



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 20, 2026 – 02:43 AM UTC

PDB ID : 6N9E / pdb_00006n9e
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 types of validation reports are described at

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

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

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

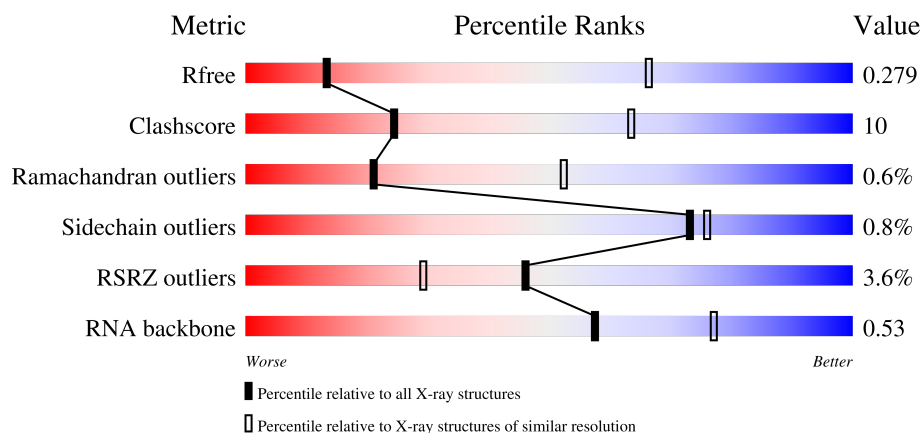
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.70 Å.

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



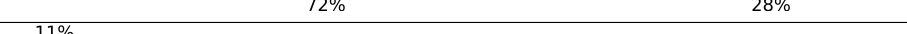
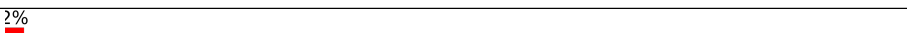
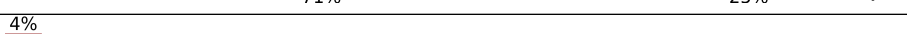
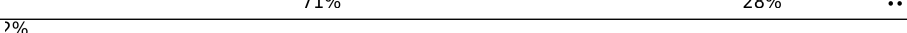
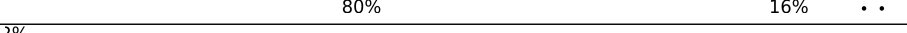
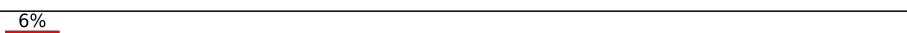
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1131 (3.80-3.60)
Clashscore	190562	1171 (3.80-3.60)
Ramachandran outliers	187476	1129 (3.80-3.60)
Sidechain outliers	187428	1126 (3.80-3.60)
RSRZ outliers	180081	1130 (3.80-3.60)
RNA backbone	3983	1007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

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

Mol	Chain	Length	Quality of chain
1	1A	2915	3% 54% 38% 7% .
1	2A	2915	3% 54% 36% 6% .
2	1B	121	58% 40% ..

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

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

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Mol	Chain	Length	Quality of chain
27	25	60	8% 75% 23% .
28	16	54	9% 76% 22% .
28	26	54	2% 78% 20% .
29	17	49	12% 82% 16% .
29	27	49	6% 71% 27% .
30	18	65	17% 74% 25% .
30	28	65	5% 75% 23% .
31	19	37	3% 81% 19% .
31	29	37	3% 76% 24% .
32	1a	1521	% 46% 44% 8% .
32	2a	1521	% 50% 42% 7% .
33	1b	256	59% 30% 10% .
33	2b	256	% 61% 27% 10% .
34	1c	239	62% 24% 14% .
34	2c	239	65% 21% 14% .
35	1d	209	9% 70% 29% .
35	2d	209	2% 73% 26% .
36	1e	162	69% 22% 9% .
36	2e	162	4% 60% 31% 9% .
37	1f	101	6% 76% 23% .
37	2f	101	71% 28% .
38	1g	156	3% 77% 21% ..
38	2g	156	3% 74% 25% ..
39	1h	138	72% 27% .
39	2h	138	3% 69% 29% ..

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

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Mol	Chain	Length	Quality of chain
52	2u	27	
53	1v	24	
53	2v	24	
54	1w	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	1A	3017	-	-	-	X
56	MG	1A	3078	-	-	-	X
56	MG	1A	3137	-	-	-	X
56	MG	1A	3224	-	-	-	X
56	MG	1A	3247	-	-	-	X
56	MG	1A	3304	-	-	-	X
56	MG	1A	3340	-	-	-	X
56	MG	1A	3414	-	-	-	X
56	MG	1A	3415	-	-	-	X
56	MG	1A	3428	-	-	-	X
56	MG	1a	1651	-	-	-	X
56	MG	2A	3141	-	-	-	X
56	MG	2A	3205	-	-	-	X
56	MG	2A	3259	-	-	-	X
56	MG	2A	3276	-	-	-	X
56	MG	2A	3373	-	-	-	X
56	MG	2A	3374	-	-	-	X
58	SF4	1d	302	-	-	X	-
58	SF4	2d	302	-	-	X	-

2 Entry composition

There are 59 unique types of molecules in this entry. The entry contains 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 (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
56	1A	498	Total	Mg	0	0
			498	498		
56	1B	12	Total	Mg	0	0
			12	12		
56	1D	1	Total	Mg	0	0
			1	1		
56	1E	6	Total	Mg	0	0
			6	6		
56	1F	1	Total	Mg	0	0
			1	1		
56	1Q	1	Total	Mg	0	0
			1	1		
56	1S	1	Total	Mg	0	0
			1	1		
56	1U	1	Total	Mg	0	0
			1	1		
56	1V	3	Total	Mg	0	0
			3	3		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
56	1W	1	Total 1	Mg 1	0	0
56	10	3	Total 3	Mg 3	0	0
56	13	1	Total 1	Mg 1	0	0
56	15	1	Total 1	Mg 1	0	0
56	16	1	Total 1	Mg 1	0	0
56	17	2	Total 2	Mg 2	0	0
56	18	1	Total 1	Mg 1	0	0
56	1a	93	Total 93	Mg 93	0	0
56	1d	1	Total 1	Mg 1	0	0
56	1l	1	Total 1	Mg 1	0	0
56	1r	1	Total 1	Mg 1	0	0
56	1x	2	Total 2	Mg 2	0	0
56	2A	385	Total 385	Mg 385	0	0
56	2B	9	Total 9	Mg 9	0	0
56	2D	1	Total 1	Mg 1	0	0
56	2E	6	Total 6	Mg 6	0	0
56	2O	1	Total 1	Mg 1	0	0
56	2Q	2	Total 2	Mg 2	0	0
56	2R	2	Total 2	Mg 2	0	0
56	2T	2	Total 2	Mg 2	0	0
56	2Y	1	Total 1	Mg 1	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
56	20	2	Total 2	Mg 2	0	0
56	21	1	Total 1	Mg 1	0	0
56	23	1	Total 1	Mg 1	0	0
56	25	1	Total 1	Mg 1	0	0
56	27	1	Total 1	Mg 1	0	0
56	28	2	Total 2	Mg 2	0	0
56	2a	103	Total 103	Mg 103	0	0
56	2d	1	Total 1	Mg 1	0	0
56	2f	1	Total 1	Mg 1	0	0
56	2l	1	Total 1	Mg 1	0	0
56	2r	1	Total 1	Mg 1	0	0

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

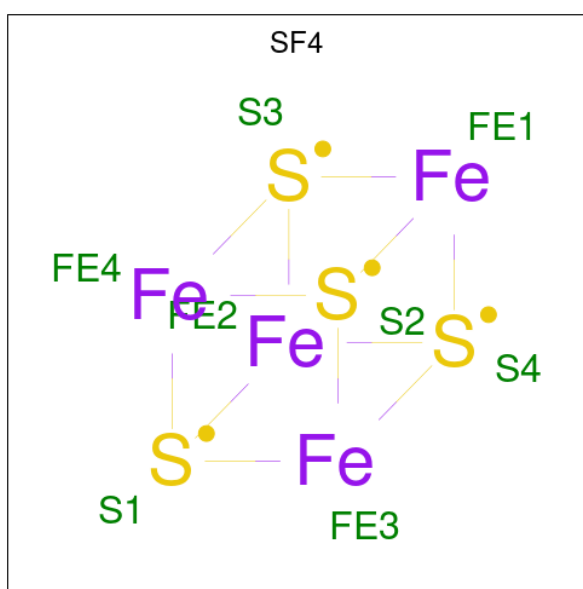
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
57	1Y	1	Total 1	Zn 1	0	0
57	14	1	Total 1	Zn 1	0	0
57	15	1	Total 1	Zn 1	0	0
57	16	1	Total 1	Zn 1	0	0
57	19	1	Total 1	Zn 1	0	0
57	1n	1	Total 1	Zn 1	0	0
57	2Y	1	Total 1	Zn 1	0	0
57	24	1	Total 1	Zn 1	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
57	25	1	Total	Zn	0	0
			1	1		
57	26	1	Total	Zn	0	0
			1	1		
57	29	1	Total	Zn	0	0
			1	1		
57	2n	1	Total	Zn	0	0
			1	1		

- Molecule 58 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe_4S_4).



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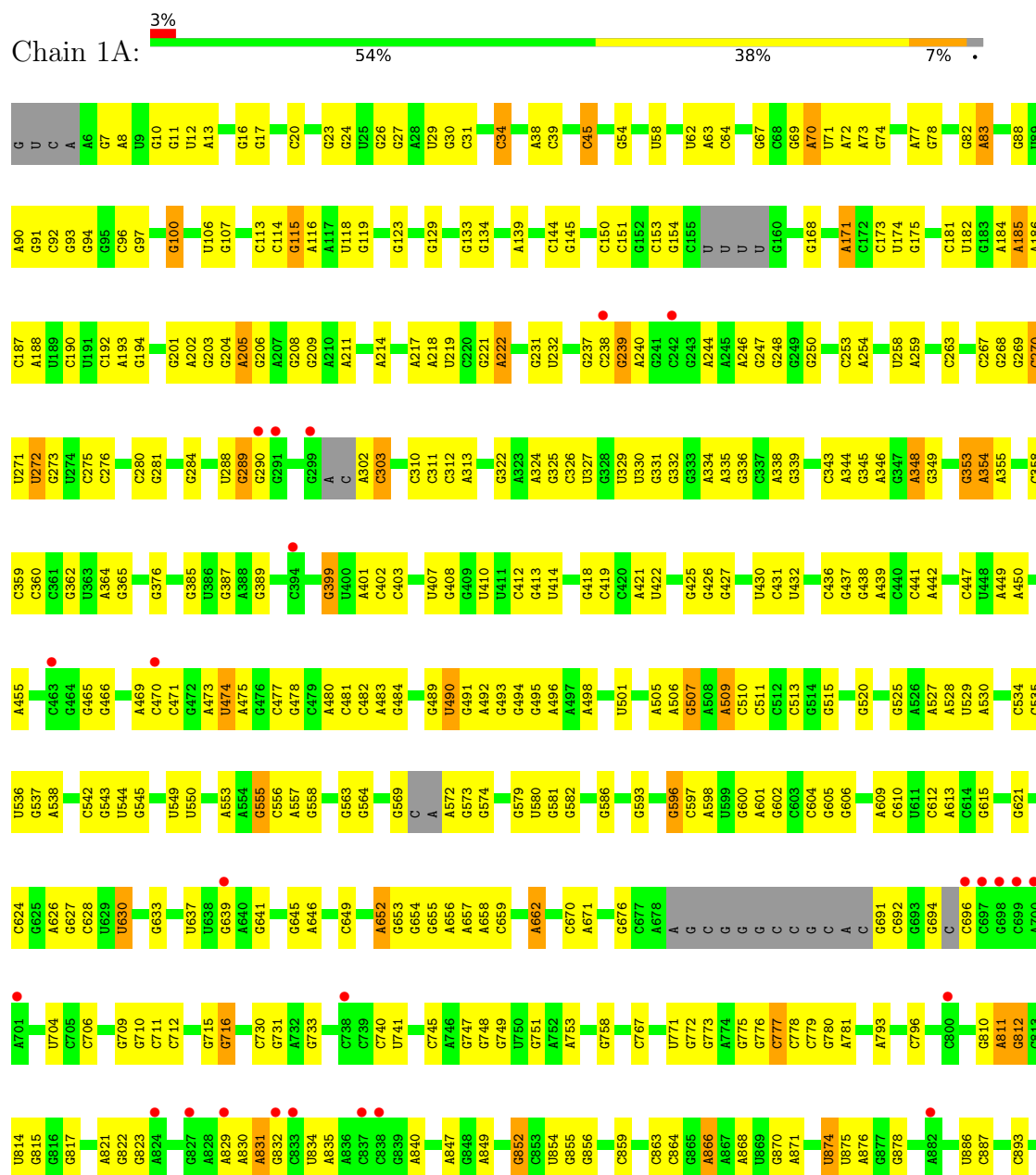
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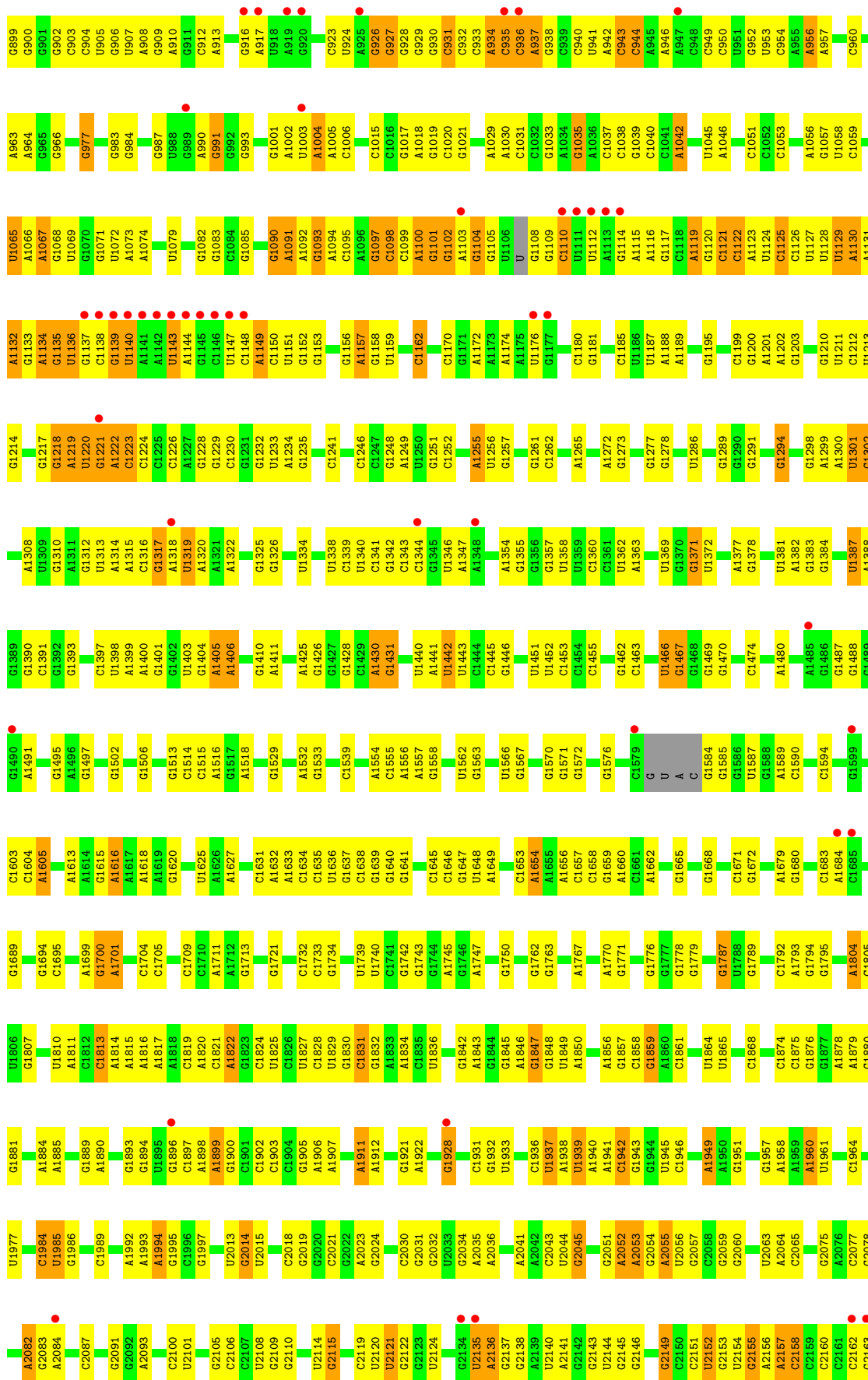
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
59	1x	2	Total 2	O 2	0	0
59	2A	32	Total 32	O 32	0	0
59	2B	1	Total 1	O 1	0	0
59	2a	19	Total 19	O 19	0	0

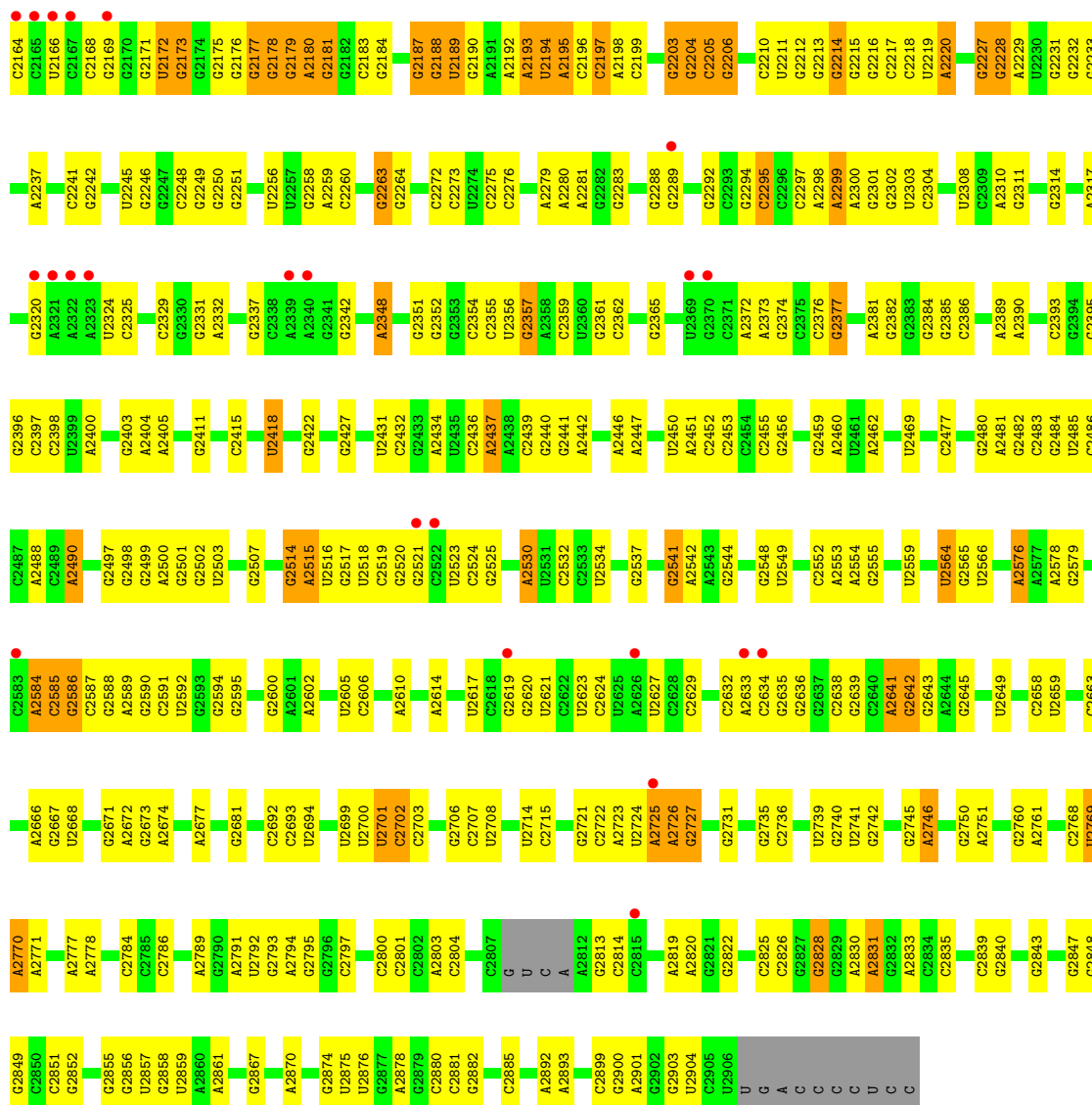
3 Residue-property plots

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

• Molecule 1: 23S Ribosomal RNA

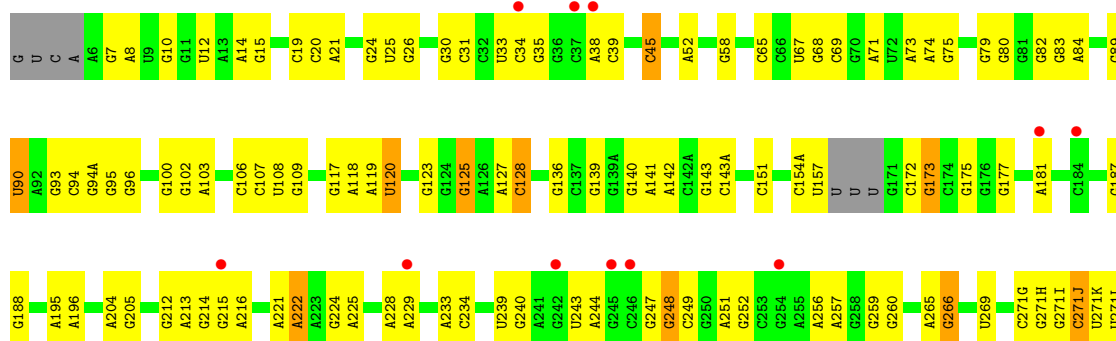






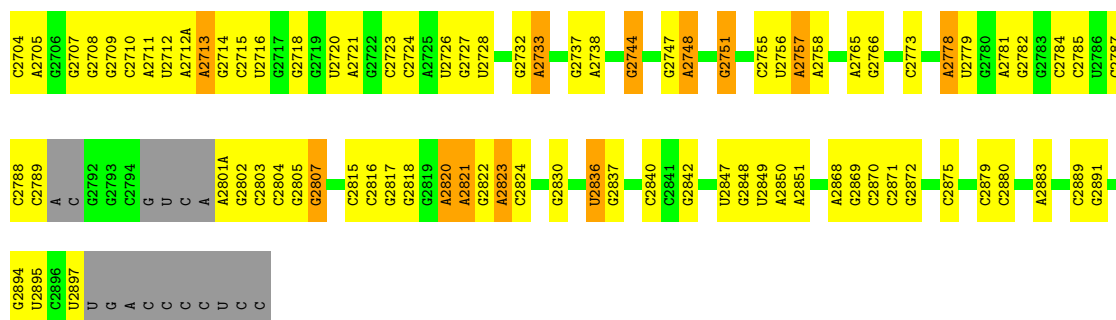
• Molecule 1: 23S Ribosomal RNA

Chain 2A: 3% 54% 36% 6%



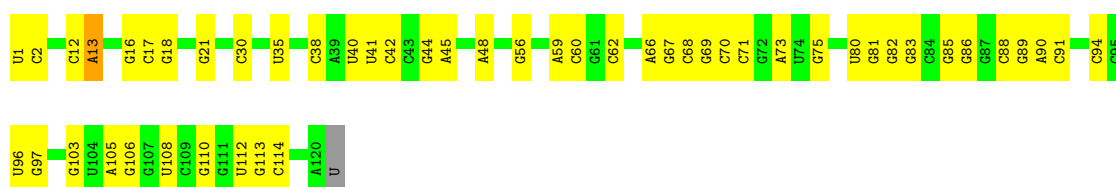
A1384	C1270	A	G1034	G969	G775	U606	G530	G430	G338	G271M
G1385	G1271	C	C1038	A872	G776	U607	C531	C435	A346	U271N
C1386	A1272	U	G1039	A670	A685	A608	A532	A347	A346	C271O
C1387	U1273	C	A953	G874	A782	G614B	G533	G438	A347	G271P
A1392	A1274	A	G953	G875	A783	G615	U534	C440	A347	G271Q
A1393	A1275	C	C955	G876	G785	G616	C540	C444	G352	G271R
G1187	U1188	U	U958	U877	A793	G621	G545	C445	U358	G271S
U1188	G1189	G	A959	A878	G796	G622	A	C446	A359	C271T
A1395	G1190	G	A960	G880	C796	G623	C	C446	U362	G272
U1396	G1191	U	C961	G881	G801	G624	A	C451	U372A	U272A
G1296	C1196	G	C964	G882	G801	C627	G549	A454	G362	G272B
C1297	G1197	A	A973	G883	G805	A627	G551	C455	A363A	G272C
U1300	U1112	C	C984	G884	G806	G629	U554	C456	G363B	G272D
A1301	U1113	C	A973	C905	G807	G629	U554	A457	G363C	G272E
A1302	G1114	A	G974	U807	G700	G630	U557	C463	G363D	U272I
U1205	G1115	G	C975	G808	G701	A631	G558	U464	C364	C272J
G1309	U1116	G	A983	A887	G702	A632	G561	C370	G370	A276
G1310	G1117	A	U989	G888	U810	A633	U562	A374	A374	C277
G1311	U1118	G	G987	A890	G710	C634	G563	C375	A374	A278
U1312	G1119	G	C989	G892	G711	A637	U568	G379	G379	C286
U1313	C1124	U	C994	G894	G713	C645	U569	U380	U380	C287
C1314	G1125	G	U995	G817	U714	A646	A571	G381	G381	A289
G1327	A1126	G	A896	A819	G716	A652B	A572	G386	G386	A294
G1334	A1127	C	C997	A820	A717	G652C	G573	U387	U387	C297
U1335	A1128	U	A899	U821	G717	G652E	A575	G388	G388	G298
A1336	A1129	U	A900	G823	C720	G	U576	G391	G391	G301
G1337	U1130	A	A901	A824	G721	G	A577	C392	C392	U302
G1338	U1131	G	C902	G825	G722	G	A578	G396	G396	G303
U1341	C1135	A	C903	U826	A722	G	C581	G397	G397	G304
G1442	G1136	G	G1003	U827	G723	C	C584	G399	G399	U305
G1443	G1139	C	C1004	U828	G729	C	G585	U403	U403	G308
G1444	G1140	A	C1006	A829	G730	C	G586	U404	U404	G309
A1445	U1141	G	C1007	G832	C732	C	C587	U405	U405	A310
G1445A	U1142	C	G1008	U839	G733	C	U588	U406	U406	A311
C1446	U1143	C	A1009	C940	G733	C	C589	C409	C409	A314
G1447	A1142A	U	G1010	A841	G742	C	C590	C410	C410	G315
G1448	G1144	U	U1012	G842	G743	C	C591	C411	C411	A322
U1357	C1147	C	U1014	G848	A746	C	C592	C412	C412	G323
G1358	A1148	U	G1015	A849	G760	C	G593	C413	C413	A324
A1359	G1149	U	U1019	G854	G753	C	U594	C414	C414	G325
A1360	C1150	A	A1020	G855	C754	C	U595	C415	C415	G326
G1364	G1151	A	A1021	C857	C755	C	G596	C419	C419	G329
U1248	C1152	G	G1022	U858	C756	C	U597	U421	U421	A330
G1250	G1153	A	U1023	G859	G760	C	U598	A422	A422	C336
C1251	G1154	G	G934	C857	A761	C	G599	C420	C420	C337
A1253	G1155	U	C935	U858	G762	C	G600	C429	C429	
U1254	G1156	U	U1024	U859	G763	C	G601	U421	U421	
U1255	C1166	G	G1025	G861	A764	C	G602	A422	A422	
G1256	U1165	A	U1026	G862	G765	C	G603	A423	A423	
U1265	G1166	U	A1027	G863	A766	C	G604			
G1266	U1166	U	G1028	A863		C	G605			
G1368	G1167	C	A1029	A866		C				
G1369	G1171	G	U1030			C				
C1370	G	U	U1033			C				
G1371	A	U				C				
U1372	A	U				C				
A1373	A	U				C				
G1465	A	U				C				
G1466	A	U				C				
C1467	A	U				C				
A1471	A	U				C				

A2590	C2591	G2592	U2593	C2594	G2595	U2596	G2597	A2602	G2603	U2604	U2605	U2611	G2612	U2613	A2614	U2615	G2616	C2617	G2618	C2619	G2627	G2628	A2629	G2630	G2631	G2634	G2635	U2636	G2637	G2638	C2646	C2651	A2654	G2656	G2657	A2659	C2660	C2661	G2665	G2666	U2667	U2668	U2669	C2690	C2691	C2695	U2696	G2697	C2703																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																														
U2491	G2495	C2496	U2500	G2501	G2502	U2504	G2505	G2506	C2507	G2508	A2518	U2519	U2520	U2521	A2530	G2531	G2532	A2533	A2534	C2540	A2541	U2547	G2548	G2549	G2550	G2551	U2552	G2553	U2554	C2559	A2564	G2565	A2566	G2567	A2572	C2573	G2574	G2575	G2576	U2577	C2578	C2579	G2582	U2583	U2584	U2585	G2586	U2687	U2688	U2689	C2690	C2691	C2695	U2696	G2697	C2703																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																							
G2399	C2402	C2403	U2406	G2407	G2410	A2411	U2419	A2420	G2421	U2422	U2423	U2424	A2425	A2426	G2427	G2428	G2429	A2430	U2431	A2432	A2435	A2436	A2439	G2440	C2441	G2442	G2443	G2444	G2447	A2448	A2451	G2454	G2455	C2465	C2466	C2467	G2468	A2469	G2472	U2473	C2474	A2475	A2476	C2477	A2478	G2485	G2486																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																



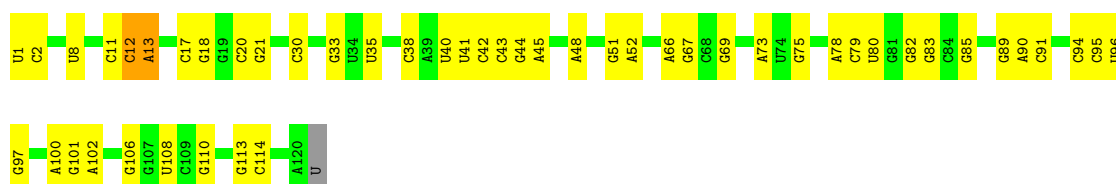
- Molecule 2: 5S Ribosomal RNA

Chain 1B: ..



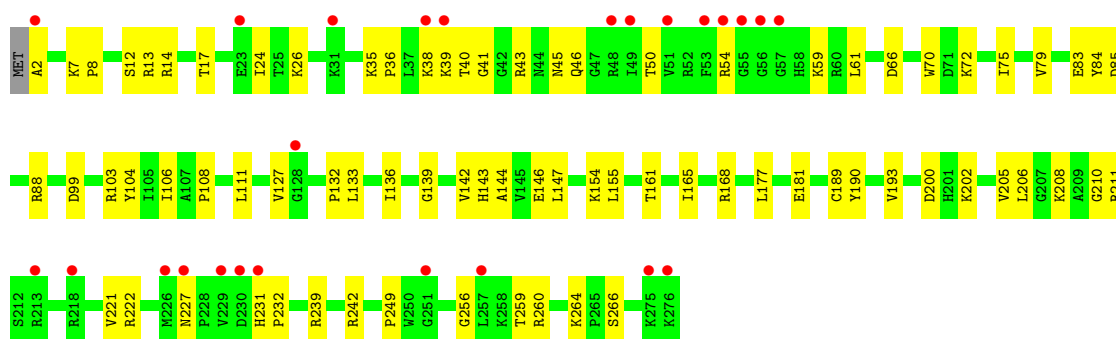
- Molecule 2: 5S Ribosomal RNA

Chain 2B: ..



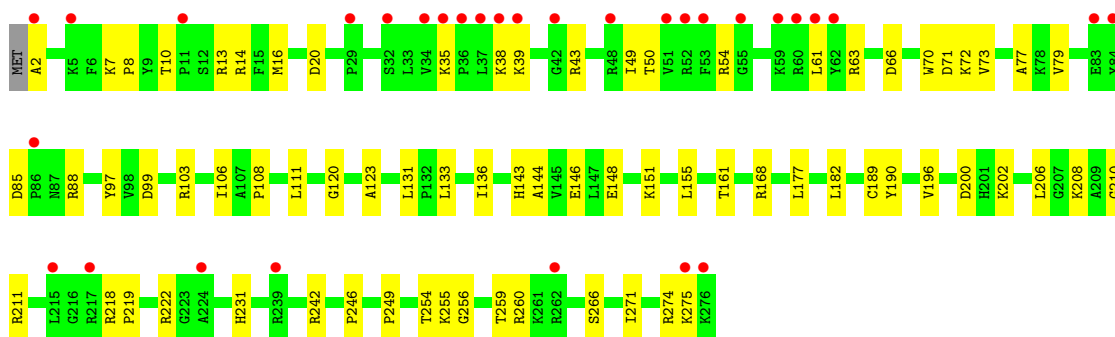
- Molecule 3: 50S Ribosomal Protein L2

Chain 1D:

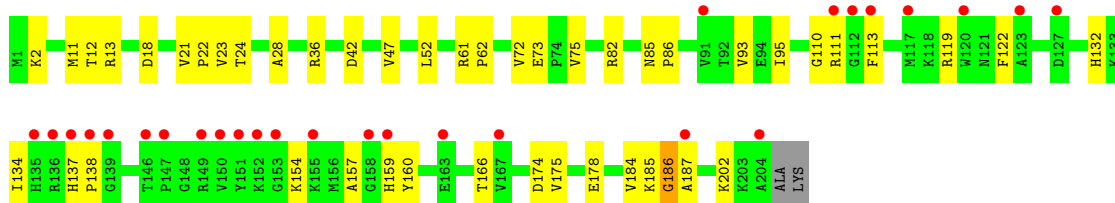
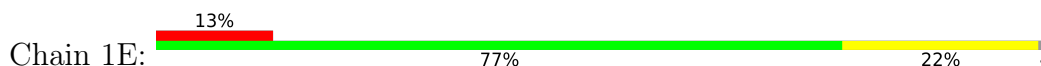


- Molecule 3: 50S Ribosomal Protein L2

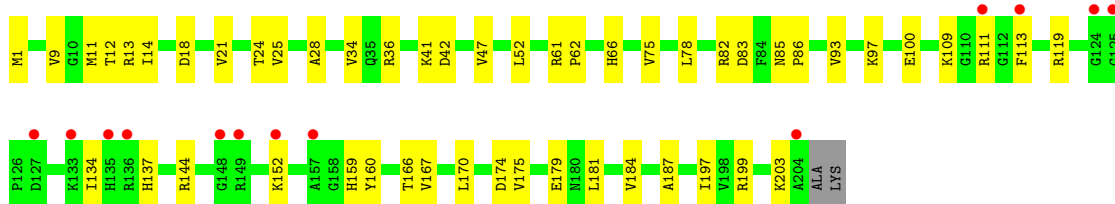
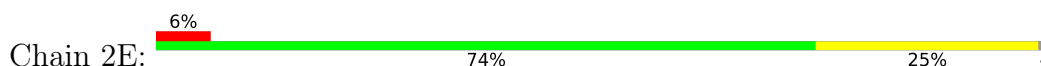
Chain 2D:



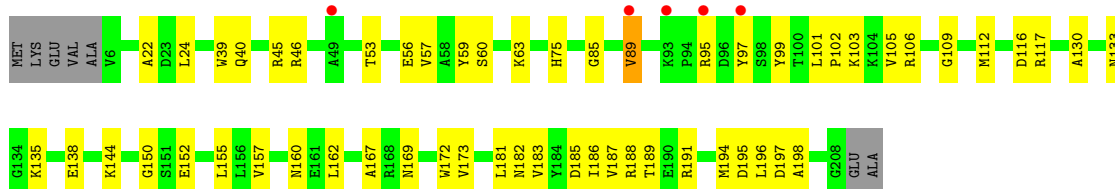
• Molecule 4: 50S Ribosomal Protein L3



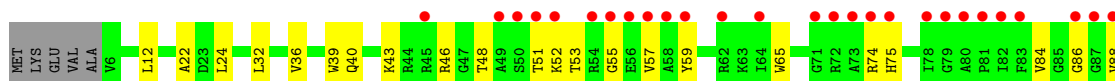
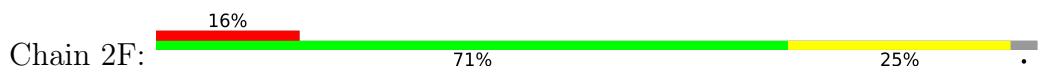
• Molecule 4: 50S Ribosomal Protein L3

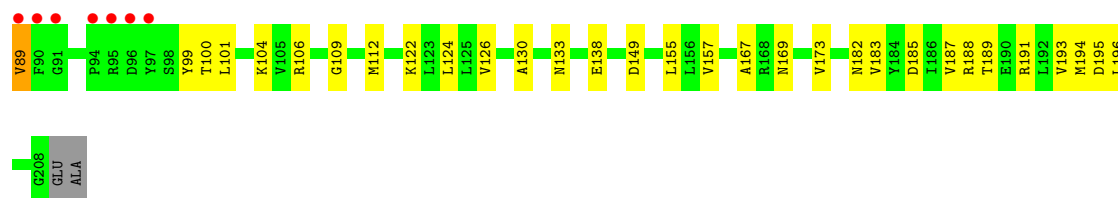


• Molecule 5: 50S Ribosomal Protein L4

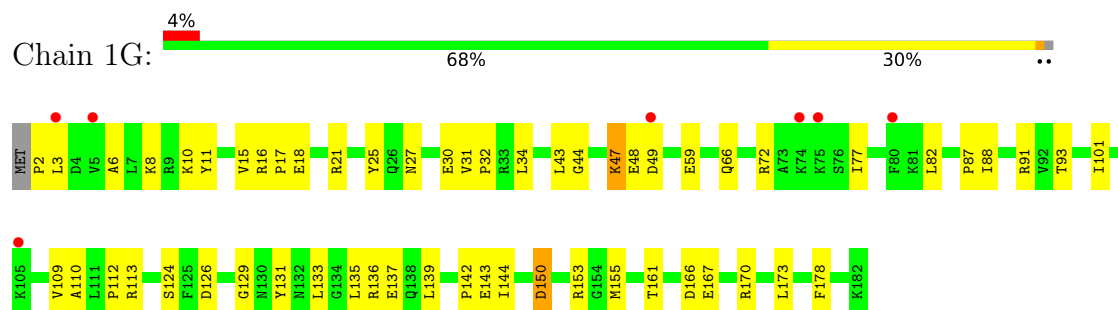


• Molecule 5: 50S Ribosomal Protein L4

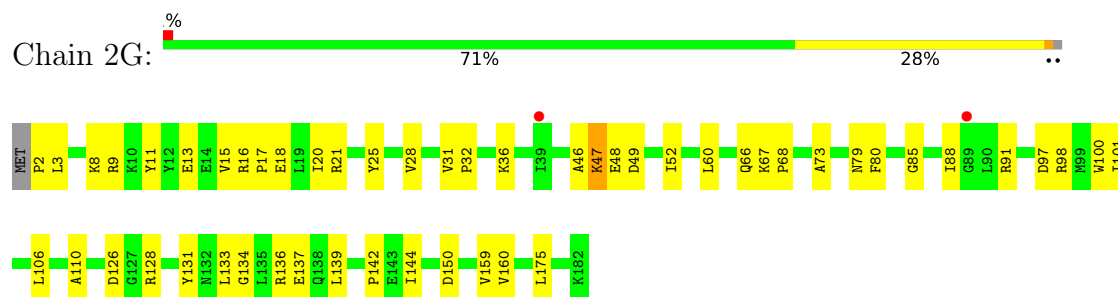




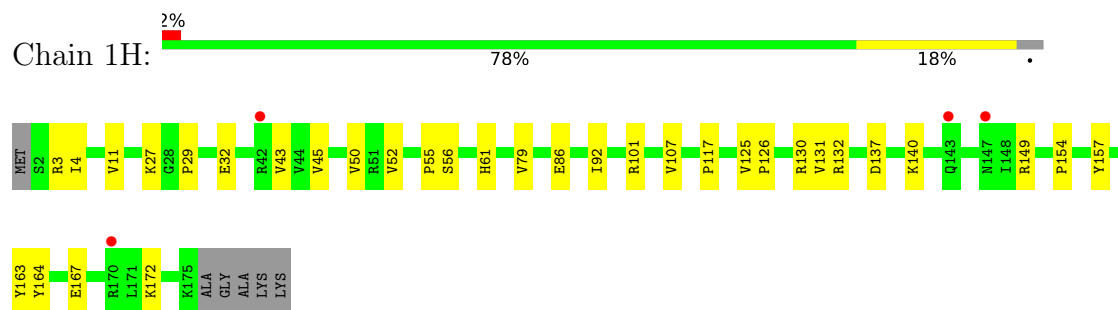
• Molecule 6: 50S Ribosomal Protein L5



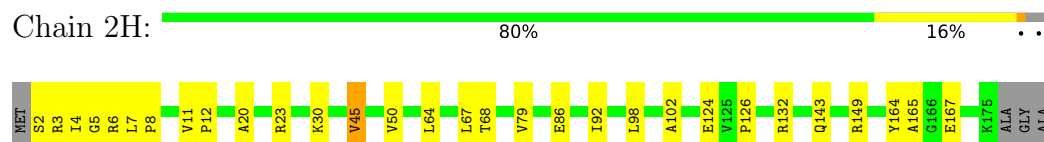
• Molecule 6: 50S Ribosomal Protein L5



• Molecule 7: 50S Ribosomal Protein L6

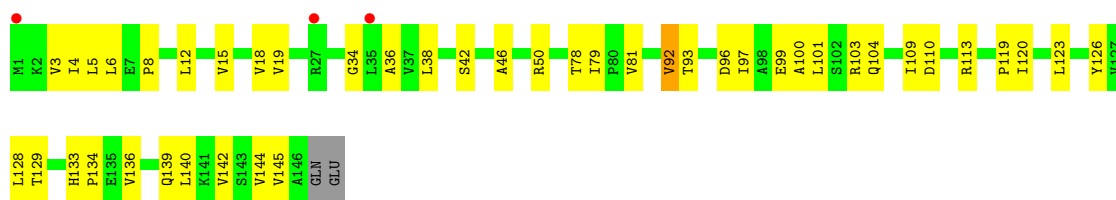


• Molecule 7: 50S Ribosomal Protein L6

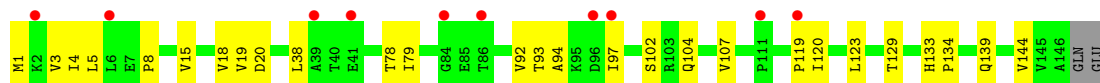
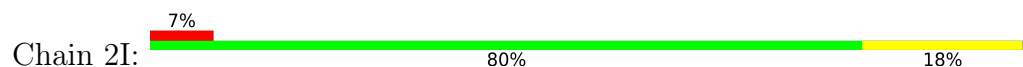


• Molecule 8: 50S Ribosomal Protein L9

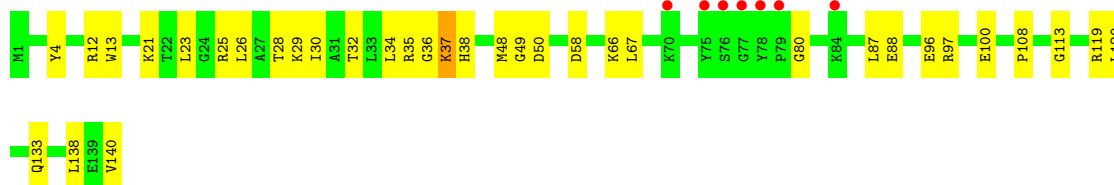
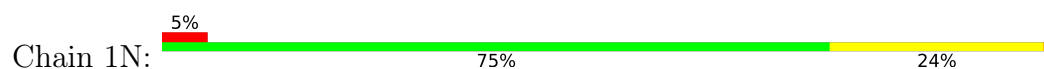




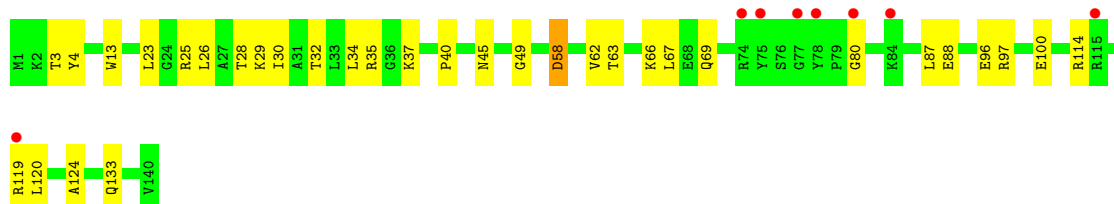
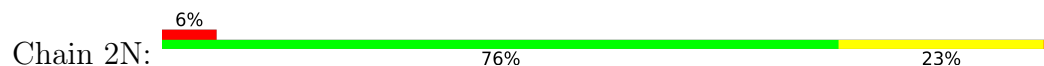
• Molecule 8: 50S Ribosomal Protein L9



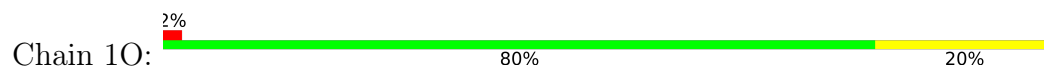
• Molecule 9: 50S Ribosomal Protein L13



• Molecule 9: 50S Ribosomal Protein L13



• Molecule 10: 50S Ribosomal Protein L14

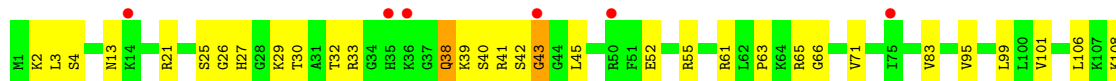


• Molecule 10: 50S Ribosomal Protein L14

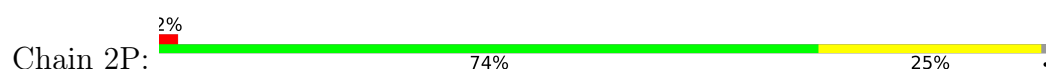




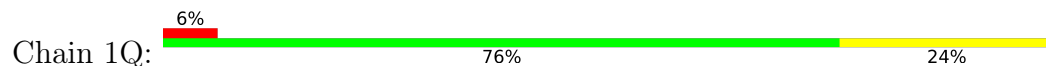
• Molecule 11: 50S Ribosomal Protein L15



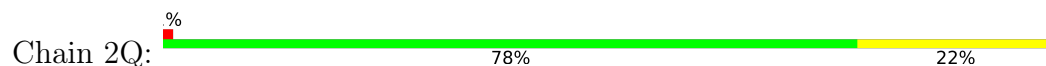
• Molecule 11: 50S Ribosomal Protein L15



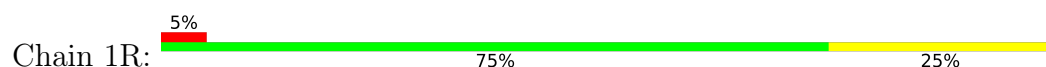
• Molecule 12: 50S Ribosomal Protein L16



• Molecule 12: 50S Ribosomal Protein L16

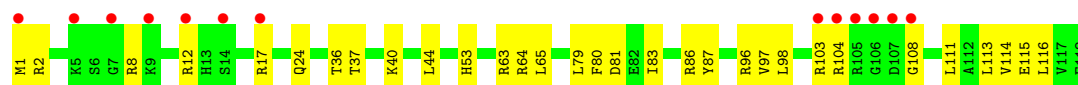
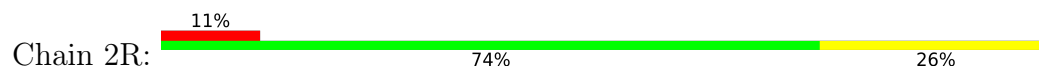


• Molecule 13: 50S Ribosomal Protein L17

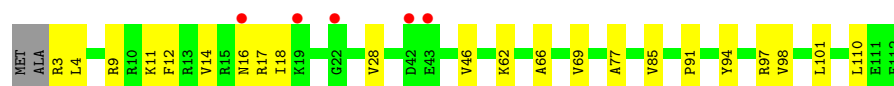
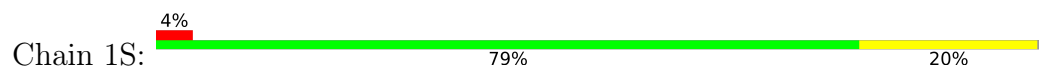


E118

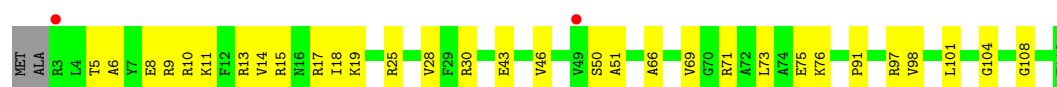
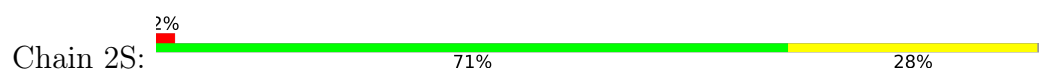
• Molecule 13: 50S Ribosomal Protein L17



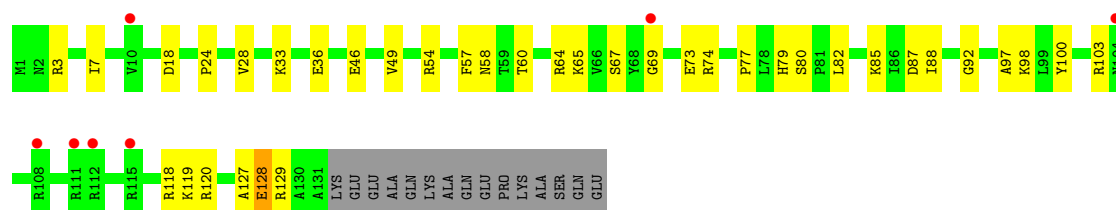
• Molecule 14: 50S Ribosomal Protein L18



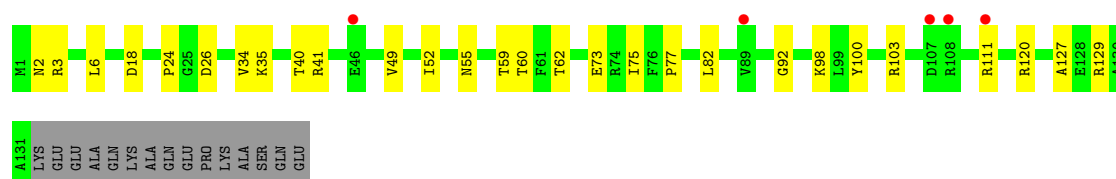
• Molecule 14: 50S Ribosomal Protein L18



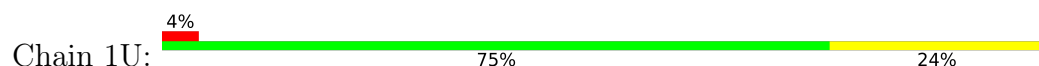
• Molecule 15: 50S Ribosomal Protein L19



• Molecule 15: 50S Ribosomal Protein L19

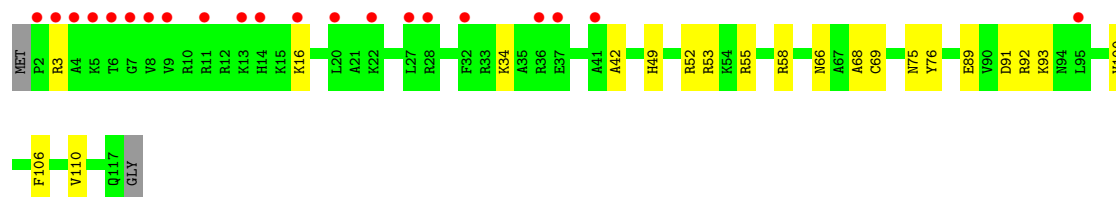
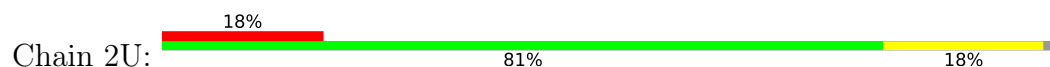


• Molecule 16: 50S Ribosomal Protein L20

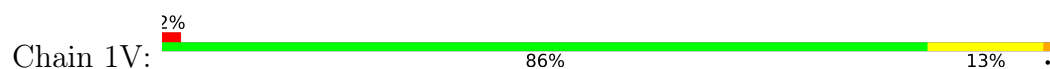




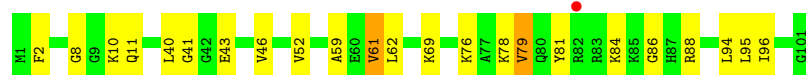
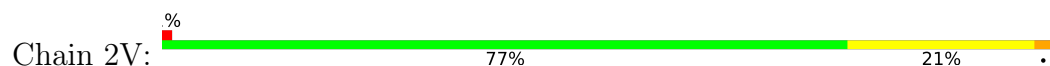
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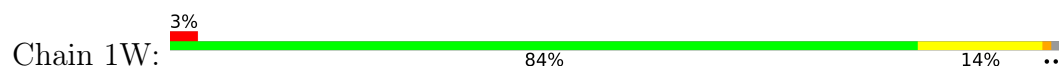
• Molecule 17: 50S Ribosomal Protein L21



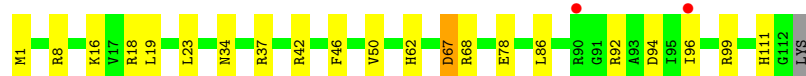
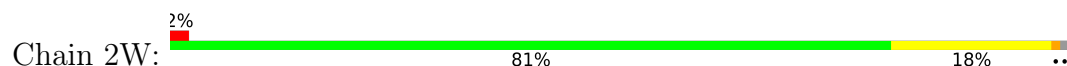
• Molecule 17: 50S Ribosomal Protein L21



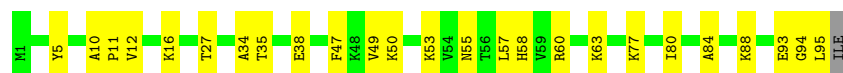
• Molecule 18: 50S Ribosomal Protein L22



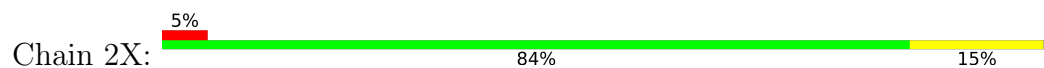
• Molecule 18: 50S Ribosomal Protein L22



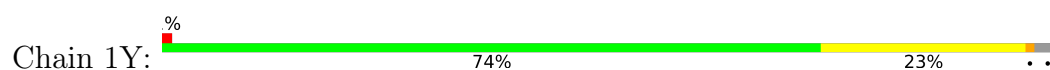
• Molecule 19: 50S Ribosomal Protein L23



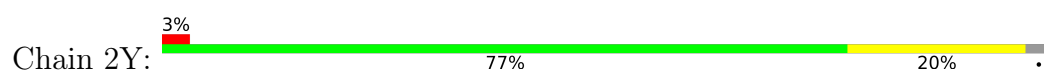
- Molecule 19: 50S Ribosomal Protein L23



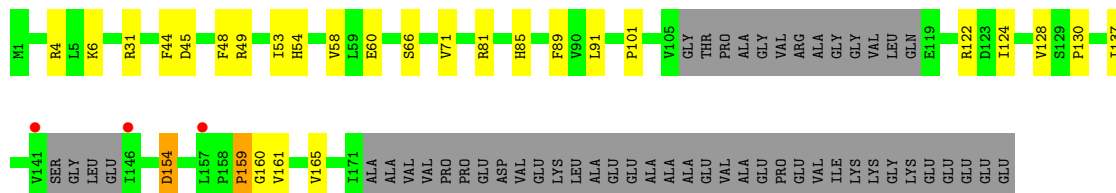
- Molecule 20: 50S ribosomal protein L24



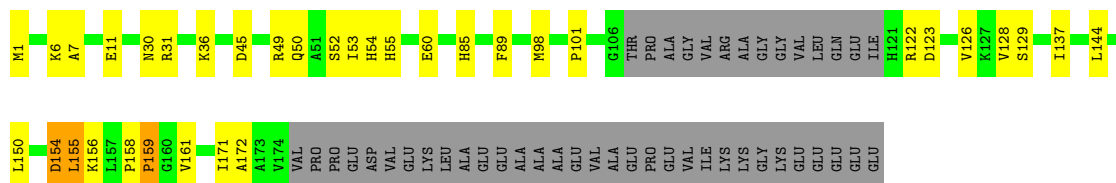
- Molecule 20: 50S ribosomal protein L24



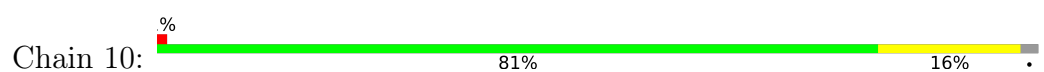
- Molecule 21: 50S ribosomal protein L25



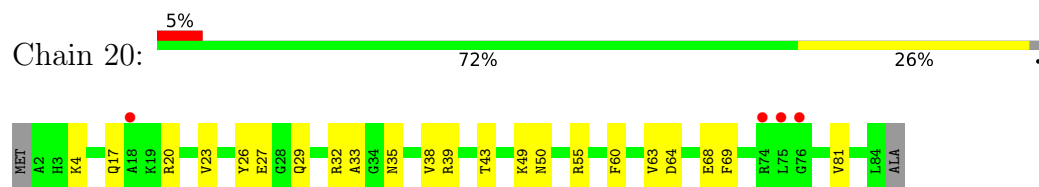
- Molecule 21: 50S ribosomal protein L25



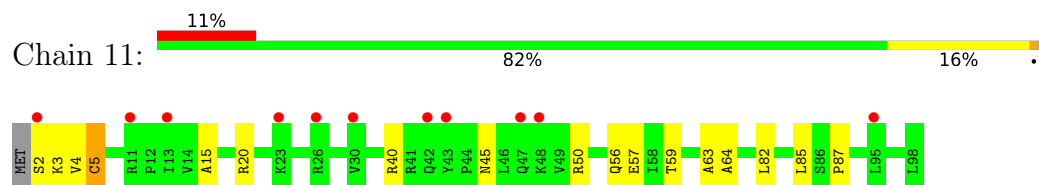
- Molecule 22: 50S ribosomal protein L27



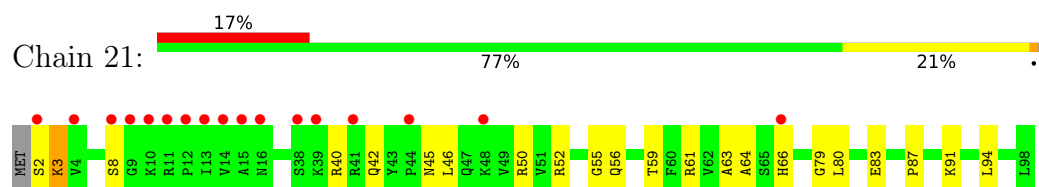
- Molecule 22: 50S ribosomal protein L27



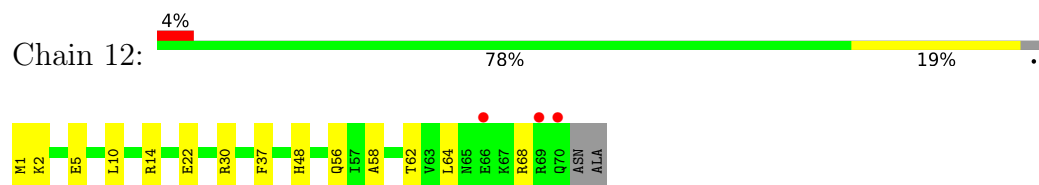
- Molecule 23: 50S ribosomal protein L28



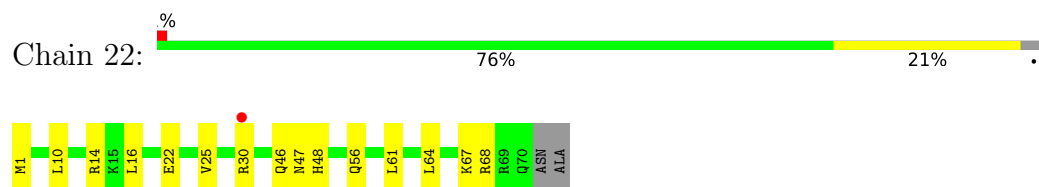
- Molecule 23: 50S ribosomal protein L28



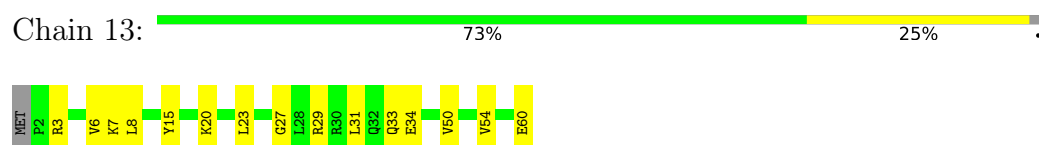
- Molecule 24: 50S ribosomal protein L29



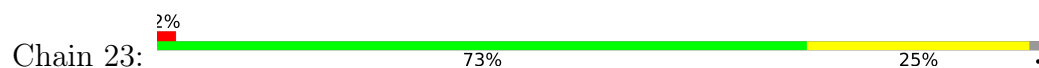
- Molecule 24: 50S ribosomal protein L29



- Molecule 25: 50S ribosomal protein L30



- Molecule 25: 50S ribosomal protein L30





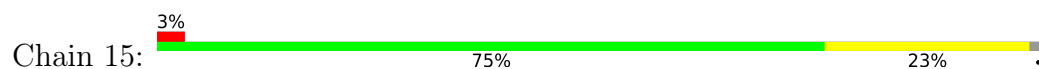
- Molecule 26: 50S ribosomal protein L31



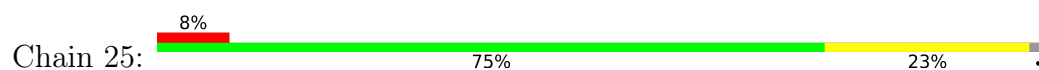
- Molecule 26: 50S ribosomal protein L31



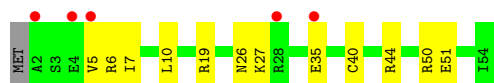
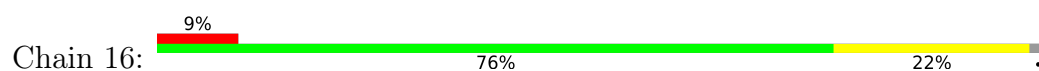
- Molecule 27: 50S ribosomal protein L32



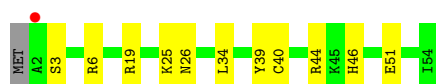
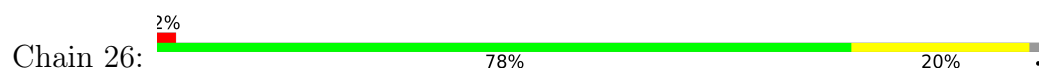
- Molecule 27: 50S ribosomal protein L32



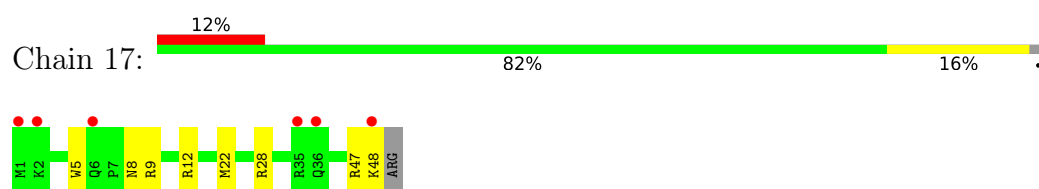
- Molecule 28: 50S ribosomal protein L33



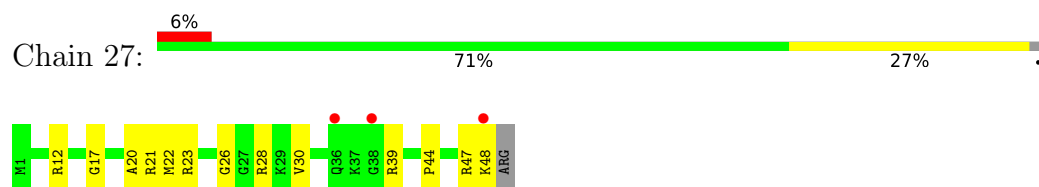
- Molecule 28: 50S ribosomal protein L33



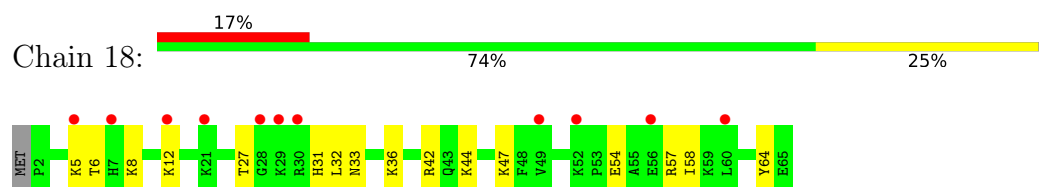
- Molecule 29: 50S ribosomal protein L34



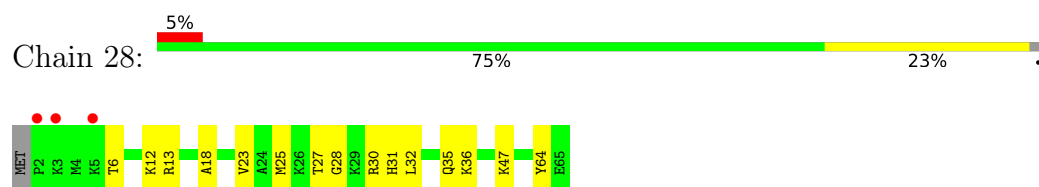
- Molecule 29: 50S ribosomal protein L34



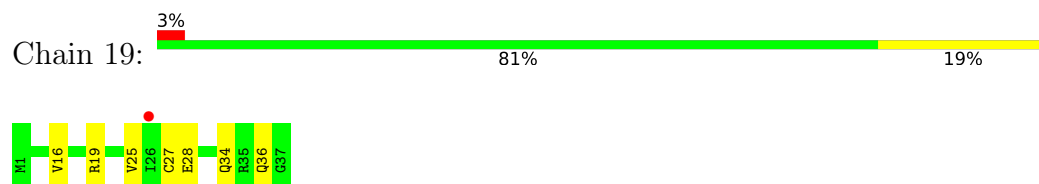
- Molecule 30: 50S Ribosomal Protein L35



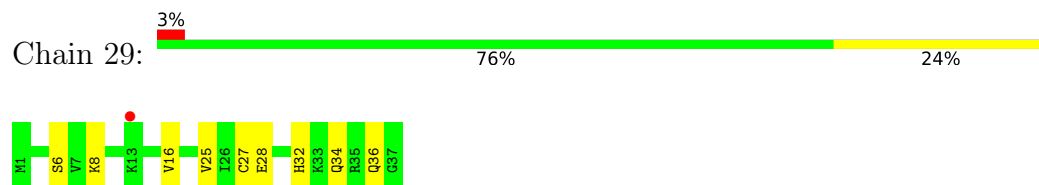
- Molecule 30: 50S Ribosomal Protein L35



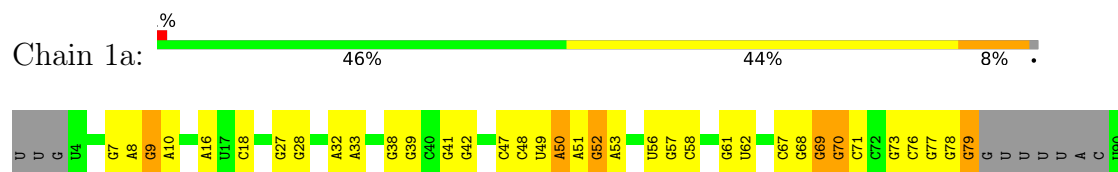
- Molecule 31: 50S Ribosomal Protein L36

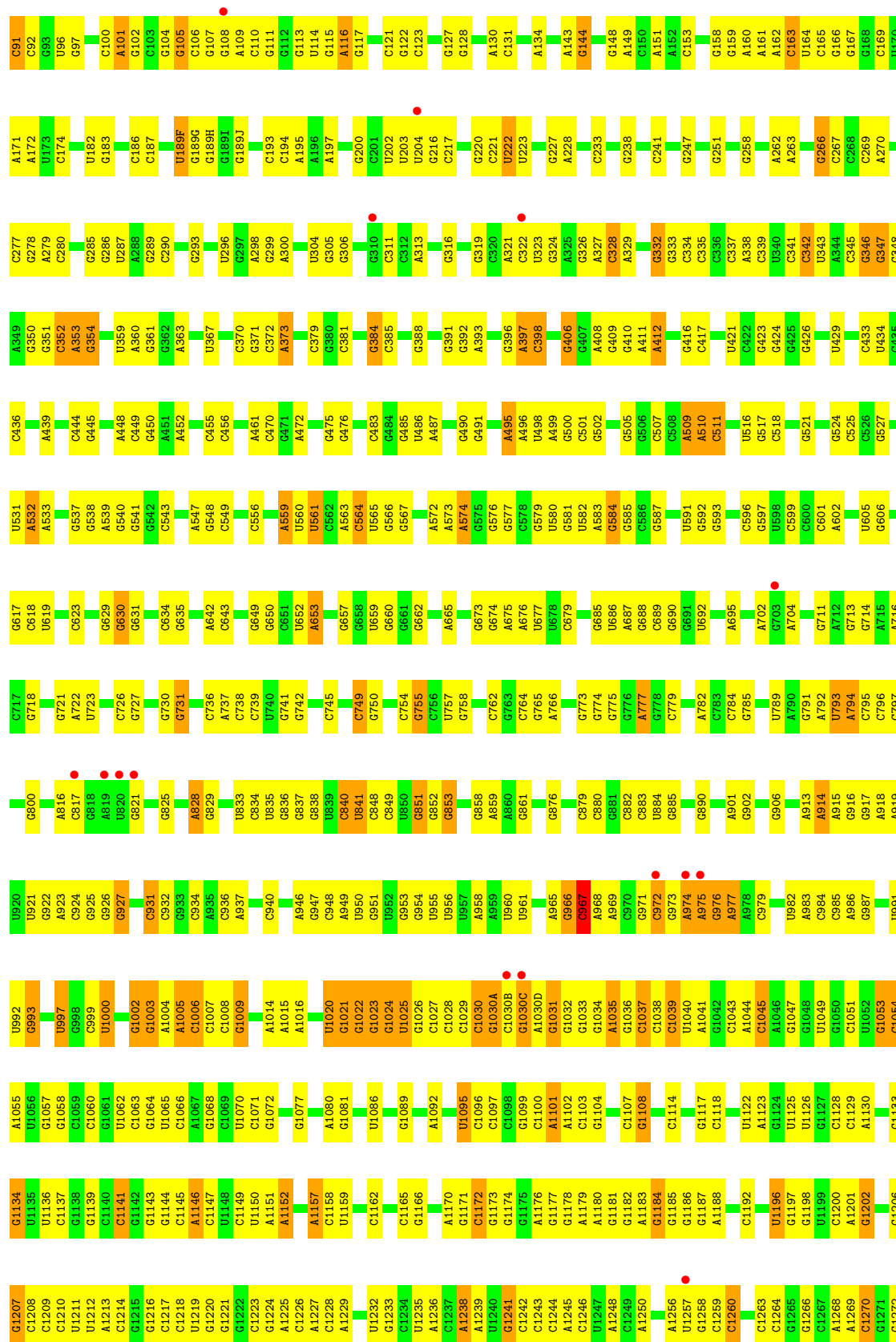


- Molecule 31: 50S Ribosomal Protein L36

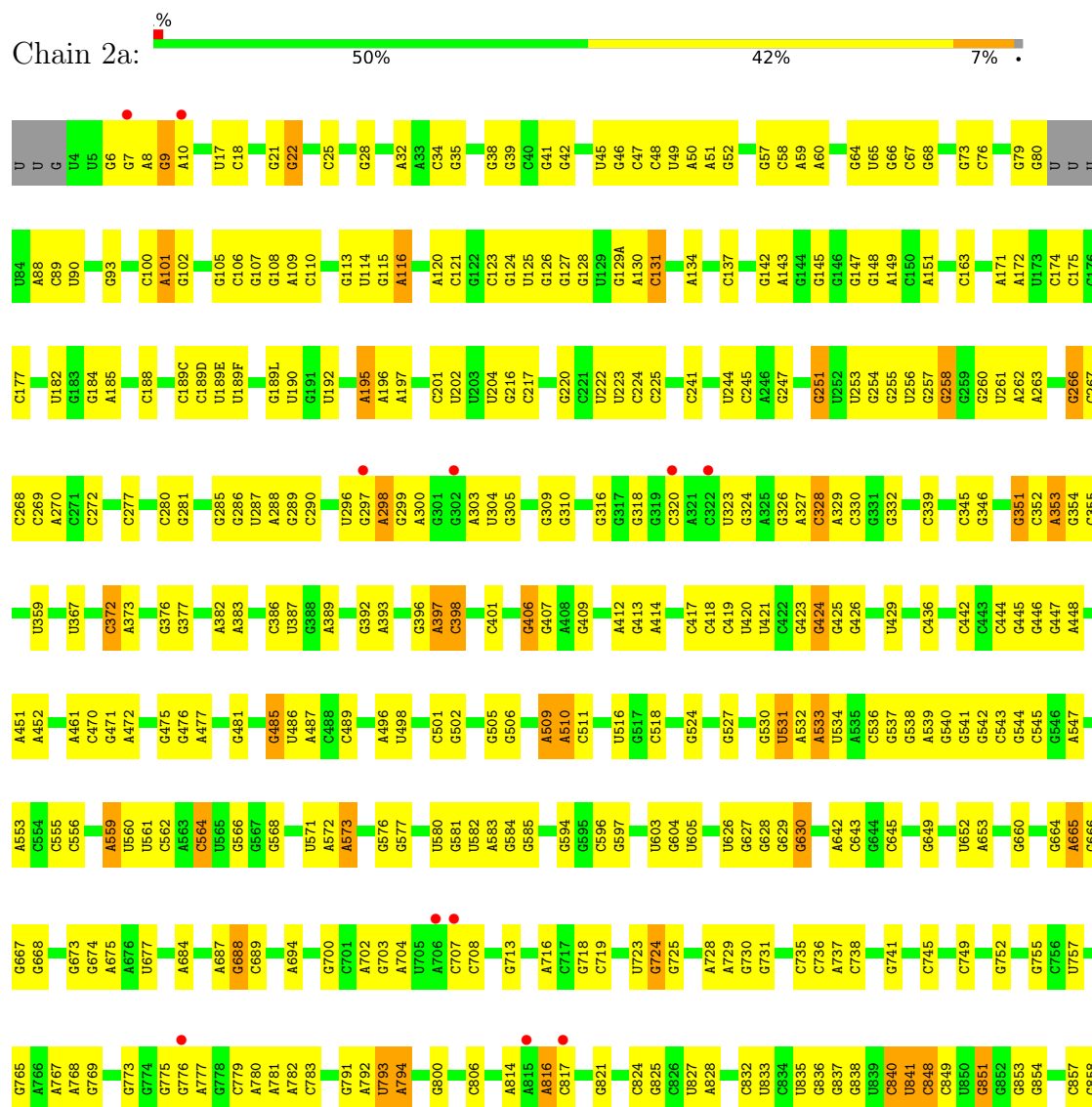


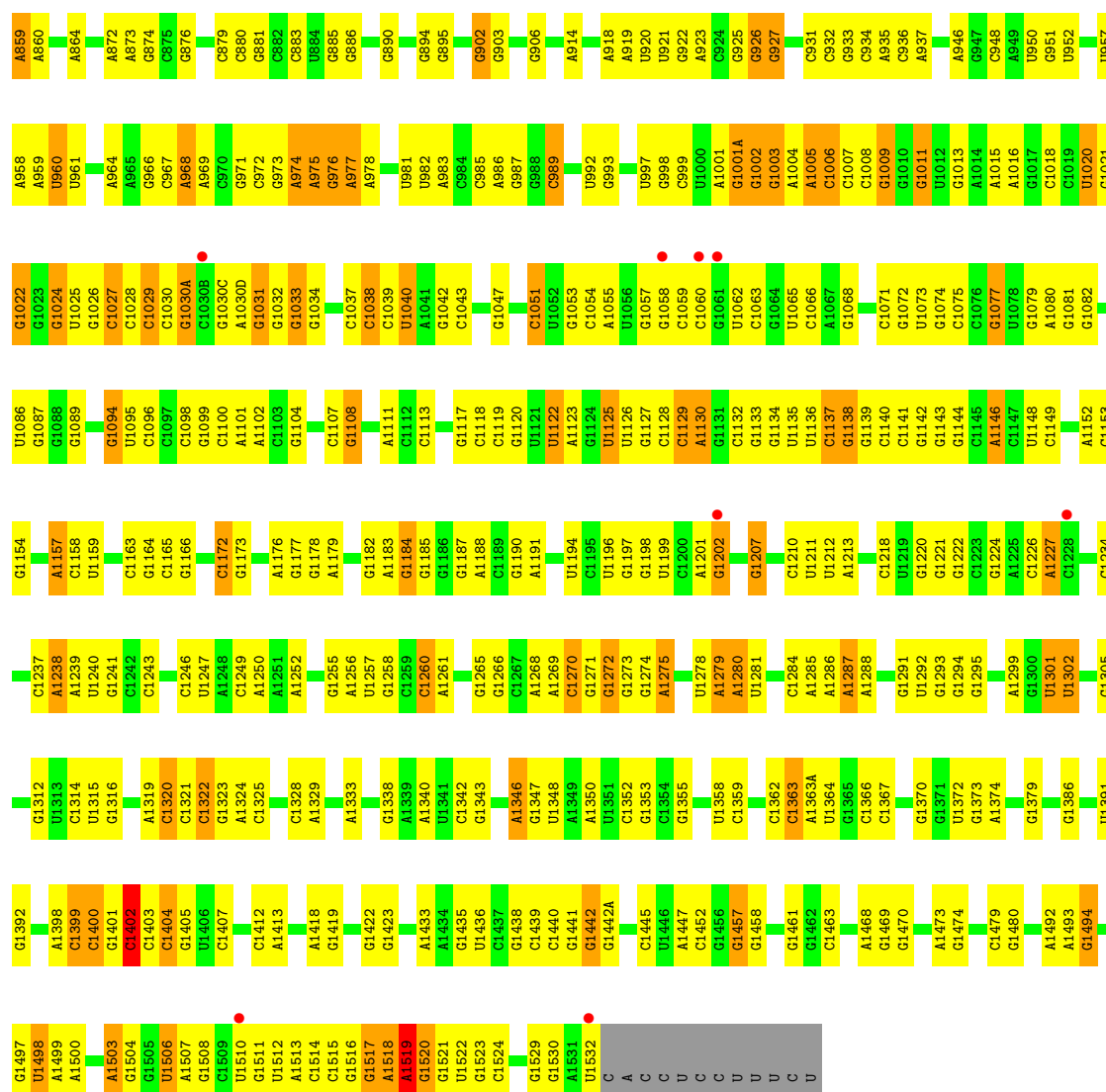
- Molecule 32: 16S Ribosomal RNA





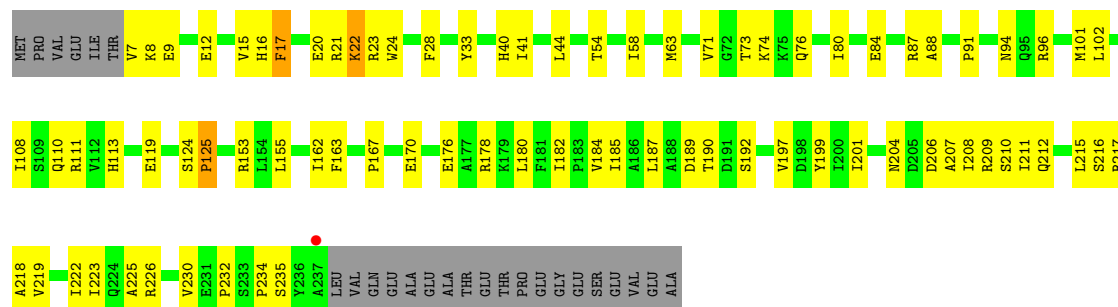
- Molecule 32: 16S Ribosomal RNA





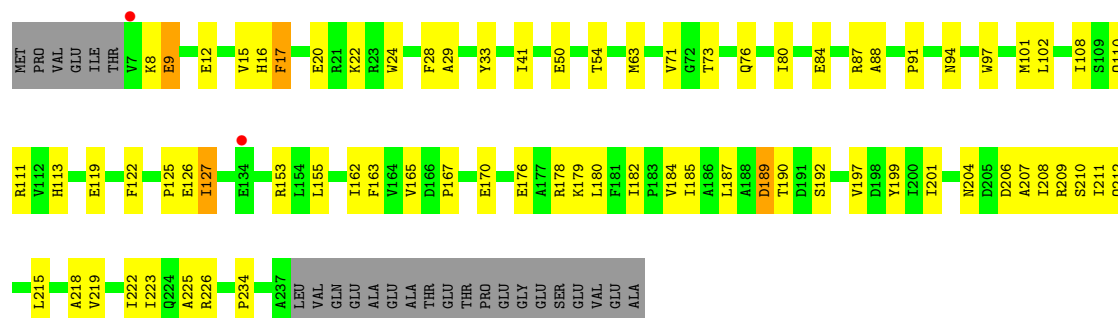
• Molecule 33: 30S Ribosomal Protein S2

Chain 1b: 59% 30% 10%



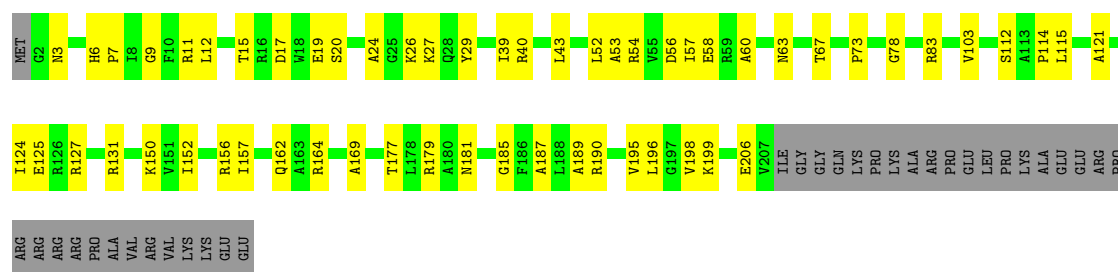
• Molecule 33: 30S Ribosomal Protein S2

Chain 2b: 61% 27% 10%



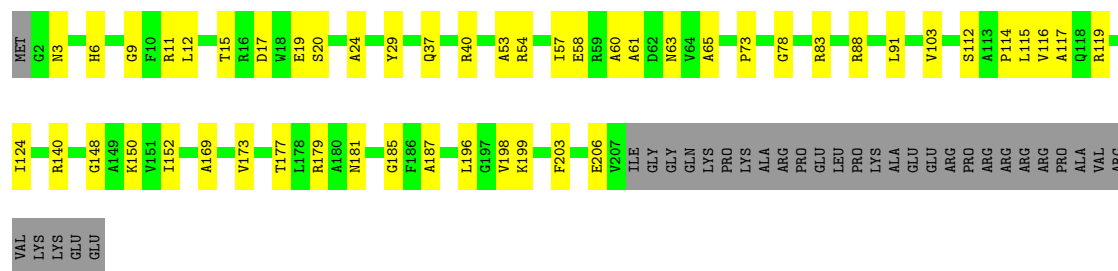
• Molecule 34: 30S Ribosomal Protein S3

Chain 1c: 62% 24% 14%



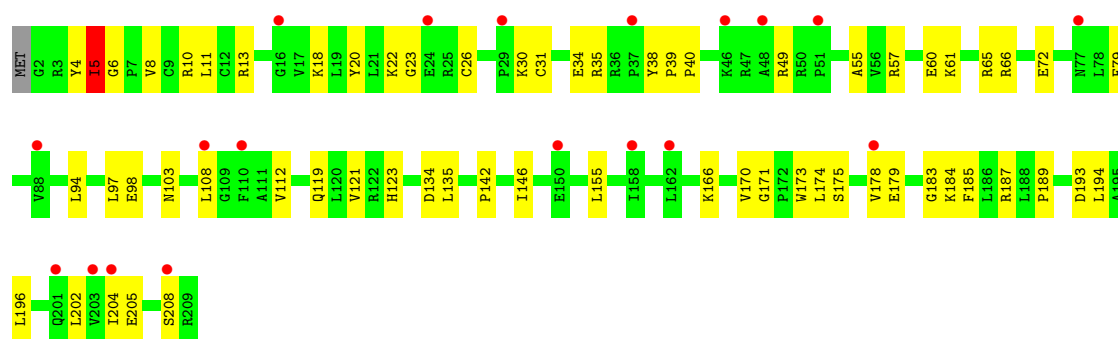
• Molecule 34: 30S Ribosomal Protein S3

Chain 2c: 65% 21% 14%

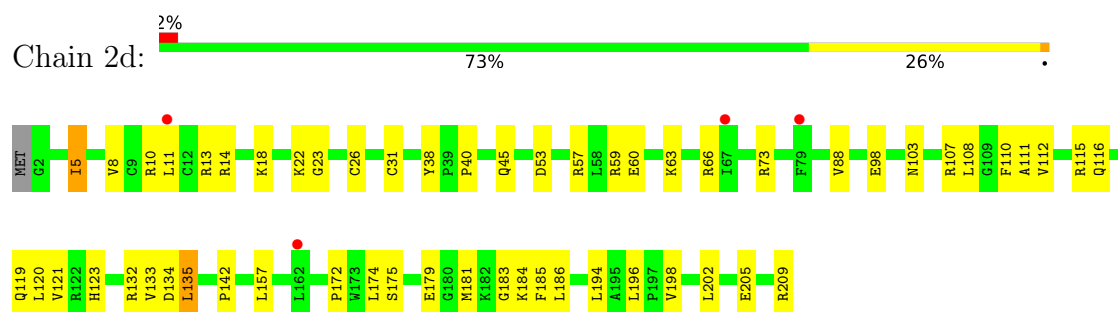


• Molecule 35: 30S Ribosomal Protein S4

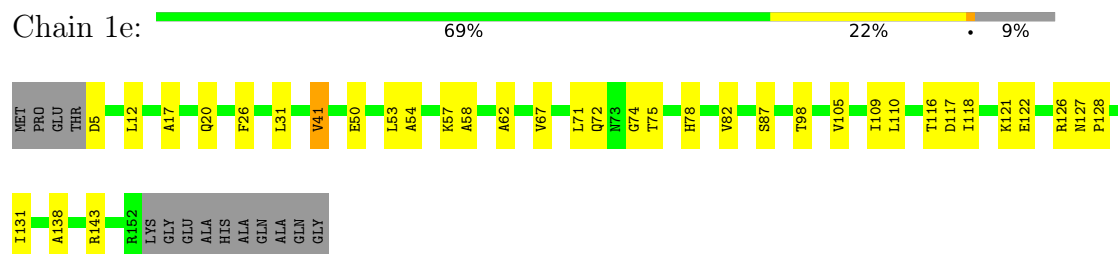
Chain 1d: 9% 70% 29%



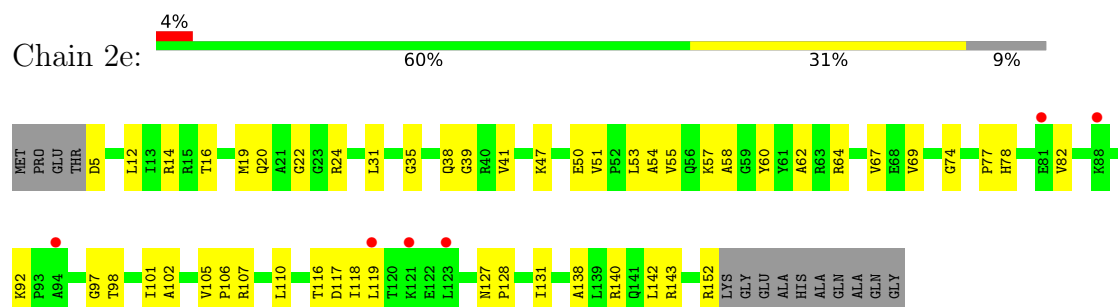
• Molecule 35: 30S Ribosomal Protein S4



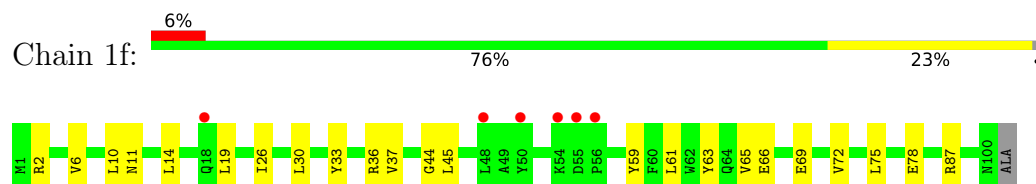
- Molecule 36: 30S Ribosomal Protein S5



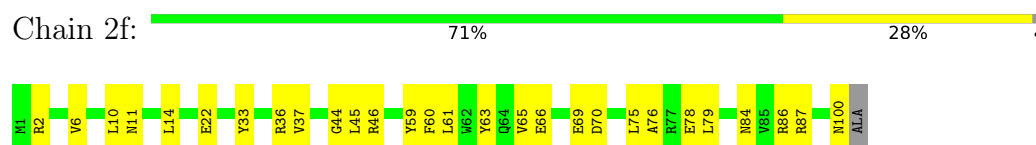
- Molecule 36: 30S Ribosomal Protein S5



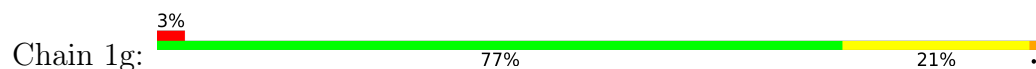
- Molecule 37: 30S Ribosomal Protein S6

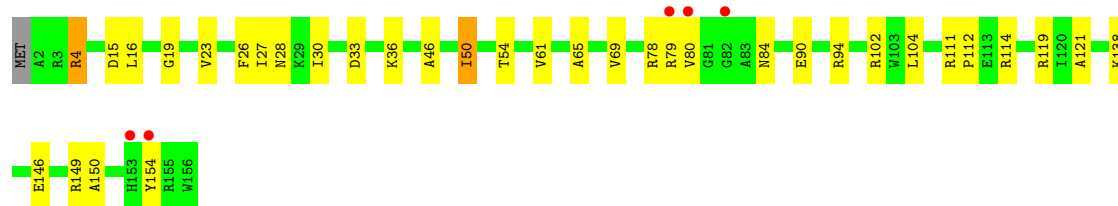


- Molecule 37: 30S Ribosomal Protein S6

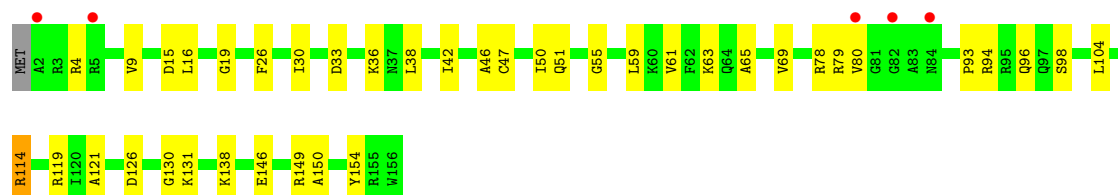
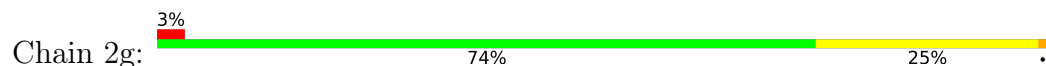


- Molecule 38: 30S Ribosomal Protein S7





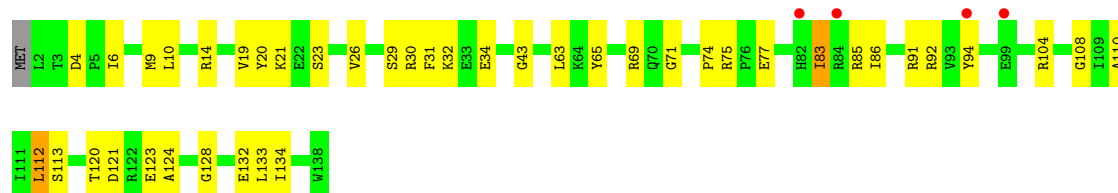
• Molecule 38: 30S Ribosomal Protein S7



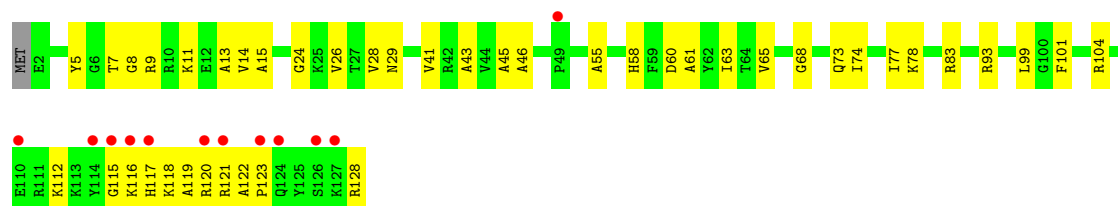
• Molecule 39: 30S Ribosomal Protein S8



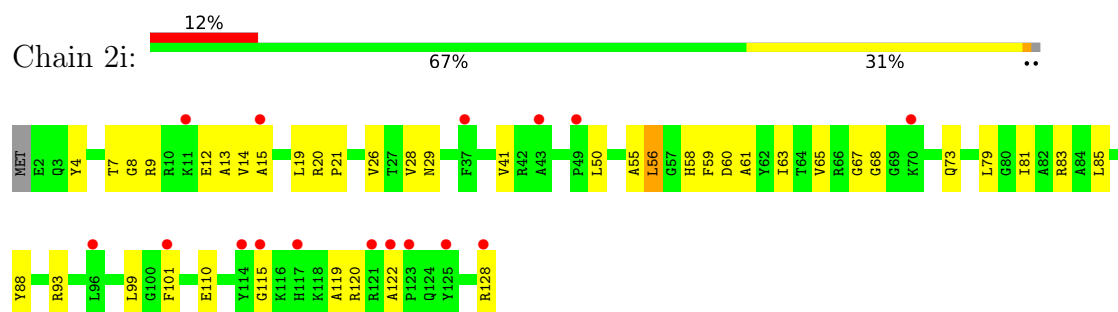
• Molecule 39: 30S Ribosomal Protein S8



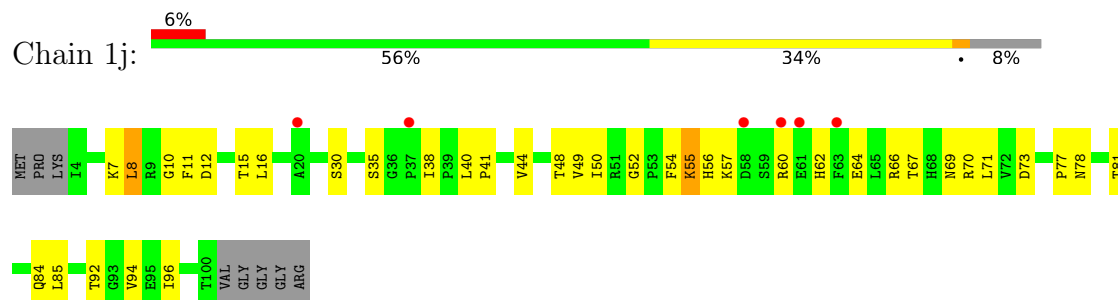
• Molecule 40: 30S ribosomal protein S9



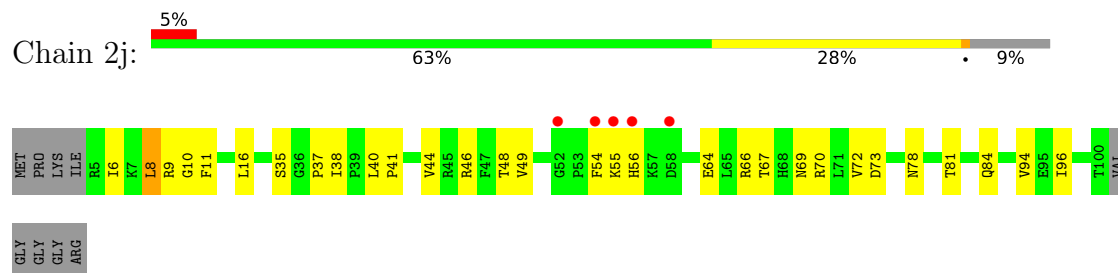
• Molecule 40: 30S ribosomal protein S9



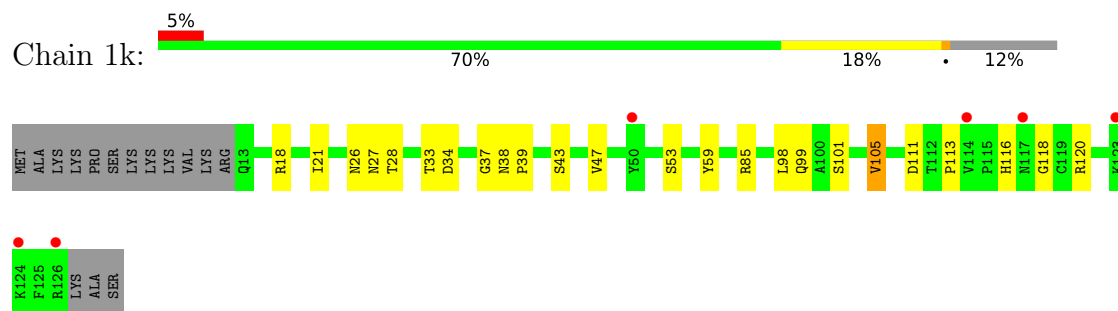
- Molecule 41: 30S ribosomal protein S10



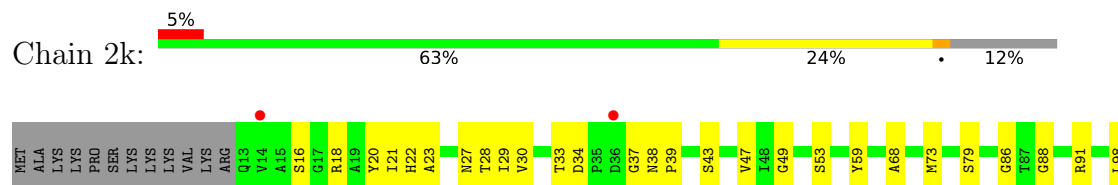
- Molecule 41: 30S ribosomal protein S10

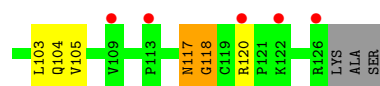


- Molecule 42: 30S ribosomal protein S11

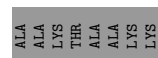


- Molecule 42: 30S ribosomal protein S11

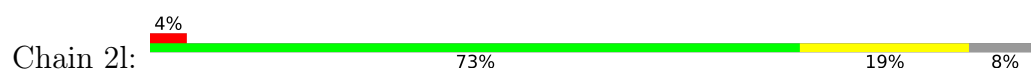




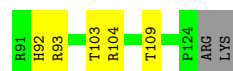
- Molecule 43: 30S ribosomal protein S12



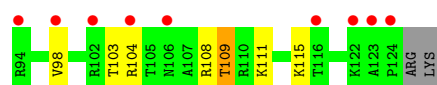
- Molecule 43: 30S ribosomal protein S12



- Molecule 44: 30S ribosomal protein S13



- Molecule 44: 30S ribosomal protein S13

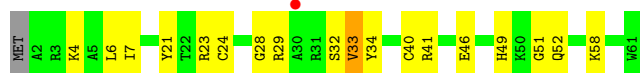


- Molecule 45: 30S ribosomal protein S14 type Z

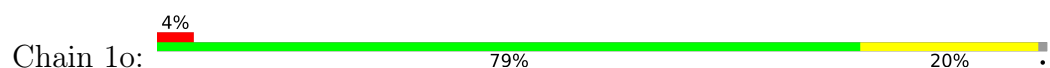




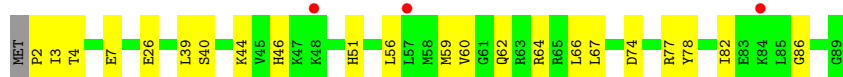
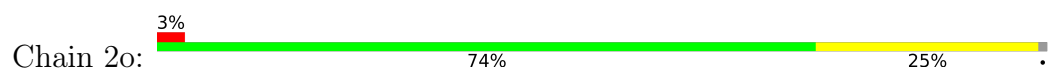
- Molecule 45: 30S ribosomal protein S14 type Z



- Molecule 46: 30S ribosomal protein S15



- Molecule 46: 30S ribosomal protein S15



- Molecule 47: 30S ribosomal protein S16

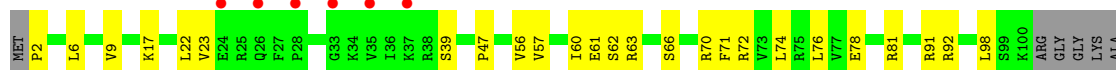


- Molecule 47: 30S ribosomal protein S16



GLY
ALA

- Molecule 48: 30S ribosomal protein S17



• Molecule 48: 30S ribosomal protein S17



• Molecule 49: 30S ribosomal protein S18



• Molecule 49: 30S ribosomal protein S18



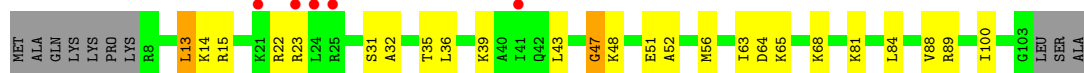
• Molecule 50: 30S Ribosomal Protein S19



• Molecule 50: 30S Ribosomal Protein S19

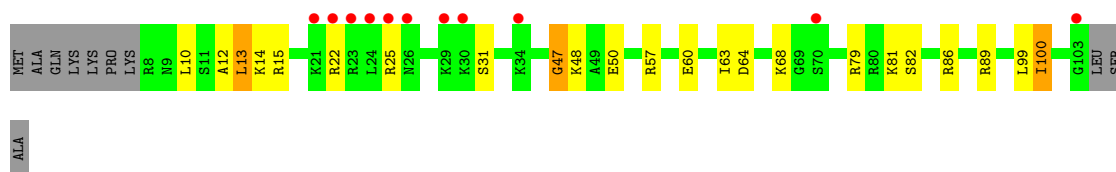


• Molecule 51: 30S Ribosomal Protein S20



• Molecule 51: 30S Ribosomal Protein S20





- Molecule 52: 30S ribosomal protein Thx



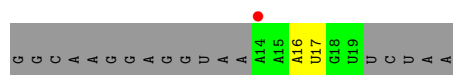
- Molecule 52: 30S ribosomal protein Thx



- 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

Chain 2x:

56%

36%

6%



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 – 3.70 146.71 – 3.70	Depositor EDS
% Data completeness (in resolution range)	99.1 (146.71-3.70) 99.1 (146.71-3.70)	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 (4.98%)	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)	0.27 , 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	0.92	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: PPU, 5MC, SF4, MA6, 5MU, 2MU, M2G, OMG, UR3, 2MA, 4SU, 4OC, 2MG, 0TD, PSU, 7MG, ZN, MG

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	0.20	0/69009	0.32	0/107712
1	2A	0.18	0/67293	0.31	0/105034
2	1B	0.15	0/2882	0.27	0/4494
2	2B	0.15	0/2879	0.27	0/4487
3	1D	0.24	0/2186	0.42	0/2944
3	2D	0.24	1/2186 (0.0%)	0.41	0/2944
4	1E	0.20	0/1592	0.42	1/2149 (0.0%)
4	2E	0.19	0/1592	0.40	0/2149
5	1F	0.20	0/1619	0.42	1/2193 (0.0%)
5	2F	0.18	0/1615	0.38	0/2188
6	1G	0.17	0/1448	0.39	0/1957
6	2G	0.18	0/1453	0.39	0/1963
7	1H	0.17	0/1356	0.34	0/1834
7	2H	0.19	0/1356	0.34	0/1834
8	1I	0.16	0/1112	0.35	0/1514
8	2I	0.18	0/1079	0.34	0/1475
9	1N	0.26	0/1144	0.51	2/1543 (0.1%)
9	2N	0.19	0/1144	0.43	1/1543 (0.1%)
10	1O	0.20	0/943	0.39	0/1269
10	2O	0.19	0/943	0.38	0/1269
11	1P	0.21	0/1152	0.55	3/1533 (0.2%)
11	2P	0.19	0/1152	0.53	3/1533 (0.2%)
12	1Q	0.19	0/1143	0.38	0/1527
12	2Q	0.17	0/1143	0.37	0/1527
13	1R	0.19	0/982	0.42	0/1312
13	2R	0.20	0/982	0.40	0/1312
14	1S	0.17	0/883	0.38	0/1176
14	2S	0.18	0/880	0.39	0/1172
15	1T	0.19	0/1105	0.42	1/1477 (0.1%)
15	2T	0.18	0/1097	0.39	0/1468
16	1U	0.19	0/977	0.35	0/1301

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
16	2U	0.18	0/977	0.35	0/1301
17	1V	0.18	0/782	0.36	0/1049
17	2V	0.19	0/782	0.37	0/1049
18	1W	0.19	0/897	0.36	0/1205
18	2W	0.19	0/897	0.41	0/1205
19	1X	0.20	0/764	0.39	0/1025
19	2X	0.17	0/764	0.36	0/1025
20	1Y	0.19	0/819	0.37	0/1095
20	2Y	0.18	0/819	0.37	0/1095
21	1Z	0.18	0/1267	0.41	0/1717
21	2Z	0.18	0/1299	0.39	0/1763
22	10	0.18	0/662	0.41	0/881
22	20	0.18	0/662	0.41	0/881
23	11	0.21	0/762	0.39	0/1014
23	21	0.18	0/762	0.36	0/1014
24	12	0.20	0/590	0.36	0/781
24	22	0.18	0/590	0.35	0/781
25	13	0.21	0/474	0.40	0/635
25	23	0.19	0/469	0.39	0/630
26	14	0.27	0/565	0.60	0/761
26	24	0.27	0/545	0.54	0/737
27	15	0.24	0/469	0.43	0/635
27	25	0.20	0/469	0.42	0/635
28	16	0.18	0/460	0.39	0/613
28	26	0.16	0/456	0.41	0/608
29	17	0.24	0/426	0.44	0/561
29	27	0.21	0/426	0.43	0/561
30	18	0.20	0/525	0.36	0/691
30	28	0.18	0/525	0.36	0/691
31	19	0.22	0/310	0.45	0/407
31	29	0.19	0/310	0.43	0/407
32	1a	0.17	0/35795	0.31	0/55864
32	2a	0.17	0/35886	0.31	0/56005
33	1b	0.21	0/1881	0.45	0/2542
33	2b	0.22	0/1860	0.42	0/2518
34	1c	0.19	0/1572	0.38	0/2126
34	2c	0.17	0/1566	0.37	0/2119
35	1d	0.25	1/1685 (0.1%)	0.45	0/2262
35	2d	0.19	0/1704	0.42	0/2284
36	1e	0.17	0/1145	0.40	0/1543
36	2e	0.18	0/1149	0.42	0/1548
37	1f	0.16	0/823	0.35	0/1115
37	2f	0.17	0/829	0.37	0/1123

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
38	1g	0.19	0/1250	0.42	1/1679 (0.1%)
38	2g	0.22	0/1254	0.38	0/1683
39	1h	0.17	0/1108	0.39	0/1494
39	2h	0.18	0/1108	0.39	0/1494
40	1i	0.23	0/1002	0.46	0/1346
40	2i	0.22	0/997	0.45	0/1343
41	1j	0.20	0/722	0.41	0/982
41	2j	0.19	0/727	0.41	0/988
42	1k	0.15	0/844	0.36	0/1145
42	2k	0.16	0/848	0.34	0/1149
43	1l	0.18	0/937	0.40	0/1260
43	2l	0.18	0/937	0.42	0/1260
44	1m	0.18	0/969	0.41	0/1302
44	2m	0.18	0/961	0.39	0/1291
45	1n	0.18	0/501	0.42	0/664
45	2n	0.17	0/501	0.37	0/664
46	1o	0.17	0/739	0.34	0/985
46	2o	0.16	0/739	0.34	0/985
47	1p	0.18	0/697	0.40	0/939
47	2p	0.17	0/693	0.39	0/935
48	1q	0.17	0/836	0.35	0/1117
48	2q	0.17	0/836	0.36	0/1117
49	1r	0.16	0/560	0.32	0/746
49	2r	0.19	0/560	0.36	0/746
50	1s	0.21	0/667	0.43	0/900
50	2s	0.18	0/661	0.42	0/893
51	1t	0.27	0/730	0.40	0/965
51	2t	0.17	0/729	0.40	0/965
52	1u	0.18	0/203	0.41	0/266
52	2u	0.18	0/203	0.38	0/266
53	1v	0.20	0/126	0.27	0/195
53	2v	0.16	0/126	0.27	0/195
54	1w	0.28	0/40	0.51	0/60
54	2w	0.20	0/40	0.48	0/60
55	1x	0.22	0/1725	0.33	0/2689
55	2x	0.21	0/1725	0.31	0/2689
All	All	0.19	2/310047 (0.0%)	0.34	13/463792 (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 (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	2D	7	LYS	C-N	-7.02	1.17	1.33
35	1d	39	PRO	CA-C	-5.64	1.48	1.51

The worst 5 of 13 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	1N	80	GLY	N-CA-C	-9.08	102.62	115.43
11	1P	26	GLY	N-CA-C	-8.32	104.42	115.40
9	2N	80	GLY	N-CA-C	-8.08	104.03	115.43
38	1g	50	ILE	N-CA-C	-8.04	103.55	112.80
11	2P	26	GLY	N-CA-C	-6.81	106.36	115.21

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	858	0
1	2A	60322	0	30425	776	0
2	1B	2577	0	1305	32	0
2	2B	2575	0	1303	31	0
3	1D	2136	0	2218	62	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	2D	2136	0	2218	62	0
4	1E	1559	0	1618	35	0
4	2E	1559	0	1618	35	0
5	1F	1584	0	1625	33	0
5	2F	1580	0	1619	38	0
6	1G	1423	0	1436	39	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	17	0
9	1N	1117	0	1184	21	0
9	2N	1117	0	1184	26	0
10	1O	933	0	996	21	0
10	2O	933	0	996	28	0
11	1P	1135	0	1212	30	0
11	2P	1135	0	1212	27	0
12	1Q	1122	0	1179	25	0
12	2Q	1122	0	1179	30	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	22	0
15	1T	1091	0	1151	31	0
15	2T	1083	0	1136	25	0
16	1U	959	0	1019	25	0
16	2U	959	0	1019	27	0
17	1V	771	0	830	7	0
17	2V	771	0	830	17	0
18	1W	886	0	940	15	0
18	2W	886	0	940	16	0
19	1X	750	0	814	18	0
19	2X	750	0	814	11	0
20	1Y	806	0	881	20	0
20	2Y	806	0	881	15	0
21	1Z	1240	0	1240	21	0
21	2Z	1271	0	1273	27	0
22	10	653	0	674	12	0
22	20	653	0	674	17	0
23	11	755	0	826	9	0
23	21	755	0	826	15	0
24	12	588	0	643	12	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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	21	0
26	24	532	0	503	24	0
27	15	455	0	465	10	0
27	25	455	0	465	12	0
28	16	453	0	473	8	0
28	26	449	0	469	8	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	14	0
31	19	307	0	335	5	0
31	29	307	0	335	7	0
32	1a	32246	0	16296	623	0
32	2a	32327	0	16339	560	0
33	1b	1846	0	1867	62	0
33	2b	1825	0	1828	53	0
34	1c	1548	0	1535	37	0
34	2c	1542	0	1517	33	0
35	1d	1655	0	1672	50	0
35	2d	1674	0	1714	48	0
36	1e	1129	0	1185	24	0
36	2e	1133	0	1191	38	0
37	1f	810	0	804	17	0
37	2f	816	0	808	22	0
38	1g	1231	0	1238	26	0
38	2g	1235	0	1249	27	0
39	1h	1088	0	1126	32	0
39	2h	1088	0	1126	33	0
40	1i	983	0	986	38	0
40	2i	978	0	966	35	0
41	1j	709	0	650	28	0
41	2j	714	0	672	20	0
42	1k	829	0	825	20	0
42	2k	833	0	836	24	0
43	1l	932	0	981	19	0
43	2l	932	0	981	19	0
44	1m	958	0	1002	34	0
44	2m	950	0	988	38	0
45	1n	492	0	529	20	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
45	2n	492	0	529	15	0
46	1o	728	0	760	13	0
46	2o	728	0	760	19	0
47	1p	681	0	697	19	0
47	2p	677	0	686	23	0
48	1q	823	0	891	21	0
48	2q	823	0	891	22	0
49	1r	555	0	618	11	0
49	2r	555	0	618	10	0
50	1s	652	0	662	22	0
50	2s	646	0	644	24	0
51	1t	728	0	798	20	0
51	2t	727	0	796	23	0
52	1u	199	0	208	9	0
52	2u	199	0	208	5	0
53	1v	113	0	54	1	0
53	2v	113	0	54	2	0
54	1w	74	0	51	6	0
54	2w	74	0	50	6	0
55	1x	1625	0	829	21	0
55	2x	1625	0	829	29	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
56	1l	1	0	0	0	0
56	1r	1	0	0	0	0
56	1x	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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	2	0
58	2d	8	0	0	2	0
59	1A	53	0	0	2	0
59	1D	3	0	0	2	0
59	1a	15	0	0	2	0
59	1x	2	0	0	0	0
59	2A	32	0	0	2	0
59	2B	1	0	0	0	0
59	2a	19	0	0	1	0
All	All	287828	0	193417	4438	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 4438 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
32:1a:78:G:N1	32:1a:91:C:C4	2.26	1.03
32:1a:931:C:N4	32:1a:1386:G:H1	1.57	1.01
32:2a:1133:G:H1	32:2a:1141:C:N4	1.56	1.01
32:2a:1352:C:H42	32:2a:1370:G:H1	1.09	1.00

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%)	24	56
4	2E	202/206 (98%)	192 (95%)	9 (4%)	1 (0%)	24	56
5	1F	201/210 (96%)	196 (98%)	3 (2%)	2 (1%)	12	43
5	2F	201/210 (96%)	194 (96%)	5 (2%)	2 (1%)	12	43
6	1G	179/182 (98%)	168 (94%)	9 (5%)	2 (1%)	11	42
6	2G	179/182 (98%)	170 (95%)	7 (4%)	2 (1%)	11	42
7	1H	172/180 (96%)	162 (94%)	8 (5%)	2 (1%)	10	40
7	2H	172/180 (96%)	165 (96%)	4 (2%)	3 (2%)	7	34
8	1I	144/148 (97%)	135 (94%)	9 (6%)	0	100	100
8	2I	144/148 (97%)	132 (92%)	12 (8%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
9	1N	138/140 (99%)	129 (94%)	8 (6%)	1 (1%)	18	50
9	2N	138/140 (99%)	129 (94%)	8 (6%)	1 (1%)	18	50
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%)	6	32
11	2P	147/150 (98%)	136 (92%)	10 (7%)	1 (1%)	18	50
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%)	14	45
14	2S	108/112 (96%)	104 (96%)	4 (4%)	0	100	100
15	1T	129/146 (88%)	123 (95%)	5 (4%)	1 (1%)	16	48
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%)	12	43
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%)	10	40
22	20	81/85 (95%)	76 (94%)	4 (5%)	1 (1%)	10	40
23	11	95/98 (97%)	94 (99%)	0	1 (1%)	11	42
23	21	95/98 (97%)	93 (98%)	1 (1%)	1 (1%)	11	42
24	12	68/72 (94%)	68 (100%)	0	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
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	6
26	24	67/71 (94%)	53 (79%)	9 (13%)	5 (8%)	1	11
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%)	7	34
33	2b	229/256 (90%)	203 (89%)	23 (10%)	3 (1%)	9	38
34	1c	204/239 (85%)	188 (92%)	15 (7%)	1 (0%)	24	56
34	2c	204/239 (85%)	190 (93%)	14 (7%)	0	100	100
35	1d	206/209 (99%)	198 (96%)	7 (3%)	1 (0%)	24	56
35	2d	206/209 (99%)	197 (96%)	8 (4%)	1 (0%)	24	56
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%)	9	38
38	2g	153/156 (98%)	139 (91%)	12 (8%)	2 (1%)	9	38
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%)	16	48
40	2i	125/128 (98%)	114 (91%)	10 (8%)	1 (1%)	16	48

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
41	1j	95/105 (90%)	88 (93%)	4 (4%)	3 (3%)	3	25
41	2j	94/105 (90%)	86 (92%)	7 (7%)	1 (1%)	11	42
42	1k	112/129 (87%)	106 (95%)	5 (4%)	1 (1%)	14	45
42	2k	112/129 (87%)	104 (93%)	4 (4%)	4 (4%)	2	23
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%)	4	29
47	2p	80/88 (91%)	72 (90%)	7 (9%)	1 (1%)	9	38
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%)	10	40
51	1t	94/106 (89%)	85 (90%)	7 (7%)	2 (2%)	5	31
51	2t	94/106 (89%)	87 (93%)	5 (5%)	2 (2%)	5	31
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%)	21	52

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%)	214 (100%)	1 (0%)	81	80
3	2D	215/218 (99%)	215 (100%)	0	100	100
4	1E	164/166 (99%)	161 (98%)	3 (2%)	51	67
4	2E	164/166 (99%)	160 (98%)	4 (2%)	43	61
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%)	59	70
6	2G	143/156 (92%)	141 (99%)	2 (1%)	59	70
7	1H	144/148 (97%)	143 (99%)	1 (1%)	76	77
7	2H	144/148 (97%)	143 (99%)	1 (1%)	76	77
8	1I	113/124 (91%)	112 (99%)	1 (1%)	70	75
8	2I	105/124 (85%)	105 (100%)	0	100	100
9	1N	118/119 (99%)	117 (99%)	1 (1%)	73	76
9	2N	118/119 (99%)	117 (99%)	1 (1%)	73	76
10	1O	100/100 (100%)	100 (100%)	0	100	100
10	2O	100/100 (100%)	99 (99%)	1 (1%)	68	74
11	1P	115/116 (99%)	112 (97%)	3 (3%)	40	60
11	2P	115/116 (99%)	113 (98%)	2 (2%)	53	67
12	1Q	111/111 (100%)	110 (99%)	1 (1%)	70	75
12	2Q	111/111 (100%)	111 (100%)	0	100	100
13	1R	101/101 (100%)	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

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
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%)	29	53
17	2V	80/82 (98%)	77 (96%)	3 (4%)	29	53
18	1W	90/92 (98%)	89 (99%)	1 (1%)	65	73
18	2W	90/92 (98%)	89 (99%)	1 (1%)	65	73
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%)	63	72
20	2Y	85/91 (93%)	85 (100%)	0	100	100
21	1Z	135/179 (75%)	133 (98%)	2 (2%)	57	68
21	2Z	137/179 (76%)	135 (98%)	2 (2%)	57	68
22	10	65/67 (97%)	65 (100%)	0	100	100
22	20	65/67 (97%)	64 (98%)	1 (2%)	57	68
23	11	80/83 (96%)	78 (98%)	2 (2%)	42	61
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%)	57 (97%)	2 (3%)	32	55
26	24	53/63 (84%)	51 (96%)	2 (4%)	29	53
27	15	50/52 (96%)	49 (98%)	1 (2%)	48	64
27	25	50/52 (96%)	50 (100%)	0	100	100
28	16	51/52 (98%)	50 (98%)	1 (2%)	48	64
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

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
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%)	185 (99%)	2 (1%)	65	73
34	1c	142/188 (76%)	140 (99%)	2 (1%)	59	70
34	2c	140/188 (74%)	139 (99%)	1 (1%)	76	77
35	1d	169/181 (93%)	167 (99%)	2 (1%)	63	72
35	2d	173/181 (96%)	171 (99%)	2 (1%)	63	72
36	1e	113/123 (92%)	112 (99%)	1 (1%)	70	75
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%)	73	76
39	1h	114/119 (96%)	113 (99%)	1 (1%)	70	75
39	2h	114/119 (96%)	112 (98%)	2 (2%)	51	67
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%)	64 (97%)	2 (3%)	36	57
41	2j	69/92 (75%)	67 (97%)	2 (3%)	37	57
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%)	91 (98%)	2 (2%)	45	63
44	2m	92/101 (91%)	91 (99%)	1 (1%)	65	73
45	1n	49/50 (98%)	48 (98%)	1 (2%)	48	64
45	2n	49/50 (98%)	48 (98%)	1 (2%)	48	64
46	1o	78/80 (98%)	78 (100%)	0	100	100
46	2o	78/80 (98%)	78 (100%)	0	100	100
47	1p	69/74 (93%)	69 (100%)	0	100	100
47	2p	68/74 (92%)	67 (98%)	1 (2%)	57	68

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
48	1q	94/97 (97%)	94 (100%)	0	100	100
48	2q	94/97 (97%)	94 (100%)	0	100	100
49	1r	59/77 (77%)	58 (98%)	1 (2%)	53	67
49	2r	59/77 (77%)	59 (100%)	0	100	100
50	1s	69/80 (86%)	67 (97%)	2 (3%)	37	57
50	2s	67/80 (84%)	65 (97%)	2 (3%)	36	57
51	1t	70/82 (85%)	69 (99%)	1 (1%)	59	70
51	2t	70/82 (85%)	69 (99%)	1 (1%)	59	70
52	1u	18/22 (82%)	18 (100%)	0	100	100
52	2u	18/22 (82%)	18 (100%)	0	100	100
All	All	9303/10064 (92%)	9226 (99%)	77 (1%)	73	76

5 of 77 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
21	2Z	155	LEU
44	2m	109	THR
26	24	50	VAL
35	2d	135	LEU
50	2s	77	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 106 such sidechains are listed below:

Mol	Chain	Res	Type
5	2F	40	GLN
14	2S	68	GLN
42	2k	93	GLN
5	2F	133	ASN
10	2O	3	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	1A	2865/2915 (98%)	439 (15%)	28 (0%)
1	2A	2791/2915 (95%)	443 (15%)	21 (0%)
2	1B	120/121 (99%)	10 (8%)	1 (0%)

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Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
2	2B	119/121 (98%)	12 (10%)	1 (0%)
32	1a	1497/1521 (98%)	245 (16%)	0
32	2a	1501/1521 (98%)	233 (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	9053/9322 (97%)	1397 (15%)	51 (0%)

5 of 1397 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
2	1B	1	U
1	2A	752	A
1	2A	2756	U
1	2A	195	A
1	2A	271(M)	G

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

58 non-standard protein/DNA/RNA residues are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
43	0TD	2l	92	43	8,9,10	4.41	1 (12%)	6,11,13	7.99	2 (33%)
32	4OC	2a	1402	32	20,23,24	0.79	0	25,32,35	0.90	1 (4%)
55	5MC	2x	32	55	19,22,23	1.61	3 (15%)	26,32,35	1.17	3 (11%)
1	PSU	2A	2605	1	18,21,22	1.35	3 (16%)	21,30,33	1.94	5 (23%)
1	5MU	1A	1961	1	19,22,23	1.41	5 (26%)	27,32,35	2.31	6 (22%)
1	2MA	1A	2515	1,56	22,25,26	1.45	4 (18%)	32,37,40	2.37	7 (21%)
1	2MU	1A	2564	1	19,22,24	1.29	3 (15%)	25,31,36	1.78	5 (20%)
1	PSU	1A	1939	1	18,21,22	1.40	2 (11%)	21,30,33	1.97	3 (14%)
32	7MG	1a	527	32	23,26,27	1.35	3 (13%)	27,39,42	2.54	5 (18%)
32	5MC	2a	1407	32	19,22,23	1.66	3 (15%)	26,32,35	1.16	3 (11%)
32	MA6	1a	1519	32	23,26,27	1.52	5 (21%)	33,38,41	2.35	13 (39%)
1	OMG	1A	2263	1,55	23,26,27	1.26	3 (13%)	32,38,41	2.03	6 (18%)
32	UR3	1a	1498	32	19,22,23	1.04	1 (5%)	26,32,35	1.72	4 (15%)
1	5MU	2A	1915	1	19,22,23	1.38	5 (26%)	27,32,35	2.06	6 (22%)
32	5MC	1a	1400	32	19,22,23	1.68	3 (15%)	26,32,35	1.11	3 (11%)
32	5MC	1a	1407	32	19,22,23	1.71	2 (10%)	26,32,35	1.21	3 (11%)
32	5MC	1a	967	32	19,22,23	1.66	2 (10%)	26,32,35	1.12	3 (11%)
55	PSU	2x	55	55	18,21,22	1.38	2 (11%)	21,30,33	2.12	4 (19%)
1	5MC	2A	1942	1	19,22,23	1.61	3 (15%)	26,32,35	1.16	3 (11%)
1	4OC	2A	1920	1	19,22,24	0.80	0	25,31,35	0.86	0
32	5MC	2a	1400	32	19,22,23	1.75	3 (15%)	26,32,35	1.08	2 (7%)
32	PSU	2a	516	32	18,21,22	1.36	2 (11%)	21,30,33	1.95	4 (19%)
32	MA6	2a	1518	32	23,26,27	1.53	5 (21%)	33,38,41	2.30	14 (42%)
32	7MG	2a	527	32	23,26,27	1.35	3 (13%)	27,39,42	2.64	7 (25%)
32	2MG	2a	1207	32	23,26,27	1.23	3 (13%)	33,38,41	2.31	9 (27%)
1	5MU	1A	1937	1	19,22,23	1.46	4 (21%)	27,32,35	2.02	6 (22%)
32	2MG	1a	1207	32	23,26,27	1.24	4 (17%)	33,38,41	2.12	7 (21%)
32	4OC	1a	1402	32	20,23,24	0.76	0	25,32,35	0.82	1 (4%)
1	5MU	2A	1939	1	19,22,23	1.34	4 (21%)	27,32,35	2.16	6 (22%)
1	5MC	2A	1962	1	19,22,23	1.50	3 (15%)	26,32,35	1.25	4 (15%)
1	2MA	2A	2503	1,56	22,25,26	1.49	4 (18%)	32,37,40	2.31	9 (28%)
54	PPU	2w	76	1,54,56	37,40,41	1.27	4 (10%)	47,57,60	2.18	13 (27%)
32	M2G	1a	966	32	24,27,28	1.32	4 (16%)	33,40,43	1.84	6 (18%)
55	4SU	2x	8	55	18,21,22	2.07	6 (33%)	25,30,33	1.63	5 (20%)
55	PSU	1x	55	55	18,21,22	1.35	2 (11%)	21,30,33	2.06	5 (23%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
32	5MC	1a	1404	32	19,22,23	1.63	3 (15%)	26,32,35	1.11	2 (7%)
32	5MC	2a	1404	32	19,22,23	1.74	3 (15%)	26,32,35	1.09	3 (11%)
1	4OC	1A	1942	1	19,22,24	0.78	0	25,31,35	0.98	1 (4%)
32	MA6	2a	1519	32	23,26,27	1.54	5 (21%)	33,38,41	2.37	13 (39%)
32	M2G	2a	966	32	24,27,28	1.33	4 (16%)	33,40,43	1.81	5 (15%)
43	0TD	1l	92	43	8,9,10	4.37	1 (12%)	6,11,13	7.53	2 (33%)
1	5MC	1A	1964	1	19,22,23	1.61	3 (15%)	26,32,35	1.06	3 (11%)
1	PSU	2A	1911	1	18,21,22	1.40	2 (11%)	21,30,33	2.02	3 (14%)
32	PSU	1a	516	56,32	18,21,22	1.41	2 (11%)	21,30,33	1.92	4 (19%)
55	5MU	2x	54	55	19,22,23	1.37	5 (26%)	27,32,35	2.07	6 (22%)
1	2MU	2A	2552	1	19,22,24	1.28	2 (10%)	25,31,36	1.90	5 (20%)
32	MA6	1a	1518	32	23,26,27	1.52	5 (21%)	33,38,41	2.29	13 (39%)
32	UR3	2a	1498	32	19,22,23	1.01	2 (10%)	26,32,35	1.67	4 (15%)
54	PPU	1w	76	1,54	37,40,41	1.25	4 (10%)	47,57,60	2.19	14 (29%)
1	5MC	1A	1984	1	19,22,23	1.66	3 (15%)	26,32,35	1.29	5 (19%)
32	5MC	2a	967	32	19,22,23	1.73	2 (10%)	26,32,35	1.06	2 (7%)
55	5MC	1x	32	55	19,22,23	1.65	3 (15%)	26,32,35	1.23	3 (11%)
1	OMG	2A	2251	1,55	23,26,27	1.24	3 (13%)	32,38,41	2.02	6 (18%)
55	5MU	1x	54	55	19,22,23	1.43	6 (31%)	27,32,35	1.90	6 (22%)
55	4SU	1x	8	55	18,21,22	1.96	5 (27%)	25,30,33	1.86	6 (24%)
1	PSU	1A	1933	1	18,21,22	1.38	2 (11%)	21,30,33	1.98	3 (14%)
1	PSU	1A	2617	1	18,21,22	1.40	2 (11%)	21,30,33	2.03	4 (19%)
1	PSU	2A	1917	1	18,21,22	1.43	3 (16%)	21,30,33	2.06	5 (23%)

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
43	0TD	2l	92	43	-	3/7/12/14	-
32	4OC	2a	1402	32	-	2/9/29/30	0/2/2/2
55	5MC	2x	32	55	-	0/7/25/26	0/2/2/2
1	PSU	2A	2605	1	-	0/7/25/26	0/2/2/2
1	5MU	1A	1961	1	-	0/7/25/26	0/2/2/2
1	2MA	1A	2515	1,56	-	0/7/25/26	0/3/3/3
1	2MU	1A	2564	1	-	0/9/27/28	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	PSU	1A	1939	1	-	0/7/25/26	0/2/2/2
32	7MG	1a	527	32	-	0/7/37/38	0/3/3/3
32	5MC	2a	1407	32	-	0/7/25/26	0/2/2/2
32	MA6	1a	1519	32	-	4/11/29/30	0/3/3/3
1	OMG	1A	2263	1,55	-	0/9/27/28	0/3/3/3
32	UR3	1a	1498	32	-	0/7/25/26	0/2/2/2
1	5MU	2A	1915	1	-	0/7/25/26	0/2/2/2
32	5MC	1a	1400	32	-	2/7/25/26	0/2/2/2
32	5MC	1a	1407	32	-	0/7/25/26	0/2/2/2
32	5MC	1a	967	32	-	2/7/25/26	0/2/2/2
55	PSU	2x	55	55	-	0/7/25/26	0/2/2/2
1	5MC	2A	1942	1	-	0/7/25/26	0/2/2/2
1	4OC	2A	1920	1	-	0/9/27/30	0/2/2/2
32	5MC	2a	1400	32	-	2/7/25/26	0/2/2/2
32	PSU	2a	516	32	-	0/7/25/26	0/2/2/2
32	MA6	2a	1518	32	-	1/11/29/30	0/3/3/3
32	7MG	2a	527	32	-	0/7/37/38	0/3/3/3
32	2MG	2a	1207	32	-	0/9/27/28	0/3/3/3
1	5MU	1A	1937	1	-	0/7/25/26	0/2/2/2
32	2MG	1a	1207	32	-	0/9/27/28	0/3/3/3
32	4OC	1a	1402	32	-	2/9/29/30	0/2/2/2
1	5MU	2A	1939	1	-	0/7/25/26	0/2/2/2
1	5MC	2A	1962	1	-	0/7/25/26	0/2/2/2
1	2MA	2A	2503	1,56	-	2/7/25/26	0/3/3/3
54	PPU	2w	76	1,54,56	-	5/25/43/44	0/4/4/4
32	M2G	1a	966	32	-	0/11/29/30	0/3/3/3
55	4SU	2x	8	55	-	0/7/25/26	0/2/2/2
55	PSU	1x	55	55	-	0/7/25/26	0/2/2/2
32	5MC	1a	1404	32	-	0/7/25/26	0/2/2/2
32	5MC	2a	1404	32	-	0/7/25/26	0/2/2/2
1	4OC	1A	1942	1	-	1/9/27/30	0/2/2/2
32	MA6	2a	1519	32	-	4/11/29/30	0/3/3/3
32	M2G	2a	966	32	-	4/11/29/30	0/3/3/3
43	0TD	1l	92	43	-	1/7/12/14	-
1	5MC	1A	1964	1	-	0/7/25/26	0/2/2/2
1	PSU	2A	1911	1	-	0/7/25/26	0/2/2/2
32	PSU	1a	516	56,32	-	2/7/25/26	0/2/2/2
55	5MU	2x	54	55	-	0/7/25/26	0/2/2/2
1	2MU	2A	2552	1	-	0/9/27/28	0/2/2/2
32	MA6	1a	1518	32	-	3/11/29/30	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
32	UR3	2a	1498	32	-	0/7/25/26	0/2/2/2
54	PPU	1w	76	1,54	-	5/25/43/44	0/4/4/4
1	5MC	1A	1984	1	-	0/7/25/26	0/2/2/2
32	5MC	2a	967	32	-	0/7/25/26	0/2/2/2
55	5MC	1x	32	55	-	0/7/25/26	0/2/2/2
1	OMG	2A	2251	1,55	-	0/9/27/28	0/3/3/3
55	5MU	1x	54	55	-	0/7/25/26	0/2/2/2
55	4SU	1x	8	55	-	0/7/25/26	0/2/2/2
1	PSU	1A	1933	1	-	0/7/25/26	0/2/2/2
1	PSU	1A	2617	1	-	0/7/25/26	0/2/2/2
1	PSU	2A	1917	1	-	0/7/25/26	0/2/2/2

The worst 5 of 174 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
43	2l	92	0TD	CB-SB	-12.17	1.70	1.82
43	1l	92	0TD	CB-SB	-12.03	1.70	1.82
32	2a	1400	5MC	C5-C4	6.46	1.49	1.44
32	2a	1404	5MC	C5-C4	6.41	1.49	1.44
32	2a	967	5MC	C5-C4	6.29	1.48	1.44

The worst 5 of 301 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
43	2l	92	0TD	CSB-SB-CB	-19.22	67.82	102.36
43	1l	92	0TD	CSB-SB-CB	-18.13	69.78	102.36
32	2a	527	7MG	N9-C4-N3	8.94	138.56	125.46
1	1A	2515	2MA	C5-C4-N3	-8.79	117.92	127.18
32	1a	527	7MG	N9-C4-N3	8.73	138.25	125.46

There are no chirality outliers.

5 of 45 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
43	2l	92	0TD	O-C-CA-CB
32	1a	516	PSU	C2'-C1'-C5-C4
32	1a	516	PSU	C2'-C1'-C5-C6
32	2a	966	M2G	N1-C2-N2-CM2
32	2a	966	M2G	N3-C2-N2-CM1

There are no ring outliers.

30 monomers are involved in 49 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
32	2a	1402	4OC	1	0
1	1A	2515	2MA	1	0
1	1A	2564	2MU	1	0
1	1A	1939	PSU	1	0
32	1a	1519	MA6	3	0
1	1A	2263	OMG	3	0
32	1a	967	5MC	1	0
32	2a	1518	MA6	2	0
32	2a	1207	2MG	3	0
1	1A	1937	5MU	1	0
32	1a	1207	2MG	2	0
32	1a	1402	4OC	3	0
1	2A	1939	5MU	1	0
1	2A	1962	5MC	1	0
1	2A	2503	2MA	2	0
54	2w	76	PPU	3	0
32	1a	966	M2G	2	0
55	2x	8	4SU	2	0
32	2a	1404	5MC	1	0
1	1A	1942	4OC	2	0
32	2a	1519	MA6	2	0
1	2A	1911	PSU	1	0
55	2x	54	5MU	2	0
1	2A	2552	2MU	1	0
32	1a	1518	MA6	4	0
32	2a	1498	UR3	1	0
54	1w	76	PPU	2	0
1	1A	1984	5MC	1	0
55	1x	54	5MU	2	0
55	1x	8	4SU	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides 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	-	-	-		
58	SF4	2d	302	35	0,12,12	-	-	-		

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
58	SF4	1d	302	35	-	-	0/6/5/5
58	SF4	2d	302	35	-	-	0/6/5/5

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 4 short contacts:

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

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
3	2D	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	2D	7:LYS	C	8:PRO	N	1.17

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%)	0.14	95 (3%)	49	31	82, 102, 143, 157	0
1	2A	2789/2915 (95%)	-0.01	81 (2%)	53	33	88, 107, 136, 157	0
2	1B	120/121 (99%)	-0.41	0	100	100	104, 121, 132, 134	0
2	2B	120/121 (99%)	-0.28	0	100	100	111, 125, 135, 152	0
3	1D	275/276 (99%)	0.59	25 (9%)	15	13	84, 95, 108, 127	0
3	2D	275/276 (99%)	0.82	31 (11%)	10	11	88, 104, 114, 123	0
4	1E	204/206 (99%)	0.55	27 (13%)	7	9	86, 108, 122, 131	0
4	2E	204/206 (99%)	0.05	13 (6%)	25	18	88, 105, 119, 129	0
5	1F	203/210 (96%)	-0.07	5 (2%)	58	36	79, 102, 120, 137	0
5	2F	203/210 (96%)	0.64	34 (16%)	4	6	90, 108, 122, 130	0
6	1G	181/182 (99%)	0.24	7 (3%)	43	28	112, 122, 131, 139	0
6	2G	181/182 (99%)	0.08	2 (1%)	78	53	113, 126, 136, 149	0
7	1H	174/180 (96%)	0.11	4 (2%)	61	38	96, 113, 124, 131	0
7	2H	174/180 (96%)	-0.15	0	100	100	105, 125, 134, 142	0
8	1I	146/148 (98%)	-0.10	3 (2%)	63	40	102, 115, 124, 134	0
8	2I	146/148 (98%)	0.55	10 (6%)	23	17	109, 124, 138, 143	0
9	1N	140/140 (100%)	0.19	7 (5%)	34	22	93, 106, 119, 122	0
9	2N	140/140 (100%)	0.49	8 (5%)	29	20	97, 111, 122, 135	0
10	1O	122/122 (100%)	0.32	2 (1%)	70	45	90, 108, 122, 128	0
10	2O	122/122 (100%)	0.36	3 (2%)	58	36	87, 102, 113, 118	0
11	1P	149/150 (99%)	0.40	6 (4%)	42	27	85, 109, 124, 130	0
11	2P	149/150 (99%)	-0.04	3 (2%)	65	41	90, 115, 126, 134	0
12	1Q	141/141 (100%)	0.34	8 (5%)	29	20	89, 108, 119, 127	0
12	2Q	141/141 (100%)	-0.09	1 (0%)	84	63	96, 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%)	0.33	6 (5%) 33 22	94, 104, 116, 125	0
13	2R	118/118 (100%)	0.57	13 (11%) 10 11	89, 103, 111, 118	0
14	1S	110/112 (98%)	0.18	5 (4%) 38 24	106, 116, 125, 131	0
14	2S	110/112 (98%)	0.17	2 (1%) 67 42	106, 119, 127, 130	0
15	1T	131/146 (89%)	0.21	7 (5%) 32 21	95, 110, 123, 138	0
15	2T	131/146 (89%)	0.14	5 (3%) 44 28	92, 106, 121, 129	0
16	1U	116/118 (98%)	0.31	5 (4%) 40 25	86, 105, 119, 134	0
16	2U	116/118 (98%)	0.84	21 (18%) 3 4	94, 109, 121, 125	0
17	1V	101/101 (100%)	0.00	2 (1%) 65 41	88, 106, 120, 127	0
17	2V	101/101 (100%)	0.02	1 (0%) 79 55	93, 114, 127, 136	0
18	1W	112/113 (99%)	0.27	3 (2%) 56 35	88, 101, 120, 131	0
18	2W	112/113 (99%)	0.06	2 (1%) 67 42	87, 101, 113, 129	0
19	1X	95/96 (98%)	0.12	0 100 100	87, 98, 116, 125	0
19	2X	95/96 (98%)	0.51	5 (5%) 32 21	98, 107, 127, 132	0
20	1Y	107/110 (97%)	0.23	1 (0%) 81 58	86, 108, 121, 126	0
20	2Y	107/110 (97%)	0.31	3 (2%) 55 34	91, 113, 126, 133	0
21	1Z	154/206 (74%)	-0.02	3 (1%) 66 42	109, 120, 132, 138	0
21	2Z	160/206 (77%)	-0.28	0 100 100	111, 123, 131, 135	0
22	10	83/85 (97%)	0.21	1 (1%) 76 51	94, 108, 116, 124	0
22	20	83/85 (97%)	0.29	4 (4%) 35 23	101, 114, 122, 125	0
23	11	97/98 (98%)	0.69	11 (11%) 10 11	87, 101, 121, 131	0
23	21	97/98 (98%)	1.13	17 (17%) 4 5	92, 110, 124, 130	0
24	12	70/72 (97%)	0.19	3 (4%) 40 25	87, 101, 111, 128	0
24	22	70/72 (97%)	0.29	1 (1%) 73 48	106, 116, 126, 129	0
25	13	59/60 (98%)	0.07	0 100 100	86, 107, 121, 139	0
25	23	59/60 (98%)	-0.01	1 (1%) 69 43	99, 108, 131, 143	0
26	14	69/71 (97%)	0.14	0 100 100	121, 130, 141, 147	0
26	24	69/71 (97%)	-0.17	0 100 100	117, 128, 137, 144	0
27	15	59/60 (98%)	0.24	2 (3%) 48 30	89, 103, 117, 122	0
27	25	59/60 (98%)	0.34	5 (8%) 16 14	90, 103, 117, 125	0
28	16	53/54 (98%)	0.34	5 (9%) 14 13	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%)	-0.18	1 (1%) 66 42	105, 114, 124, 134	0
29	17	48/49 (97%)	0.94	6 (12%) 8 10	82, 90, 107, 119	0
29	27	48/49 (97%)	0.67	3 (6%) 26 18	86, 99, 116, 124	0
30	18	64/65 (98%)	1.06	11 (17%) 4 5	89, 100, 111, 120	0
30	28	64/65 (98%)	0.37	3 (4%) 36 23	98, 106, 114, 120	0
31	19	37/37 (100%)	0.25	1 (2%) 56 35	99, 108, 113, 117	0
31	29	37/37 (100%)	0.24	1 (2%) 56 35	105, 116, 127, 130	0
32	1a	1488/1521 (97%)	-0.08	21 (1%) 73 48	92, 123, 141, 160	0
32	2a	1491/1521 (98%)	-0.14	19 (1%) 75 50	97, 119, 138, 155	0
33	1b	231/256 (90%)	-0.03	1 (0%) 88 72	113, 127, 135, 144	0
33	2b	231/256 (90%)	0.10	2 (0%) 81 58	105, 126, 137, 143	0
34	1c	206/239 (86%)	-0.03	0 100 100	113, 129, 137, 141	0
34	2c	206/239 (86%)	-0.25	0 100 100	115, 124, 132, 141	0
35	1d	208/209 (99%)	0.65	19 (9%) 15 13	104, 121, 131, 137	0
35	2d	208/209 (99%)	0.13	4 (1%) 66 42	104, 117, 128, 136	0
36	1e	148/162 (91%)	-0.03	0 100 100	103, 119, 127, 133	0
36	2e	148/162 (91%)	0.17	6 (4%) 41 26	107, 117, 128, 136	0
37	1f	100/101 (99%)	0.22	6 (6%) 27 19	101, 117, 126, 133	0
37	2f	100/101 (99%)	0.03	0 100 100	105, 118, 127, 132	0
38	1g	155/156 (99%)	-0.08	5 (3%) 50 31	111, 125, 135, 141	0
38	2g	155/156 (99%)	-0.17	5 (3%) 50 31	112, 124, 135, 145	0
39	1h	137/138 (99%)	-0.12	0 100 100	108, 122, 129, 134	0
39	2h	137/138 (99%)	0.16	4 (2%) 53 33	103, 118, 127, 135	0
40	1i	127/128 (99%)	0.60	12 (9%) 14 13	114, 128, 135, 139	0
40	2i	127/128 (99%)	0.83	16 (12%) 8 9	115, 127, 135, 144	0
41	1j	97/105 (92%)	0.44	6 (6%) 26 18	121, 131, 138, 143	0
41	2j	96/105 (91%)	0.54	5 (5%) 33 22	118, 129, 137, 142	0
42	1k	114/129 (88%)	0.22	6 (5%) 32 21	103, 117, 126, 130	0
42	2k	114/129 (88%)	0.40	7 (6%) 27 18	107, 120, 129, 137	0
43	1l	121/132 (91%)	0.09	5 (4%) 41 26	103, 117, 124, 136	0
43	2l	121/132 (91%)	0.07	5 (4%) 41 26	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%)	0.04	0 100 100	113, 125, 133, 139	0
44	2m	122/126 (96%)	0.67	12 (9%) 13 13	111, 125, 136, 147	0
45	1n	60/61 (98%)	0.37	0 100 100	118, 128, 137, 144	0
45	2n	60/61 (98%)	0.13	1 (1%) 69 43	114, 124, 130, 134	0
46	1o	88/89 (98%)	0.30	4 (4%) 38 24	101, 116, 122, 124	0
46	2o	88/89 (98%)	0.25	3 (3%) 48 30	101, 119, 127, 132	0
47	1p	82/88 (93%)	0.39	2 (2%) 59 37	115, 124, 131, 137	0
47	2p	82/88 (93%)	0.09	3 (3%) 45 28	99, 111, 118, 123	0
48	1q	99/105 (94%)	0.28	6 (6%) 27 18	103, 118, 125, 131	0
48	2q	99/105 (94%)	0.03	3 (3%) 52 32	102, 113, 122, 126	0
49	1r	68/88 (77%)	-0.15	0 100 100	109, 116, 125, 130	0
49	2r	68/88 (77%)	-0.07	0 100 100	109, 119, 126, 131	0
50	1s	83/93 (89%)	0.37	4 (4%) 35 23	117, 128, 136, 143	0
50	2s	83/93 (89%)	0.18	1 (1%) 76 51	116, 126, 135, 137	0
51	1t	96/106 (90%)	0.42	5 (5%) 33 22	111, 122, 128, 132	0
51	2t	96/106 (90%)	0.46	11 (11%) 9 11	101, 116, 126, 129	0
52	1u	23/27 (85%)	0.30	0 100 100	119, 126, 129, 131	0
52	2u	23/27 (85%)	0.29	0 100 100	123, 127, 131, 133	0
53	1v	6/24 (25%)	0.55	0 100 100	110, 116, 131, 136	0
53	2v	6/24 (25%)	0.63	1 (16%) 4 6	113, 116, 131, 147	0
54	1w	2/3 (66%)	-0.46	0 100 100	88, 88, 88, 89	0
54	2w	2/3 (66%)	2.08	1 (50%) 0 0	103, 103, 103, 106	0
55	1x	72/77 (93%)	-0.61	0 100 100	90, 118, 130, 140	0
55	2x	72/77 (93%)	-0.09	0 100 100	96, 123, 134, 144	0
All	All	20600/21450 (96%)	0.13	746 (3%) 46 29	79, 114, 134, 160	0

The worst 5 of 746 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
44	2m	124	PRO	9.4
5	2F	87	GLY	9.3
23	21	39	LYS	7.7
23	21	4	VAL	7.4
5	2F	52	LYS	7.3

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
1	5MU	2A	1915	21/22	0.78	0.09	114,120,131,143	0
55	4SU	2x	8	20/21	0.78	0.07	120,133,139,140	0
55	PSU	1x	55	20/21	0.78	0.08	109,117,129,133	0
32	PSU	1a	516	20/21	0.81	0.07	113,120,128,129	0
55	PSU	2x	55	20/21	0.83	0.10	114,125,136,143	0
1	PSU	1A	1933	20/21	0.84	0.08	90,105,108,109	0
1	5MU	2A	1939	21/22	0.84	0.15	89,98,104,114	0
55	5MU	1x	54	21/22	0.85	0.07	111,118,130,131	0
55	5MU	2x	54	21/22	0.86	0.10	108,120,136,142	0
55	5MC	1x	32	21/22	0.86	0.10	99,116,123,128	0
32	2MG	2a	1207	24/25	0.86	0.10	114,124,129,137	0
1	5MU	1A	1937	21/22	0.88	0.08	115,126,133,144	0
1	PSU	2A	1911	20/21	0.88	0.10	96,105,117,118	0
32	PSU	2a	516	20/21	0.88	0.07	117,122,126,128	0
32	5MC	2a	967	21/22	0.88	0.13	102,116,124,125	0
1	PSU	2A	1917	20/21	0.88	0.09	106,110,120,127	0
55	4SU	1x	8	20/21	0.88	0.06	111,122,128,128	0
32	5MC	1a	967	21/22	0.89	0.10	104,115,127,130	0
32	7MG	1a	527	24/25	0.89	0.10	101,115,123,126	0
1	5MC	1A	1964	21/22	0.90	0.09	82,93,104,111	0
32	5MC	1a	1407	21/22	0.90	0.09	100,110,116,121	0
32	2MG	1a	1207	24/25	0.90	0.07	114,124,132,136	0
1	4OC	2A	1920	21/23	0.91	0.11	94,114,119,120	0
32	5MC	1a	1400	21/22	0.91	0.09	106,115,124,131	0
32	5MC	2a	1400	21/22	0.91	0.13	101,114,128,132	0
32	4OC	2a	1402	22/23	0.91	0.10	104,109,115,116	0
1	4OC	1A	1942	21/23	0.91	0.09	96,108,120,123	0
32	7MG	2a	527	24/25	0.91	0.10	99,117,123,125	0
32	M2G	1a	966	25/26	0.92	0.09	104,110,120,121	0
1	5MC	2A	1962	21/22	0.92	0.15	79,100,106,110	0
1	PSU	2A	2605	20/21	0.92	0.10	81,91,98,102	0
1	5MC	2A	1942	21/22	0.92	0.11	88,97,104,108	0
1	5MU	1A	1961	21/22	0.93	0.09	85,92,100,103	0
55	5MC	2x	32	21/22	0.93	0.10	110,118,124,126	0
1	PSU	1A	2617	20/21	0.93	0.11	81,90,100,100	0
32	UR3	1a	1498	21/22	0.93	0.09	96,107,111,114	0
32	M2G	2a	966	25/26	0.93	0.14	107,119,123,126	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
32	4OC	1a	1402	22/23	0.93	0.09	104,112,120,123	0
32	MA6	2a	1518	24/25	0.94	0.13	100,109,116,117	0
54	PPU	2w	76	37/38	0.94	0.16	86,100,107,111	0
1	PSU	1A	1939	20/21	0.94	0.05	95,110,117,117	0
1	2MU	1A	2564	21/23	0.94	0.10	85,95,105,109	0
1	2MU	2A	2552	21/23	0.94	0.09	84,90,101,104	0
1	5MC	1A	1984	21/22	0.95	0.08	87,96,104,106	0
43	0TD	1l	92	10/11	0.95	0.09	110,119,124,142	0
32	5MC	1a	1404	21/22	0.95	0.09	95,106,113,115	0
32	5MC	2a	1404	21/22	0.95	0.09	101,111,116,121	0
1	2MA	1A	2515	23/24	0.95	0.12	76,84,97,103	0
32	5MC	2a	1407	21/22	0.95	0.09	90,106,116,118	0
1	2MA	2A	2503	23/24	0.95	0.13	81,92,103,114	0
43	0TD	2l	92	10/11	0.95	0.12	117,123,129,141	0
32	MA6	1a	1519	24/25	0.95	0.11	93,107,119,119	0
54	PPU	1w	76	37/38	0.96	0.12	84,91,103,108	0
32	MA6	1a	1518	24/25	0.96	0.10	103,109,113,116	0
1	OMG	1A	2263	24/25	0.96	0.10	70,88,102,105	0
32	UR3	2a	1498	21/22	0.96	0.09	95,105,114,115	0
32	MA6	2a	1519	24/25	0.96	0.11	93,107,112,116	0
1	OMG	2A	2251	24/25	0.97	0.08	85,96,109,111	0

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	1A	3416	1/1	0.17	0.30	103,103,103,103	0
56	MG	1a	1607	1/1	0.27	0.36	100,100,100,100	0
56	MG	1A	3426	1/1	0.32	0.37	89,89,89,89	0
56	MG	1A	3172	1/1	0.37	0.40	96,96,96,96	0
56	MG	1a	1629	1/1	0.38	0.13	94,94,94,94	0
56	MG	1A	3072	1/1	0.41	0.20	79,79,79,79	0
56	MG	1B	202	1/1	0.42	0.26	80,80,80,80	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	1A	3008	1/1	0.43	0.25	109,109,109,109	0
56	MG	1a	1669	1/1	0.44	0.09	102,102,102,102	0
56	MG	2A	3037	1/1	0.45	0.30	90,90,90,90	0
56	MG	2A	3305	1/1	0.45	0.36	83,83,83,83	0
56	MG	2a	3011	1/1	0.46	0.25	94,94,94,94	0
56	MG	1A	3396	1/1	0.48	0.36	84,84,84,84	0
56	MG	2A	3098	1/1	0.49	0.22	97,97,97,97	0
56	MG	2A	3181	1/1	0.50	0.18	101,101,101,101	0
56	MG	1A	3263	1/1	0.50	0.29	105,105,105,105	0
56	MG	1a	1617	1/1	0.50	0.21	91,91,91,91	0
56	MG	2a	3046	1/1	0.50	0.19	99,99,99,99	0
56	MG	2A	3245	1/1	0.51	0.38	64,64,64,64	0
56	MG	1B	203	1/1	0.51	0.19	106,106,106,106	0
56	MG	2A	3150	1/1	0.51	0.17	101,101,101,101	0
56	MG	1A	3059	1/1	0.51	0.33	92,92,92,92	0
56	MG	2A	3114	1/1	0.52	0.33	75,75,75,75	0
56	MG	2A	3205	1/1	0.52	0.41	81,81,81,81	0
56	MG	1A	3397	1/1	0.52	0.28	84,84,84,84	0
56	MG	2A	3094	1/1	0.53	0.33	83,83,83,83	0
56	MG	1a	1633	1/1	0.53	0.31	97,97,97,97	0
56	MG	2A	3151	1/1	0.53	0.23	109,109,109,109	0
56	MG	2a	3088	1/1	0.53	0.35	83,83,83,83	0
56	MG	1A	3138	1/1	0.54	0.17	108,108,108,108	0
56	MG	1a	1611	1/1	0.55	0.20	93,93,93,93	0
56	MG	2A	3078	1/1	0.55	0.35	79,79,79,79	0
56	MG	1A	3347	1/1	0.56	0.20	90,90,90,90	0
56	MG	1A	3102	1/1	0.56	0.34	74,74,74,74	0
56	MG	1A	3034	1/1	0.56	0.26	91,91,91,91	0
56	MG	2a	3008	1/1	0.57	0.14	102,102,102,102	0
56	MG	1a	1631	1/1	0.57	0.15	97,97,97,97	0
56	MG	2A	3259	1/1	0.57	0.46	72,72,72,72	0
56	MG	2A	3155	1/1	0.57	0.26	92,92,92,92	0
56	MG	1a	1647	1/1	0.58	0.13	106,106,106,106	0
56	MG	1B	201	1/1	0.58	0.20	82,82,82,82	0
56	MG	2A	3175	1/1	0.58	0.23	107,107,107,107	0
56	MG	2A	3373	1/1	0.58	0.42	69,69,69,69	0
56	MG	1A	3240	1/1	0.58	0.39	66,66,66,66	0
56	MG	2A	3198	1/1	0.58	0.26	96,96,96,96	0
56	MG	1A	3352	1/1	0.58	0.24	101,101,101,101	0
56	MG	2A	3239	1/1	0.58	0.29	68,68,68,68	0
56	MG	1A	3115	1/1	0.59	0.13	89,89,89,89	0
56	MG	2A	3336	1/1	0.59	0.31	91,91,91,91	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	1A	3027	1/1	0.59	0.28	78,78,78,78	0
56	MG	1A	3258	1/1	0.59	0.27	98,98,98,98	0
56	MG	1A	3358	1/1	0.59	0.38	75,75,75,75	0
56	MG	2A	3157	1/1	0.59	0.32	88,88,88,88	0
56	MG	1A	3479	1/1	0.59	0.38	72,72,72,72	0
56	MG	1A	3124	1/1	0.60	0.20	75,75,75,75	0
56	MG	1a	1671	1/1	0.60	0.27	99,99,99,99	0
56	MG	1a	1674	1/1	0.60	0.23	92,92,92,92	0
56	MG	2A	3014	1/1	0.60	0.15	90,90,90,90	0
56	MG	2A	3315	1/1	0.60	0.37	68,68,68,68	0
56	MG	2A	3031	1/1	0.60	0.25	89,89,89,89	0
56	MG	1a	1640	1/1	0.60	0.16	91,91,91,91	0
56	MG	2A	3039	1/1	0.60	0.30	93,93,93,93	0
56	MG	2A	3049	1/1	0.60	0.23	73,73,73,73	0
56	MG	1A	3159	1/1	0.60	0.17	81,81,81,81	0
56	MG	1a	1665	1/1	0.60	0.19	74,74,74,74	0
56	MG	1A	3377	1/1	0.61	0.30	77,77,77,77	0
56	MG	1A	3322	1/1	0.61	0.22	94,94,94,94	0
56	MG	1A	3313	1/1	0.61	0.31	70,70,70,70	0
56	MG	1A	3360	1/1	0.61	0.30	82,82,82,82	0
56	MG	2A	3101	1/1	0.61	0.36	80,80,80,80	0
56	MG	2A	3294	1/1	0.61	0.22	87,87,87,87	0
56	MG	1A	3370	1/1	0.61	0.23	88,88,88,88	0
56	MG	1A	3444	1/1	0.62	0.09	109,109,109,109	0
56	MG	1B	212	1/1	0.62	0.23	83,83,83,83	0
56	MG	2B	202	1/1	0.62	0.21	87,87,87,87	0
56	MG	1A	3289	1/1	0.62	0.28	84,84,84,84	0
56	MG	1A	3410	1/1	0.62	0.32	83,83,83,83	0
56	MG	1A	3438	1/1	0.62	0.36	84,84,84,84	0
56	MG	2A	3090	1/1	0.62	0.09	110,110,110,110	0
56	MG	2A	3208	1/1	0.63	0.18	82,82,82,82	0
56	MG	2A	3337	1/1	0.63	0.17	87,87,87,87	0
56	MG	2A	3352	1/1	0.63	0.16	107,107,107,107	0
56	MG	1A	3245	1/1	0.63	0.20	81,81,81,81	0
56	MG	1A	3343	1/1	0.63	0.32	80,80,80,80	0
56	MG	1A	3211	1/1	0.63	0.24	93,93,93,93	0
56	MG	1A	3434	1/1	0.63	0.29	72,72,72,72	0
56	MG	1A	3308	1/1	0.63	0.23	76,76,76,76	0
56	MG	2a	3066	1/1	0.63	0.22	86,86,86,86	0
56	MG	1A	3262	1/1	0.63	0.18	82,82,82,82	0
56	MG	1A	3009	1/1	0.64	0.23	84,84,84,84	0
56	MG	1A	3020	1/1	0.64	0.19	84,84,84,84	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	1A	3001	1/1	0.64	0.16	80,80,80,80	0
56	MG	2a	3022	1/1	0.64	0.22	81,81,81,81	0
56	MG	2A	3351	1/1	0.64	0.25	94,94,94,94	0
56	MG	1a	1678	1/1	0.64	0.17	89,89,89,89	0
56	MG	1a	1681	1/1	0.64	0.35	79,79,79,79	0
56	MG	1a	1632	1/1	0.65	0.34	88,88,88,88	0
56	MG	1A	3443	1/1	0.65	0.20	91,91,91,91	0
56	MG	1A	3039	1/1	0.65	0.16	71,71,71,71	0
56	MG	2A	3097	1/1	0.65	0.20	93,93,93,93	0
56	MG	2A	3235	1/1	0.65	0.31	75,75,75,75	0
56	MG	1A	3414	1/1	0.65	0.46	70,70,70,70	0
56	MG	1A	3369	1/1	0.65	0.29	76,76,76,76	0
56	MG	2A	3258	1/1	0.65	0.40	80,80,80,80	0
56	MG	2a	3097	1/1	0.65	0.19	74,74,74,74	0
56	MG	1A	3187	1/1	0.66	0.15	83,83,83,83	0
56	MG	1A	3040	1/1	0.66	0.36	79,79,79,79	0
56	MG	2A	3019	1/1	0.66	0.31	69,69,69,69	0
56	MG	2a	3029	1/1	0.66	0.21	104,104,104,104	0
56	MG	1A	3341	1/1	0.66	0.25	77,77,77,77	0
56	MG	1A	3051	1/1	0.66	0.17	89,89,89,89	0
56	MG	1a	1679	1/1	0.66	0.18	107,107,107,107	0
56	MG	2A	3306	1/1	0.66	0.28	80,80,80,80	0
56	MG	15	101	1/1	0.67	0.27	70,70,70,70	0
56	MG	2a	3041	1/1	0.67	0.15	80,80,80,80	0
56	MG	1a	1641	1/1	0.67	0.21	82,82,82,82	0
56	MG	1A	3095	1/1	0.67	0.24	69,69,69,69	0
56	MG	1A	3129	1/1	0.67	0.11	77,77,77,77	0
56	MG	1A	3260	1/1	0.67	0.26	81,81,81,81	0
56	MG	1A	3236	1/1	0.68	0.28	102,102,102,102	0
56	MG	1A	3180	1/1	0.68	0.30	61,61,61,61	0
56	MG	1A	3390	1/1	0.68	0.31	61,61,61,61	0
56	MG	2D	3100	1/1	0.68	0.25	83,83,83,83	0
56	MG	1A	3068	1/1	0.68	0.36	75,75,75,75	0
56	MG	2A	3052	1/1	0.68	0.25	86,86,86,86	0
56	MG	1A	3088	1/1	0.68	0.26	74,74,74,74	0
56	MG	1A	3361	1/1	0.68	0.24	94,94,94,94	0
56	MG	2A	3004	1/1	0.68	0.24	88,88,88,88	0
56	MG	2A	3095	1/1	0.68	0.24	81,81,81,81	0
56	MG	1A	3453	1/1	0.68	0.23	80,80,80,80	0
56	MG	1A	3303	1/1	0.68	0.21	83,83,83,83	0
56	MG	2A	3209	1/1	0.68	0.13	77,77,77,77	0
56	MG	1A	3252	1/1	0.69	0.30	80,80,80,80	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	1a	1618	1/1	0.69	0.13	96,96,96,96	0
56	MG	1A	3219	1/1	0.69	0.27	90,90,90,90	0
56	MG	1A	3140	1/1	0.69	0.24	73,73,73,73	0
56	MG	1A	3400	1/1	0.69	0.21	87,87,87,87	0
56	MG	1A	3405	1/1	0.69	0.30	93,93,93,93	0
56	MG	1a	1634	1/1	0.69	0.21	102,102,102,102	0
56	MG	1a	1686	1/1	0.69	0.27	76,76,76,76	0
56	MG	2A	3229	1/1	0.69	0.25	72,72,72,72	0
56	MG	1a	1687	1/1	0.69	0.15	100,100,100,100	0
56	MG	1a	1689	1/1	0.69	0.30	78,78,78,78	0
56	MG	1A	3086	1/1	0.69	0.21	90,90,90,90	0
56	MG	2A	3254	1/1	0.69	0.32	82,82,82,82	0
56	MG	2A	3107	1/1	0.69	0.37	81,81,81,81	0
56	MG	1A	3065	1/1	0.69	0.29	88,88,88,88	0
56	MG	2A	3266	1/1	0.69	0.23	69,69,69,69	0
56	MG	1A	3464	1/1	0.69	0.19	95,95,95,95	0
56	MG	1a	1649	1/1	0.69	0.24	106,106,106,106	0
56	MG	1A	3469	1/1	0.70	0.29	88,88,88,88	0
56	MG	2A	3030	1/1	0.70	0.09	91,91,91,91	0
56	MG	1A	3109	1/1	0.70	0.26	92,92,92,92	0
56	MG	2A	3171	1/1	0.70	0.19	94,94,94,94	0
56	MG	2A	3267	1/1	0.70	0.30	81,81,81,81	0
56	MG	1A	3454	1/1	0.70	0.22	73,73,73,73	0
56	MG	1A	3188	1/1	0.70	0.34	62,62,62,62	0
56	MG	2a	3071	1/1	0.70	0.31	75,75,75,75	0
56	MG	2B	207	1/1	0.70	0.28	84,84,84,84	0
56	MG	2A	3042	1/1	0.70	0.18	75,75,75,75	0
56	MG	1r	101	1/1	0.71	0.23	81,81,81,81	0
56	MG	2A	3001	1/1	0.71	0.29	80,80,80,80	0
56	MG	1A	3234	1/1	0.71	0.37	85,85,85,85	0
56	MG	1A	3477	1/1	0.71	0.34	61,61,61,61	0
56	MG	2A	3357	1/1	0.71	0.28	69,69,69,69	0
56	MG	2A	3371	1/1	0.71	0.27	62,62,62,62	0
56	MG	1A	3130	1/1	0.71	0.23	84,84,84,84	0
56	MG	2A	3027	1/1	0.71	0.27	83,83,83,83	0
56	MG	2A	3238	1/1	0.71	0.33	67,67,67,67	0
56	MG	1A	3137	1/1	0.71	0.40	61,61,61,61	0
56	MG	1A	3017	1/1	0.71	0.41	61,61,61,61	0
56	MG	1A	3048	1/1	0.71	0.34	69,69,69,69	0
56	MG	1B	209	1/1	0.71	0.10	122,122,122,122	0
56	MG	1A	3194	1/1	0.71	0.09	92,92,92,92	0
56	MG	10	102	1/1	0.71	0.11	73,73,73,73	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	2A	3166	1/1	0.71	0.16	94,94,94,94	0
56	MG	1A	3113	1/1	0.71	0.10	77,77,77,77	0
56	MG	2A	3173	1/1	0.71	0.32	78,78,78,78	0
56	MG	2A	3055	1/1	0.71	0.27	82,82,82,82	0
56	MG	1A	3167	1/1	0.71	0.23	80,80,80,80	0
56	MG	1B	207	1/1	0.72	0.16	106,106,106,106	0
56	MG	2A	3369	1/1	0.72	0.24	70,70,70,70	0
56	MG	1A	3449	1/1	0.72	0.30	83,83,83,83	0
56	MG	1A	3014	1/1	0.72	0.13	86,86,86,86	0
56	MG	1A	3118	1/1	0.72	0.26	75,75,75,75	0
56	MG	1A	3171	1/1	0.72	0.26	76,76,76,76	0
56	MG	1a	1603	1/1	0.72	0.20	94,94,94,94	0
56	MG	1A	3375	1/1	0.72	0.27	95,95,95,95	0
56	MG	2A	3015	1/1	0.72	0.32	76,76,76,76	0
56	MG	2A	3186	1/1	0.72	0.26	92,92,92,92	0
56	MG	1A	3349	1/1	0.72	0.17	80,80,80,80	0
56	MG	1A	3083	1/1	0.72	0.22	83,83,83,83	0
56	MG	2A	3206	1/1	0.72	0.19	78,78,78,78	0
56	MG	1A	3491	1/1	0.72	0.19	91,91,91,91	0
56	MG	1A	3355	1/1	0.72	0.13	71,71,71,71	0
56	MG	2a	3085	1/1	0.72	0.23	92,92,92,92	0
56	MG	1A	3114	1/1	0.72	0.32	82,82,82,82	0
56	MG	1A	3157	1/1	0.72	0.32	79,79,79,79	0
56	MG	2A	3093	1/1	0.73	0.25	82,82,82,82	0
56	MG	2A	3243	1/1	0.73	0.28	64,64,64,64	0
56	MG	1B	210	1/1	0.73	0.15	96,96,96,96	0
56	MG	1A	3316	1/1	0.73	0.22	63,63,63,63	0
56	MG	1A	3047	1/1	0.73	0.27	67,67,67,67	0
56	MG	2B	206	1/1	0.73	0.23	89,89,89,89	0
56	MG	1A	3447	1/1	0.73	0.30	78,78,78,78	0
56	MG	1A	3424	1/1	0.73	0.34	61,61,61,61	0
56	MG	2a	3001	1/1	0.73	0.16	80,80,80,80	0
56	MG	1A	3077	1/1	0.73	0.33	81,81,81,81	0
56	MG	2A	3281	1/1	0.73	0.24	73,73,73,73	0
56	MG	2a	3014	1/1	0.73	0.15	81,81,81,81	0
56	MG	1A	3383	1/1	0.73	0.17	73,73,73,73	0
56	MG	2A	3141	1/1	0.73	0.47	81,81,81,81	0
56	MG	2a	3034	1/1	0.73	0.15	78,78,78,78	0
56	MG	2A	3147	1/1	0.73	0.28	75,75,75,75	0
56	MG	2A	3310	1/1	0.73	0.27	67,67,67,67	0
56	MG	1A	3437	1/1	0.73	0.11	99,99,99,99	0
56	MG	2A	3084	1/1	0.73	0.17	79,79,79,79	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	1A	3144	1/1	0.73	0.32	87,87,87,87	0
56	MG	2A	3236	1/1	0.73	0.34	66,66,66,66	0
56	MG	2a	3092	1/1	0.73	0.13	82,82,82,82	0
56	MG	2A	3092	1/1	0.73	0.27	75,75,75,75	0
56	MG	2a	3099	1/1	0.73	0.23	79,79,79,79	0
56	MG	2A	3022	1/1	0.74	0.30	66,66,66,66	0
56	MG	1A	3189	1/1	0.74	0.26	82,82,82,82	0
56	MG	1A	3407	1/1	0.74	0.24	94,94,94,94	0
56	MG	1A	3339	1/1	0.74	0.25	73,73,73,73	0
56	MG	2A	3275	1/1	0.74	0.29	62,62,62,62	0
56	MG	2A	3153	1/1	0.74	0.12	100,100,100,100	0
56	MG	2A	3291	1/1	0.74	0.24	78,78,78,78	0
56	MG	2A	3293	1/1	0.74	0.24	77,77,77,77	0
56	MG	1A	3456	1/1	0.74	0.32	68,68,68,68	0
56	MG	2A	3301	1/1	0.74	0.16	77,77,77,77	0
56	MG	2A	3003	1/1	0.74	0.29	73,73,73,73	0
56	MG	1A	3241	1/1	0.74	0.31	61,61,61,61	0
56	MG	2A	3009	1/1	0.74	0.12	110,110,110,110	0
56	MG	2A	3314	1/1	0.74	0.24	78,78,78,78	0
56	MG	1A	3202	1/1	0.74	0.14	85,85,85,85	0
56	MG	2A	3318	1/1	0.74	0.29	62,62,62,62	0
56	MG	2a	3061	1/1	0.74	0.24	72,72,72,72	0
56	MG	2A	3334	1/1	0.74	0.29	77,77,77,77	0
56	MG	1A	3420	1/1	0.74	0.29	70,70,70,70	0
56	MG	2A	3180	1/1	0.74	0.16	76,76,76,76	0
56	MG	1A	3290	1/1	0.74	0.21	80,80,80,80	0
56	MG	2A	3247	1/1	0.74	0.23	81,81,81,81	0
56	MG	2a	3095	1/1	0.74	0.11	84,84,84,84	0
56	MG	2A	3185	1/1	0.74	0.20	72,72,72,72	0
56	MG	2A	3359	1/1	0.74	0.14	74,74,74,74	0
56	MG	2A	3377	1/1	0.75	0.12	92,92,92,92	0
56	MG	1A	3237	1/1	0.75	0.26	79,79,79,79	0
56	MG	2A	3202	1/1	0.75	0.27	70,70,70,70	0
56	MG	2A	3034	1/1	0.75	0.18	94,94,94,94	0
56	MG	1B	206	1/1	0.75	0.18	89,89,89,89	0
56	MG	2A	3129	1/1	0.75	0.34	61,61,61,61	0
56	MG	1A	3079	1/1	0.75	0.14	78,78,78,78	0
56	MG	1A	3398	1/1	0.75	0.32	70,70,70,70	0
56	MG	2A	3309	1/1	0.75	0.17	61,61,61,61	0
56	MG	2a	3015	1/1	0.75	0.13	80,80,80,80	0
56	MG	1A	3457	1/1	0.75	0.38	62,62,62,62	0
56	MG	1A	3075	1/1	0.75	0.10	72,72,72,72	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	1A	3292	1/1	0.75	0.23	75,75,75,75	0
56	MG	1A	3471	1/1	0.75	0.31	75,75,75,75	0
56	MG	2A	3083	1/1	0.75	0.19	77,77,77,77	0
56	MG	16	101	1/1	0.75	0.30	75,75,75,75	0
56	MG	1A	3069	1/1	0.75	0.23	81,81,81,81	0
56	MG	1A	3340	1/1	0.75	0.41	61,61,61,61	0
56	MG	1a	1609	1/1	0.75	0.10	103,103,103,103	0
56	MG	1A	3387	1/1	0.75	0.22	80,80,80,80	0
56	MG	2A	3261	1/1	0.75	0.31	72,72,72,72	0
56	MG	1A	3415	1/1	0.75	0.51	80,80,80,80	0
56	MG	2A	3029	1/1	0.75	0.25	70,70,70,70	0
56	MG	1A	3304	1/1	0.75	0.41	61,61,61,61	0
56	MG	2d	301	1/1	0.75	0.07	81,81,81,81	0
56	MG	1a	1652	1/1	0.76	0.18	74,74,74,74	0
56	MG	1A	3423	1/1	0.76	0.34	62,62,62,62	0
56	MG	2A	3063	1/1	0.76	0.20	79,79,79,79	0
56	MG	1B	208	1/1	0.76	0.13	81,81,81,81	0
56	MG	2A	3081	1/1	0.76	0.30	76,76,76,76	0
56	MG	2A	3152	1/1	0.76	0.31	81,81,81,81	0
56	MG	1A	3329	1/1	0.76	0.20	74,74,74,74	0
56	MG	1a	1621	1/1	0.76	0.31	73,73,73,73	0
56	MG	2A	3311	1/1	0.76	0.28	79,79,79,79	0
56	MG	1A	3445	1/1	0.76	0.34	78,78,78,78	0
56	MG	1A	3044	1/1	0.76	0.16	83,83,83,83	0
56	MG	1V	202	1/1	0.76	0.29	68,68,68,68	0
56	MG	2A	3320	1/1	0.76	0.26	74,74,74,74	0
56	MG	1A	3428	1/1	0.76	0.48	61,61,61,61	0
56	MG	1A	3433	1/1	0.76	0.35	75,75,75,75	0
56	MG	1A	3078	1/1	0.76	0.42	80,80,80,80	0
56	MG	1A	3032	1/1	0.76	0.21	77,77,77,77	0
56	MG	2A	3184	1/1	0.76	0.36	70,70,70,70	0
56	MG	2a	3073	1/1	0.76	0.14	76,76,76,76	0
56	MG	1x	102	1/1	0.76	0.12	85,85,85,85	0
56	MG	1A	3228	1/1	0.76	0.30	77,77,77,77	0
56	MG	2A	3365	1/1	0.76	0.38	67,67,67,67	0
56	MG	1A	3461	1/1	0.76	0.35	83,83,83,83	0
56	MG	2A	3276	1/1	0.76	0.43	74,74,74,74	0
56	MG	2A	3122	1/1	0.76	0.36	85,85,85,85	0
56	MG	2A	3376	1/1	0.76	0.17	72,72,72,72	0
56	MG	1A	3452	1/1	0.77	0.23	76,76,76,76	0
56	MG	1A	3291	1/1	0.77	0.21	77,77,77,77	0
56	MG	1A	3101	1/1	0.77	0.16	74,74,74,74	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	2Q	202	1/1	0.77	0.12	69,69,69,69	0
56	MG	1A	3226	1/1	0.77	0.12	79,79,79,79	0
56	MG	1A	3165	1/1	0.77	0.16	84,84,84,84	0
56	MG	1A	3231	1/1	0.77	0.20	65,65,65,65	0
56	MG	1A	3143	1/1	0.77	0.20	62,62,62,62	0
56	MG	2A	3007	1/1	0.77	0.22	78,78,78,78	0
56	MG	1A	3465	1/1	0.77	0.27	61,61,61,61	0
56	MG	1A	3004	1/1	0.77	0.13	89,89,89,89	0
56	MG	1a	1662	1/1	0.77	0.16	94,94,94,94	0
56	MG	1A	3435	1/1	0.77	0.23	90,90,90,90	0
56	MG	1a	1667	1/1	0.77	0.17	78,78,78,78	0
56	MG	1A	3154	1/1	0.77	0.14	77,77,77,77	0
56	MG	1A	3406	1/1	0.77	0.27	76,76,76,76	0
56	MG	1A	3325	1/1	0.77	0.39	70,70,70,70	0
56	MG	2A	3271	1/1	0.77	0.26	63,63,63,63	0
56	MG	2A	3100	1/1	0.77	0.34	74,74,74,74	0
56	MG	1A	3279	1/1	0.77	0.25	65,65,65,65	0
56	MG	1A	3336	1/1	0.77	0.31	64,64,64,64	0
56	MG	2A	3111	1/1	0.77	0.09	76,76,76,76	0
56	MG	1A	3239	1/1	0.77	0.09	90,90,90,90	0
56	MG	1A	3100	1/1	0.77	0.21	86,86,86,86	0
56	MG	2A	3297	1/1	0.77	0.30	77,77,77,77	0
56	MG	2A	3193	1/1	0.78	0.10	87,87,87,87	0
56	MG	2A	3374	1/1	0.78	0.40	62,62,62,62	0
56	MG	1A	3186	1/1	0.78	0.21	84,84,84,84	0
56	MG	1A	3264	1/1	0.78	0.18	83,83,83,83	0
56	MG	2A	3126	1/1	0.78	0.17	76,76,76,76	0
56	MG	1A	3270	1/1	0.78	0.27	62,62,62,62	0
56	MG	1A	3274	1/1	0.78	0.24	74,74,74,74	0
56	MG	1a	1651	1/1	0.78	0.42	71,71,71,71	0
56	MG	2A	3221	1/1	0.78	0.23	80,80,80,80	0
56	MG	1A	3106	1/1	0.78	0.25	73,73,73,73	0
56	MG	1a	1655	1/1	0.78	0.22	84,84,84,84	0
56	MG	1A	3285	1/1	0.78	0.23	83,83,83,83	0
56	MG	2A	3087	1/1	0.78	0.18	68,68,68,68	0
56	MG	1A	3247	1/1	0.78	0.42	69,69,69,69	0
56	MG	1A	3099	1/1	0.78	0.18	98,98,98,98	0
56	MG	2a	3025	1/1	0.78	0.34	81,81,81,81	0
56	MG	1A	3221	1/1	0.78	0.33	86,86,86,86	0
56	MG	1A	3028	1/1	0.78	0.16	107,107,107,107	0
56	MG	1A	3378	1/1	0.78	0.22	77,77,77,77	0
56	MG	1A	3293	1/1	0.78	0.24	84,84,84,84	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	2a	3056	1/1	0.78	0.21	82,82,82,82	0
56	MG	2A	3176	1/1	0.78	0.15	79,79,79,79	0
56	MG	2A	3340	1/1	0.78	0.21	86,86,86,86	0
56	MG	2a	3070	1/1	0.78	0.09	78,78,78,78	0
56	MG	1a	1630	1/1	0.78	0.14	80,80,80,80	0
56	MG	2A	3263	1/1	0.78	0.28	70,70,70,70	0
56	MG	2a	3077	1/1	0.78	0.13	95,95,95,95	0
56	MG	1A	3385	1/1	0.78	0.21	63,63,63,63	0
56	MG	2A	3358	1/1	0.78	0.29	81,81,81,81	0
56	MG	1A	3299	1/1	0.78	0.19	83,83,83,83	0
56	MG	2A	3364	1/1	0.78	0.19	80,80,80,80	0
56	MG	2A	3268	1/1	0.78	0.33	68,68,68,68	0
56	MG	1A	3122	1/1	0.78	0.16	106,106,106,106	0
56	MG	1A	3391	1/1	0.78	0.23	66,66,66,66	0
56	MG	2A	3146	1/1	0.79	0.36	79,79,79,79	0
56	MG	1d	301	1/1	0.79	0.21	91,91,91,91	0
56	MG	2A	3328	1/1	0.79	0.27	68,68,68,68	0
56	MG	2A	3330	1/1	0.79	0.14	82,82,82,82	0
56	MG	1A	3371	1/1	0.79	0.25	75,75,75,75	0
56	MG	1A	3210	1/1	0.79	0.30	81,81,81,81	0
56	MG	1A	3451	1/1	0.79	0.17	77,77,77,77	0
56	MG	2A	3002	1/1	0.79	0.20	70,70,70,70	0
56	MG	2A	3348	1/1	0.79	0.30	77,77,77,77	0
56	MG	1A	3253	1/1	0.79	0.13	79,79,79,79	0
56	MG	1A	3257	1/1	0.79	0.17	82,82,82,82	0
56	MG	2a	3037	1/1	0.79	0.06	84,84,84,84	0
56	MG	1A	3002	1/1	0.79	0.13	94,94,94,94	0
56	MG	2A	3054	1/1	0.79	0.10	78,78,78,78	0
56	MG	1a	1636	1/1	0.79	0.07	93,93,93,93	0
56	MG	1A	3046	1/1	0.79	0.20	78,78,78,78	0
56	MG	1A	3082	1/1	0.79	0.22	74,74,74,74	0
56	MG	2A	3367	1/1	0.79	0.34	62,62,62,62	0
56	MG	2A	3304	1/1	0.79	0.32	63,63,63,63	0
56	MG	1A	3224	1/1	0.79	0.44	76,76,76,76	0
56	MG	2A	3372	1/1	0.79	0.27	70,70,70,70	0
56	MG	2A	3124	1/1	0.79	0.11	94,94,94,94	0
56	MG	2A	3308	1/1	0.79	0.30	85,85,85,85	0
56	MG	2A	3248	1/1	0.79	0.28	78,78,78,78	0
56	MG	1A	3151	1/1	0.79	0.23	76,76,76,76	0
56	MG	1A	3096	1/1	0.79	0.22	76,76,76,76	0
56	MG	2A	3139	1/1	0.79	0.18	64,64,64,64	0
56	MG	1A	3031	1/1	0.79	0.19	69,69,69,69	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	2A	3212	1/1	0.80	0.14	78,78,78,78	0
56	MG	2A	3219	1/1	0.80	0.21	75,75,75,75	0
56	MG	1A	3018	1/1	0.80	0.21	77,77,77,77	0
56	MG	2A	3160	1/1	0.80	0.21	75,75,75,75	0
56	MG	2A	3354	1/1	0.80	0.27	65,65,65,65	0
56	MG	1A	3062	1/1	0.80	0.14	89,89,89,89	0
56	MG	1A	3093	1/1	0.80	0.29	76,76,76,76	0
56	MG	1A	3024	1/1	0.80	0.28	85,85,85,85	0
56	MG	2A	3123	1/1	0.80	0.28	78,78,78,78	0
56	MG	1A	3321	1/1	0.80	0.30	67,67,67,67	0
56	MG	2A	3244	1/1	0.80	0.28	61,61,61,61	0
56	MG	2A	3177	1/1	0.80	0.29	63,63,63,63	0
56	MG	2A	3125	1/1	0.80	0.11	82,82,82,82	0
56	MG	1A	3058	1/1	0.80	0.34	73,73,73,73	0
56	MG	1A	3178	1/1	0.80	0.27	65,65,65,65	0
56	MG	2A	3091	1/1	0.80	0.27	75,75,75,75	0
56	MG	1A	3216	1/1	0.80	0.31	65,65,65,65	0
56	MG	1A	3097	1/1	0.80	0.23	77,77,77,77	0
56	MG	1A	3338	1/1	0.80	0.38	61,61,61,61	0
56	MG	13	101	1/1	0.80	0.28	72,72,72,72	0
56	MG	2A	3005	1/1	0.80	0.16	85,85,85,85	0
56	MG	1A	3450	1/1	0.80	0.17	75,75,75,75	0
56	MG	2E	302	1/1	0.80	0.16	80,80,80,80	0
56	MG	1A	3156	1/1	0.80	0.20	78,78,78,78	0
56	MG	1A	3084	1/1	0.80	0.15	79,79,79,79	0
56	MG	1A	3026	1/1	0.81	0.21	75,75,75,75	0
56	MG	1A	3269	1/1	0.81	0.24	92,92,92,92	0
56	MG	2A	3174	1/1	0.81	0.12	80,80,80,80	0
56	MG	1a	1602	1/1	0.81	0.18	74,74,74,74	0
56	MG	2A	3016	1/1	0.81	0.11	72,72,72,72	0
56	MG	1A	3010	1/1	0.81	0.21	72,72,72,72	0
56	MG	2A	3179	1/1	0.81	0.28	93,93,93,93	0
56	MG	1A	3271	1/1	0.81	0.27	75,75,75,75	0
56	MG	1A	3408	1/1	0.81	0.41	61,61,61,61	0
56	MG	1A	3478	1/1	0.81	0.25	76,76,76,76	0
56	MG	2A	3103	1/1	0.81	0.22	78,78,78,78	0
56	MG	2E	301	1/1	0.81	0.11	87,87,87,87	0
56	MG	2A	3105	1/1	0.81	0.16	74,74,74,74	0
56	MG	1A	3199	1/1	0.81	0.15	84,84,84,84	0
56	MG	20	102	1/1	0.81	0.15	75,75,75,75	0
56	MG	1a	1677	1/1	0.81	0.20	85,85,85,85	0
56	MG	2A	3113	1/1	0.81	0.20	70,70,70,70	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	1A	3123	1/1	0.81	0.34	81,81,81,81	0
56	MG	1A	3206	1/1	0.81	0.31	76,76,76,76	0
56	MG	1A	3448	1/1	0.81	0.26	74,74,74,74	0
56	MG	2a	3020	1/1	0.81	0.11	105,105,105,105	0
56	MG	1a	1683	1/1	0.81	0.16	118,118,118,118	0
56	MG	1A	3353	1/1	0.81	0.12	62,62,62,62	0
56	MG	2a	3028	1/1	0.81	0.13	83,83,83,83	0
56	MG	1A	3054	1/1	0.81	0.11	75,75,75,75	0
56	MG	1A	3422	1/1	0.81	0.34	61,61,61,61	0
56	MG	2A	3133	1/1	0.81	0.28	77,77,77,77	0
56	MG	1A	3127	1/1	0.81	0.17	69,69,69,69	0
56	MG	2A	3056	1/1	0.81	0.11	79,79,79,79	0
56	MG	2A	3057	1/1	0.81	0.11	91,91,91,91	0
56	MG	1A	3395	1/1	0.81	0.23	67,67,67,67	0
56	MG	2a	3065	1/1	0.81	0.15	75,75,75,75	0
56	MG	2A	3148	1/1	0.81	0.27	72,72,72,72	0
56	MG	2A	3071	1/1	0.81	0.22	61,61,61,61	0
56	MG	1A	3425	1/1	0.81	0.33	67,67,67,67	0
56	MG	2A	3246	1/1	0.81	0.20	79,79,79,79	0
56	MG	2a	3075	1/1	0.81	0.11	92,92,92,92	0
56	MG	1B	211	1/1	0.81	0.10	72,72,72,72	0
56	MG	1A	3042	1/1	0.81	0.23	79,79,79,79	0
56	MG	2A	3253	1/1	0.81	0.26	62,62,62,62	0
56	MG	1a	1644	1/1	0.81	0.23	76,76,76,76	0
56	MG	2a	3093	1/1	0.81	0.12	77,77,77,77	0
56	MG	1A	3217	1/1	0.81	0.22	65,65,65,65	0
56	MG	1A	3460	1/1	0.81	0.32	67,67,67,67	0
56	MG	2A	3162	1/1	0.81	0.23	90,90,90,90	0
56	MG	1A	3150	1/1	0.81	0.31	90,90,90,90	0
56	MG	1A	3288	1/1	0.82	0.28	78,78,78,78	0
56	MG	2A	3045	1/1	0.82	0.13	74,74,74,74	0
56	MG	2A	3190	1/1	0.82	0.16	82,82,82,82	0
56	MG	1A	3327	1/1	0.82	0.23	83,83,83,83	0
56	MG	1A	3374	1/1	0.82	0.24	62,62,62,62	0
56	MG	2A	3339	1/1	0.82	0.10	85,85,85,85	0
56	MG	2A	3200	1/1	0.82	0.22	74,74,74,74	0
56	MG	2a	3019	1/1	0.82	0.20	77,77,77,77	0
56	MG	2A	3341	1/1	0.82	0.21	76,76,76,76	0
56	MG	1A	3043	1/1	0.82	0.08	76,76,76,76	0
56	MG	2A	3350	1/1	0.82	0.10	93,93,93,93	0
56	MG	1a	1643	1/1	0.82	0.14	71,71,71,71	0
56	MG	1A	3446	1/1	0.82	0.26	77,77,77,77	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	1A	3333	1/1	0.82	0.23	68,68,68,68	0
56	MG	2A	3058	1/1	0.82	0.30	82,82,82,82	0
56	MG	1a	1648	1/1	0.82	0.12	100,100,100,100	0
56	MG	2A	3282	1/1	0.82	0.17	74,74,74,74	0
56	MG	2A	3069	1/1	0.82	0.20	83,83,83,83	0
56	MG	2A	3021	1/1	0.82	0.13	90,90,90,90	0
56	MG	1A	3334	1/1	0.82	0.20	62,62,62,62	0
56	MG	2A	3234	1/1	0.82	0.25	68,68,68,68	0
56	MG	1A	3379	1/1	0.82	0.17	80,80,80,80	0
56	MG	1A	3111	1/1	0.82	0.30	78,78,78,78	0
56	MG	1E	303	1/1	0.82	0.31	62,62,62,62	0
56	MG	1A	3261	1/1	0.82	0.13	77,77,77,77	0
56	MG	1A	3011	1/1	0.82	0.29	72,72,72,72	0
56	MG	1A	3173	1/1	0.82	0.29	87,87,87,87	0
56	MG	2A	3136	1/1	0.82	0.30	78,78,78,78	0
56	MG	1A	3223	1/1	0.82	0.18	64,64,64,64	0
56	MG	2A	3182	1/1	0.82	0.18	76,76,76,76	0
56	MG	2A	3183	1/1	0.82	0.19	81,81,81,81	0
56	MG	2A	3250	1/1	0.82	0.35	62,62,62,62	0
56	MG	2A	3041	1/1	0.82	0.26	91,91,91,91	0
56	MG	2Q	201	1/1	0.82	0.09	93,93,93,93	0
56	MG	2l	201	1/1	0.82	0.12	80,80,80,80	0
56	MG	2r	101	1/1	0.82	0.19	77,77,77,77	0
56	MG	2A	3099	1/1	0.83	0.26	81,81,81,81	0
56	MG	2A	3194	1/1	0.83	0.15	79,79,79,79	0
56	MG	2a	3003	1/1	0.83	0.16	90,90,90,90	0
56	MG	1A	3198	1/1	0.83	0.20	64,64,64,64	0
56	MG	1A	3337	1/1	0.83	0.15	79,79,79,79	0
56	MG	1A	3357	1/1	0.83	0.10	68,68,68,68	0
56	MG	2A	3203	1/1	0.83	0.27	61,61,61,61	0
56	MG	1A	3468	1/1	0.83	0.21	63,63,63,63	0
56	MG	1A	3142	1/1	0.83	0.13	71,71,71,71	0
56	MG	2A	3158	1/1	0.83	0.10	73,73,73,73	0
56	MG	2a	3023	1/1	0.83	0.17	72,72,72,72	0
56	MG	2A	3110	1/1	0.83	0.07	88,88,88,88	0
56	MG	2a	3027	1/1	0.83	0.22	79,79,79,79	0
56	MG	1A	3050	1/1	0.83	0.12	83,83,83,83	0
56	MG	1A	3204	1/1	0.83	0.20	72,72,72,72	0
56	MG	2A	3355	1/1	0.83	0.09	86,86,86,86	0
56	MG	2A	3356	1/1	0.83	0.20	68,68,68,68	0
56	MG	1a	1624	1/1	0.83	0.09	109,109,109,109	0
56	MG	2A	3118	1/1	0.83	0.15	71,71,71,71	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	2A	3082	1/1	0.83	0.23	79,79,79,79	0
56	MG	1A	3363	1/1	0.83	0.34	77,77,77,77	0
56	MG	1A	3177	1/1	0.83	0.17	62,62,62,62	0
56	MG	2A	3237	1/1	0.83	0.15	82,82,82,82	0
56	MG	2A	3086	1/1	0.83	0.16	77,77,77,77	0
56	MG	1A	3481	1/1	0.83	0.22	68,68,68,68	0
56	MG	2A	3240	1/1	0.83	0.36	61,61,61,61	0
56	MG	1A	3121	1/1	0.83	0.30	79,79,79,79	0
56	MG	1A	3280	1/1	0.83	0.20	64,64,64,64	0
56	MG	1a	1668	1/1	0.83	0.33	78,78,78,78	0
56	MG	1A	3190	1/1	0.83	0.34	79,79,79,79	0
56	MG	1A	3134	1/1	0.83	0.23	80,80,80,80	0
56	MG	1a	1637	1/1	0.83	0.14	89,89,89,89	0
56	MG	2A	3317	1/1	0.83	0.24	65,65,65,65	0
56	MG	2A	3012	1/1	0.83	0.24	66,66,66,66	0
56	MG	2A	3251	1/1	0.83	0.26	75,75,75,75	0
56	MG	2A	3323	1/1	0.83	0.12	64,64,64,64	0
56	MG	2A	3324	1/1	0.83	0.17	82,82,82,82	0
56	MG	1a	1638	1/1	0.83	0.21	75,75,75,75	0
56	MG	1A	3169	1/1	0.84	0.14	62,62,62,62	0
56	MG	1A	3411	1/1	0.84	0.31	75,75,75,75	0
56	MG	1A	3365	1/1	0.84	0.24	69,69,69,69	0
56	MG	2A	3242	1/1	0.84	0.29	61,61,61,61	0
56	MG	1A	3366	1/1	0.84	0.25	61,61,61,61	0
56	MG	2A	3138	1/1	0.84	0.04	76,76,76,76	0
56	MG	2A	3044	1/1	0.84	0.14	81,81,81,81	0
56	MG	1A	3135	1/1	0.84	0.23	80,80,80,80	0
56	MG	1A	3392	1/1	0.84	0.26	73,73,73,73	0
56	MG	2A	3006	1/1	0.84	0.09	76,76,76,76	0
56	MG	2a	3030	1/1	0.84	0.11	74,74,74,74	0
56	MG	1A	3473	1/1	0.84	0.28	61,61,61,61	0
56	MG	1a	1670	1/1	0.84	0.14	97,97,97,97	0
56	MG	1A	3238	1/1	0.84	0.28	75,75,75,75	0
56	MG	10	103	1/1	0.84	0.20	69,69,69,69	0
56	MG	2A	3104	1/1	0.84	0.17	80,80,80,80	0
56	MG	2A	3375	1/1	0.84	0.17	66,66,66,66	0
56	MG	1A	3161	1/1	0.84	0.11	65,65,65,65	0
56	MG	1A	3373	1/1	0.84	0.29	61,61,61,61	0
56	MG	1A	3356	1/1	0.84	0.19	61,61,61,61	0
56	MG	2A	3159	1/1	0.84	0.13	83,83,83,83	0
56	MG	2a	3072	1/1	0.84	0.11	72,72,72,72	0
56	MG	2A	3333	1/1	0.84	0.72	74,74,74,74	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	1A	3488	1/1	0.84	0.20	69,69,69,69	0
56	MG	2a	3076	1/1	0.84	0.07	82,82,82,82	0
56	MG	1A	3091	1/1	0.84	0.19	77,77,77,77	0
56	MG	2A	3025	1/1	0.84	0.14	89,89,89,89	0
56	MG	2E	303	1/1	0.84	0.26	81,81,81,81	0
56	MG	2a	3090	1/1	0.84	0.23	73,73,73,73	0
56	MG	2a	3091	1/1	0.84	0.18	79,79,79,79	0
56	MG	1A	3402	1/1	0.84	0.35	62,62,62,62	0
56	MG	2A	3120	1/1	0.84	0.17	78,78,78,78	0
56	MG	1A	3232	1/1	0.84	0.18	77,77,77,77	0
56	MG	25	101	1/1	0.84	0.20	69,69,69,69	0
56	MG	1A	3310	1/1	0.84	0.75	62,62,62,62	0
56	MG	2A	3349	1/1	0.84	0.30	76,76,76,76	0
56	MG	1A	3087	1/1	0.84	0.13	82,82,82,82	0
56	MG	1A	3362	1/1	0.84	0.37	62,62,62,62	0
56	MG	2A	3213	1/1	0.85	0.19	67,67,67,67	0
56	MG	1A	3126	1/1	0.85	0.33	80,80,80,80	0
56	MG	2A	3284	1/1	0.85	0.23	71,71,71,71	0
56	MG	1A	3297	1/1	0.85	0.28	79,79,79,79	0
56	MG	1A	3298	1/1	0.85	0.23	71,71,71,71	0
56	MG	1A	3155	1/1	0.85	0.28	73,73,73,73	0
56	MG	1A	3409	1/1	0.85	0.28	82,82,82,82	0
56	MG	1A	3323	1/1	0.85	0.43	62,62,62,62	0
56	MG	1A	3227	1/1	0.85	0.11	71,71,71,71	0
56	MG	1A	3203	1/1	0.85	0.29	72,72,72,72	0
56	MG	2a	3033	1/1	0.85	0.08	72,72,72,72	0
56	MG	1A	3328	1/1	0.85	0.19	61,61,61,61	0
56	MG	2A	3178	1/1	0.85	0.16	75,75,75,75	0
56	MG	2A	3130	1/1	0.85	0.34	63,63,63,63	0
56	MG	1a	1650	1/1	0.85	0.07	82,82,82,82	0
56	MG	1a	1619	1/1	0.85	0.13	92,92,92,92	0
56	MG	2A	3137	1/1	0.85	0.36	62,62,62,62	0
56	MG	1A	3348	1/1	0.85	0.33	79,79,79,79	0
56	MG	1a	1654	1/1	0.85	0.17	71,71,71,71	0
56	MG	1A	3307	1/1	0.85	0.18	71,71,71,71	0
56	MG	2A	3145	1/1	0.85	0.20	79,79,79,79	0
56	MG	1a	1660	1/1	0.85	0.40	61,61,61,61	0
56	MG	1A	3330	1/1	0.85	0.18	69,69,69,69	0
56	MG	1A	3474	1/1	0.85	0.16	70,70,70,70	0
56	MG	2A	3257	1/1	0.85	0.24	84,84,84,84	0
56	MG	2A	3195	1/1	0.85	0.22	66,66,66,66	0
56	MG	2a	3079	1/1	0.85	0.13	62,62,62,62	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	1S	201	1/1	0.85	0.10	78,78,78,78	0
56	MG	2A	3335	1/1	0.85	0.18	68,68,68,68	0
56	MG	2A	3008	1/1	0.85	0.20	69,69,69,69	0
56	MG	1A	3372	1/1	0.85	0.14	72,72,72,72	0
56	MG	2I	101	1/1	0.85	0.24	63,63,63,63	0
56	MG	2A	3011	1/1	0.85	0.09	82,82,82,82	0
56	MG	1A	3331	1/1	0.85	0.20	63,63,63,63	0
56	MG	2A	3156	1/1	0.85	0.10	63,63,63,63	0
56	MG	1A	3266	1/1	0.85	0.10	77,77,77,77	0
56	MG	1a	1635	1/1	0.85	0.07	84,84,84,84	0
56	MG	2f	201	1/1	0.85	0.21	77,77,77,77	0
56	MG	2a	3012	1/1	0.85	0.09	104,104,104,104	0
56	MG	1A	3268	1/1	0.85	0.17	68,68,68,68	0
56	MG	2A	3112	1/1	0.86	0.15	68,68,68,68	0
56	MG	23	101	1/1	0.86	0.18	68,68,68,68	0
56	MG	1A	3430	1/1	0.86	0.19	68,68,68,68	0
56	MG	1A	3294	1/1	0.86	0.20	75,75,75,75	0
56	MG	2A	3115	1/1	0.86	0.18	84,84,84,84	0
56	MG	1A	3359	1/1	0.86	0.14	78,78,78,78	0
56	MG	2a	3009	1/1	0.86	0.13	79,79,79,79	0
56	MG	1A	3296	1/1	0.86	0.19	73,73,73,73	0
56	MG	1A	3105	1/1	0.86	0.06	108,108,108,108	0
56	MG	2a	3013	1/1	0.86	0.07	80,80,80,80	0
56	MG	1A	3248	1/1	0.86	0.17	68,68,68,68	0
56	MG	1A	3005	1/1	0.86	0.14	82,82,82,82	0
56	MG	2A	3010	1/1	0.86	0.15	87,87,87,87	0
56	MG	2A	3255	1/1	0.86	0.25	71,71,71,71	0
56	MG	1A	3484	1/1	0.86	0.18	67,67,67,67	0
56	MG	2A	3079	1/1	0.86	0.07	79,79,79,79	0
56	MG	1A	3364	1/1	0.86	0.12	81,81,81,81	0
56	MG	2a	3026	1/1	0.86	0.31	76,76,76,76	0
56	MG	2A	3131	1/1	0.86	0.19	63,63,63,63	0
56	MG	2A	3262	1/1	0.86	0.21	80,80,80,80	0
56	MG	2A	3132	1/1	0.86	0.21	71,71,71,71	0
56	MG	2A	3353	1/1	0.86	0.24	70,70,70,70	0
56	MG	2a	3032	1/1	0.86	0.08	75,75,75,75	0
56	MG	2A	3265	1/1	0.86	0.27	73,73,73,73	0
56	MG	1A	3302	1/1	0.86	0.21	62,62,62,62	0
56	MG	1a	1622	1/1	0.86	0.10	66,66,66,66	0
56	MG	1A	3015	1/1	0.86	0.19	62,62,62,62	0
56	MG	2a	3043	1/1	0.86	0.29	62,62,62,62	0
56	MG	1A	3277	1/1	0.86	0.28	61,61,61,61	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	2a	3052	1/1	0.86	0.10	68,68,68,68	0
56	MG	1A	3306	1/1	0.86	0.53	61,61,61,61	0
56	MG	2A	3361	1/1	0.86	0.22	62,62,62,62	0
56	MG	2A	3088	1/1	0.86	0.17	76,76,76,76	0
56	MG	1A	3074	1/1	0.86	0.15	77,77,77,77	0
56	MG	2a	3067	1/1	0.86	0.07	96,96,96,96	0
56	MG	1a	1675	1/1	0.86	0.08	110,110,110,110	0
56	MG	1A	3061	1/1	0.86	0.20	71,71,71,71	0
56	MG	1A	3283	1/1	0.86	0.29	61,61,61,61	0
56	MG	1A	3312	1/1	0.86	0.21	65,65,65,65	0
56	MG	2A	3210	1/1	0.86	0.30	68,68,68,68	0
56	MG	1A	3098	1/1	0.86	0.13	81,81,81,81	0
56	MG	2A	3032	1/1	0.86	0.06	85,85,85,85	0
56	MG	2a	3078	1/1	0.86	0.21	62,62,62,62	0
56	MG	1A	3152	1/1	0.86	0.19	64,64,64,64	0
56	MG	1A	3320	1/1	0.86	0.26	74,74,74,74	0
56	MG	2a	3087	1/1	0.86	0.17	61,61,61,61	0
56	MG	2A	3227	1/1	0.86	0.20	62,62,62,62	0
56	MG	2a	3089	1/1	0.86	0.20	79,79,79,79	0
56	MG	2B	203	1/1	0.86	0.20	75,75,75,75	0
56	MG	1A	3023	1/1	0.86	0.08	73,73,73,73	0
56	MG	1A	3045	1/1	0.86	0.20	74,74,74,74	0
56	MG	1A	3384	1/1	0.86	0.12	71,71,71,71	0
56	MG	1A	3090	1/1	0.86	0.12	75,75,75,75	0
56	MG	1A	3386	1/1	0.86	0.15	77,77,77,77	0
56	MG	2A	3161	1/1	0.86	0.13	72,72,72,72	0
56	MG	2E	304	1/1	0.86	0.15	63,63,63,63	0
56	MG	1A	3012	1/1	0.86	0.14	75,75,75,75	0
56	MG	2A	3051	1/1	0.86	0.33	79,79,79,79	0
56	MG	1A	3246	1/1	0.86	0.20	77,77,77,77	0
56	MG	2A	3286	1/1	0.87	0.20	62,62,62,62	0
56	MG	1A	3441	1/1	0.87	0.15	76,76,76,76	0
56	MG	1A	3071	1/1	0.87	0.14	75,75,75,75	0
56	MG	2O	201	1/1	0.87	0.18	73,73,73,73	0
56	MG	2A	3197	1/1	0.87	0.20	61,61,61,61	0
56	MG	2A	3059	1/1	0.87	0.21	82,82,82,82	0
56	MG	2O	101	1/1	0.87	0.11	75,75,75,75	0
56	MG	2A	3199	1/1	0.87	0.14	83,83,83,83	0
56	MG	2A	3302	1/1	0.87	0.15	82,82,82,82	0
56	MG	2A	3127	1/1	0.87	0.16	93,93,93,93	0
56	MG	2A	3062	1/1	0.87	0.18	72,72,72,72	0
56	MG	27	101	1/1	0.87	0.20	69,69,69,69	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	28	101	1/1	0.87	0.07	80,80,80,80	0
56	MG	1A	3220	1/1	0.87	0.17	85,85,85,85	0
56	MG	2A	3307	1/1	0.87	0.15	77,77,77,77	0
56	MG	2A	3204	1/1	0.87	0.20	68,68,68,68	0
56	MG	2A	3064	1/1	0.87	0.12	101,101,101,101	0
56	MG	2A	3066	1/1	0.87	0.20	85,85,85,85	0
56	MG	2A	3067	1/1	0.87	0.12	73,73,73,73	0
56	MG	2A	3134	1/1	0.87	0.19	82,82,82,82	0
56	MG	1A	3160	1/1	0.87	0.21	67,67,67,67	0
56	MG	1A	3354	1/1	0.87	0.16	61,61,61,61	0
56	MG	1A	3314	1/1	0.87	0.26	71,71,71,71	0
56	MG	1A	3281	1/1	0.87	0.27	63,63,63,63	0
56	MG	1A	3319	1/1	0.87	0.20	61,61,61,61	0
56	MG	1A	3033	1/1	0.87	0.10	86,86,86,86	0
56	MG	2a	3024	1/1	0.87	0.15	83,83,83,83	0
56	MG	1A	3249	1/1	0.87	0.05	90,90,90,90	0
56	MG	1A	3251	1/1	0.87	0.18	82,82,82,82	0
56	MG	1A	3003	1/1	0.87	0.42	68,68,68,68	0
56	MG	1A	3191	1/1	0.87	0.22	70,70,70,70	0
56	MG	1A	3455	1/1	0.87	0.32	63,63,63,63	0
56	MG	1A	3326	1/1	0.87	0.22	63,63,63,63	0
56	MG	1A	3067	1/1	0.87	0.20	64,64,64,64	0
56	MG	2A	3020	1/1	0.87	0.13	88,88,88,88	0
56	MG	1a	1663	1/1	0.87	0.21	68,68,68,68	0
56	MG	1A	3041	1/1	0.87	0.20	69,69,69,69	0
56	MG	1A	3128	1/1	0.87	0.19	77,77,77,77	0
56	MG	1A	3037	1/1	0.87	0.17	68,68,68,68	0
56	MG	1A	3089	1/1	0.87	0.16	74,74,74,74	0
56	MG	2a	3047	1/1	0.87	0.09	77,77,77,77	0
56	MG	2a	3051	1/1	0.87	0.14	79,79,79,79	0
56	MG	1A	3235	1/1	0.87	0.21	77,77,77,77	0
56	MG	1A	3116	1/1	0.87	0.22	68,68,68,68	0
56	MG	2A	3249	1/1	0.87	0.18	74,74,74,74	0
56	MG	2A	3165	1/1	0.87	0.26	73,73,73,73	0
56	MG	1A	3335	1/1	0.87	0.14	85,85,85,85	0
56	MG	2A	3252	1/1	0.87	0.16	77,77,77,77	0
56	MG	2A	3169	1/1	0.87	0.27	69,69,69,69	0
56	MG	2A	3102	1/1	0.87	0.05	73,73,73,73	0
56	MG	1A	3070	1/1	0.87	0.15	87,87,87,87	0
56	MG	1A	3300	1/1	0.87	0.25	63,63,63,63	0
56	MG	2A	3362	1/1	0.87	0.14	80,80,80,80	0
56	MG	1A	3136	1/1	0.87	0.22	76,76,76,76	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	1A	3181	1/1	0.87	0.22	73,73,73,73	0
56	MG	2A	3108	1/1	0.87	0.12	67,67,67,67	0
56	MG	2A	3368	1/1	0.87	0.40	62,62,62,62	0
56	MG	1A	3183	1/1	0.87	0.23	74,74,74,74	0
56	MG	1A	3480	1/1	0.87	0.37	69,69,69,69	0
56	MG	2A	3264	1/1	0.87	0.15	70,70,70,70	0
56	MG	1A	3305	1/1	0.87	0.32	61,61,61,61	0
56	MG	1A	3081	1/1	0.87	0.17	65,65,65,65	0
56	MG	1A	3346	1/1	0.87	0.28	65,65,65,65	0
56	MG	1A	3272	1/1	0.87	0.18	70,70,70,70	0
56	MG	2A	3117	1/1	0.87	0.16	74,74,74,74	0
56	MG	2a	3094	1/1	0.87	0.16	66,66,66,66	0
56	MG	2A	3053	1/1	0.87	0.14	74,74,74,74	0
56	MG	1A	3243	1/1	0.87	0.21	71,71,71,71	0
56	MG	1x	101	1/1	0.87	0.10	92,92,92,92	0
56	MG	2A	3191	1/1	0.87	0.07	78,78,78,78	0
56	MG	2B	209	1/1	0.87	0.10	91,91,91,91	0
56	MG	2A	3283	1/1	0.87	0.18	61,61,61,61	0
56	MG	1A	3388	1/1	0.87	0.20	71,71,71,71	0
56	MG	2A	3170	1/1	0.88	0.16	67,67,67,67	0
56	MG	1a	1676	1/1	0.88	0.13	77,77,77,77	0
56	MG	2A	3321	1/1	0.88	0.22	81,81,81,81	0
56	MG	1A	3060	1/1	0.88	0.20	79,79,79,79	0
56	MG	2A	3013	1/1	0.88	0.20	73,73,73,73	0
56	MG	2B	201	1/1	0.88	0.22	80,80,80,80	0
56	MG	2A	3327	1/1	0.88	0.23	70,70,70,70	0
56	MG	2a	3035	1/1	0.88	0.35	73,73,73,73	0
56	MG	1A	3367	1/1	0.88	0.20	61,61,61,61	0
56	MG	1A	3282	1/1	0.88	0.21	70,70,70,70	0
56	MG	1A	3149	1/1	0.88	0.22	72,72,72,72	0
56	MG	2a	3044	1/1	0.88	0.11	75,75,75,75	0
56	MG	1a	1616	1/1	0.88	0.20	69,69,69,69	0
56	MG	2A	3272	1/1	0.88	0.16	62,62,62,62	0
56	MG	2a	3048	1/1	0.88	0.17	80,80,80,80	0
56	MG	1A	3301	1/1	0.88	0.14	82,82,82,82	0
56	MG	1A	3267	1/1	0.88	0.16	70,70,70,70	0
56	MG	2a	3053	1/1	0.88	0.08	74,74,74,74	0
56	MG	1A	3467	1/1	0.88	0.24	66,66,66,66	0
56	MG	2a	3058	1/1	0.88	0.19	73,73,73,73	0
56	MG	2A	3023	1/1	0.88	0.08	73,73,73,73	0
56	MG	2E	305	1/1	0.88	0.08	67,67,67,67	0
56	MG	1A	3164	1/1	0.88	0.27	69,69,69,69	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	2A	3342	1/1	0.88	0.11	85,85,85,85	0
56	MG	2A	3345	1/1	0.88	0.29	62,62,62,62	0
56	MG	2R	202	1/1	0.88	0.27	67,67,67,67	0
56	MG	1A	3229	1/1	0.88	0.09	75,75,75,75	0
56	MG	1A	3421	1/1	0.88	0.17	65,65,65,65	0
56	MG	2a	3074	1/1	0.88	0.24	76,76,76,76	0
56	MG	1A	3472	1/1	0.88	0.25	67,67,67,67	0
56	MG	1A	3254	1/1	0.88	0.19	77,77,77,77	0
56	MG	2A	3073	1/1	0.88	0.19	73,73,73,73	0
56	MG	2A	3295	1/1	0.88	0.10	76,76,76,76	0
56	MG	2A	3076	1/1	0.88	0.14	69,69,69,69	0
56	MG	2A	3300	1/1	0.88	0.12	74,74,74,74	0
56	MG	1E	304	1/1	0.88	0.14	78,78,78,78	0
56	MG	1A	3230	1/1	0.88	0.26	79,79,79,79	0
56	MG	2A	3080	1/1	0.88	0.25	69,69,69,69	0
56	MG	1A	3141	1/1	0.88	0.18	83,83,83,83	0
56	MG	1A	3006	1/1	0.88	0.12	72,72,72,72	0
56	MG	1A	3403	1/1	0.88	0.20	87,87,87,87	0
56	MG	2A	3119	1/1	0.88	0.29	63,63,63,63	0
56	MG	1A	3168	1/1	0.88	0.15	71,71,71,71	0
56	MG	2A	3366	1/1	0.88	0.29	63,63,63,63	0
56	MG	2a	3096	1/1	0.88	0.14	70,70,70,70	0
56	MG	2A	3085	1/1	0.88	0.38	71,71,71,71	0
56	MG	2a	3098	1/1	0.88	0.15	85,85,85,85	0
56	MG	1A	3035	1/1	0.88	0.22	75,75,75,75	0
56	MG	1A	3431	1/1	0.88	0.17	62,62,62,62	0
56	MG	2A	3370	1/1	0.88	0.20	75,75,75,75	0
56	MG	1A	3192	1/1	0.88	0.28	61,61,61,61	0
56	MG	2A	3050	1/1	0.88	0.16	76,76,76,76	0
56	MG	1A	3259	1/1	0.89	0.11	73,73,73,73	0
56	MG	1A	3389	1/1	0.89	0.20	71,71,71,71	0
56	MG	1A	3419	1/1	0.89	0.32	72,72,72,72	0
56	MG	1a	1601	1/1	0.89	0.21	72,72,72,72	0
56	MG	2A	3313	1/1	0.89	0.17	76,76,76,76	0
56	MG	2A	3189	1/1	0.89	0.33	75,75,75,75	0
56	MG	1A	3344	1/1	0.89	0.23	73,73,73,73	0
56	MG	2A	3140	1/1	0.89	0.15	73,73,73,73	0
56	MG	2a	3038	1/1	0.89	0.08	80,80,80,80	0
56	MG	2a	3039	1/1	0.89	0.32	79,79,79,79	0
56	MG	1A	3007	1/1	0.89	0.08	74,74,74,74	0
56	MG	1A	3482	1/1	0.89	0.24	61,61,61,61	0
56	MG	1A	3201	1/1	0.89	0.19	69,69,69,69	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	2a	3045	1/1	0.89	0.12	79,79,79,79	0
56	MG	1A	3182	1/1	0.89	0.12	69,69,69,69	0
56	MG	1a	1659	1/1	0.89	0.32	67,67,67,67	0
56	MG	1a	1613	1/1	0.89	0.12	87,87,87,87	0
56	MG	1a	1661	1/1	0.89	0.18	72,72,72,72	0
56	MG	1A	3158	1/1	0.89	0.10	75,75,75,75	0
56	MG	1A	3350	1/1	0.89	0.18	78,78,78,78	0
56	MG	2a	3055	1/1	0.89	0.06	79,79,79,79	0
56	MG	1A	3120	1/1	0.89	0.28	61,61,61,61	0
56	MG	1A	3055	1/1	0.89	0.08	83,83,83,83	0
56	MG	1B	205	1/1	0.89	0.07	68,68,68,68	0
56	MG	1A	3429	1/1	0.89	0.18	79,79,79,79	0
56	MG	1a	1623	1/1	0.89	0.12	79,79,79,79	0
56	MG	1A	3030	1/1	0.89	0.28	76,76,76,76	0
56	MG	1a	1672	1/1	0.89	0.07	104,104,104,104	0
56	MG	2T	202	1/1	0.89	0.28	82,82,82,82	0
56	MG	2A	3274	1/1	0.89	0.21	61,61,61,61	0
56	MG	2A	3344	1/1	0.89	0.12	78,78,78,78	0
56	MG	2A	3116	1/1	0.89	0.25	72,72,72,72	0
56	MG	2A	3346	1/1	0.89	0.14	86,86,86,86	0
56	MG	2A	3074	1/1	0.89	0.16	71,71,71,71	0
56	MG	2A	3277	1/1	0.89	0.26	70,70,70,70	0
56	MG	2A	3278	1/1	0.89	0.23	61,61,61,61	0
56	MG	1A	3174	1/1	0.89	0.21	73,73,73,73	0
56	MG	2a	3081	1/1	0.89	0.15	64,64,64,64	0
56	MG	2A	3222	1/1	0.89	0.15	75,75,75,75	0
56	MG	2a	3005	1/1	0.89	0.08	87,87,87,87	0
56	MG	1A	3432	1/1	0.89	0.29	68,68,68,68	0
56	MG	1A	3250	1/1	0.89	0.20	71,71,71,71	0
56	MG	2A	3231	1/1	0.89	0.24	74,74,74,74	0
56	MG	1A	3175	1/1	0.89	0.14	62,62,62,62	0
56	MG	1A	3176	1/1	0.89	0.22	75,75,75,75	0
56	MG	1A	3436	1/1	0.89	0.37	61,61,61,61	0
56	MG	1A	3104	1/1	0.89	0.14	69,69,69,69	0
56	MG	2a	3016	1/1	0.89	0.16	84,84,84,84	0
56	MG	1A	3021	1/1	0.89	0.14	73,73,73,73	0
56	MG	1V	201	1/1	0.89	0.21	80,80,80,80	0
56	MG	2A	3035	1/1	0.89	0.16	76,76,76,76	0
56	MG	2A	3241	1/1	0.89	0.22	65,65,65,65	0
56	MG	1A	3275	1/1	0.89	0.30	63,63,63,63	0
56	MG	1V	203	1/1	0.89	0.18	81,81,81,81	0
56	MG	1A	3195	1/1	0.89	0.26	71,71,71,71	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	1A	3013	1/1	0.89	0.14	83,83,83,83	0
56	MG	1A	3218	1/1	0.90	0.22	66,66,66,66	0
56	MG	1A	3345	1/1	0.90	0.14	72,72,72,72	0
56	MG	2A	3385	1/1	0.90	0.12	76,76,76,76	0
56	MG	2A	3319	1/1	0.90	0.24	64,64,64,64	0
56	MG	2a	3036	1/1	0.90	0.14	76,76,76,76	0
56	MG	1A	3139	1/1	0.90	0.22	70,70,70,70	0
56	MG	1A	3076	1/1	0.90	0.30	65,65,65,65	0
56	MG	1A	3442	1/1	0.90	0.18	61,61,61,61	0
56	MG	2a	3040	1/1	0.90	0.23	78,78,78,78	0
56	MG	2A	3163	1/1	0.90	0.27	62,62,62,62	0
56	MG	2A	3207	1/1	0.90	0.11	89,89,89,89	0
56	MG	2A	3164	1/1	0.90	0.23	68,68,68,68	0
56	MG	1A	3418	1/1	0.90	0.25	76,76,76,76	0
56	MG	1D	301	1/1	0.90	0.14	73,73,73,73	0
56	MG	2A	3211	1/1	0.90	0.24	63,63,63,63	0
56	MG	2A	3167	1/1	0.90	0.22	72,72,72,72	0
56	MG	1A	3170	1/1	0.90	0.23	79,79,79,79	0
56	MG	2A	3273	1/1	0.90	0.19	62,62,62,62	0
56	MG	2A	3214	1/1	0.90	0.17	82,82,82,82	0
56	MG	2A	3046	1/1	0.90	0.17	65,65,65,65	0
56	MG	2A	3048	1/1	0.90	0.06	82,82,82,82	0
56	MG	1A	3256	1/1	0.90	0.20	78,78,78,78	0
56	MG	2a	3059	1/1	0.90	0.07	80,80,80,80	0
56	MG	1A	3394	1/1	0.90	0.30	61,61,61,61	0
56	MG	2a	3064	1/1	0.90	0.17	67,67,67,67	0
56	MG	1A	3476	1/1	0.90	0.20	62,62,62,62	0
56	MG	1A	3179	1/1	0.90	0.09	64,64,64,64	0
56	MG	1A	3351	1/1	0.90	0.09	64,64,64,64	0
56	MG	1A	3332	1/1	0.90	0.18	74,74,74,74	0
56	MG	2A	3285	1/1	0.90	0.29	73,73,73,73	0
56	MG	1A	3107	1/1	0.90	0.07	64,64,64,64	0
56	MG	2A	3288	1/1	0.90	0.17	66,66,66,66	0
56	MG	2a	3002	1/1	0.90	0.08	65,65,65,65	0
56	MG	2A	3290	1/1	0.90	0.34	72,72,72,72	0
56	MG	1A	3205	1/1	0.90	0.20	74,74,74,74	0
56	MG	2a	3007	1/1	0.90	0.07	73,73,73,73	0
56	MG	1A	3315	1/1	0.90	0.19	80,80,80,80	0
56	MG	1A	3049	1/1	0.90	0.09	104,104,104,104	0
56	MG	2a	3010	1/1	0.90	0.21	70,70,70,70	0
56	MG	1a	1639	1/1	0.90	0.13	77,77,77,77	0
56	MG	1A	3208	1/1	0.90	0.10	62,62,62,62	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	2A	3298	1/1	0.90	0.17	69,69,69,69	0
56	MG	1A	3209	1/1	0.90	0.34	61,61,61,61	0
56	MG	1a	1642	1/1	0.90	0.11	81,81,81,81	0
56	MG	2A	3188	1/1	0.90	0.20	74,74,74,74	0
56	MG	2a	3017	1/1	0.90	0.06	87,87,87,87	0
56	MG	1A	3073	1/1	0.90	0.12	86,86,86,86	0
56	MG	1A	3025	1/1	0.90	0.15	77,77,77,77	0
56	MG	2A	3024	1/1	0.90	0.06	73,73,73,73	0
56	MG	2A	3192	1/1	0.90	0.21	79,79,79,79	0
56	MG	1A	3196	1/1	0.90	0.18	65,65,65,65	0
56	MG	1A	3063	1/1	0.90	0.22	77,77,77,77	0
56	MG	1a	1612	1/1	0.90	0.10	97,97,97,97	0
56	MG	2A	3196	1/1	0.90	0.11	78,78,78,78	0
56	MG	1a	1690	1/1	0.90	0.15	84,84,84,84	0
56	MG	1A	3463	1/1	0.90	0.29	72,72,72,72	0
56	MG	1l	201	1/1	0.90	0.06	80,80,80,80	0
56	MG	1a	1615	1/1	0.91	0.13	83,83,83,83	0
56	MG	2A	3299	1/1	0.91	0.21	78,78,78,78	0
56	MG	1a	1684	1/1	0.91	0.28	74,74,74,74	0
56	MG	1E	301	1/1	0.91	0.11	71,71,71,71	0
56	MG	1A	3287	1/1	0.91	0.28	63,63,63,63	0
56	MG	1A	3197	1/1	0.91	0.29	71,71,71,71	0
56	MG	2a	3049	1/1	0.91	0.08	80,80,80,80	0
56	MG	1E	305	1/1	0.91	0.16	72,72,72,72	0
56	MG	1a	1653	1/1	0.91	0.30	63,63,63,63	0
56	MG	1F	301	1/1	0.91	0.11	72,72,72,72	0
56	MG	2A	3142	1/1	0.91	0.26	73,73,73,73	0
56	MG	1A	3404	1/1	0.91	0.20	81,81,81,81	0
56	MG	1a	1656	1/1	0.91	0.12	82,82,82,82	0
56	MG	2A	3224	1/1	0.91	0.21	61,61,61,61	0
56	MG	2a	3004	1/1	0.91	0.11	91,91,91,91	0
56	MG	2a	3062	1/1	0.91	0.14	68,68,68,68	0
56	MG	2A	3225	1/1	0.91	0.13	62,62,62,62	0
56	MG	1A	3255	1/1	0.91	0.13	77,77,77,77	0
56	MG	2A	3269	1/1	0.91	0.25	62,62,62,62	0
56	MG	1A	3276	1/1	0.91	0.18	75,75,75,75	0
56	MG	2A	3077	1/1	0.91	0.10	62,62,62,62	0
56	MG	1A	3376	1/1	0.91	0.20	61,61,61,61	0
56	MG	2A	3038	1/1	0.91	0.23	77,77,77,77	0
56	MG	1W	201	1/1	0.91	0.09	65,65,65,65	0
56	MG	2A	3322	1/1	0.91	0.09	89,89,89,89	0
56	MG	2A	3154	1/1	0.91	0.24	68,68,68,68	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	1A	3497	1/1	0.91	0.24	65,65,65,65	0
56	MG	2A	3325	1/1	0.91	0.26	67,67,67,67	0
56	MG	2A	3326	1/1	0.91	0.21	74,74,74,74	0
56	MG	1A	3148	1/1	0.91	0.30	79,79,79,79	0
56	MG	2a	3080	1/1	0.91	0.09	74,74,74,74	0
56	MG	2A	3280	1/1	0.91	0.30	61,61,61,61	0
56	MG	2a	3084	1/1	0.91	0.17	72,72,72,72	0
56	MG	2A	3382	1/1	0.91	0.11	124,124,124,124	0
56	MG	2a	3086	1/1	0.91	0.23	74,74,74,74	0
56	MG	2A	3329	1/1	0.91	0.07	82,82,82,82	0
56	MG	1A	3393	1/1	0.91	0.25	61,61,61,61	0
56	MG	2A	3332	1/1	0.91	0.31	80,80,80,80	0
56	MG	1A	3185	1/1	0.91	0.30	62,62,62,62	0
56	MG	2B	204	1/1	0.91	0.15	80,80,80,80	0
56	MG	2B	205	1/1	0.91	0.14	89,89,89,89	0
56	MG	1A	3470	1/1	0.91	0.15	68,68,68,68	0
56	MG	17	102	1/1	0.91	0.10	83,83,83,83	0
56	MG	1A	3022	1/1	0.91	0.07	89,89,89,89	0
56	MG	1A	3412	1/1	0.91	0.22	65,65,65,65	0
56	MG	1A	3413	1/1	0.91	0.19	68,68,68,68	0
56	MG	1A	3066	1/1	0.91	0.18	72,72,72,72	0
56	MG	1A	3166	1/1	0.91	0.26	69,69,69,69	0
56	MG	1A	3212	1/1	0.91	0.20	62,62,62,62	0
56	MG	1A	3057	1/1	0.91	0.07	73,73,73,73	0
56	MG	1A	3401	1/1	0.91	0.23	64,64,64,64	0
56	MG	1a	1614	1/1	0.91	0.20	76,76,76,76	0
56	MG	1a	1688	1/1	0.92	0.08	80,80,80,80	0
56	MG	1a	1657	1/1	0.92	0.11	93,93,93,93	0
56	MG	2a	3063	1/1	0.92	0.21	61,61,61,61	0
56	MG	1A	3265	1/1	0.92	0.20	72,72,72,72	0
56	MG	1A	3108	1/1	0.92	0.13	75,75,75,75	0
56	MG	2B	208	1/1	0.92	0.21	62,62,62,62	0
56	MG	1A	3440	1/1	0.92	0.27	70,70,70,70	0
56	MG	2A	3270	1/1	0.92	0.10	80,80,80,80	0
56	MG	1A	3213	1/1	0.92	0.09	72,72,72,72	0
56	MG	1A	3295	1/1	0.92	0.13	69,69,69,69	0
56	MG	1A	3019	1/1	0.92	0.12	80,80,80,80	0
56	MG	1A	3193	1/1	0.92	0.18	71,71,71,71	0
56	MG	2A	3316	1/1	0.92	0.16	62,62,62,62	0
56	MG	1A	3200	1/1	0.92	0.07	69,69,69,69	0
56	MG	1E	306	1/1	0.92	0.20	72,72,72,72	0
56	MG	1A	3466	1/1	0.92	0.17	61,61,61,61	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	2A	3072	1/1	0.92	0.11	96,96,96,96	0
56	MG	2A	3201	1/1	0.92	0.11	75,75,75,75	0
56	MG	1Q	201	1/1	0.92	0.11	75,75,75,75	0
56	MG	2a	3083	1/1	0.92	0.37	61,61,61,61	0
56	MG	1A	3110	1/1	0.92	0.22	70,70,70,70	0
56	MG	2A	3172	1/1	0.92	0.04	87,87,87,87	0
56	MG	2A	3106	1/1	0.92	0.04	83,83,83,83	0
56	MG	1A	3286	1/1	0.92	0.14	76,76,76,76	0
56	MG	1A	3184	1/1	0.92	0.19	69,69,69,69	0
56	MG	1A	3273	1/1	0.92	0.18	80,80,80,80	0
56	MG	28	102	1/1	0.92	0.24	61,61,61,61	0
56	MG	1B	204	1/1	0.92	0.10	66,66,66,66	0
56	MG	1A	3380	1/1	0.92	0.17	73,73,73,73	0
56	MG	2A	3331	1/1	0.92	0.11	73,73,73,73	0
56	MG	1A	3381	1/1	0.92	0.20	63,63,63,63	0
56	MG	1A	3064	1/1	0.92	0.17	79,79,79,79	0
56	MG	1a	1682	1/1	0.92	0.11	96,96,96,96	0
56	MG	1a	1627	1/1	0.92	0.14	80,80,80,80	0
56	MG	2A	3218	1/1	0.92	0.07	72,72,72,72	0
56	MG	1A	3242	1/1	0.92	0.19	61,61,61,61	0
56	MG	2a	3100	1/1	0.92	0.12	95,95,95,95	0
56	MG	2A	3017	1/1	0.92	0.19	69,69,69,69	0
56	MG	1A	3222	1/1	0.92	0.22	71,71,71,71	0
56	MG	2A	3223	1/1	0.92	0.16	70,70,70,70	0
56	MG	17	101	1/1	0.92	0.09	66,66,66,66	0
56	MG	2A	3226	1/1	0.93	0.12	82,82,82,82	0
56	MG	1A	3153	1/1	0.93	0.11	72,72,72,72	0
56	MG	1A	3495	1/1	0.93	0.13	98,98,98,98	0
56	MG	2A	3040	1/1	0.93	0.09	95,95,95,95	0
56	MG	2A	3232	1/1	0.93	0.17	66,66,66,66	0
56	MG	1A	3427	1/1	0.93	0.30	61,61,61,61	0
56	MG	1A	3056	1/1	0.93	0.07	85,85,85,85	0
56	MG	1A	3207	1/1	0.93	0.24	62,62,62,62	0
56	MG	1A	3214	1/1	0.93	0.33	69,69,69,69	0
56	MG	1A	3458	1/1	0.93	0.13	79,79,79,79	0
56	MG	1a	1685	1/1	0.93	0.10	76,76,76,76	0
56	MG	1A	3094	1/1	0.93	0.05	84,84,84,84	0
56	MG	1A	3317	1/1	0.93	0.08	77,77,77,77	0
56	MG	2a	3069	1/1	0.93	0.17	104,104,104,104	0
56	MG	2A	3018	1/1	0.93	0.18	73,73,73,73	0
56	MG	1A	3462	1/1	0.93	0.23	79,79,79,79	0
56	MG	1A	3318	1/1	0.93	0.24	75,75,75,75	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	2A	3287	1/1	0.93	0.33	66,66,66,66	0
56	MG	1a	1664	1/1	0.93	0.09	67,67,67,67	0
56	MG	1A	3085	1/1	0.93	0.12	79,79,79,79	0
56	MG	1a	1666	1/1	0.93	0.07	94,94,94,94	0
56	MG	2A	3292	1/1	0.93	0.20	64,64,64,64	0
56	MG	1A	3233	1/1	0.93	0.19	76,76,76,76	0
56	MG	1A	3309	1/1	0.93	0.13	62,62,62,62	0
56	MG	2A	3026	1/1	0.93	0.17	76,76,76,76	0
56	MG	2A	3060	1/1	0.93	0.07	88,88,88,88	0
56	MG	2a	3082	1/1	0.93	0.36	66,66,66,66	0
56	MG	2A	3061	1/1	0.93	0.10	69,69,69,69	0
56	MG	2A	3135	1/1	0.93	0.08	111,111,111,111	0
56	MG	2a	3031	1/1	0.93	0.06	76,76,76,76	0
56	MG	1a	1620	1/1	0.93	0.07	81,81,81,81	0
56	MG	1A	3132	1/1	0.93	0.05	74,74,74,74	0
56	MG	1A	3485	1/1	0.93	0.13	72,72,72,72	0
56	MG	2A	3303	1/1	0.93	0.13	76,76,76,76	0
56	MG	2A	3065	1/1	0.93	0.17	68,68,68,68	0
56	MG	1A	3311	1/1	0.93	0.25	62,62,62,62	0
56	MG	2A	3215	1/1	0.93	0.14	61,61,61,61	0
56	MG	1a	1673	1/1	0.93	0.08	99,99,99,99	0
56	MG	2A	3068	1/1	0.93	0.11	90,90,90,90	0
56	MG	2Y	201	1/1	0.93	0.21	71,71,71,71	0
56	MG	2a	3042	1/1	0.93	0.06	91,91,91,91	0
56	MG	2A	3220	1/1	0.93	0.27	64,64,64,64	0
56	MG	2A	3144	1/1	0.93	0.19	83,83,83,83	0
56	MG	1E	302	1/1	0.93	0.10	76,76,76,76	0
56	MG	2A	3312	1/1	0.93	0.15	64,64,64,64	0
56	MG	18	101	1/1	0.93	0.38	65,65,65,65	0
56	MG	2A	3360	1/1	0.93	0.16	61,61,61,61	0
56	MG	2A	3036	1/1	0.93	0.12	77,77,77,77	0
56	MG	1a	1628	1/1	0.93	0.31	61,61,61,61	0
56	MG	2A	3043	1/1	0.94	0.08	70,70,70,70	0
56	MG	1A	3439	1/1	0.94	0.22	67,67,67,67	0
56	MG	1a	1680	1/1	0.94	0.14	73,73,73,73	0
56	MG	1A	3163	1/1	0.94	0.07	78,78,78,78	0
56	MG	1A	3053	1/1	0.94	0.29	77,77,77,77	0
56	MG	1A	3038	1/1	0.94	0.09	61,61,61,61	0
56	MG	1A	3382	1/1	0.94	0.07	91,91,91,91	0
56	MG	1a	1605	1/1	0.94	0.06	99,99,99,99	0
56	MG	1a	1606	1/1	0.94	0.16	69,69,69,69	0
56	MG	1A	3342	1/1	0.94	0.24	62,62,62,62	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	1A	3036	1/1	0.94	0.05	83,83,83,83	0
56	MG	2A	3216	1/1	0.94	0.17	62,62,62,62	0
56	MG	1A	3399	1/1	0.94	0.23	73,73,73,73	0
56	MG	2A	3143	1/1	0.94	0.24	69,69,69,69	0
56	MG	2A	3121	1/1	0.94	0.13	66,66,66,66	0
56	MG	1A	3244	1/1	0.94	0.13	77,77,77,77	0
56	MG	2E	306	1/1	0.94	0.16	64,64,64,64	0
56	MG	1A	3103	1/1	0.94	0.28	64,64,64,64	0
56	MG	2a	3021	1/1	0.94	0.10	82,82,82,82	0
56	MG	1A	3112	1/1	0.94	0.25	63,63,63,63	0
56	MG	1A	3131	1/1	0.94	0.05	76,76,76,76	0
56	MG	2A	3149	1/1	0.94	0.14	82,82,82,82	0
56	MG	1A	3225	1/1	0.94	0.08	90,90,90,90	0
56	MG	1A	3215	1/1	0.94	0.12	67,67,67,67	0
56	MG	2A	3343	1/1	0.94	0.12	73,73,73,73	0
56	MG	2A	3228	1/1	0.94	0.12	67,67,67,67	0
56	MG	2A	3128	1/1	0.94	0.52	61,61,61,61	0
56	MG	2A	3230	1/1	0.94	0.18	62,62,62,62	0
56	MG	1A	3145	1/1	0.94	0.08	79,79,79,79	0
56	MG	2a	3103	1/1	0.94	0.06	101,101,101,101	0
56	MG	2a	3068	1/1	0.94	0.19	81,81,81,81	0
56	MG	2A	3379	1/1	0.94	0.14	77,77,77,77	0
56	MG	2A	3380	1/1	0.94	0.05	85,85,85,85	0
56	MG	1A	3162	1/1	0.94	0.13	65,65,65,65	0
57	ZN	2Y	202	1/1	0.94	0.16	176,176,176,176	0
56	MG	1A	3146	1/1	0.95	0.06	64,64,64,64	0
56	MG	2A	3279	1/1	0.95	0.21	80,80,80,80	0
56	MG	2A	3233	1/1	0.95	0.16	70,70,70,70	0
56	MG	2A	3168	1/1	0.95	0.09	68,68,68,68	0
56	MG	1A	3483	1/1	0.95	0.07	68,68,68,68	0
56	MG	2A	3109	1/1	0.95	0.22	63,63,63,63	0
56	MG	1a	1658	1/1	0.95	0.09	75,75,75,75	0
56	MG	1a	1625	1/1	0.95	0.12	102,102,102,102	0
56	MG	1A	3147	1/1	0.95	0.30	76,76,76,76	0
56	MG	1A	3324	1/1	0.95	0.07	67,67,67,67	0
56	MG	2A	3363	1/1	0.95	0.34	65,65,65,65	0
56	MG	1A	3052	1/1	0.95	0.10	85,85,85,85	0
56	MG	1a	1646	1/1	0.95	0.06	71,71,71,71	0
56	MG	2A	3096	1/1	0.95	0.06	92,92,92,92	0
56	MG	1A	3489	1/1	0.95	0.07	78,78,78,78	0
56	MG	1A	3029	1/1	0.95	0.10	86,86,86,86	0
56	MG	1A	3494	1/1	0.95	0.07	85,85,85,85	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	1A	3080	1/1	0.95	0.07	82,82,82,82	0
56	MG	2A	3296	1/1	0.95	0.15	66,66,66,66	0
56	MG	1A	3368	1/1	0.95	0.15	77,77,77,77	0
56	MG	2A	3347	1/1	0.95	0.28	61,61,61,61	0
56	MG	2a	3102	1/1	0.95	0.04	127,127,127,127	0
56	MG	1A	3119	1/1	0.95	0.16	64,64,64,64	0
56	MG	1a	1604	1/1	0.95	0.04	107,107,107,107	0
56	MG	2a	3018	1/1	0.95	0.09	86,86,86,86	0
56	MG	1A	3278	1/1	0.95	0.13	63,63,63,63	0
56	MG	2A	3047	1/1	0.95	0.10	81,81,81,81	0
56	MG	10	101	1/1	0.95	0.06	65,65,65,65	0
56	MG	2A	3187	1/1	0.96	0.08	74,74,74,74	0
56	MG	1A	3498	1/1	0.96	0.06	74,74,74,74	0
56	MG	2A	3089	1/1	0.96	0.06	87,87,87,87	0
56	MG	1a	1645	1/1	0.96	0.06	90,90,90,90	0
56	MG	1a	1608	1/1	0.96	0.10	73,73,73,73	0
56	MG	1a	1626	1/1	0.96	0.03	81,81,81,81	0
56	MG	2R	201	1/1	0.96	0.11	64,64,64,64	0
56	MG	2A	3378	1/1	0.96	0.07	83,83,83,83	0
56	MG	2a	3060	1/1	0.96	0.09	120,120,120,120	0
56	MG	1A	3092	1/1	0.96	0.08	71,71,71,71	0
56	MG	2A	3033	1/1	0.96	0.10	82,82,82,82	0
56	MG	2A	3256	1/1	0.96	0.30	66,66,66,66	0
56	MG	1A	3417	1/1	0.96	0.11	64,64,64,64	0
56	MG	2A	3070	1/1	0.96	0.10	81,81,81,81	0
56	MG	2T	201	1/1	0.97	0.06	63,63,63,63	0
56	MG	2a	3054	1/1	0.97	0.04	69,69,69,69	0
56	MG	1A	3133	1/1	0.97	0.08	72,72,72,72	0
56	MG	2A	3260	1/1	0.97	0.12	70,70,70,70	0
56	MG	2a	3057	1/1	0.97	0.05	101,101,101,101	0
56	MG	1A	3284	1/1	0.97	0.09	76,76,76,76	0
56	MG	2A	3338	1/1	0.97	0.22	75,75,75,75	0
56	MG	1A	3125	1/1	0.97	0.06	62,62,62,62	0
56	MG	2A	3384	1/1	0.97	0.04	91,91,91,91	0
56	MG	1A	3117	1/1	0.97	0.17	63,63,63,63	0
57	ZN	1Y	501	1/1	0.97	0.04	156,156,156,156	0
56	MG	2a	3006	1/1	0.97	0.05	76,76,76,76	0
56	MG	2A	3289	1/1	0.98	0.07	77,77,77,77	0
56	MG	1a	1693	1/1	0.98	0.03	127,127,127,127	0
56	MG	1A	3475	1/1	0.98	0.20	65,65,65,65	0
56	MG	2A	3383	1/1	0.98	0.05	76,76,76,76	0
56	MG	1U	201	1/1	0.98	0.11	67,67,67,67	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	1A	3486	1/1	0.98	0.04	78,78,78,78	0
56	MG	1A	3016	1/1	0.98	0.04	95,95,95,95	0
56	MG	2a	3050	1/1	0.98	0.05	88,88,88,88	0
56	MG	2A	3028	1/1	0.98	0.07	91,91,91,91	0
56	MG	1a	1610	1/1	0.98	0.06	104,104,104,104	0
57	ZN	1n	501	1/1	0.98	0.04	148,148,148,148	0
56	MG	1a	1692	1/1	0.98	0.04	114,114,114,114	0
57	ZN	24	501	1/1	0.98	0.06	182,182,182,182	0
58	SF4	1d	302	8/8	0.98	0.04	111,128,150,164	0
58	SF4	2d	302	8/8	0.98	0.06	99,114,123,127	0
56	MG	1A	3493	1/1	0.99	0.03	97,97,97,97	0
56	MG	2A	3217	1/1	0.99	0.06	78,78,78,78	0
56	MG	1A	3487	1/1	0.99	0.09	74,74,74,74	0
56	MG	1a	1691	1/1	0.99	0.05	94,94,94,94	0
56	MG	1A	3459	1/1	0.99	0.07	76,76,76,76	0
57	ZN	14	501	1/1	0.99	0.07	166,166,166,166	0
57	ZN	16	102	1/1	0.99	0.06	102,102,102,102	0
57	ZN	19	501	1/1	0.99	0.07	104,104,104,104	0
56	MG	2A	3381	1/1	0.99	0.04	76,76,76,76	0
56	MG	1A	3496	1/1	0.99	0.03	94,94,94,94	0
56	MG	2a	3101	1/1	0.99	0.03	102,102,102,102	0
57	ZN	25	102	1/1	0.99	0.04	104,104,104,104	0
57	ZN	26	501	1/1	0.99	0.03	107,107,107,107	0
57	ZN	29	501	1/1	0.99	0.05	114,114,114,114	0
57	ZN	2n	501	1/1	0.99	0.03	118,118,118,118	0
56	MG	1A	3492	1/1	0.99	0.03	95,95,95,95	0
56	MG	2A	3075	1/1	0.99	0.07	95,95,95,95	0
57	ZN	15	102	1/1	1.00	0.02	106,106,106,106	0
56	MG	1A	3490	1/1	1.00	0.03	79,79,79,79	0

6.5 Other polymers ⓘ

There are no such residues in this entry.