



wwPDB X-ray Structure Validation Summary Report ⓘ

Jun 3, 2020 – 05:50 am BST

PDB ID : 6N9E
Title : Crystal structure of the *Thermus thermophilus* 70S ribosome in complex with a short substrate mimic CC-Pmn 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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.11
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.11

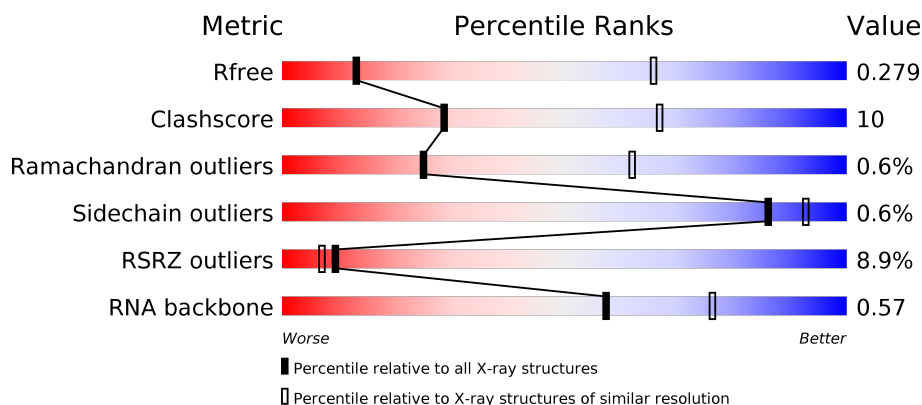
1 Overall quality at a glance

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}	130704	1049 (3.88-3.52)
Clashscore	141614	1027 (3.86-3.54)
Ramachandran outliers	138981	1069 (3.88-3.52)
Sidechain outliers	138945	1065 (3.88-3.52)
RSRZ outliers	127900	1578 (3.90-3.50)
RNA backbone	3102	1027 (4.40-3.00)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria 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	<div> <div>3%</div> <div> <div></div> <div>52%</div> <div>39%</div> <div>7%</div> <div></div> </div> </div>
1	2A	2915	<div> <div>3%</div> <div> <div></div> <div>54%</div> <div>35%</div> <div>6%</div> <div></div> </div> </div>
2	1B	121	<div> <div></div> <div> <div></div> <div>58%</div> <div>40%</div> <div></div> </div> </div>
2	2B	121	<div> <div></div> <div> <div></div> <div>59%</div> <div>37%</div> <div></div> </div> </div>

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Mol	Chain	Length	Quality of chain
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	
15	1T	146	

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Mol	Chain	Length	Quality of chain
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	
27	25	60	

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Mol	Chain	Length	Quality of chain
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	
40	1i	128	

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Mol	Chain	Length	Quality of chain
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	
52	2u	27	

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Mol	Chain	Length	Quality of chain
53	1v	24	
53	2v	24	
54	1w	3	
54	2w	3	
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	10	103	-	-	-	X
56	MG	1A	3014	-	-	-	X
56	MG	1A	3026	-	-	-	X
56	MG	1A	3034	-	-	-	X
56	MG	1A	3039	-	-	-	X
56	MG	1A	3040	-	-	-	X
56	MG	1A	3051	-	-	-	X
56	MG	1A	3054	-	-	-	X
56	MG	1A	3067	-	-	-	X
56	MG	1A	3068	-	-	-	X
56	MG	1A	3070	-	-	-	X
56	MG	1A	3075	-	-	-	X
56	MG	1A	3078	-	-	-	X
56	MG	1A	3082	-	-	-	X
56	MG	1A	3104	-	-	-	X
56	MG	1A	3115	-	-	-	X
56	MG	1A	3124	-	-	-	X
56	MG	1A	3142	-	-	-	X
56	MG	1A	3144	-	-	-	X
56	MG	1A	3146	-	-	-	X
56	MG	1A	3148	-	-	-	X
56	MG	1A	3154	-	-	-	X
56	MG	1A	3159	-	-	-	X
56	MG	1A	3165	-	-	-	X
56	MG	1A	3172	-	-	-	X
56	MG	1A	3173	-	-	-	X
56	MG	1A	3177	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
56	MG	1A	3187	-	-	-	X
56	MG	1A	3192	-	-	-	X
56	MG	1A	3197	-	-	-	X
56	MG	1A	3202	-	-	-	X
56	MG	1A	3217	-	-	-	X
56	MG	1A	3221	-	-	-	X
56	MG	1A	3224	-	-	-	X
56	MG	1A	3232	-	-	-	X
56	MG	1A	3237	-	-	-	X
56	MG	1A	3239	-	-	-	X
56	MG	1A	3245	-	-	-	X
56	MG	1A	3250	-	-	-	X
56	MG	1A	3252	-	-	-	X
56	MG	1A	3254	-	-	-	X
56	MG	1A	3255	-	-	-	X
56	MG	1A	3257	-	-	-	X
56	MG	1A	3258	-	-	-	X
56	MG	1A	3262	-	-	-	X
56	MG	1A	3264	-	-	-	X
56	MG	1A	3293	-	-	-	X
56	MG	1A	3299	-	-	-	X
56	MG	1A	3308	-	-	-	X
56	MG	1A	3312	-	-	-	X
56	MG	1A	3322	-	-	-	X
56	MG	1A	3327	-	-	-	X
56	MG	1A	3340	-	-	-	X
56	MG	1A	3341	-	-	-	X
56	MG	1A	3349	-	-	-	X
56	MG	1A	3358	-	-	-	X
56	MG	1A	3360	-	-	-	X
56	MG	1A	3402	-	-	-	X
56	MG	1A	3420	-	-	-	X
56	MG	1A	3437	-	-	-	X
56	MG	1A	3440	-	-	-	X
56	MG	1A	3445	-	-	-	X
56	MG	1A	3471	-	-	-	X
56	MG	1A	3479	-	-	-	X
56	MG	1B	201	-	-	-	X
56	MG	1B	202	-	-	-	X
56	MG	1E	304	-	-	-	X
56	MG	1Q	201	-	-	-	X
56	MG	1a	1603	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
56	MG	1a	1645	-	-	-	X
56	MG	1a	1687	-	-	-	X
56	MG	1l	201	-	-	-	X
56	MG	1x	102	-	-	-	X
56	MG	20	101	-	-	-	X
56	MG	27	101	-	-	-	X
56	MG	2A	3002	-	-	-	X
56	MG	2A	3011	-	-	-	X
56	MG	2A	3014	-	-	-	X
56	MG	2A	3015	-	-	-	X
56	MG	2A	3024	-	-	-	X
56	MG	2A	3027	-	-	-	X
56	MG	2A	3030	-	-	-	X
56	MG	2A	3039	-	-	-	X
56	MG	2A	3049	-	-	-	X
56	MG	2A	3059	-	-	-	X
56	MG	2A	3061	-	-	-	X
56	MG	2A	3113	-	-	-	X
56	MG	2A	3122	-	-	-	X
56	MG	2A	3157	-	-	-	X
56	MG	2A	3162	-	-	-	X
56	MG	2A	3183	-	-	-	X
56	MG	2A	3187	-	-	-	X
56	MG	2A	3209	-	-	-	X
56	MG	2A	3220	-	-	-	X
56	MG	2A	3253	-	-	-	X
56	MG	2A	3258	-	-	-	X
56	MG	2A	3263	-	-	-	X
56	MG	2A	3266	-	-	-	X
56	MG	2A	3276	-	-	-	X
56	MG	2A	3285	-	-	-	X
56	MG	2A	3323	-	-	-	X
56	MG	2A	3326	-	-	-	X
56	MG	2A	3327	-	-	-	X
56	MG	2A	3332	-	-	-	X
56	MG	2A	3337	-	-	-	X
56	MG	2A	3349	-	-	-	X
56	MG	2B	201	-	-	-	X
56	MG	2B	202	-	-	-	X
56	MG	2E	302	-	-	-	X
56	MG	2O	201	-	-	-	X
56	MG	2T	202	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
56	MG	2a	3068	-	-	-	X
56	MG	2a	3069	-	-	-	X

2 Entry composition

There are 59 unique types of molecules in this entry. The entry contains 287828 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	6	Total	C	N	O	P	0	0	0
			113	49	22	36	6			
53	2v	6	Total	C	N	O	P	0	0	0
			113	49	22	36	6			

- Molecule 54 is a RNA chain called CC-Pmn.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
54	1w	3	Total	C	N	O	P	0	0	0
			74	40	13	19	2			
54	2w	3	Total	C	N	O	P	0	0	0
			74	40	13	19	2			

- 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 (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
56	2E	6	Total	Mg	0	0
			6	6		
56	17	2	Total	Mg	0	0
			2	2		
56	2d	1	Total	Mg	0	0
			1	1		
56	20	2	Total	Mg	0	0
			2	2		
56	18	1	Total	Mg	0	0
			1	1		
56	13	1	Total	Mg	0	0
			1	1		
56	2B	9	Total	Mg	0	0
			9	9		
56	2a	103	Total	Mg	0	0
			103	103		
56	1E	6	Total	Mg	0	0
			6	6		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
56	2l	1	Total 1	Mg 1	0	0
56	16	1	Total 1	Mg 1	0	0
56	28	2	Total 2	Mg 2	0	0
56	1W	1	Total 1	Mg 1	0	0
56	1A	498	Total 498	Mg 498	0	0
56	21	1	Total 1	Mg 1	0	0
56	1S	1	Total 1	Mg 1	0	0
56	25	1	Total 1	Mg 1	0	0
56	2T	2	Total 2	Mg 2	0	0
56	1D	1	Total 1	Mg 1	0	0
56	2f	1	Total 1	Mg 1	0	0
56	1V	3	Total 3	Mg 3	0	0
56	1a	93	Total 93	Mg 93	0	0
56	2Q	2	Total 2	Mg 2	0	0
56	15	1	Total 1	Mg 1	0	0
56	1x	2	Total 2	Mg 2	0	0
56	2O	1	Total 1	Mg 1	0	0
56	1d	1	Total 1	Mg 1	0	0
56	2r	1	Total 1	Mg 1	0	0
56	2Y	1	Total 1	Mg 1	0	0
56	23	1	Total 1	Mg 1	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
56	2R	2	Total 2	Mg 2	0	0
56	2D	1	Total 1	Mg 1	0	0
56	1U	1	Total 1	Mg 1	0	0
56	1r	1	Total 1	Mg 1	0	0
56	1l	1	Total 1	Mg 1	0	0
56	1F	1	Total 1	Mg 1	0	0
56	10	3	Total 3	Mg 3	0	0
56	1Q	1	Total 1	Mg 1	0	0
56	2A	385	Total 385	Mg 385	0	0
56	1B	12	Total 12	Mg 12	0	0
56	27	1	Total 1	Mg 1	0	0

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

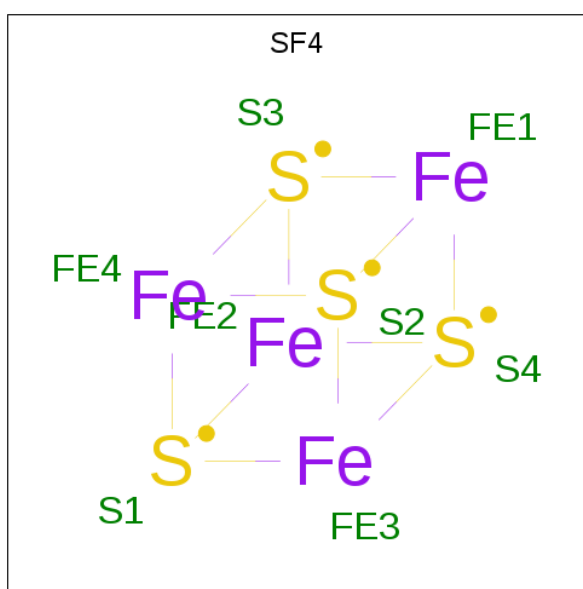
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
57	1Y	1	Total 1	Zn 1	0	0
57	14	1	Total 1	Zn 1	0	0
57	1n	1	Total 1	Zn 1	0	0
57	15	1	Total 1	Zn 1	0	0
57	29	1	Total 1	Zn 1	0	0
57	19	1	Total 1	Zn 1	0	0
57	26	1	Total 1	Zn 1	0	0
57	25	1	Total 1	Zn 1	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
57	24	1	Total	Zn	0	0
			1	1		
57	2n	1	Total	Zn	0	0
			1	1		
57	2Y	1	Total	Zn	0	0
			1	1		
57	16	1	Total	Zn	0	0
			1	1		

- Molecule 58 is IRON/SULFUR CLUSTER (three-letter code: 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.

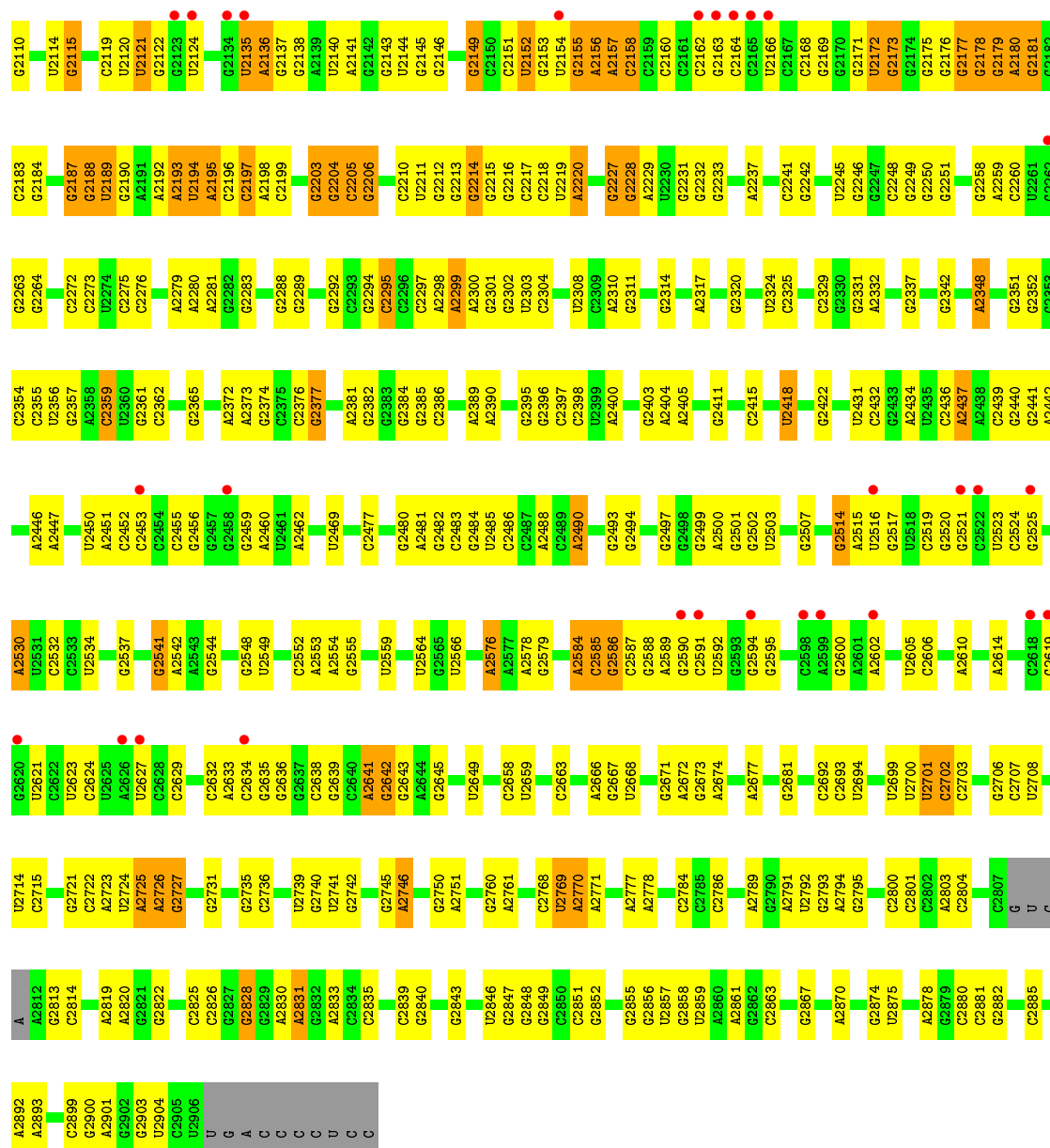
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
59	1A	53	Total	O	0	0
			53	53		
59	1D	3	Total	O	0	0
			3	3		
59	1a	15	Total	O	0	0
			15	15		

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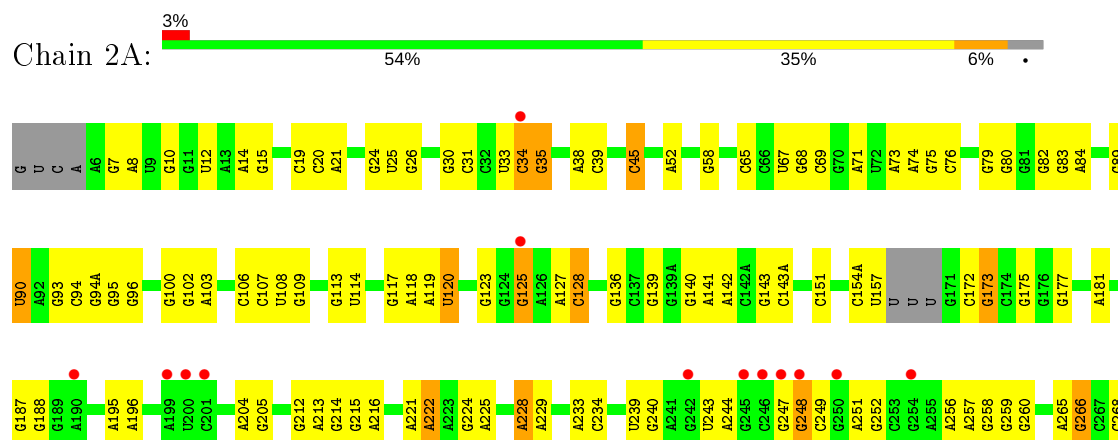
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
59	1x	2	Total 2	O 2	0	0
59	2A	32	Total 32	O 32	0	0
59	2B	1	Total 1	O 1	0	0
59	2a	19	Total 19	O 19	0	0

G2019	G1905	U1827	G1733	U1636	A1532	G1435	G1345	G1261	C1180	A1113	G1036	C944	A866
G2020	A1906	C1828	G1734	G1637	G1533	G1436	U1346	C1262	G1181	G1114	C1037	A945	A867
G2021	A1907	G1638	U1739	G1639	C1539	U1436	A1348	A1265	G1182	A1115	C1038	A946	A868
G2022	G1830	G1640	U1740	G1641	A1554	U1440	A1354	A1272	U1185	G1117	C1040	C949	U869
A2023	C1831	G1642	G1741	C1645	C1555	U1441	G1355	G1273	U1186	G1118	G1041	C950	G870
G2024	A1912	G1643	G1742	C1646	A1556	U1442	G1356	G1274	A1187	G1119	A1042	U951	A871
C2030	G1921	C1832	G1743	C1647	A1557	U1443	G1357	G1275	A1188	G1120	U1045	G952	U874
G2031	A1922	U1836	G1744	U1647	G1558	U1444	U1358	G1276	A1189	C1121	A1046	G953	U875
G2032	G1928	U1648	G1745	U1648	G1559	G1445	U1359	G1277	G1195	C1122	U1046	A954	A876
G2034	A1843	A1649	A1747	A1649	U1562	G1446	C1360	G1278	G1196	A1123	G1051	A955	G877
A2035	C1931	C1653	G1750	C1653	U1563	U1451	C1361	U1286	C1199	U1124	G1052	A956	G878
A2036	G1932	A1654	G1751	A1654	U1566	U1452	U1362	A1287	G1200	C1125	C1053	A957	U886
A2041	C1936	A1655	G1752	A1655	G1567	C1453	A1363	A1287	G1201	U1127	U1056	C960	C887
A2042	U1937	C1656	G1753	C1656	U1567	C1454	U1364	A1288	A1202	U1128	A1057	A963	G890
C2043	G1938	C1657	G1754	C1657	A1567	U1455	U1369	G1289	G1203	U1129	U1058	A964	G891
G2044	U1939	C1658	A1767	C1658	G1570	G1456	U1370	G1290	G1204	U1130	G1059	G965	G902
G2045	A1940	U1659	A1768	C1659	G1571	G1457	U1371	G1291	G1205	A1131	C1059	G966	C903
G2051	C1942	A1660	G1770	A1660	G1572	G1458	U1372	G1294	G1206	A1132	U1065	G987	C904
A2052	G1943	C1661	G1771	C1661	G1576	U1465	A1377	G1298	G1210	G1133	A1066	G976	U905
A2053	C1946	A1662	G1772	A1662	C1579	U1466	A1378	A1299	U1211	A1134	A1067	G977	G900
A2054	U1949	G1665	G1776	G1665	G	G1467	U1381	A1300	U1212	G1135	G1068	G977	G901
U2056	A1950	G1668	G1777	G1668	U	G1468	A1382	U1301	U1213	U1136	U1069	G983	G902
G2057	C1950	G1669	G1778	G1669	A	G1469	A1383	G1302	U1214	G1137	G1070	G984	C903
G2058	A1951	G1670	G1779	G1670	C	G1470	G1384	G1305	G1217	C1138	U1071	G987	C904
G2059	A1954	G1671	G1780	G1671	G1584	C1474	U1387	A1308	U1218	G1139	A1072	G987	U905
G2060	U1954	G1672	G1781	G1672	G1585	A1480	A1388	U1309	A1219	A1141	U1073	U988	U907
U2063	C1957	A1679	G1782	A1679	G1586	A1481	G1388	G1310	U1220	U1142	A990	G989	A908
A2064	A1958	G1680	G1783	G1680	U1587	G1486	G1389	U1313	A1222	U1143	G991	G990	G909
G2065	C1959	G1681	G1784	G1681	G1588	G1487	C1391	U1314	C1223	G1145	G1082	G992	G911
G2074	A1960	C1683	G1785	C1683	C1590	G1488	G1392	A1315	G1225	U1147	G1083	G993	C912
G2075	U1977	A1684	G1786	A1684	G1594	A1491	G1393	C1316	G1226	C1148	G1084	G1001	A913
A2076	C1984	G1689	G1787	G1689	C1594	A1492	C1397	G1317	U1227	A1149	U1085	U1002	G916
G2077	U1985	G1694	G1788	G1694	C1603	G1495	U1398	A1318	G1228	C1150	G1090	U1003	A917
G2078	G1986	C1695	G1789	C1695	A1604	A1496	A1399	U1319	G1229	U1151	A1091	A1004	C923
A2082	C1989	G1700	G1790	G1700	A1605	G1497	A1400	A1320	G1231	G1152	A1092	A1005	U924
A2084	U1992	A1701	G1791	A1701	G1502	G1506	G1401	A1321	G1232	G1153	A1094	C1006	A925
C2087	A1994	C1704	G1792	C1704	A1507	G1507	G1402	U1322	U1233	U1156	G1095	G1015	G926
G2091	G1995	C1705	G1793	C1705	A1508	G1508	G1403	G1323	U1234	A1157	A1096	G1016	G927
G2092	C1996	G1709	G1794	G1709	G1513	G1514	U1404	A1324	G1235	G1158	G1097	G1017	G928
A2093	G1997	C1710	G1795	C1710	C1515	C1516	G1405	G1325	U1159	U1159	C1098	G1018	G929
G2100	G2002	A1711	G1796	A1711	U1625	G1517	A1406	A1326	G1239	G1162	A1101	G1020	G930
U2101	C2012	A1712	G1797	A1712	A1627	G1518	G1407	G1326	U1246	C1165	G1102	G1021	C931
G2105	U2013	G1713	G1798	G1713	G1631	G1525	G1408	U1339	G1247	U1170	G1103	G1022	C932
C2106	C2014	A1714	G1799	A1714	A1632	G1526	G1409	U1340	G1248	G1171	G1104	G1023	A934
G2107	U2015	G1721	G1800	G1721	A1633	G1529	G1428	U1341	G1249	G1172	U1105	G1024	C935
U2108	C2018	C1732	G1801	C1732	C1634	G1529	G1429	C1342	U1256	A1173	U1106	A1029	C936
G2109			G1802		C1635		G1431	C1344		U1174	U	A1030	A937
										A175	G108	A1031	G938
										G1177	G109	G1082	C939
											G1110	G1033	C940
											U1111	A1034	U941
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													C943

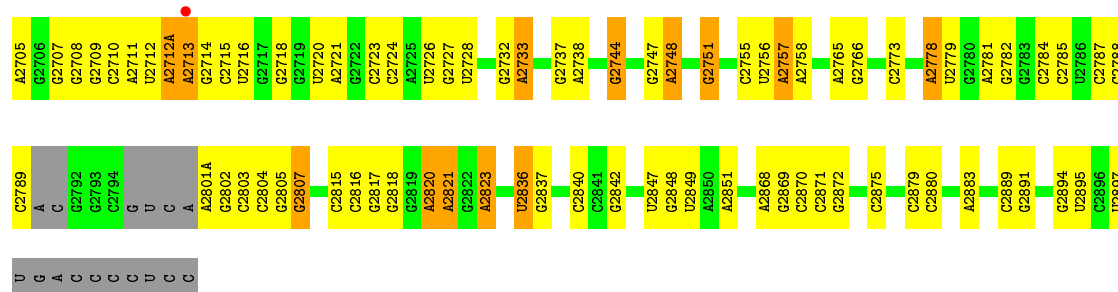


• Molecule 1: 23S Ribosomal RNA



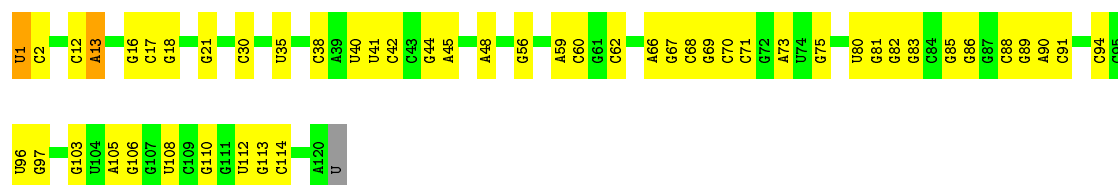
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G1370	G1371	G1166	G1025	G944	G775	G668	C605	G521	C414	G326	C271G
G1372	G1373	G1171	U1026	G945	G776	G669	U607	G522	A415	G329	G271H
A1268	A1269	G1171	A1028	G946	A782	A670	A608	C527	C419	A330	G271I
C1270	C1271	A	A1029	G947	A783	G571	G614B	A528	G420	G271J	U271K
G1271	A	A	G873	G948	A784	G572	A614C	A529	U421	C336	U271L
U1272	G	U	G874	A953	G785	G573	G615	G530	A422	C337	G271M
A1273	A	A	G875	G954	A786	A675	G616	C531	A423	G338	U271N
A1274	A	A	G876	G955	A787	A676	G617	A532	G430	A345	C271O
A1275	G	G	U877	G956	A788	A685	A621	A533	G436	A346	G271P
G1183	U	U	G879	A957	C796	G686	G622	U534	A347	A347	G271Q
G1186	C	C	G880	U958	G801	G689	G623	G540	G437	G352	G271R
G1187	A	A	G881	A959	G802	U694	A627	G545	G438	U358	C271S
U1188	C	C	G882	A960	G805	G695	G628	C	G440	A359	G271T
A1189	U	U	G883	C961	C806	G696	G629	A	C444	G362	G271U
A1287	G	G	C884	C962	U807	G700	G630	A	C445	U363	G272
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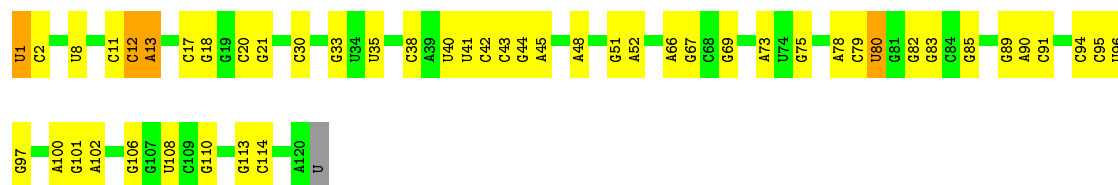
• Molecule 2: 5S Ribosomal RNA

Chain 1B: 58% 40%



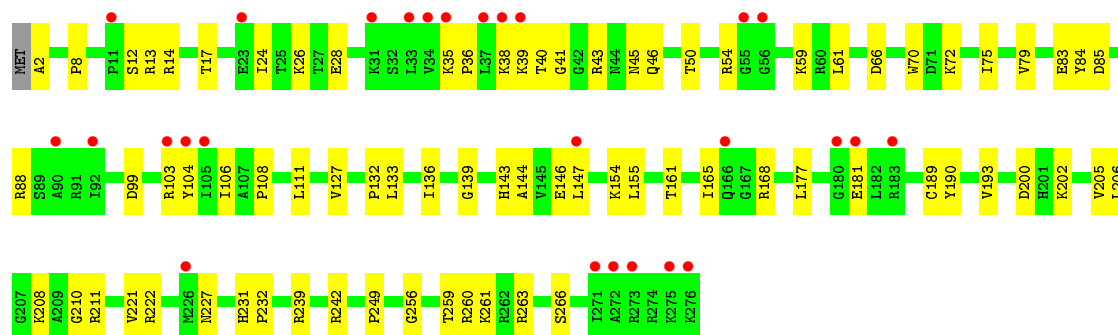
• Molecule 2: 5S Ribosomal RNA

Chain 2B: 59% 37%



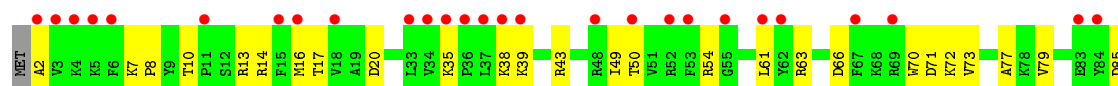
• Molecule 3: 50S Ribosomal Protein L2

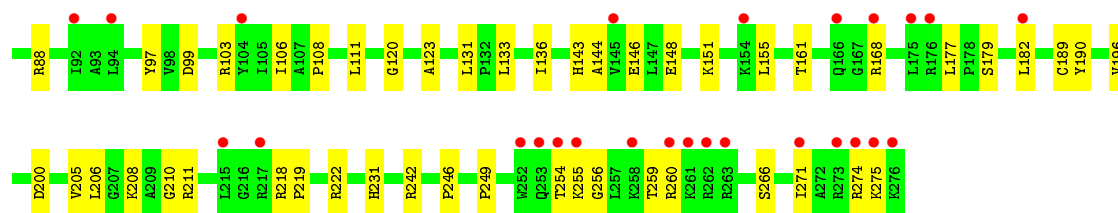
Chain 1D: 10% 72% 28%



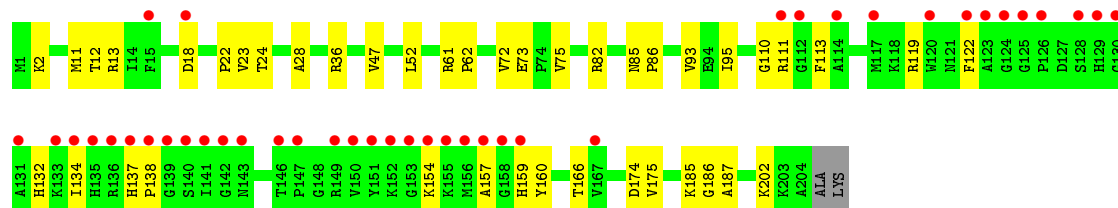
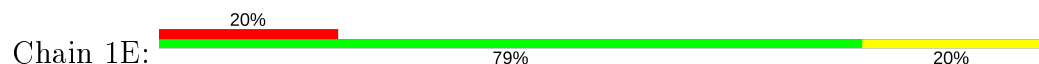
• Molecule 3: 50S Ribosomal Protein L2

Chain 2D: 19% 73% 27%

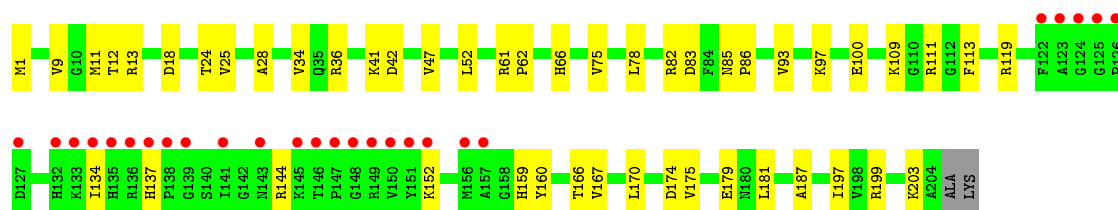
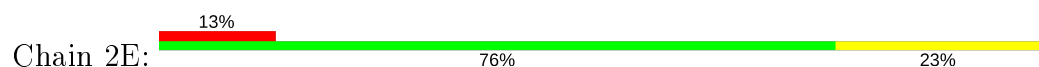




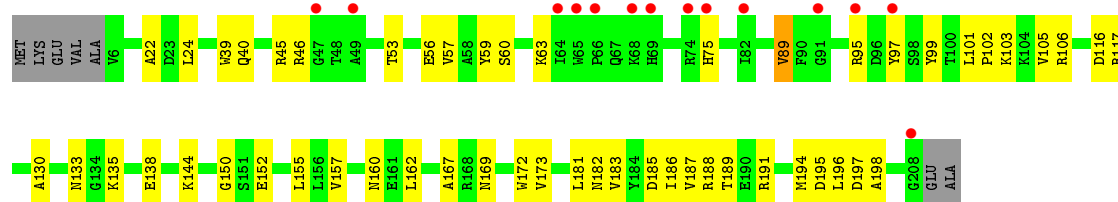
• Molecule 4: 50S Ribosomal Protein L3



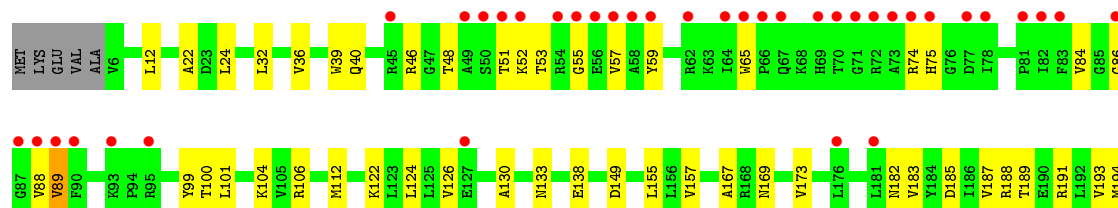
• Molecule 4: 50S Ribosomal Protein L3

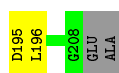


• Molecule 5: 50S Ribosomal Protein L4

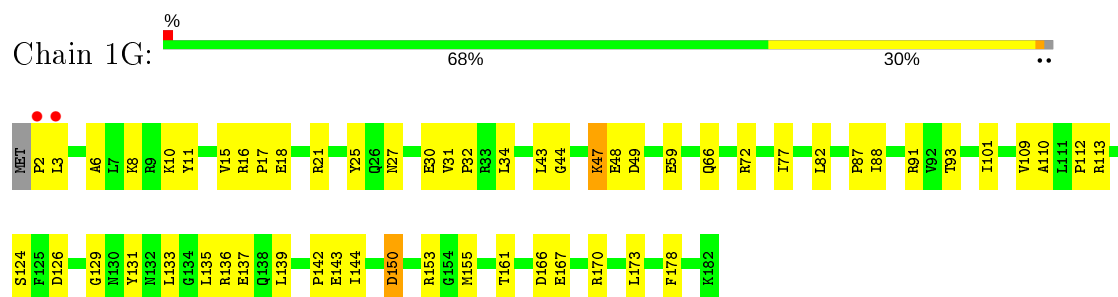


• Molecule 5: 50S Ribosomal Protein L4

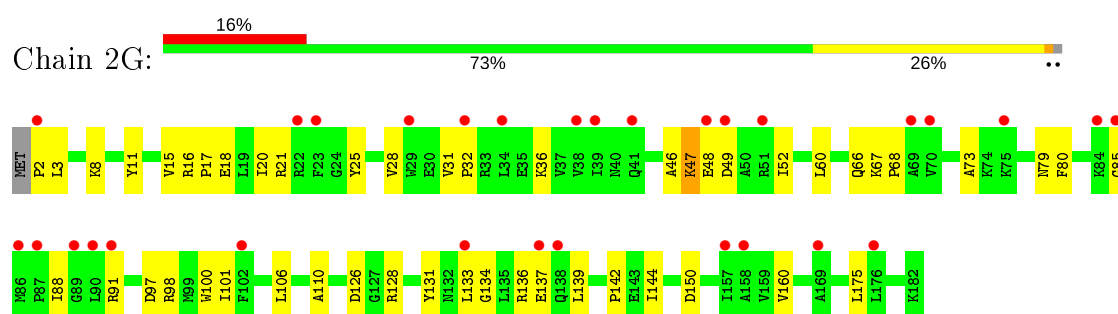




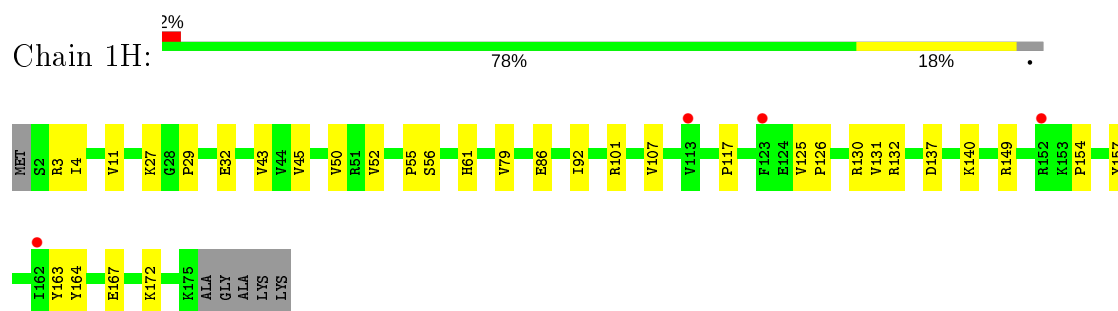
- Molecule 6: 50S Ribosomal Protein L5



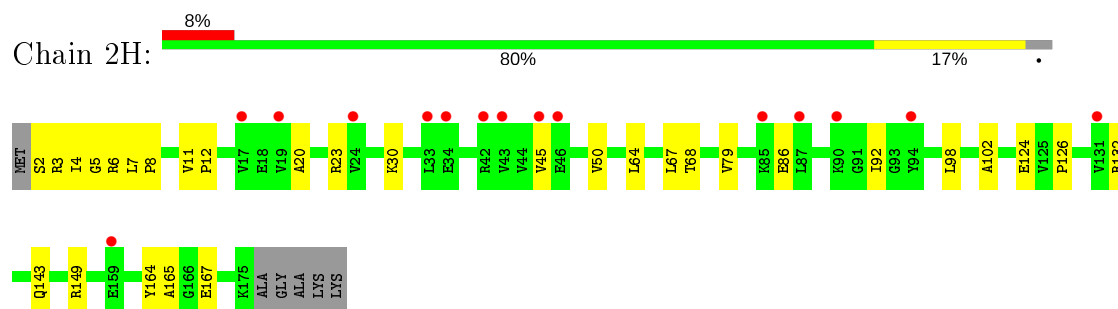
- Molecule 6: 50S Ribosomal Protein L5



- Molecule 7: 50S Ribosomal Protein L6

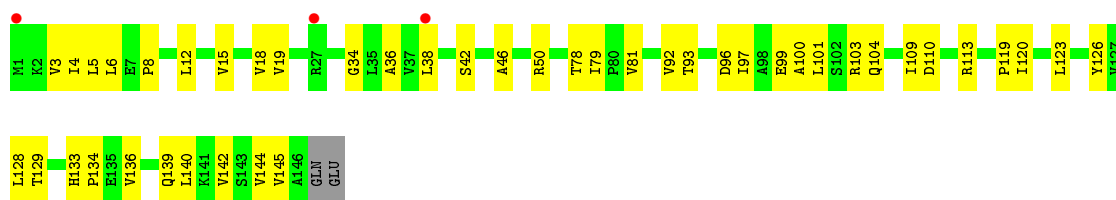


- Molecule 7: 50S Ribosomal Protein L6

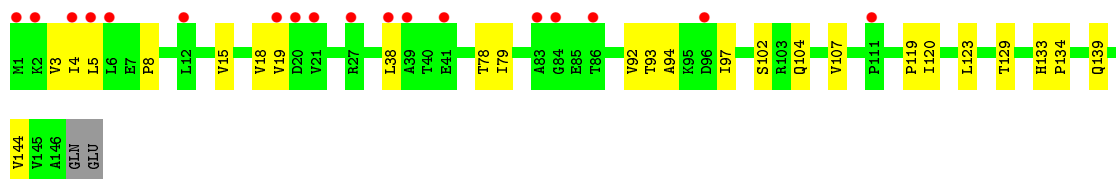
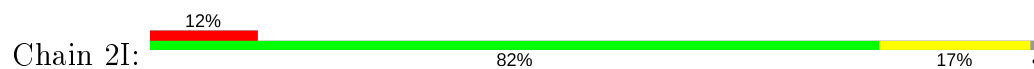


- Molecule 8: 50S Ribosomal Protein L9

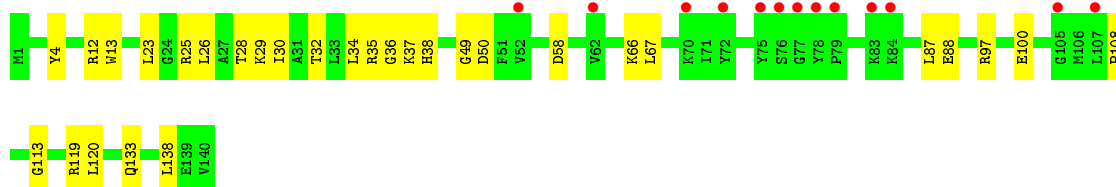
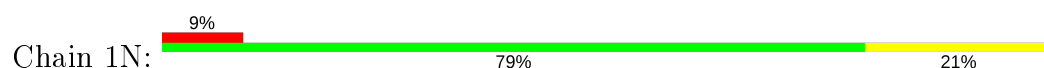




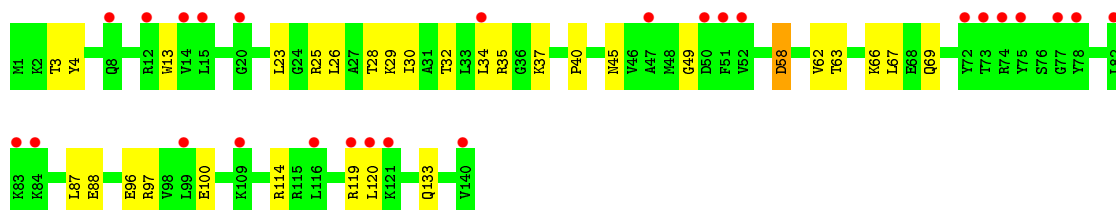
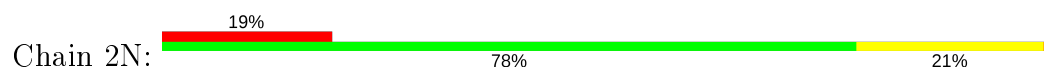
• Molecule 8: 50S Ribosomal Protein L9



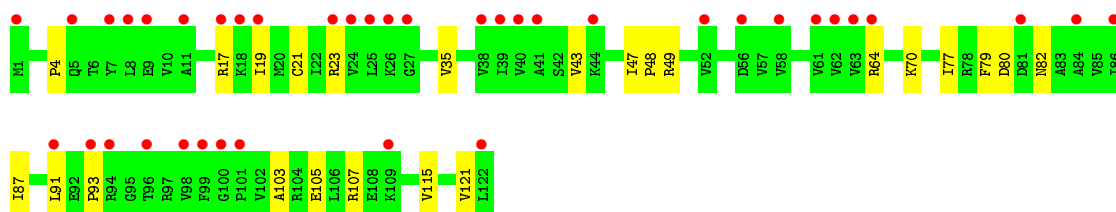
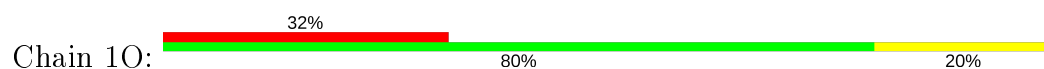
• Molecule 9: 50S Ribosomal Protein L13



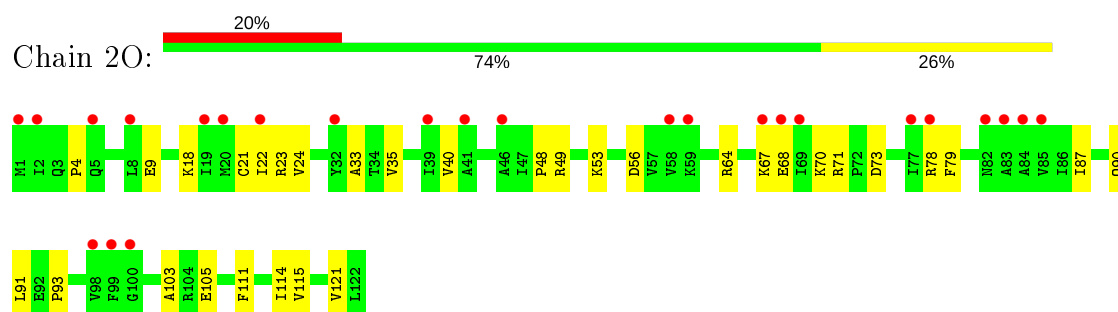
• Molecule 9: 50S Ribosomal Protein L13



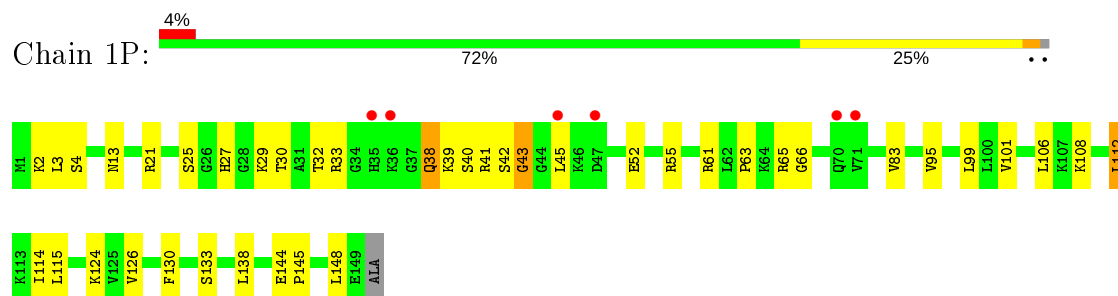
• Molecule 10: 50S Ribosomal Protein L14



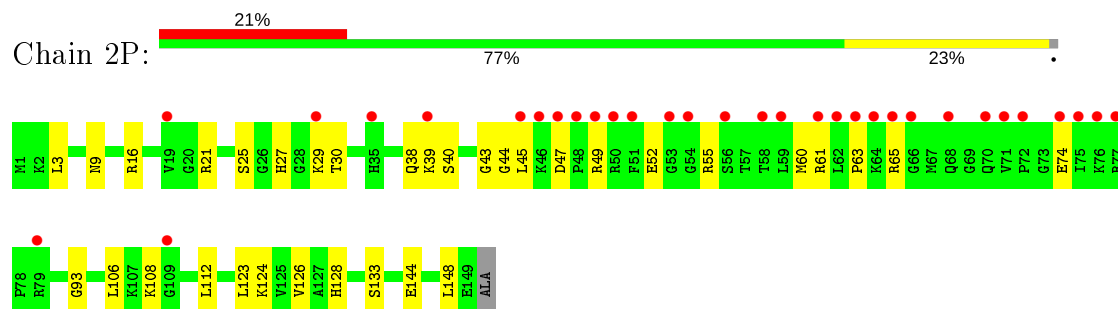
• Molecule 10: 50S Ribosomal Protein L14



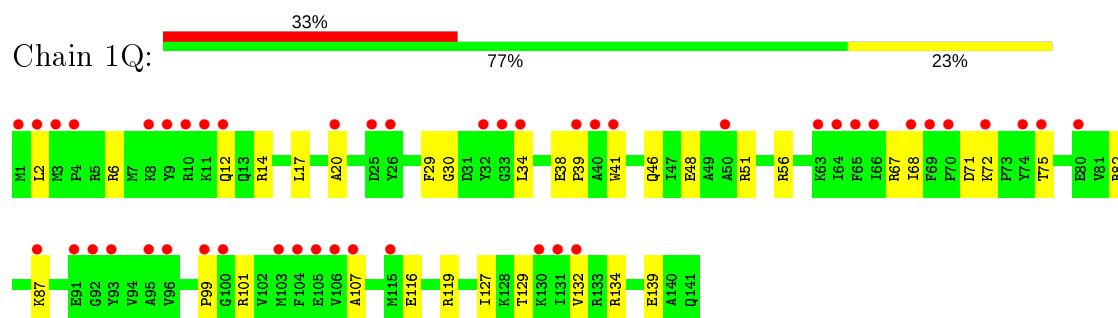
- Molecule 11: 50S Ribosomal Protein L15



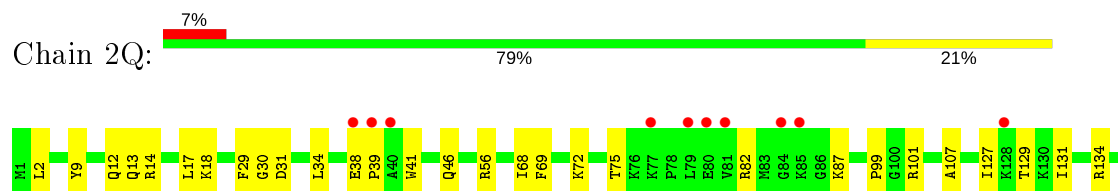
- Molecule 11: 50S Ribosomal Protein L15

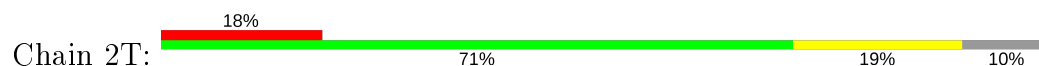


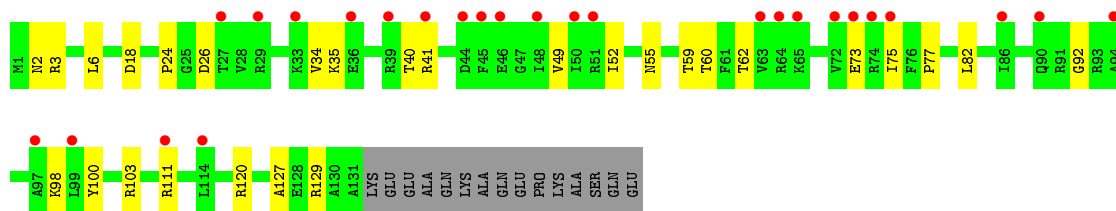
- Molecule 12: 50S Ribosomal Protein L16



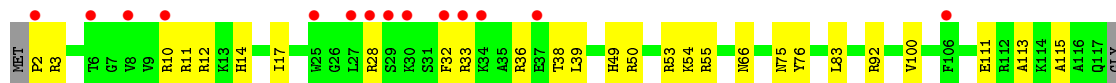
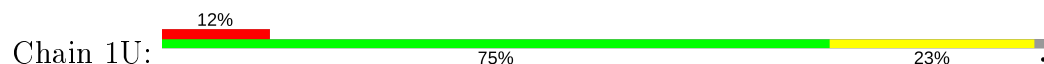
- Molecule 12: 50S Ribosomal Protein L16



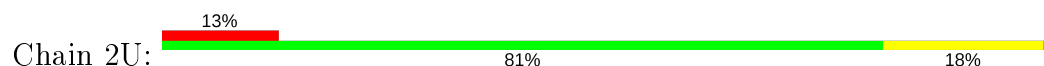




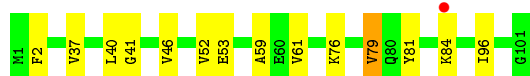
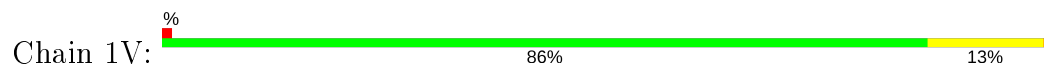
• Molecule 16: 50S Ribosomal Protein L20



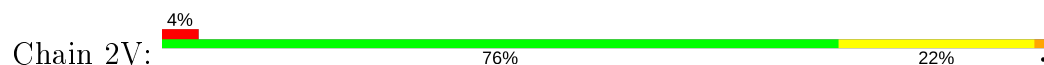
• Molecule 16: 50S Ribosomal Protein L20



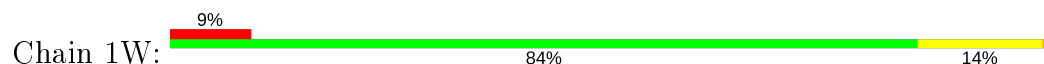
• Molecule 17: 50S Ribosomal Protein L21



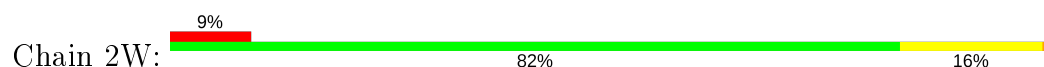
• Molecule 17: 50S Ribosomal Protein L21



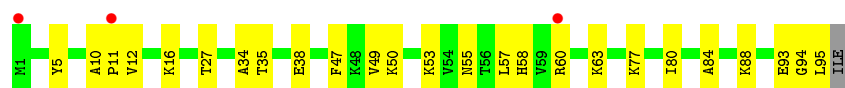
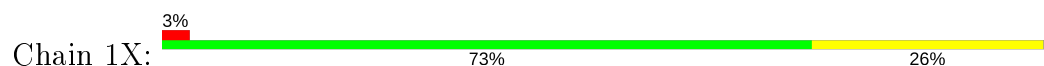
• Molecule 18: 50S Ribosomal Protein L22



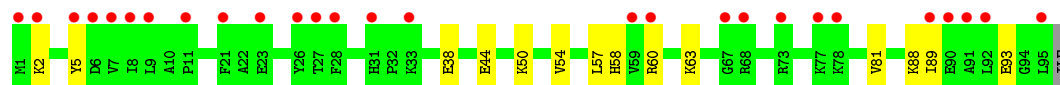
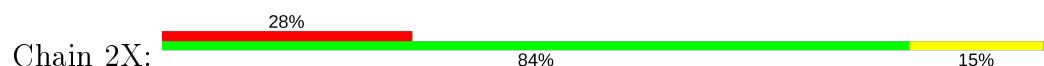
• Molecule 18: 50S Ribosomal Protein L22



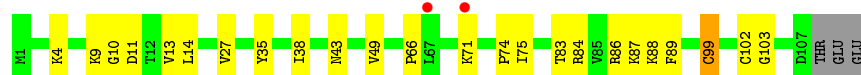
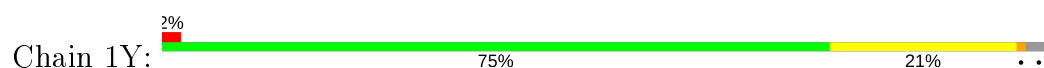
- Molecule 19: 50S Ribosomal Protein L23



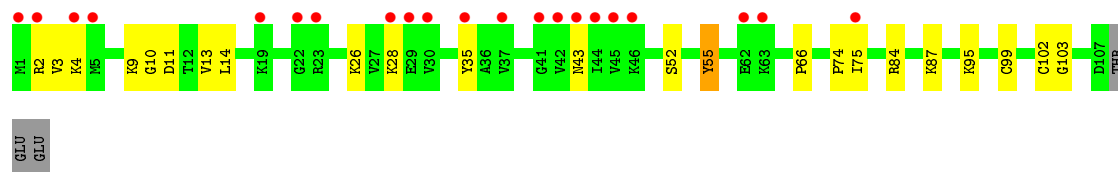
- Molecule 19: 50S Ribosomal Protein L23



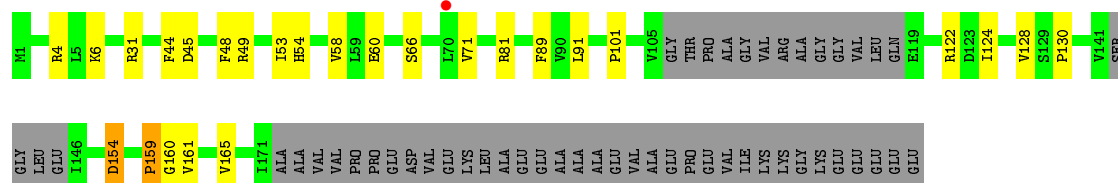
- Molecule 20: 50S ribosomal protein L24



- Molecule 20: 50S ribosomal protein L24

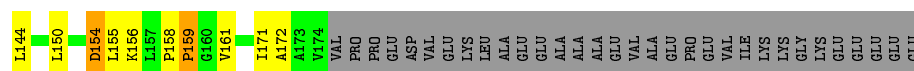


- Molecule 21: 50S ribosomal protein L25

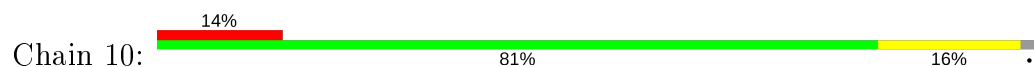


- Molecule 21: 50S ribosomal protein L25

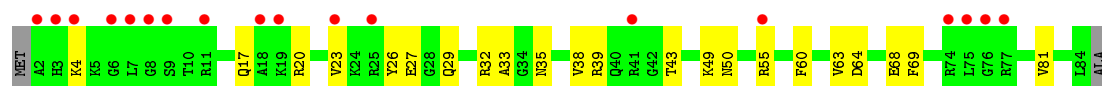
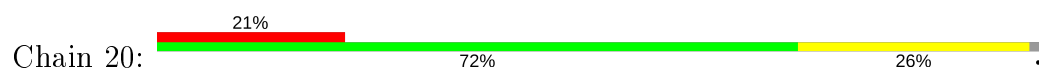




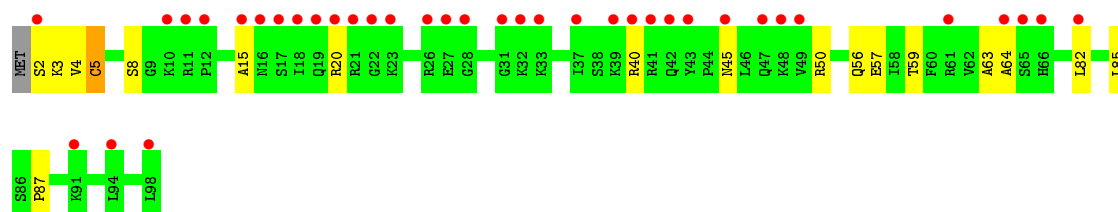
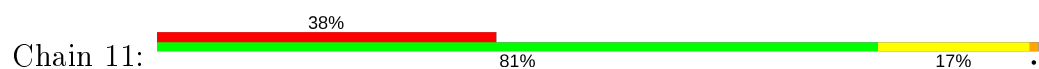
- Molecule 22: 50S ribosomal protein L27



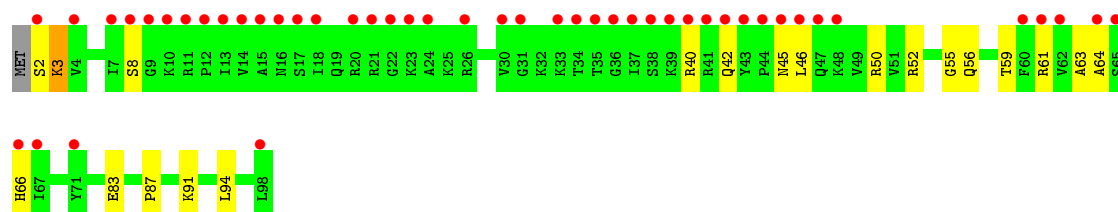
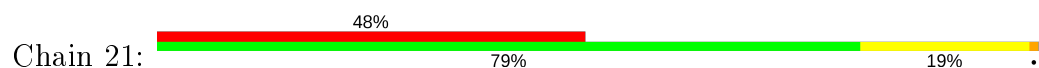
- Molecule 22: 50S ribosomal protein L27



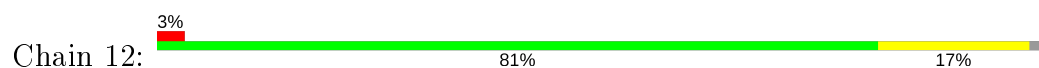
- Molecule 23: 50S ribosomal protein L28



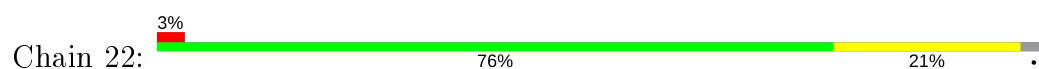
- Molecule 23: 50S ribosomal protein L28



- Molecule 24: 50S ribosomal protein L29

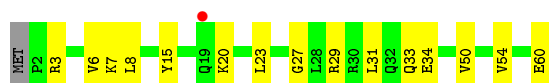
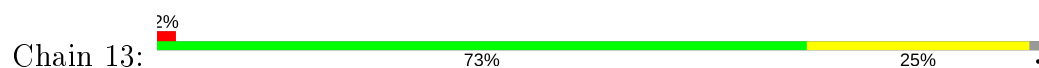


- Molecule 24: 50S ribosomal protein L29





- Molecule 25: 50S ribosomal protein L30



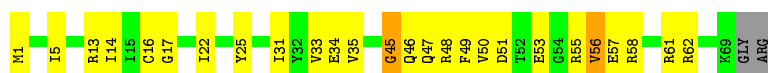
- Molecule 25: 50S ribosomal protein L30



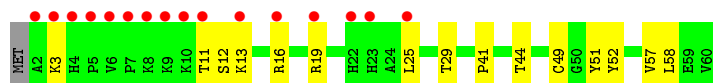
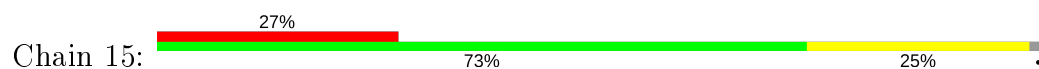
- Molecule 26: 50S ribosomal protein L31



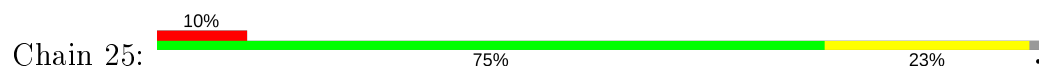
- Molecule 26: 50S ribosomal protein L31



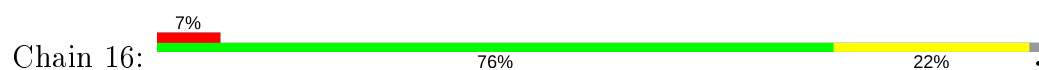
- Molecule 27: 50S ribosomal protein L32



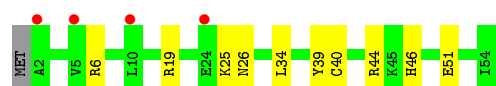
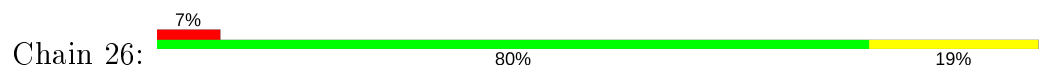
- Molecule 27: 50S ribosomal protein L32



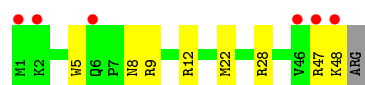
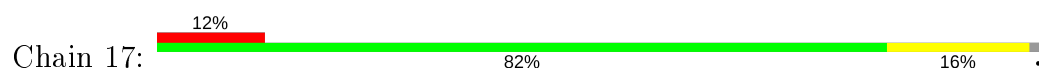
- Molecule 28: 50S ribosomal protein L33



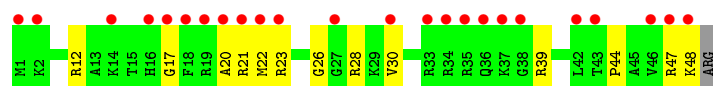
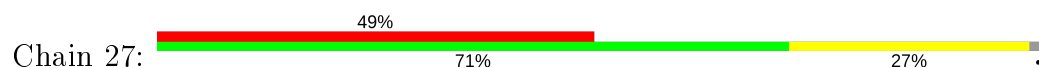
- Molecule 28: 50S ribosomal protein L33



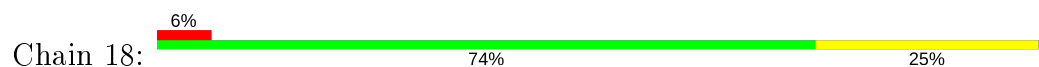
- Molecule 29: 50S ribosomal protein L34



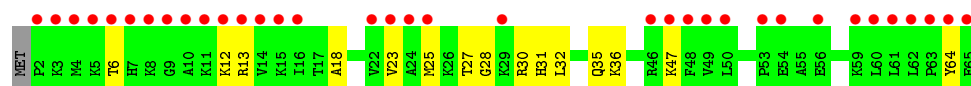
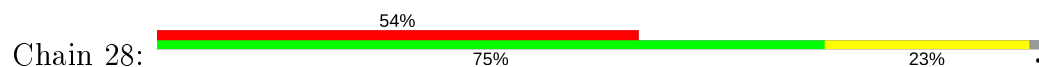
- Molecule 29: 50S ribosomal protein L34



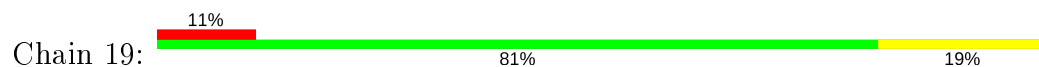
- Molecule 30: 50S Ribosomal Protein L35



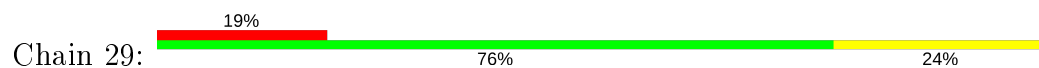
- Molecule 30: 50S Ribosomal Protein L35



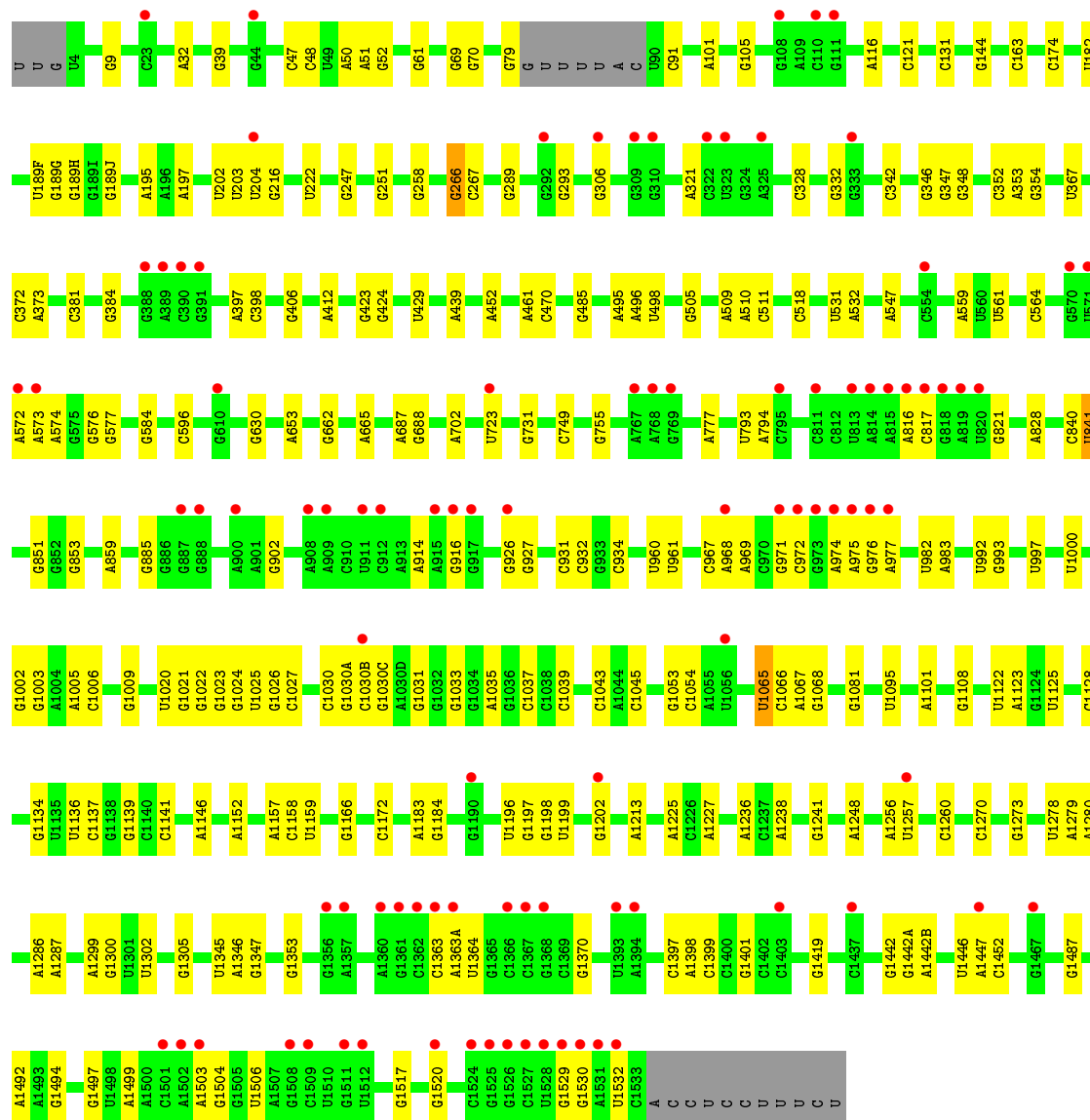
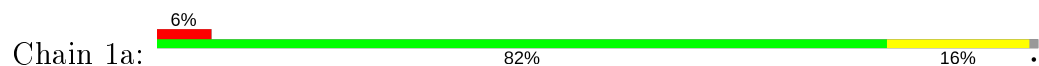
- Molecule 31: 50S Ribosomal Protein L36



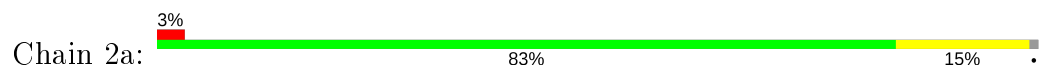
- Molecule 31: 50S Ribosomal Protein L36

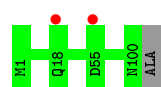


- Molecule 32: 16S Ribosomal RNA

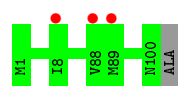


- Molecule 32: 16S Ribosomal RNA

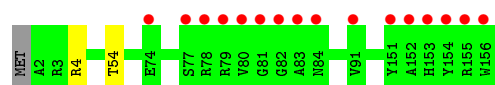




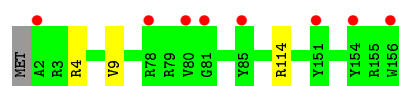
- Molecule 37: 30S Ribosomal Protein S6



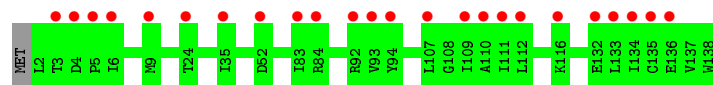
- Molecule 38: 30S Ribosomal Protein S7



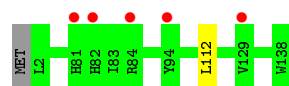
- Molecule 38: 30S Ribosomal Protein S7



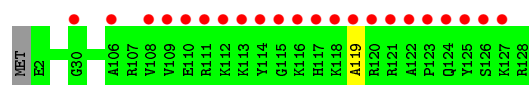
- Molecule 39: 30S Ribosomal Protein S8



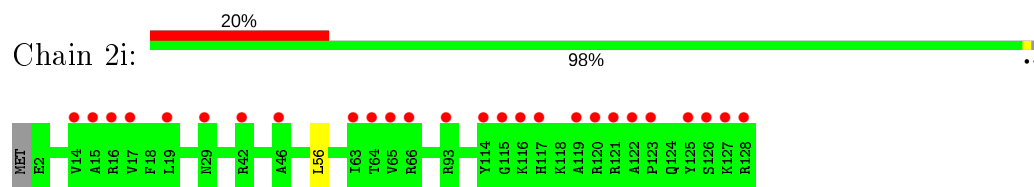
- Molecule 39: 30S Ribosomal Protein S8



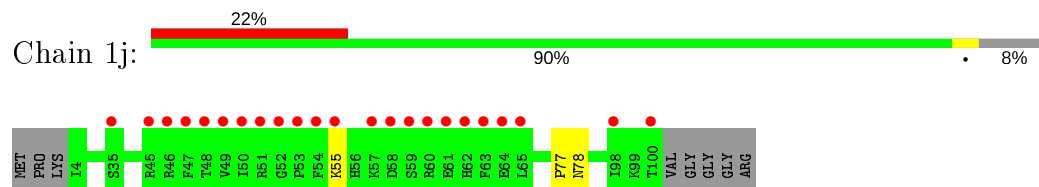
- Molecule 40: 30S ribosomal protein S9



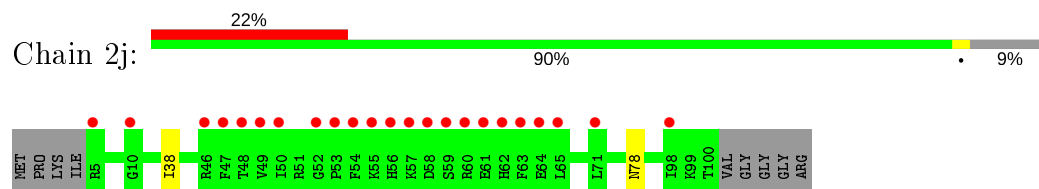
- Molecule 40: 30S ribosomal protein S9



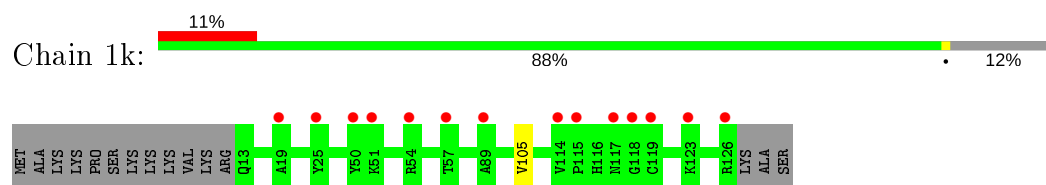
- Molecule 41: 30S ribosomal protein S10



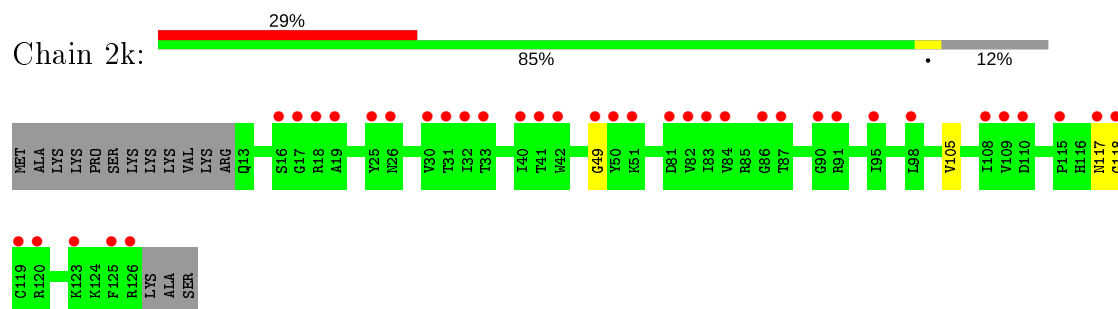
- Molecule 41: 30S ribosomal protein S10



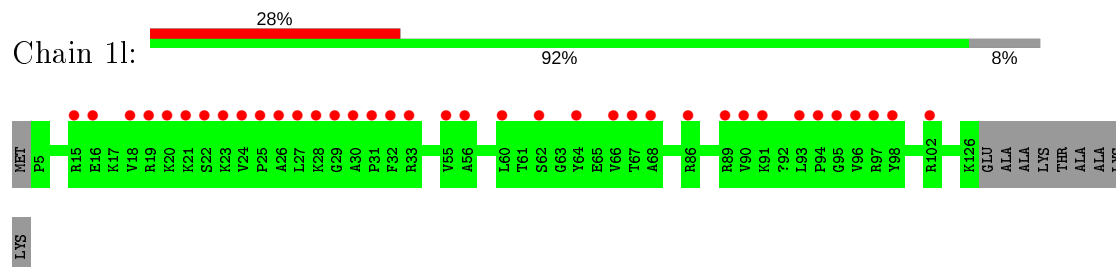
- Molecule 42: 30S ribosomal protein S11



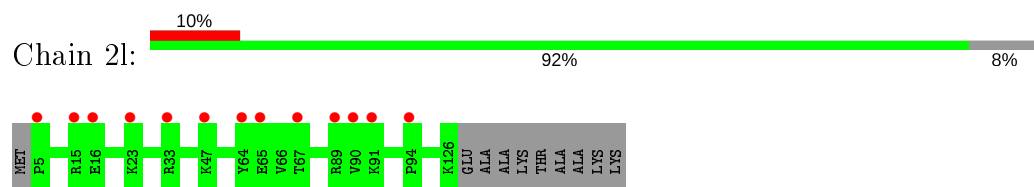
- Molecule 42: 30S ribosomal protein S11



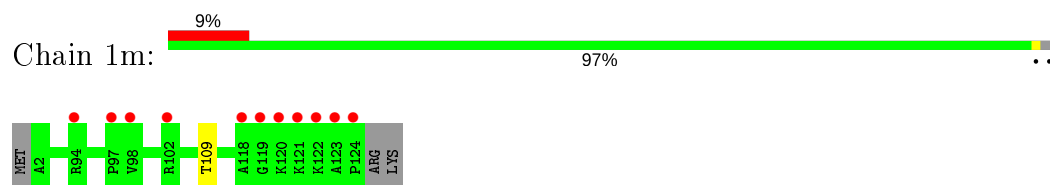
- Molecule 43: 30S ribosomal protein S12



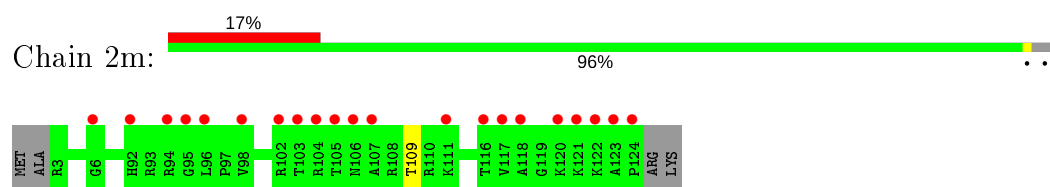
- Molecule 43: 30S ribosomal protein S12



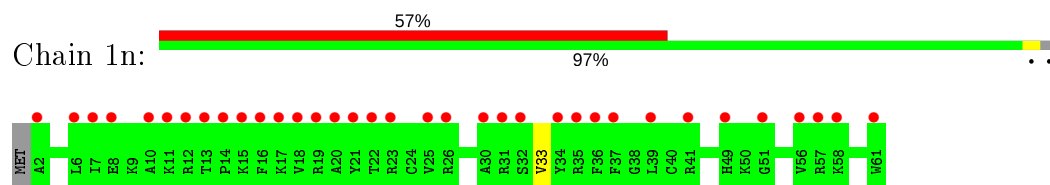
- Molecule 44: 30S ribosomal protein S13



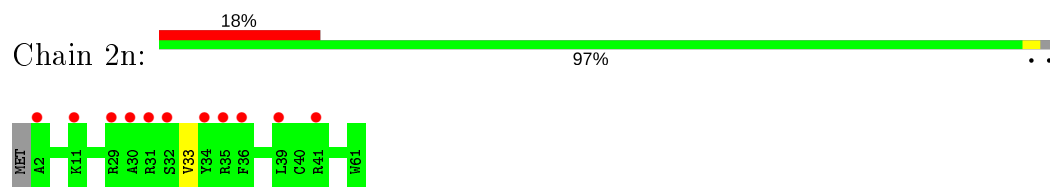
- Molecule 44: 30S ribosomal protein S13



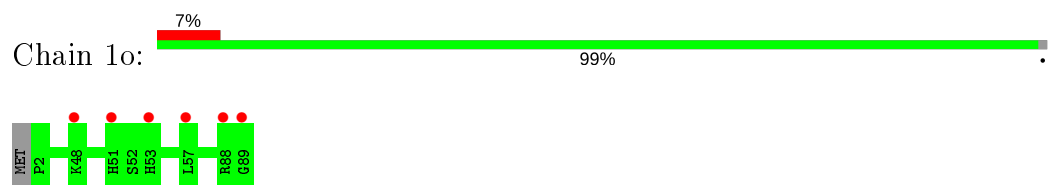
- Molecule 45: 30S ribosomal protein S14 type Z



- Molecule 45: 30S ribosomal protein S14 type Z

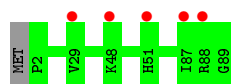


- Molecule 46: 30S ribosomal protein S15

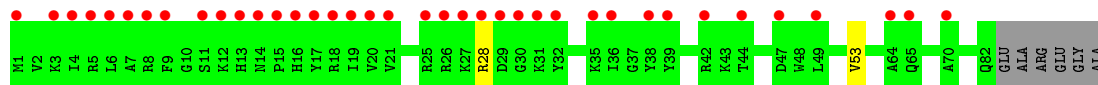
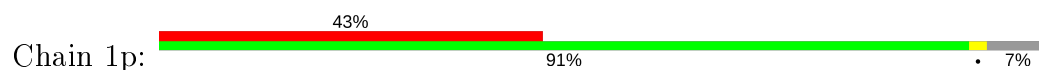


- Molecule 46: 30S ribosomal protein S15

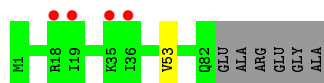




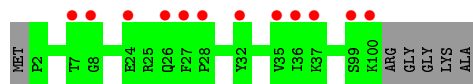
- Molecule 47: 30S ribosomal protein S16



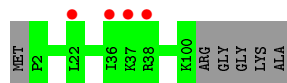
- Molecule 47: 30S ribosomal protein S16



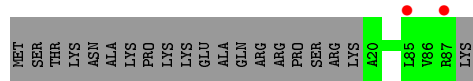
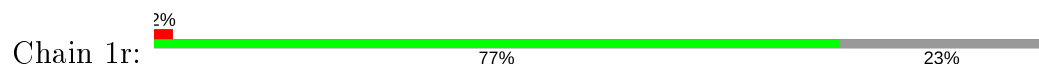
- Molecule 48: 30S ribosomal protein S17



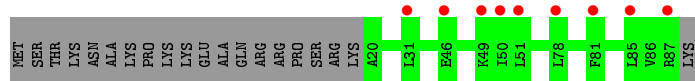
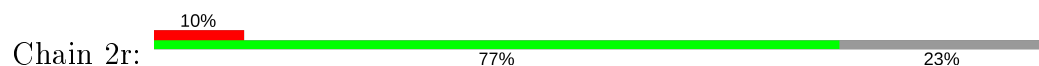
- Molecule 48: 30S ribosomal protein S17



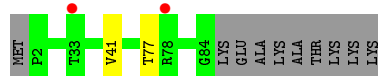
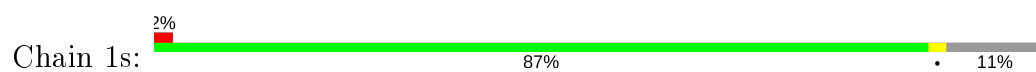
- Molecule 49: 30S ribosomal protein S18



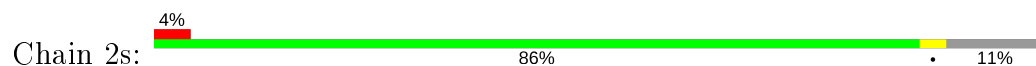
- Molecule 49: 30S ribosomal protein S18



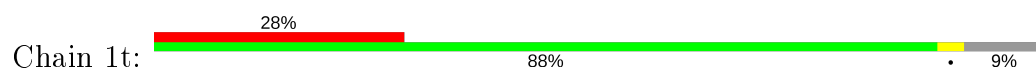
- Molecule 50: 30S Ribosomal Protein S19



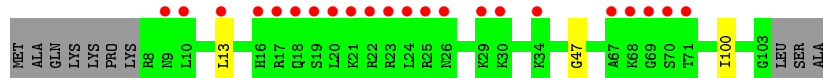
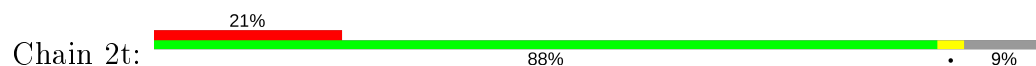
- Molecule 50: 30S Ribosomal Protein S19



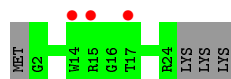
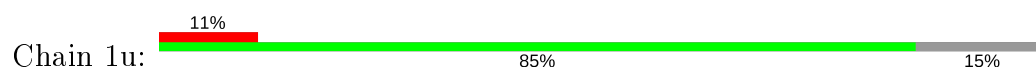
- Molecule 51: 30S Ribosomal Protein S20



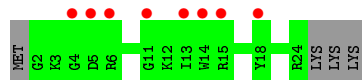
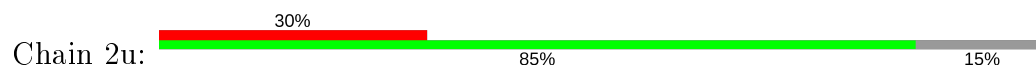
- Molecule 51: 30S Ribosomal Protein S20



- Molecule 52: 30S ribosomal protein Thx



- Molecule 52: 30S ribosomal protein Thx



- Molecule 53: mRNA



- Molecule 53: mRNA



- Molecule 54: CC-Pmn



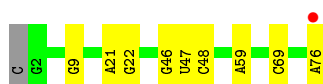
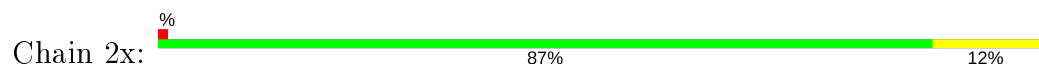
- Molecule 54: CC-Pmn



- 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	212.24Å 452.84Å 620.30Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	146.71 – 3.70 212.69 – 3.70	Depositor EDS
% Data completeness (in resolution range)	99.1 (146.71-3.70) 99.1 (212.69-3.70)	Depositor EDS
R_{merge}	0.24	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.31 (at 3.68Å)	Xtriage
Refinement program	PHENIX 1.8.2	Depositor
R, R_{free}	0.237 , 0.278 0.237 , 0.279	Depositor DCC
R_{free} test set	31415 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å ²)	135.2	Xtriage
Anisotropy	0.099	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.24 , 50.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.42$, $\langle L^2 \rangle = 0.24$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.84	EDS
Total number of atoms	287828	wwPDB-VP
Average B, all atoms (Å ²)	113.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.03% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	1A	0.37	0/69009	0.82	20/107712 (0.0%)
1	2A	0.33	0/67293	0.80	13/105034 (0.0%)
2	1B	0.33	1/2882 (0.0%)	0.76	0/4494
2	2B	0.33	1/2879 (0.0%)	0.78	1/4487 (0.0%)
3	1D	0.33	0/2186	0.48	0/2944
3	2D	0.35	1/2186 (0.0%)	0.48	0/2944
4	1E	0.29	0/1592	0.48	0/2149
4	2E	0.28	0/1592	0.46	0/2149
5	1F	0.30	0/1619	0.46	0/2193
5	2F	0.28	0/1615	0.44	0/2188
6	1G	0.27	0/1448	0.47	0/1957
6	2G	0.27	0/1453	0.46	0/1963
7	1H	0.27	0/1356	0.43	0/1834
7	2H	0.28	0/1356	0.43	0/1834
8	1I	0.26	0/1112	0.44	0/1514
8	2I	0.27	0/1079	0.45	0/1475
9	1N	0.31	0/1144	0.47	0/1543
9	2N	0.28	0/1144	0.46	0/1543
10	1O	0.31	0/943	0.47	0/1269
10	2O	0.30	0/943	0.47	0/1269
11	1P	0.28	0/1152	0.52	1/1533 (0.1%)
11	2P	0.29	0/1152	0.52	0/1533
12	1Q	0.30	0/1143	0.47	0/1527
12	2Q	0.27	0/1143	0.45	0/1527
13	1R	0.26	0/982	0.46	0/1312
13	2R	0.26	0/982	0.44	0/1312
14	1S	0.27	0/883	0.43	0/1176
14	2S	0.28	0/880	0.42	0/1172
15	1T	0.28	0/1105	0.45	0/1477
15	2T	0.28	0/1097	0.44	0/1468
16	1U	0.28	0/977	0.41	0/1301

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
16	2U	0.27	0/977	0.40	0/1301
17	1V	0.29	0/782	0.48	0/1049
17	2V	0.28	0/782	0.50	0/1049
18	1W	0.28	0/897	0.44	0/1205
18	2W	0.29	0/897	0.46	0/1205
19	1X	0.30	0/764	0.47	0/1025
19	2X	0.27	0/764	0.46	0/1025
20	1Y	0.31	0/819	0.46	0/1095
20	2Y	0.30	0/819	0.46	0/1095
21	1Z	0.27	0/1267	0.48	0/1717
21	2Z	0.27	0/1299	0.46	0/1763
22	10	0.28	0/662	0.47	0/881
22	20	0.28	0/662	0.46	0/881
23	11	0.30	0/762	0.46	0/1014
23	21	0.30	0/762	0.46	0/1014
24	12	0.27	0/590	0.39	0/781
24	22	0.27	0/590	0.37	0/781
25	13	0.29	0/474	0.43	0/635
25	23	0.26	0/469	0.43	0/630
26	14	0.30	0/565	0.56	0/761
26	24	0.35	0/545	0.50	0/737
27	15	0.33	0/469	0.48	0/635
27	25	0.32	0/469	0.47	0/635
28	16	0.27	0/460	0.47	0/613
28	26	0.26	0/456	0.46	0/608
29	17	0.29	0/426	0.43	0/561
29	27	0.26	0/426	0.44	0/561
30	18	0.28	0/525	0.45	0/691
30	28	0.27	0/525	0.45	0/691
31	19	0.33	0/310	0.50	0/407
31	29	0.30	0/310	0.48	0/407
32	1a	0.31	0/35795	0.83	19/55864 (0.0%)
32	2a	0.31	2/35886 (0.0%)	0.83	11/56005 (0.0%)
33	1b	0.28	0/1881	0.46	0/2542
33	2b	0.28	0/1860	0.45	0/2518
34	1c	0.28	0/1572	0.45	0/2126
34	2c	0.27	0/1566	0.44	0/2119
35	1d	0.29	0/1685	0.44	0/2262
35	2d	0.28	0/1704	0.44	0/2284
36	1e	0.27	0/1145	0.46	0/1543
36	2e	0.28	0/1149	0.48	0/1548
37	1f	0.27	0/823	0.46	0/1115
37	2f	0.27	0/829	0.47	0/1123

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
38	1g	0.27	0/1250	0.42	0/1679
38	2g	0.28	0/1254	0.41	0/1683
39	1h	0.26	0/1108	0.44	0/1494
39	2h	0.28	0/1108	0.44	0/1494
40	1i	0.29	0/1002	0.46	0/1346
40	2i	0.30	0/997	0.46	0/1343
41	1j	0.26	0/722	0.46	0/982
41	2j	0.26	0/727	0.46	0/988
42	1k	0.27	0/844	0.44	0/1145
42	2k	0.26	0/848	0.43	0/1149
43	1l	0.28	0/937	0.49	0/1260
43	2l	0.28	0/937	0.48	0/1260
44	1m	0.26	0/969	0.43	0/1302
44	2m	0.26	0/961	0.46	0/1291
45	1n	0.28	0/501	0.44	0/664
45	2n	0.28	0/501	0.45	0/664
46	1o	0.26	0/739	0.40	0/985
46	2o	0.25	0/739	0.40	0/985
47	1p	0.26	0/697	0.47	0/939
47	2p	0.27	0/693	0.45	0/935
48	1q	0.27	0/836	0.43	0/1117
48	2q	0.27	0/836	0.42	0/1117
49	1r	0.26	0/560	0.42	0/746
49	2r	0.27	0/560	0.44	0/746
50	1s	0.26	0/667	0.47	0/900
50	2s	0.25	0/661	0.48	0/893
51	1t	0.31	0/730	0.41	0/965
51	2t	0.25	0/729	0.39	0/965
52	1u	0.23	0/203	0.44	0/266
52	2u	0.24	0/203	0.43	0/266
53	1v	0.35	0/126	0.86	0/195
53	2v	0.33	0/126	0.81	0/195
54	1w	0.46	0/40	0.95	0/60
54	2w	0.35	0/40	1.05	0/60
55	1x	0.38	0/1725	0.97	1/2689 (0.0%)
55	2x	0.37	0/1725	0.96	3/2689 (0.1%)
All	All	0.32	5/310047 (0.0%)	0.74	69/463792 (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 (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	1B	1	U	OP3-P	-10.34	1.48	1.61
2	2B	1	U	OP3-P	-10.27	1.48	1.61
3	2D	7	LYS	C-N	-8.87	1.17	1.34
32	2a	1272	G	C6-N1	-6.71	1.34	1.39
32	2a	1272	G	N1-C2	-5.10	1.33	1.37

The worst 5 of 69 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	2a	1272	G	C5-C6-O6	13.95	136.97	128.60
32	2a	1272	G	N1-C6-O6	-11.59	112.94	119.90
32	2a	1272	G	N3-C2-N2	11.37	127.86	119.90
32	2a	1272	G	N1-C2-N2	-10.97	106.33	116.20
1	1A	1109	G	C5-C6-O6	9.10	134.06	128.60

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	9	GLU	Peptide

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	1A	61852	0	31194	902	0
1	2A	60322	0	30425	800	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	1B	2577	0	1305	30	0
2	2B	2575	0	1303	31	0
3	1D	2136	0	2218	61	0
3	2D	2136	0	2218	61	0
4	1E	1559	0	1618	33	0
4	2E	1559	0	1618	35	0
5	1F	1584	0	1625	32	0
5	2F	1580	0	1619	36	0
6	1G	1423	0	1436	40	0
6	2G	1428	0	1438	38	0
7	1H	1330	0	1407	20	0
7	2H	1330	0	1407	19	0
8	1I	1097	0	1140	29	0
8	2I	1064	0	1082	16	0
9	1N	1117	0	1184	18	0
9	2N	1117	0	1184	25	0
10	1O	933	0	996	19	0
10	2O	933	0	996	26	0
11	1P	1135	0	1212	29	0
11	2P	1135	0	1212	28	0
12	1Q	1122	0	1179	25	0
12	2Q	1122	0	1179	26	0
13	1R	968	0	1033	23	0
13	2R	968	0	1033	24	0
14	1S	873	0	927	14	0
14	2S	870	0	923	24	0
15	1T	1091	0	1151	29	0
15	2T	1083	0	1136	23	0
16	1U	959	0	1019	25	0
16	2U	959	0	1019	26	0
17	1V	771	0	830	7	0
17	2V	771	0	830	18	0
18	1W	886	0	940	15	0
18	2W	886	0	940	15	0
19	1X	750	0	814	18	0
19	2X	750	0	814	11	0
20	1Y	806	0	881	18	0
20	2Y	806	0	881	15	0
21	1Z	1240	0	1240	19	0
21	2Z	1271	0	1273	27	0
22	10	653	0	674	12	0
22	20	653	0	674	17	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
23	11	755	0	826	11	0
23	21	755	0	826	14	0
24	12	588	0	643	10	0
24	22	588	0	643	11	0
25	13	469	0	518	12	0
25	23	464	0	514	9	0
26	14	552	0	533	17	0
26	24	532	0	503	19	0
27	15	455	0	465	11	0
27	25	455	0	465	12	0
28	16	453	0	473	9	0
28	26	449	0	469	7	0
29	17	418	0	467	10	0
29	27	418	0	467	9	0
30	18	517	0	582	14	0
30	28	517	0	582	15	0
31	19	307	0	335	5	0
31	29	307	0	335	7	0
32	1a	32246	0	16296	0	0
32	2a	32327	0	16339	0	0
33	1b	1846	0	1867	0	0
33	2b	1825	0	1828	0	0
34	1c	1548	0	1535	0	0
34	2c	1542	0	1517	0	0
35	1d	1655	0	1672	0	0
35	2d	1674	0	1714	0	0
36	1e	1129	0	1185	0	0
36	2e	1133	0	1191	0	0
37	1f	810	0	804	0	0
37	2f	816	0	808	0	0
38	1g	1231	0	1238	0	0
38	2g	1235	0	1249	0	0
39	1h	1088	0	1126	0	0
39	2h	1088	0	1126	0	0
40	1i	983	0	986	0	0
40	2i	978	0	966	0	0
41	1j	709	0	650	0	0
41	2j	714	0	672	0	0
42	1k	829	0	825	0	0
42	2k	833	0	836	0	0
43	1l	932	0	981	0	0
43	2l	932	0	981	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
44	1m	958	0	1002	0	0
44	2m	950	0	988	0	0
45	1n	492	0	529	0	0
45	2n	492	0	529	0	0
46	1o	728	0	760	0	0
46	2o	728	0	760	0	0
47	1p	681	0	697	0	0
47	2p	677	0	686	0	0
48	1q	823	0	891	0	0
48	2q	823	0	891	0	0
49	1r	555	0	618	0	0
49	2r	555	0	618	0	0
50	1s	652	0	662	0	0
50	2s	646	0	644	0	0
51	1t	728	0	798	0	0
51	2t	727	0	796	0	0
52	1u	199	0	208	0	0
52	2u	199	0	208	0	0
53	1v	113	0	54	0	0
53	2v	113	0	54	0	0
54	1w	74	0	51	0	0
54	2w	74	0	50	0	0
55	1x	1625	0	829	0	0
55	2x	1625	0	829	0	0
56	10	3	0	0	0	0
56	13	1	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	1	0	0	0	0
56	1A	498	0	0	0	0
56	1B	12	0	0	0	0
56	1D	1	0	0	0	0
56	1E	6	0	0	0	0
56	1F	1	0	0	0	0
56	1Q	1	0	0	0	0
56	1S	1	0	0	0	0
56	1U	1	0	0	0	0
56	1V	3	0	0	0	0
56	1W	1	0	0	0	0
56	1a	93	0	0	0	0
56	1d	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
56	1l	1	0	0	0	0
56	1r	1	0	0	0	0
56	1x	2	0	0	0	0
56	20	2	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	385	0	0	0	0
56	2B	9	0	0	0	0
56	2D	1	0	0	0	0
56	2E	6	0	0	0	0
56	2O	1	0	0	0	0
56	2Q	2	0	0	0	0
56	2R	2	0	0	0	0
56	2T	2	0	0	0	0
56	2Y	1	0	0	0	0
56	2a	103	0	0	0	0
56	2d	1	0	0	0	0
56	2f	1	0	0	0	0
56	2l	1	0	0	0	0
56	2r	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
57	2Y	1	0	0	0	0
57	2n	1	0	0	0	0
58	1d	8	0	0	0	0
58	2d	8	0	0	0	0
59	1A	53	0	0	2	0
59	1D	3	0	0	2	0
59	1a	15	0	0	0	0
59	1x	2	0	0	0	0
59	2A	32	0	0	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
59	2B	1	0	0	0	0
59	2a	19	0	0	0	0
All	All	287828	0	193417	2518	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 2518 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:1128:U:H3	1:1A:1132:A:N6	1.47	1.12
1:2A:1011:G:H1	1:2A:1018:C:H42	18.84	1.00
1:1A:1103:A:N6	1:1A:1127:U:H3	1.59	1.00
1:1A:2121:U:H3	1:1A:2212:G:H1	1.06	1.00
1:1A:1105:G:H1	1:1A:1125:C:H42	1.04	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%)	262 (96%)	11 (4%)	0	100	100
4	1E	202/206 (98%)	191 (95%)	10 (5%)	1 (0%)	29	66
4	2E	202/206 (98%)	192 (95%)	9 (4%)	1 (0%)	29	66
5	1F	201/210 (96%)	196 (98%)	3 (2%)	2 (1%)	15	51
5	2F	201/210 (96%)	194 (96%)	5 (2%)	2 (1%)	15	51
6	1G	179/182 (98%)	168 (94%)	9 (5%)	2 (1%)	14	50
6	2G	179/182 (98%)	170 (95%)	7 (4%)	2 (1%)	14	50

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
7	1H	172/180 (96%)	162 (94%)	8 (5%)	2 (1%)	13	48
7	2H	172/180 (96%)	165 (96%)	4 (2%)	3 (2%)	9	42
8	1I	144/148 (97%)	135 (94%)	9 (6%)	0	100	100
8	2I	144/148 (97%)	132 (92%)	12 (8%)	0	100	100
9	1N	138/140 (99%)	129 (94%)	8 (6%)	1 (1%)	22	59
9	2N	138/140 (99%)	129 (94%)	8 (6%)	1 (1%)	22	59
10	1O	120/122 (98%)	111 (92%)	9 (8%)	0	100	100
10	2O	120/122 (98%)	114 (95%)	6 (5%)	0	100	100
11	1P	147/150 (98%)	136 (92%)	8 (5%)	3 (2%)	7	39
11	2P	147/150 (98%)	136 (92%)	10 (7%)	1 (1%)	22	59
12	1Q	139/141 (99%)	133 (96%)	6 (4%)	0	100	100
12	2Q	139/141 (99%)	131 (94%)	8 (6%)	0	100	100
13	1R	116/118 (98%)	110 (95%)	6 (5%)	0	100	100
13	2R	116/118 (98%)	110 (95%)	6 (5%)	0	100	100
14	1S	108/112 (96%)	104 (96%)	3 (3%)	1 (1%)	17	54
14	2S	108/112 (96%)	104 (96%)	4 (4%)	0	100	100
15	1T	129/146 (88%)	123 (95%)	5 (4%)	1 (1%)	19	56
15	2T	129/146 (88%)	126 (98%)	3 (2%)	0	100	100
16	1U	114/118 (97%)	113 (99%)	1 (1%)	0	100	100
16	2U	114/118 (97%)	114 (100%)	0	0	100	100
17	1V	99/101 (98%)	92 (93%)	6 (6%)	1 (1%)	15	51
17	2V	99/101 (98%)	93 (94%)	6 (6%)	0	100	100
18	1W	110/113 (97%)	105 (96%)	5 (4%)	0	100	100
18	2W	110/113 (97%)	106 (96%)	4 (4%)	0	100	100
19	1X	93/96 (97%)	88 (95%)	5 (5%)	0	100	100
19	2X	93/96 (97%)	90 (97%)	3 (3%)	0	100	100
20	1Y	105/110 (96%)	102 (97%)	3 (3%)	0	100	100
20	2Y	105/110 (96%)	100 (95%)	5 (5%)	0	100	100
21	1Z	148/206 (72%)	130 (88%)	18 (12%)	0	100	100
21	2Z	156/206 (76%)	142 (91%)	14 (9%)	0	100	100
22	10	81/85 (95%)	76 (94%)	4 (5%)	1 (1%)	13	48

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
22	20	81/85 (95%)	76 (94%)	4 (5%)	1 (1%)	13	48
23	11	95/98 (97%)	94 (99%)	0	1 (1%)	14	50
23	21	95/98 (97%)	93 (98%)	1 (1%)	1 (1%)	14	50
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%)	57 (100%)	0	0	100	100
25	23	57/60 (95%)	57 (100%)	0	0	100	100
26	14	67/71 (94%)	51 (76%)	9 (13%)	7 (10%)	0	7
26	24	67/71 (94%)	53 (79%)	9 (13%)	5 (8%)	1	13
27	15	57/60 (95%)	54 (95%)	3 (5%)	0	100	100
27	25	57/60 (95%)	55 (96%)	2 (4%)	0	100	100
28	16	51/54 (94%)	51 (100%)	0	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%)	45 (98%)	1 (2%)	0	100	100
30	18	62/65 (95%)	60 (97%)	2 (3%)	0	100	100
30	28	62/65 (95%)	61 (98%)	1 (2%)	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%)	201 (88%)	24 (10%)	4 (2%)	9	42
33	2b	229/256 (90%)	203 (89%)	23 (10%)	3 (1%)	12	47
34	1c	204/239 (85%)	188 (92%)	15 (7%)	1 (0%)	29	66
34	2c	204/239 (85%)	190 (93%)	14 (7%)	0	100	100
35	1d	206/209 (99%)	198 (96%)	7 (3%)	1 (0%)	29	66
35	2d	206/209 (99%)	197 (96%)	8 (4%)	1 (0%)	29	66
36	1e	146/162 (90%)	132 (90%)	14 (10%)	0	100	100
36	2e	146/162 (90%)	138 (94%)	8 (6%)	0	100	100
37	1f	98/101 (97%)	97 (99%)	1 (1%)	0	100	100
37	2f	98/101 (97%)	94 (96%)	4 (4%)	0	100	100
38	1g	153/156 (98%)	139 (91%)	12 (8%)	2 (1%)	12	47
38	2g	153/156 (98%)	139 (91%)	12 (8%)	2 (1%)	12	47

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
39	1h	135/138 (98%)	127 (94%)	8 (6%)	0	100	100
39	2h	135/138 (98%)	128 (95%)	7 (5%)	0	100	100
40	1i	125/128 (98%)	113 (90%)	11 (9%)	1 (1%)	19	56
40	2i	125/128 (98%)	114 (91%)	10 (8%)	1 (1%)	19	56
41	1j	95/105 (90%)	88 (93%)	4 (4%)	3 (3%)	4	31
41	2j	94/105 (90%)	86 (92%)	7 (7%)	1 (1%)	14	50
42	1k	112/129 (87%)	106 (95%)	5 (4%)	1 (1%)	17	54
42	2k	112/129 (87%)	104 (93%)	4 (4%)	4 (4%)	3	29
43	1l	119/132 (90%)	107 (90%)	12 (10%)	0	100	100
43	2l	119/132 (90%)	109 (92%)	10 (8%)	0	100	100
44	1m	121/126 (96%)	115 (95%)	6 (5%)	0	100	100
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%)	57 (98%)	1 (2%)	0	100	100
46	1o	86/89 (97%)	82 (95%)	4 (5%)	0	100	100
46	2o	86/89 (97%)	83 (96%)	3 (4%)	0	100	100
47	1p	80/88 (91%)	74 (92%)	4 (5%)	2 (2%)	5	35
47	2p	80/88 (91%)	72 (90%)	7 (9%)	1 (1%)	12	47
48	1q	97/105 (92%)	92 (95%)	5 (5%)	0	100	100
48	2q	97/105 (92%)	91 (94%)	6 (6%)	0	100	100
49	1r	66/88 (75%)	66 (100%)	0	0	100	100
49	2r	66/88 (75%)	66 (100%)	0	0	100	100
50	1s	81/93 (87%)	71 (88%)	10 (12%)	0	100	100
50	2s	81/93 (87%)	74 (91%)	6 (7%)	1 (1%)	13	48
51	1t	94/106 (89%)	85 (90%)	7 (7%)	2 (2%)	7	38
51	2t	94/106 (89%)	87 (93%)	5 (5%)	2 (2%)	7	38
52	1u	21/27 (78%)	20 (95%)	1 (5%)	0	100	100
52	2u	21/27 (78%)	20 (95%)	1 (5%)	0	100	100
All	All	11370/12128 (94%)	10706 (94%)	591 (5%)	73 (1%)	25	62

5 of 73 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
7	1H	92	ILE
26	14	46	GLN
26	14	51	ASP
26	14	57	GLU
33	1b	22	LYS

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	1D	215/218 (99%)	215 (100%)	0	100	100
3	2D	215/218 (99%)	215 (100%)	0	100	100
4	1E	164/166 (99%)	163 (99%)	1 (1%)	86	93
4	2E	164/166 (99%)	163 (99%)	1 (1%)	86	93
5	1F	160/166 (96%)	160 (100%)	0	100	100
5	2F	159/166 (96%)	159 (100%)	0	100	100
6	1G	143/156 (92%)	141 (99%)	2 (1%)	67	82
6	2G	143/156 (92%)	142 (99%)	1 (1%)	84	91
7	1H	144/148 (97%)	143 (99%)	1 (1%)	84	91
7	2H	144/148 (97%)	144 (100%)	0	100	100
8	1I	113/124 (91%)	113 (100%)	0	100	100
8	2I	105/124 (85%)	105 (100%)	0	100	100
9	1N	118/119 (99%)	117 (99%)	1 (1%)	81	89
9	2N	118/119 (99%)	117 (99%)	1 (1%)	81	89
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%)	113 (98%)	2 (2%)	60	79
11	2P	115/116 (99%)	115 (100%)	0	100	100
12	1Q	111/111 (100%)	111 (100%)	0	100	100
12	2Q	111/111 (100%)	111 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
13	1R	101/101 (100%)	101 (100%)	0	100	100
13	2R	101/101 (100%)	101 (100%)	0	100	100
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%)	93 (100%)	0	100	100
17	1V	80/82 (98%)	77 (96%)	3 (4%)	33	61
17	2V	80/82 (98%)	77 (96%)	3 (4%)	33	61
18	1W	90/92 (98%)	89 (99%)	1 (1%)	73	85
18	2W	90/92 (98%)	89 (99%)	1 (1%)	73	85
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%)	84 (99%)	1 (1%)	71	84
20	2Y	85/91 (93%)	83 (98%)	2 (2%)	49	71
21	1Z	135/179 (75%)	134 (99%)	1 (1%)	84	91
21	2Z	137/179 (76%)	136 (99%)	1 (1%)	84	91
22	10	65/67 (97%)	65 (100%)	0	100	100
22	20	65/67 (97%)	64 (98%)	1 (2%)	65	81
23	11	80/83 (96%)	78 (98%)	2 (2%)	47	70
23	21	80/83 (96%)	80 (100%)	0	100	100
24	12	65/67 (97%)	65 (100%)	0	100	100
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%)	56 (95%)	3 (5%)	24	55
26	24	53/63 (84%)	52 (98%)	1 (2%)	57	76
27	15	50/52 (96%)	49 (98%)	1 (2%)	55	74
27	25	50/52 (96%)	50 (100%)	0	100	100
28	16	51/52 (98%)	51 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
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%)	192 (100%)	0	100	100
33	2b	187/220 (85%)	183 (98%)	4 (2%)	53	74
34	1c	142/188 (76%)	142 (100%)	0	100	100
34	2c	140/188 (74%)	140 (100%)	0	100	100
35	1d	169/181 (93%)	168 (99%)	1 (1%)	86	93
35	2d	173/181 (96%)	171 (99%)	2 (1%)	71	84
36	1e	113/123 (92%)	112 (99%)	1 (1%)	78	88
36	2e	114/123 (93%)	114 (100%)	0	100	100
37	1f	84/90 (93%)	84 (100%)	0	100	100
37	2f	85/90 (94%)	85 (100%)	0	100	100
38	1g	119/127 (94%)	119 (100%)	0	100	100
38	2g	120/127 (94%)	119 (99%)	1 (1%)	81	89
39	1h	114/119 (96%)	114 (100%)	0	100	100
39	2h	114/119 (96%)	113 (99%)	1 (1%)	78	88
40	1i	90/99 (91%)	90 (100%)	0	100	100
40	2i	89/99 (90%)	89 (100%)	0	100	100
41	1j	66/92 (72%)	66 (100%)	0	100	100
41	2j	69/92 (75%)	68 (99%)	1 (1%)	67	82
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%)	92 (99%)	1 (1%)	73	85
44	2m	92/101 (91%)	91 (99%)	1 (1%)	73	85

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
45	1n	49/50 (98%)	48 (98%)	1 (2%)	55	74
45	2n	49/50 (98%)	48 (98%)	1 (2%)	55	74
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%)	69 (100%)	0	100	100
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%)	59 (100%)	0	100	100
49	2r	59/77 (77%)	59 (100%)	0	100	100
50	1s	69/80 (86%)	67 (97%)	2 (3%)	42	66
50	2s	67/80 (84%)	65 (97%)	2 (3%)	41	66
51	1t	70/82 (85%)	69 (99%)	1 (1%)	67	82
51	2t	70/82 (85%)	69 (99%)	1 (1%)	67	82
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%)	9251 (99%)	52 (1%)	86	93

5 of 52 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
50	1s	41	VAL
17	2V	52	VAL
45	2n	33	VAL
50	1s	77	THR
4	2E	75	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 60 such sidechains are listed below:

Mol	Chain	Res	Type
49	1r	63	GLN
6	2G	26	GLN
40	2i	58	HIS
5	2F	40	GLN
8	2I	11	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	1A	2861/2915 (98%)	438 (15%)	28 (0%)
1	2A	2788/2915 (95%)	443 (15%)	21 (0%)
2	1B	120/121 (99%)	10 (8%)	1 (0%)
2	2B	119/121 (98%)	12 (10%)	1 (0%)
32	1a	1494/1521 (98%)	243 (16%)	0
32	2a	1498/1521 (98%)	231 (15%)	0
53	1v	4/24 (16%)	0	0
53	2v	4/24 (16%)	0	0
54	1w	1/3 (33%)	1 (100%)	0
54	2w	1/3 (33%)	1 (100%)	0
55	1x	75/77 (97%)	6 (8%)	0
55	2x	75/77 (97%)	7 (9%)	0
All	All	9040/9322 (96%)	1392 (15%)	51 (0%)

5 of 1392 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	1A	12	U
1	1A	13	A
1	1A	34	C
1	1A	45	C
1	1A	62	U

5 of 51 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	1A	2418	U
2	1B	1	U
1	2A	2351	G
1	1A	2641	A
1	2A	195	A

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	1A	1961	1	15,22,23	1.12	2 (13%)	16,32,35	1.77	2 (12%)
1	5MU	1A	1937	1	15,22,23	1.09	1 (6%)	16,32,35	1.88	1 (6%)
55	4SU	2x	8	55	14,21,22	1.37	2 (14%)	15,30,33	2.21	2 (13%)
1	2MU	1A	2564	1	14,22,24	0.87	0	14,31,36	0.84	1 (7%)
1	OMG	2A	2251	1,55	18,26,27	1.20	2 (11%)	20,38,41	2.13	6 (30%)
1	5MU	2A	1915	1	15,22,23	1.05	1 (6%)	16,32,35	1.86	2 (12%)
32	5MC	2a	1404	32	15,22,23	1.37	1 (6%)	19,32,35	1.24	3 (15%)
32	MA6	2a	1519	32	19,26,27	1.01	1 (5%)	18,38,41	1.75	5 (27%)
1	5MC	1A	1964	1	15,22,23	1.29	1 (6%)	19,32,35	1.25	3 (15%)
1	5MC	1A	1984	1	15,22,23	1.35	1 (6%)	19,32,35	1.29	3 (15%)
32	PSU	2a	516	32	17,21,22	1.47	3 (17%)	20,30,33	3.16	6 (30%)
32	5MC	1a	1400	32	15,22,23	1.35	1 (6%)	19,32,35	1.25	3 (15%)
1	2MA	2A	2503	1,56	17,25,26	1.37	2 (11%)	19,37,40	2.09	3 (15%)
32	4OC	2a	1402	32	16,23,24	0.59	0	17,32,35	1.26	1 (5%)
55	5MU	2x	54	55	15,22,23	1.08	1 (6%)	16,32,35	1.83	2 (12%)
1	PSU	2A	1911	1	17,21,22	1.50	2 (11%)	20,30,33	3.12	6 (30%)
55	5MC	2x	32	55	15,22,23	1.29	1 (6%)	19,32,35	1.44	3 (15%)
1	PSU	1A	1933	1	17,21,22	1.60	3 (17%)	20,30,33	3.15	6 (30%)
32	UR3	1a	1498	32	14,22,23	0.71	0	15,32,35	0.66	0
32	5MC	2a	1400	32	15,22,23	1.37	1 (6%)	19,32,35	1.26	3 (15%)
32	PSU	1a	516	32,56	17,21,22	1.43	3 (17%)	20,30,33	3.21	6 (30%)
1	5MU	2A	1939	1	15,22,23	1.00	1 (6%)	16,32,35	1.97	2 (12%)
32	MA6	1a	1519	32	19,26,27	0.97	1 (5%)	18,38,41	1.69	6 (33%)
1	2MU	2A	2552	1	14,22,24	0.88	0	14,31,36	0.91	0
1	PSU	1A	2617	1	17,21,22	1.65	4 (23%)	20,30,33	3.06	6 (30%)
32	2MG	1a	1207	32	19,26,27	1.20	2 (10%)	21,38,41	2.08	6 (28%)
32	UR3	2a	1498	32	14,22,23	0.82	1 (7%)	15,32,35	0.80	1 (6%)
55	5MC	1x	32	55	15,22,23	1.30	1 (6%)	19,32,35	1.44	4 (21%)
32	5MC	1a	1404	32	15,22,23	1.30	1 (6%)	19,32,35	1.34	3 (15%)
55	4SU	1x	8	55	14,21,22	1.36	2 (14%)	15,30,33	1.88	2 (13%)
32	5MC	2a	967	32	15,22,23	1.34	1 (6%)	19,32,35	1.36	3 (15%)
43	0TD	1l	92	43	4,9,10	3.03	1 (25%)	3,11,13	9.45	1 (33%)
32	MA6	2a	1518	32	19,26,27	0.97	1 (5%)	18,38,41	1.77	6 (33%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
55	PSU	1x	55	55	17,21,22	1.57	3 (17%)	20,30,33	3.04	7 (35%)
1	4OC	2A	1920	1	15,22,24	0.65	0	17,31,35	1.35	2 (11%)
1	OMG	1A	2263	1,55	18,26,27	1.16	2 (11%)	20,38,41	1.96	6 (30%)
32	M2G	1a	966	32	20,27,28	1.39	3 (15%)	22,40,43	2.13	4 (18%)
1	PSU	1A	1939	1	17,21,22	1.48	2 (11%)	20,30,33	3.15	5 (25%)
1	PSU	2A	2605	1	17,21,22	1.49	3 (17%)	20,30,33	3.17	6 (30%)
32	4OC	1a	1402	32	16,23,24	0.65	0	17,32,35	1.13	1 (5%)
1	2MA	1A	2515	1,56	17,25,26	1.27	2 (11%)	19,37,40	2.09	3 (15%)
54	PPU	1w	76	1,54	32,40,41	0.92	1 (3%)	33,57,60	1.67	8 (24%)
55	5MU	1x	54	55	15,22,23	1.10	1 (6%)	16,32,35	2.01	2 (12%)
32	M2G	2a	966	32	20,27,28	1.38	3 (15%)	22,40,43	2.12	6 (27%)
32	7MG	2a	527	32	22,26,27	1.76	4 (18%)	28,39,42	2.76	10 (35%)
32	5MC	2a	1407	32	15,22,23	1.33	1 (6%)	19,32,35	1.42	3 (15%)
32	5MC	1a	1407	32	15,22,23	1.36	1 (6%)	19,32,35	1.32	2 (10%)
32	5MC	1a	967	32	15,22,23	1.30	1 (6%)	19,32,35	1.45	2 (10%)
43	0TD	2l	92	43	4,9,10	3.05	1 (25%)	3,11,13	10.02	1 (33%)
32	7MG	1a	527	32	22,26,27	1.79	4 (18%)	28,39,42	2.73	8 (28%)
55	PSU	2x	55	55	17,21,22	1.56	2 (11%)	20,30,33	3.04	6 (30%)
32	MA6	1a	1518	32	19,26,27	0.94	1 (5%)	18,38,41	1.65	4 (22%)
54	PPU	2w	76	1,54,56	32,40,41	0.90	1 (3%)	33,57,60	1.60	8 (24%)
1	5MC	2A	1962	1	15,22,23	1.24	1 (6%)	19,32,35	1.44	3 (15%)
1	PSU	2A	1917	1	17,21,22	1.57	4 (23%)	20,30,33	3.01	6 (30%)
1	5MC	2A	1942	1	15,22,23	1.28	1 (6%)	19,32,35	1.35	3 (15%)
32	2MG	2a	1207	32	19,26,27	1.33	2 (10%)	21,38,41	2.23	7 (33%)
1	4OC	1A	1942	1	15,22,24	0.67	0	17,31,35	1.33	2 (11%)

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	1A	1961	1	-	0/5/25/26	0/2/2/2
1	5MU	1A	1937	1	-	0/5/25/26	0/2/2/2
55	4SU	2x	8	55	-	0/5/25/26	0/2/2/2
1	2MU	1A	2564	1	-	0/7/27/28	0/2/2/2
1	OMG	2A	2251	1,55	-	0/5/27/28	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	5MU	2A	1915	1	-	0/5/25/26	0/2/2/2
32	5MC	2a	1404	32	-	0/5/25/26	0/2/2/2
32	MA6	2a	1519	32	-	4/7/29/30	0/3/3/3
1	5MC	1A	1964	1	-	0/5/25/26	0/2/2/2
1	5MC	1A	1984	1	-	2/5/25/26	0/2/2/2
32	PSU	2a	516	32	-	0/7/25/26	0/2/2/2
32	5MC	1a	1400	32	-	2/5/25/26	0/2/2/2
1	2MA	2A	2503	1,56	-	1/3/25/26	0/3/3/3
32	4OC	2a	1402	32	-	4/9/29/30	0/2/2/2
55	5MU	2x	54	55	-	0/5/25/26	0/2/2/2
1	PSU	2A	1911	1	-	0/7/25/26	0/2/2/2
55	5MC	2x	32	55	-	0/5/25/26	0/2/2/2
1	PSU	1A	1933	1	-	0/7/25/26	0/2/2/2
32	UR3	1a	1498	32	-	0/5/25/26	0/2/2/2
32	5MC	2a	1400	32	-	2/5/25/26	0/2/2/2
32	PSU	1a	516	32,56	-	1/7/25/26	0/2/2/2
1	5MU	2A	1939	1	-	0/5/25/26	0/2/2/2
32	MA6	1a	1519	32	-	4/7/29/30	0/3/3/3
1	2MU	2A	2552	1	-	0/7/27/28	0/2/2/2
1	PSU	1A	2617	1	-	0/7/25/26	0/2/2/2
32	2MG	1a	1207	32	-	0/5/27/28	0/3/3/3
32	UR3	2a	1498	32	-	0/5/25/26	0/2/2/2
55	5MC	1x	32	55	-	0/5/25/26	0/2/2/2
32	5MC	1a	1404	32	-	0/5/25/26	0/2/2/2
55	4SU	1x	8	55	-	0/5/25/26	0/2/2/2
32	5MC	2a	967	32	-	0/5/25/26	0/2/2/2
43	0TD	1l	92	43	-	1/3/12/14	-
32	MA6	2a	1518	32	-	1/7/29/30	0/3/3/3
55	PSU	1x	55	55	-	0/7/25/26	0/2/2/2
1	4OC	2A	1920	1	-	0/7/27/30	0/2/2/2
1	OMG	1A	2263	1,55	-	0/5/27/28	0/3/3/3
32	M2G	1a	966	32	-	0/7/29/30	0/3/3/3
1	PSU	1A	1939	1	-	0/7/25/26	0/2/2/2
1	PSU	2A	2605	1	-	0/7/25/26	0/2/2/2
32	4OC	1a	1402	32	-	4/9/29/30	0/2/2/2
1	2MA	1A	2515	1,56	-	1/3/25/26	0/3/3/3
54	PPU	1w	76	1,54	-	5/21/43/44	0/4/4/4
55	5MU	1x	54	55	-	0/5/25/26	0/2/2/2
32	M2G	2a	966	32	-	4/7/29/30	0/3/3/3
32	7MG	2a	527	32	-	0/7/37/38	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
32	5MC	2a	1407	32	-	0/5/25/26	0/2/2/2
32	5MC	1a	1407	32	-	0/5/25/26	0/2/2/2
32	5MC	1a	967	32	-	2/5/25/26	0/2/2/2
43	0TD	2l	92	43	-	2/3/12/14	-
32	7MG	1a	527	32	-	0/7/37/38	0/3/3/3
55	PSU	2x	55	55	-	0/7/25/26	0/2/2/2
32	MA6	1a	1518	32	-	3/7/29/30	0/3/3/3
54	PPU	2w	76	1,54,56	-	5/21/43/44	0/4/4/4
1	5MC	2A	1962	1	-	2/5/25/26	0/2/2/2
1	PSU	2A	1917	1	-	0/7/25/26	0/2/2/2
1	5MC	2A	1942	1	-	0/5/25/26	0/2/2/2
32	2MG	2a	1207	32	-	0/5/27/28	0/3/3/3
1	4OC	1A	1942	1	-	1/7/27/30	0/2/2/2

The worst 5 of 89 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
43	2l	92	0TD	CB-SB	-5.85	1.70	1.84
43	1l	92	0TD	CB-SB	-5.79	1.70	1.84
32	1a	527	7MG	C6-C5	5.10	1.48	1.41
32	2a	1400	5MC	C5-C4	4.94	1.49	1.41
32	2a	1404	5MC	C5-C4	4.92	1.49	1.41

The worst 5 of 222 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
43	2l	92	0TD	CSB-SB-CB	-17.30	67.82	101.85
43	1l	92	0TD	CSB-SB-CB	-16.30	69.78	101.85
1	2A	2605	PSU	N1-C2-N3	-9.19	121.13	128.43
32	2a	527	7MG	N3-C4-N9	9.07	138.56	126.91
32	1a	516	PSU	N1-C2-N3	-9.05	121.23	128.43

There are no chirality outliers.

5 of 51 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
32	2a	1519	MA6	O4'-C4'-C5'-O5'
32	2a	1519	MA6	C3'-C4'-C5'-O5'
1	1A	1984	5MC	O4'-C1'-N1-C6
1	1A	1984	5MC	C2'-C1'-N1-C6

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Mol	Chain	Res	Type	Atoms
32	2a	1402	4OC	O4'-C4'-C5'-O5'

There are no ring outliers.

13 monomers are involved in 16 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	1A	1937	5MU	1	0
1	1A	2564	2MU	1	0
1	2A	1915	5MU	1	0
1	1A	1984	5MC	1	0
1	2A	2503	2MA	2	0
1	2A	1911	PSU	1	0
1	2A	1939	5MU	1	0
1	2A	2552	2MU	1	0
1	1A	2263	OMG	2	0
1	1A	1939	PSU	1	0
1	1A	2515	2MA	1	0
1	2A	1962	5MC	1	0
1	1A	1942	4OC	2	0

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 1170 ligands modelled in this entry, 1168 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	0.00	-	-		
58	SF4	2d	302	35	0,12,12	0.00	-	-		

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.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
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	1.17

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%)	0.24	80 (2%) 53 40	82, 102, 143, 157	0
1	2A	2789/2915 (95%)	0.12	95 (3%) 45 34	88, 107, 136, 157	0
2	1B	120/121 (99%)	-0.38	0 100 100	104, 121, 132, 134	0
2	2B	120/121 (99%)	-0.57	0 100 100	111, 125, 135, 152	0
3	1D	275/276 (99%)	0.88	27 (9%) 7 6	84, 95, 108, 127	0
3	2D	275/276 (99%)	1.15	53 (19%) 1 1	88, 104, 114, 123	0
4	1E	204/206 (99%)	0.63	41 (20%) 1 0	86, 108, 122, 131	0
4	2E	204/206 (99%)	0.31	26 (12%) 3 4	89, 105, 119, 129	0
5	1F	203/210 (96%)	0.23	14 (6%) 16 11	79, 102, 120, 137	0
5	2F	203/210 (96%)	0.64	38 (18%) 1 1	90, 108, 122, 130	0
6	1G	181/182 (99%)	-0.27	2 (1%) 80 71	112, 122, 131, 139	0
6	2G	181/182 (99%)	0.72	30 (16%) 1 1	113, 126, 136, 149	0
7	1H	174/180 (96%)	0.20	4 (2%) 60 48	96, 113, 124, 131	0
7	2H	174/180 (96%)	0.49	15 (8%) 10 8	105, 125, 134, 142	0
8	1I	146/148 (98%)	-0.32	3 (2%) 63 52	102, 115, 124, 134	0
8	2I	146/148 (98%)	0.30	18 (12%) 4 4	109, 124, 138, 143	0
9	1N	140/140 (100%)	0.72	13 (9%) 8 6	93, 106, 119, 122	0
9	2N	140/140 (100%)	1.08	26 (18%) 1 1	97, 111, 122, 135	0
10	1O	122/122 (100%)	1.55	39 (31%) 0 0	90, 108, 122, 128	0
10	2O	122/122 (100%)	1.19	25 (20%) 1 0	87, 102, 113, 118	0
11	1P	149/150 (99%)	0.40	6 (4%) 38 28	85, 109, 124, 130	0
11	2P	149/150 (99%)	0.83	32 (21%) 0 0	90, 115, 126, 134	0
12	1Q	141/141 (100%)	1.58	47 (33%) 0 0	89, 108, 119, 127	0
12	2Q	141/141 (100%)	0.22	10 (7%) 16 11	97, 110, 122, 130	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
13	1R	118/118 (100%)	0.35	1 (0%) 86 78	94, 104, 116, 125	0
13	2R	118/118 (100%)	0.63	13 (11%) 5 4	89, 103, 111, 118	0
14	1S	110/112 (98%)	-0.42	0 100 100	106, 116, 125, 131	0
14	2S	110/112 (98%)	-0.16	1 (0%) 84 76	106, 119, 127, 130	0
15	1T	131/146 (89%)	0.46	15 (11%) 4 4	95, 110, 123, 138	0
15	2T	131/146 (89%)	0.86	26 (19%) 1 0	92, 106, 121, 129	0
16	1U	116/118 (98%)	0.55	14 (12%) 4 4	86, 105, 119, 134	0
16	2U	116/118 (98%)	0.81	15 (12%) 3 3	94, 109, 121, 125	0
17	1V	101/101 (100%)	0.02	1 (0%) 82 73	88, 106, 120, 127	0
17	2V	101/101 (100%)	0.21	4 (3%) 38 28	93, 114, 127, 136	0
18	1W	112/113 (99%)	0.84	10 (8%) 9 7	88, 101, 120, 131	0
18	2W	112/113 (99%)	0.47	10 (8%) 9 7	87, 101, 113, 129	0
19	1X	95/96 (98%)	0.44	3 (3%) 47 35	87, 98, 116, 125	0
19	2X	95/96 (98%)	1.41	27 (28%) 0 0	98, 107, 127, 132	0
20	1Y	107/110 (97%)	0.15	2 (1%) 66 55	86, 108, 121, 126	0
20	2Y	107/110 (97%)	0.96	21 (19%) 1 1	91, 113, 126, 133	0
21	1Z	154/206 (74%)	-0.28	1 (0%) 89 83	109, 120, 132, 138	0
21	2Z	160/206 (77%)	-0.57	0 100 100	111, 123, 131, 135	0
22	10	83/85 (97%)	0.75	12 (14%) 2 2	94, 108, 116, 124	0
22	20	83/85 (97%)	1.13	18 (21%) 0 0	101, 114, 122, 125	0
23	11	97/98 (98%)	1.52	37 (38%) 0 0	87, 101, 121, 131	0
23	21	97/98 (98%)	1.94	47 (48%) 0 0	93, 110, 124, 130	0
24	12	70/72 (97%)	0.03	2 (2%) 51 39	87, 101, 111, 128	0
24	22	70/72 (97%)	0.49	2 (2%) 51 39	106, 116, 126, 129	0
25	13	59/60 (98%)	0.08	1 (1%) 70 59	86, 107, 121, 139	0
25	23	59/60 (98%)	0.65	2 (3%) 45 34	99, 108, 131, 143	0
26	14	69/71 (97%)	-0.75	0 100 100	121, 130, 141, 147	0
26	24	69/71 (97%)	-0.29	0 100 100	117, 128, 137, 144	0
27	15	59/60 (98%)	1.11	16 (27%) 0 0	89, 103, 117, 122	0
27	25	59/60 (98%)	0.20	6 (10%) 6 5	90, 103, 117, 125	0
28	16	53/54 (98%)	0.57	4 (7%) 14 10	95, 108, 120, 126	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
28	26	53/54 (98%)	0.50	4 (7%) 14 10	105, 114, 124, 134	0
29	17	48/49 (97%)	0.93	6 (12%) 3 4	82, 90, 107, 119	0
29	27	48/49 (97%)	2.11	24 (50%) 0 0	86, 99, 116, 124	0
30	18	64/65 (98%)	0.94	4 (6%) 20 13	89, 100, 111, 120	0
30	28	64/65 (98%)	2.17	35 (54%) 0 0	98, 106, 114, 120	0
31	19	37/37 (100%)	0.77	4 (10%) 5 4	99, 108, 113, 117	0
31	29	37/37 (100%)	1.09	7 (18%) 1 1	105, 116, 127, 130	0
32	1a	1488/1521 (97%)	0.03	95 (6%) 19 13	92, 123, 141, 160	0
32	2a	1491/1521 (98%)	-0.14	41 (2%) 54 42	97, 119, 138, 155	0
33	1b	231/256 (90%)	-0.20	1 (0%) 92 88	113, 127, 135, 144	0
33	2b	231/256 (90%)	-0.04	12 (5%) 27 20	105, 126, 137, 143	0
34	1c	206/239 (86%)	0.74	41 (19%) 1 0	113, 129, 137, 141	0
34	2c	206/239 (86%)	-0.23	9 (4%) 34 25	115, 124, 132, 141	0
35	1d	208/209 (99%)	0.78	33 (15%) 1 1	104, 121, 131, 137	0
35	2d	208/209 (99%)	0.52	18 (8%) 10 7	104, 117, 128, 136	0
36	1e	148/162 (91%)	0.99	38 (25%) 0 0	103, 119, 127, 133	0
36	2e	148/162 (91%)	0.88	31 (20%) 1 0	107, 117, 128, 136	0
37	1f	100/101 (99%)	-0.18	2 (2%) 65 53	101, 117, 126, 133	0
37	2f	100/101 (99%)	-0.12	3 (3%) 50 37	105, 118, 127, 132	0
38	1g	155/156 (99%)	0.23	16 (10%) 6 5	111, 125, 135, 141	0
38	2g	155/156 (99%)	-0.05	8 (5%) 27 20	112, 124, 135, 145	0
39	1h	137/138 (99%)	0.82	24 (17%) 1 1	108, 122, 129, 134	0
39	2h	137/138 (99%)	-0.06	5 (3%) 42 32	103, 118, 127, 135	0
40	1i	127/128 (99%)	0.38	22 (17%) 1 1	114, 128, 135, 139	0
40	2i	127/128 (99%)	0.81	26 (20%) 1 0	115, 127, 135, 144	0
41	1j	97/105 (92%)	0.87	23 (23%) 0 0	121, 131, 138, 143	0
41	2j	96/105 (91%)	0.72	23 (23%) 0 0	118, 129, 137, 142	0
42	1k	114/129 (88%)	0.72	14 (12%) 4 4	103, 117, 126, 130	0
42	2k	114/129 (88%)	1.33	37 (32%) 0 0	107, 120, 129, 137	0
43	1l	121/132 (91%)	1.45	37 (30%) 0 0	103, 117, 124, 136	0
43	2l	121/132 (91%)	0.43	13 (10%) 6 5	100, 112, 122, 128	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
44	1m	123/126 (97%)	-0.11	11 (8%) 9 7	113, 125, 133, 139	0
44	2m	122/126 (96%)	0.47	21 (17%) 1 1	111, 125, 137, 147	0
45	1n	60/61 (98%)	2.21	35 (58%) 0 0	118, 128, 137, 144	0
45	2n	60/61 (98%)	0.54	11 (18%) 1 1	114, 124, 130, 134	0
46	1o	88/89 (98%)	0.23	6 (6%) 17 12	101, 116, 122, 124	0
46	2o	88/89 (98%)	0.42	5 (5%) 23 16	101, 119, 127, 132	0
47	1p	82/88 (93%)	1.81	38 (46%) 0 0	115, 124, 131, 137	0
47	2p	82/88 (93%)	0.23	4 (4%) 29 22	99, 111, 119, 123	0
48	1q	99/105 (94%)	0.43	12 (12%) 4 4	103, 118, 125, 131	0
48	2q	99/105 (94%)	0.24	4 (4%) 38 28	102, 113, 122, 126	0
49	1r	68/88 (77%)	0.22	2 (2%) 51 39	109, 117, 125, 130	0
49	2r	68/88 (77%)	0.58	9 (13%) 3 3	109, 119, 126, 131	0
50	1s	83/93 (89%)	-0.25	2 (2%) 59 47	117, 128, 136, 143	0
50	2s	83/93 (89%)	0.11	4 (4%) 30 22	116, 126, 135, 137	0
51	1t	96/106 (90%)	1.16	30 (31%) 0 0	111, 122, 128, 132	0
51	2t	96/106 (90%)	0.89	22 (22%) 0 0	101, 116, 126, 129	0
52	1u	23/27 (85%)	0.55	3 (13%) 3 3	119, 126, 129, 131	0
52	2u	23/27 (85%)	1.51	8 (34%) 0 0	123, 127, 131, 133	0
53	1v	6/24 (25%)	0.93	1 (16%) 1 1	110, 116, 131, 136	0
53	2v	6/24 (25%)	1.69	2 (33%) 0 0	113, 116, 131, 147	0
54	1w	2/3 (66%)	0.44	0 100 100	88, 88, 88, 89	0
54	2w	2/3 (66%)	0.79	0 100 100	103, 103, 103, 106	0
55	1x	72/77 (93%)	-0.41	0 100 100	90, 118, 130, 140	0
55	2x	72/77 (93%)	-0.26	1 (1%) 75 64	96, 123, 134, 144	0
All	All	20600/21450 (96%)	0.33	1842 (8%) 9 7	79, 114, 134, 160	0

The worst 5 of 1842 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
44	2m	124	PRO	10.7
41	1j	61	GLU	10.0
44	1m	124	PRO	8.6
3	2D	276	LYS	8.5
38	1g	82	GLY	8.4

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(Å ²)	Q<0.9
55	PSU	2x	55	20/21	0.84	0.23	114,125,136,143	0
55	4SU	2x	8	20/21	0.86	0.13	120,133,139,140	0
1	5MU	1A	1937	21/22	0.86	0.13	115,126,133,144	0
32	PSU	2a	516	20/21	0.87	0.14	117,122,126,128	0
32	7MG	1a	527	24/25	0.89	0.25	101,115,123,126	0
32	PSU	1a	516	20/21	0.89	0.12	113,120,128,129	0
32	5MC	2a	967	21/22	0.90	0.25	102,116,124,125	0
32	4OC	1a	1402	22/23	0.90	0.31	104,112,120,123	0
32	7MG	2a	527	24/25	0.90	0.22	99,117,123,125	0
32	4OC	2a	1402	22/23	0.90	0.26	104,109,115,116	0
32	2MG	2a	1207	24/25	0.90	0.14	114,124,129,137	0
55	4SU	1x	8	20/21	0.91	0.14	111,122,128,128	0
1	5MU	2A	1915	21/22	0.91	0.13	114,120,131,143	0
1	4OC	1A	1942	21/23	0.91	0.19	96,108,120,123	0
54	PPU	2w	76	37/38	0.92	0.45	86,100,107,111	0
55	PSU	1x	55	20/21	0.92	0.11	109,117,129,133	0
32	M2G	2a	966	25/26	0.93	0.29	107,119,123,126	0
55	5MU	2x	54	21/22	0.93	0.21	108,120,136,142	0
32	5MC	1a	967	21/22	0.93	0.33	104,115,127,130	0
1	PSU	2A	1911	20/21	0.93	0.14	96,105,117,118	0
32	UR3	1a	1498	21/22	0.93	0.24	96,107,111,114	0
32	5MC	2a	1404	21/22	0.93	0.28	101,111,116,121	0
1	PSU	2A	1917	20/21	0.93	0.15	106,110,120,127	0
1	PSU	1A	2617	20/21	0.93	0.31	81,90,100,100	0
32	M2G	1a	966	25/26	0.94	0.26	104,110,120,121	0
1	PSU	2A	2605	20/21	0.94	0.24	81,91,98,102	0
32	5MC	1a	1400	21/22	0.94	0.21	106,115,124,131	0
55	5MU	1x	54	21/22	0.94	0.12	111,118,130,131	0
55	5MC	2x	32	21/22	0.94	0.27	110,118,124,126	0
32	UR3	2a	1498	21/22	0.94	0.40	95,105,114,115	0
32	5MC	2a	1407	21/22	0.94	0.24	90,106,116,118	0
32	5MC	1a	1407	21/22	0.94	0.17	100,110,116,121	0
55	5MC	1x	32	21/22	0.94	0.18	99,116,123,128	0
1	5MC	1A	1964	21/22	0.94	0.18	82,93,104,111	0
32	2MG	1a	1207	24/25	0.94	0.15	114,124,132,136	0
32	MA6	1a	1518	24/25	0.94	0.21	103,109,113,116	0
43	0TD	1l	92	10/11	0.94	0.46	110,119,124,142	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
1	5MU	2A	1939	21/22	0.94	0.23	89,98,104,114	0
1	4OC	2A	1920	21/23	0.94	0.19	94,114,119,120	0
32	5MC	2a	1400	21/22	0.95	0.20	101,114,128,132	0
1	2MA	2A	2503	23/24	0.95	0.31	81,92,103,114	0
1	PSU	1A	1939	20/21	0.95	0.13	95,110,117,117	0
43	0TD	2l	92	10/11	0.95	0.48	117,123,129,141	0
1	2MU	1A	2564	21/23	0.95	0.37	85,95,105,109	0
1	2MU	2A	2552	21/23	0.95	0.20	84,90,101,104	0
54	PPU	1w	76	37/38	0.95	0.40	84,91,103,108	0
1	PSU	1A	1933	20/21	0.95	0.14	90,105,108,109	0
32	MA6	2a	1518	24/25	0.95	0.26	100,109,116,117	0
1	5MC	2A	1942	21/22	0.95	0.16	88,97,104,108	0
1	5MC	1A	1984	21/22	0.95	0.18	87,96,104,106	0
32	MA6	2a	1519	24/25	0.96	0.33	93,107,112,116	0
1	5MU	1A	1961	21/22	0.96	0.28	85,92,100,103	0
1	5MC	2A	1962	21/22	0.96	0.19	79,100,106,110	0
32	5MC	1a	1404	21/22	0.96	0.34	95,106,113,115	0
1	OMG	1A	2263	24/25	0.96	0.33	70,88,102,105	0
1	2MA	1A	2515	23/24	0.96	0.28	76,84,97,103	0
1	OMG	2A	2251	24/25	0.97	0.29	85,96,109,111	0
32	MA6	1a	1519	24/25	0.97	0.32	93,107,119,119	0

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. 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(\AA^2)	Q<0.9
56	MG	1a	1669	1/1	0.14	0.34	102,102,102,102	0
56	MG	1A	3124	1/1	0.30	0.42	75,75,75,75	0
56	MG	2A	3157	1/1	0.31	0.44	88,88,88,88	0
56	MG	1x	102	1/1	0.33	0.52	85,85,85,85	0
56	MG	1A	3115	1/1	0.33	0.51	89,89,89,89	0
56	MG	2a	3088	1/1	0.36	0.35	83,83,83,83	0
56	MG	2d	301	1/1	0.38	0.32	81,81,81,81	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	2A	3176	1/1	0.39	0.36	79,79,79,79	0
56	MG	2A	3105	1/1	0.40	0.35	74,74,74,74	0
56	MG	2A	3194	1/1	0.42	0.40	79,79,79,79	0
56	MG	2A	3125	1/1	0.44	0.32	82,82,82,82	0
56	MG	1A	3220	1/1	0.45	0.37	85,85,85,85	0
56	MG	2A	3301	1/1	0.47	0.29	77,77,77,77	0
56	MG	1A	3308	1/1	0.49	0.63	76,76,76,76	0
56	MG	1A	3217	1/1	0.50	0.53	65,65,65,65	0
56	MG	1A	3086	1/1	0.50	0.31	90,90,90,90	0
56	MG	1A	3358	1/1	0.51	0.65	75,75,75,75	0
56	MG	2A	3311	1/1	0.51	0.17	79,79,79,79	0
56	MG	2O	201	1/1	0.51	1.98	73,73,73,73	0
56	MG	2A	3015	1/1	0.51	0.47	76,76,76,76	0
56	MG	1A	3471	1/1	0.52	0.46	75,75,75,75	0
56	MG	1A	3299	1/1	0.52	0.50	83,83,83,83	0
56	MG	1A	3341	1/1	0.54	0.45	77,77,77,77	0
56	MG	2a	3098	1/1	0.54	0.31	85,85,85,85	0
56	MG	1A	3070	1/1	0.55	0.54	87,87,87,87	0
56	MG	2A	3187	1/1	0.55	0.81	74,74,74,74	0
56	MG	2A	3088	1/1	0.55	0.26	76,76,76,76	0
56	MG	1a	1684	1/1	0.56	0.32	74,74,74,74	0
56	MG	1A	3438	1/1	0.56	0.36	84,84,84,84	0
56	MG	2A	3052	1/1	0.56	0.24	86,86,86,86	0
56	MG	2a	3069	1/1	0.56	0.52	104,104,104,104	0
56	MG	2A	3010	1/1	0.57	0.28	87,87,87,87	0
56	MG	2A	3141	1/1	0.57	0.35	81,81,81,81	0
56	MG	2A	3114	1/1	0.57	0.18	75,75,75,75	0
56	MG	1A	3154	1/1	0.58	0.42	77,77,77,77	0
56	MG	1A	3226	1/1	0.58	0.28	79,79,79,79	0
56	MG	2A	3101	1/1	0.59	0.27	80,80,80,80	0
56	MG	2a	3051	1/1	0.59	0.27	79,79,79,79	0
56	MG	1A	3268	1/1	0.59	0.23	68,68,68,68	0
56	MG	1A	3114	1/1	0.60	0.33	82,82,82,82	0
56	MG	1A	3349	1/1	0.60	0.68	80,80,80,80	0
56	MG	2A	3205	1/1	0.60	0.26	81,81,81,81	0
56	MG	1A	3054	1/1	0.60	1.02	75,75,75,75	0
56	MG	2a	3067	1/1	0.60	0.12	96,96,96,96	0
56	MG	1a	1687	1/1	0.60	0.46	100,100,100,100	0
56	MG	1A	3264	1/1	0.60	0.60	83,83,83,83	0
56	MG	1A	3258	1/1	0.61	0.72	98,98,98,98	0
56	MG	1a	1603	1/1	0.61	0.94	94,94,94,94	0
56	MG	2a	3093	1/1	0.61	0.34	77,77,77,77	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	1a	1642	1/1	0.61	0.29	81,81,81,81	0
56	MG	1A	3088	1/1	0.61	0.28	74,74,74,74	0
56	MG	1A	3327	1/1	0.62	0.46	83,83,83,83	0
56	MG	2A	3290	1/1	0.62	0.33	72,72,72,72	0
56	MG	2a	3026	1/1	0.62	0.22	76,76,76,76	0
56	MG	10	103	1/1	0.62	0.52	69,69,69,69	0
56	MG	1a	1641	1/1	0.62	0.27	82,82,82,82	0
56	MG	2A	3061	1/1	0.63	0.43	69,69,69,69	0
56	MG	1A	3187	1/1	0.63	0.66	83,83,83,83	0
56	MG	1A	3240	1/1	0.63	0.36	66,66,66,66	0
56	MG	1A	3239	1/1	0.64	1.06	90,90,90,90	0
56	MG	1a	1689	1/1	0.64	0.36	78,78,78,78	0
56	MG	2a	3040	1/1	0.64	0.21	78,78,78,78	0
56	MG	1A	3034	1/1	0.64	0.42	91,91,91,91	0
56	MG	2A	3276	1/1	0.64	0.46	74,74,74,74	0
56	MG	1l	201	1/1	0.64	1.89	80,80,80,80	0
56	MG	1A	3165	1/1	0.64	1.11	84,84,84,84	0
56	MG	1A	3082	1/1	0.65	0.65	74,74,74,74	0
56	MG	2A	3327	1/1	0.65	0.40	70,70,70,70	0
56	MG	1A	3051	1/1	0.65	0.50	89,89,89,89	0
56	MG	1A	3221	1/1	0.65	0.56	86,86,86,86	0
56	MG	1a	1671	1/1	0.66	0.37	99,99,99,99	0
56	MG	2A	3266	1/1	0.66	0.45	69,69,69,69	0
56	MG	1A	3312	1/1	0.66	0.48	65,65,65,65	0
56	MG	1a	1611	1/1	0.66	0.13	93,93,93,93	0
56	MG	1a	1681	1/1	0.66	0.36	79,79,79,79	0
56	MG	2A	3160	1/1	0.66	0.16	75,75,75,75	0
56	MG	1A	3202	1/1	0.66	0.63	85,85,85,85	0
56	MG	2A	3306	1/1	0.67	0.21	80,80,80,80	0
56	MG	2T	201	1/1	0.67	0.38	63,63,63,63	0
56	MG	2A	3345	1/1	0.67	0.29	62,62,62,62	0
56	MG	1a	1686	1/1	0.67	0.36	76,76,76,76	0
56	MG	1A	3008	1/1	0.68	0.34	109,109,109,109	0
56	MG	2A	3030	1/1	0.68	0.40	91,91,91,91	0
56	MG	1B	201	1/1	0.68	0.59	82,82,82,82	0
56	MG	1A	3232	1/1	0.68	0.45	77,77,77,77	0
56	MG	2A	3056	1/1	0.68	0.27	79,79,79,79	0
56	MG	1a	1675	1/1	0.68	0.17	110,110,110,110	0
56	MG	2A	3335	1/1	0.68	0.26	68,68,68,68	0
56	MG	27	101	1/1	0.68	0.41	69,69,69,69	0
56	MG	2A	3352	1/1	0.68	0.40	107,107,107,107	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	1A	3245	1/1	0.68	0.59	81,81,81,81	0
56	MG	1A	3197	1/1	0.68	0.43	71,71,71,71	0
56	MG	2A	3026	1/1	0.68	0.20	76,76,76,76	0
56	MG	2A	3078	1/1	0.68	0.17	79,79,79,79	0
56	MG	1a	1629	1/1	0.69	0.15	94,94,94,94	0
56	MG	2a	3003	1/1	0.69	0.26	90,90,90,90	0
56	MG	1A	3322	1/1	0.69	0.77	94,94,94,94	0
56	MG	2A	3254	1/1	0.69	0.30	82,82,82,82	0
56	MG	2A	3337	1/1	0.69	0.76	87,87,87,87	0
56	MG	1A	3252	1/1	0.69	0.53	80,80,80,80	0
56	MG	1A	3321	1/1	0.70	0.36	67,67,67,67	0
56	MG	1Q	201	1/1	0.70	0.84	75,75,75,75	0
56	MG	2A	3113	1/1	0.70	0.52	70,70,70,70	0
56	MG	2A	3297	1/1	0.70	0.37	77,77,77,77	0
56	MG	2A	3332	1/1	0.70	0.47	80,80,80,80	0
56	MG	2A	3100	1/1	0.70	0.34	74,74,74,74	0
56	MG	2A	3175	1/1	0.70	0.25	107,107,107,107	0
56	MG	1a	1678	1/1	0.70	0.35	89,89,89,89	0
56	MG	2A	3253	1/1	0.70	0.45	62,62,62,62	0
56	MG	1A	3255	1/1	0.70	0.62	77,77,77,77	0
56	MG	2A	3161	1/1	0.70	0.27	72,72,72,72	0
56	MG	1A	3173	1/1	0.71	0.50	87,87,87,87	0
56	MG	2A	3189	1/1	0.71	0.40	75,75,75,75	0
56	MG	1A	3083	1/1	0.71	0.38	83,83,83,83	0
56	MG	2A	3305	1/1	0.71	0.19	83,83,83,83	0
56	MG	2a	3076	1/1	0.71	0.26	82,82,82,82	0
56	MG	2a	3061	1/1	0.71	0.39	72,72,72,72	0
56	MG	2A	3014	1/1	0.71	0.78	90,90,90,90	0
56	MG	2B	201	1/1	0.71	0.47	80,80,80,80	0
56	MG	1A	3224	1/1	0.71	0.47	76,76,76,76	0
56	MG	1A	3180	1/1	0.71	0.36	61,61,61,61	0
56	MG	2A	3102	1/1	0.71	0.33	73,73,73,73	0
56	MG	2A	3122	1/1	0.71	0.63	85,85,85,85	0
56	MG	1B	202	1/1	0.71	0.52	80,80,80,80	0
56	MG	2A	3239	1/1	0.72	0.23	68,68,68,68	0
56	MG	1A	3181	1/1	0.72	0.36	73,73,73,73	0
56	MG	2A	3257	1/1	0.72	0.38	84,84,84,84	0
56	MG	2A	3183	1/1	0.72	0.51	81,81,81,81	0
56	MG	20	101	1/1	0.72	0.64	75,75,75,75	0
56	MG	2A	3293	1/1	0.72	0.13	77,77,77,77	0
56	MG	1A	3480	1/1	0.72	0.37	69,69,69,69	0
56	MG	1A	3494	1/1	0.72	0.14	85,85,85,85	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	1a	1649	1/1	0.72	0.11	106,106,106,106	0
56	MG	1A	3172	1/1	0.72	0.65	96,96,96,96	0
56	MG	1A	3142	1/1	0.72	0.46	71,71,71,71	0
56	MG	1A	3177	1/1	0.72	0.50	62,62,62,62	0
56	MG	2a	3046	1/1	0.72	0.30	99,99,99,99	0
56	MG	1a	1640	1/1	0.72	0.18	91,91,91,91	0
56	MG	2A	3248	1/1	0.72	0.31	78,78,78,78	0
56	MG	1E	304	1/1	0.73	0.54	78,78,78,78	0
56	MG	2a	3080	1/1	0.73	0.26	74,74,74,74	0
56	MG	1A	3237	1/1	0.73	0.50	79,79,79,79	0
56	MG	1A	3440	1/1	0.73	0.47	70,70,70,70	0
56	MG	2A	3012	1/1	0.73	0.35	66,66,66,66	0
56	MG	1A	3140	1/1	0.73	0.20	73,73,73,73	0
56	MG	2A	3155	1/1	0.73	0.22	92,92,92,92	0
56	MG	1A	3192	1/1	0.73	0.43	61,61,61,61	0
56	MG	1a	1630	1/1	0.73	0.17	80,80,80,80	0
56	MG	2A	3057	1/1	0.73	0.28	91,91,91,91	0
56	MG	2A	3024	1/1	0.73	0.50	73,73,73,73	0
56	MG	2A	3166	1/1	0.73	0.27	94,94,94,94	0
56	MG	1A	3040	1/1	0.73	0.40	79,79,79,79	0
56	MG	1A	3078	1/1	0.73	0.81	80,80,80,80	0
56	MG	2A	3209	1/1	0.73	0.43	77,77,77,77	0
56	MG	1A	3075	1/1	0.74	0.45	72,72,72,72	0
56	MG	2A	3147	1/1	0.74	0.26	75,75,75,75	0
56	MG	2A	3315	1/1	0.74	0.33	68,68,68,68	0
56	MG	2A	3042	1/1	0.74	0.16	75,75,75,75	0
56	MG	1A	3113	1/1	0.74	0.34	77,77,77,77	0
56	MG	1A	3437	1/1	0.74	0.57	99,99,99,99	0
56	MG	2E	303	1/1	0.74	0.28	81,81,81,81	0
56	MG	2A	3011	1/1	0.74	0.48	82,82,82,82	0
56	MG	1A	3159	1/1	0.75	0.50	81,81,81,81	0
56	MG	1A	3254	1/1	0.75	0.66	77,77,77,77	0
56	MG	1A	3104	1/1	0.75	1.08	69,69,69,69	0
56	MG	2A	3139	1/1	0.75	0.34	64,64,64,64	0
56	MG	2a	3068	1/1	0.75	0.54	81,81,81,81	0
56	MG	2A	3326	1/1	0.75	0.60	74,74,74,74	0
56	MG	2A	3002	1/1	0.75	0.56	70,70,70,70	0
56	MG	2A	3374	1/1	0.75	0.24	62,62,62,62	0
56	MG	1A	3148	1/1	0.75	0.80	79,79,79,79	0
56	MG	2E	302	1/1	0.75	0.47	80,80,80,80	0
56	MG	1d	301	1/1	0.75	0.18	91,91,91,91	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	1A	3146	1/1	0.76	1.17	64,64,64,64	0
56	MG	1A	3360	1/1	0.76	0.52	82,82,82,82	0
56	MG	2a	3014	1/1	0.76	0.27	81,81,81,81	0
56	MG	1a	1631	1/1	0.76	0.20	97,97,97,97	0
56	MG	1A	3118	1/1	0.76	0.40	75,75,75,75	0
56	MG	1a	1609	1/1	0.76	0.17	103,103,103,103	0
56	MG	1A	3144	1/1	0.76	0.43	87,87,87,87	0
56	MG	1a	1645	1/1	0.76	0.44	90,90,90,90	0
56	MG	2A	3049	1/1	0.76	0.47	73,73,73,73	0
56	MG	1A	3293	1/1	0.76	0.54	84,84,84,84	0
56	MG	1A	3071	1/1	0.76	0.35	75,75,75,75	0
56	MG	2a	3011	1/1	0.76	0.26	94,94,94,94	0
56	MG	1a	1651	1/1	0.76	0.20	71,71,71,71	0
56	MG	2A	3285	1/1	0.76	0.44	73,73,73,73	0
56	MG	2a	3035	1/1	0.76	0.32	73,73,73,73	0
56	MG	1A	3291	1/1	0.76	0.28	77,77,77,77	0
56	MG	2A	3006	1/1	0.76	0.24	76,76,76,76	0
56	MG	1A	3479	1/1	0.76	0.53	72,72,72,72	0
56	MG	1A	3251	1/1	0.77	0.39	82,82,82,82	0
56	MG	2A	3263	1/1	0.77	0.48	70,70,70,70	0
56	MG	2A	3027	1/1	0.77	0.56	83,83,83,83	0
56	MG	1A	3194	1/1	0.77	0.30	92,92,92,92	0
56	MG	1A	3432	1/1	0.77	0.27	68,68,68,68	0
57	ZN	2Y	202	1/1	0.77	0.09	176,176,176,176	0
56	MG	1A	3364	1/1	0.77	0.35	81,81,81,81	0
56	MG	1a	1644	1/1	0.77	0.20	76,76,76,76	0
56	MG	2A	3377	1/1	0.77	0.25	92,92,92,92	0
56	MG	1A	3402	1/1	0.77	0.45	62,62,62,62	0
56	MG	2A	3059	1/1	0.77	0.41	82,82,82,82	0
56	MG	1A	3250	1/1	0.77	0.51	71,71,71,71	0
56	MG	2a	3086	1/1	0.77	0.36	74,74,74,74	0
56	MG	1A	3342	1/1	0.78	0.37	62,62,62,62	0
56	MG	2A	3119	1/1	0.78	0.39	63,63,63,63	0
56	MG	2B	202	1/1	0.78	0.62	87,87,87,87	0
56	MG	2A	3258	1/1	0.78	0.46	80,80,80,80	0
56	MG	1A	3056	1/1	0.78	0.15	85,85,85,85	0
56	MG	2a	3090	1/1	0.78	0.24	73,73,73,73	0
56	MG	1A	3039	1/1	0.78	0.48	71,71,71,71	0
56	MG	1A	3288	1/1	0.78	0.30	78,78,78,78	0
56	MG	2A	3110	1/1	0.78	0.32	88,88,88,88	0
56	MG	1A	3007	1/1	0.78	0.27	74,74,74,74	0
56	MG	1A	3257	1/1	0.78	0.82	82,82,82,82	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	2A	3129	1/1	0.78	0.26	61,61,61,61	0
56	MG	2A	3039	1/1	0.78	0.59	93,93,93,93	0
56	MG	2a	3023	1/1	0.78	0.38	72,72,72,72	0
56	MG	2A	3349	1/1	0.78	0.65	76,76,76,76	0
56	MG	2A	3094	1/1	0.78	0.23	83,83,83,83	0
56	MG	2A	3041	1/1	0.78	0.35	91,91,91,91	0
56	MG	2A	3085	1/1	0.78	0.27	71,71,71,71	0
56	MG	1A	3072	1/1	0.78	0.29	79,79,79,79	0
56	MG	1A	3134	1/1	0.78	0.38	80,80,80,80	0
56	MG	2A	3127	1/1	0.78	0.27	93,93,93,93	0
56	MG	2A	3300	1/1	0.78	0.26	74,74,74,74	0
56	MG	1A	3253	1/1	0.78	0.40	79,79,79,79	0
56	MG	2A	3016	1/1	0.78	0.36	72,72,72,72	0
56	MG	2A	3229	1/1	0.79	0.36	72,72,72,72	0
56	MG	1A	3068	1/1	0.79	0.44	75,75,75,75	0
56	MG	2A	3071	1/1	0.79	0.33	61,61,61,61	0
56	MG	1A	3262	1/1	0.79	0.42	82,82,82,82	0
56	MG	2A	3120	1/1	0.79	0.23	78,78,78,78	0
56	MG	1a	1636	1/1	0.79	0.29	93,93,93,93	0
56	MG	2A	3162	1/1	0.79	0.46	90,90,90,90	0
56	MG	1A	3420	1/1	0.79	0.58	70,70,70,70	0
56	MG	2T	202	1/1	0.79	0.75	82,82,82,82	0
56	MG	2a	3065	1/1	0.79	0.38	75,75,75,75	0
56	MG	1a	1667	1/1	0.79	0.15	78,78,78,78	0
56	MG	1a	1665	1/1	0.79	0.35	74,74,74,74	0
56	MG	1A	3026	1/1	0.79	0.80	75,75,75,75	0
56	MG	1A	3340	1/1	0.79	0.43	61,61,61,61	0
56	MG	1A	3445	1/1	0.79	0.70	78,78,78,78	0
56	MG	1A	3001	1/1	0.79	0.18	80,80,80,80	0
56	MG	1A	3093	1/1	0.79	0.36	76,76,76,76	0
56	MG	2A	3277	1/1	0.79	0.37	70,70,70,70	0
56	MG	2A	3031	1/1	0.79	0.13	89,89,89,89	0
56	MG	1a	1614	1/1	0.79	0.26	76,76,76,76	0
56	MG	2A	3208	1/1	0.79	0.13	82,82,82,82	0
56	MG	2E	305	1/1	0.79	0.24	67,67,67,67	0
56	MG	1A	3047	1/1	0.79	0.36	67,67,67,67	0
56	MG	2A	3323	1/1	0.79	0.47	64,64,64,64	0
56	MG	1A	3067	1/1	0.79	0.50	64,64,64,64	0
56	MG	1A	3418	1/1	0.80	0.34	76,76,76,76	0
56	MG	1A	3270	1/1	0.80	0.22	62,62,62,62	0
56	MG	1A	3171	1/1	0.80	0.30	76,76,76,76	0
56	MG	1a	1655	1/1	0.80	0.21	84,84,84,84	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	1V	203	1/1	0.80	0.81	81,81,81,81	0
56	MG	1A	3379	1/1	0.80	0.39	80,80,80,80	0
56	MG	2A	3180	1/1	0.80	0.51	76,76,76,76	0
56	MG	2A	3137	1/1	0.80	0.26	62,62,62,62	0
56	MG	1A	3062	1/1	0.80	0.23	89,89,89,89	0
56	MG	2A	3131	1/1	0.80	0.24	63,63,63,63	0
56	MG	1A	3377	1/1	0.80	0.52	77,77,77,77	0
56	MG	1A	3139	1/1	0.80	0.29	70,70,70,70	0
56	MG	1A	3099	1/1	0.80	0.69	98,98,98,98	0
56	MG	2A	3097	1/1	0.80	0.22	93,93,93,93	0
56	MG	2E	301	1/1	0.80	0.26	87,87,87,87	0
56	MG	1A	3121	1/1	0.80	0.26	79,79,79,79	0
56	MG	2A	3159	1/1	0.80	0.28	83,83,83,83	0
56	MG	2A	3334	1/1	0.80	0.28	77,77,77,77	0
56	MG	2A	3079	1/1	0.80	0.37	79,79,79,79	0
56	MG	2A	3369	1/1	0.80	0.35	70,70,70,70	0
56	MG	1A	3065	1/1	0.80	0.84	88,88,88,88	0
56	MG	20	102	1/1	0.80	0.23	75,75,75,75	0
56	MG	2A	3291	1/1	0.80	0.35	78,78,78,78	0
56	MG	2A	3220	1/1	0.80	0.40	64,64,64,64	0
56	MG	1A	3014	1/1	0.80	0.49	86,86,86,86	0
56	MG	1A	3087	1/1	0.81	0.31	82,82,82,82	0
56	MG	2A	3118	1/1	0.81	0.31	71,71,71,71	0
56	MG	1A	3211	1/1	0.81	0.57	93,93,93,93	0
56	MG	1W	201	1/1	0.81	0.81	65,65,65,65	0
56	MG	1A	3351	1/1	0.81	0.36	64,64,64,64	0
56	MG	2A	3112	1/1	0.81	0.49	68,68,68,68	0
56	MG	2a	3087	1/1	0.81	0.26	61,61,61,61	0
56	MG	17	101	1/1	0.81	0.47	66,66,66,66	0
56	MG	1A	3491	1/1	0.81	0.20	91,91,91,91	0
56	MG	1a	1664	1/1	0.81	0.90	67,67,67,67	0
56	MG	2a	3004	1/1	0.81	0.32	91,91,91,91	0
56	MG	2A	3058	1/1	0.81	0.32	82,82,82,82	0
56	MG	1A	3020	1/1	0.81	0.30	84,84,84,84	0
56	MG	2A	3109	1/1	0.81	0.35	63,63,63,63	0
56	MG	1A	3156	1/1	0.81	0.35	78,78,78,78	0
56	MG	1A	3249	1/1	0.81	0.54	90,90,90,90	0
56	MG	2R	201	1/1	0.81	0.67	64,64,64,64	0
56	MG	1A	3162	1/1	0.81	0.43	65,65,65,65	0
56	MG	2A	3091	1/1	0.81	0.17	75,75,75,75	0
56	MG	1A	3228	1/1	0.81	0.34	77,77,77,77	0
56	MG	2A	3355	1/1	0.81	0.13	86,86,86,86	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	2A	3375	1/1	0.81	0.30	66,66,66,66	0
56	MG	1A	3357	1/1	0.81	1.32	68,68,68,68	0
56	MG	1A	3236	1/1	0.81	0.34	102,102,102,102	0
56	MG	1A	3373	1/1	0.81	0.49	61,61,61,61	0
56	MG	2Q	202	1/1	0.81	0.39	69,69,69,69	0
56	MG	1B	204	1/1	0.81	0.51	66,66,66,66	0
56	MG	2A	3331	1/1	0.81	0.46	73,73,73,73	0
56	MG	1E	306	1/1	0.81	0.27	72,72,72,72	0
56	MG	1A	3497	1/1	0.81	0.33	65,65,65,65	0
56	MG	2A	3081	1/1	0.81	0.56	76,76,76,76	0
56	MG	1A	3409	1/1	0.82	0.20	82,82,82,82	0
56	MG	1a	1674	1/1	0.82	0.24	92,92,92,92	0
56	MG	2a	3009	1/1	0.82	0.19	79,79,79,79	0
56	MG	1A	3184	1/1	0.82	0.51	69,69,69,69	0
56	MG	2A	3008	1/1	0.82	1.02	69,69,69,69	0
56	MG	1A	3316	1/1	0.82	0.41	63,63,63,63	0
56	MG	1A	3028	1/1	0.82	0.42	107,107,107,107	0
56	MG	1B	209	1/1	0.82	0.60	122,122,122,122	0
56	MG	2A	3310	1/1	0.82	0.49	67,67,67,67	0
56	MG	28	102	1/1	0.82	0.36	61,61,61,61	0
56	MG	2A	3086	1/1	0.82	0.16	77,77,77,77	0
56	MG	1A	3235	1/1	0.82	0.59	77,77,77,77	0
56	MG	2A	3152	1/1	0.82	0.31	81,81,81,81	0
56	MG	1A	3498	1/1	0.82	0.79	74,74,74,74	0
56	MG	2A	3142	1/1	0.82	0.29	73,73,73,73	0
56	MG	2A	3029	1/1	0.82	0.35	70,70,70,70	0
56	MG	1F	301	1/1	0.82	0.22	72,72,72,72	0
56	MG	1a	1607	1/1	0.82	0.13	100,100,100,100	0
56	MG	1A	3161	1/1	0.82	0.29	65,65,65,65	0
56	MG	1A	3025	1/1	0.82	0.41	77,77,77,77	0
56	MG	2a	3084	1/1	0.82	0.31	72,72,72,72	0
56	MG	2A	3138	1/1	0.82	0.29	76,76,76,76	0
56	MG	1a	1635	1/1	0.82	0.26	84,84,84,84	0
56	MG	2A	3048	1/1	0.82	0.35	82,82,82,82	0
56	MG	1A	3157	1/1	0.82	0.31	79,79,79,79	0
56	MG	2A	3050	1/1	0.82	0.16	76,76,76,76	0
56	MG	1A	3443	1/1	0.82	0.81	91,91,91,91	0
56	MG	2A	3065	1/1	0.82	0.43	68,68,68,68	0
56	MG	1A	3100	1/1	0.83	0.25	86,86,86,86	0
56	MG	1A	3105	1/1	0.83	0.36	108,108,108,108	0
56	MG	2A	3134	1/1	0.83	0.31	82,82,82,82	0
56	MG	1V	202	1/1	0.83	1.03	68,68,68,68	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	2A	3098	1/1	0.83	0.09	97,97,97,97	0
56	MG	2A	3280	1/1	0.83	0.34	61,61,61,61	0
56	MG	2A	3117	1/1	0.83	0.27	74,74,74,74	0
56	MG	1E	305	1/1	0.83	0.32	72,72,72,72	0
56	MG	2A	3197	1/1	0.83	0.47	61,61,61,61	0
56	MG	2A	3124	1/1	0.83	0.14	94,94,94,94	0
56	MG	2A	3178	1/1	0.83	1.27	75,75,75,75	0
56	MG	2a	3039	1/1	0.83	0.21	79,79,79,79	0
56	MG	1A	3027	1/1	0.83	0.42	78,78,78,78	0
56	MG	1V	201	1/1	0.83	0.42	80,80,80,80	0
56	MG	1A	3213	1/1	0.83	0.29	72,72,72,72	0
56	MG	1A	3297	1/1	0.83	0.66	79,79,79,79	0
56	MG	1S	201	1/1	0.83	0.23	78,78,78,78	0
56	MG	1A	3256	1/1	0.83	0.51	78,78,78,78	0
57	ZN	24	501	1/1	0.83	0.05	182,182,182,182	0
56	MG	1A	3355	1/1	0.83	0.23	71,71,71,71	0
56	MG	1a	1615	1/1	0.83	0.23	83,83,83,83	0
56	MG	1A	3269	1/1	0.83	0.57	92,92,92,92	0
56	MG	1A	3473	1/1	0.83	0.43	61,61,61,61	0
56	MG	1A	3178	1/1	0.83	0.53	65,65,65,65	0
56	MG	2A	3115	1/1	0.83	0.23	84,84,84,84	0
56	MG	2a	3008	1/1	0.83	0.42	102,102,102,102	0
56	MG	2a	3092	1/1	0.83	0.29	82,82,82,82	0
56	MG	1A	3101	1/1	0.84	0.35	74,74,74,74	0
56	MG	1A	3279	1/1	0.84	0.17	65,65,65,65	0
56	MG	1A	3462	1/1	0.84	0.56	79,79,79,79	0
56	MG	2a	3037	1/1	0.84	0.19	84,84,84,84	0
56	MG	2A	3066	1/1	0.84	0.32	85,85,85,85	0
56	MG	1A	3057	1/1	0.84	0.49	73,73,73,73	0
56	MG	2a	3102	1/1	0.84	0.09	127,127,127,127	0
56	MG	17	102	1/1	0.84	0.74	83,83,83,83	0
56	MG	2A	3350	1/1	0.84	0.15	93,93,93,93	0
56	MG	2a	3047	1/1	0.84	0.25	77,77,77,77	0
56	MG	2a	3024	1/1	0.84	0.24	83,83,83,83	0
56	MG	1A	3043	1/1	0.84	0.21	76,76,76,76	0
56	MG	1A	3260	1/1	0.84	0.28	81,81,81,81	0
56	MG	2A	3347	1/1	0.84	0.42	61,61,61,61	0
56	MG	2A	3214	1/1	0.84	0.25	82,82,82,82	0
56	MG	1B	208	1/1	0.84	0.55	81,81,81,81	0
56	MG	2A	3062	1/1	0.84	0.36	72,72,72,72	0
56	MG	1a	1620	1/1	0.84	0.18	81,81,81,81	0
56	MG	2A	3271	1/1	0.84	0.20	63,63,63,63	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	2l	201	1/1	0.84	1.15	80,80,80,80	0
56	MG	2a	3089	1/1	0.84	0.27	79,79,79,79	0
56	MG	2a	3073	1/1	0.84	0.27	76,76,76,76	0
56	MG	2R	202	1/1	0.84	0.40	67,67,67,67	0
56	MG	2a	3010	1/1	0.84	0.30	70,70,70,70	0
56	MG	1a	1643	1/1	0.84	0.21	71,71,71,71	0
56	MG	2A	3053	1/1	0.84	0.29	74,74,74,74	0
56	MG	1B	212	1/1	0.84	0.43	83,83,83,83	0
56	MG	1A	3074	1/1	0.84	0.48	77,77,77,77	0
56	MG	2a	3096	1/1	0.84	0.32	70,70,70,70	0
56	MG	1A	3263	1/1	0.84	0.52	105,105,105,105	0
56	MG	1A	3045	1/1	0.84	0.42	74,74,74,74	0
56	MG	1A	3203	1/1	0.84	0.40	72,72,72,72	0
56	MG	1A	3320	1/1	0.84	0.51	74,74,74,74	0
56	MG	2a	3032	1/1	0.85	0.14	75,75,75,75	0
56	MG	2a	3097	1/1	0.85	0.54	74,74,74,74	0
56	MG	18	101	1/1	0.85	0.30	65,65,65,65	0
56	MG	1A	3193	1/1	0.85	0.29	71,71,71,71	0
56	MG	2A	3107	1/1	0.85	0.24	81,81,81,81	0
56	MG	2A	3348	1/1	0.85	0.46	77,77,77,77	0
56	MG	2A	3151	1/1	0.85	0.15	109,109,109,109	0
56	MG	1a	1688	1/1	0.85	0.48	80,80,80,80	0
56	MG	1A	3010	1/1	0.85	0.39	72,72,72,72	0
56	MG	2A	3262	1/1	0.85	0.26	80,80,80,80	0
56	MG	1A	3428	1/1	0.85	0.61	61,61,61,61	0
56	MG	1A	3009	1/1	0.85	0.41	84,84,84,84	0
56	MG	1A	3170	1/1	0.85	0.29	79,79,79,79	0
56	MG	2A	3259	1/1	0.85	0.38	72,72,72,72	0
56	MG	2a	3077	1/1	0.85	0.30	95,95,95,95	0
56	MG	1A	3470	1/1	0.85	1.17	68,68,68,68	0
56	MG	1B	211	1/1	0.85	0.36	72,72,72,72	0
56	MG	1A	3126	1/1	0.85	0.30	80,80,80,80	0
56	MG	1A	3247	1/1	0.85	0.32	69,69,69,69	0
56	MG	2A	3126	1/1	0.85	0.22	76,76,76,76	0
56	MG	1a	1623	1/1	0.85	0.17	79,79,79,79	0
56	MG	1A	3439	1/1	0.85	0.36	67,67,67,67	0
56	MG	1B	203	1/1	0.85	0.60	106,106,106,106	0
56	MG	1A	3222	1/1	0.85	0.35	71,71,71,71	0
56	MG	1a	1648	1/1	0.85	0.40	100,100,100,100	0
56	MG	1A	3044	1/1	0.85	0.40	83,83,83,83	0
56	MG	2A	3237	1/1	0.85	0.21	82,82,82,82	0
56	MG	1A	3198	1/1	0.85	0.34	64,64,64,64	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	1A	3123	1/1	0.85	0.31	81,81,81,81	0
56	MG	2A	3336	1/1	0.85	0.53	91,91,91,91	0
56	MG	2A	3145	1/1	0.85	0.48	79,79,79,79	0
56	MG	1A	3424	1/1	0.85	0.27	61,61,61,61	0
56	MG	1A	3275	1/1	0.85	0.42	63,63,63,63	0
56	MG	1A	3189	1/1	0.85	0.32	82,82,82,82	0
56	MG	1a	1672	1/1	0.85	0.17	104,104,104,104	0
56	MG	1A	3205	1/1	0.85	0.49	74,74,74,74	0
56	MG	2A	3268	1/1	0.85	0.53	68,68,68,68	0
56	MG	2a	3021	1/1	0.86	0.24	82,82,82,82	0
56	MG	2a	3056	1/1	0.86	0.55	82,82,82,82	0
56	MG	1a	1676	1/1	0.86	0.12	77,77,77,77	0
56	MG	1A	3463	1/1	0.86	0.49	72,72,72,72	0
56	MG	1E	302	1/1	0.86	0.35	76,76,76,76	0
56	MG	2A	3108	1/1	0.86	0.34	67,67,67,67	0
56	MG	2A	3256	1/1	0.86	0.43	66,66,66,66	0
56	MG	1A	3129	1/1	0.86	0.46	77,77,77,77	0
56	MG	1A	3434	1/1	0.86	0.24	72,72,72,72	0
56	MG	2a	3033	1/1	0.86	0.21	72,72,72,72	0
56	MG	1A	3098	1/1	0.86	0.24	81,81,81,81	0
56	MG	1A	3145	1/1	0.86	0.22	79,79,79,79	0
56	MG	2B	207	1/1	0.86	0.53	84,84,84,84	0
56	MG	1A	3415	1/1	0.86	0.23	80,80,80,80	0
56	MG	1A	3149	1/1	0.86	0.34	72,72,72,72	0
56	MG	1A	3478	1/1	0.86	0.21	76,76,76,76	0
56	MG	2Y	201	1/1	0.86	0.35	71,71,71,71	0
56	MG	2A	3210	1/1	0.86	0.23	68,68,68,68	0
56	MG	1A	3117	1/1	0.86	0.36	63,63,63,63	0
56	MG	2A	3359	1/1	0.86	0.28	74,74,74,74	0
56	MG	2A	3382	1/1	0.86	0.17	124,124,124,124	0
56	MG	2A	3080	1/1	0.86	0.52	69,69,69,69	0
56	MG	2A	3128	1/1	0.86	0.43	61,61,61,61	0
56	MG	1A	3227	1/1	0.86	0.26	71,71,71,71	0
56	MG	1A	3234	1/1	0.86	0.17	85,85,85,85	0
56	MG	1A	3449	1/1	0.86	0.96	83,83,83,83	0
56	MG	1A	3150	1/1	0.86	0.65	90,90,90,90	0
56	MG	1A	3266	1/1	0.86	0.26	77,77,77,77	0
56	MG	1A	3410	1/1	0.86	0.32	83,83,83,83	0
56	MG	2A	3023	1/1	0.86	0.29	73,73,73,73	0
57	ZN	1Y	501	1/1	0.86	0.15	156,156,156,156	0
56	MG	2A	3001	1/1	0.86	0.32	80,80,80,80	0
56	MG	1A	3073	1/1	0.86	0.28	86,86,86,86	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	2a	3094	1/1	0.86	0.26	66,66,66,66	0
56	MG	1A	3011	1/1	0.86	0.34	72,72,72,72	0
56	MG	2A	3251	1/1	0.86	0.30	75,75,75,75	0
56	MG	2A	3143	1/1	0.86	0.38	69,69,69,69	0
56	MG	1A	3378	1/1	0.86	0.63	77,77,77,77	0
56	MG	1A	3167	1/1	0.86	0.26	80,80,80,80	0
56	MG	1A	3081	1/1	0.86	0.83	65,65,65,65	0
56	MG	1a	1668	1/1	0.87	0.49	78,78,78,78	0
56	MG	2B	205	1/1	0.87	0.24	89,89,89,89	0
56	MG	1A	3425	1/1	0.87	0.58	67,67,67,67	0
56	MG	1A	3128	1/1	0.87	0.54	77,77,77,77	0
56	MG	15	101	1/1	0.87	0.20	70,70,70,70	0
56	MG	1A	3059	1/1	0.87	0.32	92,92,92,92	0
56	MG	1A	3136	1/1	0.87	0.23	76,76,76,76	0
56	MG	1A	3160	1/1	0.87	0.70	67,67,67,67	0
56	MG	1A	3037	1/1	0.87	0.80	68,68,68,68	0
56	MG	1A	3208	1/1	0.87	0.46	62,62,62,62	0
56	MG	2A	3287	1/1	0.87	0.29	66,66,66,66	0
56	MG	1a	1670	1/1	0.87	0.17	97,97,97,97	0
56	MG	1a	1650	1/1	0.87	0.22	82,82,82,82	0
56	MG	2A	3032	1/1	0.87	0.29	85,85,85,85	0
56	MG	2A	3309	1/1	0.87	0.29	61,61,61,61	0
56	MG	1A	3397	1/1	0.87	0.25	84,84,84,84	0
56	MG	2B	203	1/1	0.87	0.41	75,75,75,75	0
56	MG	1A	3038	1/1	0.87	0.45	61,61,61,61	0
56	MG	1a	1617	1/1	0.87	0.14	91,91,91,91	0
56	MG	1A	3243	1/1	0.87	0.39	71,71,71,71	0
56	MG	2a	3034	1/1	0.87	0.20	78,78,78,78	0
56	MG	2A	3044	1/1	0.87	0.47	81,81,81,81	0
56	MG	1A	3292	1/1	0.87	0.97	75,75,75,75	0
56	MG	2A	3055	1/1	0.87	0.31	82,82,82,82	0
56	MG	2a	3030	1/1	0.87	0.51	74,74,74,74	0
56	MG	1A	3168	1/1	0.87	0.69	71,71,71,71	0
56	MG	1A	3400	1/1	0.87	0.32	87,87,87,87	0
56	MG	1A	3469	1/1	0.87	0.58	88,88,88,88	0
56	MG	2A	3366	1/1	0.87	0.34	63,63,63,63	0
56	MG	1a	1604	1/1	0.87	0.18	107,107,107,107	0
56	MG	1A	3214	1/1	0.87	1.15	69,69,69,69	0
56	MG	2r	101	1/1	0.87	0.23	77,77,77,77	0
56	MG	1A	3290	1/1	0.87	0.29	80,80,80,80	0
56	MG	2A	3154	1/1	0.87	0.22	68,68,68,68	0
56	MG	2A	3177	1/1	0.87	0.26	63,63,63,63	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	1A	3356	1/1	0.87	0.24	61,61,61,61	0
56	MG	2a	3029	1/1	0.87	0.15	104,104,104,104	0
56	MG	1A	3298	1/1	0.88	0.39	71,71,71,71	0
56	MG	1A	3241	1/1	0.88	0.58	61,61,61,61	0
56	MG	2a	3022	1/1	0.88	0.40	81,81,81,81	0
56	MG	1A	3464	1/1	0.88	0.33	95,95,95,95	0
56	MG	1A	3210	1/1	0.88	0.63	81,81,81,81	0
56	MG	2A	3211	1/1	0.88	0.29	63,63,63,63	0
56	MG	1A	3018	1/1	0.88	0.37	77,77,77,77	0
56	MG	1A	3063	1/1	0.88	0.56	77,77,77,77	0
56	MG	2A	3255	1/1	0.88	0.32	71,71,71,71	0
56	MG	2A	3003	1/1	0.88	0.22	73,73,73,73	0
56	MG	2A	3380	1/1	0.88	0.18	85,85,85,85	0
56	MG	1A	3166	1/1	0.88	0.65	69,69,69,69	0
56	MG	2A	3051	1/1	0.88	1.39	79,79,79,79	0
56	MG	2A	3144	1/1	0.88	0.32	83,83,83,83	0
56	MG	1a	1634	1/1	0.88	0.11	102,102,102,102	0
56	MG	1A	3362	1/1	0.88	0.52	62,62,62,62	0
56	MG	1A	3383	1/1	0.88	0.24	73,73,73,73	0
56	MG	2a	3074	1/1	0.88	0.29	76,76,76,76	0
56	MG	2A	3103	1/1	0.88	0.49	78,78,78,78	0
56	MG	1A	3359	1/1	0.88	0.46	78,78,78,78	0
56	MG	1A	3212	1/1	0.88	0.45	62,62,62,62	0
56	MG	2A	3363	1/1	0.88	0.37	65,65,65,65	0
56	MG	1A	3436	1/1	0.88	0.52	61,61,61,61	0
56	MG	2A	3185	1/1	0.88	0.27	72,72,72,72	0
56	MG	2A	3181	1/1	0.88	0.30	101,101,101,101	0
56	MG	1a	1647	1/1	0.88	1.09	106,106,106,106	0
56	MG	1A	3274	1/1	0.88	0.36	74,74,74,74	0
56	MG	1A	3345	1/1	0.88	0.29	72,72,72,72	0
56	MG	2A	3165	1/1	0.88	0.28	73,73,73,73	0
56	MG	1A	3015	1/1	0.88	0.46	62,62,62,62	0
56	MG	2A	3292	1/1	0.88	0.34	64,64,64,64	0
56	MG	2A	3084	1/1	0.88	0.25	79,79,79,79	0
56	MG	2A	3037	1/1	0.88	0.33	90,90,90,90	0
56	MG	2A	3047	1/1	0.88	0.40	81,81,81,81	0
56	MG	1B	210	1/1	0.88	0.36	96,96,96,96	0
56	MG	1a	1626	1/1	0.88	0.28	81,81,81,81	0
56	MG	2a	3064	1/1	0.88	0.43	67,67,67,67	0
56	MG	2A	3376	1/1	0.88	0.35	72,72,72,72	0
56	MG	1A	3069	1/1	0.88	0.78	81,81,81,81	0
56	MG	2a	3015	1/1	0.88	0.15	80,80,80,80	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	2a	3078	1/1	0.88	0.44	62,62,62,62	0
56	MG	2A	3013	1/1	0.88	0.32	73,73,73,73	0
56	MG	2a	3007	1/1	0.88	0.24	73,73,73,73	0
56	MG	2A	3054	1/1	0.88	0.15	78,78,78,78	0
56	MG	1A	3206	1/1	0.88	0.53	76,76,76,76	0
56	MG	1a	1690	1/1	0.88	0.18	84,84,84,84	0
56	MG	1A	3444	1/1	0.88	0.16	109,109,109,109	0
56	MG	1A	3472	1/1	0.88	0.41	67,67,67,67	0
56	MG	2A	3320	1/1	0.88	0.40	74,74,74,74	0
56	MG	1E	303	1/1	0.88	0.35	62,62,62,62	0
56	MG	1A	3191	1/1	0.88	0.27	70,70,70,70	0
56	MG	2A	3038	1/1	0.89	0.18	77,77,77,77	0
56	MG	1A	3079	1/1	0.89	0.58	78,78,78,78	0
56	MG	1A	3371	1/1	0.89	0.49	75,75,75,75	0
56	MG	2A	3021	1/1	0.89	0.16	90,90,90,90	0
56	MG	2a	3052	1/1	0.89	0.52	68,68,68,68	0
56	MG	1A	3246	1/1	0.89	0.23	77,77,77,77	0
56	MG	1A	3248	1/1	0.89	0.51	68,68,68,68	0
56	MG	1A	3233	1/1	0.89	0.63	76,76,76,76	0
56	MG	1A	3016	1/1	0.89	0.08	95,95,95,95	0
56	MG	1A	3176	1/1	0.89	0.20	75,75,75,75	0
56	MG	2A	3351	1/1	0.89	0.29	94,94,94,94	0
56	MG	2A	3045	1/1	0.89	0.90	74,74,74,74	0
56	MG	1a	1677	1/1	0.89	0.14	85,85,85,85	0
56	MG	1A	3035	1/1	0.89	0.84	75,75,75,75	0
56	MG	2A	3302	1/1	0.89	0.27	82,82,82,82	0
56	MG	1A	3456	1/1	0.89	0.32	68,68,68,68	0
56	MG	2A	3082	1/1	0.89	0.51	79,79,79,79	0
56	MG	2a	3019	1/1	0.89	0.24	77,77,77,77	0
56	MG	1A	3475	1/1	0.89	0.68	65,65,65,65	0
56	MG	1a	1653	1/1	0.89	0.18	63,63,63,63	0
56	MG	1A	3060	1/1	0.89	0.24	79,79,79,79	0
56	MG	1A	3201	1/1	0.89	0.66	69,69,69,69	0
56	MG	1A	3347	1/1	0.89	0.27	90,90,90,90	0
56	MG	1A	3122	1/1	0.89	0.43	106,106,106,106	0
56	MG	1a	1633	1/1	0.89	0.18	97,97,97,97	0
56	MG	1A	3375	1/1	0.89	0.45	95,95,95,95	0
56	MG	1A	3204	1/1	0.89	0.69	72,72,72,72	0
56	MG	1A	3004	1/1	0.89	0.19	89,89,89,89	0
56	MG	1A	3230	1/1	0.89	0.33	79,79,79,79	0
56	MG	1A	3261	1/1	0.89	0.63	77,77,77,77	0
56	MG	1A	3175	1/1	0.89	0.30	62,62,62,62	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	28	101	1/1	0.90	0.46	80,80,80,80	0
56	MG	2a	3045	1/1	0.90	0.46	79,79,79,79	0
56	MG	1A	3024	1/1	0.90	0.22	85,85,85,85	0
56	MG	1A	3489	1/1	0.90	0.17	78,78,78,78	0
56	MG	2A	3043	1/1	0.90	0.35	70,70,70,70	0
56	MG	1A	3106	1/1	0.90	0.21	73,73,73,73	0
56	MG	2A	3184	1/1	0.90	0.29	70,70,70,70	0
56	MG	2a	3095	1/1	0.90	0.20	84,84,84,84	0
56	MG	1A	3431	1/1	0.90	0.28	62,62,62,62	0
56	MG	2A	3099	1/1	0.90	0.19	81,81,81,81	0
56	MG	2A	3364	1/1	0.90	0.19	80,80,80,80	0
56	MG	1A	3131	1/1	0.90	0.26	76,76,76,76	0
56	MG	1A	3111	1/1	0.90	0.18	78,78,78,78	0
56	MG	1A	3365	1/1	0.90	0.30	69,69,69,69	0
56	MG	2A	3146	1/1	0.90	0.15	79,79,79,79	0
56	MG	2A	3158	1/1	0.90	0.28	73,73,73,73	0
56	MG	2A	3171	1/1	0.90	0.26	94,94,94,94	0
56	MG	2a	3002	1/1	0.90	0.30	65,65,65,65	0
56	MG	2A	3106	1/1	0.90	0.14	83,83,83,83	0
56	MG	2A	3121	1/1	0.90	0.21	66,66,66,66	0
56	MG	1a	1661	1/1	0.90	0.32	72,72,72,72	0
56	MG	2A	3083	1/1	0.90	0.43	77,77,77,77	0
56	MG	2A	3022	1/1	0.90	0.31	66,66,66,66	0
56	MG	1A	3127	1/1	0.90	0.44	69,69,69,69	0
56	MG	1A	3185	1/1	0.90	0.41	62,62,62,62	0
56	MG	1A	3433	1/1	0.90	0.70	75,75,75,75	0
56	MG	2A	3232	1/1	0.90	0.20	66,66,66,66	0
56	MG	1A	3158	1/1	0.90	0.30	75,75,75,75	0
56	MG	1A	3058	1/1	0.90	0.43	73,73,73,73	0
56	MG	2A	3092	1/1	0.90	0.28	75,75,75,75	0
56	MG	2A	3230	1/1	0.90	0.42	62,62,62,62	0
56	MG	1A	3186	1/1	0.90	0.34	84,84,84,84	0
56	MG	2A	3244	1/1	0.90	0.30	61,61,61,61	0
56	MG	1a	1601	1/1	0.90	0.15	72,72,72,72	0
56	MG	1A	3411	1/1	0.90	0.44	75,75,75,75	0
56	MG	2A	3299	1/1	0.90	0.15	78,78,78,78	0
56	MG	2A	3295	1/1	0.90	0.12	76,76,76,76	0
56	MG	1A	3218	1/1	0.90	0.29	66,66,66,66	0
56	MG	2A	3182	1/1	0.90	0.29	76,76,76,76	0
56	MG	2A	3321	1/1	0.90	0.19	81,81,81,81	0
56	MG	1A	3325	1/1	0.90	0.26	70,70,70,70	0
56	MG	1a	1632	1/1	0.91	0.18	88,88,88,88	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	1A	3103	1/1	0.91	0.66	64,64,64,64	0
56	MG	2B	204	1/1	0.91	0.62	80,80,80,80	0
56	MG	2A	3261	1/1	0.91	0.22	72,72,72,72	0
56	MG	16	101	1/1	0.91	0.27	75,75,75,75	0
56	MG	2A	3338	1/1	0.91	1.37	75,75,75,75	0
56	MG	1A	3052	1/1	0.91	0.31	85,85,85,85	0
56	MG	2A	3343	1/1	0.91	0.17	73,73,73,73	0
56	MG	2A	3371	1/1	0.91	0.20	62,62,62,62	0
56	MG	1A	3147	1/1	0.91	0.34	76,76,76,76	0
56	MG	1A	3107	1/1	0.91	0.27	64,64,64,64	0
56	MG	1A	3002	1/1	0.91	0.17	94,94,94,94	0
56	MG	1A	3109	1/1	0.91	0.12	92,92,92,92	0
56	MG	2A	3199	1/1	0.91	0.23	83,83,83,83	0
56	MG	2B	206	1/1	0.91	0.44	89,89,89,89	0
56	MG	2A	3133	1/1	0.91	0.36	77,77,77,77	0
56	MG	1A	3346	1/1	0.91	0.49	65,65,65,65	0
56	MG	2a	3027	1/1	0.91	0.10	79,79,79,79	0
56	MG	1A	3151	1/1	0.91	0.23	76,76,76,76	0
56	MG	2A	3212	1/1	0.91	0.43	78,78,78,78	0
56	MG	1A	3163	1/1	0.91	0.48	78,78,78,78	0
56	MG	1A	3089	1/1	0.91	0.25	74,74,74,74	0
56	MG	1E	301	1/1	0.91	0.22	71,71,71,71	0
56	MG	1a	1628	1/1	0.91	0.51	61,61,61,61	0
56	MG	1A	3396	1/1	0.91	0.28	84,84,84,84	0
56	MG	1A	3414	1/1	0.91	0.24	70,70,70,70	0
56	MG	1A	3350	1/1	0.91	0.61	78,78,78,78	0
56	MG	1A	3317	1/1	0.91	0.89	77,77,77,77	0
56	MG	1A	3339	1/1	0.91	0.24	73,73,73,73	0
56	MG	1A	3285	1/1	0.91	0.18	83,83,83,83	0
56	MG	1A	3219	1/1	0.91	0.29	90,90,90,90	0
56	MG	2A	3191	1/1	0.91	0.18	78,78,78,78	0
56	MG	1A	3313	1/1	0.91	0.49	70,70,70,70	0
56	MG	2A	3196	1/1	0.91	0.28	78,78,78,78	0
56	MG	2A	3325	1/1	0.91	0.27	67,67,67,67	0
56	MG	1A	3450	1/1	0.91	0.21	75,75,75,75	0
56	MG	1D	301	1/1	0.91	0.24	73,73,73,73	0
56	MG	1A	3031	1/1	0.91	0.23	69,69,69,69	0
56	MG	2A	3340	1/1	0.91	0.38	86,86,86,86	0
56	MG	1A	3006	1/1	0.91	0.22	72,72,72,72	0
56	MG	2A	3330	1/1	0.91	0.23	82,82,82,82	0
56	MG	1A	3164	1/1	0.91	0.27	69,69,69,69	0
56	MG	1A	3496	1/1	0.91	0.11	94,94,94,94	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	1a	1637	1/1	0.91	0.20	89,89,89,89	0
56	MG	1A	3120	1/1	0.91	0.24	61,61,61,61	0
56	MG	1A	3077	1/1	0.91	0.86	81,81,81,81	0
56	MG	2A	3019	1/1	0.91	0.37	69,69,69,69	0
56	MG	1A	3046	1/1	0.91	0.81	78,78,78,78	0
56	MG	1A	3238	1/1	0.91	0.27	75,75,75,75	0
56	MG	1A	3363	1/1	0.91	0.47	77,77,77,77	0
56	MG	1A	3017	1/1	0.91	0.41	61,61,61,61	0
56	MG	1A	3369	1/1	0.91	0.35	76,76,76,76	0
56	MG	2a	3028	1/1	0.91	0.34	83,83,83,83	0
56	MG	13	101	1/1	0.91	0.35	72,72,72,72	0
56	MG	1A	3331	1/1	0.91	0.30	63,63,63,63	0
56	MG	25	101	1/1	0.91	0.56	69,69,69,69	0
56	MG	2A	3156	1/1	0.91	0.25	63,63,63,63	0
56	MG	1A	3403	1/1	0.91	0.46	87,87,87,87	0
56	MG	2A	3342	1/1	0.91	0.29	85,85,85,85	0
56	MG	1A	3090	1/1	0.92	0.21	75,75,75,75	0
56	MG	1A	3465	1/1	0.92	0.43	61,61,61,61	0
56	MG	2D	3100	1/1	0.92	0.19	83,83,83,83	0
56	MG	1A	3429	1/1	0.92	0.95	79,79,79,79	0
56	MG	1A	3066	1/1	0.92	0.17	72,72,72,72	0
56	MG	2A	3007	1/1	0.92	0.24	78,78,78,78	0
57	ZN	14	501	1/1	0.92	0.07	166,166,166,166	0
56	MG	1A	3055	1/1	0.92	0.68	83,83,83,83	0
56	MG	2A	3234	1/1	0.92	0.25	68,68,68,68	0
56	MG	2A	3372	1/1	0.92	0.19	70,70,70,70	0
56	MG	1a	1602	1/1	0.92	0.32	74,74,74,74	0
56	MG	1A	3306	1/1	0.92	0.53	61,61,61,61	0
56	MG	1A	3084	1/1	0.92	0.19	79,79,79,79	0
56	MG	1A	3108	1/1	0.92	0.16	75,75,75,75	0
56	MG	1A	3012	1/1	0.92	0.82	75,75,75,75	0
56	MG	2A	3218	1/1	0.92	0.14	72,72,72,72	0
56	MG	1A	3454	1/1	0.92	0.47	73,73,73,73	0
56	MG	2A	3328	1/1	0.92	0.21	68,68,68,68	0
56	MG	1A	3401	1/1	0.92	0.25	64,64,64,64	0
56	MG	23	101	1/1	0.92	0.31	68,68,68,68	0
56	MG	2A	3170	1/1	0.92	0.43	67,67,67,67	0
56	MG	2A	3322	1/1	0.92	0.17	89,89,89,89	0
56	MG	2A	3202	1/1	0.92	0.27	70,70,70,70	0
56	MG	1x	101	1/1	0.92	0.48	92,92,92,92	0
56	MG	2A	3167	1/1	0.92	0.46	72,72,72,72	0
56	MG	2Q	201	1/1	0.92	0.12	93,93,93,93	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	1A	3406	1/1	0.92	0.47	76,76,76,76	0
56	MG	1a	1652	1/1	0.92	0.17	74,74,74,74	0
56	MG	1A	3398	1/1	0.92	0.41	70,70,70,70	0
56	MG	1A	3419	1/1	0.92	0.27	72,72,72,72	0
56	MG	1A	3085	1/1	0.92	0.84	79,79,79,79	0
56	MG	2A	3384	1/1	0.92	0.10	91,91,91,91	0
56	MG	1B	205	1/1	0.92	0.42	68,68,68,68	0
56	MG	1A	3053	1/1	0.92	0.63	77,77,77,77	0
56	MG	2A	3241	1/1	0.92	0.20	65,65,65,65	0
56	MG	1a	1621	1/1	0.92	0.27	73,73,73,73	0
56	MG	2A	3219	1/1	0.92	0.28	75,75,75,75	0
56	MG	1A	3289	1/1	0.92	0.37	84,84,84,84	0
56	MG	2a	3082	1/1	0.92	0.34	66,66,66,66	0
56	MG	2A	3265	1/1	0.92	0.53	73,73,73,73	0
56	MG	2A	3188	1/1	0.92	0.30	74,74,74,74	0
57	ZN	25	102	1/1	0.92	0.19	104,104,104,104	0
56	MG	2A	3368	1/1	0.92	0.53	62,62,62,62	0
56	MG	1A	3096	1/1	0.92	0.23	76,76,76,76	0
56	MG	1A	3408	1/1	0.92	0.53	61,61,61,61	0
56	MG	1A	3033	1/1	0.92	0.28	86,86,86,86	0
56	MG	2a	3070	1/1	0.92	0.20	78,78,78,78	0
56	MG	1B	207	1/1	0.92	0.39	106,106,106,106	0
56	MG	1A	3302	1/1	0.92	0.24	62,62,62,62	0
56	MG	2A	3132	1/1	0.92	0.21	71,71,71,71	0
56	MG	2A	3373	1/1	0.93	0.36	69,69,69,69	0
56	MG	1a	1682	1/1	0.93	0.14	96,96,96,96	0
56	MG	1A	3116	1/1	0.93	0.51	68,68,68,68	0
56	MG	2A	3104	1/1	0.93	0.54	80,80,80,80	0
56	MG	1A	3352	1/1	0.93	0.30	101,101,101,101	0
56	MG	1A	3276	1/1	0.93	0.23	75,75,75,75	0
56	MG	2a	3079	1/1	0.93	0.18	62,62,62,62	0
56	MG	1A	3209	1/1	0.93	0.51	61,61,61,61	0
56	MG	2a	3099	1/1	0.93	0.58	79,79,79,79	0
56	MG	1a	1680	1/1	0.93	0.95	73,73,73,73	0
56	MG	1r	101	1/1	0.93	0.33	81,81,81,81	0
56	MG	1A	3455	1/1	0.93	0.46	63,63,63,63	0
56	MG	1A	3324	1/1	0.93	0.11	67,67,67,67	0
56	MG	1A	3348	1/1	0.93	0.36	79,79,79,79	0
56	MG	2A	3150	1/1	0.93	0.22	101,101,101,101	0
56	MG	1A	3022	1/1	0.93	0.51	89,89,89,89	0
56	MG	1a	1693	1/1	0.93	0.12	127,127,127,127	0
56	MG	1a	1608	1/1	0.93	0.20	73,73,73,73	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	1A	3336	1/1	0.93	0.27	64,64,64,64	0
56	MG	1A	3366	1/1	0.93	0.27	61,61,61,61	0
56	MG	1A	3036	1/1	0.93	0.23	83,83,83,83	0
56	MG	1A	3376	1/1	0.93	0.28	61,61,61,61	0
56	MG	1A	3169	1/1	0.93	0.33	62,62,62,62	0
56	MG	1a	1656	1/1	0.93	0.23	82,82,82,82	0
56	MG	1A	3132	1/1	0.93	0.28	74,74,74,74	0
56	MG	2E	306	1/1	0.93	0.17	64,64,64,64	0
56	MG	1A	3143	1/1	0.93	0.44	62,62,62,62	0
56	MG	1A	3265	1/1	0.93	0.50	72,72,72,72	0
56	MG	2a	3072	1/1	0.93	0.27	72,72,72,72	0
56	MG	1A	3353	1/1	0.93	0.34	62,62,62,62	0
56	MG	2A	3213	1/1	0.93	0.25	67,67,67,67	0
56	MG	1A	3354	1/1	0.93	0.29	61,61,61,61	0
56	MG	1A	3277	1/1	0.93	0.54	61,61,61,61	0
56	MG	2A	3379	1/1	0.93	0.14	77,77,77,77	0
56	MG	1a	1612	1/1	0.93	0.13	97,97,97,97	0
56	MG	2A	3316	1/1	0.93	0.30	62,62,62,62	0
56	MG	1A	3387	1/1	0.93	0.19	80,80,80,80	0
56	MG	2A	3148	1/1	0.93	0.27	72,72,72,72	0
56	MG	1A	3061	1/1	0.93	0.44	71,71,71,71	0
56	MG	1A	3395	1/1	0.93	0.24	67,67,67,67	0
56	MG	2a	3013	1/1	0.93	0.58	80,80,80,80	0
56	MG	1A	3461	1/1	0.93	0.59	83,83,83,83	0
56	MG	1A	3319	1/1	0.93	0.22	61,61,61,61	0
56	MG	2a	3083	1/1	0.93	0.29	61,61,61,61	0
56	MG	1A	3481	1/1	0.93	0.40	68,68,68,68	0
56	MG	1A	3095	1/1	0.93	0.35	69,69,69,69	0
56	MG	2A	3344	1/1	0.93	0.17	78,78,78,78	0
56	MG	2A	3060	1/1	0.93	0.17	88,88,88,88	0
56	MG	2A	3163	1/1	0.93	0.24	62,62,62,62	0
56	MG	1A	3338	1/1	0.93	0.41	61,61,61,61	0
56	MG	2a	3071	1/1	0.93	0.21	75,75,75,75	0
56	MG	1A	3097	1/1	0.93	0.54	77,77,77,77	0
56	MG	1A	3135	1/1	0.93	0.36	80,80,80,80	0
56	MG	1A	3416	1/1	0.93	0.45	103,103,103,103	0
56	MG	2a	3041	1/1	0.93	0.29	80,80,80,80	0
56	MG	1A	3399	1/1	0.93	0.30	73,73,73,73	0
56	MG	1A	3102	1/1	0.93	0.60	74,74,74,74	0
56	MG	1a	1685	1/1	0.93	0.10	76,76,76,76	0
56	MG	2a	3091	1/1	0.93	0.55	79,79,79,79	0
56	MG	2A	3111	1/1	0.93	0.36	76,76,76,76	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	1A	3451	1/1	0.94	0.15	77,77,77,77	0
56	MG	10	101	1/1	0.94	0.25	65,65,65,65	0
56	MG	2a	3044	1/1	0.94	0.66	75,75,75,75	0
56	MG	1A	3430	1/1	0.94	0.30	68,68,68,68	0
56	MG	1A	3050	1/1	0.94	0.25	83,83,83,83	0
56	MG	1A	3442	1/1	0.94	0.60	61,61,61,61	0
56	MG	1A	3259	1/1	0.94	0.22	73,73,73,73	0
56	MG	2A	3354	1/1	0.94	0.19	65,65,65,65	0
56	MG	1A	3023	1/1	0.94	0.21	73,73,73,73	0
56	MG	1A	3495	1/1	0.94	0.30	98,98,98,98	0
56	MG	2A	3339	1/1	0.94	0.06	85,85,85,85	0
56	MG	1A	3390	1/1	0.94	0.46	61,61,61,61	0
56	MG	2a	3058	1/1	0.94	0.86	73,73,73,73	0
56	MG	1A	3112	1/1	0.94	0.53	63,63,63,63	0
56	MG	1A	3323	1/1	0.94	0.39	62,62,62,62	0
56	MG	2A	3353	1/1	0.94	0.42	70,70,70,70	0
56	MG	1a	1618	1/1	0.94	0.11	96,96,96,96	0
56	MG	1A	3080	1/1	0.94	0.23	82,82,82,82	0
56	MG	1A	3216	1/1	0.94	0.37	65,65,65,65	0
56	MG	2A	3228	1/1	0.94	0.15	67,67,67,67	0
56	MG	2A	3089	1/1	0.94	0.17	87,87,87,87	0
56	MG	1A	3294	1/1	0.94	0.33	75,75,75,75	0
56	MG	1A	3476	1/1	0.94	0.42	62,62,62,62	0
56	MG	1A	3460	1/1	0.94	0.47	67,67,67,67	0
56	MG	2a	3042	1/1	0.94	0.13	91,91,91,91	0
56	MG	1A	3183	1/1	0.94	0.70	74,74,74,74	0
56	MG	2A	3028	1/1	0.94	0.44	91,91,91,91	0
56	MG	2A	3153	1/1	0.94	0.32	100,100,100,100	0
56	MG	2A	3324	1/1	0.94	0.18	82,82,82,82	0
56	MG	1A	3282	1/1	0.94	0.25	70,70,70,70	0
56	MG	1a	1666	1/1	0.94	0.27	94,94,94,94	0
56	MG	2A	3025	1/1	0.94	0.30	89,89,89,89	0
56	MG	2A	3186	1/1	0.94	0.10	92,92,92,92	0
56	MG	2a	3101	1/1	0.94	0.13	102,102,102,102	0
56	MG	2A	3203	1/1	0.94	0.34	61,61,61,61	0
56	MG	2a	3036	1/1	0.94	0.36	76,76,76,76	0
56	MG	1A	3019	1/1	0.94	0.37	80,80,80,80	0
56	MG	1A	3048	1/1	0.94	0.41	69,69,69,69	0
56	MG	2A	3307	1/1	0.94	0.25	77,77,77,77	0
56	MG	1A	3486	1/1	0.94	0.14	78,78,78,78	0
56	MG	1A	3368	1/1	0.94	0.37	77,77,77,77	0
56	MG	1A	3374	1/1	0.94	0.34	62,62,62,62	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	1A	3386	1/1	0.94	0.27	77,77,77,77	0
56	MG	1A	3441	1/1	0.94	0.25	76,76,76,76	0
56	MG	2a	3103	1/1	0.94	0.11	101,101,101,101	0
56	MG	1A	3457	1/1	0.94	0.28	62,62,62,62	0
56	MG	2A	3164	1/1	0.94	0.28	68,68,68,68	0
56	MG	1A	3389	1/1	0.94	0.17	71,71,71,71	0
56	MG	1U	201	1/1	0.94	0.37	67,67,67,67	0
56	MG	2A	3308	1/1	0.94	0.26	85,85,85,85	0
56	MG	2A	3207	1/1	0.94	0.10	89,89,89,89	0
56	MG	1A	3335	1/1	0.94	0.46	85,85,85,85	0
56	MG	1A	3041	1/1	0.94	0.59	69,69,69,69	0
56	MG	2B	209	1/1	0.94	0.13	91,91,91,91	0
56	MG	1A	3344	1/1	0.94	0.36	73,73,73,73	0
56	MG	1A	3271	1/1	0.94	0.17	75,75,75,75	0
56	MG	2A	3357	1/1	0.94	0.20	69,69,69,69	0
56	MG	2A	3192	1/1	0.94	0.49	79,79,79,79	0
56	MG	1A	3422	1/1	0.94	0.29	61,61,61,61	0
56	MG	1A	3326	1/1	0.94	0.29	63,63,63,63	0
56	MG	1a	1663	1/1	0.94	0.20	68,68,68,68	0
56	MG	1A	3225	1/1	0.94	0.11	90,90,90,90	0
56	MG	1A	3042	1/1	0.94	0.28	79,79,79,79	0
56	MG	1B	206	1/1	0.94	0.55	89,89,89,89	0
56	MG	2A	3385	1/1	0.94	0.13	76,76,76,76	0
56	MG	10	102	1/1	0.94	0.37	73,73,73,73	0
56	MG	2A	3252	1/1	0.94	0.25	77,77,77,77	0
56	MG	1A	3003	1/1	0.94	0.26	68,68,68,68	0
56	MG	2a	3031	1/1	0.94	0.11	76,76,76,76	0
56	MG	2A	3288	1/1	0.94	0.19	66,66,66,66	0
56	MG	1A	3199	1/1	0.94	0.43	84,84,84,84	0
56	MG	2A	3275	1/1	0.94	0.24	62,62,62,62	0
56	MG	2a	3075	1/1	0.94	0.26	92,92,92,92	0
56	MG	2a	3085	1/1	0.94	0.21	92,92,92,92	0
56	MG	1A	3367	1/1	0.94	0.23	61,61,61,61	0
56	MG	2A	3250	1/1	0.94	0.39	62,62,62,62	0
56	MG	2A	3069	1/1	0.94	0.23	83,83,83,83	0
56	MG	1a	1605	1/1	0.94	0.12	99,99,99,99	0
56	MG	1A	3372	1/1	0.94	0.37	72,72,72,72	0
56	MG	1A	3141	1/1	0.94	0.32	83,83,83,83	0
56	MG	2A	3169	1/1	0.94	0.60	69,69,69,69	0
56	MG	1a	1657	1/1	0.94	0.25	93,93,93,93	0
56	MG	1A	3005	1/1	0.95	0.11	82,82,82,82	0
56	MG	1A	3421	1/1	0.95	0.27	65,65,65,65	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	2a	3049	1/1	0.95	0.26	80,80,80,80	0
56	MG	1a	1639	1/1	0.95	0.53	77,77,77,77	0
56	MG	1A	3091	1/1	0.95	0.23	77,77,77,77	0
56	MG	1A	3392	1/1	0.95	0.30	73,73,73,73	0
56	MG	1A	3310	1/1	0.95	0.32	62,62,62,62	0
56	MG	2A	3370	1/1	0.95	0.16	75,75,75,75	0
56	MG	1A	3229	1/1	0.95	0.17	75,75,75,75	0
56	MG	1A	3223	1/1	0.95	0.20	64,64,64,64	0
56	MG	2A	3304	1/1	0.95	0.31	63,63,63,63	0
56	MG	2A	3190	1/1	0.95	0.18	82,82,82,82	0
56	MG	1a	1662	1/1	0.95	0.10	94,94,94,94	0
56	MG	2A	3200	1/1	0.95	0.19	74,74,74,74	0
56	MG	2A	3260	1/1	0.95	0.23	70,70,70,70	0
57	ZN	29	501	1/1	0.95	0.13	114,114,114,114	0
56	MG	1A	3490	1/1	0.95	0.11	79,79,79,79	0
56	MG	1A	3110	1/1	0.95	0.17	70,70,70,70	0
56	MG	2A	3096	1/1	0.95	0.10	92,92,92,92	0
56	MG	2A	3341	1/1	0.95	0.21	76,76,76,76	0
56	MG	2A	3095	1/1	0.95	0.26	81,81,81,81	0
56	MG	2A	3235	1/1	0.95	0.23	75,75,75,75	0
56	MG	1A	3190	1/1	0.95	0.66	79,79,79,79	0
56	MG	1A	3361	1/1	0.95	0.48	94,94,94,94	0
56	MG	1a	1616	1/1	0.95	0.77	69,69,69,69	0
56	MG	2A	3035	1/1	0.95	0.35	76,76,76,76	0
56	MG	2A	3193	1/1	0.95	0.20	87,87,87,87	0
56	MG	2A	3238	1/1	0.95	0.18	67,67,67,67	0
56	MG	2A	3136	1/1	0.95	0.38	78,78,78,78	0
56	MG	2A	3036	1/1	0.95	0.24	77,77,77,77	0
56	MG	1A	3477	1/1	0.95	0.32	61,61,61,61	0
56	MG	1A	3138	1/1	0.95	0.39	108,108,108,108	0
56	MG	1A	3303	1/1	0.95	0.36	83,83,83,83	0
56	MG	1A	3488	1/1	0.95	0.22	69,69,69,69	0
56	MG	1A	3453	1/1	0.95	0.51	80,80,80,80	0
56	MG	1A	3188	1/1	0.95	0.42	62,62,62,62	0
56	MG	1A	3013	1/1	0.95	0.26	83,83,83,83	0
56	MG	1A	3301	1/1	0.95	0.46	82,82,82,82	0
56	MG	2a	3043	1/1	0.95	0.21	62,62,62,62	0
56	MG	1A	3284	1/1	0.95	0.24	76,76,76,76	0
56	MG	2A	3093	1/1	0.95	0.10	82,82,82,82	0
56	MG	1A	3407	1/1	0.95	0.20	94,94,94,94	0
56	MG	1A	3447	1/1	0.95	0.48	78,78,78,78	0
56	MG	1A	3384	1/1	0.95	0.29	71,71,71,71	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	1a	1646	1/1	0.95	0.47	71,71,71,71	0
56	MG	2A	3317	1/1	0.95	0.27	65,65,65,65	0
56	MG	1A	3446	1/1	0.95	0.28	77,77,77,77	0
56	MG	1A	3281	1/1	0.95	0.22	63,63,63,63	0
56	MG	1A	3315	1/1	0.95	0.26	80,80,80,80	0
56	MG	2A	3246	1/1	0.95	0.13	79,79,79,79	0
56	MG	2A	3204	1/1	0.95	0.16	68,68,68,68	0
56	MG	2A	3314	1/1	0.95	0.44	78,78,78,78	0
56	MG	1a	1613	1/1	0.95	0.09	87,87,87,87	0
56	MG	2A	3298	1/1	0.95	0.21	69,69,69,69	0
56	MG	2A	3294	1/1	0.95	0.32	87,87,87,87	0
56	MG	1A	3423	1/1	0.95	0.27	62,62,62,62	0
56	MG	2A	3123	1/1	0.95	0.24	78,78,78,78	0
56	MG	1A	3133	1/1	0.95	0.26	72,72,72,72	0
56	MG	2A	3249	1/1	0.95	0.23	74,74,74,74	0
56	MG	1A	3137	1/1	0.95	0.41	61,61,61,61	0
56	MG	1a	1606	1/1	0.95	0.14	69,69,69,69	0
56	MG	2A	3075	1/1	0.95	0.21	95,95,95,95	0
56	MG	2a	3063	1/1	0.95	0.47	61,61,61,61	0
56	MG	2A	3034	1/1	0.95	0.28	94,94,94,94	0
56	MG	2A	3286	1/1	0.95	0.19	62,62,62,62	0
56	MG	2A	3179	1/1	0.95	0.22	93,93,93,93	0
56	MG	2A	3269	1/1	0.95	0.23	62,62,62,62	0
56	MG	2A	3281	1/1	0.95	0.33	73,73,73,73	0
56	MG	1A	3426	1/1	0.95	0.15	89,89,89,89	0
56	MG	1A	3474	1/1	0.95	0.35	70,70,70,70	0
56	MG	1A	3370	1/1	0.95	0.47	88,88,88,88	0
56	MG	1A	3330	1/1	0.95	0.13	69,69,69,69	0
56	MG	1A	3295	1/1	0.95	0.24	69,69,69,69	0
56	MG	1a	1619	1/1	0.95	0.21	92,92,92,92	0
56	MG	2a	3025	1/1	0.95	0.22	81,81,81,81	0
56	MG	2a	3017	1/1	0.95	0.18	87,87,87,87	0
56	MG	2a	3066	1/1	0.95	0.40	86,86,86,86	0
56	MG	1a	1622	1/1	0.95	0.26	66,66,66,66	0
56	MG	1A	3094	1/1	0.96	0.09	84,84,84,84	0
56	MG	2A	3173	1/1	0.96	0.22	78,78,78,78	0
56	MG	1A	3343	1/1	0.96	0.37	80,80,80,80	0
56	MG	1A	3334	1/1	0.96	0.14	62,62,62,62	0
56	MG	1A	3278	1/1	0.96	0.26	63,63,63,63	0
56	MG	1A	3273	1/1	0.96	0.23	80,80,80,80	0
56	MG	2A	3227	1/1	0.96	0.15	62,62,62,62	0
56	MG	1A	3304	1/1	0.96	0.42	61,61,61,61	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	2A	3073	1/1	0.96	0.38	73,73,73,73	0
56	MG	2A	3312	1/1	0.96	0.24	64,64,64,64	0
56	MG	2A	3333	1/1	0.96	0.29	74,74,74,74	0
56	MG	2A	3068	1/1	0.96	0.26	90,90,90,90	0
56	MG	2I	101	1/1	0.96	0.35	63,63,63,63	0
56	MG	1A	3485	1/1	0.96	0.12	72,72,72,72	0
56	MG	1A	3482	1/1	0.96	0.33	61,61,61,61	0
56	MG	2A	3378	1/1	0.96	0.16	83,83,83,83	0
56	MG	2f	201	1/1	0.96	0.19	77,77,77,77	0
56	MG	1A	3152	1/1	0.96	0.35	64,64,64,64	0
56	MG	2A	3245	1/1	0.96	0.45	64,64,64,64	0
56	MG	2a	3038	1/1	0.96	0.10	80,80,80,80	0
56	MG	2a	3060	1/1	0.96	0.05	120,120,120,120	0
56	MG	1a	1654	1/1	0.96	0.25	71,71,71,71	0
56	MG	2A	3365	1/1	0.96	0.22	67,67,67,67	0
56	MG	1A	3435	1/1	0.96	0.23	90,90,90,90	0
56	MG	2A	3225	1/1	0.96	0.16	62,62,62,62	0
56	MG	1A	3296	1/1	0.96	0.23	73,73,73,73	0
56	MG	1A	3466	1/1	0.96	0.18	61,61,61,61	0
56	MG	1A	3467	1/1	0.96	0.21	66,66,66,66	0
56	MG	2A	3046	1/1	0.96	0.16	65,65,65,65	0
56	MG	2A	3313	1/1	0.96	0.17	76,76,76,76	0
56	MG	1A	3314	1/1	0.96	0.17	71,71,71,71	0
56	MG	1A	3231	1/1	0.96	0.27	65,65,65,65	0
56	MG	1A	3332	1/1	0.96	0.31	74,74,74,74	0
56	MG	2A	3282	1/1	0.96	0.30	74,74,74,74	0
56	MG	2a	3059	1/1	0.96	0.14	80,80,80,80	0
56	MG	2A	3206	1/1	0.96	0.12	78,78,78,78	0
56	MG	1A	3300	1/1	0.96	0.28	63,63,63,63	0
56	MG	2a	3050	1/1	0.96	0.19	88,88,88,88	0
56	MG	2A	3174	1/1	0.96	0.18	80,80,80,80	0
56	MG	2A	3221	1/1	0.96	0.29	80,80,80,80	0
56	MG	1A	3155	1/1	0.96	0.36	73,73,73,73	0
56	MG	2A	3149	1/1	0.96	0.10	82,82,82,82	0
56	MG	2A	3090	1/1	0.96	0.05	110,110,110,110	0
56	MG	2A	3198	1/1	0.96	0.43	96,96,96,96	0
56	MG	2a	3062	1/1	0.96	0.54	68,68,68,68	0
56	MG	1A	3032	1/1	0.96	0.50	77,77,77,77	0
56	MG	1A	3076	1/1	0.96	0.20	65,65,65,65	0
56	MG	1A	3207	1/1	0.96	0.38	62,62,62,62	0
56	MG	2A	3236	1/1	0.96	0.14	66,66,66,66	0
56	MG	1A	3242	1/1	0.96	0.34	61,61,61,61	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	1A	3179	1/1	0.96	0.21	64,64,64,64	0
56	MG	2A	3242	1/1	0.96	0.32	61,61,61,61	0
56	MG	2A	3009	1/1	0.96	0.24	110,110,110,110	0
56	MG	1A	3244	1/1	0.96	0.32	77,77,77,77	0
56	MG	2A	3303	1/1	0.96	0.15	76,76,76,76	0
56	MG	2A	3140	1/1	0.96	0.46	73,73,73,73	0
56	MG	1A	3267	1/1	0.96	0.22	70,70,70,70	0
56	MG	2A	3358	1/1	0.96	0.19	81,81,81,81	0
56	MG	2a	3081	1/1	0.96	0.12	64,64,64,64	0
56	MG	2A	3195	1/1	0.96	0.24	66,66,66,66	0
56	MG	2a	3048	1/1	0.96	0.15	80,80,80,80	0
56	MG	1A	3200	1/1	0.96	0.11	69,69,69,69	0
56	MG	2A	3076	1/1	0.96	0.31	69,69,69,69	0
56	MG	1a	1691	1/1	0.96	0.09	94,94,94,94	0
56	MG	2A	3223	1/1	0.96	0.16	70,70,70,70	0
56	MG	2B	208	1/1	0.96	0.66	62,62,62,62	0
56	MG	1A	3283	1/1	0.96	0.30	61,61,61,61	0
56	MG	2A	3360	1/1	0.96	0.27	61,61,61,61	0
56	MG	1A	3021	1/1	0.97	0.15	73,73,73,73	0
56	MG	1A	3318	1/1	0.97	0.26	75,75,75,75	0
56	MG	2A	3296	1/1	0.97	0.11	66,66,66,66	0
56	MG	1A	3311	1/1	0.97	0.29	62,62,62,62	0
56	MG	2A	3274	1/1	0.97	0.22	61,61,61,61	0
56	MG	2A	3356	1/1	0.97	0.22	68,68,68,68	0
56	MG	1A	3391	1/1	0.97	0.18	66,66,66,66	0
56	MG	2a	3100	1/1	0.97	0.12	95,95,95,95	0
56	MG	1A	3404	1/1	0.97	0.30	81,81,81,81	0
56	MG	1A	3492	1/1	0.97	0.07	95,95,95,95	0
56	MG	2a	3001	1/1	0.97	0.11	80,80,80,80	0
56	MG	1a	1659	1/1	0.97	0.28	67,67,67,67	0
56	MG	1A	3182	1/1	0.97	0.18	69,69,69,69	0
56	MG	2A	3063	1/1	0.97	0.14	79,79,79,79	0
56	MG	2a	3057	1/1	0.97	0.24	101,101,101,101	0
56	MG	1a	1638	1/1	0.97	0.16	75,75,75,75	0
56	MG	2A	3004	1/1	0.97	0.07	88,88,88,88	0
56	MG	2A	3074	1/1	0.97	0.16	71,71,71,71	0
56	MG	1A	3329	1/1	0.97	0.23	74,74,74,74	0
56	MG	2A	3172	1/1	0.97	0.07	87,87,87,87	0
56	MG	1A	3030	1/1	0.97	0.16	76,76,76,76	0
56	MG	2A	3264	1/1	0.97	0.23	70,70,70,70	0
56	MG	2A	3087	1/1	0.97	0.20	68,68,68,68	0
56	MG	1A	3153	1/1	0.97	0.20	72,72,72,72	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	2A	3226	1/1	0.97	0.25	82,82,82,82	0
56	MG	1A	3381	1/1	0.97	0.30	63,63,63,63	0
56	MG	1A	3458	1/1	0.97	0.25	79,79,79,79	0
56	MG	2A	3284	1/1	0.97	0.24	71,71,71,71	0
56	MG	2A	3018	1/1	0.97	0.09	73,73,73,73	0
56	MG	2E	304	1/1	0.97	0.11	63,63,63,63	0
56	MG	2A	3116	1/1	0.97	0.14	72,72,72,72	0
56	MG	1A	3130	1/1	0.97	0.22	84,84,84,84	0
56	MG	2A	3135	1/1	0.97	0.08	111,111,111,111	0
56	MG	2a	3012	1/1	0.97	0.15	104,104,104,104	0
56	MG	1A	3388	1/1	0.97	0.23	71,71,71,71	0
56	MG	1A	3393	1/1	0.97	0.29	61,61,61,61	0
56	MG	1A	3309	1/1	0.97	0.21	62,62,62,62	0
56	MG	2a	3005	1/1	0.97	0.11	87,87,87,87	0
56	MG	2A	3222	1/1	0.97	0.32	75,75,75,75	0
56	MG	1a	1692	1/1	0.97	0.10	114,114,114,114	0
56	MG	1a	1660	1/1	0.97	0.33	61,61,61,61	0
56	MG	1A	3412	1/1	0.97	0.28	65,65,65,65	0
56	MG	1A	3487	1/1	0.97	0.18	74,74,74,74	0
57	ZN	16	102	1/1	0.97	0.16	102,102,102,102	0
56	MG	2A	3201	1/1	0.97	0.12	75,75,75,75	0
56	MG	2a	3018	1/1	0.97	0.15	86,86,86,86	0
57	ZN	1n	501	1/1	0.97	0.09	148,148,148,148	0
56	MG	2A	3270	1/1	0.97	0.09	80,80,80,80	0
56	MG	2A	3367	1/1	0.97	0.20	62,62,62,62	0
56	MG	1A	3385	1/1	0.97	0.39	63,63,63,63	0
56	MG	1A	3380	1/1	0.97	0.26	73,73,73,73	0
56	MG	2A	3267	1/1	0.97	0.23	81,81,81,81	0
56	MG	2A	3362	1/1	0.97	0.26	80,80,80,80	0
58	SF4	1d	302	8/8	0.97	0.14	111,128,150,164	0
56	MG	1A	3049	1/1	0.97	0.21	104,104,104,104	0
56	MG	1A	3493	1/1	0.97	0.09	97,97,97,97	0
57	ZN	15	102	1/1	0.98	0.21	106,106,106,106	0
57	ZN	2n	501	1/1	0.98	0.16	118,118,118,118	0
56	MG	2A	3077	1/1	0.98	0.16	62,62,62,62	0
56	MG	1A	3394	1/1	0.98	0.21	61,61,61,61	0
56	MG	2A	3329	1/1	0.98	0.23	82,82,82,82	0
56	MG	1A	3459	1/1	0.98	0.21	76,76,76,76	0
56	MG	1A	3092	1/1	0.98	0.21	71,71,71,71	0
56	MG	2a	3020	1/1	0.98	0.31	105,105,105,105	0
56	MG	1A	3427	1/1	0.98	0.62	61,61,61,61	0
56	MG	1A	3333	1/1	0.98	0.34	68,68,68,68	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	1A	3337	1/1	0.98	0.28	79,79,79,79	0
56	MG	1A	3215	1/1	0.98	0.19	67,67,67,67	0
56	MG	2A	3278	1/1	0.98	0.17	61,61,61,61	0
56	MG	1a	1679	1/1	0.98	0.26	107,107,107,107	0
56	MG	2A	3215	1/1	0.98	0.16	61,61,61,61	0
56	MG	2A	3033	1/1	0.98	0.18	82,82,82,82	0
56	MG	2A	3243	1/1	0.98	0.21	64,64,64,64	0
56	MG	1A	3452	1/1	0.98	0.22	76,76,76,76	0
56	MG	2A	3070	1/1	0.98	0.16	81,81,81,81	0
56	MG	1A	3280	1/1	0.98	0.35	64,64,64,64	0
56	MG	2A	3283	1/1	0.98	0.26	61,61,61,61	0
56	MG	1A	3413	1/1	0.98	0.17	68,68,68,68	0
56	MG	2A	3216	1/1	0.98	0.18	62,62,62,62	0
56	MG	2A	3224	1/1	0.98	0.19	61,61,61,61	0
56	MG	1a	1625	1/1	0.98	0.13	102,102,102,102	0
56	MG	2A	3168	1/1	0.98	0.16	68,68,68,68	0
56	MG	2A	3273	1/1	0.98	0.32	62,62,62,62	0
56	MG	1A	3196	1/1	0.98	0.18	65,65,65,65	0
56	MG	1A	3272	1/1	0.98	0.26	70,70,70,70	0
56	MG	1A	3125	1/1	0.98	0.20	62,62,62,62	0
56	MG	1A	3305	1/1	0.98	0.35	61,61,61,61	0
56	MG	2A	3381	1/1	0.98	0.09	76,76,76,76	0
56	MG	2A	3289	1/1	0.98	0.14	77,77,77,77	0
56	MG	2A	3247	1/1	0.98	0.27	81,81,81,81	0
56	MG	2A	3346	1/1	0.98	0.27	86,86,86,86	0
56	MG	2A	3064	1/1	0.98	0.07	101,101,101,101	0
56	MG	2A	3233	1/1	0.98	0.34	70,70,70,70	0
57	ZN	26	501	1/1	0.98	0.15	107,107,107,107	0
56	MG	1A	3029	1/1	0.98	0.10	86,86,86,86	0
56	MG	2a	3016	1/1	0.98	0.18	84,84,84,84	0
56	MG	2A	3072	1/1	0.98	0.14	96,96,96,96	0
56	MG	2A	3130	1/1	0.98	0.21	63,63,63,63	0
56	MG	2A	3272	1/1	0.98	0.16	62,62,62,62	0
56	MG	2a	3053	1/1	0.98	0.12	74,74,74,74	0
56	MG	1A	3417	1/1	0.98	0.18	64,64,64,64	0
56	MG	1A	3405	1/1	0.98	0.32	93,93,93,93	0
56	MG	1a	1624	1/1	0.98	0.28	109,109,109,109	0
56	MG	2A	3318	1/1	0.98	0.23	62,62,62,62	0
56	MG	2a	3055	1/1	0.98	0.24	79,79,79,79	0
56	MG	1A	3287	1/1	0.98	0.33	63,63,63,63	0
56	MG	1A	3483	1/1	0.98	0.19	68,68,68,68	0
56	MG	2A	3231	1/1	0.98	0.19	74,74,74,74	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	1A	3328	1/1	0.98	0.32	61,61,61,61	0
56	MG	2A	3067	1/1	0.98	0.24	73,73,73,73	0
56	MG	2a	3054	1/1	0.98	0.22	69,69,69,69	0
56	MG	1A	3468	1/1	0.98	0.16	63,63,63,63	0
56	MG	1a	1627	1/1	0.98	0.09	80,80,80,80	0
56	MG	1A	3484	1/1	0.98	0.31	67,67,67,67	0
56	MG	1a	1658	1/1	0.98	0.15	75,75,75,75	0
56	MG	2A	3319	1/1	0.98	0.21	64,64,64,64	0
56	MG	1A	3119	1/1	0.98	0.22	64,64,64,64	0
56	MG	2A	3217	1/1	0.98	0.18	78,78,78,78	0
56	MG	1A	3064	1/1	0.98	0.13	79,79,79,79	0
56	MG	1a	1683	1/1	0.98	0.23	118,118,118,118	0
57	ZN	19	501	1/1	0.98	0.20	104,104,104,104	0
56	MG	2a	3006	1/1	0.98	0.14	76,76,76,76	0
56	MG	2A	3017	1/1	0.98	0.44	69,69,69,69	0
56	MG	1A	3307	1/1	0.99	0.34	71,71,71,71	0
58	SF4	2d	302	8/8	0.99	0.16	99,114,123,127	0
56	MG	2A	3020	1/1	0.99	0.27	88,88,88,88	0
56	MG	1A	3195	1/1	0.99	0.20	71,71,71,71	0
56	MG	1a	1673	1/1	0.99	0.06	99,99,99,99	0
56	MG	2A	3361	1/1	0.99	0.31	62,62,62,62	0
56	MG	2A	3240	1/1	0.99	0.27	61,61,61,61	0
56	MG	2A	3279	1/1	0.99	0.14	80,80,80,80	0
56	MG	1A	3448	1/1	0.99	0.37	74,74,74,74	0
56	MG	2A	3040	1/1	0.99	0.20	95,95,95,95	0
56	MG	2A	3005	1/1	0.99	0.15	85,85,85,85	0
56	MG	1A	3174	1/1	0.99	0.67	73,73,73,73	0
56	MG	2A	3383	1/1	0.99	0.18	76,76,76,76	0
56	MG	1A	3286	1/1	0.99	0.40	76,76,76,76	0
56	MG	1A	3382	1/1	0.99	0.11	91,91,91,91	0
56	MG	1a	1610	1/1	1.00	0.16	104,104,104,104	0

6.5 Other polymers

There are no such residues in this entry.