



wwPDB X-ray Structure Validation Summary Report ⓘ

Aug 5, 2026 – 11:54 PM EDT

PDB ID : 7JQM / pdb_00007jqm
Title : Crystal structure of the Thermus thermophilus 70S ribosome in complex with Bac7-002, mRNA, and deacylated P-site tRNA at 3.05Å resolution
Authors : Mardirossian, M.; Sola, R.; Beckert, B.; Valencic, E.; Collis, D.W.P.; Borisek, J.; Armas, F.; Di Stasi, A.; Buchmann, J.; Syroegin, E.A.; Polikanov, Y.S.; Magistrato, A.; Hilpert, K.; Wilson, D.N.; Scocchi, M.
Deposited on : 2020-08-11
Resolution : 3.05 Å(reported)

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

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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	:	9.0.015 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.50

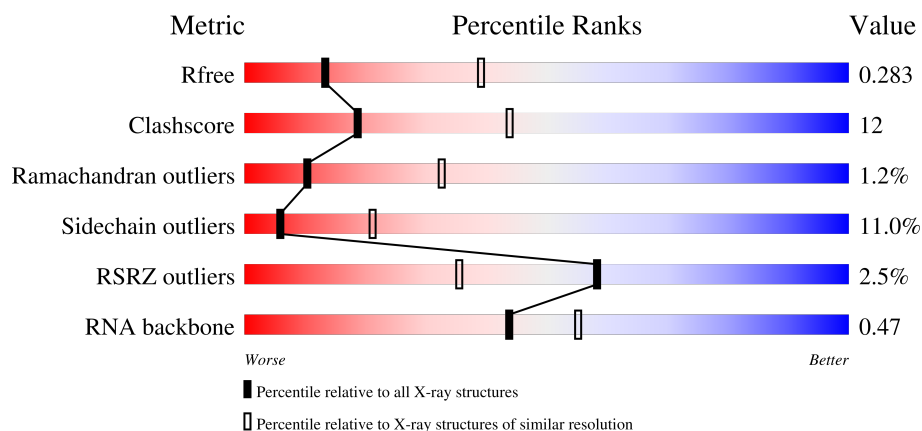
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.05 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	2469 (3.10-3.02)
Clashscore	190562	2569 (3.10-3.02)
Ramachandran outliers	187476	2424 (3.10-3.02)
Sidechain outliers	187428	2423 (3.10-3.02)
RSRZ outliers	180081	2469 (3.10-3.02)
RNA backbone	3983	1079 (3.30-2.82)

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	
1	2A	2915	
2	1B	121	

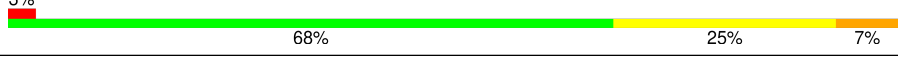
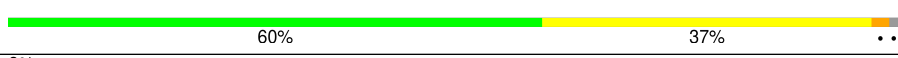
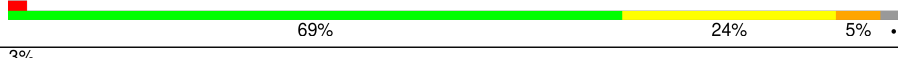
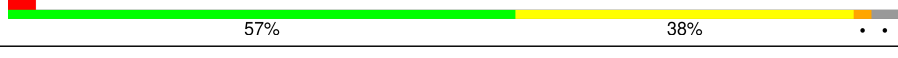
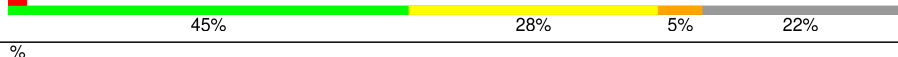
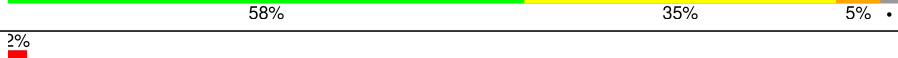
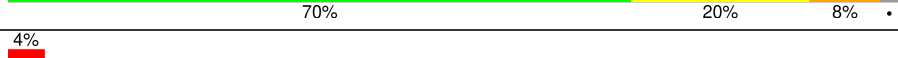
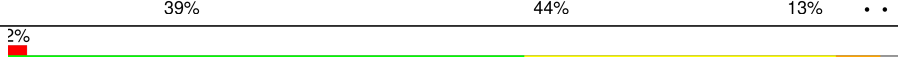
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Mol	Chain	Length	Quality of chain
2	2B	121	
3	1D	276	
3	2D	276	
4	1E	206	
4	2E	206	
5	1F	210	
5	2F	210	
6	1G	182	
6	2G	182	
7	1H	180	
7	2H	180	
8	1I	148	
8	2I	148	
9	1N	140	
9	2N	140	
10	1O	122	
10	2O	122	
11	1P	150	
11	2P	150	
12	1Q	141	
12	2Q	141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

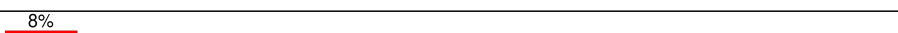
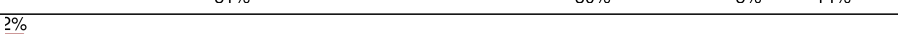
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Mol	Chain	Length	Quality of chain
15	1T	146	
15	2T	146	
16	1U	118	
16	2U	118	
17	1V	101	
17	2V	101	
18	1W	113	
18	2W	113	
19	1X	96	
19	2X	96	
20	1Y	110	
20	2Y	110	
21	1Z	206	
21	2Z	206	
22	10	85	
22	20	85	
23	11	98	
23	21	98	
24	12	72	
24	22	72	
25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

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

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

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Mol	Chain	Length	Quality of chain
52	2u	27	
53	1v	24	
53	2v	24	
54	1x	77	
54	2x	77	
55	1z	16	
55	2z	16	

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	3388	-	-	-	X
56	MG	1a	1744	-	-	-	X
56	MG	1a	1759	-	-	-	X
56	MG	2a	3082	-	-	-	X
56	MG	2a	3119	-	-	-	X
56	MG	2a	3145	-	-	-	X
58	SF4	1d	302	-	-	X	-

2 Entry composition

There are 60 unique types of molecules in this entry. The entry contains 290774 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	76	Total	C	N	O	S	0	0	0
			604	373	128	102	1			
22	20	76	Total	C	N	O	S	0	0	0
			604	373	128	102	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	13	Total	C	N	O	P	0	0	0
			277	125	51	88	13			
53	2v	13	Total	C	N	O	P	0	0	0
			277	125	51	88	13			

- Molecule 54 is a RNA chain called P-site tRNA.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
54	1x	76	Total	C	N	O	P	S	0	0	0
			1625	725	294	529	76	1			
54	2x	76	Total	C	N	O	P	S	0	0	0
			1625	725	294	529	76	1			

- Molecule 55 is a protein called Bac7-002.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
55	1z	16	Total	C	N	O	0	0	0
			147	93	38	16			
55	2z	16	Total	C	N	O	0	0	0
			141	90	35	16			

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
56	1A	848	Total	Mg	0	0
			848	848		
56	1B	25	Total	Mg	0	0
			25	25		
56	1D	8	Total	Mg	0	0
			8	8		
56	1E	8	Total	Mg	0	0
			8	8		
56	1F	12	Total	Mg	0	0
			12	12		
56	1G	4	Total	Mg	0	0
			4	4		
56	1H	1	Total	Mg	0	0
			1	1		
56	1I	1	Total	Mg	0	0
			1	1		
56	1N	3	Total	Mg	0	0
			3	3		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
56	1O	1	Total 1	Mg 1	0	0
56	1P	5	Total 5	Mg 5	0	0
56	1Q	4	Total 4	Mg 4	0	0
56	1R	6	Total 6	Mg 6	0	0
56	1S	1	Total 1	Mg 1	0	0
56	1T	2	Total 2	Mg 2	0	0
56	1U	6	Total 6	Mg 6	0	0
56	1V	5	Total 5	Mg 5	0	0
56	1W	6	Total 6	Mg 6	0	0
56	1X	3	Total 3	Mg 3	0	0
56	1Y	1	Total 1	Mg 1	0	0
56	1Z	3	Total 3	Mg 3	0	0
56	10	5	Total 5	Mg 5	0	0
56	11	2	Total 2	Mg 2	0	0
56	12	2	Total 2	Mg 2	0	0
56	13	3	Total 3	Mg 3	0	0
56	14	1	Total 1	Mg 1	0	0
56	15	5	Total 5	Mg 5	0	0
56	17	6	Total 6	Mg 6	0	0
56	18	4	Total 4	Mg 4	0	0
56	19	1	Total 1	Mg 1	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
56	1a	167	Total 167	Mg 167	0	0
56	1d	1	Total 1	Mg 1	0	0
56	1e	2	Total 2	Mg 2	0	0
56	1f	2	Total 2	Mg 2	0	0
56	1h	1	Total 1	Mg 1	0	0
56	1l	3	Total 3	Mg 3	0	0
56	1m	1	Total 1	Mg 1	0	0
56	1n	2	Total 2	Mg 2	0	0
56	1s	1	Total 1	Mg 1	0	0
56	1v	1	Total 1	Mg 1	0	0
56	1x	10	Total 10	Mg 10	0	0
56	1z	1	Total 1	Mg 1	0	0
56	2A	625	Total 625	Mg 625	0	0
56	2B	12	Total 12	Mg 12	0	0
56	2D	2	Total 2	Mg 2	0	0
56	2E	5	Total 5	Mg 5	0	0
56	2F	4	Total 4	Mg 4	0	0
56	2N	1	Total 1	Mg 1	0	0
56	2O	1	Total 1	Mg 1	0	0
56	2P	3	Total 3	Mg 3	0	0
56	2Q	2	Total 2	Mg 2	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
56	2R	1	Total 1	Mg 1	0	0
56	2T	2	Total 2	Mg 2	0	0
56	2V	2	Total 2	Mg 2	0	0
56	2W	1	Total 1	Mg 1	0	0
56	2Y	1	Total 1	Mg 1	0	0
56	2Z	1	Total 1	Mg 1	0	0
56	20	1	Total 1	Mg 1	0	0
56	21	1	Total 1	Mg 1	0	0
56	23	2	Total 2	Mg 2	0	0
56	25	2	Total 2	Mg 2	0	0
56	26	1	Total 1	Mg 1	0	0
56	27	2	Total 2	Mg 2	0	0
56	28	3	Total 3	Mg 3	0	0
56	2a	145	Total 145	Mg 145	0	0
56	2d	1	Total 1	Mg 1	0	0
56	2f	1	Total 1	Mg 1	0	0
56	2j	1	Total 1	Mg 1	0	0
56	2k	1	Total 1	Mg 1	0	0
56	2l	2	Total 2	Mg 2	0	0
56	2q	2	Total 2	Mg 2	0	0
56	2r	1	Total 1	Mg 1	0	0

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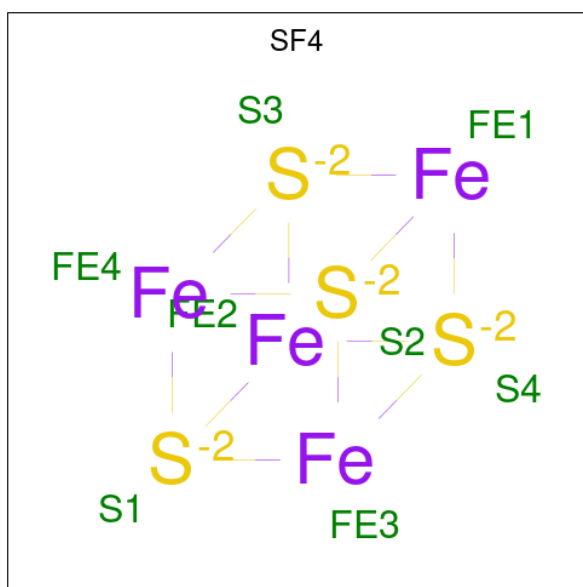
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
56	2t	1	Total 1	Mg 1	0	0
56	2v	2	Total 2	Mg 2	0	0
56	2x	3	Total 3	Mg 3	0	0

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

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

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



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

- Molecule 59 is POTASSIUM ION (CCD ID: K) (formula: K).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
59	2x	1	Total	K	0	0
			1	1		

- Molecule 60 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
60	1A	1222	Total	O	0	0
			1222	1222		
60	1B	27	Total	O	0	0
			27	27		
60	1D	21	Total	O	0	0
			21	21		
60	1E	11	Total	O	0	0
			11	11		
60	1F	9	Total	O	0	0
			9	9		
60	1N	1	Total	O	0	0
			1	1		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
60	1O	1	Total 1	O 1	0	0
60	1P	14	Total 14	O 14	0	0
60	1Q	2	Total 2	O 2	0	0
60	1R	3	Total 3	O 3	0	0
60	1S	2	Total 2	O 2	0	0
60	1T	4	Total 4	O 4	0	0
60	1U	4	Total 4	O 4	0	0
60	1V	4	Total 4	O 4	0	0
60	1W	3	Total 3	O 3	0	0
60	10	2	Total 2	O 2	0	0
60	11	2	Total 2	O 2	0	0
60	12	2	Total 2	O 2	0	0
60	13	2	Total 2	O 2	0	0
60	18	2	Total 2	O 2	0	0
60	1a	26	Total 26	O 26	0	0
60	1d	1	Total 1	O 1	0	0
60	1z	1	Total 1	O 1	0	0
60	2A	416	Total 416	O 416	0	0
60	2B	3	Total 3	O 3	0	0
60	2D	12	Total 12	O 12	0	0
60	2E	4	Total 4	O 4	0	0

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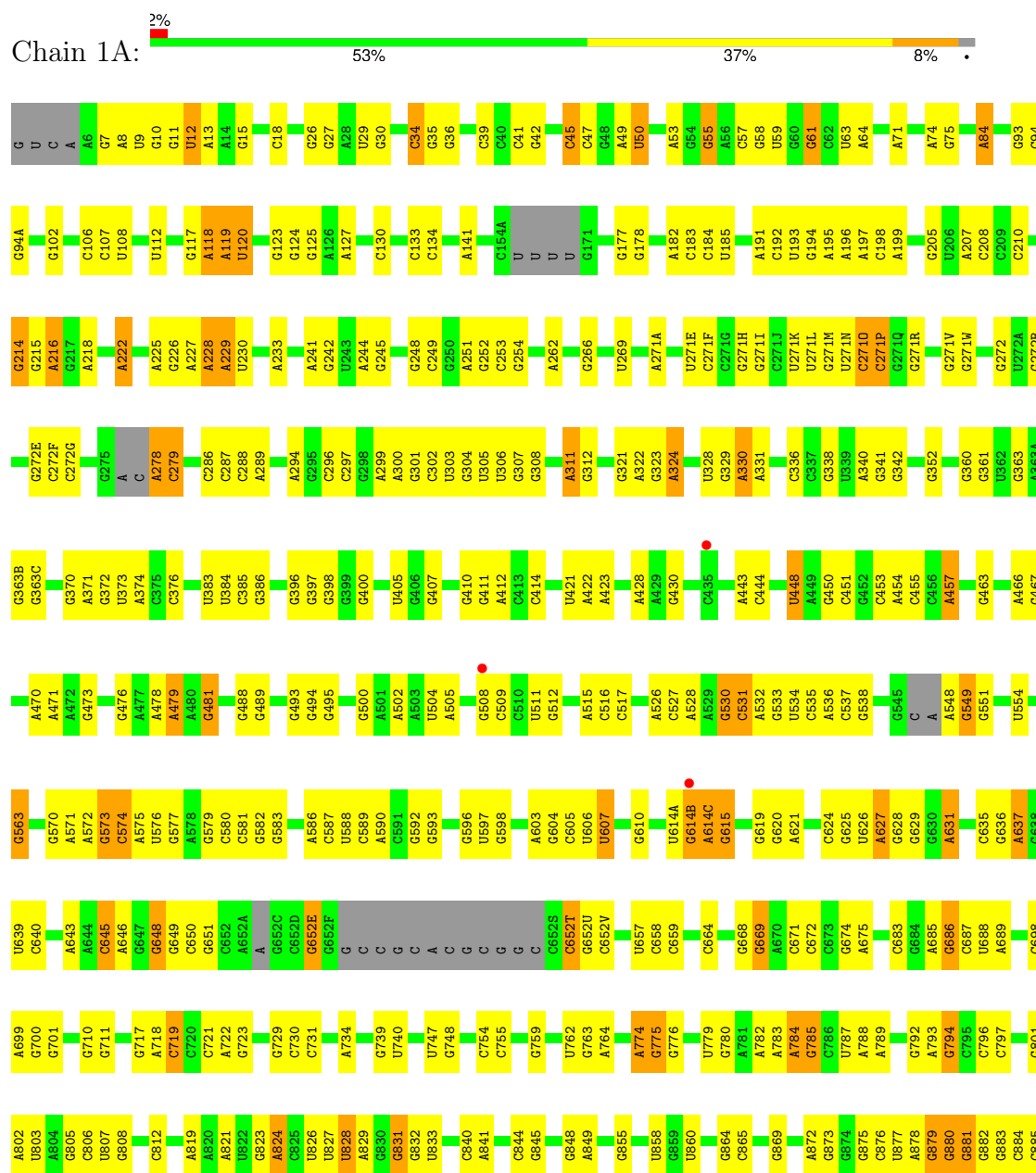
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
60	2F	6	Total 6	O 6	0	0
60	2I	1	Total 1	O 1	0	0
60	2O	3	Total 3	O 3	0	0
60	2P	4	Total 4	O 4	0	0
60	2Q	1	Total 1	O 1	0	0
60	2R	1	Total 1	O 1	0	0
60	2T	1	Total 1	O 1	0	0
60	2V	1	Total 1	O 1	0	0
60	2W	2	Total 2	O 2	0	0
60	20	1	Total 1	O 1	0	0
60	21	2	Total 2	O 2	0	0
60	28	2	Total 2	O 2	0	0
60	2a	17	Total 17	O 17	0	0
60	2l	1	Total 1	O 1	0	0
60	2n	1	Total 1	O 1	0	0
60	2t	1	Total 1	O 1	0	0
60	2x	1	Total 1	O 1	0	0

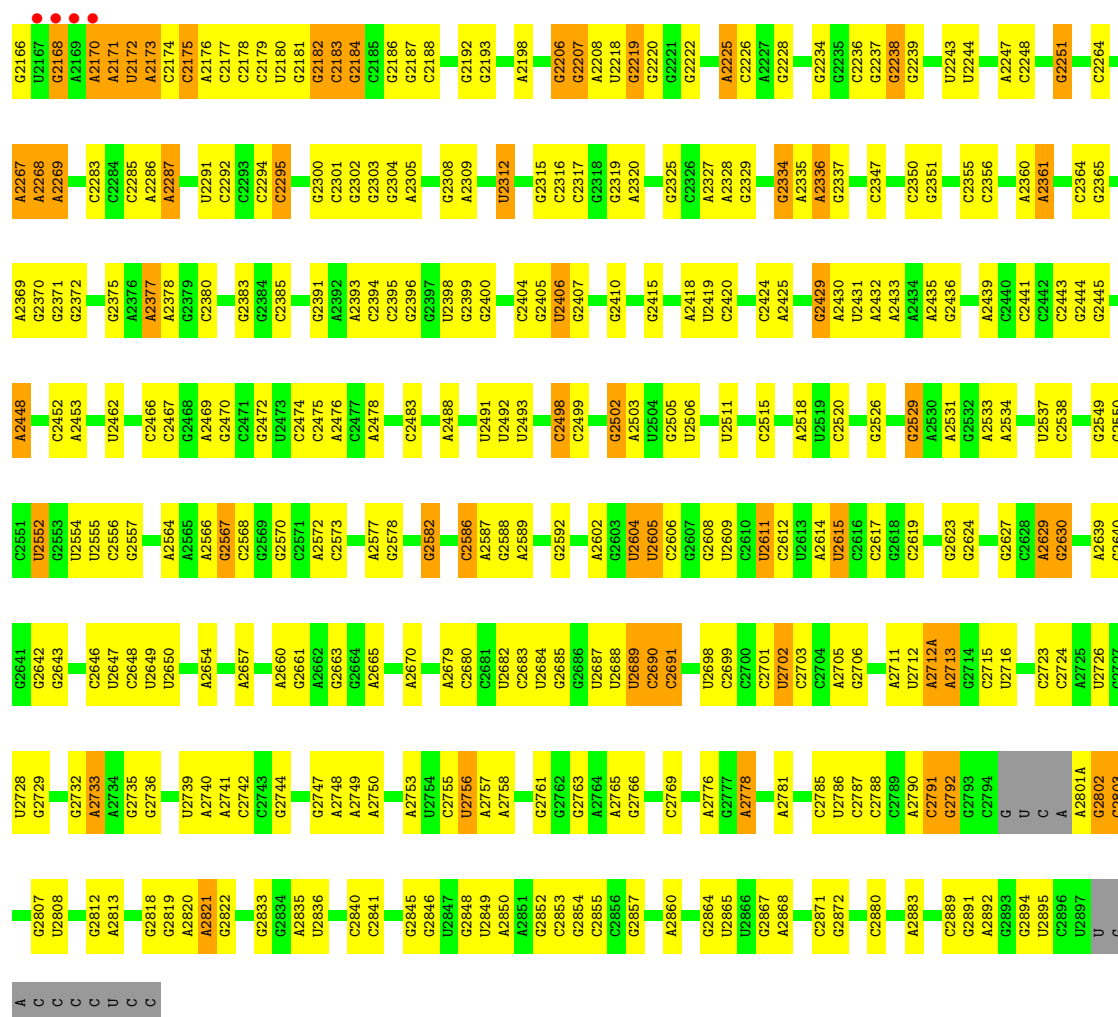
3 Residue-property plots [i](#)

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.

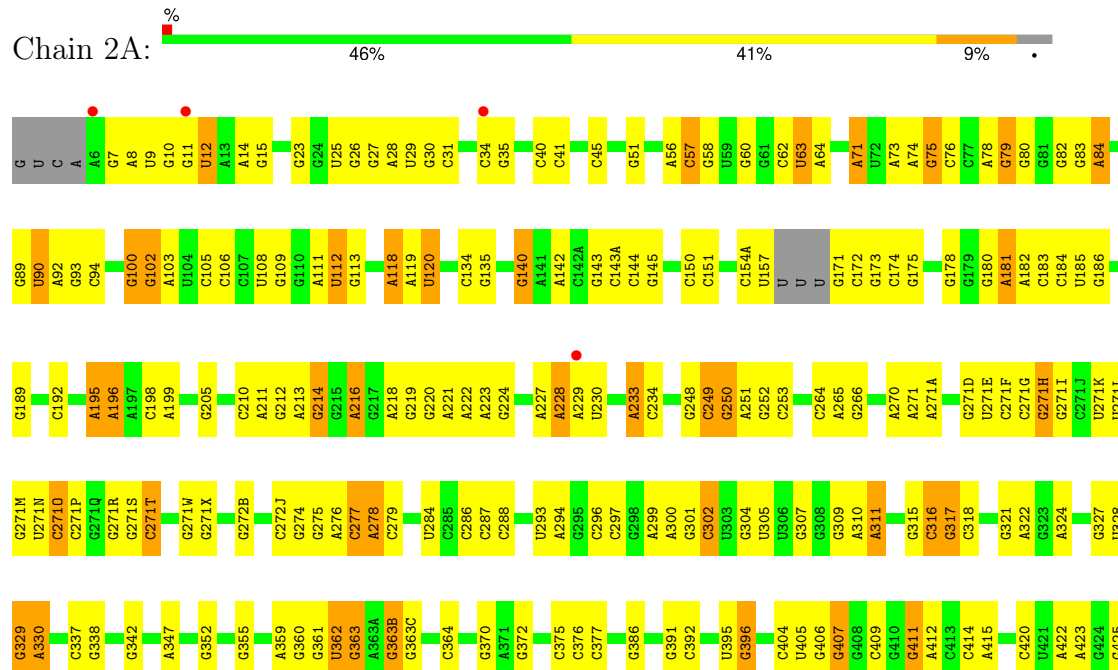
• Molecule 1: 23S Ribosomal RNA



C2104	C2105	C2106	C2107	C2108	U2109	C2110	C2111	C2112	U2113	C2114	C2115	C2116	C2117	A2042	C2043	C2044	U2047	C2048	A2051	C2052	C2053	A2054	C2055	C2056	C2057	A2060	C2061	A2062	C2065	C2066	C2067	C2068	C2069	C2070	C2071	C2072	C2073	U2074	U2075	U2076	C2077	C2078	C2079	C2080	C2081	C2082	C2083	C2084	C2085	C2086	C2087	C2088	C2089	C2090	C2091	C2092	C2093	C2094	C2095	C2096	C2097	C2098	C2099	C2100	C2101	C2102	C2103
G1816	G1817	G1823	G1826	A1829	C1830	G1831	C1832	U1833	G1842	C1843	C1844	A1847	G1858	A1859	U1864	G1865	A1877	C1878	C1879	C1882	G1883	A1889	A1890	G1897	U1898	G1899	A1900	G1906	U1911	A1912	A1913	C1914	U1915	C1916	U1917	C1918	A1919	C1920	A1927	U1928	C1929	A2001	C2002	C2012	A2013	A2014	A2015	U2016	U2017	C2018	A2019	G2020	C2021	U2022	C2023												
G1721	A1722	U1739	G1746	G1753	C1754	G1756	A1759	A1762	C1763	G1764	C1765	U1766	C1767	G1770	C1771	G1772	A1773	C1774	U1778	U1779	U1780	C1781	G1782	A1783	A1784	A1785	A1786	A1787	C1788	A1789	C1790	A1791	G1792	C1793	U1794	C1795	U1796	C1797	U1798	G1799	C1800	A1803	C1804	U1805	A1810	C1811	G1814	A1815																			
C1636	A1637	C1638	U1639	C1640	A1641	G1642	C1646	G1647	A1648	G1649	G1653	A1654	A1655	A1656	A1657	G1667	A1668	C1669	U1670	U1671	G1674	C1675	A1676	A1677	C1683	C1684	C1685	C1686	G1687	A1688	A1689	U1692	U1693	C1694	G1697	A1698	G1699	A1700	A1701	G1702	G1703	G1704	G1705	U1706	U1709	C1710	C1711	C1712	U1713	G1628	U1629																
A1528A	C1532	G1533	U1540	A1541	A1542	C1543	A1544	A1545	C1546	C1547	C1548	C1557	A1558	G1561	A1566	A1567	A1568	A1569	A1570	C1577	U1578	A1579	A1580	G1581	C1584	A1586	A1587	C1588	C1589	U1590	G1593	G1594	G1595	C1604	C1607	A1608	A1609	A1610	A1614	C1615	A1616	G1628	U1629																								
A1434	G1435	G1436	C1437	G1441	G1442	A1445	C1446	C1447	G1448	A1449	G1450	U1453	G1455	G1461	C1464	G1465	G1466	C1467	A1472	G1473	G1482	G1484	G1485	A1486	G1487	C1493	A1494	A1495	A1496	U1497	G1500	A1507	A1508	C1509	A1509A	A1509B	G1510	U1514	G1515	U1518	G1519	G1525	G1526	G1527	A1528																						
A1342	G1343	C1344	C1345	A1349	U1352	A1353	U1357	G1358	A1359	A1360	G1364	A1365	G1369	C1370	G1371	U1372	G1377	A1378	A1379	G1380	A1384	G1385	C1386	A1392	A1393	A1394	A1395	U1396	C1398	U1405	U1406	C1407	G1416	C1417	G1418	A1419	U1420	G1421	G1424	G1425	U1428	C1429	C1430	U1431	C1432	U1433																					
U1130	C1135	G1136	G1137	G1138	G1139	C1140	U1141	A1142A	A1143	C1153	G1154	A1155	A1156	G1164	U1165	C1166	G1167	G1168	G1169	G1170	G1171	A1174	U1175	G1176	A1177	C1178	C1179	C1180	G1183	G1186	G1187	U1188	A1189	C1201	C1202	G1203	C1218	G1219	A1220	U1227	U1234	G1235	G1239	U1240	G1243	G1244																					
G1245	C1250	G1251	A1253	G1256	G1264	A1265	G1266	U1267	A1268	A1269	C1270	A1271	U1272	U1273	A1274	A1275	A1278	A1287	U1288	U1292	C1293	U1294	C1295	G1296	C1297	U1300	A1301	A1302	G1310	G1311	C1315	U1316	A1317	C1320	A1321	A1322	U1329	C1330	G1332	A1336	G1337	G1338	U1339	G1340	U1341																						
G1062	G1063	C1064	U1065	A1066	A1067	G1068	A1069	A1070	G1071	C1072	A1073	G1074	C1075	A1076	A1077	U1078	C1079	U1080	U1081	U1082	U1083	A1084	A1085	A1086	U1087	U1088	G1089	U1090	G1091	C1092	G1093	U1094	A1095	U1096	A1097	A1098	G1099	C1100	U1101	C1102	A1103	C1104	U1105	G1106	U1107	U1108	C1109	G1110	A1111	G1112	U1113	G1114	G1115	C1116	G1125	A1129											
C987	A988	G989	G993	C994	C995	A996	A1000	C997	C998	A899	C894	U907	A910	A918	G919	C923	C924	C925	G928	G932	U1020	A1021	U1022	U1023	G1024	G1025	U1026	A1027	G1028	U1029	U1030	A1031	U1032	A1033	U1034	U1035	C1038	G1039	C1040	A957	U958	A959	A960	C961	G968	C971	G972	A973	C974	C975	C976	G977	A980	U983													

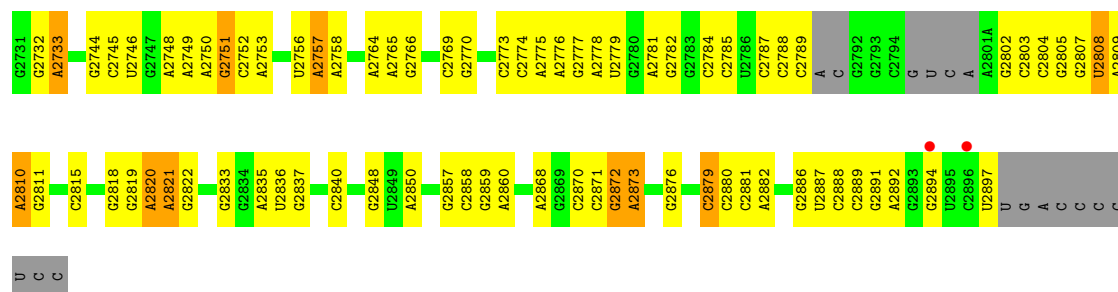


• Molecule 1: 23S Ribosomal RNA



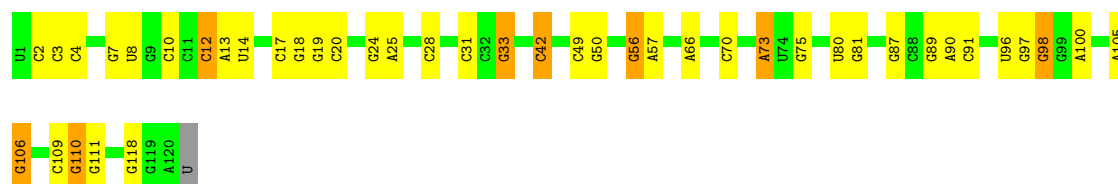


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U2853	A2855	A2856	A2488	U2401	C2316	G2235	G2156	U2011	U1926	G1828	G1740	C1647	A1566
G2855	G2856	G2857	G2489	C2404	C2317	G2238	A2158	G2012	A1927	C1829	C1745	C1648	A1567
U2856	U2857	G2858	G2490	G2405	G2319	G2239	G2159	A2013	G1928	G1830	G1746	G1650	A1568
G2857	G2858	A2859	U2406	U2406	A2320	U2243	C2161	A2014	G1930	G1835	G1758	G1651	A1569
G2858	G2859	A2860	G2495	U2407	G2325	U2244	C2162	G2018	U1931	C1836	A1755	G1652	A1570
U2859	C2860	U2861	C2498	U2408	C2326	U2245	C2163	A2019	A1932	C1837	G1756	A1652	A1571
G2860	U2861	U2862	G2499	G2410	A2327	G2246	G2164	G2020	G1933	G1842	U1757	G1653	A1572
G2861	G2862	G2863	G2502	A2418	A2328	A2247	G2165	G2021	G1934	G1843	G1758	A1654	C1574
G2862	G2863	G2864	G2503	U2419	G2329	G2248	G2166	U2022	A1936	A1847	C1758	C1657	U1578
U2863	U2864	U2865	A2503	U2419	G2330	G2251	U2167	G2023	A1937	A1848	A1762	C1658	A1579
G2864	G2865	G2866	U2504	C2420	G2331	G2251	G2168	G2027	U1938	G1849	G1763	U1659	A1580
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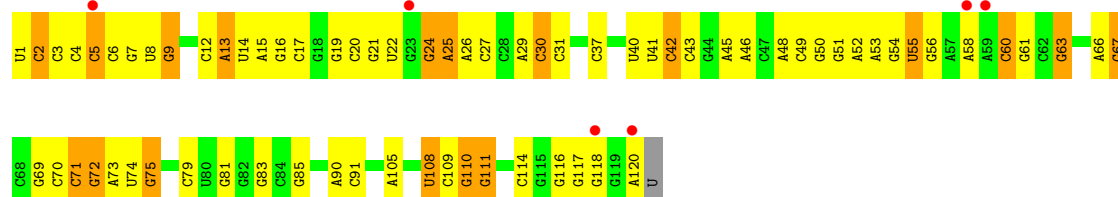
• Molecule 2: 5S Ribosomal RNA

Chain 1B: 64% 29% 7% .



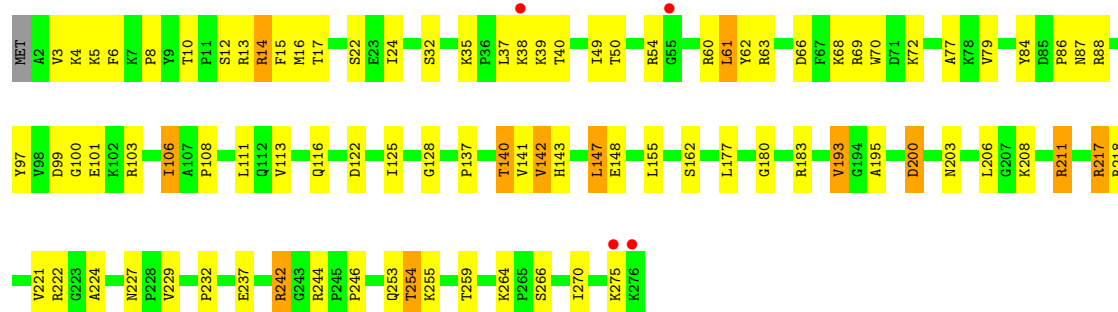
• Molecule 2: 5S Ribosomal RNA

Chain 2B: 5% 40% 44% 15% .



• Molecule 3: 50S ribosomal protein L2

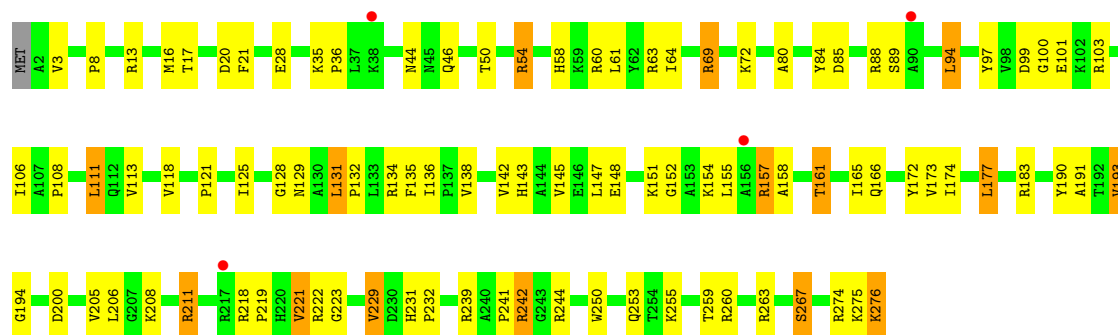
Chain 1D: 67% 28% .



• Molecule 3: 50S ribosomal protein L2

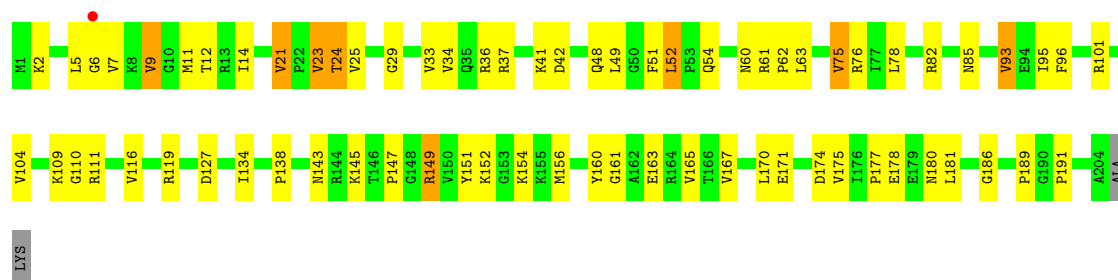
Chain 2D: 64% 30% 5% .





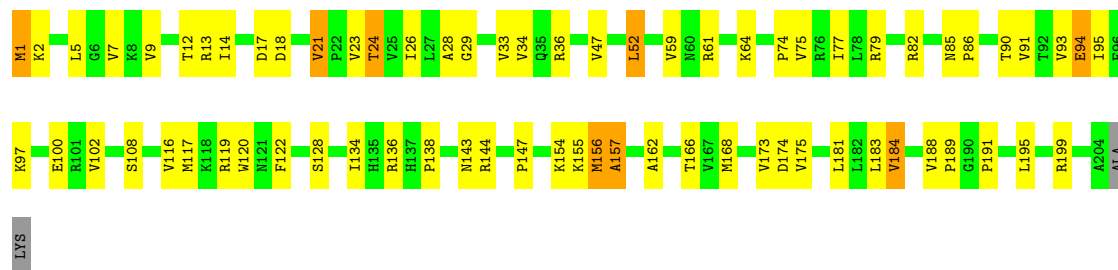
• Molecule 4: 50S ribosomal protein L3

Chain 1E: 65% 30% ..



• Molecule 4: 50S ribosomal protein L3

Chain 2E: 65% 30% ..



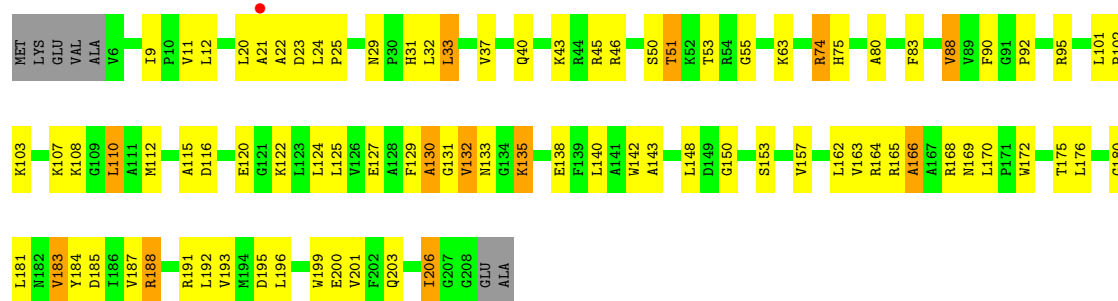
• Molecule 5: 50S ribosomal protein L4

Chain 1F: 61% 30% 6% .



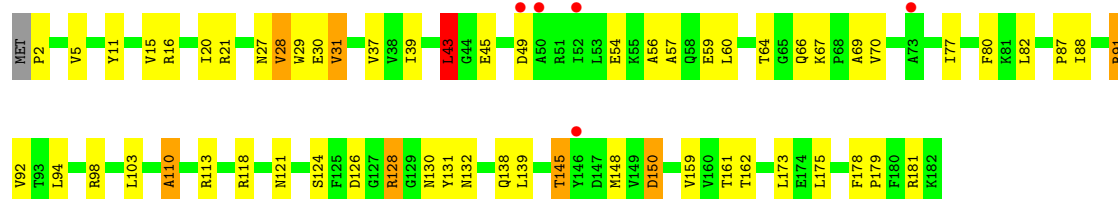
• Molecule 5: 50S ribosomal protein L4

Chain 2F: 



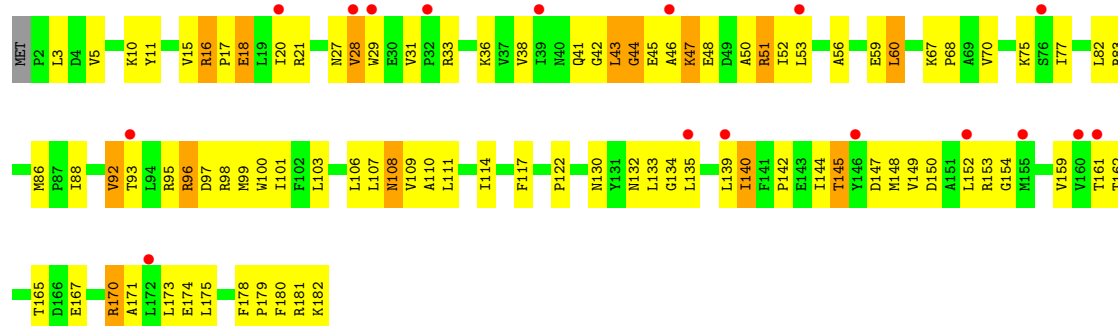
• Molecule 6: 50S ribosomal protein L5

Chain 1G: 



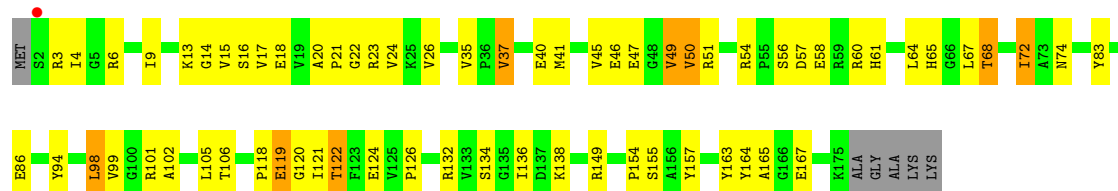
• Molecule 6: 50S ribosomal protein L5

Chain 2G: 

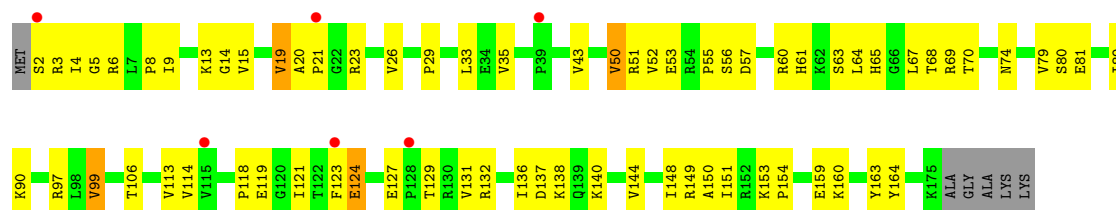


• Molecule 7: 50S ribosomal protein L6

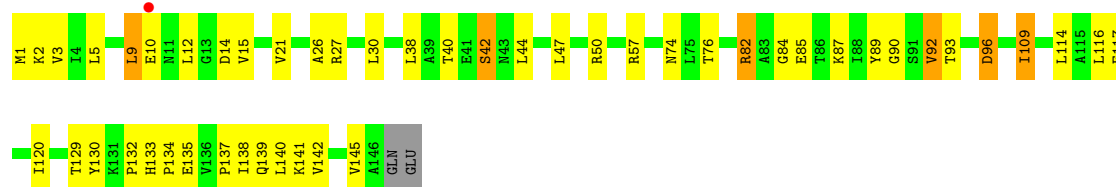
Chain 1H: 



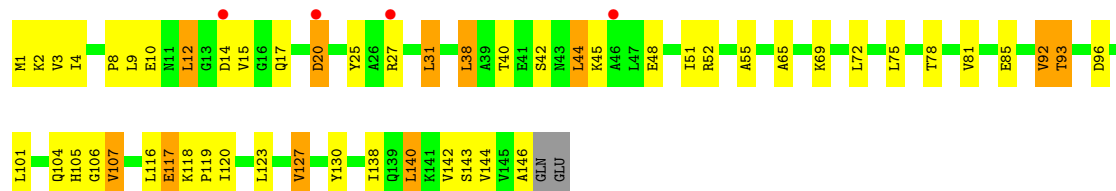
• Molecule 7: 50S ribosomal protein L6



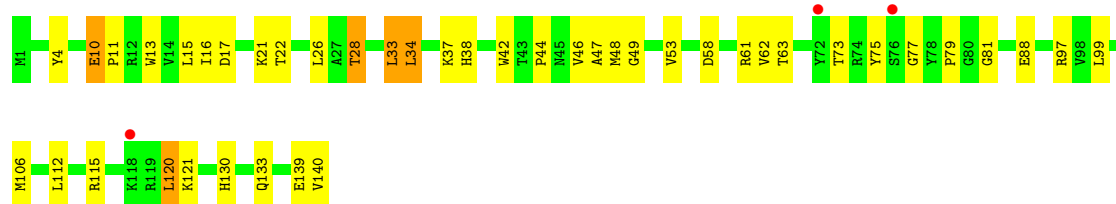
• Molecule 8: 50S ribosomal protein L9



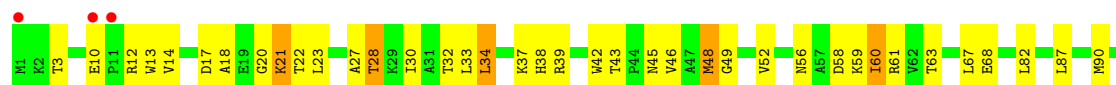
• Molecule 8: 50S ribosomal protein L9

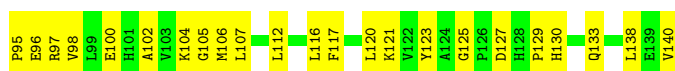


• Molecule 9: 50S ribosomal protein L13

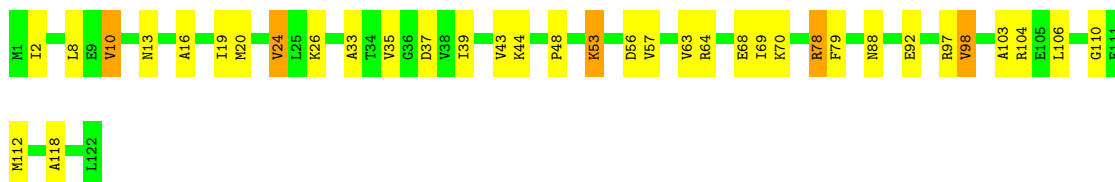


• Molecule 9: 50S ribosomal protein L13





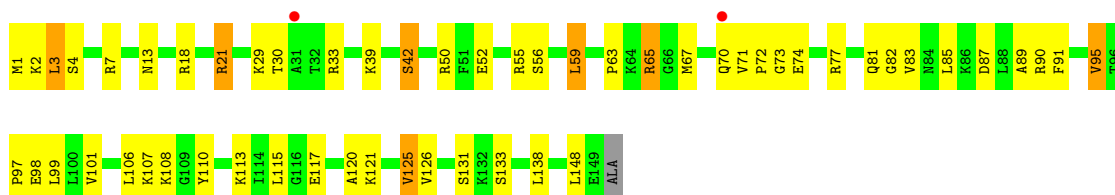
- Molecule 10: 50S ribosomal protein L14



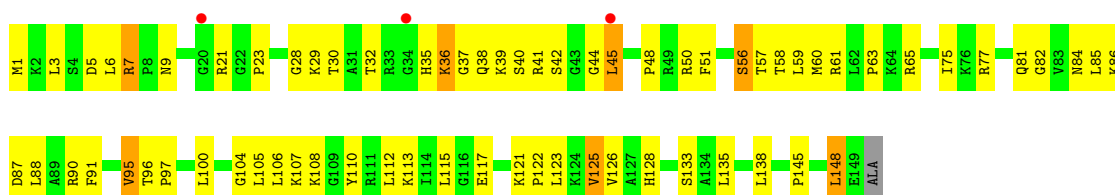
- Molecule 10: 50S ribosomal protein L14



- Molecule 11: 50S ribosomal protein L15

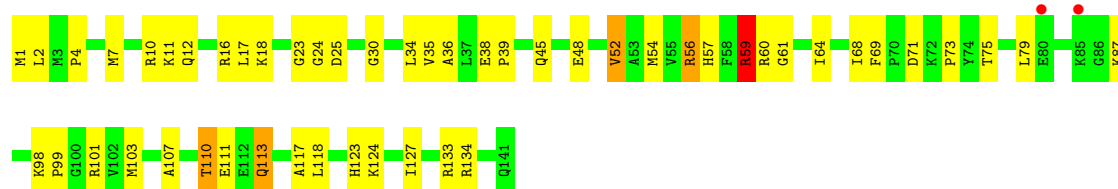


- Molecule 11: 50S ribosomal protein L15

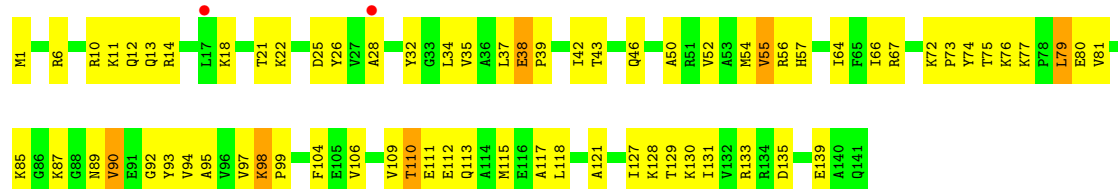


- Molecule 12: 50S ribosomal protein L16

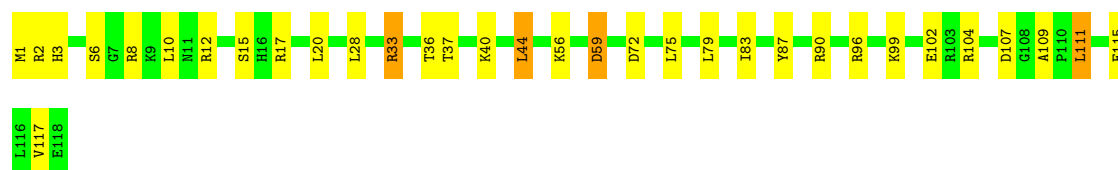




• Molecule 12: 50S ribosomal protein L16



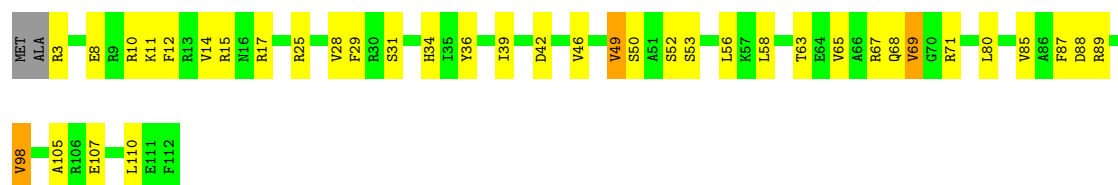
• Molecule 13: 50S ribosomal protein L17



• Molecule 13: 50S ribosomal protein L17

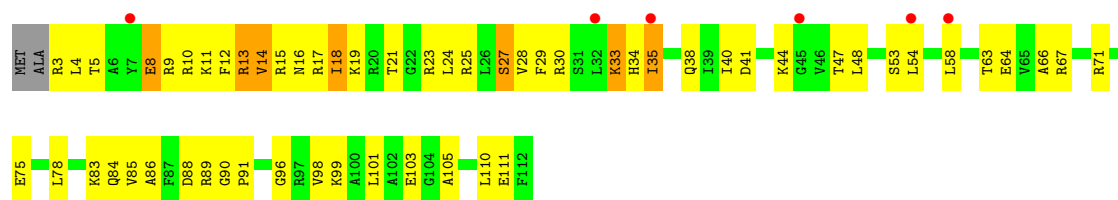


• Molecule 14: 50S ribosomal protein L18

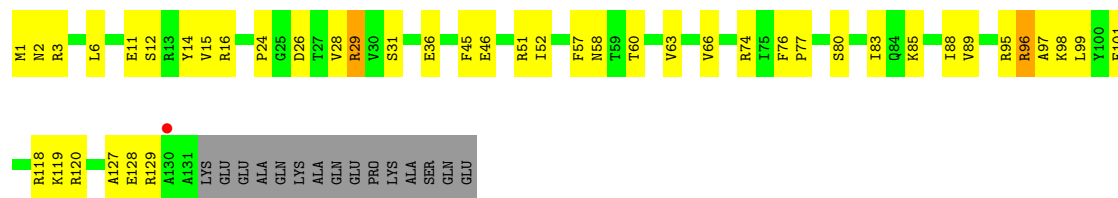


• Molecule 14: 50S ribosomal protein L18

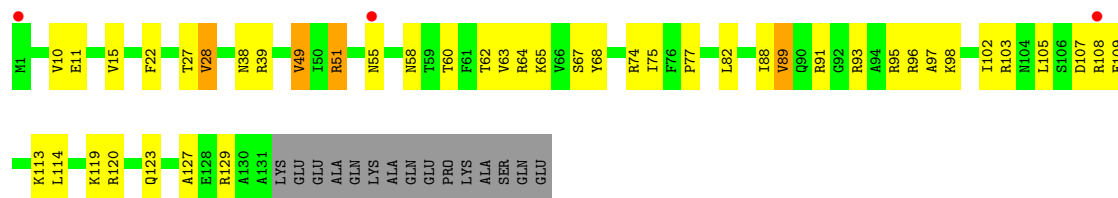




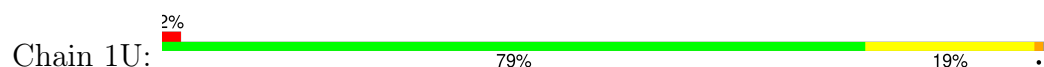
- Molecule 15: 50S ribosomal protein L19



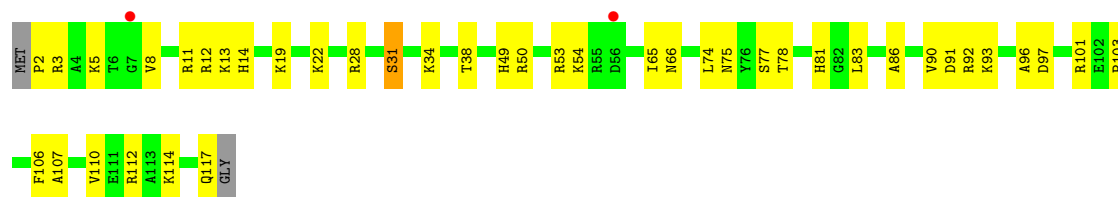
- Molecule 15: 50S ribosomal protein L19



- Molecule 16: 50S ribosomal protein L20



- Molecule 16: 50S ribosomal protein L20



- Molecule 17: 50S ribosomal protein L21





- Molecule 17: 50S ribosomal protein L21



- Molecule 18: 50S ribosomal protein L22



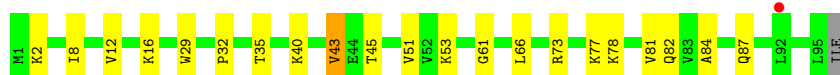
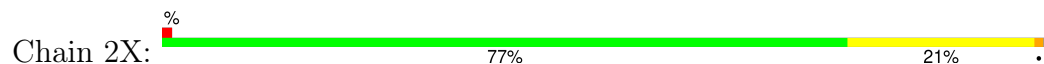
- Molecule 18: 50S ribosomal protein L22



- Molecule 19: 50S ribosomal protein L23



- Molecule 19: 50S ribosomal protein L23

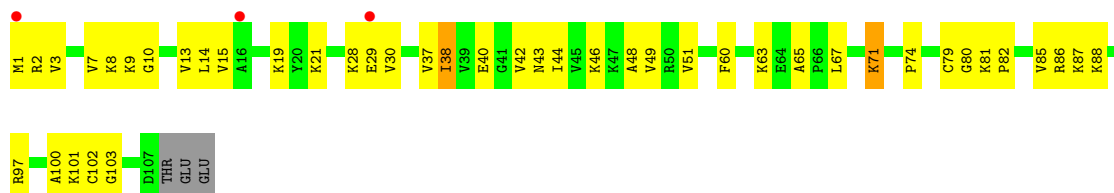


- Molecule 20: 50S ribosomal protein L24

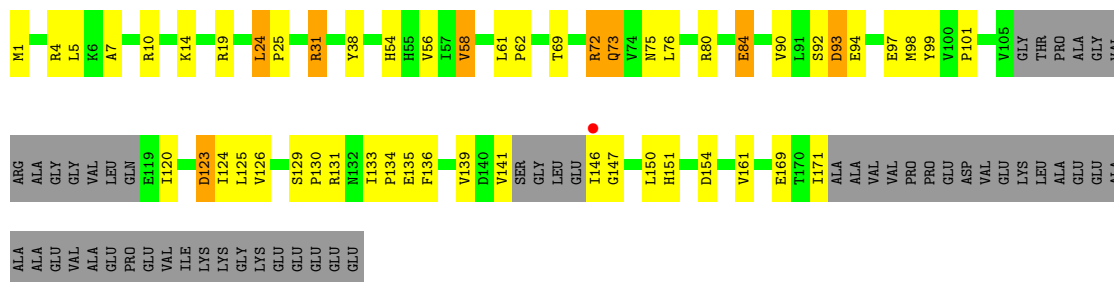




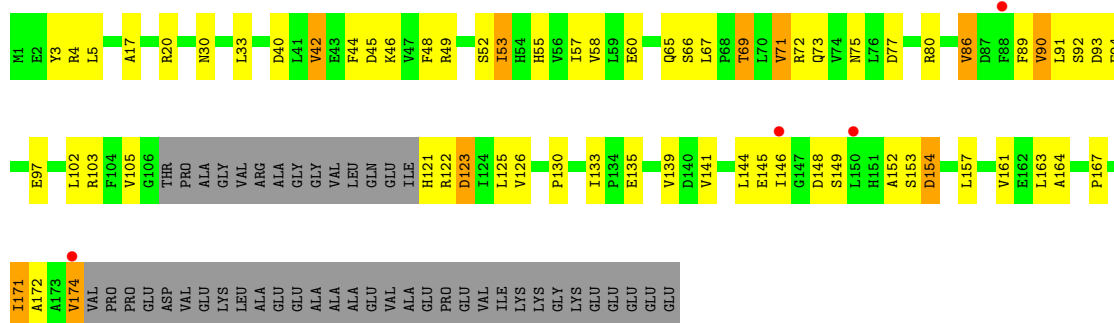
- Molecule 20: 50S ribosomal protein L24



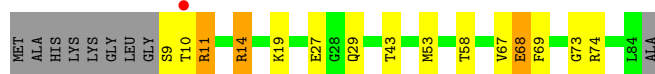
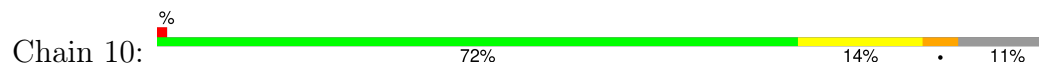
- Molecule 21: 50S ribosomal protein L25



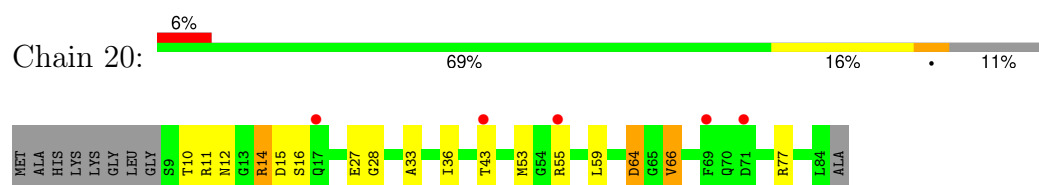
- Molecule 21: 50S ribosomal protein L25



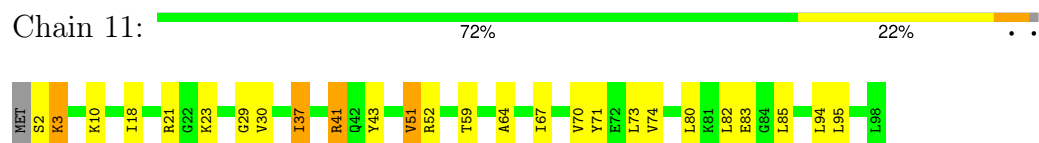
- Molecule 22: 50S ribosomal protein L27



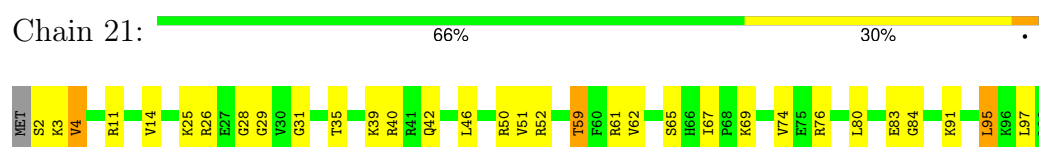
- Molecule 22: 50S ribosomal protein L27



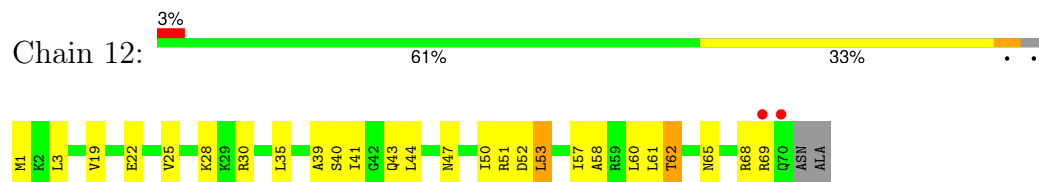
- Molecule 23: 50S ribosomal protein L28



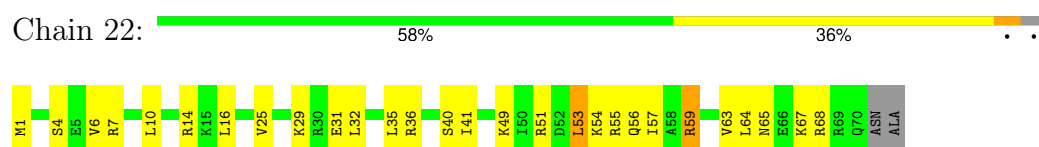
- Molecule 23: 50S ribosomal protein L28



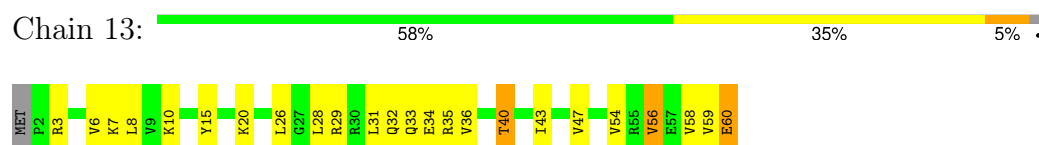
- Molecule 24: 50S ribosomal protein L29



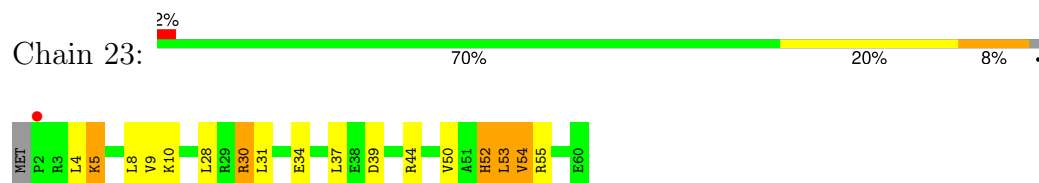
- Molecule 24: 50S ribosomal protein L29



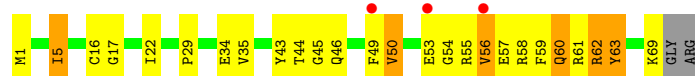
- Molecule 25: 50S ribosomal protein L30



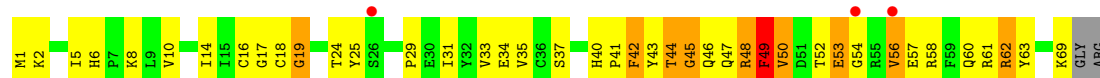
- Molecule 25: 50S ribosomal protein L30



- Molecule 26: 50S ribosomal protein L31



- Molecule 26: 50S ribosomal protein L31



- Molecule 27: 50S ribosomal protein L32



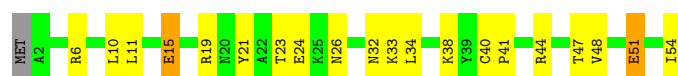
- Molecule 27: 50S ribosomal protein L32



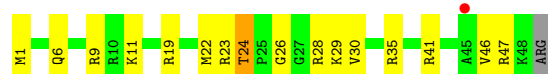
- Molecule 28: 50S ribosomal protein L33



- Molecule 28: 50S ribosomal protein L33



- Molecule 29: 50S ribosomal protein L34



- Molecule 29: 50S ribosomal protein L34



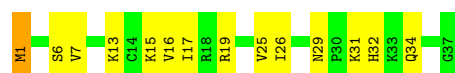
- Molecule 30: 50S ribosomal protein L35



- Molecule 30: 50S ribosomal protein L35



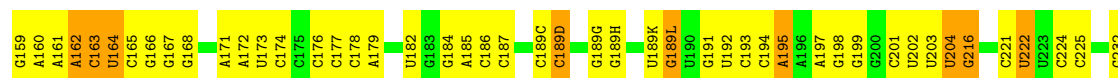
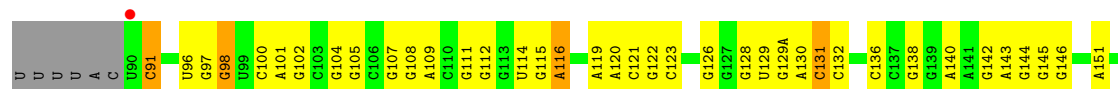
- Molecule 31: 50S ribosomal protein L36



- Molecule 31: 50S ribosomal protein L36



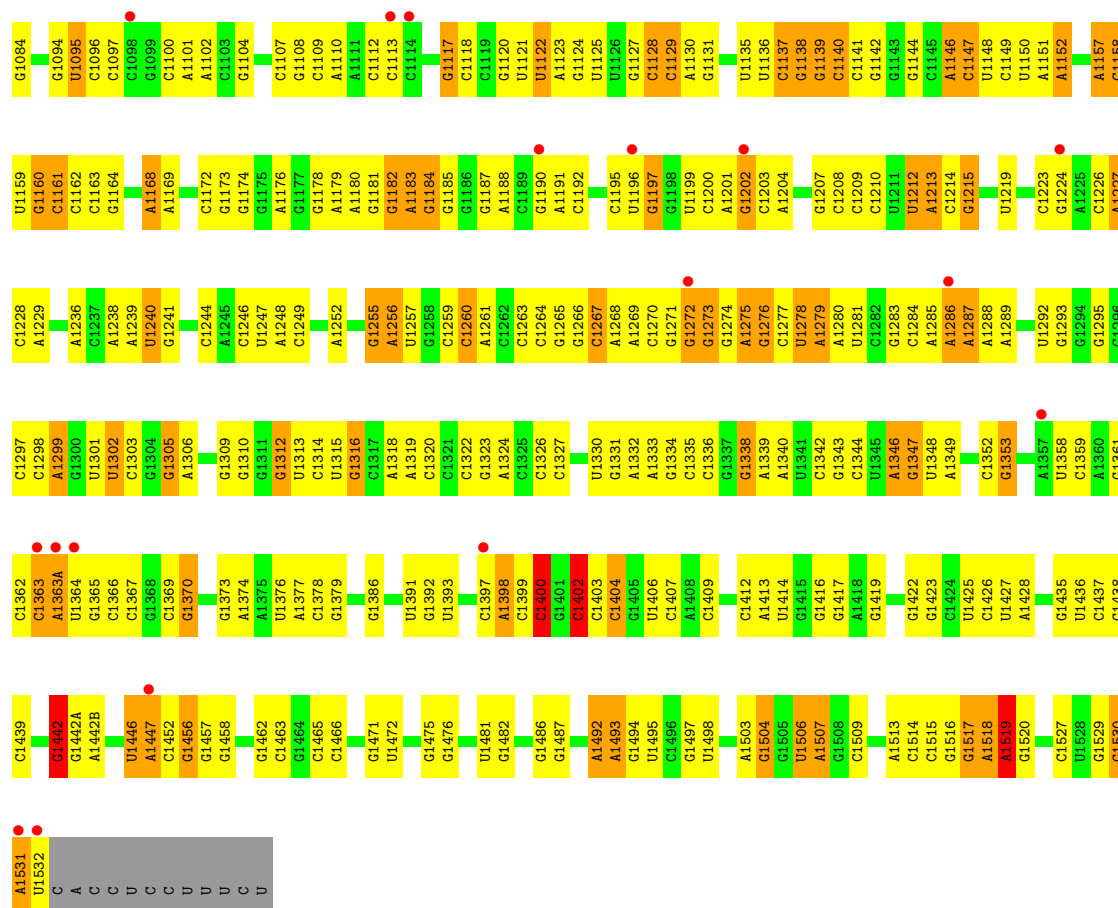
- Molecule 32: 16S Ribosomal RNA



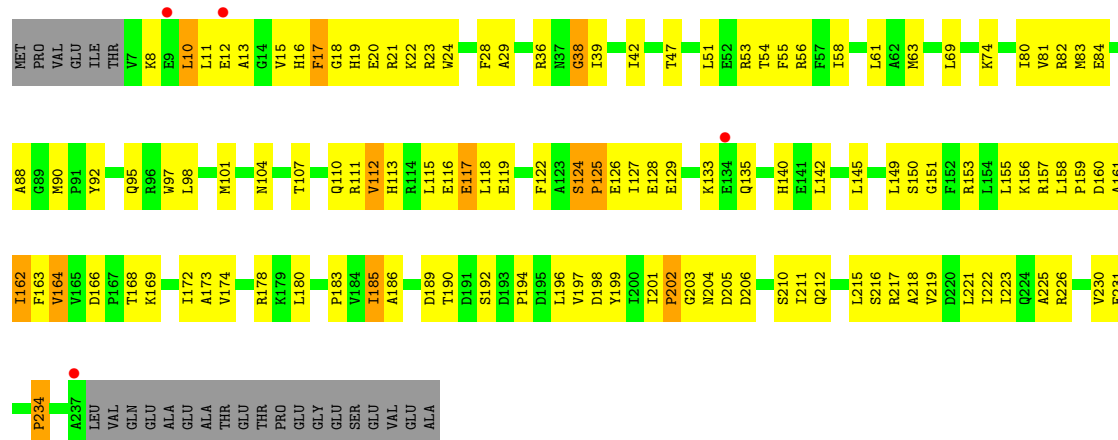
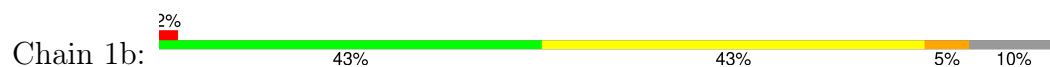


Chain 2a:



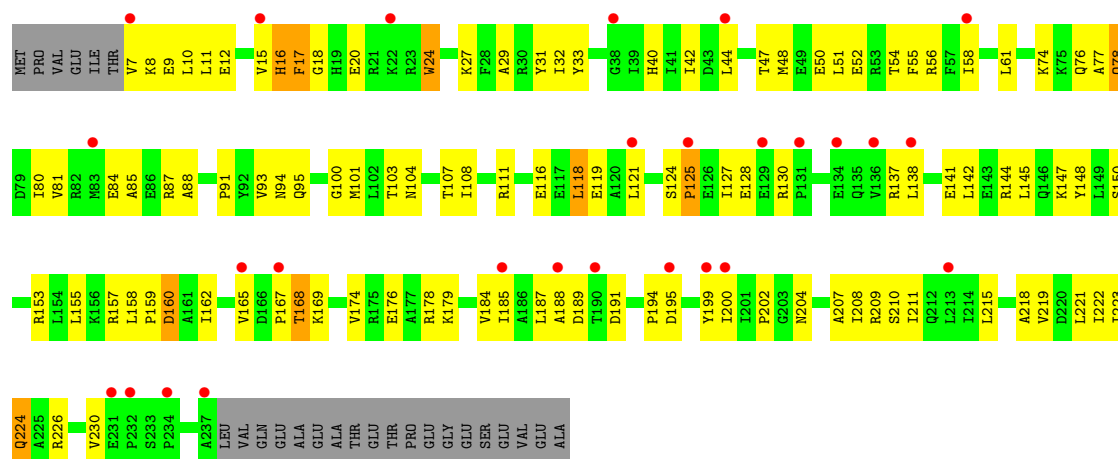


• Molecule 33: 30S ribosomal protein S2



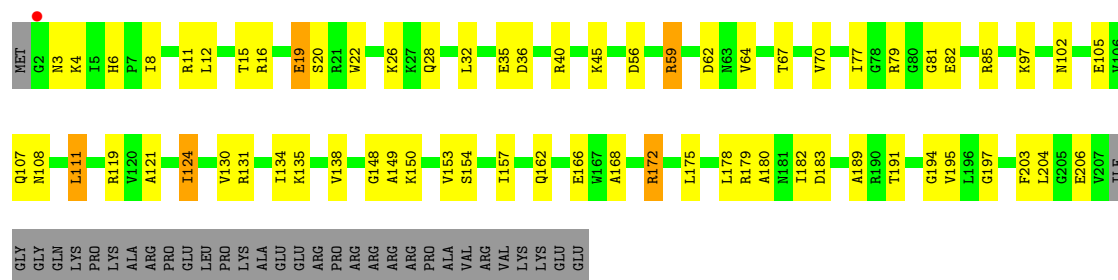
• Molecule 33: 30S ribosomal protein S2





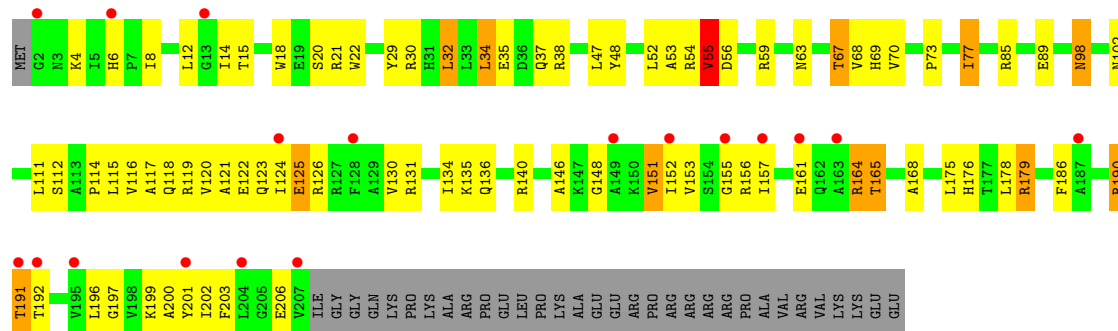
• Molecule 34: 30S ribosomal protein S3

Chain 1c: 58% 26% 14%



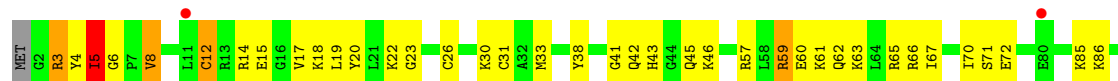
• Molecule 34: 30S ribosomal protein S3

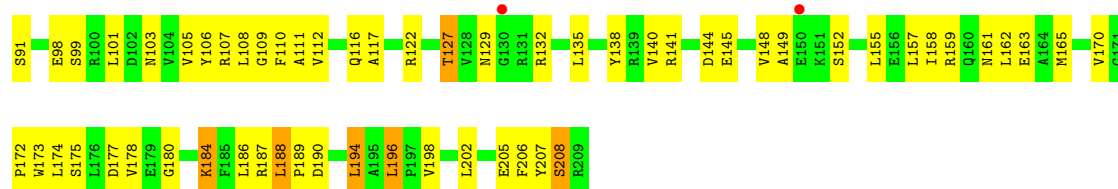
Chain 2c: 8% 51% 30% 5% 14%



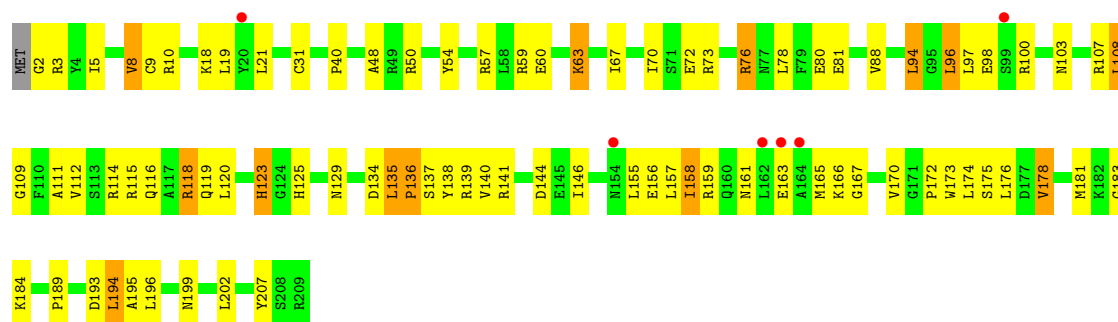
• Molecule 35: 30S ribosomal protein S4

Chain 1d: 2% 54% 41% 5%

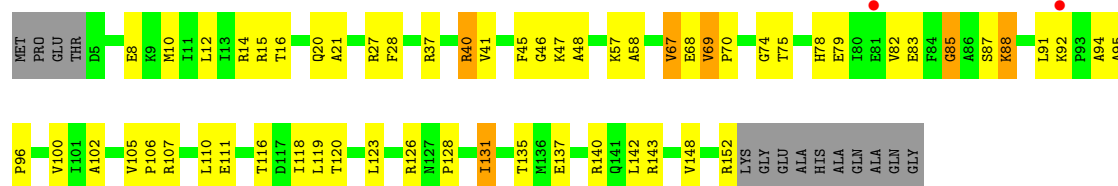




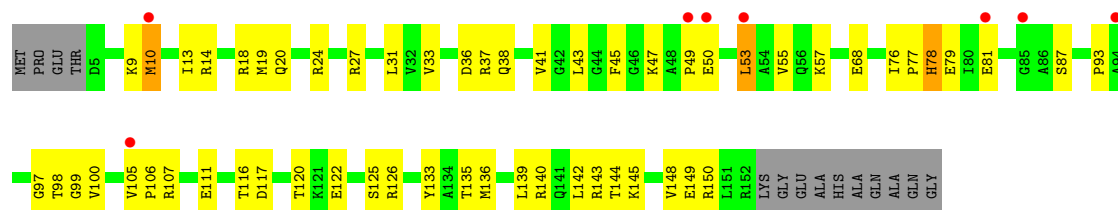
• Molecule 35: 30S ribosomal protein S4



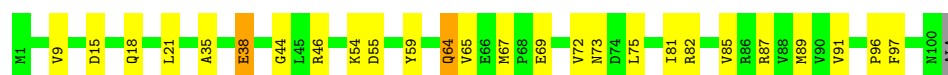
• Molecule 36: 30S ribosomal protein S5



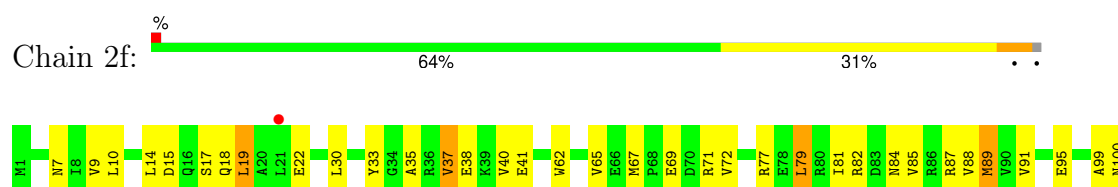
• Molecule 36: 30S ribosomal protein S5



• Molecule 37: 30S ribosomal protein S6

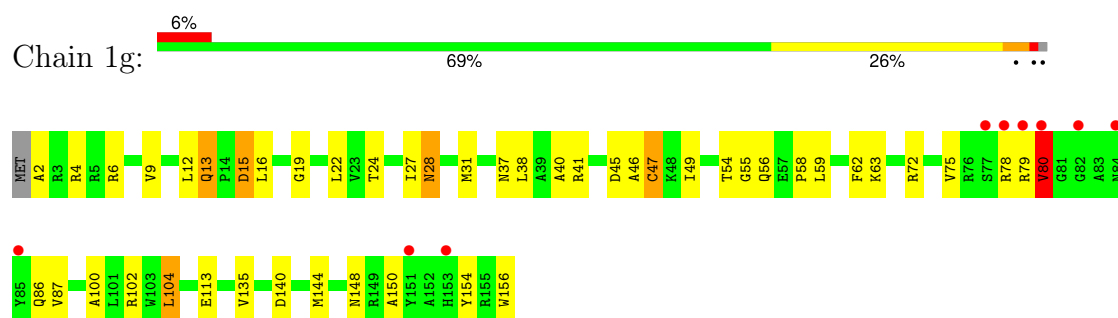


• Molecule 37: 30S ribosomal protein S6

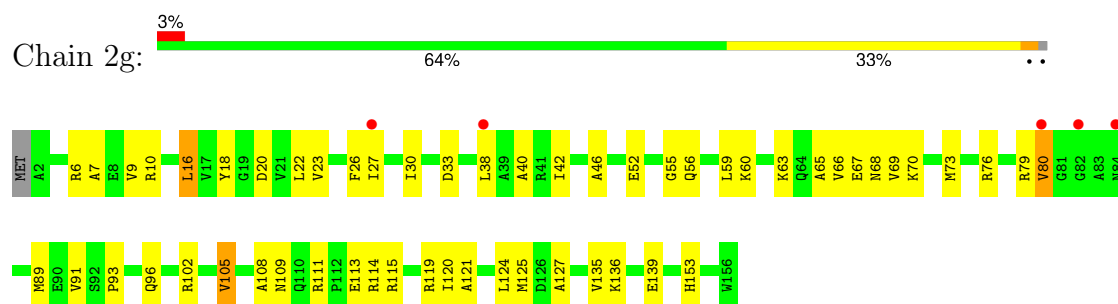


ALA

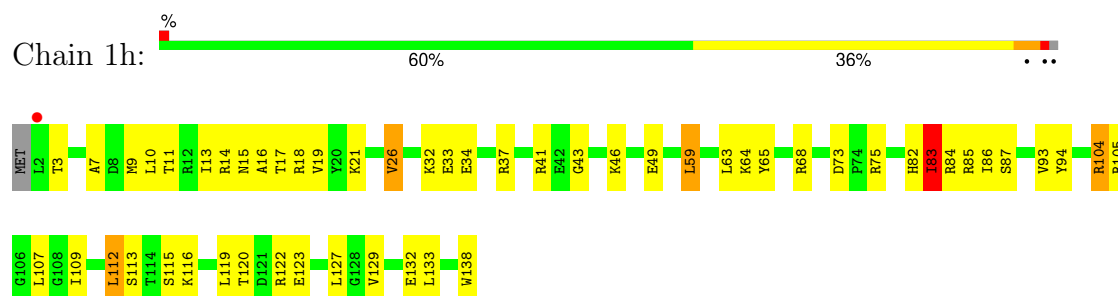
- Molecule 38: 30S ribosomal protein S7



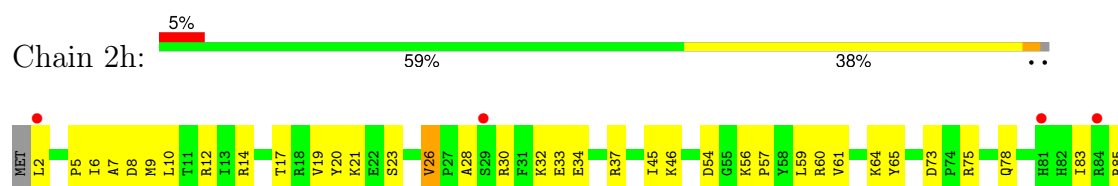
- Molecule 38: 30S ribosomal protein S7



- Molecule 39: 30S ribosomal protein S8

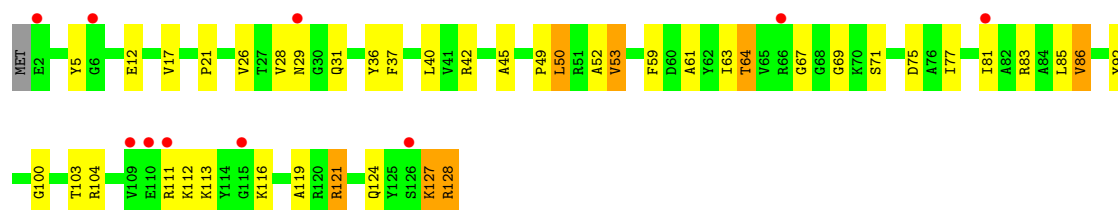


- Molecule 39: 30S ribosomal protein S8

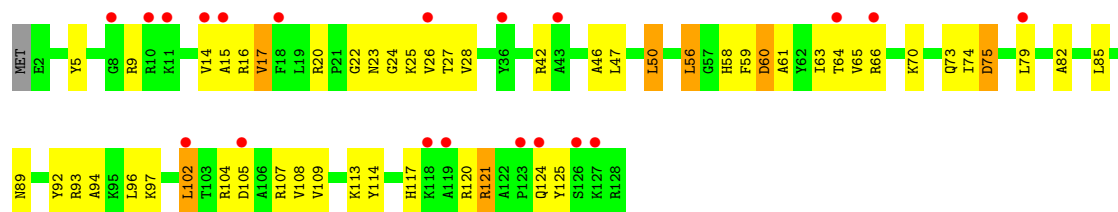




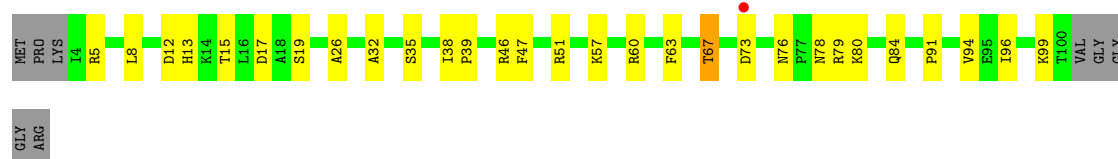
- Molecule 40: 30S ribosomal protein S9



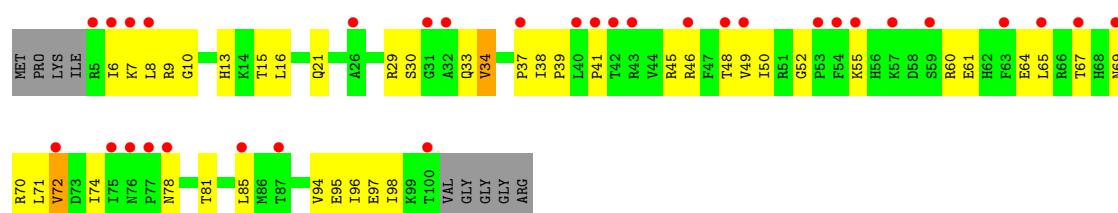
- Molecule 40: 30S ribosomal protein S9



- Molecule 41: 30S ribosomal protein S10

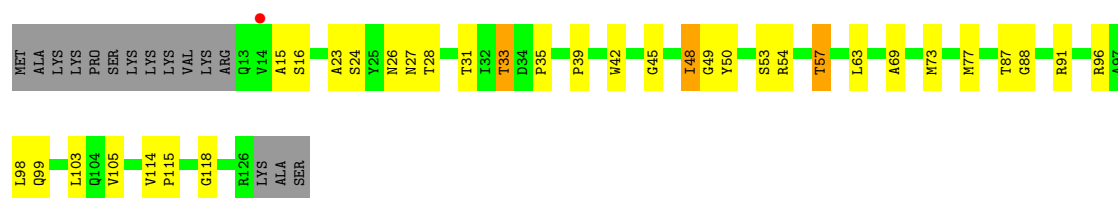


- Molecule 41: 30S ribosomal protein S10

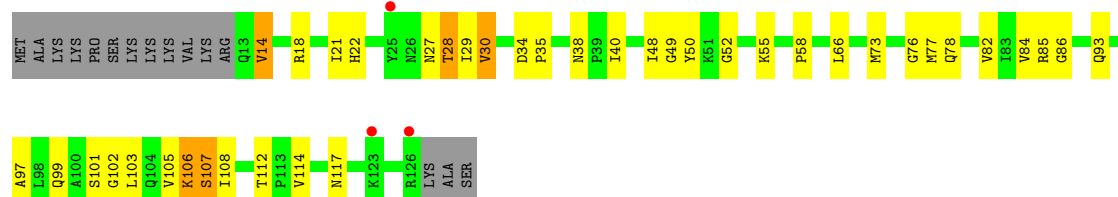


- Molecule 42: 30S ribosomal protein S11

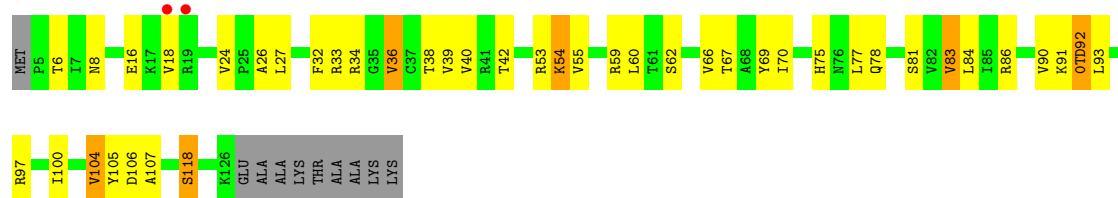




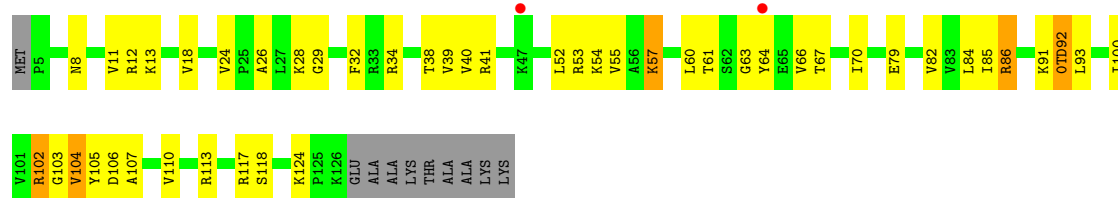
• Molecule 42: 30S ribosomal protein S11



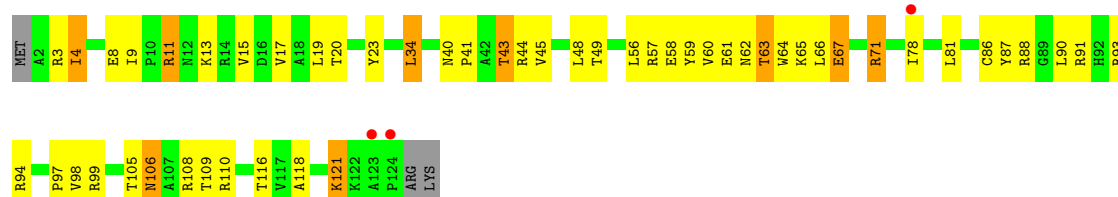
• Molecule 43: 30S ribosomal protein S12



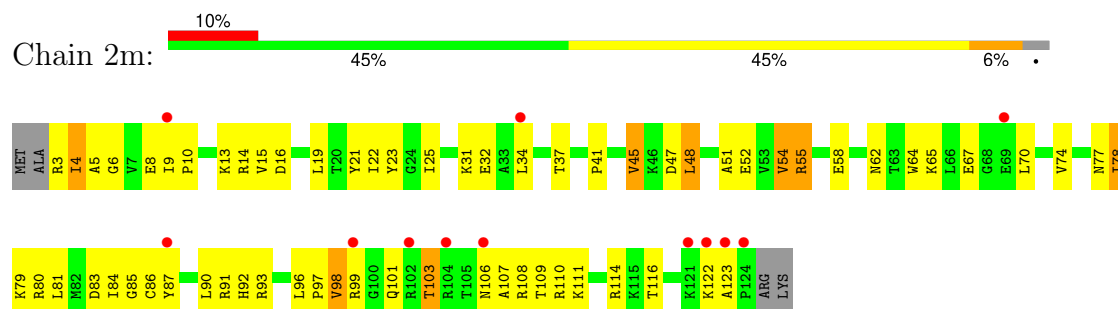
• Molecule 43: 30S ribosomal protein S12



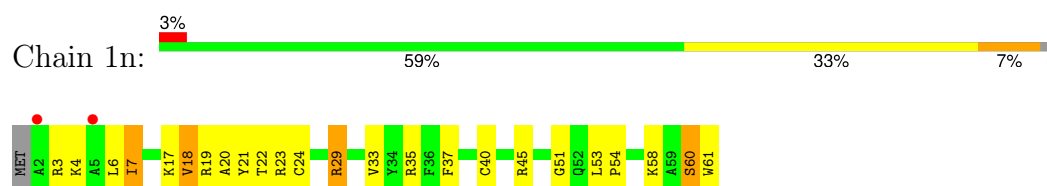
• Molecule 44: 30S ribosomal protein S13



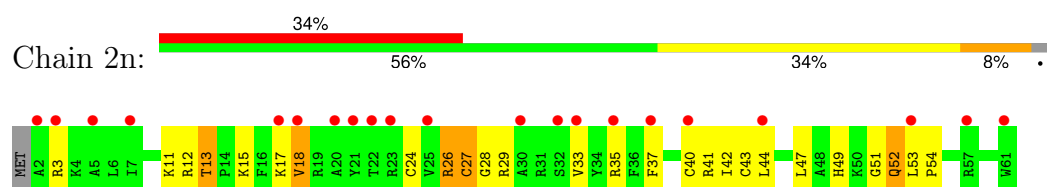
- Molecule 44: 30S ribosomal protein S13



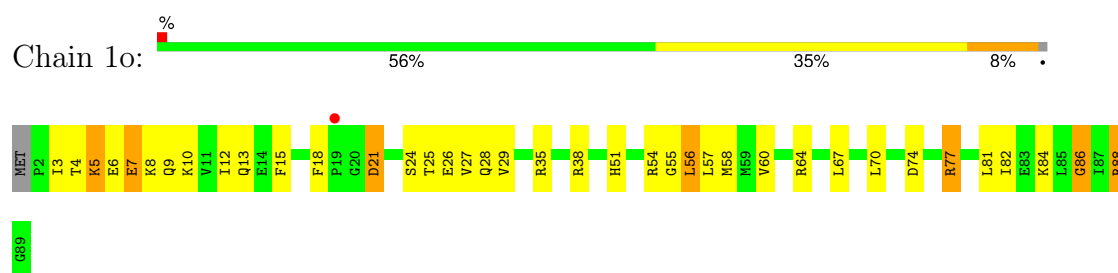
- Molecule 45: 30S ribosomal protein S14 type Z



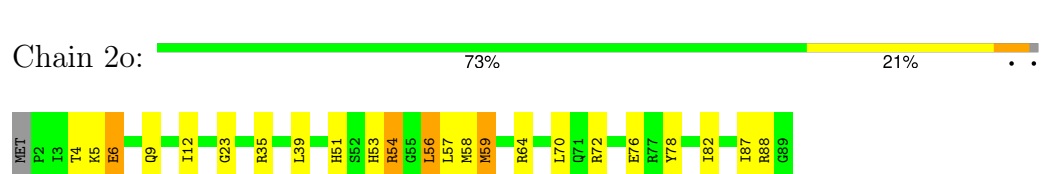
- Molecule 45: 30S ribosomal protein S14 type Z



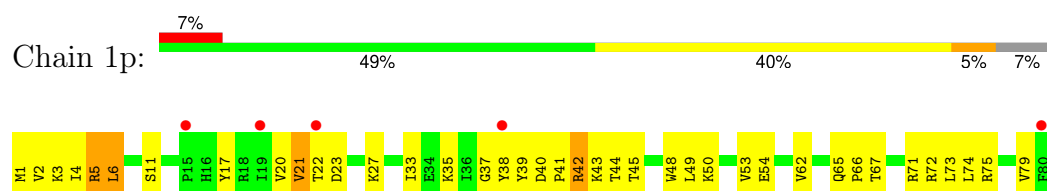
- Molecule 46: 30S ribosomal protein S15



- Molecule 46: 30S ribosomal protein S15



- Molecule 47: 30S ribosomal protein S16



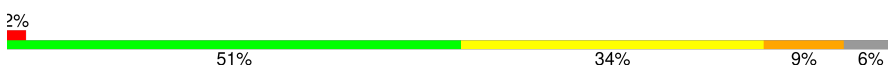
ARG
GLU
GLY
ALA

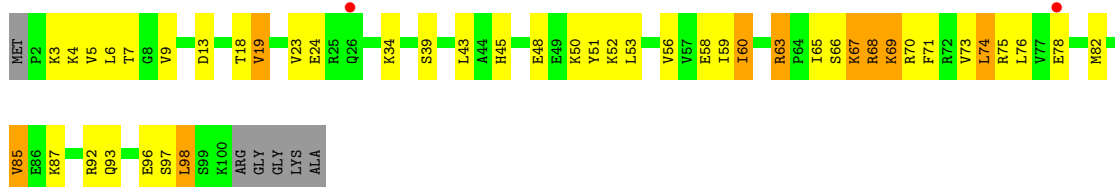
• Molecule 47: 30S ribosomal protein S16

Chain 2p: 



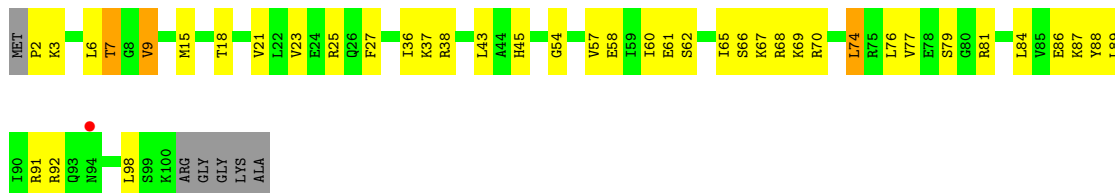
• Molecule 48: 30S ribosomal protein S17

Chain 1q: 



• Molecule 48: 30S ribosomal protein S17

Chain 2q: 



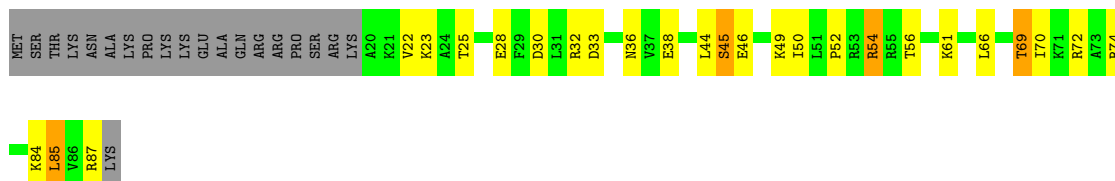
• Molecule 49: 30S ribosomal protein S18

Chain 1r: 

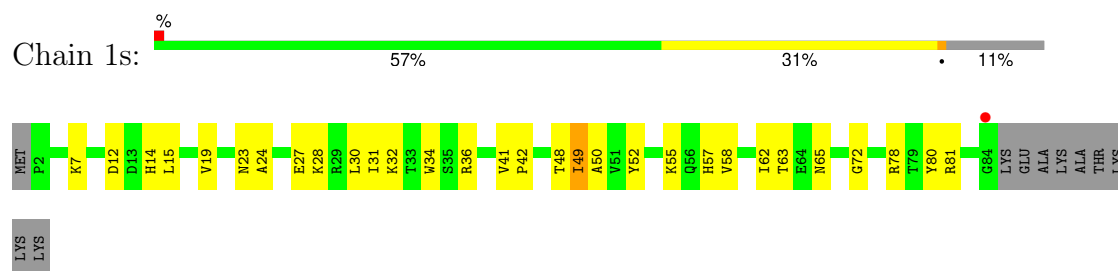


• Molecule 49: 30S ribosomal protein S18

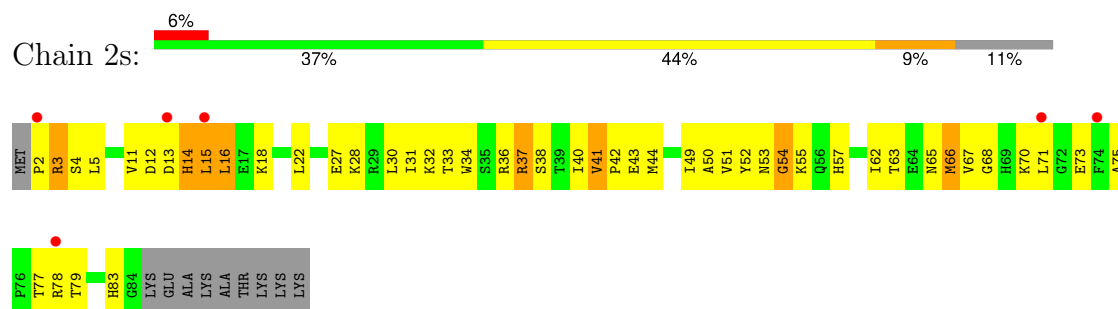
Chain 2r: 



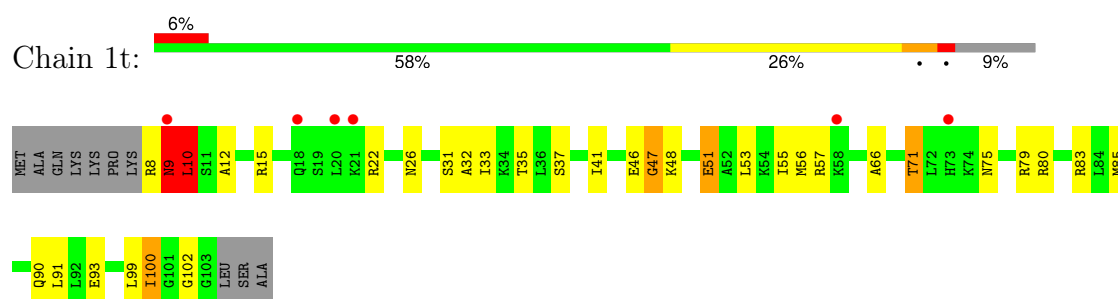
- Molecule 50: 30S ribosomal protein S19



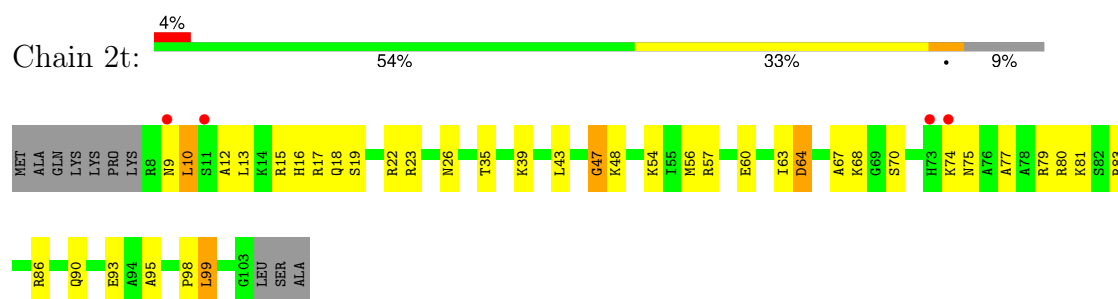
- Molecule 50: 30S ribosomal protein S19



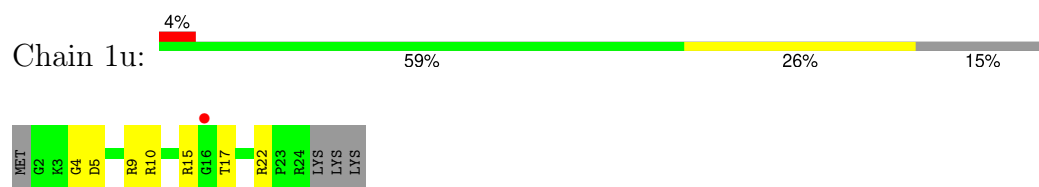
- Molecule 51: 30S ribosomal protein S20



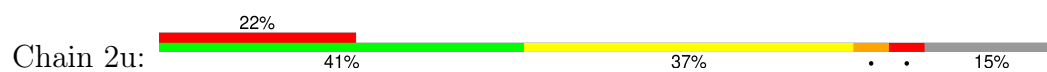
- Molecule 51: 30S ribosomal protein S20



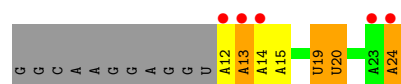
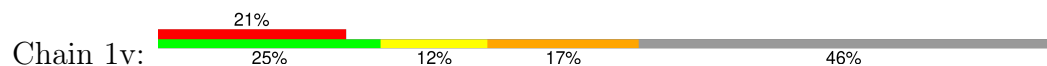
- Molecule 52: 30S ribosomal protein Thx



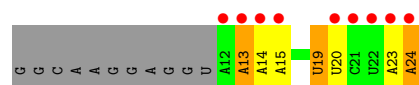
- Molecule 52: 30S ribosomal protein Thx



• Molecule 53: mRNA



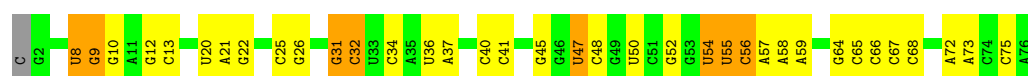
• Molecule 53: mRNA



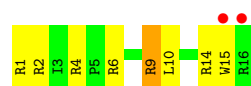
• Molecule 54: P-site tRNA



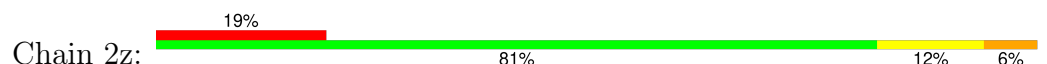
• Molecule 54: P-site tRNA



• Molecule 55: Bac7-002



• Molecule 55: Bac7-002



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	208.64Å 447.57Å 619.73Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	151.79 – 3.05 151.79 – 3.05	Depositor EDS
% Data completeness (in resolution range)	98.7 (151.79-3.05) 98.7 (151.79-3.05)	Depositor EDS
R_{merge}	0.28	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.26 (at 3.07Å)	Xtriage
Refinement program	PHENIX 1.8.2	Depositor
R, R_{free}	0.227 , 0.283 0.226 , 0.283	Depositor DCC
R_{free} test set	53845 reflections (4.94%)	wwPDB-VP
Wilson B-factor (Å ²)	62.7	Xtriage
Anisotropy	0.294	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.27 , 50.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.41$, $\langle L^2 \rangle = 0.23$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	290774	wwPDB-VP
Average B, all atoms (Å ²)	60.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.52% 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: M2G, 2MA, 5MU, ZN, 0TD, K, 4SU, 2MG, UR3, 5MC, MG, SF4, 2MU, PSU, OMG, MA6, 7MG, 4OC

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	0.26	0/69009	0.43	2/107712 (0.0%)
1	2A	0.22	0/67293	0.40	1/105034 (0.0%)
2	1B	0.22	0/2882	0.39	0/4494
2	2B	0.21	0/2879	0.41	0/4487
3	1D	0.26	0/2186	0.50	0/2944
3	2D	0.23	0/2186	0.48	0/2944
4	1E	0.25	0/1592	0.48	0/2149
4	2E	0.22	0/1592	0.44	0/2149
5	1F	0.25	0/1619	0.47	0/2193
5	2F	0.23	0/1615	0.47	0/2188
6	1G	0.22	0/1448	0.49	0/1957
6	2G	0.21	0/1453	0.44	0/1963
7	1H	0.21	0/1356	0.40	0/1834
7	2H	0.20	0/1356	0.39	0/1834
8	1I	0.20	0/1112	0.40	0/1514
8	2I	0.18	0/1079	0.42	0/1475
9	1N	0.24	0/1144	0.45	0/1543
9	2N	0.20	0/1144	0.41	0/1543
10	1O	0.24	0/943	0.47	0/1269
10	2O	0.21	0/943	0.48	0/1269
11	1P	0.25	0/1152	0.48	0/1533
11	2P	0.22	0/1152	0.52	0/1533
12	1Q	0.25	0/1143	0.51	0/1527
12	2Q	0.21	0/1143	0.46	0/1527
13	1R	0.23	0/982	0.46	0/1312
13	2R	0.22	0/982	0.44	0/1312
14	1S	0.21	0/883	0.46	0/1176
14	2S	0.22	0/880	0.46	0/1172
15	1T	0.23	0/1105	0.45	0/1477
15	2T	0.21	0/1097	0.47	0/1468
16	1U	0.26	0/977	0.46	0/1301

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
16	2U	0.20	0/977	0.43	0/1301
17	1V	0.24	0/782	0.45	0/1049
17	2V	0.19	0/782	0.38	0/1049
18	1W	0.25	0/897	0.41	0/1205
18	2W	0.21	0/897	0.46	0/1205
19	1X	0.25	0/764	0.45	0/1025
19	2X	0.19	0/764	0.41	0/1025
20	1Y	0.21	0/819	0.47	0/1095
20	2Y	0.18	0/819	0.44	0/1095
21	1Z	0.22	0/1267	0.47	0/1717
21	2Z	0.22	0/1299	0.45	0/1763
22	10	0.25	0/612	0.51	0/816
22	20	0.22	0/612	0.47	0/816
23	11	0.25	0/762	0.44	0/1014
23	21	0.22	0/762	0.43	0/1014
24	12	0.24	0/590	0.42	0/781
24	22	0.21	0/590	0.43	1/781 (0.1%)
25	13	0.23	0/474	0.46	0/635
25	23	0.20	0/469	0.44	0/630
26	14	0.25	0/565	0.53	0/761
26	24	0.26	0/545	0.62	0/737
27	15	0.26	0/469	0.46	0/635
27	25	0.24	0/469	0.46	0/635
28	16	0.25	0/460	0.52	0/613
28	26	0.21	0/456	0.42	0/608
29	17	0.28	0/426	0.50	0/561
29	27	0.26	0/426	0.47	0/561
30	18	0.26	0/525	0.44	0/691
30	28	0.22	0/525	0.43	0/691
31	19	0.27	0/310	0.44	0/407
31	29	0.21	0/310	0.46	0/407
32	1a	0.20	1/35795 (0.0%)	0.39	0/55864
32	2a	0.20	0/35886	0.39	1/56005 (0.0%)
33	1b	0.26	0/1881	0.53	3/2542 (0.1%)
33	2b	0.25	0/1860	0.50	0/2518
34	1c	0.20	0/1572	0.41	0/2126
34	2c	0.22	0/1566	0.43	0/2119
35	1d	0.21	0/1685	0.46	0/2262
35	2d	0.21	0/1704	0.45	0/2284
36	1e	0.21	0/1145	0.45	0/1543
36	2e	0.23	0/1149	0.47	0/1548
37	1f	0.22	0/823	0.41	0/1115
37	2f	0.21	0/829	0.39	0/1123

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
38	1g	0.19	0/1250	0.40	0/1679
38	2g	0.21	0/1254	0.45	0/1683
39	1h	0.20	0/1108	0.44	0/1494
39	2h	0.21	0/1108	0.45	0/1494
40	1i	0.19	0/1002	0.47	1/1346 (0.1%)
40	2i	0.22	0/997	0.47	0/1343
41	1j	0.20	0/722	0.45	0/982
41	2j	0.25	0/727	0.46	0/988
42	1k	0.19	0/844	0.47	0/1145
42	2k	0.18	0/848	0.34	0/1149
43	1l	0.23	0/937	0.45	0/1260
43	2l	0.21	0/937	0.46	0/1260
44	1m	0.22	0/969	0.46	0/1302
44	2m	0.24	0/961	0.53	0/1291
45	1n	0.22	0/501	0.42	0/664
45	2n	0.23	0/501	0.43	0/664
46	1o	0.20	0/739	0.40	0/985
46	2o	0.19	0/739	0.42	0/985
47	1p	0.21	0/697	0.49	0/939
47	2p	0.20	0/693	0.43	0/935
48	1q	0.21	0/836	0.44	0/1117
48	2q	0.19	0/836	0.42	0/1117
49	1r	0.19	0/560	0.41	0/746
49	2r	0.20	0/560	0.44	0/746
50	1s	0.19	0/667	0.49	0/900
50	2s	0.23	0/661	0.57	0/893
51	1t	0.20	0/730	0.52	0/965
51	2t	0.21	0/729	0.45	0/965
52	1u	0.21	0/203	0.50	0/266
52	2u	0.22	0/203	0.50	0/266
53	1v	0.23	0/310	0.37	0/480
53	2v	0.27	0/310	0.37	0/480
54	1x	0.27	0/1725	0.44	0/2689
54	2x	0.25	1/1725 (0.1%)	0.41	0/2689
55	1z	0.29	0/153	0.66	0/207
55	2z	0.29	0/147	0.49	0/200
All	All	0.23	2/310535 (0.0%)	0.42	9/464519 (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
12	1Q	0	1
51	1t	0	1
All	All	0	2

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
54	2x	8	4SU	O3'-P	5.28	1.61	1.56
32	1a	1498	UR3	O3'-P	5.07	1.61	1.56

The worst 5 of 9 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
33	1b	38	GLY	N-CA-C	-5.57	107.28	115.30
33	1b	128	GLU	CA-C-N	5.50	132.05	121.54
33	1b	128	GLU	C-N-CA	5.50	132.05	121.54
1	1A	1992	G	C2'-C3'-O3'	5.34	117.52	109.50
1	2A	1992	G	C2'-C3'-O3'	5.34	117.50	109.50

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
12	1Q	59	ARG	Peptide
51	1t	9	ASN	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	31189	917	0
1	2A	60322	0	30423	1007	0
2	1B	2577	0	1305	36	0
2	2B	2575	0	1303	54	0
3	1D	2136	0	2217	65	0
3	2D	2136	0	2218	69	0
4	1E	1559	0	1618	45	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	2E	1559	0	1618	45	0
5	1F	1584	0	1625	58	0
5	2F	1580	0	1619	65	0
6	1G	1423	0	1436	38	0
6	2G	1428	0	1438	68	0
7	1H	1330	0	1407	44	0
7	2H	1330	0	1407	44	0
8	1I	1097	0	1140	35	0
8	2I	1064	0	1082	27	0
9	1N	1117	0	1184	30	0
9	2N	1117	0	1184	41	0
10	1O	933	0	996	26	0
10	2O	933	0	996	35	0
11	1P	1135	0	1212	44	0
11	2P	1135	0	1212	51	0
12	1Q	1122	0	1179	32	0
12	2Q	1122	0	1179	46	0
13	1R	968	0	1033	21	0
13	2R	968	0	1033	26	0
14	1S	873	0	927	20	0
14	2S	870	0	923	44	0
15	1T	1091	0	1151	28	0
15	2T	1083	0	1136	30	0
16	1U	959	0	1018	18	0
16	2U	959	0	1019	31	0
17	1V	771	0	829	17	0
17	2V	771	0	829	20	0
18	1W	886	0	940	35	0
18	2W	886	0	940	20	0
19	1X	750	0	814	19	0
19	2X	750	0	814	13	0
20	1Y	806	0	881	18	0
20	2Y	806	0	881	24	0
21	1Z	1240	0	1240	28	0
21	2Z	1271	0	1273	47	0
22	10	604	0	619	13	0
22	20	604	0	619	12	0
23	11	755	0	826	19	0
23	21	755	0	826	24	0
24	12	588	0	643	13	0
24	22	588	0	643	21	0
25	13	469	0	518	13	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
25	23	464	0	514	12	0
26	14	552	0	533	15	0
26	24	532	0	503	35	0
27	15	455	0	465	18	0
27	25	455	0	465	15	0
28	16	453	0	473	9	0
28	26	449	0	469	13	0
29	17	418	0	467	12	0
29	27	418	0	467	13	0
30	18	517	0	582	15	0
30	28	517	0	582	20	0
31	19	307	0	335	12	0
31	29	307	0	335	12	0
32	1a	32246	0	16295	536	0
32	2a	32327	0	16338	639	0
33	1b	1846	0	1867	80	0
33	2b	1825	0	1828	79	0
34	1c	1548	0	1535	44	0
34	2c	1542	0	1517	63	0
35	1d	1655	0	1672	75	0
35	2d	1674	0	1714	72	0
36	1e	1129	0	1185	34	0
36	2e	1133	0	1191	41	0
37	1f	810	0	804	17	0
37	2f	816	0	808	22	0
38	1g	1231	0	1238	31	0
38	2g	1235	0	1249	27	0
39	1h	1088	0	1126	31	0
39	2h	1088	0	1126	38	0
40	1i	983	0	986	32	0
40	2i	978	0	966	36	0
41	1j	709	0	650	23	0
41	2j	714	0	672	32	0
42	1k	829	0	825	24	0
42	2k	833	0	836	23	0
43	1l	932	0	981	22	0
43	2l	932	0	981	30	0
44	1m	958	0	1002	34	0
44	2m	950	0	988	55	0
45	1n	492	0	529	22	0
45	2n	492	0	529	23	0
46	1o	728	0	760	25	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
46	2o	728	0	760	16	0
47	1p	681	0	697	23	0
47	2p	677	0	686	30	0
48	1q	823	0	891	35	0
48	2q	823	0	891	31	0
49	1r	555	0	618	15	0
49	2r	555	0	618	19	0
50	1s	652	0	662	19	0
50	2s	646	0	644	39	0
51	1t	728	0	798	26	0
51	2t	727	0	796	26	0
52	1u	199	0	208	6	0
52	2u	199	0	208	8	0
53	1v	277	0	140	9	0
53	2v	277	0	140	5	0
54	1x	1625	0	829	21	0
54	2x	1625	0	828	23	0
55	1z	147	0	162	8	0
55	2z	141	0	151	2	0
56	10	5	0	0	0	0
56	11	2	0	0	0	0
56	12	2	0	0	0	0
56	13	3	0	0	0	0
56	14	1	0	0	0	0
56	15	5	0	0	0	0
56	17	6	0	0	0	0
56	18	4	0	0	0	0
56	19	1	0	0	0	0
56	1A	848	0	0	0	0
56	1B	25	0	0	0	0
56	1D	8	0	0	0	0
56	1E	8	0	0	0	0
56	1F	12	0	0	0	0
56	1G	4	0	0	0	0
56	1H	1	0	0	0	0
56	1I	1	0	0	0	0
56	1N	3	0	0	0	0
56	1O	1	0	0	0	0
56	1P	5	0	0	0	0
56	1Q	4	0	0	0	0
56	1R	6	0	0	0	0
56	1S	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
56	1T	2	0	0	0	0
56	1U	6	0	0	0	0
56	1V	5	0	0	0	0
56	1W	6	0	0	0	0
56	1X	3	0	0	0	0
56	1Y	1	0	0	0	0
56	1Z	3	0	0	0	0
56	1a	167	0	0	0	0
56	1d	1	0	0	0	0
56	1e	2	0	0	0	0
56	1f	2	0	0	0	0
56	1h	1	0	0	0	0
56	1l	3	0	0	0	0
56	1m	1	0	0	0	0
56	1n	2	0	0	0	0
56	1s	1	0	0	0	0
56	1v	1	0	0	0	0
56	1x	10	0	0	0	0
56	1z	1	0	0	0	0
56	20	1	0	0	0	0
56	21	1	0	0	0	0
56	23	2	0	0	0	0
56	25	2	0	0	0	0
56	26	1	0	0	0	0
56	27	2	0	0	0	0
56	28	3	0	0	0	0
56	2A	625	0	0	0	0
56	2B	12	0	0	0	0
56	2D	2	0	0	0	0
56	2E	5	0	0	0	0
56	2F	4	0	0	0	0
56	2N	1	0	0	0	0
56	2O	1	0	0	0	0
56	2P	3	0	0	0	0
56	2Q	2	0	0	0	0
56	2R	1	0	0	0	0
56	2T	2	0	0	0	0
56	2V	2	0	0	0	0
56	2W	1	0	0	0	0
56	2Y	1	0	0	0	0
56	2Z	1	0	0	0	0
56	2a	145	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
56	2d	1	0	0	0	0
56	2f	1	0	0	0	0
56	2j	1	0	0	0	0
56	2k	1	0	0	0	0
56	2l	2	0	0	0	0
56	2q	2	0	0	0	0
56	2r	1	0	0	0	0
56	2t	1	0	0	0	0
56	2v	2	0	0	0	0
56	2x	3	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	3	0
58	2d	8	0	0	0	0
59	2x	1	0	0	0	0
60	10	2	0	0	1	0
60	11	2	0	0	0	0
60	12	2	0	0	0	0
60	13	2	0	0	0	0
60	18	2	0	0	0	0
60	1A	1222	0	0	109	0
60	1B	27	0	0	3	0
60	1D	21	0	0	1	0
60	1E	11	0	0	1	0
60	1F	9	0	0	1	0
60	1N	1	0	0	0	0
60	1O	1	0	0	0	0
60	1P	14	0	0	1	0
60	1Q	2	0	0	0	0
60	1R	3	0	0	0	0
60	1S	2	0	0	0	0
60	1T	4	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
60	1U	4	0	0	0	0
60	1V	4	0	0	0	0
60	1W	3	0	0	1	0
60	1a	26	0	0	4	0
60	1d	1	0	0	0	0
60	1z	1	0	0	0	0
60	20	1	0	0	0	0
60	21	2	0	0	0	0
60	28	2	0	0	0	0
60	2A	416	0	0	59	0
60	2B	3	0	0	0	0
60	2D	12	0	0	1	0
60	2E	4	0	0	0	0
60	2F	6	0	0	0	0
60	2I	1	0	0	0	0
60	2O	3	0	0	0	0
60	2P	4	0	0	1	0
60	2Q	1	0	0	0	0
60	2R	1	0	0	0	0
60	2T	1	0	0	0	0
60	2V	1	0	0	0	0
60	2W	2	0	0	0	0
60	2a	17	0	0	0	0
60	2l	1	0	0	0	0
60	2n	1	0	0	0	0
60	2t	1	0	0	0	0
60	2x	1	0	0	1	0
All	All	290774	0	193677	5438	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 12.

The worst 5 of 5438 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:1082:U:H3	1:1A:1086:A:N6	1.41	1.19
32:1a:987:G:H1	32:1a:1218:C:N4	1.56	1.02
1:2A:2137:C:N4	1:2A:2154:G:H1	1.54	1.02
1:1A:2124:G:H1	1:1A:2174:C:N4	1.57	1.01
1:2A:2137:C:H42	1:2A:2154:G:H1	1.03	0.99

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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%)	252 (92%)	21 (8%)	0	100	100
3	2D	273/276 (99%)	245 (90%)	28 (10%)	0	100	100
4	1E	202/206 (98%)	188 (93%)	13 (6%)	1 (0%)	24	52
4	2E	202/206 (98%)	187 (93%)	13 (6%)	2 (1%)	12	37
5	1F	201/210 (96%)	190 (94%)	10 (5%)	1 (0%)	24	52
5	2F	201/210 (96%)	181 (90%)	17 (8%)	3 (2%)	8	28
6	1G	179/182 (98%)	161 (90%)	16 (9%)	2 (1%)	11	34
6	2G	179/182 (98%)	153 (86%)	22 (12%)	4 (2%)	5	20
7	1H	172/180 (96%)	154 (90%)	17 (10%)	1 (1%)	21	48
7	2H	172/180 (96%)	145 (84%)	25 (14%)	2 (1%)	10	32
8	1I	144/148 (97%)	123 (85%)	19 (13%)	2 (1%)	9	29
8	2I	144/148 (97%)	131 (91%)	10 (7%)	3 (2%)	5	21
9	1N	138/140 (99%)	130 (94%)	8 (6%)	0	100	100
9	2N	138/140 (99%)	123 (89%)	15 (11%)	0	100	100
10	1O	120/122 (98%)	108 (90%)	12 (10%)	0	100	100
10	2O	120/122 (98%)	103 (86%)	15 (12%)	2 (2%)	7	25
11	1P	147/150 (98%)	132 (90%)	15 (10%)	0	100	100
11	2P	147/150 (98%)	128 (87%)	16 (11%)	3 (2%)	6	21
12	1Q	139/141 (99%)	126 (91%)	10 (7%)	3 (2%)	5	20
12	2Q	139/141 (99%)	125 (90%)	14 (10%)	0	100	100
13	1R	116/118 (98%)	111 (96%)	5 (4%)	0	100	100
13	2R	116/118 (98%)	104 (90%)	12 (10%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
14	1S	108/112 (96%)	102 (94%)	6 (6%)	0	100	100
14	2S	108/112 (96%)	95 (88%)	12 (11%)	1 (1%)	14	39
15	1T	129/146 (88%)	117 (91%)	12 (9%)	0	100	100
15	2T	129/146 (88%)	119 (92%)	10 (8%)	0	100	100
16	1U	114/118 (97%)	112 (98%)	2 (2%)	0	100	100
16	2U	114/118 (97%)	110 (96%)	4 (4%)	0	100	100
17	1V	99/101 (98%)	93 (94%)	5 (5%)	1 (1%)	12	37
17	2V	99/101 (98%)	87 (88%)	10 (10%)	2 (2%)	6	21
18	1W	110/113 (97%)	108 (98%)	2 (2%)	0	100	100
18	2W	110/113 (97%)	105 (96%)	5 (4%)	0	100	100
19	1X	93/96 (97%)	86 (92%)	5 (5%)	2 (2%)	5	20
19	2X	93/96 (97%)	78 (84%)	15 (16%)	0	100	100
20	1Y	105/110 (96%)	92 (88%)	11 (10%)	2 (2%)	6	23
20	2Y	105/110 (96%)	90 (86%)	13 (12%)	2 (2%)	6	23
21	1Z	148/206 (72%)	128 (86%)	17 (12%)	3 (2%)	6	21
21	2Z	156/206 (76%)	130 (83%)	25 (16%)	1 (1%)	21	48
22	10	74/85 (87%)	72 (97%)	2 (3%)	0	100	100
22	20	74/85 (87%)	67 (90%)	6 (8%)	1 (1%)	9	29
23	11	95/98 (97%)	88 (93%)	6 (6%)	1 (1%)	11	34
23	21	95/98 (97%)	87 (92%)	8 (8%)	0	100	100
24	12	68/72 (94%)	63 (93%)	5 (7%)	0	100	100
24	22	68/72 (94%)	63 (93%)	5 (7%)	0	100	100
25	13	57/60 (95%)	55 (96%)	2 (4%)	0	100	100
25	23	57/60 (95%)	50 (88%)	7 (12%)	0	100	100
26	14	67/71 (94%)	52 (78%)	10 (15%)	5 (8%)	1	3
26	24	67/71 (94%)	48 (72%)	14 (21%)	5 (8%)	1	3
27	15	57/60 (95%)	56 (98%)	1 (2%)	0	100	100
27	25	57/60 (95%)	53 (93%)	3 (5%)	1 (2%)	6	24
28	16	51/54 (94%)	47 (92%)	4 (8%)	0	100	100
28	26	51/54 (94%)	47 (92%)	4 (8%)	0	100	100
29	17	46/49 (94%)	44 (96%)	2 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
29	27	46/49 (94%)	43 (94%)	2 (4%)	1 (2%)	5	20
30	18	62/65 (95%)	62 (100%)	0	0	100	100
30	28	62/65 (95%)	59 (95%)	3 (5%)	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%)	193 (84%)	25 (11%)	11 (5%)	2	9
33	2b	229/256 (90%)	185 (81%)	38 (17%)	6 (3%)	4	17
34	1c	204/239 (85%)	187 (92%)	16 (8%)	1 (0%)	24	52
34	2c	204/239 (85%)	166 (81%)	37 (18%)	1 (0%)	24	52
35	1d	206/209 (99%)	194 (94%)	11 (5%)	1 (0%)	24	52
35	2d	206/209 (99%)	178 (86%)	24 (12%)	4 (2%)	6	23
36	1e	146/162 (90%)	129 (88%)	15 (10%)	2 (1%)	9	29
36	2e	146/162 (90%)	127 (87%)	17 (12%)	2 (1%)	9	29
37	1f	98/101 (97%)	90 (92%)	7 (7%)	1 (1%)	12	37
37	2f	98/101 (97%)	88 (90%)	9 (9%)	1 (1%)	12	37
38	1g	153/156 (98%)	138 (90%)	10 (6%)	5 (3%)	3	13
38	2g	153/156 (98%)	131 (86%)	18 (12%)	4 (3%)	4	17
39	1h	135/138 (98%)	126 (93%)	8 (6%)	1 (1%)	18	45
39	2h	135/138 (98%)	120 (89%)	15 (11%)	0	100	100
40	1i	125/128 (98%)	110 (88%)	15 (12%)	0	100	100
40	2i	125/128 (98%)	109 (87%)	16 (13%)	0	100	100
41	1j	95/105 (90%)	81 (85%)	11 (12%)	3 (3%)	3	14
41	2j	94/105 (90%)	88 (94%)	5 (5%)	1 (1%)	11	34
42	1k	112/129 (87%)	99 (88%)	12 (11%)	1 (1%)	14	39
42	2k	112/129 (87%)	102 (91%)	7 (6%)	3 (3%)	4	16
43	1l	119/132 (90%)	111 (93%)	6 (5%)	2 (2%)	7	25
43	2l	119/132 (90%)	101 (85%)	16 (13%)	2 (2%)	7	25
44	1m	121/126 (96%)	105 (87%)	14 (12%)	2 (2%)	7	25
44	2m	120/126 (95%)	99 (82%)	18 (15%)	3 (2%)	4	17
45	1n	58/61 (95%)	55 (95%)	2 (3%)	1 (2%)	7	25
45	2n	58/61 (95%)	51 (88%)	5 (9%)	2 (3%)	3	13

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
46	1o	86/89 (97%)	76 (88%)	8 (9%)	2 (2%)	5	19
46	2o	86/89 (97%)	80 (93%)	6 (7%)	0	100	100
47	1p	80/88 (91%)	67 (84%)	13 (16%)	0	100	100
47	2p	80/88 (91%)	71 (89%)	8 (10%)	1 (1%)	9	31
48	1q	97/105 (92%)	84 (87%)	11 (11%)	2 (2%)	5	21
48	2q	97/105 (92%)	90 (93%)	7 (7%)	0	100	100
49	1r	66/88 (75%)	59 (89%)	7 (11%)	0	100	100
49	2r	66/88 (75%)	62 (94%)	4 (6%)	0	100	100
50	1s	81/93 (87%)	69 (85%)	10 (12%)	2 (2%)	4	17
50	2s	81/93 (87%)	68 (84%)	12 (15%)	1 (1%)	10	32
51	1t	94/106 (89%)	84 (89%)	8 (8%)	2 (2%)	5	21
51	2t	94/106 (89%)	83 (88%)	8 (8%)	3 (3%)	3	14
52	1u	21/27 (78%)	18 (86%)	3 (14%)	0	100	100
52	2u	21/27 (78%)	15 (71%)	4 (19%)	2 (10%)	0	2
55	1z	14/16 (88%)	12 (86%)	1 (7%)	1 (7%)	1	4
55	2z	14/16 (88%)	13 (93%)	1 (7%)	0	100	100
All	All	11384/12160 (94%)	10190 (90%)	1061 (9%)	133 (1%)	10	32

5 of 133 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
5	1F	130	ALA
6	1G	43	LEU
7	1H	126	PRO
12	1Q	24	GLY
12	1Q	60	ARG

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%)	191 (89%)	24 (11%)	6	20
3	2D	215/218 (99%)	185 (86%)	30 (14%)	3	13
4	1E	164/166 (99%)	142 (87%)	22 (13%)	4	14
4	2E	164/166 (99%)	143 (87%)	21 (13%)	4	15
5	1F	160/166 (96%)	141 (88%)	19 (12%)	5	18
5	2F	159/166 (96%)	141 (89%)	18 (11%)	5	20
6	1G	143/156 (92%)	129 (90%)	14 (10%)	7	26
6	2G	143/156 (92%)	120 (84%)	23 (16%)	2	9
7	1H	144/148 (97%)	125 (87%)	19 (13%)	4	14
7	2H	144/148 (97%)	134 (93%)	10 (7%)	14	38
8	1I	113/124 (91%)	100 (88%)	13 (12%)	5	19
8	2I	105/124 (85%)	87 (83%)	18 (17%)	2	8
9	1N	118/119 (99%)	104 (88%)	14 (12%)	5	18
9	2N	118/119 (99%)	101 (86%)	17 (14%)	3	12
10	1O	100/100 (100%)	93 (93%)	7 (7%)	14	38
10	2O	100/100 (100%)	96 (96%)	4 (4%)	28	56
11	1P	115/116 (99%)	99 (86%)	16 (14%)	3	13
11	2P	115/116 (99%)	99 (86%)	16 (14%)	3	13
12	1Q	111/111 (100%)	101 (91%)	10 (9%)	9	29
12	2Q	111/111 (100%)	96 (86%)	15 (14%)	4	14
13	1R	101/101 (100%)	92 (91%)	9 (9%)	9	29
13	2R	101/101 (100%)	98 (97%)	3 (3%)	36	62
14	1S	86/88 (98%)	72 (84%)	14 (16%)	2	9
14	2S	85/88 (97%)	70 (82%)	15 (18%)	2	7
15	1T	115/127 (91%)	107 (93%)	8 (7%)	14	38
15	2T	113/127 (89%)	102 (90%)	11 (10%)	8	26
16	1U	93/94 (99%)	88 (95%)	5 (5%)	20	46
16	2U	93/94 (99%)	90 (97%)	3 (3%)	34	60
17	1V	80/82 (98%)	71 (89%)	9 (11%)	5	20
17	2V	80/82 (98%)	69 (86%)	11 (14%)	3	13
18	1W	90/92 (98%)	85 (94%)	5 (6%)	19	45
18	2W	90/92 (98%)	82 (91%)	8 (9%)	9	29

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
19	1X	77/78 (99%)	74 (96%)	3 (4%)	28	56
19	2X	77/78 (99%)	74 (96%)	3 (4%)	28	56
20	1Y	85/91 (93%)	75 (88%)	10 (12%)	5	18
20	2Y	85/91 (93%)	77 (91%)	8 (9%)	8	27
21	1Z	135/179 (75%)	118 (87%)	17 (13%)	4	16
21	2Z	137/179 (76%)	120 (88%)	17 (12%)	4	16
22	10	61/67 (91%)	55 (90%)	6 (10%)	7	26
22	20	61/67 (91%)	56 (92%)	5 (8%)	10	32
23	11	80/83 (96%)	72 (90%)	8 (10%)	7	25
23	21	80/83 (96%)	73 (91%)	7 (9%)	9	30
24	12	65/67 (97%)	57 (88%)	8 (12%)	4	16
24	22	65/67 (97%)	61 (94%)	4 (6%)	16	42
25	13	51/52 (98%)	43 (84%)	8 (16%)	2	10
25	23	50/52 (96%)	45 (90%)	5 (10%)	7	25
26	14	59/63 (94%)	51 (86%)	8 (14%)	3	13
26	24	53/63 (84%)	42 (79%)	11 (21%)	1	4
27	15	50/52 (96%)	44 (88%)	6 (12%)	5	17
27	25	50/52 (96%)	46 (92%)	4 (8%)	11	33
28	16	51/52 (98%)	45 (88%)	6 (12%)	5	18
28	26	50/52 (96%)	44 (88%)	6 (12%)	5	17
29	17	41/42 (98%)	36 (88%)	5 (12%)	5	17
29	27	41/42 (98%)	38 (93%)	3 (7%)	13	36
30	18	54/55 (98%)	52 (96%)	2 (4%)	30	57
30	28	54/55 (98%)	51 (94%)	3 (6%)	19	45
31	19	34/34 (100%)	33 (97%)	1 (3%)	37	62
31	29	34/34 (100%)	31 (91%)	3 (9%)	9	30
33	1b	192/220 (87%)	172 (90%)	20 (10%)	7	23
33	2b	187/220 (85%)	169 (90%)	18 (10%)	8	26
34	1c	142/188 (76%)	124 (87%)	18 (13%)	4	16
34	2c	140/188 (74%)	120 (86%)	20 (14%)	3	12
35	1d	169/181 (93%)	148 (88%)	21 (12%)	4	16

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
35	2d	173/181 (96%)	157 (91%)	16 (9%)	8	28
36	1e	113/123 (92%)	100 (88%)	13 (12%)	5	19
36	2e	114/123 (93%)	99 (87%)	15 (13%)	4	14
37	1f	84/90 (93%)	77 (92%)	7 (8%)	10	32
37	2f	85/90 (94%)	78 (92%)	7 (8%)	10	32
38	1g	119/127 (94%)	105 (88%)	14 (12%)	5	18
38	2g	120/127 (94%)	107 (89%)	13 (11%)	6	22
39	1h	114/119 (96%)	100 (88%)	14 (12%)	4	16
39	2h	114/119 (96%)	104 (91%)	10 (9%)	9	30
40	1i	90/99 (91%)	80 (89%)	10 (11%)	6	21
40	2i	89/99 (90%)	76 (85%)	13 (15%)	3	12
41	1j	66/92 (72%)	61 (92%)	5 (8%)	12	35
41	2j	69/92 (75%)	59 (86%)	10 (14%)	3	12
42	1k	82/99 (83%)	77 (94%)	5 (6%)	17	42
42	2k	83/99 (84%)	76 (92%)	7 (8%)	10	31
43	1l	96/108 (89%)	83 (86%)	13 (14%)	4	14
43	2l	96/108 (89%)	85 (88%)	11 (12%)	5	19
44	1m	93/101 (92%)	78 (84%)	15 (16%)	2	9
44	2m	92/101 (91%)	79 (86%)	13 (14%)	3	12
45	1n	49/50 (98%)	42 (86%)	7 (14%)	3	12
45	2n	49/50 (98%)	43 (88%)	6 (12%)	5	17
46	1o	78/80 (98%)	71 (91%)	7 (9%)	9	29
46	2o	78/80 (98%)	71 (91%)	7 (9%)	9	29
47	1p	69/74 (93%)	55 (80%)	14 (20%)	1	4
47	2p	68/74 (92%)	57 (84%)	11 (16%)	2	9
48	1q	94/97 (97%)	80 (85%)	14 (15%)	3	11
48	2q	94/97 (97%)	87 (93%)	7 (7%)	13	36
49	1r	59/77 (77%)	54 (92%)	5 (8%)	10	31
49	2r	59/77 (77%)	52 (88%)	7 (12%)	5	18
50	1s	69/80 (86%)	65 (94%)	4 (6%)	18	44
50	2s	67/80 (84%)	54 (81%)	13 (19%)	1	5

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
51	1t	70/82 (85%)	60 (86%)	10 (14%)	3	12
51	2t	70/82 (85%)	66 (94%)	4 (6%)	18	45
52	1u	18/22 (82%)	17 (94%)	1 (6%)	19	45
52	2u	18/22 (82%)	15 (83%)	3 (17%)	2	8
55	1z	15/16 (94%)	14 (93%)	1 (7%)	15	39
55	2z	14/16 (88%)	13 (93%)	1 (7%)	13	37
All	All	9324/10096 (92%)	8296 (89%)	1028 (11%)	6	21

5 of 1028 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
40	2i	121	ARG
43	2l	105	TYR
40	2i	117	HIS
38	1g	140	ASP
38	1g	28	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 135 such sidechains are listed below:

Mol	Chain	Res	Type
34	2c	118	GLN
35	2d	123	HIS
50	2s	14	HIS
35	1d	160	GLN
35	1d	123	HIS

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	1A	2863/2915 (98%)	473 (16%)	26 (0%)
1	2A	2791/2915 (95%)	507 (18%)	22 (0%)
2	1B	119/121 (98%)	11 (9%)	0
2	2B	118/121 (97%)	32 (27%)	0
32	1a	1497/1521 (98%)	262 (17%)	0
32	2a	1501/1521 (98%)	307 (20%)	0
53	1v	12/24 (50%)	5 (41%)	0
53	2v	12/24 (50%)	5 (41%)	0
54	1x	75/77 (97%)	9 (12%)	0

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Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
54	2x	75/77 (97%)	11 (14%)	0
All	All	9063/9316 (97%)	1622 (17%)	48 (0%)

5 of 1622 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	50	U

5 of 48 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	2A	266	G
1	2A	856	C
1	2A	271(K)	U
1	2A	479	A
1	2A	900	A

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

56 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
32	MA6	1a	1518	32	23,26,27	1.56	4 (17%)	33,38,41	2.34	14 (42%)
1	PSU	2A	2605	1	18,21,22	1.39	3 (16%)	21,30,33	2.10	5 (23%)
32	MA6	2a	1518	32	23,26,27	1.53	5 (21%)	33,38,41	2.30	14 (42%)
54	5MU	2x	54	54	19,22,23	1.33	5 (26%)	27,32,35	2.20	7 (25%)
54	PSU	2x	55	54	18,21,22	1.37	2 (11%)	21,30,33	1.84	4 (19%)
1	5MC	1A	1942	1	19,22,23	1.61	3 (15%)	26,32,35	1.18	2 (7%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
32	5MC	2a	1404	32	19,22,23	1.68	3 (15%)	26,32,35	1.21	3 (11%)
54	5MC	2x	32	54	19,22,23	1.53	2 (10%)	26,32,35	1.15	3 (11%)
1	5MU	1A	1915	1	19,22,23	1.39	5 (26%)	27,32,35	2.16	7 (25%)
1	PSU	1A	2605	56,1	18,21,22	1.36	3 (16%)	21,30,33	2.00	5 (23%)
32	5MC	1a	1407	32	19,22,23	1.59	3 (15%)	26,32,35	1.18	3 (11%)
1	2MA	1A	2503	56,1	22,25,26	1.43	5 (22%)	32,37,40	2.35	9 (28%)
43	0TD	1l	92	43	8,9,10	4.61	1 (12%)	6,11,13	2.22	3 (50%)
54	5MC	1x	32	54	19,22,23	1.76	3 (15%)	26,32,35	1.19	3 (11%)
32	5MC	2a	1407	32	19,22,23	1.59	3 (15%)	26,32,35	1.16	3 (11%)
32	MA6	1a	1519	32	23,26,27	1.55	4 (17%)	33,38,41	2.36	12 (36%)
1	4OC	2A	1920	1	19,22,24	0.79	0	25,31,35	0.92	1 (4%)
32	M2G	1a	966	32	24,27,28	1.29	4 (16%)	33,40,43	1.85	6 (18%)
32	5MC	2a	1400	32	19,22,23	1.84	3 (15%)	26,32,35	1.32	3 (11%)
32	M2G	2a	966	32	24,27,28	1.35	4 (16%)	33,40,43	1.93	6 (18%)
1	5MU	2A	1915	56,1	19,22,23	1.50	6 (31%)	27,32,35	2.06	6 (22%)
32	7MG	2a	527	32	23,26,27	1.38	4 (17%)	27,39,42	2.50	6 (22%)
54	4SU	1x	8	54	18,21,22	2.05	4 (22%)	25,30,33	1.35	5 (20%)
1	PSU	2A	1917	1	18,21,22	1.41	2 (11%)	21,30,33	2.08	4 (19%)
32	4OC	1a	1402	32	20,23,24	0.75	0	25,32,35	1.12	3 (12%)
32	PSU	1a	516	56,32	18,21,22	1.36	2 (11%)	21,30,33	2.01	3 (14%)
1	5MC	2A	1962	56,1	19,22,23	1.63	3 (15%)	26,32,35	1.19	3 (11%)
1	PSU	1A	1911	1	18,21,22	1.36	2 (11%)	21,30,33	1.89	3 (14%)
1	5MU	2A	1939	1	19,22,23	1.38	6 (31%)	27,32,35	2.30	6 (22%)
1	5MU	1A	1939	56,1	19,22,23	1.48	5 (26%)	27,32,35	2.02	7 (25%)
54	PSU	1x	55	54,56	18,21,22	1.36	2 (11%)	21,30,33	2.12	5 (23%)
32	MA6	2a	1519	32	23,26,27	1.58	4 (17%)	33,38,41	2.27	11 (33%)
32	5MC	1a	967	32	19,22,23	1.54	3 (15%)	26,32,35	1.03	2 (7%)
1	PSU	1A	1917	1	18,21,22	1.37	2 (11%)	21,30,33	2.10	3 (14%)
1	5MC	2A	1942	1	19,22,23	1.71	3 (15%)	26,32,35	1.15	2 (7%)
1	5MC	1A	1962	56,1	19,22,23	1.67	3 (15%)	26,32,35	1.14	3 (11%)
32	UR3	1a	1498	32	19,22,23	1.08	1 (5%)	26,32,35	1.81	4 (15%)
1	2MU	1A	2552	56,1	19,22,24	1.21	2 (10%)	25,31,36	2.04	5 (20%)
32	2MG	2a	1207	32	23,26,27	1.22	3 (13%)	33,38,41	2.16	8 (24%)
32	5MC	1a	1400	32	19,22,23	1.72	3 (15%)	26,32,35	1.15	3 (11%)
54	5MU	1x	54	54	19,22,23	1.42	5 (26%)	27,32,35	1.96	6 (22%)

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	1.57	2 (10%)	26,32,35	1.07	2 (7%)
1	2MA	2A	2503	56,1	22,25,26	1.52	4 (18%)	32,37,40	2.41	7 (21%)
32	UR3	2a	1498	56,32	19,22,23	1.09	2 (10%)	26,32,35	1.68	4 (15%)
43	0TD	2l	92	43	8,9,10	4.65	1 (12%)	6,11,13	1.95	2 (33%)
32	2MG	1a	1207	32	23,26,27	1.23	3 (13%)	33,38,41	2.09	6 (18%)
1	PSU	2A	1911	1	18,21,22	1.37	2 (11%)	21,30,33	1.97	3 (14%)
32	4OC	2a	1402	32	20,23,24	0.81	0	25,32,35	1.06	2 (8%)
1	OMG	1A	2251	54,56,1	23,26,27	1.24	3 (13%)	32,38,41	2.08	6 (18%)
1	2MU	2A	2552	56,1	19,22,24	1.17	1 (5%)	25,31,36	1.99	6 (24%)
32	PSU	2a	516	56,32	18,21,22	1.35	3 (16%)	21,30,33	1.99	5 (23%)
32	7MG	1a	527	56,32	23,26,27	1.41	4 (17%)	27,39,42	2.59	7 (25%)
54	4SU	2x	8	54	18,21,22	1.94	5 (27%)	25,30,33	1.66	7 (28%)
1	4OC	1A	1920	1	19,22,24	0.83	1 (5%)	25,31,35	1.07	2 (8%)
32	5MC	2a	967	32	19,22,23	1.75	3 (15%)	26,32,35	1.12	3 (11%)
1	OMG	2A	2251	54,56,1	23,26,27	1.23	3 (13%)	32,38,41	1.93	5 (15%)

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
32	MA6	1a	1518	32	-	2/11/29/30	0/3/3/3
1	PSU	2A	2605	1	-	0/7/25/26	0/2/2/2
32	MA6	2a	1518	32	-	1/11/29/30	0/3/3/3
54	5MU	2x	54	54	-	0/7/25/26	0/2/2/2
54	PSU	2x	55	54	-	0/7/25/26	0/2/2/2
1	5MC	1A	1942	1	-	0/7/25/26	0/2/2/2
32	5MC	2a	1404	32	-	0/7/25/26	0/2/2/2
54	5MC	2x	32	54	-	0/7/25/26	0/2/2/2
1	5MU	1A	1915	1	-	0/7/25/26	0/2/2/2
1	PSU	1A	2605	56,1	-	0/7/25/26	0/2/2/2
32	5MC	1a	1407	32	-	0/7/25/26	0/2/2/2
1	2MA	1A	2503	56,1	-	2/7/25/26	0/3/3/3
43	0TD	1l	92	43	-	1/7/12/14	-
54	5MC	1x	32	54	-	0/7/25/26	0/2/2/2
32	5MC	2a	1407	32	-	0/7/25/26	0/2/2/2
32	MA6	1a	1519	32	-	3/11/29/30	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	4OC	2A	1920	1	-	1/9/27/30	0/2/2/2
32	M2G	1a	966	32	-	0/11/29/30	0/3/3/3
32	5MC	2a	1400	32	-	2/7/25/26	0/2/2/2
32	M2G	2a	966	32	-	0/11/29/30	0/3/3/3
1	5MU	2A	1915	56,1	-	0/7/25/26	0/2/2/2
32	7MG	2a	527	32	-	2/7/37/38	0/3/3/3
54	4SU	1x	8	54	-	0/7/25/26	0/2/2/2
1	PSU	2A	1917	1	-	1/7/25/26	0/2/2/2
32	4OC	1a	1402	32	-	1/9/29/30	0/2/2/2
32	PSU	1a	516	56,32	-	2/7/25/26	0/2/2/2
1	5MC	2A	1962	56,1	-	1/7/25/26	0/2/2/2
1	PSU	1A	1911	1	-	0/7/25/26	0/2/2/2
1	5MU	2A	1939	1	-	0/7/25/26	0/2/2/2
1	5MU	1A	1939	56,1	-	0/7/25/26	0/2/2/2
54	PSU	1x	55	54,56	-	0/7/25/26	0/2/2/2
32	MA6	2a	1519	32	-	4/11/29/30	0/3/3/3
32	5MC	1a	967	32	-	1/7/25/26	0/2/2/2
1	PSU	1A	1917	1	-	0/7/25/26	0/2/2/2
1	5MC	2A	1942	1	-	0/7/25/26	0/2/2/2
1	5MC	1A	1962	56,1	-	4/7/25/26	0/2/2/2
32	UR3	1a	1498	32	-	0/7/25/26	0/2/2/2
1	2MU	1A	2552	56,1	-	0/9/27/28	0/2/2/2
32	2MG	2a	1207	32	-	0/9/27/28	0/3/3/3
32	5MC	1a	1400	32	-	2/7/25/26	0/2/2/2
54	5MU	1x	54	54	-	0/7/25/26	0/2/2/2
32	5MC	1a	1404	32	-	0/7/25/26	0/2/2/2
1	2MA	2A	2503	56,1	-	0/7/25/26	0/3/3/3
32	UR3	2a	1498	56,32	-	0/7/25/26	0/2/2/2
43	0TD	2l	92	43	-	1/7/12/14	-
32	2MG	1a	1207	32	-	2/9/27/28	0/3/3/3
1	PSU	2A	1911	1	-	0/7/25/26	0/2/2/2
32	4OC	2a	1402	32	-	3/9/29/30	0/2/2/2
1	OMG	1A	2251	54,56,1	-	0/9/27/28	0/3/3/3
1	2MU	2A	2552	56,1	-	1/9/27/28	0/2/2/2
32	PSU	2a	516	56,32	-	0/7/25/26	0/2/2/2
32	7MG	1a	527	56,32	-	2/7/37/38	0/3/3/3
54	4SU	2x	8	54	-	1/7/25/26	0/2/2/2
1	4OC	1A	1920	1	-	1/9/27/30	0/2/2/2
32	5MC	2a	967	32	-	1/7/25/26	0/2/2/2
1	OMG	2A	2251	54,56,1	-	0/9/27/28	0/3/3/3

The worst 5 of 167 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
43	1l	92	0TD	CB-SB	-12.67	1.69	1.82
43	2l	92	0TD	CB-SB	-12.66	1.69	1.82
32	2a	1400	5MC	C5-C4	6.75	1.49	1.44
54	1x	32	5MC	C5-C4	6.39	1.49	1.44
32	2a	967	5MC	C5-C4	6.37	1.48	1.44

The worst 5 of 278 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	2A	2503	2MA	C5-C4-N3	-9.08	117.62	127.18
32	1a	527	7MG	N9-C4-N3	8.95	138.57	125.46
32	2a	527	7MG	N9-C4-N3	8.40	137.77	125.46
1	1A	2503	2MA	C5-C4-N3	-8.13	118.62	127.18
32	1a	1498	UR3	C4-N3-C2	-7.03	118.92	124.58

There are no chirality outliers.

5 of 42 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
32	1a	1207	2MG	N1-C2-N2-CM2
32	1a	1207	2MG	N3-C2-N2-CM2
32	1a	1400	5MC	O4'-C4'-C5'-O5'
32	1a	1519	MA6	O4'-C4'-C5'-O5'
32	2a	1402	4OC	O4'-C4'-C5'-O5'

There are no ring outliers.

34 monomers are involved in 47 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
32	1a	1518	MA6	1	0
32	2a	1518	MA6	5	0
54	2x	54	5MU	1	0
54	2x	55	PSU	1	0
32	2a	1404	5MC	1	0
54	2x	32	5MC	1	0
1	1A	2605	PSU	1	0
43	1l	92	0TD	1	0
32	1a	1519	MA6	1	0
1	2A	1920	4OC	1	0
32	1a	966	M2G	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
32	2a	1400	5MC	1	0
32	2a	966	M2G	1	0
1	2A	1915	5MU	1	0
54	1x	8	4SU	3	0
32	1a	1402	4OC	4	0
1	2A	1939	5MU	1	0
1	1A	1939	5MU	1	0
54	1x	55	PSU	1	0
32	2a	1519	MA6	4	0
32	1a	967	5MC	1	0
1	2A	1942	5MC	1	0
1	1A	2552	2MU	2	0
32	1a	1400	5MC	1	0
32	1a	1404	5MC	2	0
1	2A	2503	2MA	1	0
43	2l	92	0TD	1	0
32	1a	1207	2MG	3	0
32	2a	1402	4OC	1	0
1	1A	2251	OMG	1	0
1	2A	2552	2MU	2	0
54	2x	8	4SU	1	0
32	2a	967	5MC	3	0
1	2A	2251	OMG	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 2024 ligands modelled in this entry, 2022 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

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.

1 monomer is involved in 3 short contacts:

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

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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%)	-0.34	50 (1%) 69 46	26, 42, 92, 108	0
1	2A	2789/2915 (95%)	-0.05	35 (1%) 75 53	35, 59, 90, 106	0
2	1B	120/121 (99%)	-0.47	0 100 100	36, 51, 67, 83	0
2	2B	120/121 (99%)	0.62	6 (5%) 34 17	64, 81, 90, 98	0
3	1D	275/276 (99%)	0.03	4 (1%) 72 50	29, 41, 54, 77	0
3	2D	275/276 (99%)	0.30	4 (1%) 72 50	35, 50, 62, 71	0
4	1E	204/206 (99%)	-0.00	1 (0%) 87 72	26, 45, 60, 73	0
4	2E	204/206 (99%)	0.05	0 100 100	37, 57, 67, 77	0
5	1F	203/210 (96%)	-0.10	0 100 100	28, 47, 65, 79	0
5	2F	203/210 (96%)	0.16	1 (0%) 87 72	37, 65, 77, 81	0
6	1G	181/182 (99%)	0.33	5 (2%) 55 32	42, 58, 70, 83	0
6	2G	181/182 (99%)	0.97	17 (9%) 14 7	69, 79, 86, 92	0
7	1H	174/180 (96%)	0.01	1 (0%) 85 69	45, 55, 66, 74	0
7	2H	174/180 (96%)	0.68	6 (3%) 48 27	64, 79, 87, 97	0
8	1I	146/148 (98%)	0.36	1 (0%) 84 66	45, 69, 78, 82	0
8	2I	146/148 (98%)	0.54	4 (2%) 56 33	57, 72, 81, 87	0
9	1N	140/140 (100%)	0.06	3 (2%) 63 40	34, 45, 62, 72	0
9	2N	140/140 (100%)	0.37	3 (2%) 63 40	46, 63, 76, 84	0
10	1O	122/122 (100%)	-0.16	0 100 100	34, 44, 58, 64	0
10	2O	122/122 (100%)	0.17	0 100 100	45, 56, 69, 74	0
11	1P	149/150 (99%)	0.16	2 (1%) 75 53	28, 49, 67, 86	0
11	2P	149/150 (99%)	0.31	3 (2%) 65 42	43, 66, 81, 84	0
12	1Q	141/141 (100%)	-0.07	2 (1%) 73 51	32, 46, 58, 67	0
12	2Q	141/141 (100%)	0.46	2 (1%) 73 51	47, 63, 75, 80	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
13	1R	118/118 (100%)	-0.10	0 100 100	34, 41, 55, 63	0
13	2R	118/118 (100%)	0.18	1 (0%) 82 63	40, 53, 61, 67	0
14	1S	110/112 (98%)	0.08	0 100 100	42, 51, 60, 66	0
14	2S	110/112 (98%)	0.95	6 (5%) 30 16	63, 73, 82, 85	0
15	1T	131/146 (89%)	-0.01	1 (0%) 82 63	34, 48, 68, 83	0
15	2T	131/146 (89%)	0.35	3 (2%) 61 38	48, 58, 75, 85	0
16	1U	116/118 (98%)	0.01	2 (1%) 69 46	31, 41, 53, 66	0
16	2U	116/118 (98%)	0.35	2 (1%) 69 46	43, 60, 74, 81	0
17	1V	101/101 (100%)	-0.10	0 100 100	32, 47, 60, 73	0
17	2V	101/101 (100%)	0.37	3 (2%) 52 30	43, 68, 77, 81	0
18	1W	112/113 (99%)	-0.11	0 100 100	32, 40, 55, 76	0
18	2W	112/113 (99%)	0.19	3 (2%) 56 33	42, 52, 64, 87	0
19	1X	95/96 (98%)	-0.05	1 (1%) 78 57	32, 41, 58, 70	0
19	2X	95/96 (98%)	0.50	1 (1%) 78 57	53, 63, 74, 84	0
20	1Y	107/110 (97%)	0.01	2 (1%) 66 43	38, 52, 68, 73	0
20	2Y	107/110 (97%)	0.46	3 (2%) 55 32	58, 69, 78, 83	0
21	1Z	154/206 (74%)	0.04	1 (0%) 85 69	46, 62, 77, 80	0
21	2Z	160/206 (77%)	0.54	4 (2%) 58 35	66, 77, 85, 90	0
22	10	76/85 (89%)	-0.01	1 (1%) 75 53	33, 43, 55, 63	0
22	20	76/85 (89%)	0.61	5 (6%) 24 12	46, 63, 71, 80	0
23	11	97/98 (98%)	0.05	0 100 100	33, 46, 65, 71	0
23	21	97/98 (98%)	0.36	0 100 100	43, 55, 72, 76	0
24	12	70/72 (97%)	0.04	2 (2%) 53 31	38, 50, 60, 72	0
24	22	70/72 (97%)	0.31	0 100 100	61, 70, 75, 79	0
25	13	59/60 (98%)	0.00	0 100 100	31, 43, 61, 80	0
25	23	59/60 (98%)	0.23	1 (1%) 69 46	51, 65, 74, 82	0
26	14	69/71 (97%)	0.41	3 (4%) 40 21	55, 69, 83, 89	0
26	24	69/71 (97%)	0.71	3 (4%) 40 21	76, 85, 91, 95	0
27	15	59/60 (98%)	-0.10	1 (1%) 69 46	28, 40, 54, 66	0
27	25	59/60 (98%)	0.03	0 100 100	40, 52, 63, 72	0
28	16	53/54 (98%)	-0.32	0 100 100	36, 42, 54, 59	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
28	26	53/54 (98%)	0.27	0 100 100	52, 60, 66, 77	0
29	17	48/49 (97%)	-0.03	1 (2%) 63 40	29, 36, 58, 63	0
29	27	48/49 (97%)	0.18	1 (2%) 63 40	37, 45, 66, 74	0
30	18	64/65 (98%)	0.12	1 (1%) 70 47	29, 39, 48, 57	0
30	28	64/65 (98%)	0.38	0 100 100	49, 55, 63, 68	0
31	19	37/37 (100%)	-0.02	0 100 100	39, 46, 60, 66	0
31	29	37/37 (100%)	0.59	1 (2%) 56 33	60, 67, 74, 75	0
32	1a	1488/1521 (97%)	-0.04	16 (1%) 78 57	39, 65, 89, 105	0
32	2a	1491/1521 (98%)	0.37	33 (2%) 62 39	49, 75, 93, 105	0
33	1b	231/256 (90%)	0.38	4 (1%) 69 46	62, 75, 84, 94	0
33	2b	231/256 (90%)	0.92	27 (11%) 9 5	68, 81, 88, 95	0
34	1c	206/239 (86%)	0.07	1 (0%) 87 72	52, 67, 76, 83	0
34	2c	206/239 (86%)	0.80	18 (8%) 16 9	69, 81, 86, 92	0
35	1d	208/209 (99%)	0.29	4 (1%) 66 43	54, 67, 76, 80	0
35	2d	208/209 (99%)	0.74	6 (2%) 53 31	59, 72, 81, 86	0
36	1e	148/162 (91%)	0.31	2 (1%) 73 51	51, 63, 72, 77	0
36	2e	148/162 (91%)	0.68	8 (5%) 31 16	62, 73, 80, 85	0
37	1f	100/101 (99%)	-0.07	0 100 100	53, 62, 73, 74	0
37	2f	100/101 (99%)	0.12	1 (1%) 79 59	58, 70, 77, 81	0
38	1g	155/156 (99%)	0.30	9 (5%) 29 15	56, 66, 78, 86	0
38	2g	155/156 (99%)	0.42	5 (3%) 50 28	67, 77, 83, 88	0
39	1h	137/138 (99%)	0.22	1 (0%) 84 66	57, 66, 73, 79	0
39	2h	137/138 (99%)	0.71	7 (5%) 33 17	61, 72, 79, 80	0
40	1i	127/128 (99%)	0.72	10 (7%) 18 9	51, 71, 80, 85	0
40	2i	127/128 (99%)	1.17	20 (15%) 5 2	72, 82, 87, 91	0
41	1j	97/105 (92%)	0.49	1 (1%) 79 59	59, 72, 82, 85	0
41	2j	96/105 (91%)	1.62	32 (33%) 1 0	71, 83, 89, 92	0
42	1k	114/129 (88%)	0.09	1 (0%) 81 61	48, 65, 75, 81	0
42	2k	114/129 (88%)	0.52	3 (2%) 57 34	61, 70, 77, 86	0
43	1l	121/132 (91%)	0.05	2 (1%) 69 46	43, 56, 67, 75	0
43	2l	121/132 (91%)	0.54	2 (1%) 69 46	55, 65, 73, 79	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
44	1m	123/126 (97%)	0.48	3 (2%) 59 37	54, 66, 77, 95	0
44	2m	122/126 (96%)	1.07	12 (9%) 13 6	71, 81, 86, 93	0
45	1n	60/61 (98%)	0.48	2 (3%) 49 28	52, 62, 69, 72	0
45	2n	60/61 (98%)	1.65	21 (35%) 1 0	72, 81, 86, 88	0
46	1o	88/89 (98%)	0.16	1 (1%) 78 57	48, 63, 75, 81	0
46	2o	88/89 (98%)	0.55	0 100 100	61, 71, 78, 85	0
47	1p	82/88 (93%)	0.94	6 (7%) 21 10	58, 66, 76, 86	0
47	2p	82/88 (93%)	0.86	2 (2%) 59 37	54, 68, 76, 82	0
48	1q	99/105 (94%)	0.46	2 (2%) 65 42	53, 65, 74, 77	0
48	2q	99/105 (94%)	0.47	1 (1%) 79 59	60, 68, 75, 80	0
49	1r	68/88 (77%)	-0.04	0 100 100	57, 65, 74, 80	0
49	2r	68/88 (77%)	0.27	0 100 100	61, 69, 78, 81	0
50	1s	83/93 (89%)	0.35	1 (1%) 76 55	57, 66, 77, 82	0
50	2s	83/93 (89%)	0.99	6 (7%) 21 11	75, 82, 89, 93	0
51	1t	96/106 (90%)	0.62	6 (6%) 26 13	58, 68, 79, 83	0
51	2t	96/106 (90%)	0.44	4 (4%) 40 21	56, 68, 79, 82	0
52	1u	23/27 (85%)	0.69	1 (4%) 40 21	59, 64, 69, 71	0
52	2u	23/27 (85%)	1.41	6 (26%) 1 1	72, 78, 83, 88	0
53	1v	13/24 (54%)	1.70	5 (38%) 1 0	52, 88, 95, 95	0
53	2v	13/24 (54%)	2.38	9 (69%) 0 0	65, 95, 100, 102	0
54	1x	72/77 (93%)	-0.12	1 (1%) 73 51	37, 63, 80, 94	0
54	2x	72/77 (93%)	0.08	0 100 100	51, 77, 89, 94	0
55	1z	16/16 (100%)	0.52	2 (12%) 8 4	37, 43, 62, 75	0
55	2z	16/16 (100%)	0.89	3 (18%) 3 2	48, 52, 72, 77	0
All	All	20628/21476 (96%)	0.17	510 (2%) 58 35	26, 62, 86, 108	0

The worst 5 of 510 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
32	2a	1532	U	7.4
44	2m	123	ALA	6.0
44	1m	123	ALA	5.8
1	2A	2133	G	5.4
53	1v	24	A	5.3

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

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. 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
54	PSU	2x	55	20/21	0.71	0.14	75,83,93,101	0
54	5MU	2x	54	21/22	0.81	0.12	79,82,89,97	0
54	4SU	2x	8	20/21	0.81	0.11	77,86,93,93	0
32	2MG	2a	1207	24/25	0.84	0.11	76,83,88,95	0
1	5MU	2A	1915	21/22	0.84	0.09	74,78,84,97	0
32	5MC	2a	967	21/22	0.85	0.16	67,72,81,85	0
32	5MC	2a	1400	21/22	0.86	0.16	56,70,78,81	0
54	5MC	2x	32	21/22	0.88	0.13	68,74,76,78	0
1	PSU	2A	1911	20/21	0.88	0.12	64,69,77,77	0
32	M2G	2a	966	25/26	0.88	0.15	64,71,81,85	0
32	PSU	2a	516	20/21	0.89	0.09	66,74,81,82	0
54	5MU	1x	54	21/22	0.89	0.10	60,66,70,74	0
54	PSU	1x	55	20/21	0.89	0.09	62,65,72,76	0
32	4OC	2a	1402	22/23	0.90	0.12	64,69,76,79	0
43	0TD	2l	92	10/11	0.90	0.12	57,62,66,79	0
32	7MG	2a	527	24/25	0.90	0.14	65,69,75,76	0
32	2MG	1a	1207	24/25	0.91	0.09	54,66,75,81	0
1	PSU	2A	1917	20/21	0.91	0.08	58,69,74,76	0
1	5MC	2A	1942	21/22	0.91	0.10	49,62,66,67	0
54	4SU	1x	8	20/21	0.92	0.08	60,67,74,76	0
1	PSU	1A	1917	20/21	0.92	0.08	55,61,66,68	0
32	5MC	2a	1404	21/22	0.92	0.12	56,64,71,74	0
1	5MU	1A	1915	21/22	0.92	0.08	52,64,73,80	0
1	4OC	2A	1920	21/23	0.93	0.12	55,64,71,78	0
32	7MG	1a	527	24/25	0.93	0.11	40,50,56,60	0
32	4OC	1a	1402	22/23	0.93	0.12	48,54,61,63	0
1	5MC	2A	1962	21/22	0.94	0.10	45,55,59,64	0
1	5MC	1A	1942	21/22	0.94	0.09	39,45,50,58	0
32	MA6	2a	1518	24/25	0.94	0.11	53,63,68,75	0
32	PSU	1a	516	20/21	0.94	0.08	54,64,68,71	0
32	5MC	1a	1404	21/22	0.94	0.12	40,50,54,56	0
1	PSU	1A	1911	20/21	0.94	0.08	46,57,61,64	0
54	5MC	1x	32	21/22	0.94	0.10	47,53,58,64	0
32	M2G	1a	966	25/26	0.94	0.11	54,58,61,66	0
32	MA6	2a	1519	24/25	0.95	0.13	54,61,67,73	0
43	0TD	1l	92	10/11	0.95	0.08	53,56,59,62	0
32	5MC	1a	1400	21/22	0.95	0.11	49,55,62,70	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
32	5MC	1a	967	21/22	0.95	0.11	55,63,65,65	0
32	UR3	2a	1498	21/22	0.95	0.11	46,54,62,69	0
1	4OC	1A	1920	21/23	0.95	0.10	39,52,55,65	0
1	5MU	2A	1939	21/22	0.96	0.09	32,48,52,55	0
1	OMG	1A	2251	24/25	0.96	0.10	26,37,40,44	0
32	5MC	1a	1407	21/22	0.96	0.08	39,45,49,51	0
1	OMG	2A	2251	24/25	0.96	0.09	35,44,49,50	0
1	2MA	2A	2503	23/24	0.96	0.10	39,46,49,52	0
1	2MU	2A	2552	21/23	0.96	0.10	33,42,49,52	0
32	MA6	1a	1519	24/25	0.96	0.10	44,52,54,55	0
32	5MC	2a	1407	21/22	0.96	0.07	49,61,69,71	0
1	2MU	1A	2552	21/23	0.97	0.07	26,37,42,48	0
1	PSU	1A	2605	20/21	0.97	0.07	28,36,41,42	0
1	5MC	1A	1962	21/22	0.97	0.07	35,44,48,50	0
1	PSU	2A	2605	20/21	0.97	0.07	35,42,46,46	0
32	UR3	1a	1498	21/22	0.97	0.08	42,49,56,60	0
32	MA6	1a	1518	24/25	0.97	0.10	34,49,55,55	0
1	5MU	1A	1939	21/22	0.97	0.08	28,36,41,43	0
1	2MA	1A	2503	23/24	0.98	0.07	24,32,35,41	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	2A	3483	1/1	0.44	0.22	73,73,73,73	0
56	MG	1A	3176	1/1	0.56	0.37	69,69,69,69	0
56	MG	2A	3351	1/1	0.63	0.17	59,59,59,59	0
56	MG	1A	3512	1/1	0.63	0.14	50,50,50,50	0
56	MG	2A	3197	1/1	0.64	0.24	73,73,73,73	0
56	MG	2a	3112	1/1	0.65	0.25	64,64,64,64	0
56	MG	1A	3837	1/1	0.66	0.29	64,64,64,64	0
56	MG	1a	1697	1/1	0.66	0.29	72,72,72,72	0
56	MG	1A	3802	1/1	0.69	0.20	37,37,37,37	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	1x	105	1/1	0.69	0.21	60,60,60,60	0
56	MG	1A	3399	1/1	0.69	0.17	70,70,70,70	0
56	MG	2a	3055	1/1	0.70	0.22	61,61,61,61	0
56	MG	1a	1681	1/1	0.70	0.19	55,55,55,55	0
56	MG	2A	3550	1/1	0.71	0.19	61,61,61,61	0
56	MG	1a	1717	1/1	0.72	0.23	67,67,67,67	0
56	MG	2a	3061	1/1	0.72	0.27	51,51,51,51	0
56	MG	1A	3480	1/1	0.72	0.19	28,28,28,28	0
56	MG	2a	3140	1/1	0.72	0.25	64,64,64,64	0
56	MG	1a	1686	1/1	0.73	0.33	64,64,64,64	0
56	MG	1a	1723	1/1	0.74	0.24	57,57,57,57	0
56	MG	1A	3388	1/1	0.74	0.70	35,35,35,35	0
56	MG	2A	3506	1/1	0.74	0.23	68,68,68,68	0
56	MG	1A	3575	1/1	0.74	0.20	72,72,72,72	0
56	MG	1A	3179	1/1	0.75	0.26	59,59,59,59	0
56	MG	2A	3407	1/1	0.75	0.15	75,75,75,75	0
56	MG	1A	3461	1/1	0.75	0.27	52,52,52,52	0
56	MG	2a	3145	1/1	0.75	0.43	66,66,66,66	0
56	MG	2v	101	1/1	0.75	0.15	77,77,77,77	0
56	MG	2A	3312	1/1	0.76	0.09	53,53,53,53	0
56	MG	1a	1763	1/1	0.76	0.23	59,59,59,59	0
56	MG	1A	3763	1/1	0.76	0.20	68,68,68,68	0
56	MG	1A	3408	1/1	0.76	0.33	65,65,65,65	0
56	MG	1a	1759	1/1	0.77	0.41	65,65,65,65	0
56	MG	2A	3585	1/1	0.77	0.17	66,66,66,66	0
56	MG	2a	3003	1/1	0.77	0.29	61,61,61,61	0
56	MG	1A	3347	1/1	0.77	0.17	62,62,62,62	0
56	MG	2A	3395	1/1	0.77	0.27	52,52,52,52	0
56	MG	2a	3082	1/1	0.77	0.43	61,61,61,61	0
56	MG	1A	3712	1/1	0.77	0.33	43,43,43,43	0
56	MG	2A	3409	1/1	0.77	0.35	60,60,60,60	0
56	MG	1a	1744	1/1	0.77	0.48	58,58,58,58	0
56	MG	2A	3206	1/1	0.77	0.20	52,52,52,52	0
56	MG	2A	3082	1/1	0.78	0.29	52,52,52,52	0
56	MG	2A	3090	1/1	0.78	0.35	72,72,72,72	0
56	MG	1B	219	1/1	0.78	0.19	66,66,66,66	0
56	MG	1A	3284	1/1	0.78	0.17	51,51,51,51	0
56	MG	2F	302	1/1	0.78	0.15	45,45,45,45	0
56	MG	2Z	301	1/1	0.78	0.15	60,60,60,60	0
56	MG	1a	1756	1/1	0.78	0.35	54,54,54,54	0
56	MG	2A	3317	1/1	0.78	0.17	59,59,59,59	0
56	MG	2A	3326	1/1	0.78	0.17	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	3081	1/1	0.78	0.24	55,55,55,55	0
56	MG	1A	3687	1/1	0.78	0.20	58,58,58,58	0
56	MG	2a	3105	1/1	0.78	0.31	53,53,53,53	0
56	MG	1A	3383	1/1	0.78	0.27	69,69,69,69	0
56	MG	2a	3123	1/1	0.78	0.24	62,62,62,62	0
56	MG	1B	213	1/1	0.78	0.25	58,58,58,58	0
56	MG	2A	3054	1/1	0.78	0.20	51,51,51,51	0
56	MG	2A	3413	1/1	0.78	0.18	57,57,57,57	0
56	MG	1A	3553	1/1	0.79	0.17	65,65,65,65	0
56	MG	2a	3025	1/1	0.79	0.11	73,73,73,73	0
56	MG	2a	3053	1/1	0.79	0.20	67,67,67,67	0
56	MG	2A	3344	1/1	0.79	0.18	66,66,66,66	0
56	MG	2a	3059	1/1	0.79	0.24	58,58,58,58	0
56	MG	2A	3421	1/1	0.79	0.27	54,54,54,54	0
56	MG	1A	3696	1/1	0.79	0.10	67,67,67,67	0
56	MG	2A	3368	1/1	0.79	0.30	70,70,70,70	0
56	MG	2A	3375	1/1	0.79	0.12	51,51,51,51	0
56	MG	2A	3391	1/1	0.79	0.13	94,94,94,94	0
56	MG	2a	3117	1/1	0.79	0.18	50,50,50,50	0
56	MG	2a	3122	1/1	0.79	0.26	65,65,65,65	0
56	MG	2A	3602	1/1	0.79	0.20	55,55,55,55	0
56	MG	1a	1612	1/1	0.79	0.24	45,45,45,45	0
56	MG	2N	201	1/1	0.79	0.08	49,49,49,49	0
56	MG	1A	3151	1/1	0.79	0.28	72,72,72,72	0
56	MG	1a	1659	1/1	0.80	0.25	64,64,64,64	0
56	MG	1A	3083	1/1	0.80	0.25	52,52,52,52	0
56	MG	1U	205	1/1	0.80	0.15	39,39,39,39	0
56	MG	2A	3471	1/1	0.80	0.12	54,54,54,54	0
56	MG	1A	3241	1/1	0.80	0.11	54,54,54,54	0
56	MG	2A	3492	1/1	0.80	0.25	69,69,69,69	0
56	MG	2a	3009	1/1	0.80	0.11	49,49,49,49	0
56	MG	2a	3119	1/1	0.80	0.51	76,76,76,76	0
56	MG	2A	3401	1/1	0.80	0.37	53,53,53,53	0
56	MG	2a	3029	1/1	0.80	0.19	47,47,47,47	0
56	MG	2a	3033	1/1	0.80	0.22	57,57,57,57	0
56	MG	2A	3217	1/1	0.80	0.26	48,48,48,48	0
56	MG	2A	3552	1/1	0.80	0.14	60,60,60,60	0
56	MG	2A	3416	1/1	0.81	0.18	63,63,63,63	0
56	MG	1A	3501	1/1	0.81	0.11	58,58,58,58	0
56	MG	2A	3429	1/1	0.81	0.42	59,59,59,59	0
56	MG	1A	3737	1/1	0.81	0.09	47,47,47,47	0
56	MG	1A	3594	1/1	0.81	0.17	64,64,64,64	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	1A	3767	1/1	0.81	0.16	51,51,51,51	0
56	MG	1A	3784	1/1	0.81	0.24	60,60,60,60	0
56	MG	2A	3357	1/1	0.81	0.32	54,54,54,54	0
56	MG	1A	3648	1/1	0.81	0.29	62,62,62,62	0
56	MG	2A	3566	1/1	0.81	0.19	62,62,62,62	0
56	MG	2A	3077	1/1	0.81	0.25	54,54,54,54	0
56	MG	1A	3187	1/1	0.81	0.13	49,49,49,49	0
56	MG	2B	205	1/1	0.81	0.22	79,79,79,79	0
56	MG	1A	3844	1/1	0.81	0.20	50,50,50,50	0
56	MG	2A	3143	1/1	0.81	0.22	56,56,56,56	0
56	MG	1A	3373	1/1	0.81	0.16	47,47,47,47	0
56	MG	1a	1724	1/1	0.81	0.26	52,52,52,52	0
56	MG	1a	1725	1/1	0.81	0.20	67,67,67,67	0
56	MG	1A	3254	1/1	0.82	0.18	64,64,64,64	0
56	MG	1a	1753	1/1	0.82	0.32	59,59,59,59	0
56	MG	1a	1691	1/1	0.82	0.25	42,42,42,42	0
56	MG	2A	3537	1/1	0.82	0.20	57,57,57,57	0
56	MG	2A	3210	1/1	0.82	0.11	76,76,76,76	0
56	MG	1A	3259	1/1	0.82	0.16	60,60,60,60	0
56	MG	2A	3560	1/1	0.82	0.20	75,75,75,75	0
56	MG	2A	3406	1/1	0.82	0.22	50,50,50,50	0
56	MG	1A	3660	1/1	0.82	0.14	63,63,63,63	0
56	MG	2a	3094	1/1	0.82	0.24	57,57,57,57	0
56	MG	1a	1621	1/1	0.82	0.25	51,51,51,51	0
56	MG	2a	3111	1/1	0.82	0.24	66,66,66,66	0
56	MG	1A	3667	1/1	0.82	0.13	33,33,33,33	0
56	MG	1A	3113	1/1	0.82	0.30	58,58,58,58	0
56	MG	1a	1728	1/1	0.82	0.27	63,63,63,63	0
56	MG	2A	3356	1/1	0.82	0.23	61,61,61,61	0
56	MG	2A	3450	1/1	0.82	0.19	41,41,41,41	0
56	MG	2a	3127	1/1	0.82	0.20	65,65,65,65	0
56	MG	2a	3139	1/1	0.82	0.19	54,54,54,54	0
56	MG	2a	3006	1/1	0.82	0.32	63,63,63,63	0
56	MG	2a	3142	1/1	0.82	0.27	49,49,49,49	0
56	MG	1a	1742	1/1	0.82	0.26	60,60,60,60	0
56	MG	2a	3018	1/1	0.82	0.22	59,59,59,59	0
56	MG	1A	3715	1/1	0.83	0.15	53,53,53,53	0
56	MG	1A	3302	1/1	0.83	0.23	55,55,55,55	0
56	MG	2a	3012	1/1	0.83	0.24	52,52,52,52	0
56	MG	2A	3102	1/1	0.83	0.21	50,50,50,50	0
56	MG	1A	3081	1/1	0.83	0.15	57,57,57,57	0
56	MG	1E	306	1/1	0.83	0.12	43,43,43,43	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	1H	201	1/1	0.83	0.12	40,40,40,40	0
56	MG	2A	3207	1/1	0.83	0.09	55,55,55,55	0
56	MG	1A	3407	1/1	0.83	0.56	103,103,103,103	0
56	MG	1a	1606	1/1	0.83	0.14	54,54,54,54	0
56	MG	2A	3289	1/1	0.83	0.21	45,45,45,45	0
56	MG	1A	3230	1/1	0.83	0.12	49,49,49,49	0
56	MG	2A	3313	1/1	0.83	0.15	51,51,51,51	0
56	MG	2a	3085	1/1	0.83	0.33	52,52,52,52	0
56	MG	1a	1618	1/1	0.83	0.25	61,61,61,61	0
56	MG	1a	1752	1/1	0.83	0.17	60,60,60,60	0
56	MG	1A	3430	1/1	0.83	0.25	64,64,64,64	0
56	MG	1a	1628	1/1	0.83	0.18	43,43,43,43	0
56	MG	1a	1634	1/1	0.83	0.18	49,49,49,49	0
56	MG	1a	1644	1/1	0.83	0.23	54,54,54,54	0
56	MG	2A	3359	1/1	0.83	0.25	52,52,52,52	0
56	MG	1A	3826	1/1	0.83	0.15	51,51,51,51	0
56	MG	2A	3016	1/1	0.83	0.42	65,65,65,65	0
56	MG	2a	3136	1/1	0.83	0.15	62,62,62,62	0
56	MG	2A	3376	1/1	0.83	0.14	52,52,52,52	0
56	MG	1A	3827	1/1	0.83	0.16	51,51,51,51	0
56	MG	2T	201	1/1	0.83	0.10	33,33,33,33	0
56	MG	2A	3394	1/1	0.83	0.16	60,60,60,60	0
56	MG	1A	3002	1/1	0.83	0.15	56,56,56,56	0
56	MG	2v	102	1/1	0.83	0.51	57,57,57,57	0
56	MG	2x	102	1/1	0.83	0.17	47,47,47,47	0
56	MG	2A	3521	1/1	0.84	0.19	60,60,60,60	0
56	MG	1A	3738	1/1	0.84	0.11	44,44,44,44	0
56	MG	1A	3212	1/1	0.84	0.18	45,45,45,45	0
56	MG	1A	3221	1/1	0.84	0.15	36,36,36,36	0
56	MG	2a	3078	1/1	0.84	0.23	71,71,71,71	0
56	MG	1A	3842	1/1	0.84	0.23	42,42,42,42	0
56	MG	1A	3679	1/1	0.84	0.15	52,52,52,52	0
56	MG	2A	3037	1/1	0.84	0.20	50,50,50,50	0
56	MG	2a	3093	1/1	0.84	0.13	50,50,50,50	0
56	MG	2A	3291	1/1	0.84	0.28	43,43,43,43	0
56	MG	2a	3097	1/1	0.84	0.21	68,68,68,68	0
56	MG	1A	3785	1/1	0.84	0.13	53,53,53,53	0
56	MG	2A	3060	1/1	0.84	0.27	62,62,62,62	0
56	MG	2A	3069	1/1	0.84	0.25	53,53,53,53	0
56	MG	1B	218	1/1	0.84	0.26	52,52,52,52	0
56	MG	2A	3419	1/1	0.84	0.26	30,30,30,30	0
56	MG	2A	3329	1/1	0.84	0.18	55,55,55,55	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	1A	3786	1/1	0.84	0.14	58,58,58,58	0
56	MG	2a	3008	1/1	0.84	0.09	46,46,46,46	0
56	MG	1A	3795	1/1	0.84	0.11	39,39,39,39	0
56	MG	2a	3138	1/1	0.84	0.27	67,67,67,67	0
56	MG	1F	306	1/1	0.84	0.09	47,47,47,47	0
56	MG	2a	3016	1/1	0.84	0.19	76,76,76,76	0
56	MG	2A	3135	1/1	0.84	0.13	52,52,52,52	0
56	MG	1A	3269	1/1	0.84	0.08	34,34,34,34	0
56	MG	2A	3174	1/1	0.84	0.17	49,49,49,49	0
56	MG	2A	3516	1/1	0.84	0.18	67,67,67,67	0
56	MG	2a	3046	1/1	0.84	0.22	49,49,49,49	0
56	MG	2A	3545	1/1	0.85	0.28	53,53,53,53	0
56	MG	2A	3215	1/1	0.85	0.25	60,60,60,60	0
56	MG	2A	3384	1/1	0.85	0.25	45,45,45,45	0
56	MG	1a	1605	1/1	0.85	0.15	54,54,54,54	0
56	MG	2a	3064	1/1	0.85	0.29	64,64,64,64	0
56	MG	2A	3282	1/1	0.85	0.26	58,58,58,58	0
56	MG	1a	1737	1/1	0.85	0.18	41,41,41,41	0
56	MG	2A	3597	1/1	0.85	0.18	49,49,49,49	0
56	MG	1a	1740	1/1	0.85	0.28	35,35,35,35	0
56	MG	2a	3086	1/1	0.85	0.17	69,69,69,69	0
56	MG	2A	3620	1/1	0.85	0.25	61,61,61,61	0
56	MG	1A	3339	1/1	0.85	0.14	55,55,55,55	0
56	MG	2B	209	1/1	0.85	0.27	50,50,50,50	0
56	MG	2a	3103	1/1	0.85	0.20	65,65,65,65	0
56	MG	1A	3500	1/1	0.85	0.15	59,59,59,59	0
56	MG	2a	3106	1/1	0.85	0.24	60,60,60,60	0
56	MG	1A	3289	1/1	0.85	0.14	46,46,46,46	0
56	MG	2A	3325	1/1	0.85	0.14	52,52,52,52	0
56	MG	1a	1692	1/1	0.85	0.31	43,43,43,43	0
56	MG	28	103	1/1	0.85	0.25	60,60,60,60	0
56	MG	1A	3389	1/1	0.85	0.12	50,50,50,50	0
56	MG	2A	3343	1/1	0.85	0.18	69,69,69,69	0
56	MG	1a	1757	1/1	0.85	0.25	51,51,51,51	0
56	MG	1A	3437	1/1	0.85	0.25	53,53,53,53	0
56	MG	2A	3355	1/1	0.85	0.12	61,61,61,61	0
56	MG	1A	3072	1/1	0.85	0.29	52,52,52,52	0
56	MG	1a	1767	1/1	0.85	0.19	47,47,47,47	0
56	MG	1a	1637	1/1	0.85	0.21	46,46,46,46	0
56	MG	2A	3010	1/1	0.85	0.14	56,56,56,56	0
56	MG	2A	3370	1/1	0.85	0.32	51,51,51,51	0
56	MG	17	3106	1/1	0.85	0.25	58,58,58,58	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	2a	3049	1/1	0.85	0.20	54,54,54,54	0
56	MG	2A	3399	1/1	0.86	0.23	47,47,47,47	0
56	MG	1A	3337	1/1	0.86	0.14	31,31,31,31	0
56	MG	2A	3212	1/1	0.86	0.20	62,62,62,62	0
56	MG	2a	3023	1/1	0.86	0.17	59,59,59,59	0
56	MG	1A	3404	1/1	0.86	0.18	52,52,52,52	0
56	MG	1A	3184	1/1	0.86	0.10	46,46,46,46	0
56	MG	2A	3260	1/1	0.86	0.19	53,53,53,53	0
56	MG	1T	201	1/1	0.86	0.15	44,44,44,44	0
56	MG	2a	3048	1/1	0.86	0.18	61,61,61,61	0
56	MG	2A	3005	1/1	0.86	0.21	42,42,42,42	0
56	MG	2a	3051	1/1	0.86	0.17	56,56,56,56	0
56	MG	1A	3150	1/1	0.86	0.12	35,35,35,35	0
56	MG	1a	1709	1/1	0.86	0.19	36,36,36,36	0
56	MG	2A	3435	1/1	0.86	0.35	49,49,49,49	0
56	MG	2A	3034	1/1	0.86	0.10	34,34,34,34	0
56	MG	1X	103	1/1	0.86	0.11	40,40,40,40	0
56	MG	2a	3065	1/1	0.86	0.24	56,56,56,56	0
56	MG	2a	3072	1/1	0.86	0.33	55,55,55,55	0
56	MG	2A	3051	1/1	0.86	0.17	54,54,54,54	0
56	MG	1A	3825	1/1	0.86	0.15	46,46,46,46	0
56	MG	1A	3276	1/1	0.86	0.13	45,45,45,45	0
56	MG	2A	3333	1/1	0.86	0.33	51,51,51,51	0
56	MG	2A	3334	1/1	0.86	0.13	51,51,51,51	0
56	MG	2a	3091	1/1	0.86	0.15	43,43,43,43	0
56	MG	2A	3340	1/1	0.86	0.22	60,60,60,60	0
56	MG	2A	3341	1/1	0.86	0.22	56,56,56,56	0
56	MG	2A	3063	1/1	0.86	0.14	46,46,46,46	0
56	MG	1A	3233	1/1	0.86	0.14	62,62,62,62	0
56	MG	1A	3627	1/1	0.86	0.11	36,36,36,36	0
56	MG	1a	1735	1/1	0.86	0.26	57,57,57,57	0
56	MG	1A	3841	1/1	0.86	0.17	57,57,57,57	0
56	MG	1A	3646	1/1	0.86	0.09	56,56,56,56	0
56	MG	1A	3739	1/1	0.86	0.19	66,66,66,66	0
56	MG	2A	3606	1/1	0.86	0.10	54,54,54,54	0
56	MG	2A	3364	1/1	0.86	0.24	53,53,53,53	0
56	MG	2A	3366	1/1	0.86	0.17	53,53,53,53	0
56	MG	1A	3074	1/1	0.86	0.13	55,55,55,55	0
56	MG	2a	3131	1/1	0.86	0.33	60,60,60,60	0
56	MG	2a	3132	1/1	0.86	0.39	55,55,55,55	0
56	MG	2A	3152	1/1	0.86	0.18	64,64,64,64	0
56	MG	1A	3214	1/1	0.86	0.06	46,46,46,46	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	2A	3179	1/1	0.86	0.29	54,54,54,54	0
56	MG	2A	3377	1/1	0.86	0.15	47,47,47,47	0
56	MG	2A	3185	1/1	0.86	0.14	49,49,49,49	0
56	MG	2A	3386	1/1	0.86	0.39	63,63,63,63	0
56	MG	1A	3666	1/1	0.86	0.14	48,48,48,48	0
56	MG	1B	221	1/1	0.86	0.10	63,63,63,63	0
56	MG	1a	1672	1/1	0.86	0.17	49,49,49,49	0
56	MG	1a	1665	1/1	0.87	0.23	40,40,40,40	0
56	MG	1A	3445	1/1	0.87	0.21	46,46,46,46	0
56	MG	1a	1675	1/1	0.87	0.33	53,53,53,53	0
56	MG	1A	3460	1/1	0.87	0.26	49,49,49,49	0
56	MG	1A	3120	1/1	0.87	0.11	46,46,46,46	0
56	MG	2a	3007	1/1	0.87	0.20	50,50,50,50	0
56	MG	1A	3469	1/1	0.87	0.22	48,48,48,48	0
56	MG	1A	3692	1/1	0.87	0.13	48,48,48,48	0
56	MG	2A	3096	1/1	0.87	0.19	49,49,49,49	0
56	MG	1a	1694	1/1	0.87	0.20	35,35,35,35	0
56	MG	1A	3024	1/1	0.87	0.16	76,76,76,76	0
56	MG	1a	1701	1/1	0.87	0.17	49,49,49,49	0
56	MG	2A	3148	1/1	0.87	0.11	45,45,45,45	0
56	MG	1A	3706	1/1	0.87	0.13	41,41,41,41	0
56	MG	2A	3165	1/1	0.87	0.15	44,44,44,44	0
56	MG	2A	3173	1/1	0.87	0.09	47,47,47,47	0
56	MG	2a	3047	1/1	0.87	0.09	67,67,67,67	0
56	MG	2A	3397	1/1	0.87	0.18	69,69,69,69	0
56	MG	1a	1715	1/1	0.87	0.15	42,42,42,42	0
56	MG	1A	3270	1/1	0.87	0.15	50,50,50,50	0
56	MG	1B	222	1/1	0.87	0.11	47,47,47,47	0
56	MG	1A	3274	1/1	0.87	0.21	52,52,52,52	0
56	MG	2a	3057	1/1	0.87	0.33	59,59,59,59	0
56	MG	2A	3201	1/1	0.87	0.14	46,46,46,46	0
56	MG	1E	307	1/1	0.87	0.17	38,38,38,38	0
56	MG	1A	3716	1/1	0.87	0.21	53,53,53,53	0
56	MG	1A	3728	1/1	0.87	0.12	58,58,58,58	0
56	MG	2a	3067	1/1	0.87	0.15	58,58,58,58	0
56	MG	1A	3503	1/1	0.87	0.17	49,49,49,49	0
56	MG	1A	3094	1/1	0.87	0.15	42,42,42,42	0
56	MG	1W	204	1/1	0.87	0.26	53,53,53,53	0
56	MG	1A	3530	1/1	0.87	0.12	34,34,34,34	0
56	MG	2a	3084	1/1	0.87	0.29	67,67,67,67	0
56	MG	2A	3267	1/1	0.87	0.28	51,51,51,51	0
56	MG	2A	3270	1/1	0.87	0.32	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	3090	1/1	0.87	0.36	52,52,52,52	0
56	MG	1a	1748	1/1	0.87	0.23	49,49,49,49	0
56	MG	2a	3092	1/1	0.87	0.20	58,58,58,58	0
56	MG	2A	3495	1/1	0.87	0.30	44,44,44,44	0
56	MG	2A	3283	1/1	0.87	0.44	47,47,47,47	0
56	MG	1A	3239	1/1	0.87	0.19	53,53,53,53	0
56	MG	1a	1603	1/1	0.87	0.19	59,59,59,59	0
56	MG	2A	3305	1/1	0.87	0.32	43,43,43,43	0
56	MG	1A	3175	1/1	0.87	0.30	58,58,58,58	0
56	MG	2a	3108	1/1	0.87	0.21	48,48,48,48	0
56	MG	1A	3585	1/1	0.87	0.11	50,50,50,50	0
56	MG	1A	3296	1/1	0.87	0.21	61,61,61,61	0
56	MG	1A	3244	1/1	0.87	0.08	49,49,49,49	0
56	MG	1a	1765	1/1	0.87	0.16	62,62,62,62	0
56	MG	2A	3570	1/1	0.87	0.16	79,79,79,79	0
56	MG	2A	3573	1/1	0.87	0.10	55,55,55,55	0
56	MG	1A	3638	1/1	0.87	0.19	64,64,64,64	0
56	MG	2A	3587	1/1	0.87	0.14	56,56,56,56	0
56	MG	2A	3591	1/1	0.87	0.14	36,36,36,36	0
56	MG	1a	1627	1/1	0.87	0.34	60,60,60,60	0
56	MG	1x	110	1/1	0.87	0.09	53,53,53,53	0
56	MG	1A	3308	1/1	0.87	0.17	47,47,47,47	0
56	MG	1A	3821	1/1	0.87	0.30	54,54,54,54	0
56	MG	1A	3324	1/1	0.87	0.11	56,56,56,56	0
56	MG	2a	3144	1/1	0.87	0.11	45,45,45,45	0
56	MG	1A	3017	1/1	0.87	0.14	37,37,37,37	0
56	MG	2q	201	1/1	0.87	0.10	54,54,54,54	0
56	MG	2B	210	1/1	0.87	0.20	58,58,58,58	0
56	MG	1a	1657	1/1	0.87	0.34	58,58,58,58	0
56	MG	1A	3662	1/1	0.87	0.19	61,61,61,61	0
56	MG	1A	3215	1/1	0.88	0.28	49,49,49,49	0
56	MG	2A	3563	1/1	0.88	0.18	59,59,59,59	0
56	MG	2A	3565	1/1	0.88	0.07	44,44,44,44	0
56	MG	2A	3223	1/1	0.88	0.14	37,37,37,37	0
56	MG	1a	1602	1/1	0.88	0.16	51,51,51,51	0
56	MG	2A	3261	1/1	0.88	0.38	53,53,53,53	0
56	MG	1A	3774	1/1	0.88	0.16	80,80,80,80	0
56	MG	1a	1750	1/1	0.88	0.27	52,52,52,52	0
56	MG	2A	3590	1/1	0.88	0.18	49,49,49,49	0
56	MG	2A	3274	1/1	0.88	0.24	51,51,51,51	0
56	MG	2A	3276	1/1	0.88	0.21	39,39,39,39	0
56	MG	2A	3601	1/1	0.88	0.13	52,52,52,52	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	1a	1751	1/1	0.88	0.44	60,60,60,60	0
56	MG	2A	3603	1/1	0.88	0.14	61,61,61,61	0
56	MG	1A	3643	1/1	0.88	0.11	34,34,34,34	0
56	MG	2A	3610	1/1	0.88	0.21	46,46,46,46	0
56	MG	2A	3612	1/1	0.88	0.09	42,42,42,42	0
56	MG	1A	3475	1/1	0.88	0.13	29,29,29,29	0
56	MG	1A	3477	1/1	0.88	0.14	35,35,35,35	0
56	MG	1a	1615	1/1	0.88	0.16	52,52,52,52	0
56	MG	1A	3659	1/1	0.88	0.23	56,56,56,56	0
56	MG	2B	211	1/1	0.88	0.25	54,54,54,54	0
56	MG	2F	301	1/1	0.88	0.08	44,44,44,44	0
56	MG	1A	3216	1/1	0.88	0.19	58,58,58,58	0
56	MG	1A	3497	1/1	0.88	0.12	45,45,45,45	0
56	MG	2O	201	1/1	0.88	0.16	52,52,52,52	0
56	MG	2A	3318	1/1	0.88	0.17	51,51,51,51	0
56	MG	1A	3406	1/1	0.88	0.17	57,57,57,57	0
56	MG	26	101	1/1	0.88	0.12	56,56,56,56	0
56	MG	1n	102	1/1	0.88	0.16	47,47,47,47	0
56	MG	1A	3342	1/1	0.88	0.20	53,53,53,53	0
56	MG	2A	3332	1/1	0.88	0.15	56,56,56,56	0
56	MG	1x	106	1/1	0.88	0.09	72,72,72,72	0
56	MG	1A	3078	1/1	0.88	0.15	43,43,43,43	0
56	MG	2A	3339	1/1	0.88	0.25	63,63,63,63	0
56	MG	1A	3830	1/1	0.88	0.13	52,52,52,52	0
56	MG	2a	3013	1/1	0.88	0.23	56,56,56,56	0
56	MG	1a	1650	1/1	0.88	0.23	45,45,45,45	0
56	MG	2a	3017	1/1	0.88	0.13	50,50,50,50	0
56	MG	1a	1654	1/1	0.88	0.17	53,53,53,53	0
56	MG	2A	3021	1/1	0.88	0.12	53,53,53,53	0
56	MG	2A	3345	1/1	0.88	0.25	56,56,56,56	0
56	MG	1A	3426	1/1	0.88	0.35	29,29,29,29	0
56	MG	2A	3036	1/1	0.88	0.12	55,55,55,55	0
56	MG	2a	3040	1/1	0.88	0.14	50,50,50,50	0
56	MG	1A	3691	1/1	0.88	0.14	46,46,46,46	0
56	MG	1a	1662	1/1	0.88	0.14	37,37,37,37	0
56	MG	1A	3371	1/1	0.88	0.31	47,47,47,47	0
56	MG	1A	3536	1/1	0.88	0.22	63,63,63,63	0
56	MG	2A	3365	1/1	0.88	0.16	69,69,69,69	0
56	MG	2A	3062	1/1	0.88	0.13	47,47,47,47	0
56	MG	2a	3054	1/1	0.88	0.20	63,63,63,63	0
56	MG	1B	212	1/1	0.88	0.32	51,51,51,51	0
56	MG	1A	3540	1/1	0.88	0.13	28,28,28,28	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	1B	215	1/1	0.88	0.27	44,44,44,44	0
56	MG	1A	3545	1/1	0.88	0.13	48,48,48,48	0
56	MG	2a	3063	1/1	0.88	0.33	64,64,64,64	0
56	MG	1A	3222	1/1	0.88	0.11	40,40,40,40	0
56	MG	1A	3439	1/1	0.88	0.38	50,50,50,50	0
56	MG	1a	1695	1/1	0.88	0.16	59,59,59,59	0
56	MG	2A	3388	1/1	0.88	0.20	67,67,67,67	0
56	MG	2A	3389	1/1	0.88	0.19	45,45,45,45	0
56	MG	2A	3126	1/1	0.88	0.17	51,51,51,51	0
56	MG	2A	3130	1/1	0.88	0.06	29,29,29,29	0
56	MG	1A	3209	1/1	0.88	0.29	40,40,40,40	0
56	MG	2A	3139	1/1	0.88	0.07	30,30,30,30	0
56	MG	1B	224	1/1	0.88	0.10	42,42,42,42	0
56	MG	2A	3147	1/1	0.88	0.17	59,59,59,59	0
56	MG	1a	1705	1/1	0.88	0.23	52,52,52,52	0
56	MG	1A	3734	1/1	0.88	0.13	45,45,45,45	0
56	MG	2A	3153	1/1	0.88	0.13	49,49,49,49	0
56	MG	2A	3155	1/1	0.88	0.38	61,61,61,61	0
56	MG	1A	3152	1/1	0.88	0.23	47,47,47,47	0
56	MG	2a	3100	1/1	0.88	0.16	35,35,35,35	0
56	MG	2a	3102	1/1	0.88	0.17	53,53,53,53	0
56	MG	1A	3618	1/1	0.88	0.15	23,23,23,23	0
56	MG	1a	1719	1/1	0.88	0.40	53,53,53,53	0
56	MG	2A	3177	1/1	0.88	0.09	53,53,53,53	0
56	MG	2a	3107	1/1	0.88	0.34	36,36,36,36	0
56	MG	2A	3432	1/1	0.88	0.24	30,30,30,30	0
56	MG	1A	3115	1/1	0.88	0.09	31,31,31,31	0
56	MG	2A	3443	1/1	0.88	0.22	39,39,39,39	0
56	MG	2a	3115	1/1	0.88	0.31	58,58,58,58	0
56	MG	2A	3184	1/1	0.88	0.10	67,67,67,67	0
56	MG	2a	3118	1/1	0.88	0.28	61,61,61,61	0
56	MG	2A	3464	1/1	0.88	0.10	39,39,39,39	0
56	MG	1N	203	1/1	0.88	0.07	31,31,31,31	0
56	MG	2A	3187	1/1	0.88	0.17	56,56,56,56	0
56	MG	2a	3126	1/1	0.88	0.28	66,66,66,66	0
56	MG	1Q	202	1/1	0.88	0.07	40,40,40,40	0
56	MG	1A	3741	1/1	0.88	0.32	42,42,42,42	0
56	MG	1a	1732	1/1	0.88	0.19	42,42,42,42	0
56	MG	2A	3512	1/1	0.88	0.10	39,39,39,39	0
56	MG	2A	3515	1/1	0.88	0.17	39,39,39,39	0
56	MG	1A	3753	1/1	0.88	0.12	31,31,31,31	0
56	MG	2A	3208	1/1	0.88	0.19	60,60,60,60	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	2A	3523	1/1	0.88	0.13	62,62,62,62	0
56	MG	1A	3633	1/1	0.88	0.08	34,34,34,34	0
56	MG	2A	3211	1/1	0.88	0.09	51,51,51,51	0
56	MG	1a	1739	1/1	0.88	0.14	48,48,48,48	0
56	MG	2t	201	1/1	0.88	0.13	49,49,49,49	0
56	MG	1A	3765	1/1	0.88	0.12	45,45,45,45	0
56	MG	2A	3554	1/1	0.88	0.14	65,65,65,65	0
56	MG	2A	3557	1/1	0.88	0.17	47,47,47,47	0
56	MG	2A	3089	1/1	0.89	0.12	51,51,51,51	0
56	MG	2A	3346	1/1	0.89	0.23	45,45,45,45	0
56	MG	1A	3295	1/1	0.89	0.19	45,45,45,45	0
56	MG	1A	3393	1/1	0.89	0.15	40,40,40,40	0
56	MG	1A	3543	1/1	0.89	0.14	29,29,29,29	0
56	MG	2A	3109	1/1	0.89	0.27	53,53,53,53	0
56	MG	1a	1706	1/1	0.89	0.13	48,48,48,48	0
56	MG	2A	3128	1/1	0.89	0.09	47,47,47,47	0
56	MG	1A	3735	1/1	0.89	0.10	56,56,56,56	0
56	MG	1N	201	1/1	0.89	0.17	45,45,45,45	0
56	MG	1a	1716	1/1	0.89	0.33	43,43,43,43	0
56	MG	1A	3395	1/1	0.89	0.16	45,45,45,45	0
56	MG	1A	3197	1/1	0.89	0.09	43,43,43,43	0
56	MG	1Q	204	1/1	0.89	0.13	41,41,41,41	0
56	MG	1A	3297	1/1	0.89	0.12	55,55,55,55	0
56	MG	1A	3245	1/1	0.89	0.11	41,41,41,41	0
56	MG	1A	3591	1/1	0.89	0.14	46,46,46,46	0
56	MG	2A	3156	1/1	0.89	0.15	48,48,48,48	0
56	MG	1A	3307	1/1	0.89	0.12	52,52,52,52	0
56	MG	2A	3167	1/1	0.89	0.17	61,61,61,61	0
56	MG	2A	3170	1/1	0.89	0.21	46,46,46,46	0
56	MG	1A	3597	1/1	0.89	0.09	34,34,34,34	0
56	MG	1A	3599	1/1	0.89	0.12	59,59,59,59	0
56	MG	2a	3043	1/1	0.89	0.20	64,64,64,64	0
56	MG	2a	3044	1/1	0.89	0.16	67,67,67,67	0
56	MG	1A	3040	1/1	0.89	0.18	49,49,49,49	0
56	MG	1A	3413	1/1	0.89	0.10	38,38,38,38	0
56	MG	1A	3309	1/1	0.89	0.10	50,50,50,50	0
56	MG	1A	3311	1/1	0.89	0.20	60,60,60,60	0
56	MG	1A	3318	1/1	0.89	0.12	38,38,38,38	0
56	MG	2A	3190	1/1	0.89	0.16	55,55,55,55	0
56	MG	1A	3033	1/1	0.89	0.12	43,43,43,43	0
56	MG	2A	3199	1/1	0.89	0.21	46,46,46,46	0
56	MG	2a	3056	1/1	0.89	0.29	59,59,59,59	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	1A	3819	1/1	0.89	0.14	61,61,61,61	0
56	MG	2A	3426	1/1	0.89	0.45	45,45,45,45	0
56	MG	2A	3203	1/1	0.89	0.14	45,45,45,45	0
56	MG	1A	3326	1/1	0.89	0.14	51,51,51,51	0
56	MG	1A	3649	1/1	0.89	0.07	36,36,36,36	0
56	MG	2A	3438	1/1	0.89	0.18	30,30,30,30	0
56	MG	1A	3084	1/1	0.89	0.11	48,48,48,48	0
56	MG	2a	3069	1/1	0.89	0.19	53,53,53,53	0
56	MG	2A	3447	1/1	0.89	0.17	47,47,47,47	0
56	MG	1A	3234	1/1	0.89	0.13	44,44,44,44	0
56	MG	1A	3271	1/1	0.89	0.22	47,47,47,47	0
56	MG	1a	1647	1/1	0.89	0.09	49,49,49,49	0
56	MG	1a	1648	1/1	0.89	0.15	52,52,52,52	0
56	MG	2A	3484	1/1	0.89	0.10	44,44,44,44	0
56	MG	1A	3832	1/1	0.89	0.17	54,54,54,54	0
56	MG	1a	1652	1/1	0.89	0.23	51,51,51,51	0
56	MG	2A	3236	1/1	0.89	0.20	46,46,46,46	0
56	MG	2A	3245	1/1	0.89	0.17	46,46,46,46	0
56	MG	2A	3249	1/1	0.89	0.18	49,49,49,49	0
56	MG	2A	3254	1/1	0.89	0.16	40,40,40,40	0
56	MG	1A	3664	1/1	0.89	0.12	58,58,58,58	0
56	MG	1a	1655	1/1	0.89	0.19	56,56,56,56	0
56	MG	2A	3265	1/1	0.89	0.19	53,53,53,53	0
56	MG	1A	3345	1/1	0.89	0.16	50,50,50,50	0
56	MG	2a	3104	1/1	0.89	0.27	45,45,45,45	0
56	MG	1A	3273	1/1	0.89	0.13	59,59,59,59	0
56	MG	2A	3009	1/1	0.89	0.21	50,50,50,50	0
56	MG	1a	1660	1/1	0.89	0.09	48,48,48,48	0
56	MG	2A	3012	1/1	0.89	0.21	47,47,47,47	0
56	MG	1A	3479	1/1	0.89	0.07	41,41,41,41	0
56	MG	2A	3019	1/1	0.89	0.18	51,51,51,51	0
56	MG	2a	3113	1/1	0.89	0.26	59,59,59,59	0
56	MG	1A	3352	1/1	0.89	0.20	48,48,48,48	0
56	MG	2A	3023	1/1	0.89	0.15	45,45,45,45	0
56	MG	2A	3567	1/1	0.89	0.25	51,51,51,51	0
56	MG	2A	3024	1/1	0.89	0.24	49,49,49,49	0
56	MG	2a	3120	1/1	0.89	0.21	37,37,37,37	0
56	MG	2A	3025	1/1	0.89	0.10	53,53,53,53	0
56	MG	1a	1666	1/1	0.89	0.24	31,31,31,31	0
56	MG	1a	1669	1/1	0.89	0.18	38,38,38,38	0
56	MG	1A	3368	1/1	0.89	0.12	51,51,51,51	0
56	MG	1A	3117	1/1	0.89	0.17	46,46,46,46	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	2A	3328	1/1	0.89	0.24	57,57,57,57	0
56	MG	1A	3240	1/1	0.89	0.14	55,55,55,55	0
56	MG	2A	3057	1/1	0.89	0.15	44,44,44,44	0
56	MG	1A	3705	1/1	0.89	0.09	45,45,45,45	0
56	MG	1a	1688	1/1	0.89	0.24	61,61,61,61	0
56	MG	2A	3336	1/1	0.89	0.09	64,64,64,64	0
56	MG	2A	3337	1/1	0.89	0.14	56,56,56,56	0
56	MG	1A	3380	1/1	0.89	0.09	53,53,53,53	0
56	MG	1A	3158	1/1	0.89	0.35	36,36,36,36	0
56	MG	2B	208	1/1	0.89	0.08	68,68,68,68	0
56	MG	2A	3070	1/1	0.89	0.15	42,42,42,42	0
56	MG	1A	3243	1/1	0.89	0.22	46,46,46,46	0
56	MG	1E	305	1/1	0.89	0.16	52,52,52,52	0
56	MG	2x	103	1/1	0.89	0.18	51,51,51,51	0
56	MG	1A	3360	1/1	0.90	0.19	29,29,29,29	0
56	MG	2A	3071	1/1	0.90	0.12	46,46,46,46	0
56	MG	2A	3613	1/1	0.90	0.25	53,53,53,53	0
56	MG	1A	3257	1/1	0.90	0.12	52,52,52,52	0
56	MG	2A	3622	1/1	0.90	0.18	55,55,55,55	0
56	MG	2B	202	1/1	0.90	0.18	57,57,57,57	0
56	MG	2A	3335	1/1	0.90	0.11	58,58,58,58	0
56	MG	2B	207	1/1	0.90	0.09	57,57,57,57	0
56	MG	1A	3605	1/1	0.90	0.11	29,29,29,29	0
56	MG	2A	3087	1/1	0.90	0.26	53,53,53,53	0
56	MG	1A	3746	1/1	0.90	0.17	48,48,48,48	0
56	MG	1a	1713	1/1	0.90	0.20	50,50,50,50	0
56	MG	1A	3752	1/1	0.90	0.11	73,73,73,73	0
56	MG	1A	3614	1/1	0.90	0.10	47,47,47,47	0
56	MG	1V	201	1/1	0.90	0.07	38,38,38,38	0
56	MG	2A	3118	1/1	0.90	0.15	42,42,42,42	0
56	MG	2A	3121	1/1	0.90	0.16	47,47,47,47	0
56	MG	1A	3754	1/1	0.90	0.10	61,61,61,61	0
56	MG	23	102	1/1	0.90	0.08	50,50,50,50	0
56	MG	1A	3617	1/1	0.90	0.15	48,48,48,48	0
56	MG	11	102	1/1	0.90	0.17	37,37,37,37	0
56	MG	17	3101	1/1	0.90	0.09	33,33,33,33	0
56	MG	2a	3004	1/1	0.90	0.12	60,60,60,60	0
56	MG	2A	3136	1/1	0.90	0.12	24,24,24,24	0
56	MG	1A	3455	1/1	0.90	0.20	50,50,50,50	0
56	MG	1a	1730	1/1	0.90	0.20	67,67,67,67	0
56	MG	2A	3146	1/1	0.90	0.07	42,42,42,42	0
56	MG	2A	3367	1/1	0.90	0.12	52,52,52,52	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	18	103	1/1	0.90	0.25	62,62,62,62	0
56	MG	1a	1734	1/1	0.90	0.27	45,45,45,45	0
56	MG	2A	3373	1/1	0.90	0.14	34,34,34,34	0
56	MG	2A	3150	1/1	0.90	0.13	51,51,51,51	0
56	MG	1A	3228	1/1	0.90	0.15	59,59,59,59	0
56	MG	1A	3007	1/1	0.90	0.17	54,54,54,54	0
56	MG	1A	3377	1/1	0.90	0.12	61,61,61,61	0
56	MG	1A	3098	1/1	0.90	0.12	54,54,54,54	0
56	MG	2a	3035	1/1	0.90	0.21	61,61,61,61	0
56	MG	2A	3387	1/1	0.90	0.09	38,38,38,38	0
56	MG	2A	3158	1/1	0.90	0.06	50,50,50,50	0
56	MG	1A	3203	1/1	0.90	0.22	41,41,41,41	0
56	MG	1a	1613	1/1	0.90	0.12	51,51,51,51	0
56	MG	2A	3392	1/1	0.90	0.12	31,31,31,31	0
56	MG	1A	3313	1/1	0.90	0.20	34,34,34,34	0
56	MG	2A	3172	1/1	0.90	0.16	51,51,51,51	0
56	MG	1A	3043	1/1	0.90	0.20	45,45,45,45	0
56	MG	1A	3813	1/1	0.90	0.09	36,36,36,36	0
56	MG	1a	1625	1/1	0.90	0.14	52,52,52,52	0
56	MG	1A	3125	1/1	0.90	0.21	49,49,49,49	0
56	MG	2A	3183	1/1	0.90	0.13	50,50,50,50	0
56	MG	1a	1755	1/1	0.90	0.30	46,46,46,46	0
56	MG	1A	3172	1/1	0.90	0.09	52,52,52,52	0
56	MG	1A	3335	1/1	0.90	0.07	44,44,44,44	0
56	MG	1a	1758	1/1	0.90	0.34	49,49,49,49	0
56	MG	2A	3195	1/1	0.90	0.17	50,50,50,50	0
56	MG	2A	3425	1/1	0.90	0.31	41,41,41,41	0
56	MG	2a	3066	1/1	0.90	0.22	48,48,48,48	0
56	MG	1A	3502	1/1	0.90	0.22	30,30,30,30	0
56	MG	1a	1642	1/1	0.90	0.26	41,41,41,41	0
56	MG	1A	3401	1/1	0.90	0.20	55,55,55,55	0
56	MG	2a	3073	1/1	0.90	0.20	60,60,60,60	0
56	MG	1A	3829	1/1	0.90	0.09	54,54,54,54	0
56	MG	2A	3437	1/1	0.90	0.21	33,33,33,33	0
56	MG	1e	201	1/1	0.90	0.09	73,73,73,73	0
56	MG	1f	201	1/1	0.90	0.12	61,61,61,61	0
56	MG	1A	3506	1/1	0.90	0.10	41,41,41,41	0
56	MG	2A	3449	1/1	0.90	0.22	61,61,61,61	0
56	MG	2a	3087	1/1	0.90	0.20	67,67,67,67	0
56	MG	1x	103	1/1	0.90	0.21	55,55,55,55	0
56	MG	1A	3670	1/1	0.90	0.12	38,38,38,38	0
56	MG	1A	3673	1/1	0.90	0.11	64,64,64,64	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	1A	3127	1/1	0.90	0.12	52,52,52,52	0
56	MG	2A	3002	1/1	0.90	0.20	47,47,47,47	0
56	MG	1A	3129	1/1	0.90	0.07	45,45,45,45	0
56	MG	2a	3099	1/1	0.90	0.23	45,45,45,45	0
56	MG	2A	3232	1/1	0.90	0.28	63,63,63,63	0
56	MG	1A	3690	1/1	0.90	0.23	58,58,58,58	0
56	MG	1A	3845	1/1	0.90	0.33	47,47,47,47	0
56	MG	1A	3848	1/1	0.90	0.21	46,46,46,46	0
56	MG	1A	3341	1/1	0.90	0.14	54,54,54,54	0
56	MG	1A	3291	1/1	0.90	0.19	33,33,33,33	0
56	MG	2A	3020	1/1	0.90	0.23	40,40,40,40	0
56	MG	2A	3535	1/1	0.90	0.15	54,54,54,54	0
56	MG	1A	3694	1/1	0.90	0.13	40,40,40,40	0
56	MG	2A	3543	1/1	0.90	0.10	58,58,58,58	0
56	MG	1A	3143	1/1	0.90	0.08	41,41,41,41	0
56	MG	2A	3546	1/1	0.90	0.19	59,59,59,59	0
56	MG	2a	3116	1/1	0.90	0.23	51,51,51,51	0
56	MG	1A	3252	1/1	0.90	0.24	58,58,58,58	0
56	MG	1a	1673	1/1	0.90	0.29	47,47,47,47	0
56	MG	1A	3349	1/1	0.90	0.15	46,46,46,46	0
56	MG	1a	1678	1/1	0.90	0.06	45,45,45,45	0
56	MG	1A	3557	1/1	0.90	0.19	43,43,43,43	0
56	MG	2A	3040	1/1	0.90	0.28	55,55,55,55	0
56	MG	2a	3125	1/1	0.90	0.33	46,46,46,46	0
56	MG	2A	3042	1/1	0.90	0.13	31,31,31,31	0
56	MG	2A	3293	1/1	0.90	0.30	34,34,34,34	0
56	MG	2A	3299	1/1	0.90	0.11	46,46,46,46	0
56	MG	2A	3043	1/1	0.90	0.11	44,44,44,44	0
56	MG	2A	3308	1/1	0.90	0.16	55,55,55,55	0
56	MG	2A	3574	1/1	0.90	0.15	60,60,60,60	0
56	MG	2A	3584	1/1	0.90	0.13	78,78,78,78	0
56	MG	1A	3567	1/1	0.90	0.16	59,59,59,59	0
56	MG	1A	3432	1/1	0.90	0.22	40,40,40,40	0
56	MG	2A	3314	1/1	0.90	0.08	40,40,40,40	0
56	MG	1A	3582	1/1	0.90	0.08	72,72,72,72	0
56	MG	1A	3434	1/1	0.90	0.17	53,53,53,53	0
56	MG	2q	202	1/1	0.90	0.15	77,77,77,77	0
56	MG	2A	3598	1/1	0.90	0.14	49,49,49,49	0
56	MG	1A	3146	1/1	0.90	0.24	40,40,40,40	0
56	MG	1F	308	1/1	0.90	0.15	33,33,33,33	0
56	MG	2A	3065	1/1	0.90	0.16	57,57,57,57	0
56	MG	1A	3438	1/1	0.90	0.39	60,60,60,60	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	1A	3358	1/1	0.91	0.19	54,54,54,54	0
56	MG	1A	3225	1/1	0.91	0.16	35,35,35,35	0
56	MG	1A	3363	1/1	0.91	0.10	28,28,28,28	0
56	MG	2A	3621	1/1	0.91	0.10	58,58,58,58	0
56	MG	1A	3364	1/1	0.91	0.07	40,40,40,40	0
56	MG	1a	1619	1/1	0.91	0.28	53,53,53,53	0
56	MG	2B	203	1/1	0.91	0.14	46,46,46,46	0
56	MG	1A	3835	1/1	0.91	0.17	48,48,48,48	0
56	MG	1a	1743	1/1	0.91	0.28	34,34,34,34	0
56	MG	1A	3583	1/1	0.91	0.18	63,63,63,63	0
56	MG	1a	1747	1/1	0.91	0.26	46,46,46,46	0
56	MG	1A	3700	1/1	0.91	0.12	47,47,47,47	0
56	MG	2A	3353	1/1	0.91	0.14	30,30,30,30	0
56	MG	2E	303	1/1	0.91	0.10	42,42,42,42	0
56	MG	1A	3704	1/1	0.91	0.08	45,45,45,45	0
56	MG	1a	1633	1/1	0.91	0.22	56,56,56,56	0
56	MG	1A	3124	1/1	0.91	0.09	46,46,46,46	0
56	MG	1A	3196	1/1	0.91	0.14	44,44,44,44	0
56	MG	1a	1638	1/1	0.91	0.14	54,54,54,54	0
56	MG	1A	3079	1/1	0.91	0.07	32,32,32,32	0
56	MG	1B	210	1/1	0.91	0.11	41,41,41,41	0
56	MG	1a	1645	1/1	0.91	0.12	35,35,35,35	0
56	MG	2A	3160	1/1	0.91	0.15	56,56,56,56	0
56	MG	2a	3001	1/1	0.91	0.29	55,55,55,55	0
56	MG	1A	3714	1/1	0.91	0.18	51,51,51,51	0
56	MG	2A	3166	1/1	0.91	0.10	72,72,72,72	0
56	MG	2a	3005	1/1	0.91	0.12	52,52,52,52	0
56	MG	1a	1761	1/1	0.91	0.34	36,36,36,36	0
56	MG	1A	3595	1/1	0.91	0.10	56,56,56,56	0
56	MG	1A	3312	1/1	0.91	0.11	51,51,51,51	0
56	MG	2A	3378	1/1	0.91	0.26	57,57,57,57	0
56	MG	2A	3380	1/1	0.91	0.17	44,44,44,44	0
56	MG	1A	3126	1/1	0.91	0.25	48,48,48,48	0
56	MG	1A	3019	1/1	0.91	0.21	39,39,39,39	0
56	MG	1A	3160	1/1	0.91	0.09	34,34,34,34	0
56	MG	1h	201	1/1	0.91	0.20	54,54,54,54	0
56	MG	2a	3022	1/1	0.91	0.08	68,68,68,68	0
56	MG	2A	3180	1/1	0.91	0.09	48,48,48,48	0
56	MG	1A	3325	1/1	0.91	0.11	52,52,52,52	0
56	MG	1x	101	1/1	0.91	0.24	26,26,26,26	0
56	MG	1x	102	1/1	0.91	0.12	45,45,45,45	0
56	MG	1a	1658	1/1	0.91	0.14	59,59,59,59	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	1x	104	1/1	0.91	0.20	58,58,58,58	0
56	MG	2A	3192	1/1	0.91	0.12	43,43,43,43	0
56	MG	1A	3057	1/1	0.91	0.18	20,20,20,20	0
56	MG	2a	3045	1/1	0.91	0.20	49,49,49,49	0
56	MG	1A	3277	1/1	0.91	0.16	61,61,61,61	0
56	MG	1A	3740	1/1	0.91	0.19	49,49,49,49	0
56	MG	1a	1663	1/1	0.91	0.21	53,53,53,53	0
56	MG	2A	3411	1/1	0.91	0.26	46,46,46,46	0
56	MG	2A	3202	1/1	0.91	0.14	44,44,44,44	0
56	MG	1A	3396	1/1	0.91	0.22	43,43,43,43	0
56	MG	2A	3006	1/1	0.91	0.21	46,46,46,46	0
56	MG	1E	308	1/1	0.91	0.17	39,39,39,39	0
56	MG	1a	1667	1/1	0.91	0.28	49,49,49,49	0
56	MG	1A	3484	1/1	0.91	0.10	51,51,51,51	0
56	MG	2A	3428	1/1	0.91	0.20	50,50,50,50	0
56	MG	2a	3060	1/1	0.91	0.20	49,49,49,49	0
56	MG	1A	3242	1/1	0.91	0.06	43,43,43,43	0
56	MG	2A	3431	1/1	0.91	0.25	44,44,44,44	0
56	MG	1G	201	1/1	0.91	0.15	32,32,32,32	0
56	MG	1A	3400	1/1	0.91	0.14	54,54,54,54	0
56	MG	1A	3141	1/1	0.91	0.07	41,41,41,41	0
56	MG	2A	3219	1/1	0.91	0.18	47,47,47,47	0
56	MG	2A	3221	1/1	0.91	0.22	42,42,42,42	0
56	MG	1A	3142	1/1	0.91	0.20	29,29,29,29	0
56	MG	2A	3448	1/1	0.91	0.11	51,51,51,51	0
56	MG	2A	3225	1/1	0.91	0.16	51,51,51,51	0
56	MG	2A	3229	1/1	0.91	0.21	56,56,56,56	0
56	MG	2A	3460	1/1	0.91	0.12	56,56,56,56	0
56	MG	1A	3076	1/1	0.91	0.13	46,46,46,46	0
56	MG	1A	3059	1/1	0.91	0.19	58,58,58,58	0
56	MG	2A	3030	1/1	0.91	0.22	54,54,54,54	0
56	MG	1R	203	1/1	0.91	0.19	50,50,50,50	0
56	MG	2A	3485	1/1	0.91	0.11	58,58,58,58	0
56	MG	2A	3489	1/1	0.91	0.09	54,54,54,54	0
56	MG	1A	3224	1/1	0.91	0.11	33,33,33,33	0
56	MG	2A	3259	1/1	0.91	0.07	40,40,40,40	0
56	MG	2A	3497	1/1	0.91	0.17	45,45,45,45	0
56	MG	2a	3096	1/1	0.91	0.30	58,58,58,58	0
56	MG	2A	3500	1/1	0.91	0.08	58,58,58,58	0
56	MG	1A	3301	1/1	0.91	0.34	33,33,33,33	0
56	MG	2A	3039	1/1	0.91	0.06	42,42,42,42	0
56	MG	2A	3263	1/1	0.91	0.52	51,51,51,51	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	1A	3414	1/1	0.91	0.20	40,40,40,40	0
56	MG	2A	3517	1/1	0.91	0.09	49,49,49,49	0
56	MG	2A	3266	1/1	0.91	0.21	38,38,38,38	0
56	MG	1a	1696	1/1	0.91	0.23	51,51,51,51	0
56	MG	2A	3526	1/1	0.91	0.19	61,61,61,61	0
56	MG	1W	201	1/1	0.91	0.12	35,35,35,35	0
56	MG	2A	3273	1/1	0.91	0.32	47,47,47,47	0
56	MG	2A	3044	1/1	0.91	0.16	50,50,50,50	0
56	MG	1a	1698	1/1	0.91	0.24	42,42,42,42	0
56	MG	1A	3417	1/1	0.91	0.12	30,30,30,30	0
56	MG	1a	1703	1/1	0.91	0.21	48,48,48,48	0
56	MG	2A	3284	1/1	0.91	0.28	47,47,47,47	0
56	MG	1A	3792	1/1	0.91	0.10	25,25,25,25	0
56	MG	1Z	302	1/1	0.91	0.04	39,39,39,39	0
56	MG	10	104	1/1	0.91	0.42	42,42,42,42	0
56	MG	10	105	1/1	0.91	0.18	35,35,35,35	0
56	MG	2A	3303	1/1	0.91	0.15	48,48,48,48	0
56	MG	11	101	1/1	0.91	0.07	36,36,36,36	0
56	MG	1A	3669	1/1	0.91	0.15	38,38,38,38	0
56	MG	15	102	1/1	0.91	0.23	31,31,31,31	0
56	MG	1A	3420	1/1	0.91	0.24	41,41,41,41	0
56	MG	1a	1721	1/1	0.91	0.08	49,49,49,49	0
56	MG	2A	3575	1/1	0.91	0.10	48,48,48,48	0
56	MG	2a	3137	1/1	0.91	0.18	58,58,58,58	0
56	MG	2A	3315	1/1	0.91	0.22	51,51,51,51	0
56	MG	2A	3083	1/1	0.91	0.08	49,49,49,49	0
56	MG	1A	3811	1/1	0.91	0.21	17,17,17,17	0
56	MG	1A	3423	1/1	0.91	0.25	24,24,24,24	0
56	MG	1A	3675	1/1	0.91	0.24	59,59,59,59	0
56	MG	2A	3595	1/1	0.91	0.19	52,52,52,52	0
56	MG	2d	301	1/1	0.91	0.31	58,58,58,58	0
56	MG	1A	3678	1/1	0.91	0.08	35,35,35,35	0
56	MG	2A	3097	1/1	0.91	0.18	54,54,54,54	0
56	MG	2r	101	1/1	0.91	0.24	65,65,65,65	0
56	MG	2A	3330	1/1	0.91	0.13	50,50,50,50	0
56	MG	2A	3101	1/1	0.91	0.26	65,65,65,65	0
56	MG	1A	3549	1/1	0.91	0.13	54,54,54,54	0
56	MG	2A	3104	1/1	0.91	0.16	38,38,38,38	0
56	MG	1A	3256	1/1	0.91	0.11	49,49,49,49	0
56	MG	2A	3614	1/1	0.92	0.11	38,38,38,38	0
56	MG	2A	3164	1/1	0.92	0.07	35,35,35,35	0
56	MG	1n	101	1/1	0.92	0.20	45,45,45,45	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	1A	3457	1/1	0.92	0.37	45,45,45,45	0
56	MG	1O	201	1/1	0.92	0.17	43,43,43,43	0
56	MG	2A	3168	1/1	0.92	0.18	54,54,54,54	0
56	MG	1A	3574	1/1	0.92	0.11	61,61,61,61	0
56	MG	2A	3171	1/1	0.92	0.11	45,45,45,45	0
56	MG	1A	3676	1/1	0.92	0.31	67,67,67,67	0
56	MG	1A	3459	1/1	0.92	0.23	25,25,25,25	0
56	MG	1a	1670	1/1	0.92	0.22	34,34,34,34	0
56	MG	1A	3794	1/1	0.92	0.08	45,45,45,45	0
56	MG	1A	3080	1/1	0.92	0.17	45,45,45,45	0
56	MG	1A	3681	1/1	0.92	0.11	57,57,57,57	0
56	MG	1A	3685	1/1	0.92	0.07	56,56,56,56	0
56	MG	1a	1680	1/1	0.92	0.43	60,60,60,60	0
56	MG	1A	3159	1/1	0.92	0.14	37,37,37,37	0
56	MG	1a	1683	1/1	0.92	0.15	53,53,53,53	0
56	MG	2V	202	1/1	0.92	0.07	53,53,53,53	0
56	MG	2Y	201	1/1	0.92	0.22	41,41,41,41	0
56	MG	2A	3189	1/1	0.92	0.20	49,49,49,49	0
56	MG	1a	1684	1/1	0.92	0.09	51,51,51,51	0
56	MG	2A	3382	1/1	0.92	0.23	53,53,53,53	0
56	MG	27	101	1/1	0.92	0.13	44,44,44,44	0
56	MG	2A	3191	1/1	0.92	0.15	50,50,50,50	0
56	MG	1A	3817	1/1	0.92	0.07	47,47,47,47	0
56	MG	2A	3193	1/1	0.92	0.20	45,45,45,45	0
56	MG	1A	3131	1/1	0.92	0.10	32,32,32,32	0
56	MG	2A	3196	1/1	0.92	0.10	53,53,53,53	0
56	MG	10	102	1/1	0.92	0.07	49,49,49,49	0
56	MG	10	103	1/1	0.92	0.33	58,58,58,58	0
56	MG	1A	3167	1/1	0.92	0.14	63,63,63,63	0
56	MG	1A	3824	1/1	0.92	0.11	56,56,56,56	0
56	MG	2A	3396	1/1	0.92	0.23	52,52,52,52	0
56	MG	1A	3116	1/1	0.92	0.16	44,44,44,44	0
56	MG	2a	3015	1/1	0.92	0.18	63,63,63,63	0
56	MG	2A	3028	1/1	0.92	0.24	57,57,57,57	0
56	MG	1A	3315	1/1	0.92	0.10	46,46,46,46	0
56	MG	2A	3402	1/1	0.92	0.14	45,45,45,45	0
56	MG	2A	3404	1/1	0.92	0.25	38,38,38,38	0
56	MG	1A	3066	1/1	0.92	0.15	39,39,39,39	0
56	MG	2a	3024	1/1	0.92	0.28	59,59,59,59	0
56	MG	1A	3697	1/1	0.92	0.08	25,25,25,25	0
56	MG	17	3103	1/1	0.92	0.15	37,37,37,37	0
56	MG	2a	3031	1/1	0.92	0.12	46,46,46,46	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	2a	3032	1/1	0.92	0.14	56,56,56,56	0
56	MG	1A	3366	1/1	0.92	0.13	46,46,46,46	0
56	MG	2a	3034	1/1	0.92	0.33	57,57,57,57	0
56	MG	18	102	1/1	0.92	0.26	42,42,42,42	0
56	MG	2a	3036	1/1	0.92	0.14	58,58,58,58	0
56	MG	2a	3038	1/1	0.92	0.21	52,52,52,52	0
56	MG	2A	3414	1/1	0.92	0.15	45,45,45,45	0
56	MG	1a	1708	1/1	0.92	0.31	42,42,42,42	0
56	MG	2A	3218	1/1	0.92	0.26	49,49,49,49	0
56	MG	1A	3703	1/1	0.92	0.11	52,52,52,52	0
56	MG	1a	1601	1/1	0.92	0.19	61,61,61,61	0
56	MG	2A	3045	1/1	0.92	0.09	47,47,47,47	0
56	MG	1A	3492	1/1	0.92	0.14	50,50,50,50	0
56	MG	2A	3052	1/1	0.92	0.17	32,32,32,32	0
56	MG	1A	3609	1/1	0.92	0.08	37,37,37,37	0
56	MG	2a	3052	1/1	0.92	0.27	56,56,56,56	0
56	MG	2A	3234	1/1	0.92	0.13	41,41,41,41	0
56	MG	2A	3434	1/1	0.92	0.11	45,45,45,45	0
56	MG	2A	3235	1/1	0.92	0.11	48,48,48,48	0
56	MG	1a	1604	1/1	0.92	0.16	49,49,49,49	0
56	MG	2A	3237	1/1	0.92	0.23	57,57,57,57	0
56	MG	2A	3442	1/1	0.92	0.29	54,54,54,54	0
56	MG	2A	3238	1/1	0.92	0.11	45,45,45,45	0
56	MG	2A	3241	1/1	0.92	0.28	42,42,42,42	0
56	MG	2A	3242	1/1	0.92	0.14	57,57,57,57	0
56	MG	1A	3495	1/1	0.92	0.09	49,49,49,49	0
56	MG	2A	3061	1/1	0.92	0.21	46,46,46,46	0
56	MG	2A	3252	1/1	0.92	0.26	38,38,38,38	0
56	MG	1A	3048	1/1	0.92	0.18	50,50,50,50	0
56	MG	1a	1722	1/1	0.92	0.39	49,49,49,49	0
56	MG	2A	3473	1/1	0.92	0.11	35,35,35,35	0
56	MG	1A	3055	1/1	0.92	0.09	48,48,48,48	0
56	MG	2a	3076	1/1	0.92	0.38	48,48,48,48	0
56	MG	1A	3249	1/1	0.92	0.08	58,58,58,58	0
56	MG	2a	3079	1/1	0.92	0.28	52,52,52,52	0
56	MG	1A	3332	1/1	0.92	0.07	50,50,50,50	0
56	MG	1a	1727	1/1	0.92	0.37	54,54,54,54	0
56	MG	2A	3490	1/1	0.92	0.19	47,47,47,47	0
56	MG	1B	203	1/1	0.92	0.13	61,61,61,61	0
56	MG	2A	3493	1/1	0.92	0.14	45,45,45,45	0
56	MG	2A	3080	1/1	0.92	0.14	44,44,44,44	0
56	MG	2a	3089	1/1	0.92	0.16	57,57,57,57	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	1A	3727	1/1	0.92	0.09	30,30,30,30	0
56	MG	1A	3027	1/1	0.92	0.19	30,30,30,30	0
56	MG	2A	3505	1/1	0.92	0.18	59,59,59,59	0
56	MG	1a	1622	1/1	0.92	0.12	32,32,32,32	0
56	MG	2A	3507	1/1	0.92	0.12	68,68,68,68	0
56	MG	1a	1624	1/1	0.92	0.27	60,60,60,60	0
56	MG	2A	3278	1/1	0.92	0.23	23,23,23,23	0
56	MG	2A	3281	1/1	0.92	0.14	38,38,38,38	0
56	MG	1A	3013	1/1	0.92	0.17	34,34,34,34	0
56	MG	1A	3431	1/1	0.92	0.16	42,42,42,42	0
56	MG	1A	3385	1/1	0.92	0.20	38,38,38,38	0
56	MG	2A	3524	1/1	0.92	0.17	55,55,55,55	0
56	MG	2A	3099	1/1	0.92	0.21	44,44,44,44	0
56	MG	1a	1629	1/1	0.92	0.15	58,58,58,58	0
56	MG	1A	3193	1/1	0.92	0.27	34,34,34,34	0
56	MG	1A	3654	1/1	0.92	0.09	42,42,42,42	0
56	MG	2a	3109	1/1	0.92	0.22	60,60,60,60	0
56	MG	2a	3110	1/1	0.92	0.17	60,60,60,60	0
56	MG	1a	1635	1/1	0.92	0.29	57,57,57,57	0
56	MG	2A	3112	1/1	0.92	0.26	51,51,51,51	0
56	MG	2A	3114	1/1	0.92	0.11	46,46,46,46	0
56	MG	2a	3114	1/1	0.92	0.23	59,59,59,59	0
56	MG	2A	3115	1/1	0.92	0.07	53,53,53,53	0
56	MG	1A	3656	1/1	0.92	0.11	52,52,52,52	0
56	MG	1A	3340	1/1	0.92	0.20	49,49,49,49	0
56	MG	2A	3123	1/1	0.92	0.13	51,51,51,51	0
56	MG	1a	1641	1/1	0.92	0.15	57,57,57,57	0
56	MG	1D	306	1/1	0.92	0.17	47,47,47,47	0
56	MG	2A	3319	1/1	0.92	0.35	51,51,51,51	0
56	MG	2A	3322	1/1	0.92	0.22	44,44,44,44	0
56	MG	2A	3568	1/1	0.92	0.12	64,64,64,64	0
56	MG	2A	3323	1/1	0.92	0.11	50,50,50,50	0
56	MG	1D	308	1/1	0.92	0.18	41,41,41,41	0
56	MG	1E	303	1/1	0.92	0.17	33,33,33,33	0
56	MG	2A	3327	1/1	0.92	0.14	40,40,40,40	0
56	MG	2a	3135	1/1	0.92	0.19	64,64,64,64	0
56	MG	2A	3577	1/1	0.92	0.12	65,65,65,65	0
56	MG	1E	304	1/1	0.92	0.08	42,42,42,42	0
56	MG	1A	3390	1/1	0.92	0.10	50,50,50,50	0
56	MG	2A	3142	1/1	0.92	0.16	44,44,44,44	0
56	MG	1A	3062	1/1	0.92	0.11	28,28,28,28	0
56	MG	1A	3663	1/1	0.92	0.50	41,41,41,41	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	1A	3232	1/1	0.92	0.11	46,46,46,46	0
56	MG	1A	3551	1/1	0.92	0.09	30,30,30,30	0
56	MG	1A	3155	1/1	0.92	0.07	47,47,47,47	0
56	MG	2j	201	1/1	0.92	0.20	58,58,58,58	0
56	MG	1A	3456	1/1	0.92	0.43	49,49,49,49	0
56	MG	1A	3772	1/1	0.92	0.09	59,59,59,59	0
56	MG	1I	201	1/1	0.92	0.12	55,55,55,55	0
56	MG	1A	3563	1/1	0.92	0.19	57,57,57,57	0
56	MG	1l	202	1/1	0.92	0.20	53,53,53,53	0
56	MG	2A	3611	1/1	0.92	0.17	41,41,41,41	0
56	MG	1l	203	1/1	0.92	0.12	41,41,41,41	0
56	MG	2A	3161	1/1	0.92	0.10	48,48,48,48	0
56	MG	2x	104	1/1	0.92	0.26	41,41,41,41	0
59	K	2x	101	1/1	0.92	0.19	78,78,78,78	0
56	MG	2A	3111	1/1	0.93	0.20	38,38,38,38	0
56	MG	1A	3330	1/1	0.93	0.08	48,48,48,48	0
56	MG	1A	3052	1/1	0.93	0.17	47,47,47,47	0
56	MG	2A	3605	1/1	0.93	0.11	59,59,59,59	0
56	MG	1A	3200	1/1	0.93	0.12	46,46,46,46	0
56	MG	2A	3607	1/1	0.93	0.23	49,49,49,49	0
56	MG	2A	3609	1/1	0.93	0.17	42,42,42,42	0
56	MG	2A	3117	1/1	0.93	0.32	53,53,53,53	0
56	MG	1A	3604	1/1	0.93	0.15	51,51,51,51	0
56	MG	15	104	1/1	0.93	0.10	44,44,44,44	0
56	MG	1A	3202	1/1	0.93	0.23	38,38,38,38	0
56	MG	2A	3124	1/1	0.93	0.10	47,47,47,47	0
56	MG	2A	3619	1/1	0.93	0.17	35,35,35,35	0
56	MG	1A	3053	1/1	0.93	0.08	32,32,32,32	0
56	MG	17	3105	1/1	0.93	0.08	28,28,28,28	0
56	MG	1A	3206	1/1	0.93	0.16	32,32,32,32	0
56	MG	2A	3625	1/1	0.93	0.26	51,51,51,51	0
56	MG	2B	201	1/1	0.93	0.27	67,67,67,67	0
56	MG	2A	3131	1/1	0.93	0.14	53,53,53,53	0
56	MG	1A	3001	1/1	0.93	0.07	39,39,39,39	0
56	MG	1A	3265	1/1	0.93	0.11	45,45,45,45	0
56	MG	2B	206	1/1	0.93	0.28	64,64,64,64	0
56	MG	2A	3138	1/1	0.93	0.06	32,32,32,32	0
56	MG	1A	3623	1/1	0.93	0.10	65,65,65,65	0
56	MG	1A	3211	1/1	0.93	0.33	38,38,38,38	0
56	MG	1A	3442	1/1	0.93	0.25	36,36,36,36	0
56	MG	1A	3038	1/1	0.93	0.29	43,43,43,43	0
56	MG	2E	301	1/1	0.93	0.19	42,42,42,42	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	1A	3213	1/1	0.93	0.11	33,33,33,33	0
56	MG	1A	3272	1/1	0.93	0.10	42,42,42,42	0
56	MG	1A	3353	1/1	0.93	0.12	49,49,49,49	0
56	MG	1A	3026	1/1	0.93	0.09	45,45,45,45	0
56	MG	1a	1614	1/1	0.93	0.19	52,52,52,52	0
56	MG	2Q	201	1/1	0.93	0.15	57,57,57,57	0
56	MG	1A	3818	1/1	0.93	0.16	28,28,28,28	0
56	MG	2A	3361	1/1	0.93	0.11	49,49,49,49	0
56	MG	1a	1616	1/1	0.93	0.12	53,53,53,53	0
56	MG	1A	3653	1/1	0.93	0.33	43,43,43,43	0
56	MG	20	101	1/1	0.93	0.32	63,63,63,63	0
56	MG	1A	3041	1/1	0.93	0.09	38,38,38,38	0
56	MG	1a	1620	1/1	0.93	0.15	55,55,55,55	0
56	MG	2A	3162	1/1	0.93	0.13	68,68,68,68	0
56	MG	27	102	1/1	0.93	0.13	42,42,42,42	0
56	MG	1A	3014	1/1	0.93	0.07	24,24,24,24	0
56	MG	2A	3372	1/1	0.93	0.23	62,62,62,62	0
56	MG	1A	3219	1/1	0.93	0.08	48,48,48,48	0
56	MG	1A	3069	1/1	0.93	0.17	36,36,36,36	0
56	MG	1A	3661	1/1	0.93	0.10	47,47,47,47	0
56	MG	1A	3286	1/1	0.93	0.09	39,39,39,39	0
56	MG	2A	3169	1/1	0.93	0.10	42,42,42,42	0
56	MG	1A	3478	1/1	0.93	0.15	52,52,52,52	0
56	MG	1A	3831	1/1	0.93	0.18	71,71,71,71	0
56	MG	1a	1630	1/1	0.93	0.16	38,38,38,38	0
56	MG	1a	1632	1/1	0.93	0.14	49,49,49,49	0
56	MG	1A	3369	1/1	0.93	0.07	42,42,42,42	0
56	MG	1A	3165	1/1	0.93	0.12	29,29,29,29	0
56	MG	2A	3178	1/1	0.93	0.06	47,47,47,47	0
56	MG	2A	3390	1/1	0.93	0.17	46,46,46,46	0
56	MG	2a	3020	1/1	0.93	0.14	49,49,49,49	0
56	MG	1A	3482	1/1	0.93	0.13	37,37,37,37	0
56	MG	1A	3090	1/1	0.93	0.07	27,27,27,27	0
56	MG	1A	3128	1/1	0.93	0.19	51,51,51,51	0
56	MG	1A	3173	1/1	0.93	0.12	52,52,52,52	0
56	MG	2a	3026	1/1	0.93	0.13	54,54,54,54	0
56	MG	2a	3028	1/1	0.93	0.20	49,49,49,49	0
56	MG	1A	3382	1/1	0.93	0.27	57,57,57,57	0
56	MG	2A	3186	1/1	0.93	0.14	52,52,52,52	0
56	MG	1a	1643	1/1	0.93	0.07	45,45,45,45	0
56	MG	1A	3498	1/1	0.93	0.11	47,47,47,47	0
56	MG	1A	3677	1/1	0.93	0.07	50,50,50,50	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	1B	209	1/1	0.93	0.07	48,48,48,48	0
56	MG	1x	109	1/1	0.93	0.23	60,60,60,60	0
56	MG	2a	3037	1/1	0.93	0.07	57,57,57,57	0
56	MG	1A	3174	1/1	0.93	0.12	41,41,41,41	0
56	MG	2A	3408	1/1	0.93	0.32	43,43,43,43	0
56	MG	2a	3041	1/1	0.93	0.33	58,58,58,58	0
56	MG	1A	3299	1/1	0.93	0.12	31,31,31,31	0
56	MG	2A	3003	1/1	0.93	0.14	45,45,45,45	0
56	MG	1a	1651	1/1	0.93	0.18	44,44,44,44	0
56	MG	1A	3680	1/1	0.93	0.14	38,38,38,38	0
56	MG	1a	1653	1/1	0.93	0.18	42,42,42,42	0
56	MG	1A	3070	1/1	0.93	0.07	32,32,32,32	0
56	MG	2A	3420	1/1	0.93	0.28	42,42,42,42	0
56	MG	2a	3050	1/1	0.93	0.21	31,31,31,31	0
56	MG	1A	3130	1/1	0.93	0.10	54,54,54,54	0
56	MG	2A	3204	1/1	0.93	0.21	50,50,50,50	0
56	MG	2A	3014	1/1	0.93	0.16	56,56,56,56	0
56	MG	1A	3504	1/1	0.93	0.11	49,49,49,49	0
56	MG	1B	220	1/1	0.93	0.11	53,53,53,53	0
56	MG	1A	3303	1/1	0.93	0.20	58,58,58,58	0
56	MG	1A	3391	1/1	0.93	0.32	35,35,35,35	0
56	MG	1A	3029	1/1	0.93	0.16	47,47,47,47	0
56	MG	1A	3235	1/1	0.93	0.05	15,15,15,15	0
56	MG	2A	3436	1/1	0.93	0.23	40,40,40,40	0
56	MG	2a	3062	1/1	0.93	0.22	62,62,62,62	0
56	MG	1A	3236	1/1	0.93	0.17	45,45,45,45	0
56	MG	2A	3026	1/1	0.93	0.15	60,60,60,60	0
56	MG	2A	3441	1/1	0.93	0.26	21,21,21,21	0
56	MG	2A	3027	1/1	0.93	0.15	34,34,34,34	0
56	MG	1E	302	1/1	0.93	0.12	34,34,34,34	0
56	MG	2a	3068	1/1	0.93	0.25	48,48,48,48	0
56	MG	1A	3398	1/1	0.93	0.24	48,48,48,48	0
56	MG	1A	3180	1/1	0.93	0.10	38,38,38,38	0
56	MG	1A	3181	1/1	0.93	0.10	34,34,34,34	0
56	MG	1A	3104	1/1	0.93	0.10	54,54,54,54	0
56	MG	1A	3402	1/1	0.93	0.14	46,46,46,46	0
56	MG	2A	3463	1/1	0.93	0.11	47,47,47,47	0
56	MG	2a	3080	1/1	0.93	0.26	37,37,37,37	0
56	MG	1A	3403	1/1	0.93	0.22	56,56,56,56	0
56	MG	2A	3041	1/1	0.93	0.06	35,35,35,35	0
56	MG	1F	302	1/1	0.93	0.09	45,45,45,45	0
56	MG	1A	3711	1/1	0.93	0.18	42,42,42,42	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	1A	3562	1/1	0.93	0.10	61,61,61,61	0
56	MG	1A	3713	1/1	0.93	0.13	51,51,51,51	0
56	MG	2a	3088	1/1	0.93	0.17	48,48,48,48	0
56	MG	2A	3486	1/1	0.93	0.10	41,41,41,41	0
56	MG	2A	3243	1/1	0.93	0.19	54,54,54,54	0
56	MG	2A	3048	1/1	0.93	0.28	58,58,58,58	0
56	MG	2A	3246	1/1	0.93	0.20	45,45,45,45	0
56	MG	2A	3248	1/1	0.93	0.10	40,40,40,40	0
56	MG	1G	204	1/1	0.93	0.21	44,44,44,44	0
56	MG	2A	3250	1/1	0.93	0.20	38,38,38,38	0
56	MG	2A	3498	1/1	0.93	0.15	50,50,50,50	0
56	MG	2A	3251	1/1	0.93	0.12	50,50,50,50	0
56	MG	1A	3107	1/1	0.93	0.12	29,29,29,29	0
56	MG	2A	3253	1/1	0.93	0.17	63,63,63,63	0
56	MG	2A	3053	1/1	0.93	0.31	53,53,53,53	0
56	MG	1A	3565	1/1	0.93	0.14	45,45,45,45	0
56	MG	1A	3317	1/1	0.93	0.12	46,46,46,46	0
56	MG	1A	3717	1/1	0.93	0.11	33,33,33,33	0
56	MG	2A	3262	1/1	0.93	0.17	46,46,46,46	0
56	MG	2A	3518	1/1	0.93	0.16	55,55,55,55	0
56	MG	1A	3719	1/1	0.93	0.11	50,50,50,50	0
56	MG	2A	3522	1/1	0.93	0.09	41,41,41,41	0
56	MG	1Q	201	1/1	0.93	0.20	34,34,34,34	0
56	MG	1A	3725	1/1	0.93	0.09	32,32,32,32	0
56	MG	1A	3572	1/1	0.93	0.10	71,71,71,71	0
56	MG	2A	3067	1/1	0.93	0.11	55,55,55,55	0
56	MG	1A	3189	1/1	0.93	0.14	44,44,44,44	0
56	MG	2A	3538	1/1	0.93	0.08	44,44,44,44	0
56	MG	1a	1699	1/1	0.93	0.23	27,27,27,27	0
56	MG	1A	3319	1/1	0.93	0.09	52,52,52,52	0
56	MG	2A	3073	1/1	0.93	0.09	43,43,43,43	0
56	MG	2A	3549	1/1	0.93	0.10	57,57,57,57	0
56	MG	2A	3076	1/1	0.93	0.14	43,43,43,43	0
56	MG	1a	1702	1/1	0.93	0.16	42,42,42,42	0
56	MG	1A	3411	1/1	0.93	0.44	54,54,54,54	0
56	MG	2A	3555	1/1	0.93	0.13	37,37,37,37	0
56	MG	1a	1704	1/1	0.93	0.28	41,41,41,41	0
56	MG	2a	3129	1/1	0.93	0.09	46,46,46,46	0
56	MG	2A	3558	1/1	0.93	0.15	46,46,46,46	0
56	MG	2A	3285	1/1	0.93	0.22	36,36,36,36	0
56	MG	2A	3562	1/1	0.93	0.13	53,53,53,53	0
56	MG	2A	3286	1/1	0.93	0.21	29,29,29,29	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	1A	3320	1/1	0.93	0.25	59,59,59,59	0
56	MG	2A	3290	1/1	0.93	0.23	36,36,36,36	0
56	MG	2A	3084	1/1	0.93	0.12	68,68,68,68	0
56	MG	1A	3110	1/1	0.93	0.15	42,42,42,42	0
56	MG	1W	203	1/1	0.93	0.15	48,48,48,48	0
56	MG	1A	3589	1/1	0.93	0.09	67,67,67,67	0
56	MG	2A	3095	1/1	0.93	0.11	38,38,38,38	0
56	MG	1a	1711	1/1	0.93	0.17	48,48,48,48	0
56	MG	1A	3144	1/1	0.93	0.05	34,34,34,34	0
56	MG	2k	201	1/1	0.93	0.08	63,63,63,63	0
56	MG	2l	201	1/1	0.93	0.09	43,43,43,43	0
56	MG	2A	3578	1/1	0.93	0.14	60,60,60,60	0
56	MG	1A	3592	1/1	0.93	0.10	27,27,27,27	0
56	MG	1A	3593	1/1	0.93	0.10	34,34,34,34	0
56	MG	1A	3747	1/1	0.93	0.13	65,65,65,65	0
56	MG	2A	3316	1/1	0.93	0.22	44,44,44,44	0
56	MG	2A	3103	1/1	0.93	0.30	57,57,57,57	0
56	MG	1A	3248	1/1	0.93	0.09	49,49,49,49	0
56	MG	2A	3596	1/1	0.93	0.26	50,50,50,50	0
56	MG	2A	3106	1/1	0.93	0.13	33,33,33,33	0
56	MG	1a	1720	1/1	0.93	0.18	54,54,54,54	0
56	MG	2A	3600	1/1	0.94	0.13	43,43,43,43	0
56	MG	1A	3452	1/1	0.94	0.20	44,44,44,44	0
56	MG	1A	3183	1/1	0.94	0.21	55,55,55,55	0
56	MG	2A	3320	1/1	0.94	0.11	45,45,45,45	0
56	MG	2A	3604	1/1	0.94	0.11	51,51,51,51	0
56	MG	13	102	1/1	0.94	0.10	40,40,40,40	0
56	MG	1A	3287	1/1	0.94	0.19	44,44,44,44	0
56	MG	2A	3324	1/1	0.94	0.18	53,53,53,53	0
56	MG	1A	3773	1/1	0.94	0.09	69,69,69,69	0
56	MG	2A	3122	1/1	0.94	0.19	54,54,54,54	0
56	MG	15	105	1/1	0.94	0.18	37,37,37,37	0
56	MG	1a	1731	1/1	0.94	0.20	34,34,34,34	0
56	MG	2A	3125	1/1	0.94	0.19	49,49,49,49	0
56	MG	1A	3231	1/1	0.94	0.18	53,53,53,53	0
56	MG	2A	3331	1/1	0.94	0.23	42,42,42,42	0
56	MG	1A	3777	1/1	0.94	0.07	45,45,45,45	0
56	MG	2A	3129	1/1	0.94	0.06	42,42,42,42	0
56	MG	17	3104	1/1	0.94	0.17	39,39,39,39	0
56	MG	1A	3778	1/1	0.94	0.07	35,35,35,35	0
56	MG	2A	3132	1/1	0.94	0.25	58,58,58,58	0
56	MG	1A	3458	1/1	0.94	0.34	45,45,45,45	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	18	101	1/1	0.94	0.08	39,39,39,39	0
56	MG	2B	204	1/1	0.94	0.07	62,62,62,62	0
56	MG	1a	1741	1/1	0.94	0.31	46,46,46,46	0
56	MG	1A	3365	1/1	0.94	0.16	30,30,30,30	0
56	MG	2A	3141	1/1	0.94	0.07	39,39,39,39	0
56	MG	1A	3148	1/1	0.94	0.17	38,38,38,38	0
56	MG	1A	3119	1/1	0.94	0.08	44,44,44,44	0
56	MG	1a	1745	1/1	0.94	0.28	44,44,44,44	0
56	MG	1A	3793	1/1	0.94	0.10	40,40,40,40	0
56	MG	1A	3463	1/1	0.94	0.07	44,44,44,44	0
56	MG	2E	302	1/1	0.94	0.16	29,29,29,29	0
56	MG	2A	3149	1/1	0.94	0.27	55,55,55,55	0
56	MG	2E	304	1/1	0.94	0.27	52,52,52,52	0
56	MG	1A	3089	1/1	0.94	0.39	51,51,51,51	0
56	MG	2A	3151	1/1	0.94	0.42	53,53,53,53	0
56	MG	2F	303	1/1	0.94	0.15	56,56,56,56	0
56	MG	2A	3358	1/1	0.94	0.18	43,43,43,43	0
56	MG	1A	3034	1/1	0.94	0.14	41,41,41,41	0
56	MG	2P	202	1/1	0.94	0.11	34,34,34,34	0
56	MG	1A	3036	1/1	0.94	0.18	42,42,42,42	0
56	MG	2R	201	1/1	0.94	0.08	31,31,31,31	0
56	MG	2A	3362	1/1	0.94	0.19	30,30,30,30	0
56	MG	2T	202	1/1	0.94	0.22	50,50,50,50	0
56	MG	2A	3363	1/1	0.94	0.18	43,43,43,43	0
56	MG	2W	201	1/1	0.94	0.10	45,45,45,45	0
56	MG	1A	3237	1/1	0.94	0.06	45,45,45,45	0
56	MG	1A	3814	1/1	0.94	0.11	39,39,39,39	0
56	MG	1A	3816	1/1	0.94	0.10	55,55,55,55	0
56	MG	2I	101	1/1	0.94	0.18	62,62,62,62	0
56	MG	1A	3012	1/1	0.94	0.07	38,38,38,38	0
56	MG	1A	3381	1/1	0.94	0.15	45,45,45,45	0
56	MG	1a	1617	1/1	0.94	0.20	47,47,47,47	0
56	MG	2A	3163	1/1	0.94	0.24	30,30,30,30	0
56	MG	1A	3199	1/1	0.94	0.11	74,74,74,74	0
56	MG	1A	3305	1/1	0.94	0.08	32,32,32,32	0
56	MG	2a	3002	1/1	0.94	0.10	55,55,55,55	0
56	MG	1A	3306	1/1	0.94	0.30	48,48,48,48	0
56	MG	1A	3387	1/1	0.94	0.20	42,42,42,42	0
56	MG	1A	3101	1/1	0.94	0.09	36,36,36,36	0
56	MG	2A	3379	1/1	0.94	0.31	34,34,34,34	0
56	MG	1e	202	1/1	0.94	0.15	47,47,47,47	0
56	MG	2A	3381	1/1	0.94	0.16	44,44,44,44	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	1A	3665	1/1	0.94	0.06	33,33,33,33	0
56	MG	2a	3010	1/1	0.94	0.17	44,44,44,44	0
56	MG	1A	3102	1/1	0.94	0.08	42,42,42,42	0
56	MG	2A	3385	1/1	0.94	0.18	53,53,53,53	0
56	MG	2a	3014	1/1	0.94	0.17	35,35,35,35	0
56	MG	1a	1626	1/1	0.94	0.08	35,35,35,35	0
56	MG	1A	3161	1/1	0.94	0.22	36,36,36,36	0
56	MG	1A	3204	1/1	0.94	0.17	25,25,25,25	0
56	MG	2A	3175	1/1	0.94	0.09	44,44,44,44	0
56	MG	1A	3205	1/1	0.94	0.18	27,27,27,27	0
56	MG	1v	101	1/1	0.94	0.30	41,41,41,41	0
56	MG	1A	3247	1/1	0.94	0.06	46,46,46,46	0
56	MG	2A	3393	1/1	0.94	0.23	30,30,30,30	0
56	MG	1A	3836	1/1	0.94	0.17	45,45,45,45	0
56	MG	2A	3181	1/1	0.94	0.04	57,57,57,57	0
56	MG	1A	3028	1/1	0.94	0.07	44,44,44,44	0
56	MG	1A	3208	1/1	0.94	0.23	41,41,41,41	0
56	MG	2a	3030	1/1	0.94	0.07	56,56,56,56	0
56	MG	1A	3250	1/1	0.94	0.20	30,30,30,30	0
56	MG	1A	3527	1/1	0.94	0.09	23,23,23,23	0
56	MG	1x	108	1/1	0.94	0.21	44,44,44,44	0
56	MG	2A	3403	1/1	0.94	0.07	48,48,48,48	0
56	MG	2A	3188	1/1	0.94	0.14	56,56,56,56	0
56	MG	1A	3009	1/1	0.94	0.16	33,33,33,33	0
56	MG	1a	1639	1/1	0.94	0.12	40,40,40,40	0
56	MG	1z	101	1/1	0.94	0.20	49,49,49,49	0
56	MG	2a	3039	1/1	0.94	0.12	58,58,58,58	0
56	MG	1a	1640	1/1	0.94	0.08	42,42,42,42	0
56	MG	1A	3847	1/1	0.94	0.12	36,36,36,36	0
56	MG	1A	3531	1/1	0.94	0.09	46,46,46,46	0
56	MG	1B	201	1/1	0.94	0.06	31,31,31,31	0
56	MG	1B	202	1/1	0.94	0.14	30,30,30,30	0
56	MG	1A	3534	1/1	0.94	0.12	54,54,54,54	0
56	MG	1A	3683	1/1	0.94	0.13	55,55,55,55	0
56	MG	1A	3171	1/1	0.94	0.11	49,49,49,49	0
56	MG	2A	3423	1/1	0.94	0.25	34,34,34,34	0
56	MG	1A	3032	1/1	0.94	0.23	44,44,44,44	0
56	MG	1A	3689	1/1	0.94	0.06	43,43,43,43	0
56	MG	2A	3205	1/1	0.94	0.11	40,40,40,40	0
56	MG	1A	3137	1/1	0.94	0.11	33,33,33,33	0
56	MG	2A	3430	1/1	0.94	0.23	20,20,20,20	0
56	MG	1A	3138	1/1	0.94	0.13	36,36,36,36	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	1A	3547	1/1	0.94	0.15	47,47,47,47	0
56	MG	2A	3433	1/1	0.94	0.26	47,47,47,47	0
56	MG	1A	3260	1/1	0.94	0.21	48,48,48,48	0
56	MG	1A	3112	1/1	0.94	0.11	36,36,36,36	0
56	MG	1A	3333	1/1	0.94	0.24	37,37,37,37	0
56	MG	2A	3214	1/1	0.94	0.22	36,36,36,36	0
56	MG	1A	3409	1/1	0.94	0.15	38,38,38,38	0
56	MG	2A	3216	1/1	0.94	0.19	41,41,41,41	0
56	MG	1A	3558	1/1	0.94	0.08	49,49,49,49	0
56	MG	1a	1661	1/1	0.94	0.05	45,45,45,45	0
56	MG	2A	3031	1/1	0.94	0.05	44,44,44,44	0
56	MG	1A	3561	1/1	0.94	0.08	26,26,26,26	0
56	MG	1A	3266	1/1	0.94	0.11	47,47,47,47	0
56	MG	1A	3412	1/1	0.94	0.07	28,28,28,28	0
56	MG	2A	3451	1/1	0.94	0.11	45,45,45,45	0
56	MG	2A	3455	1/1	0.94	0.07	39,39,39,39	0
56	MG	2A	3227	1/1	0.94	0.11	28,28,28,28	0
56	MG	2A	3228	1/1	0.94	0.40	45,45,45,45	0
56	MG	1A	3710	1/1	0.94	0.06	50,50,50,50	0
56	MG	1A	3336	1/1	0.94	0.11	53,53,53,53	0
56	MG	1A	3566	1/1	0.94	0.12	38,38,38,38	0
56	MG	2a	3083	1/1	0.94	0.24	40,40,40,40	0
56	MG	1A	3267	1/1	0.94	0.29	61,61,61,61	0
56	MG	1A	3570	1/1	0.94	0.12	48,48,48,48	0
56	MG	1A	3338	1/1	0.94	0.13	39,39,39,39	0
56	MG	1a	1674	1/1	0.94	0.15	48,48,48,48	0
56	MG	1A	3573	1/1	0.94	0.07	53,53,53,53	0
56	MG	1F	307	1/1	0.94	0.18	45,45,45,45	0
56	MG	1A	3046	1/1	0.94	0.27	46,46,46,46	0
56	MG	1F	312	1/1	0.94	0.21	46,46,46,46	0
56	MG	1A	3422	1/1	0.94	0.16	27,27,27,27	0
56	MG	1G	202	1/1	0.94	0.19	37,37,37,37	0
56	MG	1A	3218	1/1	0.94	0.14	39,39,39,39	0
56	MG	1a	1687	1/1	0.94	0.16	37,37,37,37	0
56	MG	1A	3177	1/1	0.94	0.14	53,53,53,53	0
56	MG	2a	3098	1/1	0.94	0.18	45,45,45,45	0
56	MG	1A	3584	1/1	0.94	0.09	40,40,40,40	0
56	MG	1A	3731	1/1	0.94	0.07	65,65,65,65	0
56	MG	2A	3066	1/1	0.94	0.12	51,51,51,51	0
56	MG	2A	3513	1/1	0.94	0.10	57,57,57,57	0
56	MG	1a	1693	1/1	0.94	0.23	34,34,34,34	0
56	MG	1A	3733	1/1	0.94	0.11	34,34,34,34	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	1A	3428	1/1	0.94	0.38	58,58,58,58	0
56	MG	1A	3178	1/1	0.94	0.10	54,54,54,54	0
56	MG	1A	3344	1/1	0.94	0.14	32,32,32,32	0
56	MG	1A	3082	1/1	0.94	0.08	44,44,44,44	0
56	MG	1A	3018	1/1	0.94	0.20	48,48,48,48	0
56	MG	2A	3078	1/1	0.94	0.06	54,54,54,54	0
56	MG	1A	3435	1/1	0.94	0.24	45,45,45,45	0
56	MG	2A	3272	1/1	0.94	0.20	46,46,46,46	0
56	MG	1U	202	1/1	0.94	0.09	32,32,32,32	0
56	MG	1U	203	1/1	0.94	0.18	41,41,41,41	0
56	MG	2A	3541	1/1	0.94	0.20	38,38,38,38	0
56	MG	2A	3275	1/1	0.94	0.14	56,56,56,56	0
56	MG	1A	3049	1/1	0.94	0.27	47,47,47,47	0
56	MG	2A	3085	1/1	0.94	0.14	42,42,42,42	0
56	MG	2A	3280	1/1	0.94	0.17	49,49,49,49	0
56	MG	2a	3121	1/1	0.94	0.25	48,48,48,48	0
56	MG	2A	3086	1/1	0.94	0.10	36,36,36,36	0
56	MG	2A	3551	1/1	0.94	0.10	57,57,57,57	0
56	MG	1A	3744	1/1	0.94	0.11	22,22,22,22	0
56	MG	1V	204	1/1	0.94	0.06	44,44,44,44	0
56	MG	1a	1707	1/1	0.94	0.24	37,37,37,37	0
56	MG	2A	3091	1/1	0.94	0.12	34,34,34,34	0
56	MG	1A	3745	1/1	0.94	0.19	51,51,51,51	0
56	MG	2A	3559	1/1	0.94	0.11	64,64,64,64	0
56	MG	2a	3133	1/1	0.94	0.24	55,55,55,55	0
56	MG	1A	3351	1/1	0.94	0.15	49,49,49,49	0
56	MG	1a	1710	1/1	0.94	0.45	55,55,55,55	0
56	MG	2A	3098	1/1	0.94	0.26	35,35,35,35	0
56	MG	2A	3292	1/1	0.94	0.24	32,32,32,32	0
56	MG	1A	3226	1/1	0.94	0.18	47,47,47,47	0
56	MG	2A	3297	1/1	0.94	0.29	57,57,57,57	0
56	MG	2a	3141	1/1	0.94	0.22	46,46,46,46	0
56	MG	1X	102	1/1	0.94	0.10	58,58,58,58	0
56	MG	2a	3143	1/1	0.94	0.12	49,49,49,49	0
56	MG	2A	3301	1/1	0.94	0.23	47,47,47,47	0
56	MG	2A	3572	1/1	0.94	0.11	56,56,56,56	0
56	MG	2A	3302	1/1	0.94	0.19	42,42,42,42	0
56	MG	1A	3283	1/1	0.94	0.14	53,53,53,53	0
56	MG	2A	3304	1/1	0.94	0.25	49,49,49,49	0
56	MG	1Y	201	1/1	0.94	0.05	61,61,61,61	0
56	MG	2l	202	1/1	0.94	0.08	44,44,44,44	0
56	MG	2A	3307	1/1	0.94	0.21	31,31,31,31	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	1A	3182	1/1	0.94	0.12	47,47,47,47	0
56	MG	2A	3310	1/1	0.94	0.11	44,44,44,44	0
56	MG	2A	3311	1/1	0.94	0.26	54,54,54,54	0
56	MG	2A	3105	1/1	0.94	0.09	37,37,37,37	0
56	MG	1A	3449	1/1	0.94	0.20	45,45,45,45	0
56	MG	1A	3759	1/1	0.94	0.07	50,50,50,50	0
56	MG	1A	3760	1/1	0.94	0.12	50,50,50,50	0
56	MG	1A	3613	1/1	0.94	0.08	27,27,27,27	0
57	ZN	24	501	1/1	0.94	0.09	130,130,130,130	0
56	MG	2A	3113	1/1	0.94	0.19	68,68,68,68	0
56	MG	2A	3213	1/1	0.95	0.23	55,55,55,55	0
56	MG	14	101	1/1	0.95	0.28	56,56,56,56	0
56	MG	1A	3051	1/1	0.95	0.09	43,43,43,43	0
56	MG	2D	301	1/1	0.95	0.06	35,35,35,35	0
56	MG	1A	3217	1/1	0.95	0.11	53,53,53,53	0
56	MG	1A	3833	1/1	0.95	0.17	56,56,56,56	0
56	MG	2A	3068	1/1	0.95	0.18	44,44,44,44	0
56	MG	1A	3834	1/1	0.95	0.14	39,39,39,39	0
56	MG	1A	3606	1/1	0.95	0.20	32,32,32,32	0
56	MG	1a	1714	1/1	0.95	0.22	32,32,32,32	0
56	MG	2A	3224	1/1	0.95	0.23	48,48,48,48	0
56	MG	1A	3134	1/1	0.95	0.11	32,32,32,32	0
56	MG	2A	3226	1/1	0.95	0.19	27,27,27,27	0
56	MG	1A	3610	1/1	0.95	0.08	35,35,35,35	0
56	MG	2A	3400	1/1	0.95	0.13	38,38,38,38	0
56	MG	1A	3838	1/1	0.95	0.11	36,36,36,36	0
56	MG	1a	1718	1/1	0.95	0.12	53,53,53,53	0
56	MG	2A	3230	1/1	0.95	0.17	46,46,46,46	0
56	MG	2A	3079	1/1	0.95	0.12	53,53,53,53	0
56	MG	1A	3612	1/1	0.95	0.06	34,34,34,34	0
56	MG	2A	3081	1/1	0.95	0.16	57,57,57,57	0
56	MG	1A	3424	1/1	0.95	0.17	31,31,31,31	0
56	MG	1A	3136	1/1	0.95	0.05	32,32,32,32	0
56	MG	1A	3327	1/1	0.95	0.14	41,41,41,41	0
56	MG	1A	3720	1/1	0.95	0.11	49,49,49,49	0
56	MG	1A	3328	1/1	0.95	0.07	34,34,34,34	0
56	MG	1A	3726	1/1	0.95	0.07	36,36,36,36	0
56	MG	2A	3417	1/1	0.95	0.13	27,27,27,27	0
56	MG	2A	3418	1/1	0.95	0.19	37,37,37,37	0
56	MG	2A	3244	1/1	0.95	0.13	46,46,46,46	0
56	MG	1A	3620	1/1	0.95	0.15	29,29,29,29	0
56	MG	1A	3220	1/1	0.95	0.07	48,48,48,48	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	2A	3422	1/1	0.95	0.17	34,34,34,34	0
56	MG	2A	3247	1/1	0.95	0.25	50,50,50,50	0
56	MG	1a	1607	1/1	0.95	0.17	47,47,47,47	0
56	MG	2A	3092	1/1	0.95	0.13	49,49,49,49	0
56	MG	1a	1609	1/1	0.95	0.21	41,41,41,41	0
56	MG	1a	1610	1/1	0.95	0.16	28,28,28,28	0
56	MG	1B	204	1/1	0.95	0.12	38,38,38,38	0
56	MG	1B	205	1/1	0.95	0.21	53,53,53,53	0
56	MG	1B	208	1/1	0.95	0.12	55,55,55,55	0
56	MG	2A	3256	1/1	0.95	0.10	46,46,46,46	0
56	MG	2A	3100	1/1	0.95	0.10	34,34,34,34	0
56	MG	1A	3624	1/1	0.95	0.13	60,60,60,60	0
56	MG	1A	3293	1/1	0.95	0.12	41,41,41,41	0
56	MG	1B	211	1/1	0.95	0.27	39,39,39,39	0
56	MG	1A	3524	1/1	0.95	0.06	51,51,51,51	0
56	MG	2a	3021	1/1	0.95	0.10	68,68,68,68	0
56	MG	2A	3439	1/1	0.95	0.25	47,47,47,47	0
56	MG	2A	3440	1/1	0.95	0.28	38,38,38,38	0
56	MG	1A	3190	1/1	0.95	0.19	37,37,37,37	0
56	MG	1B	214	1/1	0.95	0.18	45,45,45,45	0
56	MG	2A	3108	1/1	0.95	0.10	55,55,55,55	0
56	MG	1A	3639	1/1	0.95	0.08	67,67,67,67	0
56	MG	2A	3110	1/1	0.95	0.11	49,49,49,49	0
56	MG	1B	217	1/1	0.95	0.08	43,43,43,43	0
56	MG	1a	1623	1/1	0.95	0.20	56,56,56,56	0
56	MG	1A	3010	1/1	0.95	0.07	42,42,42,42	0
56	MG	1A	3436	1/1	0.95	0.22	36,36,36,36	0
56	MG	1A	3095	1/1	0.95	0.07	37,37,37,37	0
56	MG	2A	3279	1/1	0.95	0.26	27,27,27,27	0
56	MG	1A	3298	1/1	0.95	0.14	55,55,55,55	0
56	MG	2A	3467	1/1	0.95	0.06	33,33,33,33	0
56	MG	1A	3651	1/1	0.95	0.07	41,41,41,41	0
56	MG	2A	3472	1/1	0.95	0.10	33,33,33,33	0
56	MG	1A	3140	1/1	0.95	0.11	37,37,37,37	0
56	MG	1D	303	1/1	0.95	0.09	55,55,55,55	0
56	MG	2a	3042	1/1	0.95	0.12	51,51,51,51	0
56	MG	1D	305	1/1	0.95	0.12	43,43,43,43	0
56	MG	1A	3541	1/1	0.95	0.09	30,30,30,30	0
56	MG	1A	3542	1/1	0.95	0.08	36,36,36,36	0
56	MG	2A	3287	1/1	0.95	0.12	38,38,38,38	0
56	MG	1a	1762	1/1	0.95	0.12	50,50,50,50	0
56	MG	2A	3491	1/1	0.95	0.20	36,36,36,36	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	1E	301	1/1	0.95	0.16	49,49,49,49	0
56	MG	1A	3657	1/1	0.95	0.07	45,45,45,45	0
56	MG	2A	3494	1/1	0.95	0.07	50,50,50,50	0
56	MG	1A	3198	1/1	0.95	0.06	41,41,41,41	0
56	MG	1A	3443	1/1	0.95	0.22	33,33,33,33	0
56	MG	2A	3294	1/1	0.95	0.30	51,51,51,51	0
56	MG	2A	3295	1/1	0.95	0.25	38,38,38,38	0
56	MG	2A	3504	1/1	0.95	0.08	43,43,43,43	0
56	MG	2A	3296	1/1	0.95	0.18	44,44,44,44	0
56	MG	1A	3169	1/1	0.95	0.20	50,50,50,50	0
56	MG	2A	3133	1/1	0.95	0.13	47,47,47,47	0
56	MG	2A	3508	1/1	0.95	0.20	53,53,53,53	0
56	MG	1A	3447	1/1	0.95	0.18	47,47,47,47	0
56	MG	1f	202	1/1	0.95	0.13	54,54,54,54	0
56	MG	2A	3137	1/1	0.95	0.15	54,54,54,54	0
56	MG	1A	3448	1/1	0.95	0.05	17,17,17,17	0
56	MG	1A	3394	1/1	0.95	0.25	42,42,42,42	0
56	MG	2A	3306	1/1	0.95	0.19	35,35,35,35	0
56	MG	1F	301	1/1	0.95	0.13	52,52,52,52	0
56	MG	1A	3555	1/1	0.95	0.12	35,35,35,35	0
56	MG	2a	3070	1/1	0.95	0.26	43,43,43,43	0
56	MG	2a	3071	1/1	0.95	0.23	44,44,44,44	0
56	MG	1F	303	1/1	0.95	0.15	36,36,36,36	0
56	MG	2A	3144	1/1	0.95	0.14	35,35,35,35	0
56	MG	2a	3074	1/1	0.95	0.18	40,40,40,40	0
56	MG	1A	3096	1/1	0.95	0.08	41,41,41,41	0
56	MG	2a	3077	1/1	0.95	0.26	46,46,46,46	0
56	MG	2A	3530	1/1	0.95	0.06	39,39,39,39	0
56	MG	1a	1649	1/1	0.95	0.13	51,51,51,51	0
56	MG	1A	3304	1/1	0.95	0.14	41,41,41,41	0
56	MG	1A	3047	1/1	0.95	0.09	49,49,49,49	0
56	MG	2A	3540	1/1	0.95	0.15	39,39,39,39	0
56	MG	1F	311	1/1	0.95	0.14	47,47,47,47	0
56	MG	2A	3542	1/1	0.95	0.10	50,50,50,50	0
56	MG	1A	3042	1/1	0.95	0.21	33,33,33,33	0
56	MG	2A	3544	1/1	0.95	0.15	54,54,54,54	0
56	MG	1A	3071	1/1	0.95	0.15	38,38,38,38	0
56	MG	1A	3779	1/1	0.95	0.07	33,33,33,33	0
56	MG	2A	3548	1/1	0.95	0.13	67,67,67,67	0
56	MG	1A	3780	1/1	0.95	0.14	64,64,64,64	0
56	MG	1A	3348	1/1	0.95	0.23	34,34,34,34	0
56	MG	1A	3103	1/1	0.95	0.13	25,25,25,25	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	1A	3056	1/1	0.95	0.15	33,33,33,33	0
56	MG	2A	3553	1/1	0.95	0.11	62,62,62,62	0
56	MG	2a	3095	1/1	0.95	0.29	57,57,57,57	0
56	MG	1A	3789	1/1	0.95	0.11	29,29,29,29	0
56	MG	1A	3790	1/1	0.95	0.08	34,34,34,34	0
56	MG	1A	3310	1/1	0.95	0.09	46,46,46,46	0
56	MG	2A	3007	1/1	0.95	0.15	49,49,49,49	0
56	MG	1A	3464	1/1	0.95	0.06	59,59,59,59	0
56	MG	1A	3466	1/1	0.95	0.10	45,45,45,45	0
56	MG	1A	3106	1/1	0.95	0.20	35,35,35,35	0
56	MG	1a	1668	1/1	0.95	0.21	31,31,31,31	0
56	MG	2A	3564	1/1	0.95	0.07	47,47,47,47	0
56	MG	1R	204	1/1	0.95	0.28	51,51,51,51	0
56	MG	2A	3018	1/1	0.95	0.05	44,44,44,44	0
56	MG	1R	206	1/1	0.95	0.17	34,34,34,34	0
56	MG	1A	3471	1/1	0.95	0.15	44,44,44,44	0
56	MG	1T	202	1/1	0.95	0.07	43,43,43,43	0
56	MG	2A	3022	1/1	0.95	0.18	43,43,43,43	0
56	MG	1A	3805	1/1	0.95	0.07	54,54,54,54	0
56	MG	1A	3808	1/1	0.95	0.10	45,45,45,45	0
56	MG	2A	3342	1/1	0.95	0.19	21,21,21,21	0
56	MG	1A	3579	1/1	0.95	0.06	41,41,41,41	0
56	MG	1a	1679	1/1	0.95	0.21	47,47,47,47	0
56	MG	2A	3581	1/1	0.95	0.07	81,81,81,81	0
56	MG	1A	3472	1/1	0.95	0.12	27,27,27,27	0
56	MG	1V	203	1/1	0.95	0.21	41,41,41,41	0
56	MG	2A	3348	1/1	0.95	0.19	30,30,30,30	0
56	MG	2A	3182	1/1	0.95	0.24	58,58,58,58	0
56	MG	1a	1682	1/1	0.95	0.25	35,35,35,35	0
56	MG	2A	3593	1/1	0.95	0.19	45,45,45,45	0
56	MG	2A	3594	1/1	0.95	0.15	42,42,42,42	0
56	MG	2A	3354	1/1	0.95	0.10	46,46,46,46	0
56	MG	1A	3356	1/1	0.95	0.17	45,45,45,45	0
56	MG	1A	3815	1/1	0.95	0.10	30,30,30,30	0
56	MG	1A	3005	1/1	0.95	0.13	53,53,53,53	0
56	MG	1A	3086	1/1	0.95	0.11	33,33,33,33	0
56	MG	2A	3038	1/1	0.95	0.05	54,54,54,54	0
56	MG	2a	3134	1/1	0.95	0.22	58,58,58,58	0
56	MG	2A	3360	1/1	0.95	0.15	32,32,32,32	0
56	MG	1W	205	1/1	0.95	0.07	38,38,38,38	0
56	MG	1X	101	1/1	0.95	0.08	35,35,35,35	0
56	MG	1A	3410	1/1	0.95	0.29	45,45,45,45	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	1A	3314	1/1	0.95	0.26	38,38,38,38	0
56	MG	1A	3820	1/1	0.95	0.19	41,41,41,41	0
56	MG	1Z	301	1/1	0.95	0.08	41,41,41,41	0
56	MG	1A	3153	1/1	0.95	0.06	33,33,33,33	0
56	MG	2A	3047	1/1	0.95	0.15	52,52,52,52	0
56	MG	2A	3369	1/1	0.95	0.17	58,58,58,58	0
56	MG	2A	3198	1/1	0.95	0.27	47,47,47,47	0
56	MG	2A	3371	1/1	0.95	0.16	34,34,34,34	0
56	MG	2A	3615	1/1	0.95	0.18	59,59,59,59	0
56	MG	2A	3618	1/1	0.95	0.09	54,54,54,54	0
56	MG	10	101	1/1	0.95	0.07	41,41,41,41	0
56	MG	2A	3050	1/1	0.95	0.10	30,30,30,30	0
56	MG	2A	3374	1/1	0.95	0.34	47,47,47,47	0
56	MG	1A	3822	1/1	0.95	0.14	40,40,40,40	0
56	MG	1A	3050	1/1	0.95	0.28	49,49,49,49	0
56	MG	1A	3487	1/1	0.95	0.10	47,47,47,47	0
56	MG	1A	3156	1/1	0.95	0.26	51,51,51,51	0
56	MG	2A	3056	1/1	0.95	0.15	52,52,52,52	0
56	MG	1A	3494	1/1	0.95	0.07	24,24,24,24	0
56	MG	2A	3059	1/1	0.95	0.15	44,44,44,44	0
56	MG	1A	3157	1/1	0.95	0.10	46,46,46,46	0
56	MG	12	101	1/1	0.95	0.05	37,37,37,37	0
56	MG	1A	3602	1/1	0.95	0.07	56,56,56,56	0
56	MG	2A	3220	1/1	0.96	0.18	33,33,33,33	0
56	MG	1A	3075	1/1	0.96	0.14	28,28,28,28	0
56	MG	2A	3222	1/1	0.96	0.04	47,47,47,47	0
56	MG	1A	3645	1/1	0.96	0.08	50,50,50,50	0
56	MG	1V	202	1/1	0.96	0.33	34,34,34,34	0
56	MG	1A	3039	1/1	0.96	0.17	44,44,44,44	0
56	MG	1A	3499	1/1	0.96	0.16	23,23,23,23	0
56	MG	2A	3398	1/1	0.96	0.23	52,52,52,52	0
56	MG	1A	3343	1/1	0.96	0.12	34,34,34,34	0
56	MG	2B	212	1/1	0.96	0.19	49,49,49,49	0
56	MG	1A	3650	1/1	0.96	0.09	29,29,29,29	0
56	MG	2D	302	1/1	0.96	0.14	32,32,32,32	0
56	MG	1A	3246	1/1	0.96	0.11	34,34,34,34	0
56	MG	1A	3797	1/1	0.96	0.08	34,34,34,34	0
56	MG	2A	3231	1/1	0.96	0.19	50,50,50,50	0
56	MG	1W	206	1/1	0.96	0.06	25,25,25,25	0
56	MG	2E	305	1/1	0.96	0.18	32,32,32,32	0
56	MG	2A	3405	1/1	0.96	0.20	47,47,47,47	0
56	MG	1A	3799	1/1	0.96	0.06	49,49,49,49	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	0.96	0.08	54,54,54,54	0
56	MG	1A	3008	1/1	0.96	0.06	22,22,22,22	0
56	MG	2A	3074	1/1	0.96	0.09	57,57,57,57	0
56	MG	1A	3346	1/1	0.96	0.15	22,22,22,22	0
56	MG	2A	3412	1/1	0.96	0.10	34,34,34,34	0
56	MG	2A	3239	1/1	0.96	0.11	56,56,56,56	0
56	MG	2A	3240	1/1	0.96	0.30	41,41,41,41	0
56	MG	1A	3806	1/1	0.96	0.05	32,32,32,32	0
56	MG	1A	3060	1/1	0.96	0.11	40,40,40,40	0
56	MG	1A	3505	1/1	0.96	0.13	48,48,48,48	0
56	MG	1A	3061	1/1	0.96	0.18	32,32,32,32	0
56	MG	1A	3300	1/1	0.96	0.10	30,30,30,30	0
56	MG	1A	3516	1/1	0.96	0.07	25,25,25,25	0
56	MG	1A	3517	1/1	0.96	0.05	43,43,43,43	0
56	MG	23	101	1/1	0.96	0.07	45,45,45,45	0
56	MG	1A	3520	1/1	0.96	0.08	37,37,37,37	0
56	MG	25	101	1/1	0.96	0.14	43,43,43,43	0
56	MG	1A	3419	1/1	0.96	0.18	18,18,18,18	0
56	MG	1A	3132	1/1	0.96	0.24	40,40,40,40	0
56	MG	2A	3427	1/1	0.96	0.33	42,42,42,42	0
56	MG	1A	3251	1/1	0.96	0.15	48,48,48,48	0
56	MG	2A	3088	1/1	0.96	0.11	35,35,35,35	0
56	MG	12	102	1/1	0.96	0.15	50,50,50,50	0
56	MG	1A	3133	1/1	0.96	0.03	31,31,31,31	0
56	MG	2A	3255	1/1	0.96	0.07	65,65,65,65	0
56	MG	13	103	1/1	0.96	0.06	38,38,38,38	0
56	MG	2A	3257	1/1	0.96	0.34	51,51,51,51	0
56	MG	1A	3533	1/1	0.96	0.09	27,27,27,27	0
56	MG	1A	3354	1/1	0.96	0.10	40,40,40,40	0
56	MG	15	103	1/1	0.96	0.15	41,41,41,41	0
56	MG	1A	3672	1/1	0.96	0.17	46,46,46,46	0
56	MG	2a	3011	1/1	0.96	0.14	62,62,62,62	0
56	MG	1A	3355	1/1	0.96	0.36	45,45,45,45	0
56	MG	2A	3264	1/1	0.96	0.19	47,47,47,47	0
56	MG	1a	1726	1/1	0.96	0.16	39,39,39,39	0
56	MG	1A	3674	1/1	0.96	0.08	58,58,58,58	0
56	MG	17	3102	1/1	0.96	0.07	27,27,27,27	0
56	MG	2A	3445	1/1	0.96	0.15	48,48,48,48	0
56	MG	2A	3446	1/1	0.96	0.11	35,35,35,35	0
56	MG	2a	3019	1/1	0.96	0.16	55,55,55,55	0
56	MG	2A	3269	1/1	0.96	0.18	26,26,26,26	0
56	MG	1A	3253	1/1	0.96	0.09	44,44,44,44	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	1A	3429	1/1	0.96	0.20	31,31,31,31	0
56	MG	1A	3021	1/1	0.96	0.14	37,37,37,37	0
56	MG	1a	1733	1/1	0.96	0.20	25,25,25,25	0
56	MG	2A	3452	1/1	0.96	0.14	48,48,48,48	0
56	MG	1A	3135	1/1	0.96	0.10	38,38,38,38	0
56	MG	2A	3458	1/1	0.96	0.15	42,42,42,42	0
56	MG	2A	3459	1/1	0.96	0.16	46,46,46,46	0
56	MG	2A	3107	1/1	0.96	0.06	51,51,51,51	0
56	MG	1A	3362	1/1	0.96	0.24	46,46,46,46	0
56	MG	1A	3433	1/1	0.96	0.08	41,41,41,41	0
56	MG	1A	3191	1/1	0.96	0.19	41,41,41,41	0
56	MG	18	104	1/1	0.96	0.13	18,18,18,18	0
56	MG	1A	3682	1/1	0.96	0.05	39,39,39,39	0
56	MG	1A	3223	1/1	0.96	0.06	41,41,41,41	0
56	MG	2A	3474	1/1	0.96	0.10	41,41,41,41	0
56	MG	2A	3481	1/1	0.96	0.06	47,47,47,47	0
56	MG	2A	3482	1/1	0.96	0.09	52,52,52,52	0
56	MG	1A	3684	1/1	0.96	0.07	30,30,30,30	0
56	MG	1A	3840	1/1	0.96	0.18	59,59,59,59	0
56	MG	2A	3116	1/1	0.96	0.10	49,49,49,49	0
56	MG	1A	3552	1/1	0.96	0.06	14,14,14,14	0
56	MG	1a	1746	1/1	0.96	0.26	34,34,34,34	0
56	MG	2A	3119	1/1	0.96	0.12	42,42,42,42	0
56	MG	1A	3686	1/1	0.96	0.07	61,61,61,61	0
56	MG	1A	3843	1/1	0.96	0.15	43,43,43,43	0
56	MG	1a	1749	1/1	0.96	0.24	31,31,31,31	0
56	MG	1A	3063	1/1	0.96	0.06	32,32,32,32	0
56	MG	1A	3263	1/1	0.96	0.26	38,38,38,38	0
56	MG	2A	3496	1/1	0.96	0.14	41,41,41,41	0
56	MG	1a	1611	1/1	0.96	0.12	49,49,49,49	0
56	MG	1A	3556	1/1	0.96	0.07	48,48,48,48	0
56	MG	2A	3298	1/1	0.96	0.25	44,44,44,44	0
56	MG	1a	1754	1/1	0.96	0.24	49,49,49,49	0
56	MG	1A	3367	1/1	0.96	0.11	41,41,41,41	0
56	MG	1A	3162	1/1	0.96	0.17	36,36,36,36	0
56	MG	2a	3058	1/1	0.96	0.35	53,53,53,53	0
56	MG	1A	3559	1/1	0.96	0.09	44,44,44,44	0
56	MG	1A	3440	1/1	0.96	0.23	46,46,46,46	0
56	MG	2A	3510	1/1	0.96	0.11	56,56,56,56	0
56	MG	2A	3134	1/1	0.96	0.10	37,37,37,37	0
56	MG	1A	3441	1/1	0.96	0.14	32,32,32,32	0
56	MG	2A	3514	1/1	0.96	0.09	44,44,44,44	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	1a	1760	1/1	0.96	0.25	37,37,37,37	0
56	MG	1A	3698	1/1	0.96	0.08	34,34,34,34	0
56	MG	2A	3309	1/1	0.96	0.08	65,65,65,65	0
56	MG	1B	207	1/1	0.96	0.13	44,44,44,44	0
56	MG	1A	3064	1/1	0.96	0.05	58,58,58,58	0
56	MG	1A	3166	1/1	0.96	0.16	40,40,40,40	0
56	MG	1A	3444	1/1	0.96	0.06	33,33,33,33	0
56	MG	1d	301	1/1	0.96	0.29	57,57,57,57	0
56	MG	2A	3525	1/1	0.96	0.17	45,45,45,45	0
56	MG	1A	3268	1/1	0.96	0.15	43,43,43,43	0
56	MG	2a	3075	1/1	0.96	0.09	39,39,39,39	0
56	MG	2A	3527	1/1	0.96	0.09	44,44,44,44	0
56	MG	2A	3145	1/1	0.96	0.09	44,44,44,44	0
56	MG	2A	3533	1/1	0.96	0.14	44,44,44,44	0
56	MG	2A	3534	1/1	0.96	0.10	36,36,36,36	0
56	MG	1A	3375	1/1	0.96	0.24	44,44,44,44	0
56	MG	1A	3709	1/1	0.96	0.10	41,41,41,41	0
56	MG	1A	3376	1/1	0.96	0.12	25,25,25,25	0
56	MG	1A	3229	1/1	0.96	0.09	46,46,46,46	0
56	MG	1A	3450	1/1	0.96	0.07	34,34,34,34	0
56	MG	1A	3379	1/1	0.96	0.18	38,38,38,38	0
56	MG	1A	3577	1/1	0.96	0.06	61,61,61,61	0
56	MG	1a	1631	1/1	0.96	0.17	56,56,56,56	0
56	MG	1s	101	1/1	0.96	0.21	55,55,55,55	0
56	MG	1A	3453	1/1	0.96	0.27	48,48,48,48	0
56	MG	1A	3454	1/1	0.96	0.18	56,56,56,56	0
56	MG	1A	3316	1/1	0.96	0.19	45,45,45,45	0
56	MG	1A	3035	1/1	0.96	0.06	33,33,33,33	0
56	MG	1D	302	1/1	0.96	0.07	32,32,32,32	0
56	MG	1A	3067	1/1	0.96	0.13	40,40,40,40	0
56	MG	1A	3201	1/1	0.96	0.12	40,40,40,40	0
56	MG	1A	3384	1/1	0.96	0.15	41,41,41,41	0
56	MG	1A	3170	1/1	0.96	0.20	33,33,33,33	0
56	MG	1A	3323	1/1	0.96	0.22	48,48,48,48	0
56	MG	1A	3030	1/1	0.96	0.21	32,32,32,32	0
56	MG	1A	3045	1/1	0.96	0.09	46,46,46,46	0
56	MG	1A	3465	1/1	0.96	0.07	26,26,26,26	0
56	MG	2A	3561	1/1	0.96	0.09	51,51,51,51	0
56	MG	1a	1646	1/1	0.96	0.21	42,42,42,42	0
56	MG	1A	3092	1/1	0.96	0.12	36,36,36,36	0
56	MG	1A	3278	1/1	0.96	0.10	46,46,46,46	0
56	MG	1A	3603	1/1	0.96	0.04	55,55,55,55	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	1A	3470	1/1	0.96	0.17	40,40,40,40	0
56	MG	2A	3011	1/1	0.96	0.17	28,28,28,28	0
56	MG	1A	3392	1/1	0.96	0.12	23,23,23,23	0
56	MG	2A	3349	1/1	0.96	0.09	33,33,33,33	0
56	MG	2A	3350	1/1	0.96	0.14	42,42,42,42	0
56	MG	1A	3282	1/1	0.96	0.09	40,40,40,40	0
56	MG	2A	3352	1/1	0.96	0.19	44,44,44,44	0
56	MG	1A	3329	1/1	0.96	0.22	34,34,34,34	0
56	MG	1F	304	1/1	0.96	0.16	38,38,38,38	0
56	MG	1F	305	1/1	0.96	0.13	40,40,40,40	0
56	MG	2A	3579	1/1	0.96	0.10	68,68,68,68	0
56	MG	2A	3580	1/1	0.96	0.06	31,31,31,31	0
56	MG	1a	1656	1/1	0.96	0.21	44,44,44,44	0
56	MG	2A	3583	1/1	0.96	0.12	63,63,63,63	0
56	MG	1A	3054	1/1	0.96	0.11	55,55,55,55	0
56	MG	1A	3037	1/1	0.96	0.17	27,27,27,27	0
56	MG	2a	3124	1/1	0.96	0.25	56,56,56,56	0
56	MG	2A	3586	1/1	0.96	0.08	50,50,50,50	0
56	MG	1A	3073	1/1	0.96	0.13	30,30,30,30	0
56	MG	1A	3751	1/1	0.96	0.10	53,53,53,53	0
56	MG	2a	3128	1/1	0.96	0.27	47,47,47,47	0
56	MG	1A	3334	1/1	0.96	0.13	34,34,34,34	0
56	MG	1A	3615	1/1	0.96	0.08	31,31,31,31	0
56	MG	1A	3210	1/1	0.96	0.28	48,48,48,48	0
56	MG	1a	1664	1/1	0.96	0.08	31,31,31,31	0
56	MG	2A	3029	1/1	0.96	0.16	38,38,38,38	0
56	MG	1G	203	1/1	0.96	0.06	53,53,53,53	0
56	MG	1A	3288	1/1	0.96	0.18	52,52,52,52	0
56	MG	2A	3599	1/1	0.96	0.11	45,45,45,45	0
56	MG	1A	3485	1/1	0.96	0.07	34,34,34,34	0
56	MG	1A	3761	1/1	0.96	0.06	48,48,48,48	0
56	MG	1A	3622	1/1	0.96	0.07	39,39,39,39	0
56	MG	1A	3149	1/1	0.96	0.10	58,58,58,58	0
56	MG	1a	1671	1/1	0.96	0.26	34,34,34,34	0
56	MG	1A	3488	1/1	0.96	0.07	47,47,47,47	0
56	MG	1P	201	1/1	0.96	0.13	36,36,36,36	0
56	MG	1A	3290	1/1	0.96	0.26	45,45,45,45	0
56	MG	1A	3628	1/1	0.96	0.06	68,68,68,68	0
56	MG	2f	201	1/1	0.96	0.06	54,54,54,54	0
56	MG	1Q	203	1/1	0.96	0.14	24,24,24,24	0
56	MG	1A	3629	1/1	0.96	0.14	54,54,54,54	0
56	MG	2A	3046	1/1	0.96	0.13	36,36,36,36	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	1R	202	1/1	0.96	0.08	52,52,52,52	0
56	MG	1A	3776	1/1	0.96	0.07	34,34,34,34	0
56	MG	1A	3630	1/1	0.96	0.07	33,33,33,33	0
56	MG	2A	3383	1/1	0.96	0.19	25,25,25,25	0
56	MG	1A	3023	1/1	0.96	0.24	42,42,42,42	0
56	MG	1A	3292	1/1	0.96	0.05	33,33,33,33	0
56	MG	1A	3496	1/1	0.96	0.09	58,58,58,58	0
56	MG	1U	201	1/1	0.96	0.15	42,42,42,42	0
56	MG	2A	3624	1/1	0.96	0.04	34,34,34,34	0
56	MG	1A	3640	1/1	0.96	0.07	30,30,30,30	0
56	MG	1a	1689	1/1	0.96	0.32	48,48,48,48	0
56	MG	1A	3642	1/1	0.96	0.07	21,21,21,21	0
56	MG	1P	203	1/1	0.97	0.27	25,25,25,25	0
56	MG	1P	204	1/1	0.97	0.19	44,44,44,44	0
56	MG	1P	205	1/1	0.97	0.05	36,36,36,36	0
56	MG	1A	3701	1/1	0.97	0.07	47,47,47,47	0
56	MG	1A	3702	1/1	0.97	0.05	31,31,31,31	0
56	MG	1A	3087	1/1	0.97	0.08	23,23,23,23	0
56	MG	1A	3625	1/1	0.97	0.08	24,24,24,24	0
56	MG	1R	201	1/1	0.97	0.07	42,42,42,42	0
56	MG	1A	3626	1/1	0.97	0.08	28,28,28,28	0
56	MG	1A	3554	1/1	0.97	0.05	25,25,25,25	0
56	MG	1A	3114	1/1	0.97	0.11	37,37,37,37	0
56	MG	1A	3359	1/1	0.97	0.24	49,49,49,49	0
56	MG	1S	201	1/1	0.97	0.06	58,58,58,58	0
56	MG	2A	3233	1/1	0.97	0.17	45,45,45,45	0
56	MG	1A	3100	1/1	0.97	0.07	51,51,51,51	0
56	MG	2A	3529	1/1	0.97	0.12	41,41,41,41	0
56	MG	1A	3631	1/1	0.97	0.04	69,69,69,69	0
56	MG	2A	3531	1/1	0.97	0.15	31,31,31,31	0
56	MG	1A	3361	1/1	0.97	0.10	46,46,46,46	0
56	MG	1A	3635	1/1	0.97	0.06	53,53,53,53	0
56	MG	1l	201	1/1	0.97	0.04	56,56,56,56	0
56	MG	2a	3027	1/1	0.97	0.16	47,47,47,47	0
56	MG	1A	3637	1/1	0.97	0.12	58,58,58,58	0
56	MG	1U	204	1/1	0.97	0.11	43,43,43,43	0
56	MG	2A	3539	1/1	0.97	0.09	68,68,68,68	0
56	MG	1A	3088	1/1	0.97	0.15	41,41,41,41	0
56	MG	1A	3022	1/1	0.97	0.07	29,29,29,29	0
56	MG	1A	3489	1/1	0.97	0.10	19,19,19,19	0
56	MG	1A	3275	1/1	0.97	0.18	55,55,55,55	0
56	MG	1A	3723	1/1	0.97	0.13	20,20,20,20	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	1V	205	1/1	0.97	0.09	47,47,47,47	0
56	MG	2A	3120	1/1	0.97	0.11	39,39,39,39	0
56	MG	2A	3547	1/1	0.97	0.10	56,56,56,56	0
56	MG	1A	3724	1/1	0.97	0.05	26,26,26,26	0
56	MG	1W	202	1/1	0.97	0.23	40,40,40,40	0
56	MG	1A	3564	1/1	0.97	0.07	20,20,20,20	0
56	MG	1A	3644	1/1	0.97	0.06	41,41,41,41	0
56	MG	1A	3168	1/1	0.97	0.06	50,50,50,50	0
56	MG	1A	3185	1/1	0.97	0.19	34,34,34,34	0
56	MG	2A	3127	1/1	0.97	0.20	44,44,44,44	0
56	MG	1A	3730	1/1	0.97	0.15	39,39,39,39	0
56	MG	1A	3647	1/1	0.97	0.06	59,59,59,59	0
56	MG	1A	3732	1/1	0.97	0.08	40,40,40,40	0
56	MG	2A	3258	1/1	0.97	0.17	32,32,32,32	0
56	MG	1A	3186	1/1	0.97	0.09	53,53,53,53	0
56	MG	1a	1676	1/1	0.97	0.04	46,46,46,46	0
56	MG	1A	3568	1/1	0.97	0.19	47,47,47,47	0
56	MG	1A	3569	1/1	0.97	0.06	43,43,43,43	0
56	MG	1A	3846	1/1	0.97	0.16	30,30,30,30	0
56	MG	1A	3279	1/1	0.97	0.06	33,33,33,33	0
56	MG	1A	3405	1/1	0.97	0.18	43,43,43,43	0
56	MG	1A	3280	1/1	0.97	0.18	34,34,34,34	0
56	MG	2A	3013	1/1	0.97	0.12	24,24,24,24	0
56	MG	2A	3569	1/1	0.97	0.15	41,41,41,41	0
56	MG	2A	3268	1/1	0.97	0.15	19,19,19,19	0
56	MG	1A	3370	1/1	0.97	0.05	39,39,39,39	0
56	MG	1a	1685	1/1	0.97	0.16	53,53,53,53	0
56	MG	1A	3281	1/1	0.97	0.08	45,45,45,45	0
56	MG	1A	3372	1/1	0.97	0.18	34,34,34,34	0
56	MG	2A	3576	1/1	0.97	0.08	23,23,23,23	0
56	MG	1A	3118	1/1	0.97	0.11	38,38,38,38	0
56	MG	1B	206	1/1	0.97	0.09	42,42,42,42	0
56	MG	1a	1690	1/1	0.97	0.23	35,35,35,35	0
56	MG	2A	3277	1/1	0.97	0.24	37,37,37,37	0
56	MG	13	101	1/1	0.97	0.05	42,42,42,42	0
56	MG	2A	3582	1/1	0.97	0.08	49,49,49,49	0
56	MG	2A	3410	1/1	0.97	0.22	32,32,32,32	0
56	MG	1A	3188	1/1	0.97	0.17	29,29,29,29	0
56	MG	1A	3077	1/1	0.97	0.16	36,36,36,36	0
56	MG	1A	3750	1/1	0.97	0.08	58,58,58,58	0
56	MG	15	101	1/1	0.97	0.07	46,46,46,46	0
56	MG	2A	3588	1/1	0.97	0.07	47,47,47,47	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	1A	3285	1/1	0.97	0.07	35,35,35,35	0
56	MG	2A	3154	1/1	0.97	0.04	31,31,31,31	0
56	MG	1A	3507	1/1	0.97	0.07	38,38,38,38	0
56	MG	1A	3587	1/1	0.97	0.08	44,44,44,44	0
56	MG	2A	3157	1/1	0.97	0.07	57,57,57,57	0
56	MG	2A	3288	1/1	0.97	0.10	38,38,38,38	0
56	MG	1A	3588	1/1	0.97	0.06	41,41,41,41	0
56	MG	1A	3756	1/1	0.97	0.06	29,29,29,29	0
56	MG	2A	3424	1/1	0.97	0.30	43,43,43,43	0
56	MG	1A	3510	1/1	0.97	0.11	33,33,33,33	0
56	MG	1B	216	1/1	0.97	0.08	46,46,46,46	0
56	MG	1A	3668	1/1	0.97	0.10	37,37,37,37	0
56	MG	1A	3378	1/1	0.97	0.08	29,29,29,29	0
56	MG	1A	3415	1/1	0.97	0.21	36,36,36,36	0
56	MG	1A	3671	1/1	0.97	0.06	41,41,41,41	0
56	MG	1A	3003	1/1	0.97	0.09	29,29,29,29	0
56	MG	1A	3768	1/1	0.97	0.06	52,52,52,52	0
56	MG	1A	3418	1/1	0.97	0.13	28,28,28,28	0
56	MG	2A	3300	1/1	0.97	0.14	29,29,29,29	0
56	MG	1B	225	1/1	0.97	0.06	29,29,29,29	0
56	MG	1a	1712	1/1	0.97	0.28	40,40,40,40	0
56	MG	1D	301	1/1	0.97	0.10	37,37,37,37	0
56	MG	1A	3522	1/1	0.97	0.08	26,26,26,26	0
56	MG	2a	3101	1/1	0.97	0.21	27,27,27,27	0
56	MG	2A	3049	1/1	0.97	0.07	41,41,41,41	0
56	MG	2A	3616	1/1	0.97	0.21	25,25,25,25	0
56	MG	2A	3617	1/1	0.97	0.13	41,41,41,41	0
56	MG	1A	3596	1/1	0.97	0.07	40,40,40,40	0
56	MG	2A	3176	1/1	0.97	0.07	56,56,56,56	0
56	MG	1A	3154	1/1	0.97	0.07	42,42,42,42	0
56	MG	1A	3598	1/1	0.97	0.09	40,40,40,40	0
56	MG	2A	3444	1/1	0.97	0.27	34,34,34,34	0
56	MG	1D	307	1/1	0.97	0.07	46,46,46,46	0
56	MG	1a	1608	1/1	0.97	0.05	50,50,50,50	0
56	MG	2A	3055	1/1	0.97	0.12	50,50,50,50	0
56	MG	1A	3258	1/1	0.97	0.09	26,26,26,26	0
56	MG	1A	3462	1/1	0.97	0.06	32,32,32,32	0
56	MG	1A	3421	1/1	0.97	0.06	21,21,21,21	0
56	MG	1A	3781	1/1	0.97	0.05	39,39,39,39	0
56	MG	1A	3782	1/1	0.97	0.11	39,39,39,39	0
56	MG	1A	3121	1/1	0.97	0.14	22,22,22,22	0
56	MG	2A	3457	1/1	0.97	0.11	60,60,60,60	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	1A	3194	1/1	0.97	0.10	52,52,52,52	0
56	MG	2A	3064	1/1	0.97	0.17	37,37,37,37	0
56	MG	2A	3321	1/1	0.97	0.10	35,35,35,35	0
56	MG	2A	3461	1/1	0.97	0.07	46,46,46,46	0
56	MG	2A	3462	1/1	0.97	0.13	60,60,60,60	0
56	MG	1A	3238	1/1	0.97	0.18	43,43,43,43	0
56	MG	1A	3788	1/1	0.97	0.11	33,33,33,33	0
56	MG	2A	3465	1/1	0.97	0.05	37,37,37,37	0
56	MG	1A	3608	1/1	0.97	0.07	32,32,32,32	0
56	MG	2A	3469	1/1	0.97	0.07	34,34,34,34	0
56	MG	2a	3130	1/1	0.97	0.15	53,53,53,53	0
56	MG	1A	3539	1/1	0.97	0.07	32,32,32,32	0
56	MG	1A	3467	1/1	0.97	0.10	30,30,30,30	0
56	MG	1A	3468	1/1	0.97	0.06	29,29,29,29	0
56	MG	1A	3425	1/1	0.97	0.16	24,24,24,24	0
56	MG	2F	304	1/1	0.97	0.09	56,56,56,56	0
56	MG	1A	3350	1/1	0.97	0.17	36,36,36,36	0
56	MG	1A	3796	1/1	0.97	0.07	69,69,69,69	0
56	MG	1a	1738	1/1	0.97	0.28	46,46,46,46	0
56	MG	2A	3075	1/1	0.97	0.08	34,34,34,34	0
56	MG	2Q	202	1/1	0.97	0.19	33,33,33,33	0
56	MG	1A	3105	1/1	0.97	0.32	35,35,35,35	0
56	MG	1F	310	1/1	0.97	0.12	31,31,31,31	0
56	MG	2A	3487	1/1	0.97	0.05	59,59,59,59	0
56	MG	2A	3488	1/1	0.97	0.05	36,36,36,36	0
56	MG	1A	3798	1/1	0.97	0.08	27,27,27,27	0
56	MG	1A	3616	1/1	0.97	0.06	37,37,37,37	0
56	MG	1A	3093	1/1	0.97	0.08	41,41,41,41	0
56	MG	1A	3803	1/1	0.97	0.14	39,39,39,39	0
56	MG	2A	3209	1/1	0.97	0.05	63,63,63,63	0
56	MG	1A	3804	1/1	0.97	0.05	35,35,35,35	0
56	MG	1A	3695	1/1	0.97	0.12	42,42,42,42	0
56	MG	1A	3548	1/1	0.97	0.18	29,29,29,29	0
56	MG	1A	3015	1/1	0.97	0.13	40,40,40,40	0
56	MG	1A	3809	1/1	0.97	0.06	46,46,46,46	0
56	MG	1a	1636	1/1	0.97	0.09	48,48,48,48	0
56	MG	28	102	1/1	0.97	0.14	48,48,48,48	0
56	MG	2A	3503	1/1	0.97	0.10	41,41,41,41	0
56	MG	2A	3347	1/1	0.97	0.34	28,28,28,28	0
56	MG	1N	202	1/1	0.97	0.11	41,41,41,41	0
56	MG	1A	3810	1/1	0.97	0.05	25,25,25,25	0
56	MG	1A	3085	1/1	0.97	0.21	34,34,34,34	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	ZN	2n	501	1/1	0.97	0.04	96,96,96,96	0
56	MG	1A	3006	1/1	0.97	0.07	36,36,36,36	0
56	MG	1A	3397	1/1	0.98	0.06	25,25,25,25	0
56	MG	1A	3576	1/1	0.98	0.06	46,46,46,46	0
56	MG	1A	3147	1/1	0.98	0.10	48,48,48,48	0
56	MG	2A	3466	1/1	0.98	0.05	56,56,56,56	0
56	MG	1A	3578	1/1	0.98	0.04	33,33,33,33	0
56	MG	1A	3255	1/1	0.98	0.08	41,41,41,41	0
56	MG	2A	3470	1/1	0.98	0.09	39,39,39,39	0
56	MG	1A	3801	1/1	0.98	0.04	47,47,47,47	0
56	MG	1A	3581	1/1	0.98	0.04	28,28,28,28	0
56	MG	1A	3044	1/1	0.98	0.06	35,35,35,35	0
56	MG	2A	3159	1/1	0.98	0.06	44,44,44,44	0
56	MG	2A	3476	1/1	0.98	0.04	48,48,48,48	0
56	MG	2A	3478	1/1	0.98	0.10	56,56,56,56	0
56	MG	1A	3523	1/1	0.98	0.04	35,35,35,35	0
56	MG	1A	3099	1/1	0.98	0.13	26,26,26,26	0
56	MG	1A	3525	1/1	0.98	0.05	25,25,25,25	0
56	MG	1A	3807	1/1	0.98	0.05	24,24,24,24	0
56	MG	1A	3586	1/1	0.98	0.06	44,44,44,44	0
56	MG	1A	3721	1/1	0.98	0.04	35,35,35,35	0
56	MG	1A	3722	1/1	0.98	0.07	35,35,35,35	0
56	MG	1A	3526	1/1	0.98	0.06	16,16,16,16	0
56	MG	1A	3655	1/1	0.98	0.10	45,45,45,45	0
56	MG	2A	3271	1/1	0.98	0.16	33,33,33,33	0
56	MG	1A	3004	1/1	0.98	0.15	35,35,35,35	0
56	MG	1A	3528	1/1	0.98	0.07	28,28,28,28	0
56	MG	1a	1677	1/1	0.98	0.20	30,30,30,30	0
56	MG	1a	1764	1/1	0.98	0.06	52,52,52,52	0
56	MG	1A	3658	1/1	0.98	0.05	48,48,48,48	0
56	MG	1a	1766	1/1	0.98	0.04	32,32,32,32	0
56	MG	2A	3623	1/1	0.98	0.03	39,39,39,39	0
56	MG	1A	3590	1/1	0.98	0.05	56,56,56,56	0
56	MG	1A	3729	1/1	0.98	0.05	52,52,52,52	0
56	MG	1F	309	1/1	0.98	0.07	40,40,40,40	0
56	MG	2A	3502	1/1	0.98	0.04	40,40,40,40	0
56	MG	1A	3011	1/1	0.98	0.17	31,31,31,31	0
56	MG	19	101	1/1	0.98	0.10	52,52,52,52	0
56	MG	1A	3016	1/1	0.98	0.07	32,32,32,32	0
56	MG	1A	3262	1/1	0.98	0.11	40,40,40,40	0
56	MG	1A	3091	1/1	0.98	0.06	39,39,39,39	0
56	MG	1A	3823	1/1	0.98	0.11	46,46,46,46	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	2A	3509	1/1	0.98	0.05	57,57,57,57	0
56	MG	1A	3374	1/1	0.98	0.17	43,43,43,43	0
56	MG	2A	3511	1/1	0.98	0.05	37,37,37,37	0
56	MG	1A	3537	1/1	0.98	0.06	32,32,32,32	0
56	MG	1A	3538	1/1	0.98	0.08	33,33,33,33	0
56	MG	1A	3264	1/1	0.98	0.09	47,47,47,47	0
56	MG	1A	3828	1/1	0.98	0.06	40,40,40,40	0
56	MG	1A	3481	1/1	0.98	0.07	31,31,31,31	0
56	MG	1A	3600	1/1	0.98	0.06	60,60,60,60	0
56	MG	1A	3020	1/1	0.98	0.07	19,19,19,19	0
56	MG	2A	3519	1/1	0.98	0.08	29,29,29,29	0
56	MG	1A	3483	1/1	0.98	0.06	49,49,49,49	0
56	MG	1P	202	1/1	0.98	0.23	31,31,31,31	0
56	MG	2A	3194	1/1	0.98	0.19	43,43,43,43	0
56	MG	2A	3093	1/1	0.98	0.17	30,30,30,30	0
56	MG	2A	3094	1/1	0.98	0.13	45,45,45,45	0
56	MG	1A	3025	1/1	0.98	0.07	48,48,48,48	0
56	MG	2P	201	1/1	0.98	0.14	47,47,47,47	0
56	MG	1x	107	1/1	0.98	0.26	48,48,48,48	0
56	MG	2P	203	1/1	0.98	0.05	60,60,60,60	0
56	MG	1A	3544	1/1	0.98	0.08	30,30,30,30	0
56	MG	1a	1700	1/1	0.98	0.28	24,24,24,24	0
56	MG	1A	3031	1/1	0.98	0.07	43,43,43,43	0
56	MG	1A	3748	1/1	0.98	0.04	77,77,77,77	0
56	MG	2A	3001	1/1	0.98	0.17	35,35,35,35	0
56	MG	2V	201	1/1	0.98	0.14	48,48,48,48	0
56	MG	1A	3486	1/1	0.98	0.09	34,34,34,34	0
56	MG	2A	3536	1/1	0.98	0.06	35,35,35,35	0
56	MG	1A	3446	1/1	0.98	0.17	22,22,22,22	0
56	MG	2A	3004	1/1	0.98	0.26	48,48,48,48	0
56	MG	1A	3839	1/1	0.98	0.08	46,46,46,46	0
56	MG	1A	3122	1/1	0.98	0.11	27,27,27,27	0
56	MG	2A	3415	1/1	0.98	0.21	35,35,35,35	0
56	MG	1A	3611	1/1	0.98	0.05	42,42,42,42	0
56	MG	2A	3008	1/1	0.98	0.04	47,47,47,47	0
56	MG	25	102	1/1	0.98	0.14	50,50,50,50	0
56	MG	1A	3550	1/1	0.98	0.06	31,31,31,31	0
56	MG	1A	3294	1/1	0.98	0.04	27,27,27,27	0
56	MG	1R	205	1/1	0.98	0.15	29,29,29,29	0
56	MG	1A	3490	1/1	0.98	0.06	28,28,28,28	0
56	MG	1A	3321	1/1	0.98	0.06	43,43,43,43	0
56	MG	1A	3493	1/1	0.98	0.11	30,30,30,30	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	2A	3015	1/1	0.98	0.10	39,39,39,39	0
56	MG	1A	3322	1/1	0.98	0.14	38,38,38,38	0
56	MG	2A	3017	1/1	0.98	0.14	45,45,45,45	0
56	MG	1A	3451	1/1	0.98	0.16	20,20,20,20	0
56	MG	1A	3416	1/1	0.98	0.14	19,19,19,19	0
56	MG	1A	3621	1/1	0.98	0.04	16,16,16,16	0
56	MG	1A	3770	1/1	0.98	0.04	65,65,65,65	0
56	MG	1A	3771	1/1	0.98	0.06	37,37,37,37	0
56	MG	1A	3688	1/1	0.98	0.04	47,47,47,47	0
56	MG	1A	3123	1/1	0.98	0.03	23,23,23,23	0
56	MG	1A	3058	1/1	0.98	0.04	29,29,29,29	0
56	MG	1A	3775	1/1	0.98	0.06	54,54,54,54	0
56	MG	1A	3560	1/1	0.98	0.08	33,33,33,33	0
56	MG	1A	3108	1/1	0.98	0.15	50,50,50,50	0
56	MG	1A	3068	1/1	0.98	0.04	24,24,24,24	0
56	MG	1A	3111	1/1	0.98	0.10	42,42,42,42	0
56	MG	1A	3357	1/1	0.98	0.12	26,26,26,26	0
56	MG	2A	3032	1/1	0.98	0.16	33,33,33,33	0
56	MG	2A	3338	1/1	0.98	0.19	45,45,45,45	0
56	MG	2A	3033	1/1	0.98	0.15	39,39,39,39	0
56	MG	1a	1729	1/1	0.98	0.25	38,38,38,38	0
56	MG	2A	3035	1/1	0.98	0.07	37,37,37,37	0
56	MG	1A	3163	1/1	0.98	0.14	38,38,38,38	0
56	MG	1A	3227	1/1	0.98	0.10	34,34,34,34	0
56	MG	1A	3699	1/1	0.98	0.09	61,61,61,61	0
56	MG	1A	3164	1/1	0.98	0.04	49,49,49,49	0
56	MG	1A	3331	1/1	0.98	0.07	56,56,56,56	0
56	MG	1A	3207	1/1	0.98	0.12	26,26,26,26	0
56	MG	1a	1736	1/1	0.98	0.09	27,27,27,27	0
56	MG	2A	3453	1/1	0.98	0.10	35,35,35,35	0
56	MG	2A	3454	1/1	0.98	0.07	37,37,37,37	0
56	MG	1A	3509	1/1	0.98	0.05	45,45,45,45	0
56	MG	2A	3456	1/1	0.98	0.04	39,39,39,39	0
56	MG	1A	3145	1/1	0.98	0.13	53,53,53,53	0
56	MG	1Z	303	1/1	0.98	0.05	35,35,35,35	0
56	MG	1A	3791	1/1	0.98	0.05	41,41,41,41	0
56	MG	1A	3097	1/1	0.98	0.13	38,38,38,38	0
56	MG	2A	3589	1/1	0.98	0.05	32,32,32,32	0
56	MG	1A	3514	1/1	0.98	0.08	25,25,25,25	0
58	SF4	1d	302	8/8	0.98	0.04	57,68,71,74	0
58	SF4	2d	302	8/8	0.98	0.05	71,76,86,97	0
56	MG	1A	3708	1/1	0.98	0.05	49,49,49,49	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	1A	3707	1/1	0.99	0.08	48,48,48,48	0
56	MG	1A	3743	1/1	0.99	0.02	33,33,33,33	0
56	MG	1A	3192	1/1	0.99	0.05	44,44,44,44	0
56	MG	2A	3468	1/1	0.99	0.06	29,29,29,29	0
56	MG	1A	3787	1/1	0.99	0.04	42,42,42,42	0
56	MG	2A	3528	1/1	0.99	0.02	43,43,43,43	0
56	MG	1A	3065	1/1	0.99	0.04	33,33,33,33	0
56	MG	1D	304	1/1	0.99	0.04	35,35,35,35	0
56	MG	1A	3619	1/1	0.99	0.03	39,39,39,39	0
56	MG	2A	3532	1/1	0.99	0.04	46,46,46,46	0
56	MG	1A	3529	1/1	0.99	0.10	20,20,20,20	0
56	MG	1A	3511	1/1	0.99	0.03	36,36,36,36	0
56	MG	2A	3475	1/1	0.99	0.14	35,35,35,35	0
56	MG	1A	3749	1/1	0.99	0.06	78,78,78,78	0
56	MG	2A	3477	1/1	0.99	0.09	28,28,28,28	0
56	MG	1A	3427	1/1	0.99	0.25	39,39,39,39	0
56	MG	2A	3479	1/1	0.99	0.08	36,36,36,36	0
56	MG	2A	3480	1/1	0.99	0.08	36,36,36,36	0
56	MG	1A	3652	1/1	0.99	0.03	31,31,31,31	0
56	MG	1m	3001	1/1	0.99	0.11	51,51,51,51	0
56	MG	1A	3532	1/1	0.99	0.04	22,22,22,22	0
56	MG	1A	3513	1/1	0.99	0.07	26,26,26,26	0
56	MG	2A	3608	1/1	0.99	0.10	37,37,37,37	0
56	MG	1A	3139	1/1	0.99	0.11	32,32,32,32	0
56	MG	28	101	1/1	0.99	0.33	50,50,50,50	0
56	MG	1A	3755	1/1	0.99	0.04	55,55,55,55	0
56	MG	1A	3601	1/1	0.99	0.03	36,36,36,36	0
56	MG	1A	3758	1/1	0.99	0.03	26,26,26,26	0
56	MG	1U	206	1/1	0.99	0.23	37,37,37,37	0
56	MG	1A	3515	1/1	0.99	0.04	30,30,30,30	0
56	MG	1A	3580	1/1	0.99	0.06	39,39,39,39	0
56	MG	1A	3386	1/1	0.99	0.09	30,30,30,30	0
56	MG	1A	3762	1/1	0.99	0.05	54,54,54,54	0
56	MG	2A	3140	1/1	0.99	0.05	34,34,34,34	0
56	MG	1A	3491	1/1	0.99	0.04	25,25,25,25	0
56	MG	2A	3556	1/1	0.99	0.05	68,68,68,68	0
56	MG	1A	3764	1/1	0.99	0.04	62,62,62,62	0
56	MG	1A	3518	1/1	0.99	0.13	27,27,27,27	0
56	MG	1A	3766	1/1	0.99	0.03	57,57,57,57	0
56	MG	2A	3499	1/1	0.99	0.03	33,33,33,33	0
56	MG	1A	3632	1/1	0.99	0.05	36,36,36,36	0
56	MG	2A	3501	1/1	0.99	0.03	42,42,42,42	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	1A	3693	1/1	0.99	0.10	23,23,23,23	0
56	MG	1A	3812	1/1	0.99	0.03	26,26,26,26	0
56	MG	1A	3769	1/1	0.99	0.03	52,52,52,52	0
56	MG	1A	3607	1/1	0.99	0.04	35,35,35,35	0
56	MG	1A	3634	1/1	0.99	0.07	40,40,40,40	0
56	MG	2A	3200	1/1	0.99	0.04	46,46,46,46	0
56	MG	1A	3519	1/1	0.99	0.04	31,31,31,31	0
56	MG	1A	3636	1/1	0.99	0.03	29,29,29,29	0
56	MG	2A	3571	1/1	0.99	0.06	53,53,53,53	0
56	MG	1A	3195	1/1	0.99	0.06	32,32,32,32	0
56	MG	1A	3521	1/1	0.99	0.03	22,22,22,22	0
56	MG	2A	3058	1/1	0.99	0.05	30,30,30,30	0
56	MG	1A	3261	1/1	0.99	0.04	38,38,38,38	0
56	MG	1A	3109	1/1	0.99	0.04	33,33,33,33	0
56	MG	1A	3641	1/1	0.99	0.07	23,23,23,23	0
56	MG	1A	3473	1/1	0.99	0.05	26,26,26,26	0
56	MG	1A	3546	1/1	0.99	0.06	12,12,12,12	0
57	ZN	14	102	1/1	0.99	0.04	88,88,88,88	0
57	ZN	15	106	1/1	0.99	0.03	44,44,44,44	0
57	ZN	1n	103	1/1	0.99	0.03	72,72,72,72	0
57	ZN	2Y	202	1/1	0.99	0.03	76,76,76,76	0
56	MG	1A	3474	1/1	0.99	0.06	33,33,33,33	0
57	ZN	25	103	1/1	0.99	0.03	51,51,51,51	0
57	ZN	26	102	1/1	0.99	0.06	64,64,64,64	0
57	ZN	29	501	1/1	0.99	0.04	67,67,67,67	0
56	MG	1A	3508	1/1	0.99	0.07	26,26,26,26	0
56	MG	2A	3520	1/1	0.99	0.12	39,39,39,39	0
56	MG	1A	3783	1/1	0.99	0.10	32,32,32,32	0
56	MG	1B	223	1/1	0.99	0.04	34,34,34,34	0
57	ZN	16	501	1/1	1.00	0.02	45,45,45,45	0
57	ZN	19	102	1/1	1.00	0.01	42,42,42,42	0
56	MG	1A	3800	1/1	1.00	0.02	30,30,30,30	0
56	MG	1A	3718	1/1	1.00	0.02	17,17,17,17	0
56	MG	1A	3571	1/1	1.00	0.05	29,29,29,29	0
56	MG	1A	3736	1/1	1.00	0.02	35,35,35,35	0
56	MG	1A	3742	1/1	1.00	0.06	29,29,29,29	0
56	MG	1A	3535	1/1	1.00	0.04	20,20,20,20	0
56	MG	2A	3592	1/1	1.00	0.05	38,38,38,38	0
57	ZN	1Y	202	1/1	1.00	0.02	57,57,57,57	0
56	MG	1A	3476	1/1	1.00	0.06	33,33,33,33	0
56	MG	1A	3757	1/1	1.00	0.06	24,24,24,24	0

6.5 Other polymers [i](#)

There are no such residues in this entry.