MG	1A	3358	1/1	0.93	0.26	60,60,60,60	0
56	MG	1A	3510	1/1	0.93	0.11	66,66,66,66	0
56	MG	1A	3452	1/1	0.93	0.23	51,51,51,51	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	2A	3188	1/1	0.93	0.30	50,50,50,50	0
56	MG	1A	3514	1/1	0.93	0.10	68,68,68,68	0
56	MG	2A	3192	1/1	0.93	0.18	50,50,50,50	0
56	MG	1A	3281	1/1	0.93	0.22	50,50,50,50	0
56	MG	2a	1617	1/1	0.93	0.09	81,81,81,81	0
56	MG	1a	1656	1/1	0.93	0.09	68,68,68,68	0
56	MG	1D	304	1/1	0.93	0.09	68,68,68,68	0
56	MG	2A	3392	1/1	0.93	0.13	73,73,73,73	0
56	MG	1E	301	1/1	0.93	0.10	76,76,76,76	0
56	MG	1A	3520	1/1	0.93	0.10	63,63,63,63	0
56	MG	1A	3126	1/1	0.93	0.14	55,55,55,55	0
56	MG	2A	3002	1/1	0.93	0.33	61,61,61,61	0
56	MG	2A	3460	1/1	0.93	0.26	59,59,59,59	0
56	MG	1F	301	1/1	0.93	0.18	65,65,65,65	0
56	MG	1A	3180	1/1	0.93	0.10	66,66,66,66	0
56	MG	1A	3302	1/1	0.93	0.13	64,64,64,64	0
56	MG	1A	3057	1/1	0.93	0.08	61,61,61,61	0
56	MG	1A	3140	1/1	0.93	0.20	67,67,67,67	0
56	MG	1A	3546	1/1	0.93	0.16	54,54,54,54	0
56	MG	1R	201	1/1	0.93	0.09	52,52,52,52	0
56	MG	1T	202	1/1	0.93	0.16	58,58,58,58	0
56	MG	1T	203	1/1	0.93	0.26	78,78,78,78	0
56	MG	1A	3241	1/1	0.93	0.14	52,52,52,52	0
56	MG	2A	3212	1/1	0.93	0.10	64,64,64,64	0
56	MG	1V	203	1/1	0.93	0.18	75,75,75,75	0
56	MG	1A	3325	1/1	0.93	0.12	63,63,63,63	0
56	MG	1A	3290	1/1	0.93	0.23	50,50,50,50	0
56	MG	2a	1642	1/1	0.93	0.09	68,68,68,68	0
56	MG	1A	3169	1/1	0.93	0.10	64,64,64,64	0
56	MG	2a	1644	1/1	0.93	0.17	63,63,63,63	0
56	MG	1A	3417	1/1	0.93	0.32	50,50,50,50	0
56	MG	2I	101	1/1	0.94	0.12	56,56,56,56	0
56	MG	1A	3124	1/1	0.94	0.13	51,51,51,51	0
56	MG	2A	3328	1/1	0.94	0.17	52,52,52,52	0
56	MG	2a	1659	1/1	0.94	0.16	53,53,53,53	0
56	MG	2A	3136	1/1	0.94	0.17	50,50,50,50	0
56	MG	1A	3261	1/1	0.94	0.13	60,60,60,60	0
56	MG	1A	3381	1/1	0.94	0.23	67,67,67,67	0
56	MG	1A	3384	1/1	0.94	0.08	55,55,55,55	0
56	MG	2A	3333	1/1	0.94	0.09	51,51,51,51	0
56	MG	2A	3390	1/1	0.94	0.16	65,65,65,65	0
56	MG	1A	3032	1/1	0.94	0.10	69,69,69,69	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	1A	3247	1/1	0.94	0.16	62,62,62,62	0
56	MG	1A	3316	1/1	0.94	0.11	58,58,58,58	0
56	MG	1A	3264	1/1	0.94	0.14	58,58,58,58	0
56	MG	2A	3395	1/1	0.94	0.14	81,81,81,81	0
56	MG	1A	3544	1/1	0.94	0.07	62,62,62,62	0
56	MG	2A	3061	1/1	0.94	0.07	87,87,87,87	0
56	MG	1A	3545	1/1	0.94	0.11	99,99,99,99	0
56	MG	1F	302	1/1	0.94	0.09	68,68,68,68	0
56	MG	2A	3343	1/1	0.94	0.29	67,67,67,67	0
56	MG	2A	3344	1/1	0.94	0.14	64,64,64,64	0
56	MG	1A	3318	1/1	0.94	0.20	50,50,50,50	0
56	MG	1A	3220	1/1	0.94	0.24	51,51,51,51	0
56	MG	1A	3391	1/1	0.94	0.14	62,62,62,62	0
56	MG	1a	1688	1/1	0.94	0.11	93,93,93,93	0
56	MG	1a	1650	1/1	0.94	0.20	62,62,62,62	0
56	MG	1a	1651	1/1	0.94	0.14	50,50,50,50	0
56	MG	1A	3159	1/1	0.94	0.13	68,68,68,68	0
56	MG	1A	3066	1/1	0.94	0.28	63,63,63,63	0
56	MG	1A	3046	1/1	0.94	0.06	56,56,56,56	0
56	MG	1R	202	1/1	0.94	0.11	59,59,59,59	0
56	MG	2A	3412	1/1	0.94	0.30	68,68,68,68	0
56	MG	1A	3181	1/1	0.94	0.29	50,50,50,50	0
56	MG	2A	3116	1/1	0.94	0.05	59,59,59,59	0
56	MG	2a	1629	1/1	0.94	0.06	87,87,87,87	0
56	MG	2A	3358	1/1	0.94	0.25	62,62,62,62	0
56	MG	1A	3499	1/1	0.94	0.21	52,52,52,52	0
56	MG	1A	3470	1/1	0.94	0.23	53,53,53,53	0
56	MG	2A	3361	1/1	0.94	0.09	54,54,54,54	0
56	MG	1A	3418	1/1	0.94	0.28	57,57,57,57	0
56	MG	1W	201	1/1	0.94	0.19	69,69,69,69	0
56	MG	1A	3289	1/1	0.94	0.36	50,50,50,50	0
56	MG	1Y	201	1/1	0.94	0.40	77,77,77,77	0
56	MG	2A	3263	1/1	0.94	0.20	54,54,54,54	0
56	MG	2A	3216	1/1	0.94	0.12	64,64,64,64	0
56	MG	1A	3107	1/1	0.94	0.10	69,69,69,69	0
56	MG	1A	3307	1/1	0.94	0.22	88,88,88,88	0
56	MG	2A	3315	1/1	0.94	0.23	52,52,52,52	0
56	MG	1A	3227	1/1	0.94	0.24	51,51,51,51	0
56	MG	2A	3268	1/1	0.94	0.26	51,51,51,51	0
56	MG	10	104	1/1	0.94	0.12	99,99,99,99	0
56	MG	1A	3423	1/1	0.94	0.15	50,50,50,50	0
56	MG	1A	3207	1/1	0.94	0.13	51,51,51,51	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	1A	3117	1/1	0.94	0.06	50,50,50,50	0
56	MG	2R	202	1/1	0.94	0.24	54,54,54,54	0
56	MG	2I	201	1/1	0.94	0.05	68,68,68,68	0
56	MG	2I	202	1/1	0.94	0.07	53,53,53,53	0
56	MG	1A	3244	1/1	0.94	0.15	50,50,50,50	0
56	MG	2A	3274	1/1	0.94	0.11	57,57,57,57	0
56	MG	1A	3513	1/1	0.94	0.18	63,63,63,63	0
56	MG	1A	3233	1/1	0.95	0.17	50,50,50,50	0
56	MG	1x	101	1/1	0.95	0.16	50,50,50,50	0
56	MG	1A	3364	1/1	0.95	0.12	77,77,77,77	0
56	MG	1A	3532	1/1	0.95	0.08	113,113,113,113	0
56	MG	1A	3067	1/1	0.95	0.04	65,65,65,65	0
56	MG	1A	3537	1/1	0.95	0.07	93,93,93,93	0
56	MG	1A	3539	1/1	0.95	0.09	77,77,77,77	0
56	MG	1A	3541	1/1	0.95	0.06	116,116,116,116	0
56	MG	2a	1653	1/1	0.95	0.20	51,51,51,51	0
56	MG	1a	1658	1/1	0.95	0.06	92,92,92,92	0
56	MG	2a	1655	1/1	0.95	0.13	70,70,70,70	0
56	MG	2A	3044	1/1	0.95	0.11	77,77,77,77	0
56	MG	2A	3209	1/1	0.95	0.10	62,62,62,62	0
56	MG	2A	3045	1/1	0.95	0.10	78,78,78,78	0
56	MG	2E	304	1/1	0.95	0.05	61,61,61,61	0
56	MG	1A	3491	1/1	0.95	0.17	73,73,73,73	0
56	MG	1A	3236	1/1	0.95	0.24	61,61,61,61	0
56	MG	1Q	202	1/1	0.95	0.21	56,56,56,56	0
56	MG	1A	3222	1/1	0.95	0.09	68,68,68,68	0
56	MG	1A	3253	1/1	0.95	0.07	51,51,51,51	0
56	MG	1T	201	1/1	0.95	0.05	99,99,99,99	0
56	MG	2A	3283	1/1	0.95	0.20	50,50,50,50	0
56	MG	1A	3271	1/1	0.95	0.14	78,78,78,78	0
56	MG	2A	3054	1/1	0.95	0.09	50,50,50,50	0
56	MG	1A	3167	1/1	0.95	0.20	61,61,61,61	0
56	MG	1A	3147	1/1	0.95	0.13	50,50,50,50	0
56	MG	1A	3156	1/1	0.95	0.19	51,51,51,51	0
56	MG	1A	3104	1/1	0.95	0.13	56,56,56,56	0
56	MG	1A	3082	1/1	0.95	0.10	56,56,56,56	0
56	MG	1A	3065	1/1	0.95	0.10	75,75,75,75	0
56	MG	1A	3331	1/1	0.95	0.11	54,54,54,54	0
56	MG	2A	3167	1/1	0.95	0.06	77,77,77,77	0
56	MG	10	101	1/1	0.95	0.11	51,51,51,51	0
56	MG	2A	3229	1/1	0.95	0.07	52,52,52,52	0
56	MG	2A	3064	1/1	0.95	0.09	78,78,78,78	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	2A	3297	1/1	0.95	0.11	63,63,63,63	0
56	MG	1A	3503	1/1	0.95	0.12	71,71,71,71	0
56	MG	2a	1682	1/1	0.95	0.21	56,56,56,56	0
56	MG	2A	3440	1/1	0.95	0.30	50,50,50,50	0
56	MG	1A	3474	1/1	0.95	0.39	50,50,50,50	0
56	MG	1A	3112	1/1	0.95	0.07	65,65,65,65	0
56	MG	1A	3506	1/1	0.95	0.11	50,50,50,50	0
56	MG	2A	3119	1/1	0.95	0.12	86,86,86,86	0
56	MG	1a	1636	1/1	0.95	0.06	55,55,55,55	0
56	MG	2A	3237	1/1	0.95	0.14	67,67,67,67	0
56	MG	2A	3020	1/1	0.95	0.12	93,93,93,93	0
56	MG	1A	3144	1/1	0.95	0.08	84,84,84,84	0
56	MG	1A	3450	1/1	0.95	0.38	66,66,66,66	0
56	MG	1A	3334	1/1	0.95	0.07	77,77,77,77	0
56	MG	2A	3309	1/1	0.95	0.36	50,50,50,50	0
56	MG	2A	3125	1/1	0.95	0.13	67,67,67,67	0
56	MG	2A	3243	1/1	0.95	0.06	62,62,62,62	0
56	MG	2A	3244	1/1	0.95	0.10	74,74,74,74	0
56	MG	1A	3175	1/1	0.95	0.09	57,57,57,57	0
56	MG	1A	3102	1/1	0.95	0.07	56,56,56,56	0
56	MG	1A	3512	1/1	0.95	0.16	60,60,60,60	0
56	MG	1A	3338	1/1	0.95	0.13	58,58,58,58	0
56	MG	1A	3248	1/1	0.95	0.28	52,52,52,52	0
56	MG	2A	3318	1/1	0.95	0.21	50,50,50,50	0
56	MG	2A	3187	1/1	0.95	0.05	80,80,80,80	0
56	MG	1A	3483	1/1	0.95	0.08	50,50,50,50	0
56	MG	2A	3189	1/1	0.95	0.12	50,50,50,50	0
56	MG	2a	1708	1/1	0.95	0.07	110,110,110,110	0
56	MG	1a	1605	1/1	0.95	0.10	117,117,117,117	0
56	MG	2a	1712	1/1	0.95	0.07	100,100,100,100	0
56	MG	2A	3191	1/1	0.95	0.25	78,78,78,78	0
56	MG	1A	3456	1/1	0.95	0.07	75,75,75,75	0
56	MG	2A	3193	1/1	0.95	0.10	56,56,56,56	0
56	MG	1A	3340	1/1	0.95	0.23	50,50,50,50	0
56	MG	1A	3459	1/1	0.95	0.30	50,50,50,50	0
56	MG	1E	302	1/1	0.95	0.22	50,50,50,50	0
56	MG	2A	3261	1/1	0.95	0.20	50,50,50,50	0
56	MG	2A	3085	1/1	0.95	0.09	73,73,73,73	0
56	MG	2A	3139	1/1	0.95	0.10	51,51,51,51	0
56	MG	1B	219	1/1	0.96	0.04	116,116,116,116	0
56	MG	2A	3322	1/1	0.96	0.17	50,50,50,50	0
56	MG	2A	3276	1/1	0.96	0.17	50,50,50,50	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	1a	1672	1/1	0.96	0.07	51,51,51,51	0
56	MG	1A	3034	1/1	0.96	0.07	90,90,90,90	0
56	MG	1A	3382	1/1	0.96	0.10	70,70,70,70	0
56	MG	1A	3383	1/1	0.96	0.21	62,62,62,62	0
56	MG	1A	3530	1/1	0.96	0.09	98,98,98,98	0
56	MG	1A	3372	1/1	0.96	0.15	51,51,51,51	0
56	MG	2A	3215	1/1	0.96	0.12	57,57,57,57	0
56	MG	1A	3235	1/1	0.96	0.07	60,60,60,60	0
56	MG	1A	3038	1/1	0.96	0.07	80,80,80,80	0
56	MG	2A	3463	1/1	0.96	0.09	115,115,115,115	0
56	MG	1A	3160	1/1	0.96	0.08	56,56,56,56	0
56	MG	2a	1618	1/1	0.96	0.10	89,89,89,89	0
56	MG	1A	3284	1/1	0.96	0.10	73,73,73,73	0
56	MG	1A	3540	1/1	0.96	0.10	91,91,91,91	0
56	MG	2a	1707	1/1	0.96	0.06	114,114,114,114	0
56	MG	1A	3377	1/1	0.96	0.12	50,50,50,50	0
56	MG	1A	3165	1/1	0.96	0.10	52,52,52,52	0
56	MG	2a	1651	1/1	0.96	0.08	83,83,83,83	0
56	MG	2A	3416	1/1	0.96	0.07	100,100,100,100	0
56	MG	1A	3335	1/1	0.96	0.10	55,55,55,55	0
56	MG	2A	3099	1/1	0.96	0.15	54,54,54,54	0
56	MG	1A	3286	1/1	0.96	0.20	54,54,54,54	0
56	MG	2A	3367	1/1	0.96	0.14	68,68,68,68	0
56	MG	1A	3518	1/1	0.96	0.07	71,71,71,71	0
56	MG	2A	3184	1/1	0.96	0.10	53,53,53,53	0
56	MG	1A	3519	1/1	0.96	0.08	73,73,73,73	0
56	MG	1A	3490	1/1	0.96	0.19	53,53,53,53	0
56	MG	2x	101	1/1	0.96	0.07	56,56,56,56	0
57	ZN	2Y	501	1/1	0.96	0.11	166,166,166,166	0
56	MG	2A	3142	1/1	0.97	0.31	65,65,65,65	0
56	MG	2A	3383	1/1	0.97	0.07	64,64,64,64	0
56	MG	1A	3370	1/1	0.97	0.18	52,52,52,52	0
56	MG	2A	3340	1/1	0.97	0.13	53,53,53,53	0
56	MG	2a	1709	1/1	0.97	0.05	110,110,110,110	0
56	MG	2R	201	1/1	0.97	0.19	55,55,55,55	0
56	MG	1A	3345	1/1	0.97	0.12	52,52,52,52	0
56	MG	2a	1713	1/1	0.97	0.04	64,64,64,64	0
56	MG	1A	3535	1/1	0.97	0.07	91,91,91,91	0
56	MG	1A	3536	1/1	0.97	0.05	67,67,67,67	0
56	MG	1V	201	1/1	0.97	0.16	55,55,55,55	0
56	MG	1A	3081	1/1	0.97	0.07	54,54,54,54	0
56	MG	1A	3538	1/1	0.97	0.10	73,73,73,73	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	1A	3050	1/1	0.97	0.09	50,50,50,50	0
56	MG	1A	3458	1/1	0.97	0.12	59,59,59,59	0
56	MG	2A	3471	1/1	0.97	0.09	75,75,75,75	0
56	MG	1A	3162	1/1	0.97	0.17	55,55,55,55	0
56	MG	1A	3039	1/1	0.97	0.07	82,82,82,82	0
56	MG	1a	1601	1/1	0.97	0.17	56,56,56,56	0
57	ZN	24	501	1/1	0.97	0.06	171,171,171,171	0
58	SF4	1d	302	8/8	0.97	0.06	107,123,153,161	0
56	MG	1A	3517	1/1	0.98	0.07	72,72,72,72	0
56	MG	1A	3076	1/1	0.98	0.09	75,75,75,75	0
56	MG	2a	1711	1/1	0.98	0.04	87,87,87,87	0
56	MG	1a	1689	1/1	0.98	0.06	109,109,109,109	0
56	MG	2A	3135	1/1	0.98	0.06	92,92,92,92	0
56	MG	2A	3466	1/1	0.98	0.12	71,71,71,71	0
56	MG	1A	3524	1/1	0.98	0.04	93,93,93,93	0
56	MG	1A	3543	1/1	0.98	0.06	75,75,75,75	0
56	MG	2A	3349	1/1	0.98	0.13	55,55,55,55	0
56	MG	1A	3534	1/1	0.98	0.04	89,89,89,89	0
56	MG	2A	3259	1/1	0.98	0.06	50,50,50,50	0
56	MG	2A	3472	1/1	0.98	0.05	107,107,107,107	0
56	MG	2A	3380	1/1	0.98	0.11	61,61,61,61	0
56	MG	1A	3526	1/1	0.98	0.05	88,88,88,88	0
56	MG	1A	3528	1/1	0.98	0.04	101,101,101,101	0
57	ZN	1Y	202	1/1	0.98	0.04	138,138,138,138	0
57	ZN	14	501	1/1	0.98	0.05	157,157,157,157	0
57	ZN	1n	501	1/1	0.98	0.06	140,140,140,140	0
56	MG	1A	3122	1/1	0.98	0.05	60,60,60,60	0
56	MG	2A	3052	1/1	0.98	0.08	80,80,80,80	0
57	ZN	26	501	1/1	0.98	0.04	111,111,111,111	0
56	MG	1A	3269	1/1	0.98	0.07	89,89,89,89	0
58	SF4	2d	302	8/8	0.98	0.05	90,106,116,116	0
57	ZN	15	102	1/1	0.99	0.02	91,91,91,91	0
57	ZN	16	102	1/1	0.99	0.03	91,91,91,91	0
57	ZN	19	102	1/1	0.99	0.07	98,98,98,98	0
56	MG	2A	3464	1/1	0.99	0.16	81,81,81,81	0
56	MG	1A	3525	1/1	0.99	0.04	81,81,81,81	0
56	MG	2A	3055	1/1	0.99	0.07	67,67,67,67	0
57	ZN	25	102	1/1	0.99	0.03	81,81,81,81	0
56	MG	1A	3516	1/1	0.99	0.07	79,79,79,79	0
57	ZN	29	501	1/1	0.99	0.03	96,96,96,96	0
57	ZN	2n	102	1/1	0.99	0.05	120,120,120,120	0
56	MG	1A	3542	1/1	0.99	0.05	98,98,98,98	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	1A	3527	1/1	0.99	0.05	52,52,52,52	0
56	MG	1A	3521	1/1	1.00	0.11	63,63,63,63	0

6.5 Other polymers [i](#)

There are no such residues in this entry.