



wwPDB X-ray Structure Validation Summary Report ⓘ

Sep 15, 2026 – 08:25 PM EDT

PDB ID : 6ND5 / pdb_00006nd5
Title : Crystal structure of the *Thermus thermophilus* 70S ribosome in complex with chloramphenicol and bound to mRNA and A-, P-, and E-site tRNAs at 2.60Å resolution
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Deposited on : 2018-12-13
Resolution : 2.60 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

The following versions of software and data (see [references](#) ①) 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
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
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

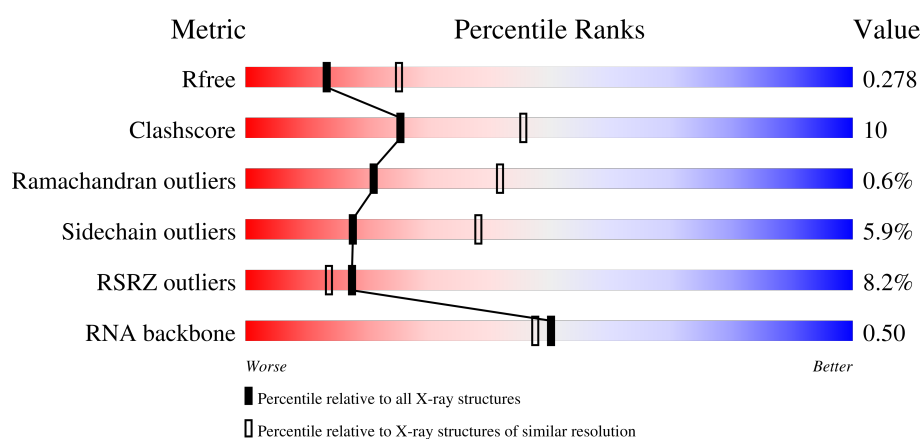
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.60 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.



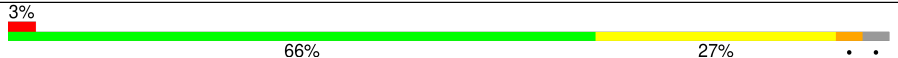
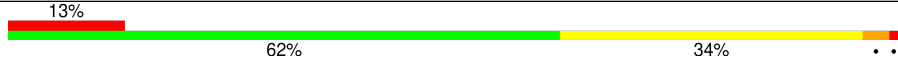
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	4008 (2.60-2.60)
Clashscore	190562	4347 (2.60-2.60)
Ramachandran outliers	187476	4277 (2.60-2.60)
Sidechain outliers	187428	4277 (2.60-2.60)
RSRZ outliers	180081	4008 (2.60-2.60)
RNA backbone	3983	1014 (2.84-2.36)

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

Mol	Chain	Length	Quality of chain
1	1A	2915	3% 61% 31% 7% .
1	2A	2915	3% 54% 35% 7% .
2	1B	121	71% 24% . .
2	2B	121	7% 44% 44% 12% .

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Mol	Chain	Length	Quality of chain
3	1D	276	
3	2D	276	
4	1E	206	
4	2E	206	
5	1F	210	
5	2F	210	
6	1G	182	
6	2G	182	
7	1H	180	
7	2H	180	
8	1I	148	
8	2I	148	
9	1N	140	
9	2N	140	
10	1O	122	
10	2O	122	
11	1P	150	
11	2P	150	
12	1Q	141	
12	2Q	141	
13	1R	118	
13	2R	118	
14	1S	112	
14	2S	112	
15	1T	146	

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

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Mol	Chain	Length	Quality of chain
28	16	54	
28	26	54	
29	17	49	
29	27	49	
30	18	65	
30	28	65	
31	19	37	
31	29	37	
32	1a	1521	
32	2a	1521	
33	1b	256	
33	2b	256	
34	1c	239	
34	2c	239	
35	1d	209	
35	2d	209	
36	1e	162	
36	2e	162	
37	1f	101	
37	2f	101	
38	1g	156	
38	2g	156	
39	1h	138	
39	2h	138	
40	1i	128	

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

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Mol	Chain	Length	Quality of chain
53	1v	24	
53	2v	24	
54	1w	76	
54	1y	76	
54	2w	76	
54	2y	76	
55	1x	77	
55	2x	77	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
60	SF4	1d	302	-	-	X	-
60	SF4	2d	302	-	-	X	-

2 Entry composition

There are 61 unique types of molecules in this entry. The entry contains 300833 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a RNA chain called 23S Ribosomal RNA.

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

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

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

- Molecule 3 is a protein called 50S ribosomal protein L2.

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

- Molecule 4 is a protein called 50S ribosomal protein L3.

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

- Molecule 5 is a protein called 50S ribosomal protein L4.

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

- Molecule 6 is a protein called 50S ribosomal protein L5.

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

- Molecule 7 is a protein called 50S ribosomal protein L6.

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

- Molecule 8 is a protein called 50S ribosomal protein L9.

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

- Molecule 9 is a protein called 50S ribosomal protein L13.

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

- Molecule 10 is a protein called 50S ribosomal protein L14.

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

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

- Molecule 11 is a protein called 50S ribosomal protein L15.

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

- Molecule 12 is a protein called 50S ribosomal protein L16.

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

- Molecule 13 is a protein called 50S ribosomal protein L17.

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

- Molecule 14 is a protein called 50S ribosomal protein L18.

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

- Molecule 15 is a protein called 50S ribosomal protein L19.

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

- Molecule 16 is a protein called 50S ribosomal protein L20.

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

- Molecule 17 is a protein called 50S ribosomal protein L21.

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

- Molecule 18 is a protein called 50S ribosomal protein L22.

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

- Molecule 19 is a protein called 50S ribosomal protein L23.

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

- Molecule 30 is a protein called 50S ribosomal protein L35.

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

- Molecule 31 is a protein called 50S ribosomal protein L36.

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

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

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

- Molecule 33 is a protein called 30S ribosomal protein S2.

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

- Molecule 34 is a protein called 30S ribosomal protein S3.

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

- Molecule 35 is a protein called 30S ribosomal protein S4.

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

- Molecule 36 is a protein called 30S ribosomal protein S5.

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

- Molecule 37 is a protein called 30S ribosomal protein S6.

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

- Molecule 38 is a protein called 30S ribosomal protein S7.

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

- Molecule 39 is a protein called 30S ribosomal protein S8.

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

- Molecule 50 is a protein called 30S ribosomal protein S19.

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

- Molecule 51 is a protein called 30S ribosomal protein S20.

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

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

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

- Molecule 53 is a RNA chain called mRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
53	1v	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 A-site and E-site tRNAs.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
54	1w	74	Total	C	N	O	P	S	0	0	0
			1592	713	285	518	74	2			
54	1y	74	Total	C	N	O	P	S	0	0	0
			1585	707	285	518	74	1			
54	2w	72	Total	C	N	O	P	S	0	0	0
			1544	690	278	502	72	2			
54	2y	73	Total	C	N	O	P	S	0	0	0
			1565	698	283	510	73	1			

- Molecule 55 is a RNA chain called P-site tRNA.

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

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
56	1A	1101	Total	Mg	0	0
			1101	1101		
56	1B	39	Total	Mg	0	0
			39	39		
56	1D	13	Total	Mg	0	0
			13	13		
56	1E	15	Total	Mg	0	0
			15	15		
56	1F	10	Total	Mg	0	0
			10	10		
56	1G	4	Total	Mg	0	0
			4	4		
56	1I	1	Total	Mg	0	0
			1	1		
56	1N	6	Total	Mg	0	0
			6	6		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
56	1O	5	Total 5	Mg 5	0	0
56	1P	9	Total 9	Mg 9	0	0
56	1Q	8	Total 8	Mg 8	0	0
56	1R	3	Total 3	Mg 3	0	0
56	1S	3	Total 3	Mg 3	0	0
56	1T	4	Total 4	Mg 4	0	0
56	1U	12	Total 12	Mg 12	0	0
56	1V	7	Total 7	Mg 7	0	0
56	1W	5	Total 5	Mg 5	0	0
56	1X	5	Total 5	Mg 5	0	0
56	1Y	3	Total 3	Mg 3	0	0
56	1Z	3	Total 3	Mg 3	0	0
56	10	6	Total 6	Mg 6	0	0
56	11	5	Total 5	Mg 5	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	16	3	Total 3	Mg 3	0	0
56	17	8	Total 8	Mg 8	0	0
56	18	7	Total 7	Mg 7	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
56	19	1	Total 1	Mg 1	0	0
56	1a	233	Total 233	Mg 233	0	0
56	1b	2	Total 2	Mg 2	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	2	Total 2	Mg 2	0	0
56	1m	2	Total 2	Mg 2	0	0
56	1n	1	Total 1	Mg 1	0	0
56	1s	1	Total 1	Mg 1	0	0
56	1t	1	Total 1	Mg 1	0	0
56	1v	1	Total 1	Mg 1	0	0
56	1w	12	Total 12	Mg 12	0	0
56	1x	18	Total 18	Mg 18	0	0
56	2A	887	Total 887	Mg 887	0	0
56	2B	20	Total 20	Mg 20	0	0
56	2D	10	Total 10	Mg 10	0	0
56	2E	4	Total 4	Mg 4	0	0
56	2F	6	Total 6	Mg 6	0	0
56	2G	1	Total 1	Mg 1	0	0

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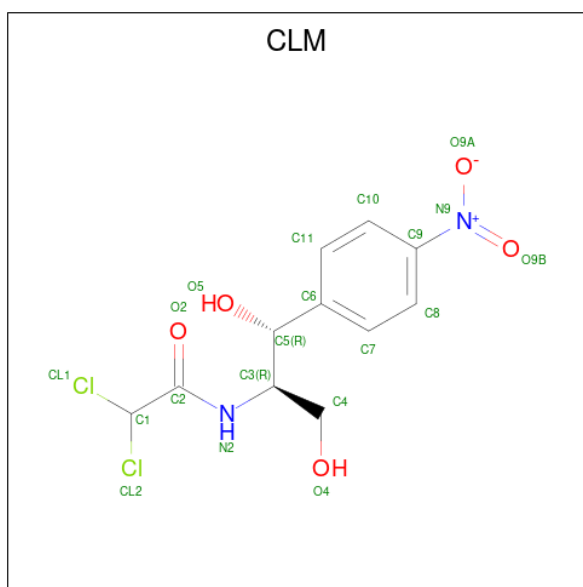
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
56	2N	1	Total 1	Mg 1	0	0
56	2O	1	Total 1	Mg 1	0	0
56	2P	4	Total 4	Mg 4	0	0
56	2Q	4	Total 4	Mg 4	0	0
56	2R	2	Total 2	Mg 2	0	0
56	2T	4	Total 4	Mg 4	0	0
56	2U	3	Total 3	Mg 3	0	0
56	2V	3	Total 3	Mg 3	0	0
56	2W	3	Total 3	Mg 3	0	0
56	2X	1	Total 1	Mg 1	0	0
56	2Z	1	Total 1	Mg 1	0	0
56	20	3	Total 3	Mg 3	0	0
56	21	1	Total 1	Mg 1	0	0
56	23	3	Total 3	Mg 3	0	0
56	25	5	Total 5	Mg 5	0	0
56	27	2	Total 2	Mg 2	0	0
56	28	3	Total 3	Mg 3	0	0
56	2a	241	Total 241	Mg 241	0	0
56	2d	1	Total 1	Mg 1	0	0
56	2e	1	Total 1	Mg 1	0	0
56	2f	2	Total 2	Mg 2	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
56	2g	1	Total 1	Mg 1	0	0
56	2i	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	4	Total 4	Mg 4	0	0
56	2m	1	Total 1	Mg 1	0	0
56	2q	2	Total 2	Mg 2	0	0
56	2r	1	Total 1	Mg 1	0	0
56	2t	1	Total 1	Mg 1	0	0
56	2v	1	Total 1	Mg 1	0	0
56	2w	4	Total 4	Mg 4	0	0
56	2x	5	Total 5	Mg 5	0	0
56	2y	6	Total 6	Mg 6	0	0

- Molecule 57 is CHLORAMPHENICOL (CCD ID: CLM) (formula: $C_{11}H_{12}Cl_2N_2O_5$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
57	1A	1	Total	C	Cl	N	O	0	0
			20	11	2	2	5		
57	2A	1	Total	C	Cl	N	O	0	0
			20	11	2	2	5		

- Molecule 58 is POTASSIUM ION (CCD ID: K) (formula: K).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
58	1A	1	Total	K	0	0
			1	1		
58	2A	1	Total	K	0	0
			1	1		

- Molecule 59 is ZINC ION (CCD ID: ZN) (formula: Zn).

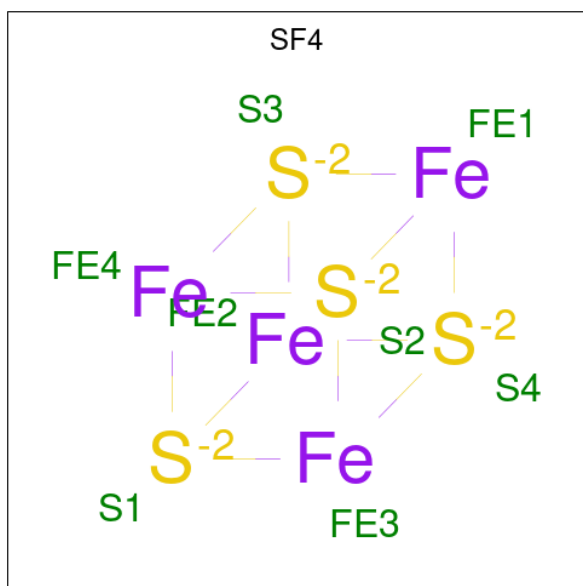
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
59	1Y	1	Total	Zn	0	0
			1	1		
59	14	1	Total	Zn	0	0
			1	1		
59	15	1	Total	Zn	0	0
			1	1		
59	16	1	Total	Zn	0	0
			1	1		
59	19	1	Total	Zn	0	0
			1	1		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
59	1n	1	Total	Zn	0	0
			1	1		
59	2Y	1	Total	Zn	0	0
			1	1		
59	24	1	Total	Zn	0	0
			1	1		
59	25	1	Total	Zn	0	0
			1	1		
59	26	1	Total	Zn	0	0
			1	1		
59	29	1	Total	Zn	0	0
			1	1		
59	2n	1	Total	Zn	0	0
			1	1		

- Molecule 60 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe_4S_4).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
60	1d	1	Total	Fe	S	0	0
			8	4	4		
60	2d	1	Total	Fe	S	0	0
			8	4	4		

- Molecule 61 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
61	1A	3	Total O 3 3	0	0
61	1A	1	Total O 1 1	0	0
61	1A	5	Total O 5 5	0	0
61	1A	5	Total O 5 5	0	0
61	1A	2	Total O 2 2	0	0
61	1A	4	Total O 4 4	0	0
61	1A	1	Total O 1 1	0	0
61	1A	4	Total O 4 4	0	0
61	1A	3	Total O 3 3	0	0
61	1A	4	Total O 4 4	0	0
61	1A	2	Total O 2 2	0	0
61	1A	2	Total O 2 2	0	0
61	1A	2	Total O 2 2	0	0
61	1A	2	Total O 2 2	0	0
61	1A	5	Total O 5 5	0	0
61	1A	4	Total O 4 4	0	0
61	1A	6	Total O 6 6	0	0
61	1A	1	Total O 1 1	0	0
61	1A	2	Total O 2 2	0	0
61	1A	1	Total O 1 1	0	0
61	1A	1	Total O 1 1	0	0
61	1A	5	Total O 5 5	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
61	1A	1	Total 1	O 1	0	0
61	1A	2	Total 2	O 2	0	0
61	1A	2	Total 2	O 2	0	0
61	1A	5	Total 5	O 5	0	0
61	1A	4	Total 4	O 4	0	0
61	1A	5	Total 5	O 5	0	0
61	1A	5	Total 5	O 5	0	0
61	1A	5	Total 5	O 5	0	0
61	1A	5	Total 5	O 5	0	0
61	1A	5	Total 5	O 5	0	0
61	1A	2	Total 2	O 2	0	0
61	1A	4	Total 4	O 4	0	0
61	1A	2	Total 2	O 2	0	0
61	1A	2	Total 2	O 2	0	0
61	1A	2	Total 2	O 2	0	0
61	1A	4	Total 4	O 4	0	0
61	1A	2	Total 2	O 2	0	0
61	1A	4	Total 4	O 4	0	0
61	1A	1	Total 1	O 1	0	0
61	1A	2	Total 2	O 2	0	0
61	1A	2	Total 2	O 2	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
61	1A	1	Total	O	0	0
			1	1		
61	1A	5	Total	O	0	0
			5	5		
61	1A	1	Total	O	0	0
			1	1		
61	1A	4	Total	O	0	0
			4	4		
61	1A	1	Total	O	0	0
			1	1		
61	1A	3	Total	O	0	0
			3	3		
61	1A	1	Total	O	0	0
			1	1		
61	1A	1	Total	O	0	0
			1	1		
61	1A	2	Total	O	0	0
			2	2		
61	1A	1	Total	O	0	0
			1	1		
61	1A	4	Total	O	0	0
			4	4		
61	1A	3	Total	O	0	0
			3	3		
61	1A	4	Total	O	0	0
			4	4		
61	1A	2	Total	O	0	0
			2	2		
61	1A	1	Total	O	0	0
			1	1		
61	1A	2	Total	O	0	0
			2	2		
61	1A	4	Total	O	0	0
			4	4		
61	1A	4	Total	O	0	0
			4	4		
61	1A	5	Total	O	0	0
			5	5		
61	1A	3	Total	O	0	0
			3	3		
61	1A	4	Total	O	0	0
			4	4		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
61	1A	5	Total 5	O 5	0	0
61	1A	4	Total 4	O 4	0	0
61	1A	5	Total 5	O 5	0	0
61	1A	5	Total 5	O 5	0	0
61	1A	4	Total 4	O 4	0	0
61	1A	5	Total 5	O 5	0	0
61	1A	5	Total 5	O 5	0	0
61	1A	4	Total 4	O 4	0	0
61	1A	4	Total 4	O 4	0	0
61	1A	5	Total 5	O 5	0	0
61	1A	4	Total 4	O 4	0	0
61	1A	5	Total 5	O 5	0	0
61	1A	5	Total 5	O 5	0	0
61	1A	2	Total 2	O 2	0	0
61	1A	2	Total 2	O 2	0	0
61	1A	4	Total 4	O 4	0	0
61	1A	1	Total 1	O 1	0	0
61	1A	5	Total 5	O 5	0	0
61	1A	1	Total 1	O 1	0	0
61	1A	4	Total 4	O 4	0	0
61	1A	1	Total 1	O 1	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
61	1A	5	Total	O	0	0
			5	5		
61	1A	4	Total	O	0	0
			4	4		
61	1A	4	Total	O	0	0
			4	4		
61	1A	4	Total	O	0	0
			4	4		
61	1A	4	Total	O	0	0
			4	4		
61	1A	3	Total	O	0	0
			3	3		
61	1A	3	Total	O	0	0
			3	3		
61	1A	4	Total	O	0	0
			4	4		
61	1A	4	Total	O	0	0
			4	4		
61	1A	4	Total	O	0	0
			4	4		
61	1A	3	Total	O	0	0
			3	3		
61	1A	1	Total	O	0	0
			1	1		
61	1A	1	Total	O	0	0
			1	1		
61	1A	5	Total	O	0	0
			5	5		
61	1A	5	Total	O	0	0
			5	5		
61	1A	3	Total	O	0	0
			3	3		
61	1A	1	Total	O	0	0
			1	1		
61	1A	1	Total	O	0	0
			1	1		
61	1A	3	Total	O	0	0
			3	3		
61	1A	3	Total	O	0	0
			3	3		
61	1A	1	Total	O	0	0
			1	1		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
61	1A	2	Total 2	O 2	0	0
61	1A	1	Total 1	O 1	0	0
61	1A	2	Total 2	O 2	0	0
61	1A	1	Total 1	O 1	0	0
61	1A	4	Total 4	O 4	0	0
61	1A	1	Total 1	O 1	0	0
61	1A	2	Total 2	O 2	0	0
61	1A	2	Total 2	O 2	0	0
61	1A	2	Total 2	O 2	0	0
61	1A	3	Total 3	O 3	0	0
61	1A	1	Total 1	O 1	0	0
61	1A	3	Total 3	O 3	0	0
61	1A	2	Total 2	O 2	0	0
61	1A	6	Total 6	O 6	0	0
61	1A	3	Total 3	O 3	0	0
61	1A	2	Total 2	O 2	0	0
61	1A	1	Total 1	O 1	0	0
61	1A	2	Total 2	O 2	0	0
61	1A	5	Total 5	O 5	0	0
61	1A	2	Total 2	O 2	0	0
61	1A	3	Total 3	O 3	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
61	1A	2	Total	O	0	0
			2	2		
61	1A	6	Total	O	0	0
			6	6		
61	1A	6	Total	O	0	0
			6	6		
61	1A	4	Total	O	0	0
			4	4		
61	1A	3	Total	O	0	0
			3	3		
61	1A	3	Total	O	0	0
			3	3		
61	1A	4	Total	O	0	0
			4	4		
61	1A	3	Total	O	0	0
			3	3		
61	1A	4	Total	O	0	0
			4	4		
61	1A	2	Total	O	0	0
			2	2		
61	1A	2	Total	O	0	0
			2	2		
61	1A	6	Total	O	0	0
			6	6		
61	1A	3	Total	O	0	0
			3	3		
61	1A	4	Total	O	0	0
			4	4		
61	1A	1	Total	O	0	0
			1	1		
61	1A	5	Total	O	0	0
			5	5		
61	1A	2	Total	O	0	0
			2	2		
61	1A	2	Total	O	0	0
			2	2		
61	1A	4	Total	O	0	0
			4	4		
61	1A	2	Total	O	0	0
			2	2		
61	1A	1	Total	O	0	0
			1	1		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
61	1A	5	Total	O	0	0
			5	5		
61	1A	4	Total	O	0	0
			4	4		
61	1A	5	Total	O	0	0
			5	5		
61	1A	6	Total	O	0	0
			6	6		
61	1A	6	Total	O	0	0
			6	6		
61	1A	5	Total	O	0	0
			5	5		
61	1A	2	Total	O	0	0
			2	2		
61	1A	2	Total	O	0	0
			2	2		
61	1A	3	Total	O	0	0
			3	3		
61	1A	4	Total	O	0	0
			4	4		
61	1A	3	Total	O	0	0
			3	3		
61	1A	6	Total	O	0	0
			6	6		
61	1A	4	Total	O	0	0
			4	4		
61	1A	3	Total	O	0	0
			3	3		
61	1A	5	Total	O	0	0
			5	5		
61	1A	3	Total	O	0	0
			3	3		
61	1A	4	Total	O	0	0
			4	4		
61	1A	4	Total	O	0	0
			4	4		
61	1A	4	Total	O	0	0
			4	4		
61	1A	3	Total	O	0	0
			3	3		
61	1A	5	Total	O	0	0
			5	5		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
61	1A	3	Total 3	O 3	0	0
61	1A	4	Total 4	O 4	0	0
61	1A	4	Total 4	O 4	0	0
61	1A	3	Total 3	O 3	0	0
61	1A	5	Total 5	O 5	0	0
61	1A	5	Total 5	O 5	0	0
61	1A	4	Total 4	O 4	0	0
61	1A	5	Total 5	O 5	0	0
61	1A	5	Total 5	O 5	0	0
61	1A	4	Total 4	O 4	0	0
61	1A	3	Total 3	O 3	0	0
61	1A	3	Total 3	O 3	0	0
61	1A	1	Total 1	O 1	0	0
61	1A	5	Total 5	O 5	0	0
61	1A	4	Total 4	O 4	0	0
61	1A	1	Total 1	O 1	0	0
61	1A	5	Total 5	O 5	0	0
61	1A	5	Total 5	O 5	0	0
61	1A	5	Total 5	O 5	0	0
61	1A	5	Total 5	O 5	0	0
61	1A	2	Total 2	O 2	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
61	1A	2	Total	O	0	0
			2	2		
61	1A	2	Total	O	0	0
			2	2		
61	1A	2	Total	O	0	0
			2	2		
61	1A	6	Total	O	0	0
			6	6		
61	1A	4	Total	O	0	0
			4	4		
61	1A	3	Total	O	0	0
			3	3		
61	1A	4	Total	O	0	0
			4	4		
61	1A	4	Total	O	0	0
			4	4		
61	1A	3	Total	O	0	0
			3	3		
61	1A	5	Total	O	0	0
			5	5		
61	1A	2	Total	O	0	0
			2	2		
61	1A	2	Total	O	0	0
			2	2		
61	1A	1	Total	O	0	0
			1	1		
61	1A	5	Total	O	0	0
			5	5		
61	1A	6	Total	O	0	0
			6	6		
61	1A	2	Total	O	0	0
			2	2		
61	1A	1	Total	O	0	0
			1	1		
61	1A	1	Total	O	0	0
			1	1		
61	1A	3	Total	O	0	0
			3	3		
61	1A	1	Total	O	0	0
			1	1		
61	1A	5	Total	O	0	0
			5	5		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
61	1A	1	Total	O	0	0
			1	1		
61	1A	3	Total	O	0	0
			3	3		
61	1A	1	Total	O	0	0
			1	1		
61	1A	1	Total	O	0	0
			1	1		
61	1A	2	Total	O	0	0
			2	2		
61	1A	2	Total	O	0	0
			2	2		
61	1A	1	Total	O	0	0
			1	1		
61	1A	2	Total	O	0	0
			2	2		
61	1A	1	Total	O	0	0
			1	1		
61	1A	1	Total	O	0	0
			1	1		
61	1A	1	Total	O	0	0
			1	1		
61	1A	1	Total	O	0	0
			1	1		
61	1A	1	Total	O	0	0
			1	1		
61	1A	1	Total	O	0	0
			1	1		
61	1A	1	Total	O	0	0
			1	1		
61	1A	2	Total	O	0	0
			2	2		
61	1A	1	Total	O	0	0
			1	1		
61	1A	2	Total	O	0	0
			2	2		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
61	1A	2	Total 2	O 2	0	0
61	1A	4	Total 4	O 4	0	0
61	1A	1	Total 1	O 1	0	0
61	1A	1	Total 1	O 1	0	0
61	1A	1	Total 1	O 1	0	0
61	1A	3	Total 3	O 3	0	0
61	1A	4	Total 4	O 4	0	0
61	1A	1	Total 1	O 1	0	0
61	1A	1	Total 1	O 1	0	0
61	1A	3	Total 3	O 3	0	0
61	1A	6	Total 6	O 6	0	0
61	1A	2	Total 2	O 2	0	0
61	1A	3	Total 3	O 3	0	0
61	1A	3	Total 3	O 3	0	0
61	1A	2	Total 2	O 2	0	0
61	1A	2	Total 2	O 2	0	0
61	1A	2	Total 2	O 2	0	0
61	1A	5	Total 5	O 5	0	0
61	1A	1	Total 1	O 1	0	0
61	1A	2	Total 2	O 2	0	0
61	1A	3	Total 3	O 3	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
61	1A	3	Total 3	O 3	0	0
61	1A	2	Total 2	O 2	0	0
61	1A	1	Total 1	O 1	0	0
61	1A	2	Total 2	O 2	0	0
61	1A	1	Total 1	O 1	0	0
61	1A	1	Total 1	O 1	0	0
61	1A	2	Total 2	O 2	0	0
61	1A	6	Total 6	O 6	0	0
61	1A	1	Total 1	O 1	0	0
61	1A	2	Total 2	O 2	0	0
61	1A	1	Total 1	O 1	0	0
61	1A	1	Total 1	O 1	0	0
61	1A	2	Total 2	O 2	0	0
61	1A	4	Total 4	O 4	0	0
61	1A	1	Total 1	O 1	0	0
61	1A	2	Total 2	O 2	0	0
61	1A	5	Total 5	O 5	0	0
61	1A	1	Total 1	O 1	0	0
61	1A	1	Total 1	O 1	0	0
61	1A	1	Total 1	O 1	0	0
61	1A	1	Total 1	O 1	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
61	1A	1	Total	O	0	0
			1	1		
61	1A	1	Total	O	0	0
			1	1		
61	1A	1	Total	O	0	0
			1	1		
61	1A	2	Total	O	0	0
			2	2		
61	1A	2	Total	O	0	0
			2	2		
61	1A	6	Total	O	0	0
			6	6		
61	1A	1	Total	O	0	0
			1	1		
61	1A	3	Total	O	0	0
			3	3		
61	1A	5	Total	O	0	0
			5	5		
61	1A	6	Total	O	0	0
			6	6		
61	1A	3	Total	O	0	0
			3	3		
61	1A	1	Total	O	0	0
			1	1		
61	1A	3	Total	O	0	0
			3	3		
61	1A	5	Total	O	0	0
			5	5		
61	1A	4	Total	O	0	0
			4	4		
61	1A	4	Total	O	0	0
			4	4		
61	1A	5	Total	O	0	0
			5	5		
61	1A	5	Total	O	0	0
			5	5		
61	1A	2	Total	O	0	0
			2	2		
61	1A	2	Total	O	0	0
			2	2		
61	1A	1	Total	O	0	0
			1	1		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
61	1A	1	Total 1	O 1	0	0
61	1A	3	Total 3	O 3	0	0
61	1A	1	Total 1	O 1	0	0
61	1A	5	Total 5	O 5	0	0
61	1A	1	Total 1	O 1	0	0
61	1A	1	Total 1	O 1	0	0
61	1A	1	Total 1	O 1	0	0
61	1A	2	Total 2	O 2	0	0
61	1A	2	Total 2	O 2	0	0
61	1A	3	Total 3	O 3	0	0
61	1A	6	Total 6	O 6	0	0
61	1A	1	Total 1	O 1	0	0
61	1A	1	Total 1	O 1	0	0
61	1A	1	Total 1	O 1	0	0
61	1A	1	Total 1	O 1	0	0
61	1A	1	Total 1	O 1	0	0
61	1A	6	Total 6	O 6	0	0
61	1A	6	Total 6	O 6	0	0
61	1A	3	Total 3	O 3	0	0
61	1A	2	Total 2	O 2	0	0
61	1A	1	Total 1	O 1	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
61	1A	1	Total 1	O 1	0	0
61	1A	1	Total 1	O 1	0	0
61	1A	4	Total 4	O 4	0	0
61	1A	6	Total 6	O 6	0	0
61	1A	6	Total 6	O 6	0	0
61	1A	6	Total 6	O 6	0	0
61	1A	4	Total 4	O 4	0	0
61	1A	6	Total 6	O 6	0	0
61	1A	6	Total 6	O 6	0	0
61	1A	6	Total 6	O 6	0	0
61	1A	4	Total 4	O 4	0	0
61	1A	3	Total 3	O 3	0	0
61	1A	5	Total 5	O 5	0	0
61	1A	4	Total 4	O 4	0	0
61	1A	5	Total 5	O 5	0	0
61	1A	5	Total 5	O 5	0	0
61	1A	6	Total 6	O 6	0	0
61	1A	3	Total 3	O 3	0	0
61	1A	4	Total 4	O 4	0	0
61	1A	6	Total 6	O 6	0	0
61	1A	6	Total 6	O 6	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
61	1A	6	Total	O	0	0
			6	6		
61	1A	5	Total	O	0	0
			5	5		
61	1A	5	Total	O	0	0
			5	5		
61	1A	5	Total	O	0	0
			5	5		
61	1A	6	Total	O	0	0
			6	6		
61	1A	6	Total	O	0	0
			6	6		
61	1A	6	Total	O	0	0
			6	6		
61	1A	3	Total	O	0	0
			3	3		
61	1A	3	Total	O	0	0
			3	3		
61	1A	5	Total	O	0	0
			5	5		
61	1A	4	Total	O	0	0
			4	4		
61	1A	6	Total	O	0	0
			6	6		
61	1A	6	Total	O	0	0
			6	6		
61	1A	6	Total	O	0	0
			6	6		
61	1A	5	Total	O	0	0
			5	5		
61	1A	5	Total	O	0	0
			5	5		
61	1A	3	Total	O	0	0
			3	3		
61	1A	6	Total	O	0	0
			6	6		
61	1A	5	Total	O	0	0
			5	5		
61	1A	5	Total	O	0	0
			5	5		
61	1A	5	Total	O	0	0
			5	5		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
61	1A	5	Total	O	0	0
			5	5		
61	1A	4	Total	O	0	0
			4	4		
61	1A	5	Total	O	0	0
			5	5		
61	1A	5	Total	O	0	0
			5	5		
61	1A	6	Total	O	0	0
			6	6		
61	1A	4	Total	O	0	0
			4	4		
61	1A	6	Total	O	0	0
			6	6		
61	1A	3	Total	O	0	0
			3	3		
61	1A	2	Total	O	0	0
			2	2		
61	1A	4	Total	O	0	0
			4	4		
61	1A	2	Total	O	0	0
			2	2		
61	1A	1	Total	O	0	0
			1	1		
61	1A	1	Total	O	0	0
			1	1		
61	1A	5	Total	O	0	0
			5	5		
61	1A	5	Total	O	0	0
			5	5		
61	1A	6	Total	O	0	0
			6	6		
61	1A	6	Total	O	0	0
			6	6		
61	1A	4	Total	O	0	0
			4	4		
61	1A	5	Total	O	0	0
			5	5		
61	1A	6	Total	O	0	0
			6	6		
61	1A	6	Total	O	0	0
			6	6		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
61	1A	6	Total 6	O 6	0	0
61	1A	5	Total 5	O 5	0	0
61	1A	5	Total 5	O 5	0	0
61	1A	5	Total 5	O 5	0	0
61	1A	6	Total 6	O 6	0	0
61	1A	6	Total 6	O 6	0	0
61	1A	5	Total 5	O 5	0	0
61	1A	4	Total 4	O 4	0	0
61	1A	5	Total 5	O 5	0	0
61	1A	4	Total 4	O 4	0	0
61	1A	4	Total 4	O 4	0	0
61	1A	4	Total 4	O 4	0	0
61	1A	6	Total 6	O 6	0	0
61	1A	6	Total 6	O 6	0	0
61	1A	6	Total 6	O 6	0	0
61	1A	6	Total 6	O 6	0	0
61	1A	6	Total 6	O 6	0	0
61	1A	6	Total 6	O 6	0	0
61	1A	4	Total 4	O 4	0	0
61	1A	5	Total 5	O 5	0	0
61	1A	5	Total 5	O 5	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
61	1A	6	Total 6	O 6	0	0
61	1A	4	Total 4	O 4	0	0
61	1A	3	Total 3	O 3	0	0
61	1A	2	Total 2	O 2	0	0
61	1A	2	Total 2	O 2	0	0
61	1A	3	Total 3	O 3	0	0
61	1A	6	Total 6	O 6	0	0
61	1A	6	Total 6	O 6	0	0
61	1A	6	Total 6	O 6	0	0
61	1A	6	Total 6	O 6	0	0
61	1A	6	Total 6	O 6	0	0
61	1A	5	Total 5	O 5	0	0
61	1A	5	Total 5	O 5	0	0
61	1A	4	Total 4	O 4	0	0
61	1A	4	Total 4	O 4	0	0
61	1A	5	Total 5	O 5	0	0
61	1A	6	Total 6	O 6	0	0
61	1A	5	Total 5	O 5	0	0
61	1A	4	Total 4	O 4	0	0
61	1A	5	Total 5	O 5	0	0
61	1A	6	Total 6	O 6	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
61	1A	4	Total 4	O 4	0	0
61	1A	6	Total 6	O 6	0	0
61	1A	5	Total 5	O 5	0	0
61	1A	5	Total 5	O 5	0	0
61	1A	6	Total 6	O 6	0	0
61	1A	4	Total 4	O 4	0	0
61	1A	5	Total 5	O 5	0	0
61	1A	5	Total 5	O 5	0	0
61	1A	6	Total 6	O 6	0	0
61	1A	6	Total 6	O 6	0	0
61	1A	6	Total 6	O 6	0	0
61	1A	5	Total 5	O 5	0	0
61	1A	6	Total 6	O 6	0	0
61	1A	4	Total 4	O 4	0	0
61	1A	4	Total 4	O 4	0	0
61	1A	4	Total 4	O 4	0	0
61	1A	6	Total 6	O 6	0	0
61	1A	5	Total 5	O 5	0	0
61	1A	6	Total 6	O 6	0	0
61	1A	6	Total 6	O 6	0	0
61	1A	6	Total 6	O 6	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
61	1A	6	Total	O	0	0
			6	6		
61	1A	5	Total	O	0	0
			5	5		
61	1A	6	Total	O	0	0
			6	6		
61	1A	6	Total	O	0	0
			6	6		
61	1A	5	Total	O	0	0
			5	5		
61	1A	4	Total	O	0	0
			4	4		
61	1A	6	Total	O	0	0
			6	6		
61	1A	4	Total	O	0	0
			4	4		
61	1A	2	Total	O	0	0
			2	2		
61	1A	5	Total	O	0	0
			5	5		
61	1A	5	Total	O	0	0
			5	5		
61	1A	1	Total	O	0	0
			1	1		
61	1A	3	Total	O	0	0
			3	3		
61	1A	4	Total	O	0	0
			4	4		
61	1A	4	Total	O	0	0
			4	4		
61	1A	6	Total	O	0	0
			6	6		
61	1A	5	Total	O	0	0
			5	5		
61	1A	5	Total	O	0	0
			5	5		
61	1A	5	Total	O	0	0
			5	5		
61	1A	6	Total	O	0	0
			6	6		
61	1A	5	Total	O	0	0
			5	5		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
61	1A	5	Total	O	0	0
			5	5		
61	1A	5	Total	O	0	0
			5	5		
61	1A	3	Total	O	0	0
			3	3		
61	1A	4	Total	O	0	0
			4	4		
61	1A	5	Total	O	0	0
			5	5		
61	1A	5	Total	O	0	0
			5	5		
61	1A	4	Total	O	0	0
			4	4		
61	1A	3	Total	O	0	0
			3	3		
61	1A	1	Total	O	0	0
			1	1		
61	1A	1	Total	O	0	0
			1	1		
61	1A	4	Total	O	0	0
			4	4		
61	1A	3	Total	O	0	0
			3	3		
61	1A	6	Total	O	0	0
			6	6		
61	1A	5	Total	O	0	0
			5	5		
61	1A	6	Total	O	0	0
			6	6		
61	1A	6	Total	O	0	0
			6	6		
61	1A	6	Total	O	0	0
			6	6		
61	1A	1	Total	O	0	0
			1	1		
61	1A	5	Total	O	0	0
			5	5		
61	1A	6	Total	O	0	0
			6	6		
61	1A	1	Total	O	0	0
			1	1		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
61	1A	1	Total 1	O 1	0	0
61	1A	6	Total 6	O 6	0	0
61	1A	2	Total 2	O 2	0	0
61	1A	1	Total 1	O 1	0	0
61	1A	6	Total 6	O 6	0	0
61	1A	2	Total 2	O 2	0	0
61	1A	2	Total 2	O 2	0	0
61	1A	6	Total 6	O 6	0	0
61	1A	2	Total 2	O 2	0	0
61	1A	1	Total 1	O 1	0	0
61	1A	6	Total 6	O 6	0	0
61	1A	500	Total 500	O 500	0	0
61	1B	3	Total 3	O 3	0	0
61	1B	1	Total 1	O 1	0	0
61	1B	5	Total 5	O 5	0	0
61	1B	4	Total 4	O 4	0	0
61	1B	3	Total 3	O 3	0	0
61	1B	1	Total 1	O 1	0	0
61	1B	1	Total 1	O 1	0	0
61	1B	1	Total 1	O 1	0	0
61	1B	1	Total 1	O 1	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
61	1B	1	Total 1	O 1	0	0
61	1B	2	Total 2	O 2	0	0
61	1B	2	Total 2	O 2	0	0
61	1B	1	Total 1	O 1	0	0
61	1B	2	Total 2	O 2	0	0
61	1B	1	Total 1	O 1	0	0
61	1B	6	Total 6	O 6	0	0
61	1B	1	Total 1	O 1	0	0
61	1B	2	Total 2	O 2	0	0
61	1B	1	Total 1	O 1	0	0
61	1B	1	Total 1	O 1	0	0
61	1B	3	Total 3	O 3	0	0
61	1B	2	Total 2	O 2	0	0
61	1B	1	Total 1	O 1	0	0
61	1B	2	Total 2	O 2	0	0
61	1B	1	Total 1	O 1	0	0
61	1B	3	Total 3	O 3	0	0
61	1B	5	Total 5	O 5	0	0
61	1B	16	Total 16	O 16	0	0
61	1D	5	Total 5	O 5	0	0
61	1D	2	Total 2	O 2	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
61	1D	1	Total 1	O 1	0	0
61	1D	1	Total 1	O 1	0	0
61	1D	15	Total 15	O 15	0	0
61	1E	2	Total 2	O 2	0	0
61	1E	2	Total 2	O 2	0	0
61	1E	2	Total 2	O 2	0	0
61	1E	2	Total 2	O 2	0	0
61	1E	6	Total 6	O 6	0	0
61	1E	13	Total 13	O 13	0	0
61	1F	1	Total 1	O 1	0	0
61	1F	8	Total 8	O 8	0	0
61	1G	2	Total 2	O 2	0	0
61	1G	3	Total 3	O 3	0	0
61	1H	1	Total 1	O 1	0	0
61	1I	2	Total 2	O 2	0	0
61	1N	4	Total 4	O 4	0	0
61	1O	2	Total 2	O 2	0	0
61	1O	1	Total 1	O 1	0	0
61	1O	4	Total 4	O 4	0	0
61	1P	5	Total 5	O 5	0	0
61	1P	2	Total 2	O 2	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
61	1P	2	Total 2	O 2	0	0
61	1P	1	Total 1	O 1	0	0
61	1P	6	Total 6	O 6	0	0
61	1P	5	Total 5	O 5	0	0
61	1Q	6	Total 6	O 6	0	0
61	1Q	1	Total 1	O 1	0	0
61	1Q	4	Total 4	O 4	0	0
61	1R	1	Total 1	O 1	0	0
61	1R	7	Total 7	O 7	0	0
61	1S	2	Total 2	O 2	0	0
61	1S	2	Total 2	O 2	0	0
61	1T	1	Total 1	O 1	0	0
61	1T	1	Total 1	O 1	0	0
61	1T	4	Total 4	O 4	0	0
61	1U	9	Total 9	O 9	0	0
61	1V	1	Total 1	O 1	0	0
61	1V	6	Total 6	O 6	0	0
61	1W	9	Total 9	O 9	0	0
61	1X	4	Total 4	O 4	0	0
61	1X	3	Total 3	O 3	0	0
61	1Y	3	Total 3	O 3	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
61	1Z	1	Total 1	O 1	0	0
61	10	3	Total 3	O 3	0	0
61	10	2	Total 2	O 2	0	0
61	10	7	Total 7	O 7	0	0
61	11	1	Total 1	O 1	0	0
61	11	1	Total 1	O 1	0	0
61	11	8	Total 8	O 8	0	0
61	12	4	Total 4	O 4	0	0
61	13	1	Total 1	O 1	0	0
61	13	3	Total 3	O 3	0	0
61	14	2	Total 2	O 2	0	0
61	15	2	Total 2	O 2	0	0
61	15	5	Total 5	O 5	0	0
61	16	1	Total 1	O 1	0	0
61	17	2	Total 2	O 2	0	0
61	17	5	Total 5	O 5	0	0
61	18	5	Total 5	O 5	0	0
61	18	2	Total 2	O 2	0	0
61	18	1	Total 1	O 1	0	0
61	18	2	Total 2	O 2	0	0
61	18	6	Total 6	O 6	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
61	18	3	Total 3	O 3	0	0
61	1a	2	Total 2	O 2	0	0
61	1a	3	Total 3	O 3	0	0
61	1a	4	Total 4	O 4	0	0
61	1a	1	Total 1	O 1	0	0
61	1a	2	Total 2	O 2	0	0
61	1a	2	Total 2	O 2	0	0
61	1a	1	Total 1	O 1	0	0
61	1a	5	Total 5	O 5	0	0
61	1a	4	Total 4	O 4	0	0
61	1a	4	Total 4	O 4	0	0
61	1a	5	Total 5	O 5	0	0
61	1a	4	Total 4	O 4	0	0
61	1a	4	Total 4	O 4	0	0
61	1a	1	Total 1	O 1	0	0
61	1a	2	Total 2	O 2	0	0
61	1a	1	Total 1	O 1	0	0
61	1a	3	Total 3	O 3	0	0
61	1a	2	Total 2	O 2	0	0
61	1a	3	Total 3	O 3	0	0
61	1a	5	Total 5	O 5	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
61	1a	6	Total 6	O 6	0	0
61	1a	3	Total 3	O 3	0	0
61	1a	5	Total 5	O 5	0	0
61	1a	5	Total 5	O 5	0	0
61	1a	3	Total 3	O 3	0	0
61	1a	1	Total 1	O 1	0	0
61	1a	5	Total 5	O 5	0	0
61	1a	2	Total 2	O 2	0	0
61	1a	4	Total 4	O 4	0	0
61	1a	1	Total 1	O 1	0	0
61	1a	1	Total 1	O 1	0	0
61	1a	6	Total 6	O 6	0	0
61	1a	5	Total 5	O 5	0	0
61	1a	4	Total 4	O 4	0	0
61	1a	1	Total 1	O 1	0	0
61	1a	4	Total 4	O 4	0	0
61	1a	2	Total 2	O 2	0	0
61	1a	1	Total 1	O 1	0	0
61	1a	1	Total 1	O 1	0	0
61	1a	1	Total 1	O 1	0	0
61	1a	6	Total 6	O 6	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
61	1a	3	Total 3	O 3	0	0
61	1a	1	Total 1	O 1	0	0
61	1a	6	Total 6	O 6	0	0
61	1a	3	Total 3	O 3	0	0
61	1a	1	Total 1	O 1	0	0
61	1a	3	Total 3	O 3	0	0
61	1a	1	Total 1	O 1	0	0
61	1a	4	Total 4	O 4	0	0
61	1a	4	Total 4	O 4	0	0
61	1a	6	Total 6	O 6	0	0
61	1a	5	Total 5	O 5	0	0
61	1a	5	Total 5	O 5	0	0
61	1a	5	Total 5	O 5	0	0
61	1a	5	Total 5	O 5	0	0
61	1a	6	Total 6	O 6	0	0
61	1a	4	Total 4	O 4	0	0
61	1a	4	Total 4	O 4	0	0
61	1a	6	Total 6	O 6	0	0
61	1a	4	Total 4	O 4	0	0
61	1a	4	Total 4	O 4	0	0
61	1a	2	Total 2	O 2	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
61	1a	4	Total 4	O 4	0	0
61	1a	6	Total 6	O 6	0	0
61	1a	4	Total 4	O 4	0	0
61	1a	6	Total 6	O 6	0	0
61	1a	6	Total 6	O 6	0	0
61	1a	6	Total 6	O 6	0	0
61	1a	6	Total 6	O 6	0	0
61	1a	6	Total 6	O 6	0	0
61	1a	5	Total 5	O 5	0	0
61	1a	4	Total 4	O 4	0	0
61	1a	6	Total 6	O 6	0	0
61	1a	6	Total 6	O 6	0	0
61	1a	6	Total 6	O 6	0	0
61	1a	6	Total 6	O 6	0	0
61	1a	6	Total 6	O 6	0	0
61	1a	6	Total 6	O 6	0	0
61	1a	6	Total 6	O 6	0	0
61	1a	2	Total 2	O 2	0	0
61	1a	4	Total 4	O 4	0	0
61	1a	5	Total 5	O 5	0	0
61	1a	6	Total 6	O 6	0	0
61	1a	6	Total 6	O 6	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
61	1a	4	Total 4	O 4	0	0
61	1a	6	Total 6	O 6	0	0
61	1a	5	Total 5	O 5	0	0
61	1a	6	Total 6	O 6	0	0
61	1a	2	Total 2	O 2	0	0
61	1a	1	Total 1	O 1	0	0
61	1a	1	Total 1	O 1	0	0
61	1a	1	Total 1	O 1	0	0
61	1a	2	Total 2	O 2	0	0
61	1a	1	Total 1	O 1	0	0
61	1a	1	Total 1	O 1	0	0
61	1a	2	Total 2	O 2	0	0
61	1a	1	Total 1	O 1	0	0
61	1a	78	Total 78	O 78	0	0
61	1b	1	Total 1	O 1	0	0
61	1d	1	Total 1	O 1	0	0
61	1f	1	Total 1	O 1	0	0
61	1l	6	Total 6	O 6	0	0
61	1l	1	Total 1	O 1	0	0
61	1q	4	Total 4	O 4	0	0
61	1w	6	Total 6	O 6	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
61	1w	1	Total 1	O 1	0	0
61	1w	9	Total 9	O 9	0	0
61	1x	3	Total 3	O 3	0	0
61	1x	2	Total 2	O 2	0	0
61	1x	1	Total 1	O 1	0	0
61	1x	2	Total 2	O 2	0	0
61	1x	1	Total 1	O 1	0	0
61	1x	1	Total 1	O 1	0	0
61	1x	5	Total 5	O 5	0	0
61	1y	1	Total 1	O 1	0	0
61	2A	6	Total 6	O 6	0	0
61	2A	5	Total 5	O 5	0	0
61	2A	6	Total 6	O 6	0	0
61	2A	1	Total 1	O 1	0	0
61	2A	1	Total 1	O 1	0	0
61	2A	5	Total 5	O 5	0	0
61	2A	4	Total 4	O 4	0	0
61	2A	3	Total 3	O 3	0	0
61	2A	1	Total 1	O 1	0	0
61	2A	3	Total 3	O 3	0	0
61	2A	1	Total 1	O 1	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
61	2A	1	Total 1	O 1	0	0
61	2A	5	Total 5	O 5	0	0
61	2A	3	Total 3	O 3	0	0
61	2A	6	Total 6	O 6	0	0
61	2A	1	Total 1	O 1	0	0
61	2A	5	Total 5	O 5	0	0
61	2A	3	Total 3	O 3	0	0
61	2A	1	Total 1	O 1	0	0
61	2A	1	Total 1	O 1	0	0
61	2A	2	Total 2	O 2	0	0
61	2A	5	Total 5	O 5	0	0
61	2A	1	Total 1	O 1	0	0
61	2A	1	Total 1	O 1	0	0
61	2A	4	Total 4	O 4	0	0
61	2A	5	Total 5	O 5	0	0
61	2A	2	Total 2	O 2	0	0
61	2A	5	Total 5	O 5	0	0
61	2A	5	Total 5	O 5	0	0
61	2A	5	Total 5	O 5	0	0
61	2A	2	Total 2	O 2	0	0
61	2A	1	Total 1	O 1	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
61	2A	1	Total O 1 1	0	0
61	2A	1	Total O 1 1	0	0
61	2A	2	Total O 2 2	0	0
61	2A	2	Total O 2 2	0	0
61	2A	2	Total O 2 2	0	0
61	2A	2	Total O 2 2	0	0
61	2A	1	Total O 1 1	0	0
61	2A	1	Total O 1 1	0	0
61	2A	1	Total O 1 1	0	0
61	2A	1	Total O 1 1	0	0
61	2A	3	Total O 3 3	0	0
61	2A	5	Total O 5 5	0	0
61	2A	4	Total O 4 4	0	0
61	2A	5	Total O 5 5	0	0
61	2A	5	Total O 5 5	0	0
61	2A	3	Total O 3 3	0	0
61	2A	1	Total O 1 1	0	0
61	2A	4	Total O 4 4	0	0
61	2A	5	Total O 5 5	0	0
61	2A	5	Total O 5 5	0	0
61	2A	3	Total O 3 3	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
61	2A	4	Total 4	O 4	0	0
61	2A	4	Total 4	O 4	0	0
61	2A	3	Total 3	O 3	0	0
61	2A	1	Total 1	O 1	0	0
61	2A	4	Total 4	O 4	0	0
61	2A	4	Total 4	O 4	0	0
61	2A	3	Total 3	O 3	0	0
61	2A	5	Total 5	O 5	0	0
61	2A	5	Total 5	O 5	0	0
61	2A	3	Total 3	O 3	0	0
61	2A	2	Total 2	O 2	0	0
61	2A	3	Total 3	O 3	0	0
61	2A	4	Total 4	O 4	0	0
61	2A	5	Total 5	O 5	0	0
61	2A	4	Total 4	O 4	0	0
61	2A	4	Total 4	O 4	0	0
61	2A	5	Total 5	O 5	0	0
61	2A	2	Total 2	O 2	0	0
61	2A	1	Total 1	O 1	0	0
61	2A	4	Total 4	O 4	0	0
61	2A	2	Total 2	O 2	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
61	2A	4	Total 4	O 4	0	0
61	2A	3	Total 3	O 3	0	0
61	2A	5	Total 5	O 5	0	0
61	2A	3	Total 3	O 3	0	0
61	2A	2	Total 2	O 2	0	0
61	2A	1	Total 1	O 1	0	0
61	2A	1	Total 1	O 1	0	0
61	2A	1	Total 1	O 1	0	0
61	2A	1	Total 1	O 1	0	0
61	2A	2	Total 2	O 2	0	0
61	2A	1	Total 1	O 1	0	0
61	2A	1	Total 1	O 1	0	0
61	2A	2	Total 2	O 2	0	0
61	2A	2	Total 2	O 2	0	0
61	2A	6	Total 6	O 6	0	0
61	2A	1	Total 1	O 1	0	0
61	2A	5	Total 5	O 5	0	0
61	2A	1	Total 1	O 1	0	0
61	2A	4	Total 4	O 4	0	0
61	2A	2	Total 2	O 2	0	0
61	2A	6	Total 6	O 6	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
61	2A	6	Total 6	O 6	0	0
61	2A	2	Total 2	O 2	0	0
61	2A	1	Total 1	O 1	0	0
61	2A	1	Total 1	O 1	0	0
61	2A	1	Total 1	O 1	0	0
61	2A	2	Total 2	O 2	0	0
61	2A	2	Total 2	O 2	0	0
61	2A	4	Total 4	O 4	0	0
61	2A	2	Total 2	O 2	0	0
61	2A	2	Total 2	O 2	0	0
61	2A	1	Total 1	O 1	0	0
61	2A	2	Total 2	O 2	0	0
61	2A	1	Total 1	O 1	0	0
61	2A	1	Total 1	O 1	0	0
61	2A	6	Total 6	O 6	0	0
61	2A	5	Total 5	O 5	0	0
61	2A	4	Total 4	O 4	0	0
61	2A	3	Total 3	O 3	0	0
61	2A	2	Total 2	O 2	0	0
61	2A	4	Total 4	O 4	0	0
61	2A	4	Total 4	O 4	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
61	2A	4	Total 4	O 4	0	0
61	2A	4	Total 4	O 4	0	0
61	2A	3	Total 3	O 3	0	0
61	2A	5	Total 5	O 5	0	0
61	2A	2	Total 2	O 2	0	0
61	2A	1	Total 1	O 1	0	0
61	2A	3	Total 3	O 3	0	0
61	2A	1	Total 1	O 1	0	0
61	2A	5	Total 5	O 5	0	0
61	2A	5	Total 5	O 5	0	0
61	2A	1	Total 1	O 1	0	0
61	2A	1	Total 1	O 1	0	0
61	2A	3	Total 3	O 3	0	0
61	2A	1	Total 1	O 1	0	0
61	2A	1	Total 1	O 1	0	0
61	2A	3	Total 3	O 3	0	0
61	2A	4	Total 4	O 4	0	0
61	2A	3	Total 3	O 3	0	0
61	2A	2	Total 2	O 2	0	0
61	2A	5	Total 5	O 5	0	0
61	2A	1	Total 1	O 1	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
61	2A	1	Total 1	O 1	0	0
61	2A	4	Total 4	O 4	0	0
61	2A	4	Total 4	O 4	0	0
61	2A	1	Total 1	O 1	0	0
61	2A	2	Total 2	O 2	0	0
61	2A	2	Total 2	O 2	0	0
61	2A	4	Total 4	O 4	0	0
61	2A	1	Total 1	O 1	0	0
61	2A	2	Total 2	O 2	0	0
61	2A	1	Total 1	O 1	0	0
61	2A	1	Total 1	O 1	0	0
61	2A	5	Total 5	O 5	0	0
61	2A	2	Total 2	O 2	0	0
61	2A	1	Total 1	O 1	0	0
61	2A	1	Total 1	O 1	0	0
61	2A	2	Total 2	O 2	0	0
61	2A	1	Total 1	O 1	0	0
61	2A	1	Total 1	O 1	0	0
61	2A	3	Total 3	O 3	0	0
61	2A	3	Total 3	O 3	0	0
61	2A	2	Total 2	O 2	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
61	2A	1	Total 1	O 1	0	0
61	2A	2	Total 2	O 2	0	0
61	2A	1	Total 1	O 1	0	0
61	2A	1	Total 1	O 1	0	0
61	2A	2	Total 2	O 2	0	0
61	2A	3	Total 3	O 3	0	0
61	2A	1	Total 1	O 1	0	0
61	2A	2	Total 2	O 2	0	0
61	2A	2	Total 2	O 2	0	0
61	2A	1	Total 1	O 1	0	0
61	2A	1	Total 1	O 1	0	0
61	2A	3	Total 3	O 3	0	0
61	2A	1	Total 1	O 1	0	0
61	2A	2	Total 2	O 2	0	0
61	2A	2	Total 2	O 2	0	0
61	2A	1	Total 1	O 1	0	0
61	2A	1	Total 1	O 1	0	0
61	2A	1	Total 1	O 1	0	0
61	2A	2	Total 2	O 2	0	0
61	2A	4	Total 4	O 4	0	0
61	2A	3	Total 3	O 3	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
61	2A	2	Total 2	O 2	0	0
61	2A	2	Total 2	O 2	0	0
61	2A	2	Total 2	O 2	0	0
61	2A	1	Total 1	O 1	0	0
61	2A	5	Total 5	O 5	0	0
61	2A	1	Total 1	O 1	0	0
61	2A	1	Total 1	O 1	0	0
61	2A	1	Total 1	O 1	0	0
61	2A	4	Total 4	O 4	0	0
61	2A	2	Total 2	O 2	0	0
61	2A	2	Total 2	O 2	0	0
61	2A	1	Total 1	O 1	0	0
61	2A	2	Total 2	O 2	0	0
61	2A	1	Total 1	O 1	0	0
61	2A	1	Total 1	O 1	0	0
61	2A	2	Total 2	O 2	0	0
61	2A	2	Total 2	O 2	0	0
61	2A	1	Total 1	O 1	0	0
61	2A	4	Total 4	O 4	0	0
61	2A	4	Total 4	O 4	0	0
61	2A	2	Total 2	O 2	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
61	2A	2	Total	O	0	0
			2	2		
61	2A	3	Total	O	0	0
			3	3		
61	2A	3	Total	O	0	0
			3	3		
61	2A	1	Total	O	0	0
			1	1		
61	2A	2	Total	O	0	0
			2	2		
61	2A	2	Total	O	0	0
			2	2		
61	2A	6	Total	O	0	0
			6	6		
61	2A	3	Total	O	0	0
			3	3		
61	2A	4	Total	O	0	0
			4	4		
61	2A	2	Total	O	0	0
			2	2		
61	2A	1	Total	O	0	0
			1	1		
61	2A	4	Total	O	0	0
			4	4		
61	2A	3	Total	O	0	0
			3	3		
61	2A	3	Total	O	0	0
			3	3		
61	2A	6	Total	O	0	0
			6	6		
61	2A	2	Total	O	0	0
			2	2		
61	2A	4	Total	O	0	0
			4	4		
61	2A	2	Total	O	0	0
			2	2		
61	2A	2	Total	O	0	0
			2	2		
61	2A	1	Total	O	0	0
			1	1		
61	2A	2	Total	O	0	0
			2	2		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
61	2A	2	Total	O	0	0
			2	2		
61	2A	6	Total	O	0	0
			6	6		
61	2A	4	Total	O	0	0
			4	4		
61	2A	1	Total	O	0	0
			1	1		
61	2A	5	Total	O	0	0
			5	5		
61	2A	4	Total	O	0	0
			4	4		
61	2A	1	Total	O	0	0
			1	1		
61	2A	1	Total	O	0	0
			1	1		
61	2A	2	Total	O	0	0
			2	2		
61	2A	2	Total	O	0	0
			2	2		
61	2A	6	Total	O	0	0
			6	6		
61	2A	2	Total	O	0	0
			2	2		
61	2A	1	Total	O	0	0
			1	1		
61	2A	3	Total	O	0	0
			3	3		
61	2A	1	Total	O	0	0
			1	1		
61	2A	2	Total	O	0	0
			2	2		
61	2A	2	Total	O	0	0
			2	2		
61	2A	2	Total	O	0	0
			2	2		
61	2A	3	Total	O	0	0
			3	3		
61	2A	4	Total	O	0	0
			4	4		
61	2A	4	Total	O	0	0
			4	4		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
61	2A	1	Total 1	O 1	0	0
61	2A	2	Total 2	O 2	0	0
61	2A	1	Total 1	O 1	0	0
61	2A	1	Total 1	O 1	0	0
61	2A	6	Total 6	O 6	0	0
61	2A	1	Total 1	O 1	0	0
61	2A	3	Total 3	O 3	0	0
61	2A	1	Total 1	O 1	0	0
61	2A	1	Total 1	O 1	0	0
61	2A	2	Total 2	O 2	0	0
61	2A	2	Total 2	O 2	0	0
61	2A	1	Total 1	O 1	0	0
61	2A	2	Total 2	O 2	0	0
61	2A	2	Total 2	O 2	0	0
61	2A	3	Total 3	O 3	0	0
61	2A	3	Total 3	O 3	0	0
61	2A	1	Total 1	O 1	0	0
61	2A	4	Total 4	O 4	0	0
61	2A	1	Total 1	O 1	0	0
61	2A	1	Total 1	O 1	0	0
61	2A	1	Total 1	O 1	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
61	2A	1	Total 1	O 1	0	0
61	2A	1	Total 1	O 1	0	0
61	2A	2	Total 2	O 2	0	0
61	2A	4	Total 4	O 4	0	0
61	2A	1	Total 1	O 1	0	0
61	2A	1	Total 1	O 1	0	0
61	2A	3	Total 3	O 3	0	0
61	2A	1	Total 1	O 1	0	0
61	2A	1	Total 1	O 1	0	0
61	2A	2	Total 2	O 2	0	0
61	2A	2	Total 2	O 2	0	0
61	2A	5	Total 5	O 5	0	0
61	2A	4	Total 4	O 4	0	0
61	2A	1	Total 1	O 1	0	0
61	2A	1	Total 1	O 1	0	0
61	2A	1	Total 1	O 1	0	0
61	2A	3	Total 3	O 3	0	0
61	2A	2	Total 2	O 2	0	0
61	2A	1	Total 1	O 1	0	0
61	2A	5	Total 5	O 5	0	0
61	2A	1	Total 1	O 1	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
61	2A	2	Total 2	O 2	0	0
61	2A	5	Total 5	O 5	0	0
61	2A	6	Total 6	O 6	0	0
61	2A	3	Total 3	O 3	0	0
61	2A	6	Total 6	O 6	0	0
61	2A	6	Total 6	O 6	0	0
61	2A	5	Total 5	O 5	0	0
61	2A	3	Total 3	O 3	0	0
61	2A	6	Total 6	O 6	0	0
61	2A	6	Total 6	O 6	0	0
61	2A	3	Total 3	O 3	0	0
61	2A	4	Total 4	O 4	0	0
61	2A	3	Total 3	O 3	0	0
61	2A	1	Total 1	O 1	0	0
61	2A	6	Total 6	O 6	0	0
61	2A	6	Total 6	O 6	0	0
61	2A	6	Total 6	O 6	0	0
61	2A	5	Total 5	O 5	0	0
61	2A	4	Total 4	O 4	0	0
61	2A	5	Total 5	O 5	0	0
61	2A	6	Total 6	O 6	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
61	2A	4	Total 4	O 4	0	0
61	2A	6	Total 6	O 6	0	0
61	2A	5	Total 5	O 5	0	0
61	2A	3	Total 3	O 3	0	0
61	2A	3	Total 3	O 3	0	0
61	2A	5	Total 5	O 5	0	0
61	2A	5	Total 5	O 5	0	0
61	2A	4	Total 4	O 4	0	0
61	2A	5	Total 5	O 5	0	0
61	2A	2	Total 2	O 2	0	0
61	2A	3	Total 3	O 3	0	0
61	2A	4	Total 4	O 4	0	0
61	2A	5	Total 5	O 5	0	0
61	2A	6	Total 6	O 6	0	0
61	2A	4	Total 4	O 4	0	0
61	2A	4	Total 4	O 4	0	0
61	2A	3	Total 3	O 3	0	0
61	2A	3	Total 3	O 3	0	0
61	2A	5	Total 5	O 5	0	0
61	2A	6	Total 6	O 6	0	0
61	2A	6	Total 6	O 6	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
61	2A	6	Total	O	0	0
			6	6		
61	2A	4	Total	O	0	0
			4	4		
61	2A	6	Total	O	0	0
			6	6		
61	2A	4	Total	O	0	0
			4	4		
61	2A	6	Total	O	0	0
			6	6		
61	2A	5	Total	O	0	0
			5	5		
61	2A	4	Total	O	0	0
			4	4		
61	2A	4	Total	O	0	0
			4	4		
61	2A	4	Total	O	0	0
			4	4		
61	2A	6	Total	O	0	0
			6	6		
61	2A	5	Total	O	0	0
			5	5		
61	2A	5	Total	O	0	0
			5	5		
61	2A	5	Total	O	0	0
			5	5		
61	2A	4	Total	O	0	0
			4	4		
61	2A	5	Total	O	0	0
			5	5		
61	2A	5	Total	O	0	0
			5	5		
61	2A	4	Total	O	0	0
			4	4		
61	2A	6	Total	O	0	0
			6	6		
61	2A	3	Total	O	0	0
			3	3		
61	2A	4	Total	O	0	0
			4	4		
61	2A	6	Total	O	0	0
			6	6		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
61	2A	5	Total	O	0	0
			5	5		
61	2A	5	Total	O	0	0
			5	5		
61	2A	6	Total	O	0	0
			6	6		
61	2A	6	Total	O	0	0
			6	6		
61	2A	6	Total	O	0	0
			6	6		
61	2A	4	Total	O	0	0
			4	4		
61	2A	6	Total	O	0	0
			6	6		
61	2A	5	Total	O	0	0
			5	5		
61	2A	4	Total	O	0	0
			4	4		
61	2A	5	Total	O	0	0
			5	5		
61	2A	5	Total	O	0	0
			5	5		
61	2A	5	Total	O	0	0
			5	5		
61	2A	4	Total	O	0	0
			4	4		
61	2A	6	Total	O	0	0
			6	6		
61	2A	6	Total	O	0	0
			6	6		
61	2A	6	Total	O	0	0
			6	6		
61	2A	6	Total	O	0	0
			6	6		
61	2A	5	Total	O	0	0
			5	5		
61	2A	5	Total	O	0	0
			5	5		
61	2A	5	Total	O	0	0
			5	5		
61	2A	6	Total	O	0	0
			6	6		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
61	2A	5	Total 5	O 5	0	0
61	2A	3	Total 3	O 3	0	0
61	2A	6	Total 6	O 6	0	0
61	2A	6	Total 6	O 6	0	0
61	2A	4	Total 4	O 4	0	0
61	2A	4	Total 4	O 4	0	0
61	2A	1	Total 1	O 1	0	0
61	2A	4	Total 4	O 4	0	0
61	2A	2	Total 2	O 2	0	0
61	2A	3	Total 3	O 3	0	0
61	2A	2	Total 2	O 2	0	0
61	2A	2	Total 2	O 2	0	0
61	2A	2	Total 2	O 2	0	0
61	2A	2	Total 2	O 2	0	0
61	2A	1	Total 1	O 1	0	0
61	2A	1	Total 1	O 1	0	0
61	2A	2	Total 2	O 2	0	0
61	2A	1	Total 1	O 1	0	0
61	2A	2	Total 2	O 2	0	0
61	2A	2	Total 2	O 2	0	0
61	2A	2	Total 2	O 2	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
61	2A	6	Total 6	O 6	0	0
61	2A	222	Total 222	O 222	0	0
61	2B	2	Total 2	O 2	0	0
61	2B	3	Total 3	O 3	0	0
61	2B	3	Total 3	O 3	0	0
61	2B	1	Total 1	O 1	0	0
61	2B	2	Total 2	O 2	0	0
61	2B	1	Total 1	O 1	0	0
61	2B	1	Total 1	O 1	0	0
61	2B	12	Total 12	O 12	0	0
61	2D	5	Total 5	O 5	0	0
61	2D	3	Total 3	O 3	0	0
61	2D	2	Total 2	O 2	0	0
61	2D	7	Total 7	O 7	0	0
61	2E	3	Total 3	O 3	0	0
61	2F	6	Total 6	O 6	0	0
61	2I	3	Total 3	O 3	0	0
61	2N	1	Total 1	O 1	0	0
61	2O	1	Total 1	O 1	0	0
61	2P	5	Total 5	O 5	0	0
61	2P	2	Total 2	O 2	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
61	2P	4	Total 4	O 4	0	0
61	2Q	1	Total 1	O 1	0	0
61	2Q	1	Total 1	O 1	0	0
61	2R	1	Total 1	O 1	0	0
61	2R	2	Total 2	O 2	0	0
61	2T	2	Total 2	O 2	0	0
61	2T	3	Total 3	O 3	0	0
61	2U	2	Total 2	O 2	0	0
61	2W	3	Total 3	O 3	0	0
61	2Z	1	Total 1	O 1	0	0
61	20	6	Total 6	O 6	0	0
61	20	2	Total 2	O 2	0	0
61	20	2	Total 2	O 2	0	0
61	21	6	Total 6	O 6	0	0
61	22	1	Total 1	O 1	0	0
61	25	4	Total 4	O 4	0	0
61	27	1	Total 1	O 1	0	0
61	27	1	Total 1	O 1	0	0
61	28	4	Total 4	O 4	0	0
61	28	1	Total 1	O 1	0	0
61	28	1	Total 1	O 1	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
61	29	1	Total	O	0	0
			1	1		
61	2a	6	Total	O	0	0
			6	6		
61	2a	6	Total	O	0	0
			6	6		
61	2a	5	Total	O	0	0
			5	5		
61	2a	5	Total	O	0	0
			5	5		
61	2a	4	Total	O	0	0
			4	4		
61	2a	6	Total	O	0	0
			6	6		
61	2a	6	Total	O	0	0
			6	6		
61	2a	6	Total	O	0	0
			6	6		
61	2a	5	Total	O	0	0
			5	5		
61	2a	5	Total	O	0	0
			5	5		
61	2a	3	Total	O	0	0
			3	3		
61	2a	5	Total	O	0	0
			5	5		
61	2a	4	Total	O	0	0
			4	4		
61	2a	6	Total	O	0	0
			6	6		
61	2a	3	Total	O	0	0
			3	3		
61	2a	5	Total	O	0	0
			5	5		
61	2a	6	Total	O	0	0
			6	6		
61	2a	4	Total	O	0	0
			4	4		
61	2a	4	Total	O	0	0
			4	4		
61	2a	2	Total	O	0	0
			2	2		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
61	2a	6	Total 6	O 6	0	0
61	2a	5	Total 5	O 5	0	0
61	2a	3	Total 3	O 3	0	0
61	2a	6	Total 6	O 6	0	0
61	2a	3	Total 3	O 3	0	0
61	2a	6	Total 6	O 6	0	0
61	2a	5	Total 5	O 5	0	0
61	2a	4	Total 4	O 4	0	0
61	2a	3	Total 3	O 3	0	0
61	2a	5	Total 5	O 5	0	0
61	2a	6	Total 6	O 6	0	0
61	2a	6	Total 6	O 6	0	0
61	2a	5	Total 5	O 5	0	0
61	2a	5	Total 5	O 5	0	0
61	2a	2	Total 2	O 2	0	0
61	2a	4	Total 4	O 4	0	0
61	2a	6	Total 6	O 6	0	0
61	2a	6	Total 6	O 6	0	0
61	2a	5	Total 5	O 5	0	0
61	2a	5	Total 5	O 5	0	0
61	2a	4	Total 4	O 4	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
61	2a	5	Total 5	O 5	0	0
61	2a	6	Total 6	O 6	0	0
61	2a	5	Total 5	O 5	0	0
61	2a	6	Total 6	O 6	0	0
61	2a	3	Total 3	O 3	0	0
61	2a	6	Total 6	O 6	0	0
61	2a	1	Total 1	O 1	0	0
61	2a	2	Total 2	O 2	0	0
61	2a	3	Total 3	O 3	0	0
61	2a	2	Total 2	O 2	0	0
61	2a	5	Total 5	O 5	0	0
61	2a	4	Total 4	O 4	0	0
61	2a	2	Total 2	O 2	0	0
61	2a	2	Total 2	O 2	0	0
61	2a	1	Total 1	O 1	0	0
61	2a	2	Total 2	O 2	0	0
61	2a	1	Total 1	O 1	0	0
61	2a	5	Total 5	O 5	0	0
61	2a	1	Total 1	O 1	0	0
61	2a	4	Total 4	O 4	0	0
61	2a	1	Total 1	O 1	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
61	2a	2	Total 2	O 2	0	0
61	2a	1	Total 1	O 1	0	0
61	2a	2	Total 2	O 2	0	0
61	2a	2	Total 2	O 2	0	0
61	2a	1	Total 1	O 1	0	0
61	2a	2	Total 2	O 2	0	0
61	2a	1	Total 1	O 1	0	0
61	2a	1	Total 1	O 1	0	0
61	2a	3	Total 3	O 3	0	0
61	2a	3	Total 3	O 3	0	0
61	2a	1	Total 1	O 1	0	0
61	2a	1	Total 1	O 1	0	0
61	2a	3	Total 3	O 3	0	0
61	2a	2	Total 2	O 2	0	0
61	2a	3	Total 3	O 3	0	0
61	2a	4	Total 4	O 4	0	0
61	2a	1	Total 1	O 1	0	0
61	2a	1	Total 1	O 1	0	0
61	2a	4	Total 4	O 4	0	0
61	2a	4	Total 4	O 4	0	0
61	2a	2	Total 2	O 2	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
61	2a	2	Total	O	0	0
			2	2		
61	2a	2	Total	O	0	0
			2	2		
61	2a	1	Total	O	0	0
			1	1		
61	2a	1	Total	O	0	0
			1	1		
61	2a	1	Total	O	0	0
			1	1		
61	2a	1	Total	O	0	0
			1	1		
61	2a	1	Total	O	0	0
			1	1		
61	2a	1	Total	O	0	0
			1	1		
61	2a	1	Total	O	0	0
			1	1		
61	2a	1	Total	O	0	0
			1	1		
61	2a	1	Total	O	0	0
			1	1		
61	2a	2	Total	O	0	0
			2	2		
61	2a	2	Total	O	0	0
			2	2		
61	2a	2	Total	O	0	0
			2	2		
61	2a	1	Total	O	0	0
			1	1		
61	2a	2	Total	O	0	0
			2	2		
61	2a	1	Total	O	0	0
			1	1		
61	2a	2	Total	O	0	0
			2	2		

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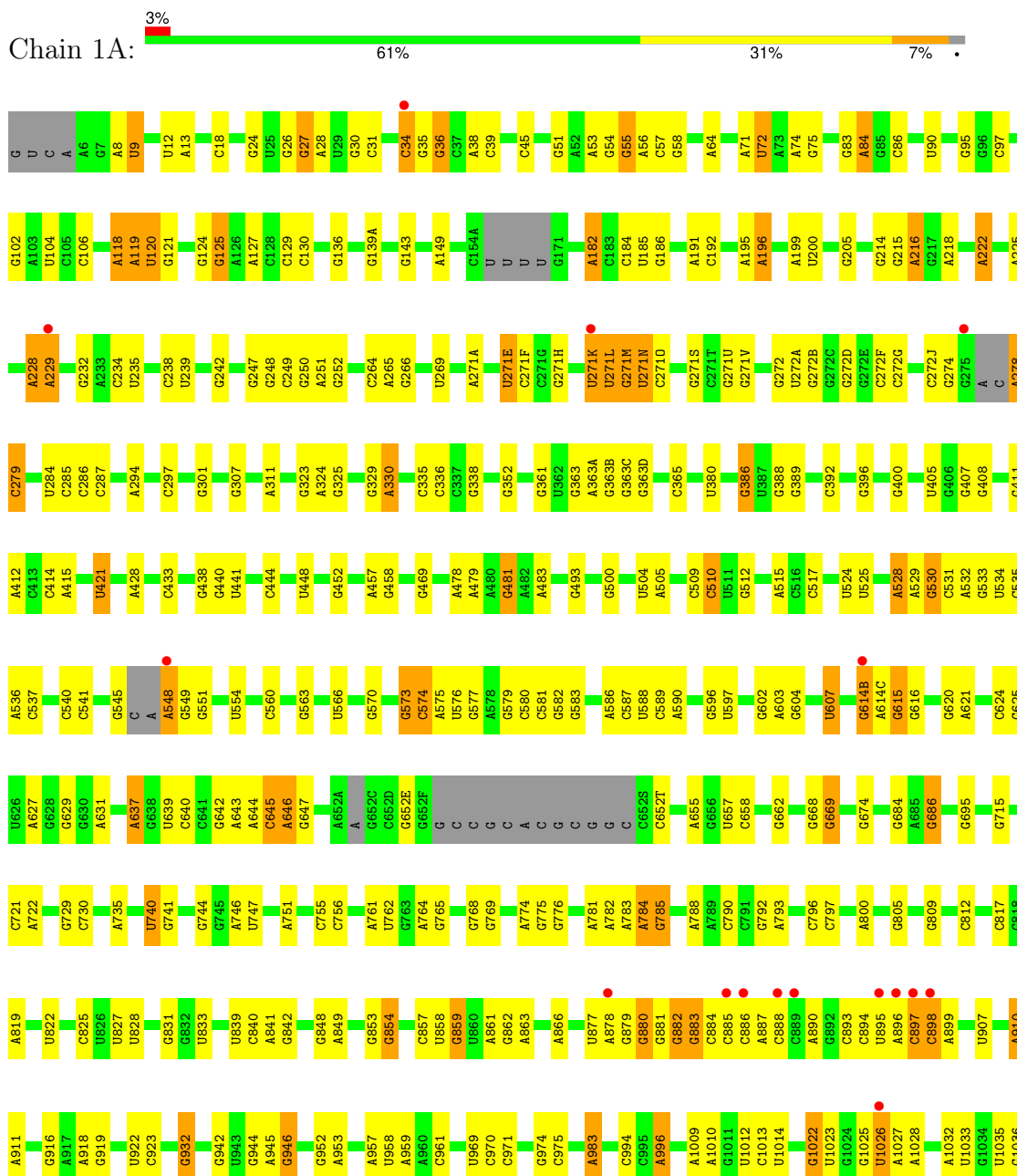
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
61	2a	2	Total 2	O 2	0	0
61	2a	2	Total 2	O 2	0	0
61	2a	40	Total 40	O 40	0	0
61	2d	1	Total 1	O 1	0	0
61	2g	1	Total 1	O 1	0	0
61	2i	1	Total 1	O 1	0	0
61	2j	2	Total 2	O 2	0	0
61	2j	1	Total 1	O 1	0	0
61	2l	1	Total 1	O 1	0	0
61	2l	1	Total 1	O 1	0	0
61	2p	1	Total 1	O 1	0	0
61	2r	1	Total 1	O 1	0	0
61	2t	2	Total 2	O 2	0	0
61	2x	2	Total 2	O 2	0	0
61	2x	2	Total 2	O 2	0	0
61	2x	3	Total 3	O 3	0	0
61	2y	6	Total 6	O 6	0	0
61	2y	1	Total 1	O 1	0	0
61	2y	6	Total 6	O 6	0	0

3 Residue-property plots

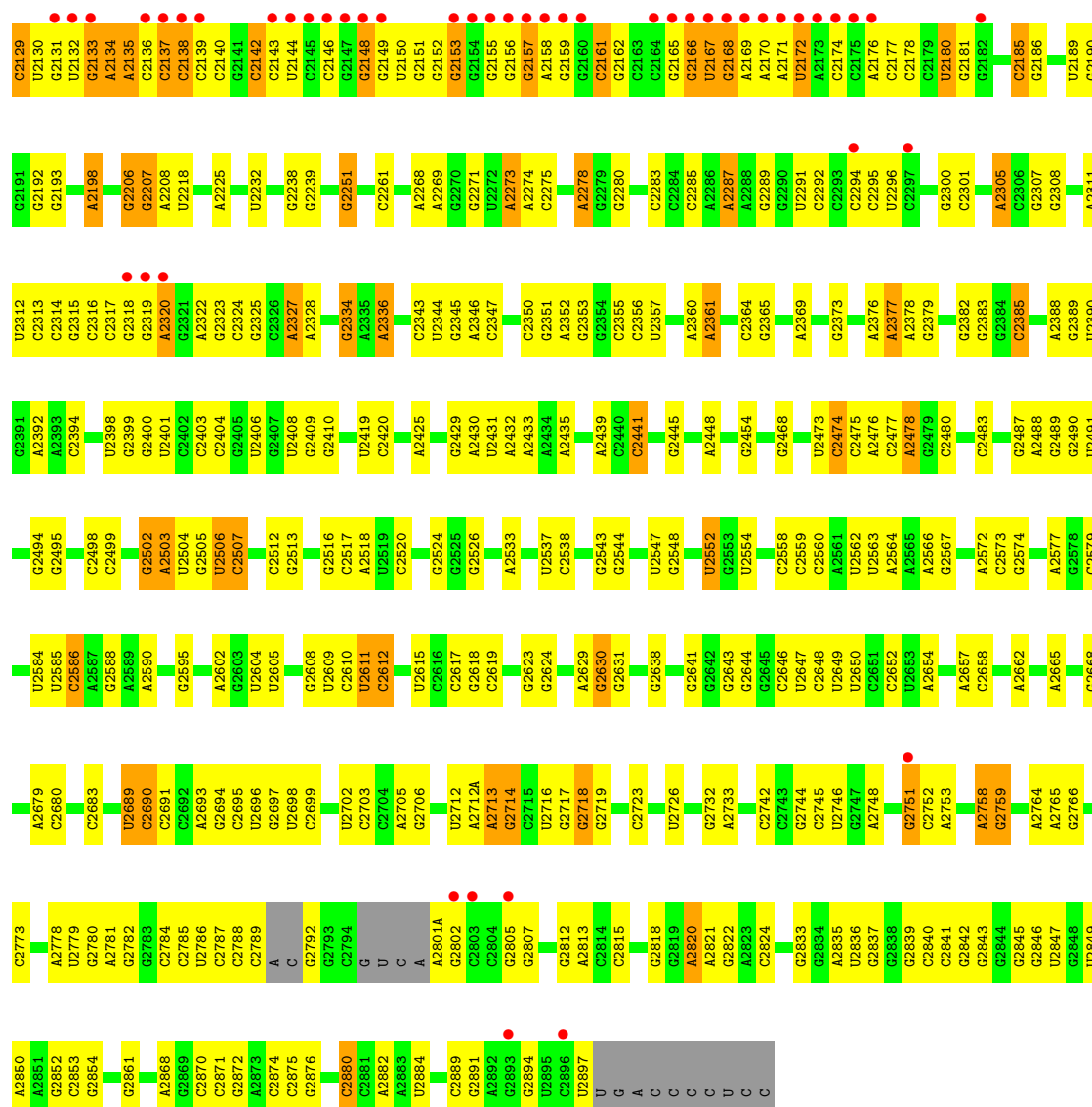
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

• Molecule 1: 23S Ribosomal RNA



G2400	G2308	G2187	A2033	C1924	G1799	A1545	G1429	A1302	U1205	G1100	G1037
G2406	A2309	C2188	G2038	G1929	C1800	A1558	C1430	G1303	U1210	U1101	C1038
G2407	A2311	U2189	C2039	G1930	G1801	G1559	C1431	G1309	A1210	C1102	G1039
U2408	G2312	G2190	C2040	A1932	A1802	U1692	C1432	G1309	U1211	A1103	C1040
G2409	G2313	G2191	U2041	A1932	A1803	U1693	U1433	G1310	G1212	C1104	C1041
G2410	G2314	G2192	A2042	G1933	G1816	A1566	A1439	U1312	G1216	U1105	G1044
	G2315	G2193	C2043	G1934	U1817	A1569	G1440	U1313	C2127	G1106	A1045
A2418		A2198	C2049	G1935	U1818	A1570	G1441	U1329	G1218	G1107	A1046
U2419	G2320	C2136	G2052	A1936	A1821	A1571	G1442	U1336	C1219	U1108	A1047
A2422	G2325	C2137	G2053	A1938	G1702	A1572		A1220	A1220	G1109	A1048
A2425	G2326	G2138	G2054	U1939	G1703	U1578	A1445	G1337	G1223	A1111	G1052
	G2327	U2140	A2054	C1942	C1712	G1581	G1447	U1352	A1226	U1113	C1053
G2429	A2328	C2141	G2056		U1713	G1582	G1448	A1352	A1226	G1114	A1054
A2430	G2329	C2142	G2056	G1952	G1714	C1584	A1449	A1353	A1226	G1115	G1055
U2431	G2330	G2143	A2060	A1953	C1830	C1584	G1450	A1354	G1230	G1116	G1056
A2432	G2331	U2144	G2061	A1953	G1718	A1586	G1450	G1355	G1231	G1117	A1057
		C2145	G2061	G1954	C1837	C1587	A1452	A1357	G1239	G1118	G1058
		C2146	G2065	U1955	A1722	C1588	U1453	G1358	U1240	G1119	G1059
		G2147	C2066	C1957	G1840	C1589	G1455	A1359	U1240	G1122	U1060
		G2228	C2066	C1957	A1847	G1593	G1465	A1360	G1244	G1125	G1062
		G2228	C2066	C1958	G1750	G1594	G1466	G1364	G1247	G1128	C1064
		G2232	G2070	C1962	A1853	G1594	G1467	A1365	A1247	A1129	U1065
		U2233	A2071	U1963	A1854	A1608	C1468	U1372	G1250	U1130	U1066
		G2234	G2086	G1964	G1858	A1609	A1469	A1373	C1251	G1135	A1067
		G2238	G2087	C1965	G1858	C1611	G1470	G1376	G1252	G1136	G1068
		G2243	G2087	A1966	G1861	G1619	G1478	G1376	A1253		A1069
		U2244	G2090	C1967	C1862	G1619	G1482	A1379	G1266		A1070
			G2096	U1968	G1863	C1636	G1488	G1380	U1267		G1071
			U2096	A1969	C1863	A1637	C1504	A1384	A1268		G1072
			G2100	A1970	C1866	C1638	C1505	G1385	A1269		A1073
			G2101	A1971	A1876	C1638	C1506	G1386	G1270		G1074
			U2102	A1972	C1877	A1641	A1507	U1396	G1271		C1075
			U2102	C1973	A1878	G1642	A1508	G1401	G1272		C1076
			U2102	U1993	C1881	G1645	A1509	C1402	A1273		A1077
			C2105	C1996	G1881	G1646	A1509A	U1405	U1274		A1078
			G2106	G1987	A1889	G1647	A1509B	U1406	A1275		U1079
			C2107	C1998	A1890	C1648	A1509B	C1407	A1276		C1080
			C2108	G2000	G1899	C1648	G1520	U1409	A1277		U1081
			U2109	A2001	A1900	A1652	G1520	U1409	A1278		U1082
			G2110	G2002	G1906	G1653	G1520	U1409	A1278		A1083
			C2111	U2011	G1906	A1654	G1520	U1409	A1278		A1084
			U2113	U2011	G1906	A1655	G1520	U1409	A1278		A1085
			A2114	G2012	U1911	C1656	G1520	U1409	A1278		A1086
			G2115	A2013	A1912	C1656	G1520	U1409	A1278		A1087
			G2116	A2014	A1913	C1656	G1520	U1409	A1278		A1088
			A2117	A2014	C1914	C1656	G1520	U1409	A1278		U1089
			U2118	A2020	U1915	C1656	G1520	U1409	A1278		U1090
			A2119	C2021	A1916	C1656	G1520	U1409	A1278		G1091
			G2120	G2022	U1917	C1656	G1520	U1409	A1278		C1092
			G2121	U2023	U1918	C1656	G1520	U1409	A1278		G1093
			U2122	G2023	A1918	C1656	G1520	U1409	A1278		U1094
			G2125	A2030	A1919	C1656	G1520	U1409	A1278		A1095
			G2125	A2031	C1920	C1656	G1520	U1409	A1278		A1096
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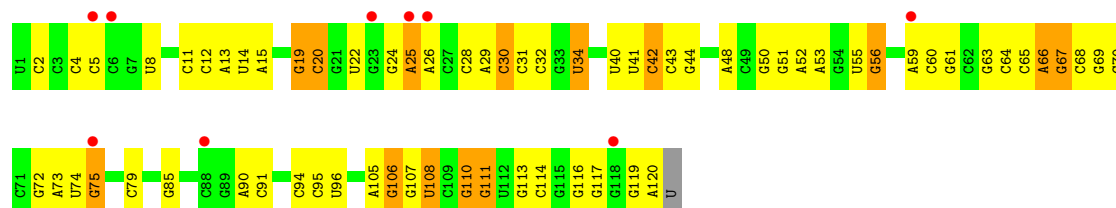
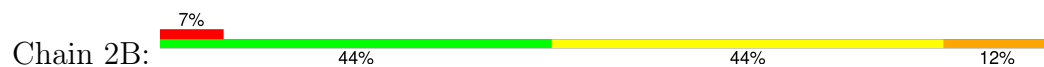




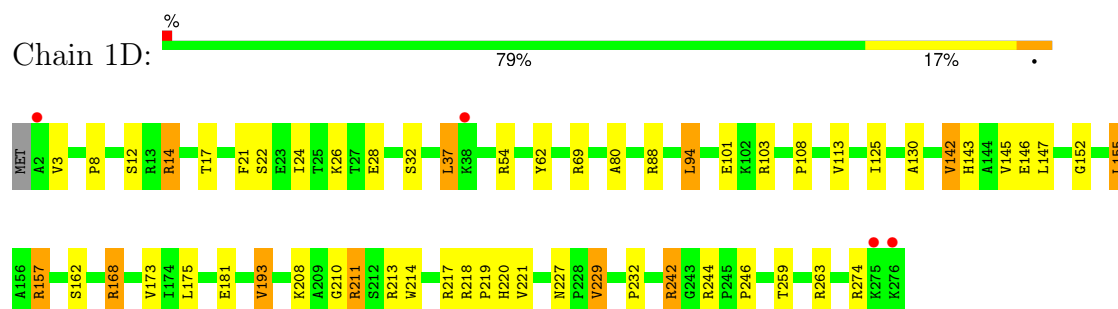
• Molecule 2: 5S Ribosomal RNA



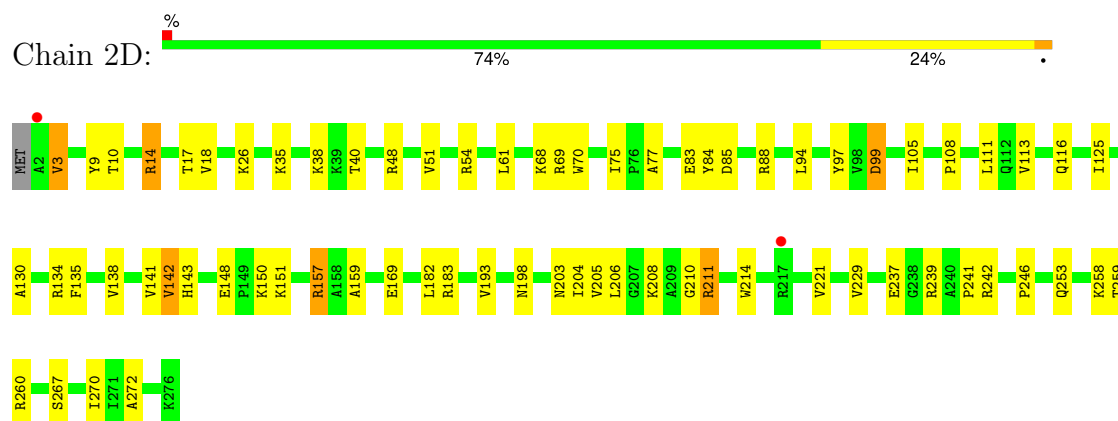
• Molecule 2: 5S Ribosomal RNA



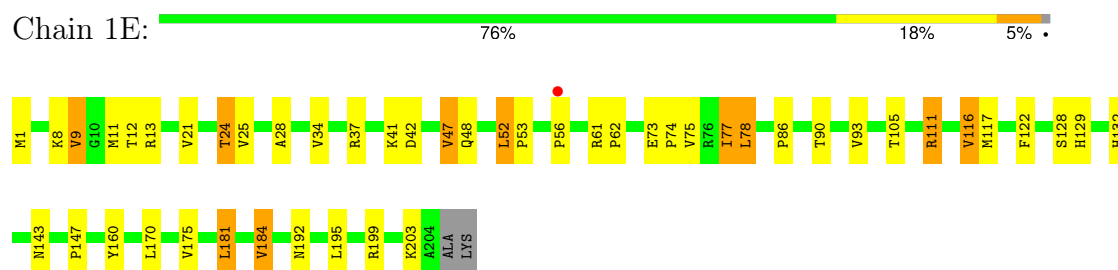
- Molecule 3: 50S ribosomal protein L2



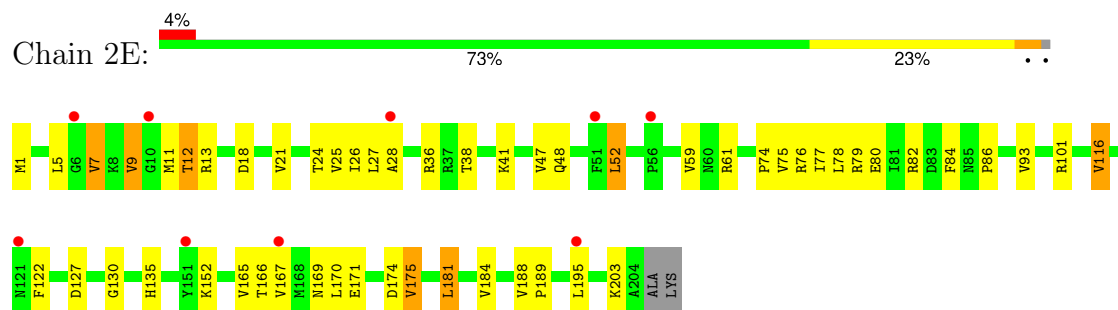
- Molecule 3: 50S ribosomal protein L2



- Molecule 4: 50S ribosomal protein L3

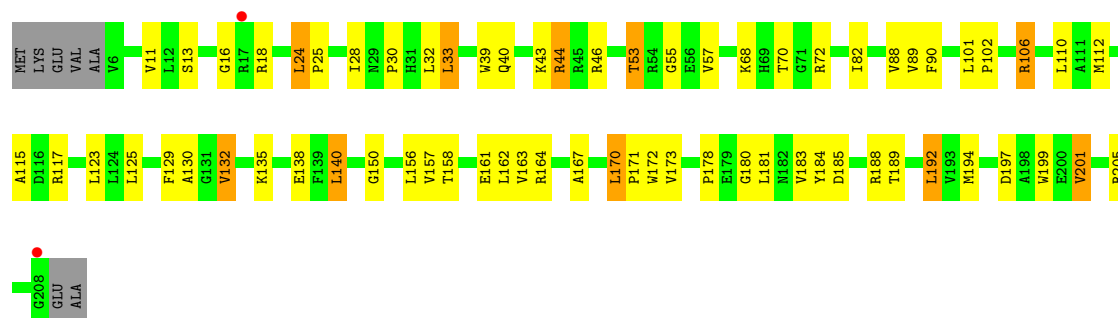


- Molecule 4: 50S ribosomal protein L3

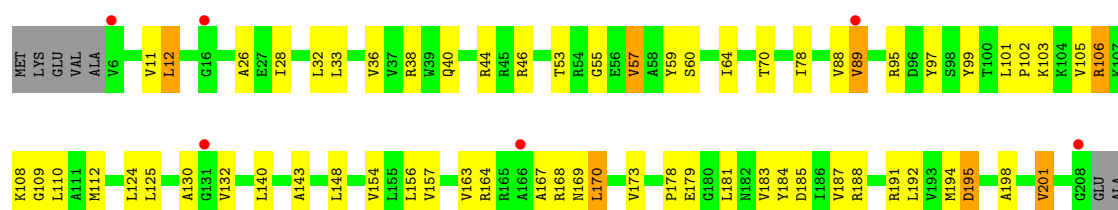


- Molecule 5: 50S ribosomal protein L4

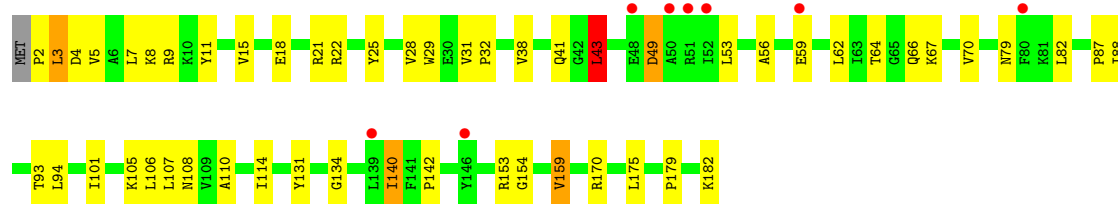




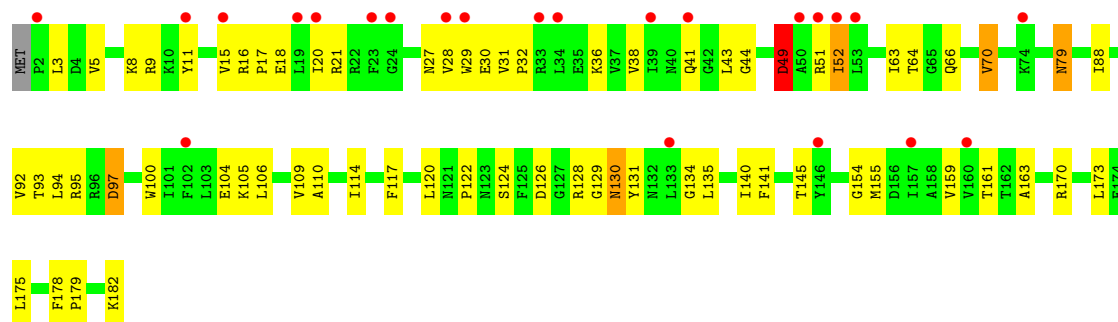
• Molecule 5: 50S ribosomal protein L4



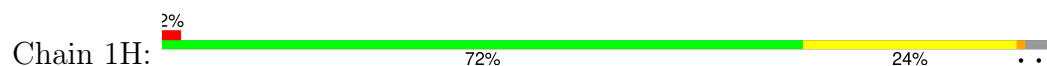
• Molecule 6: 50S ribosomal protein L5

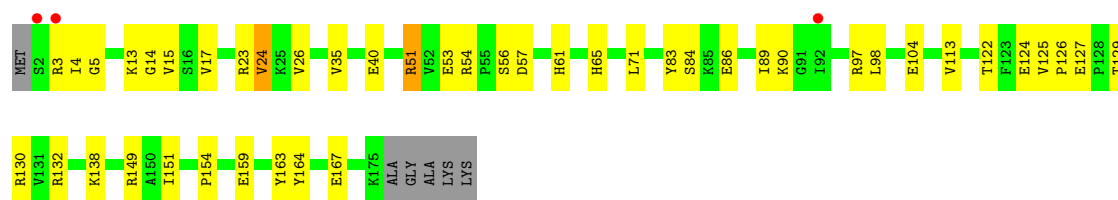


• Molecule 6: 50S ribosomal protein L5

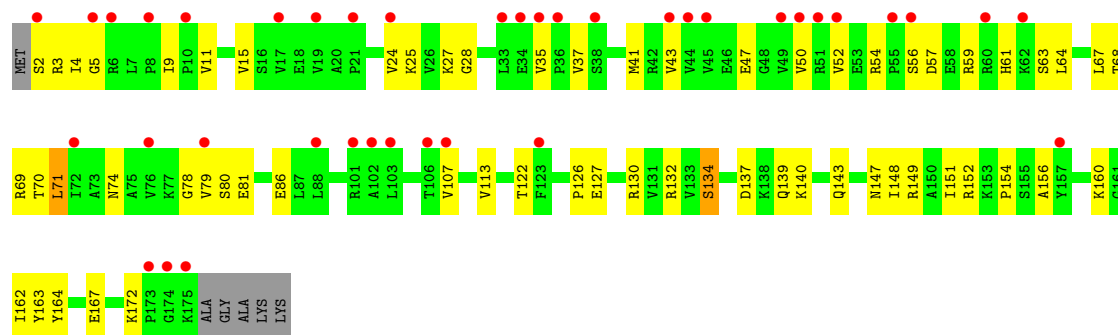


• Molecule 7: 50S ribosomal protein L6

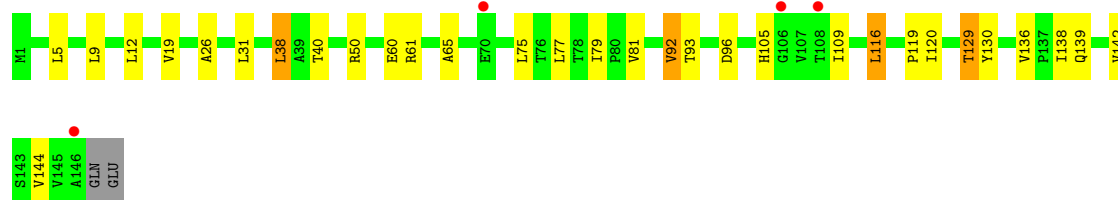
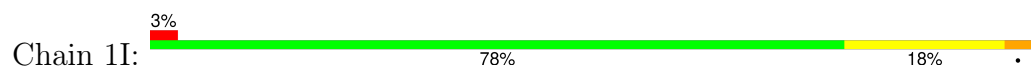




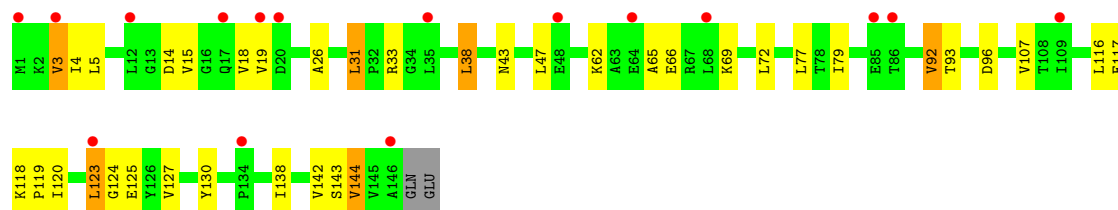
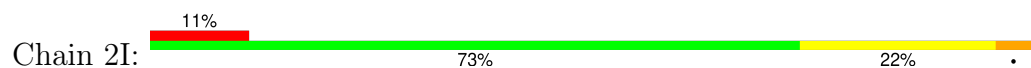
• Molecule 7: 50S ribosomal protein L6



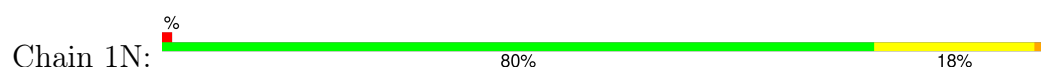
• Molecule 8: 50S ribosomal protein L9



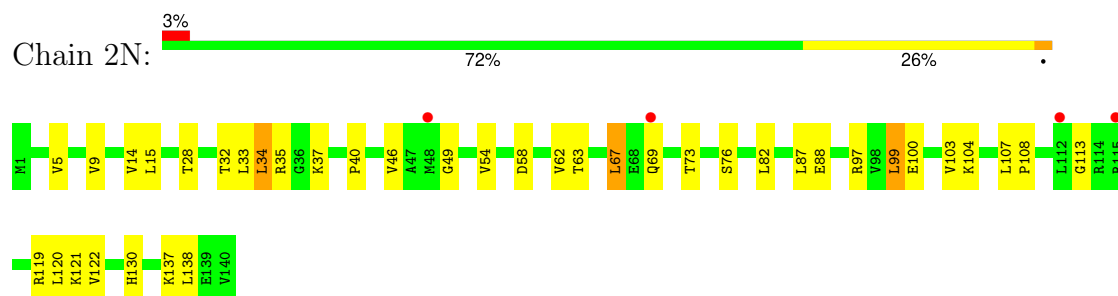
• Molecule 8: 50S ribosomal protein L9



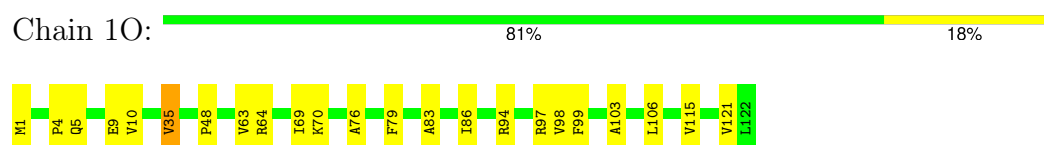
• Molecule 9: 50S ribosomal protein L13



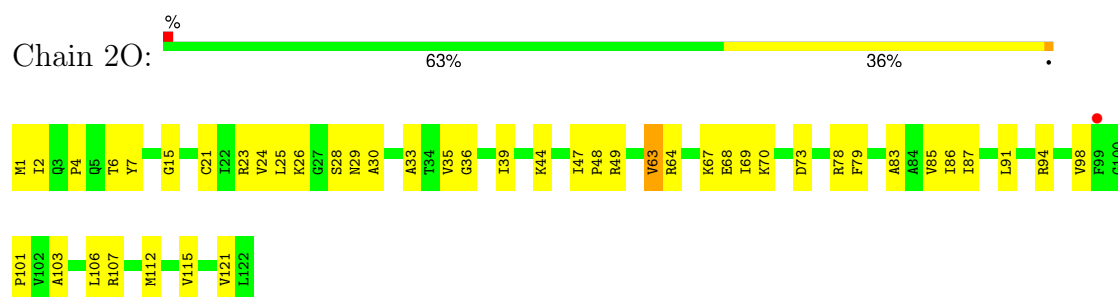
- Molecule 9: 50S ribosomal protein L13



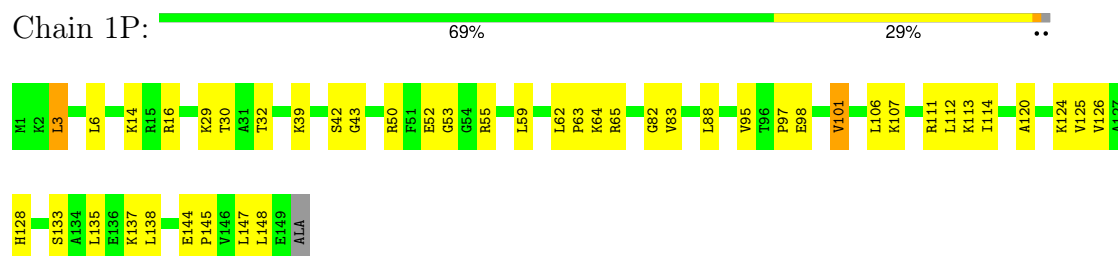
- Molecule 10: 50S ribosomal protein L14



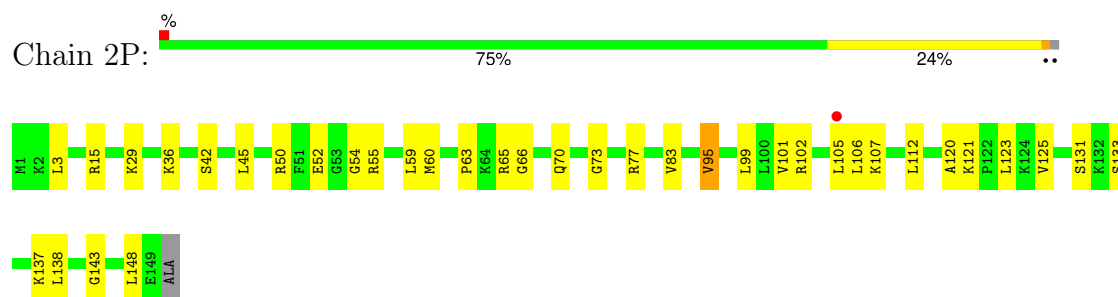
- Molecule 10: 50S ribosomal protein L14



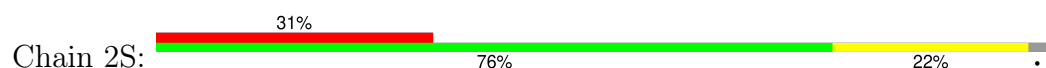
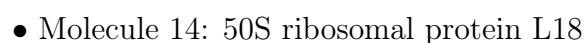
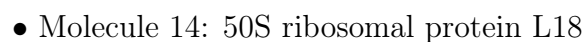
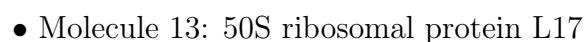
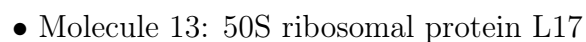
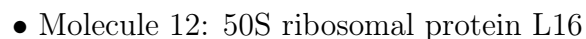
- Molecule 11: 50S ribosomal protein L15

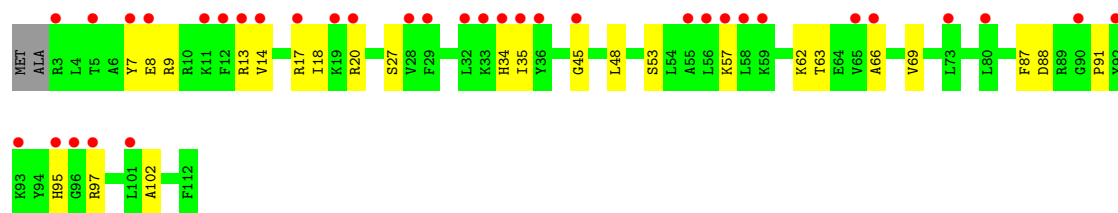


- Molecule 11: 50S ribosomal protein L15

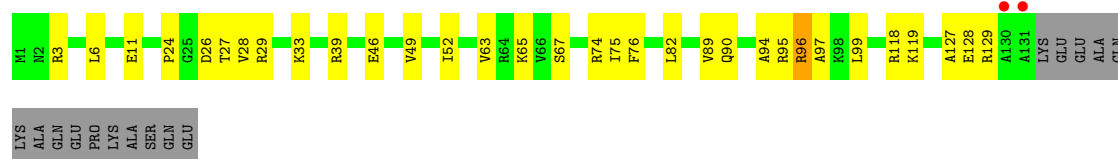


- Molecule 12: 50S ribosomal protein L16

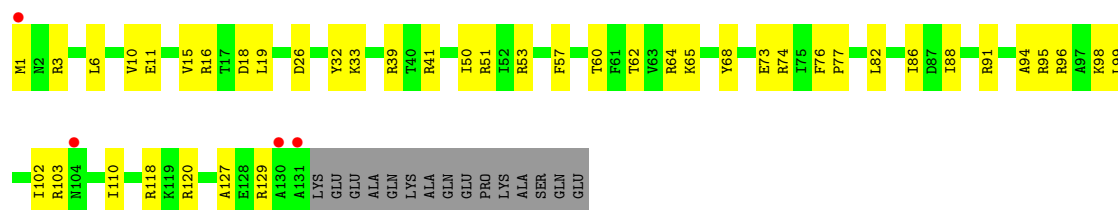




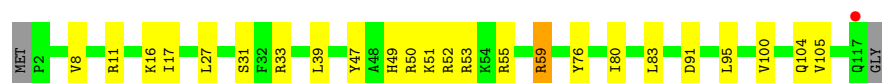
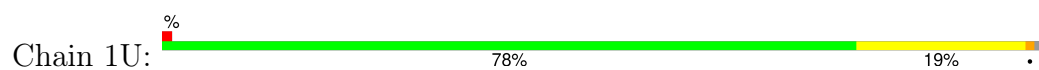
• Molecule 15: 50S ribosomal protein L19



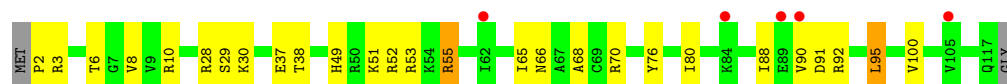
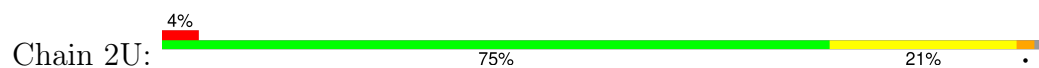
• Molecule 15: 50S ribosomal protein L19



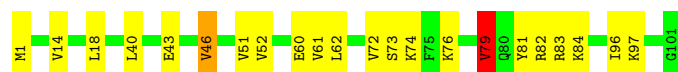
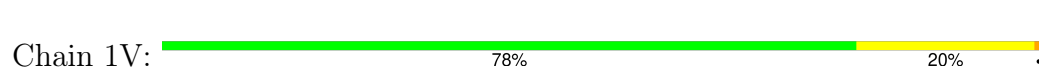
• Molecule 16: 50S ribosomal protein L20



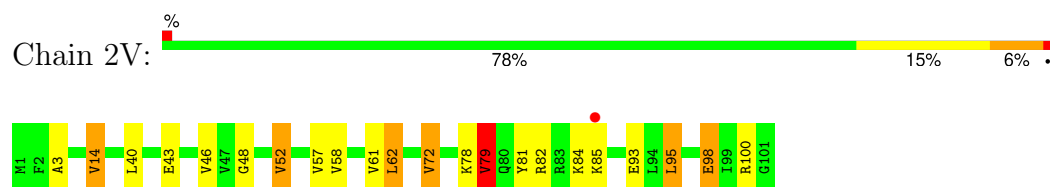
• Molecule 16: 50S ribosomal protein L20



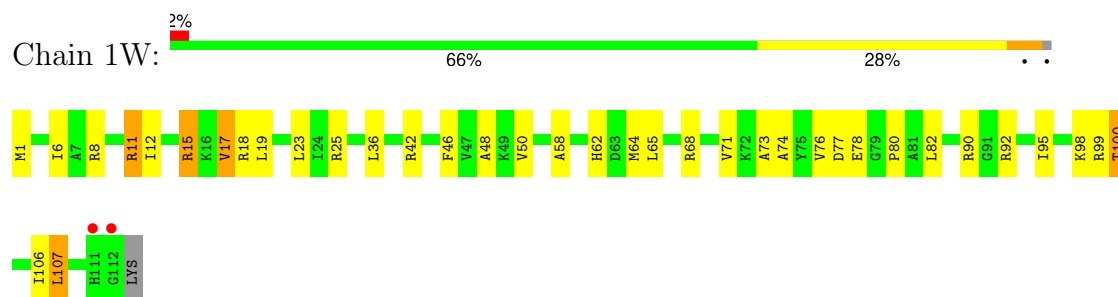
• Molecule 17: 50S ribosomal protein L21



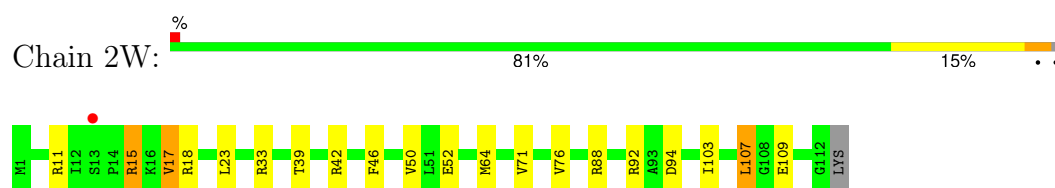
- Molecule 17: 50S ribosomal protein L21



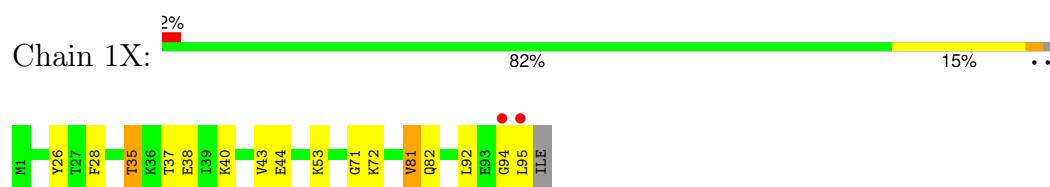
- Molecule 18: 50S ribosomal protein L22



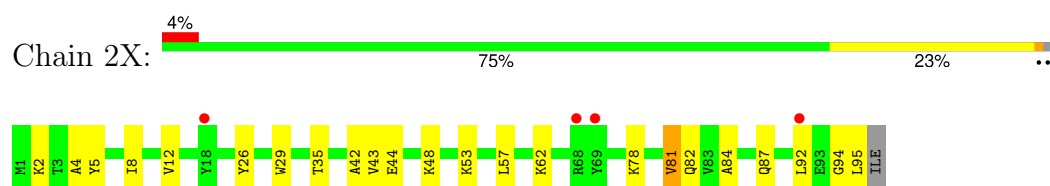
- Molecule 18: 50S ribosomal protein L22



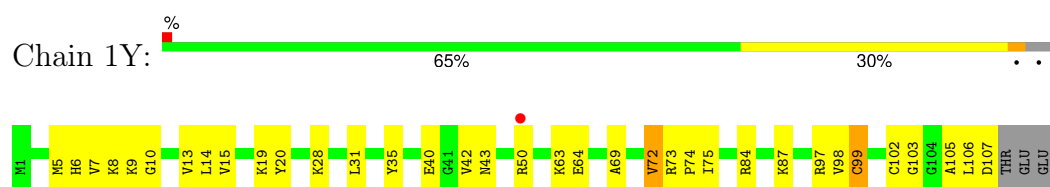
- Molecule 19: 50S ribosomal protein L23



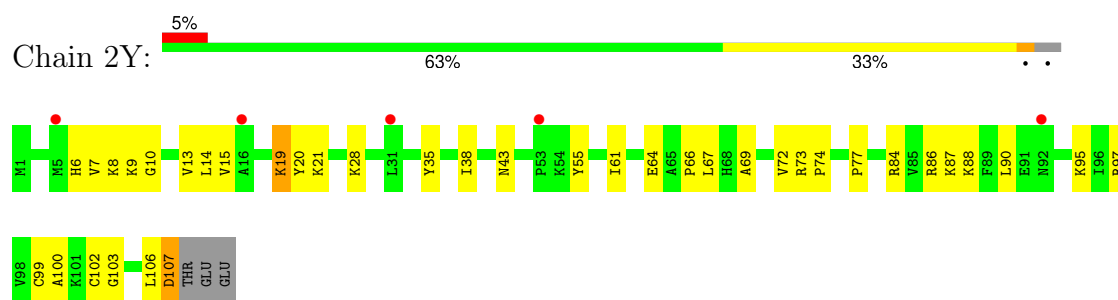
- Molecule 19: 50S ribosomal protein L23



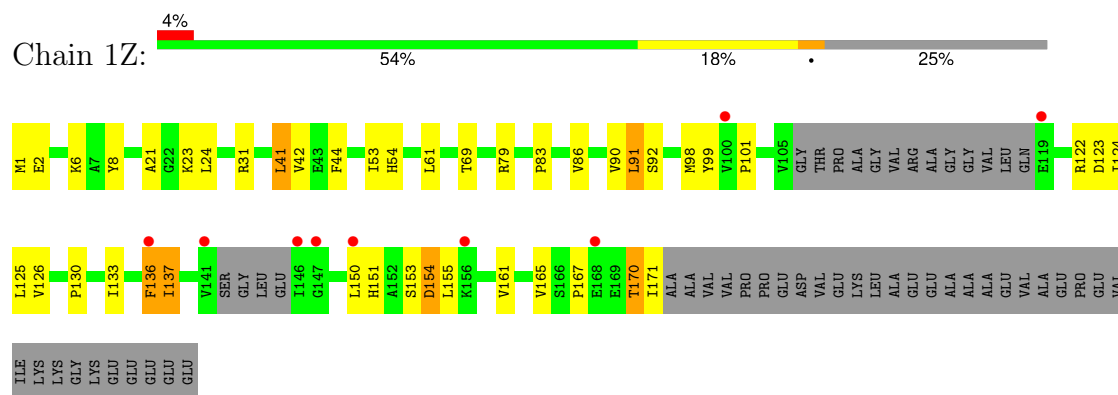
- Molecule 20: 50S ribosomal protein L24



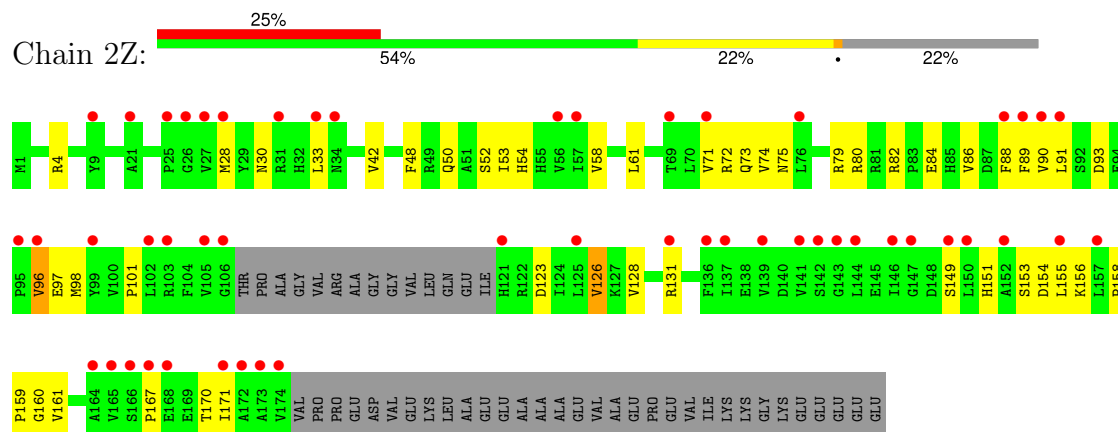
- Molecule 20: 50S ribosomal protein L24



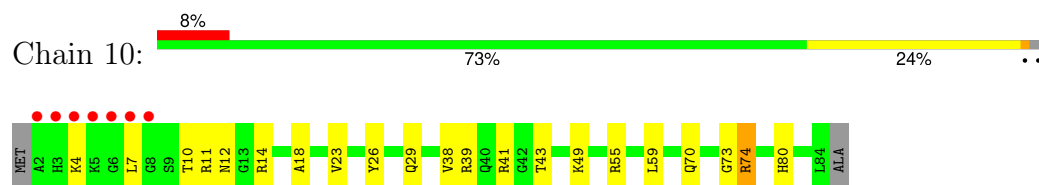
- Molecule 21: 50S ribosomal protein L25



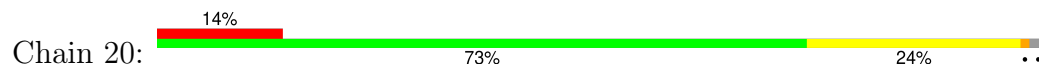
- Molecule 21: 50S ribosomal protein L25

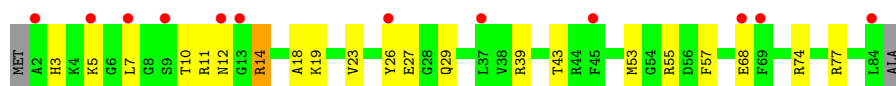


- Molecule 22: 50S ribosomal protein L27

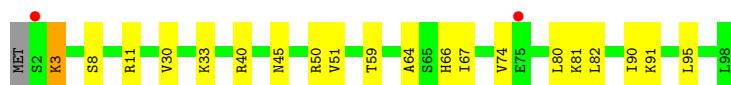
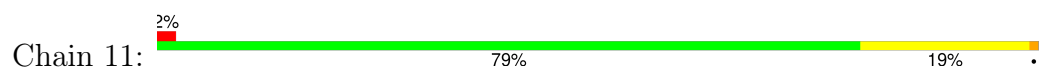


- Molecule 22: 50S ribosomal protein L27

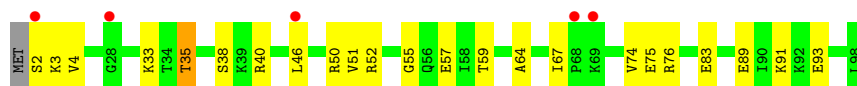
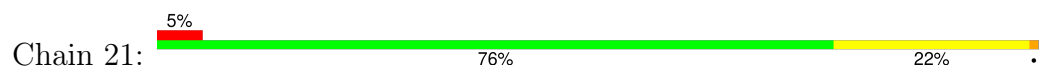




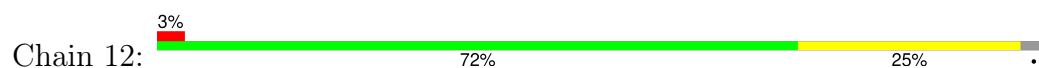
- Molecule 23: 50S ribosomal protein L28



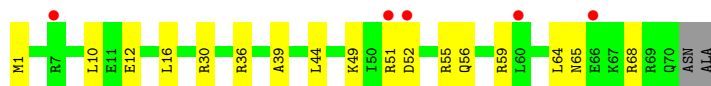
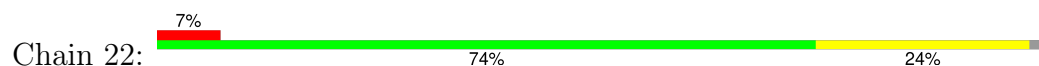
- Molecule 23: 50S ribosomal protein L28



- Molecule 24: 50S ribosomal protein L29



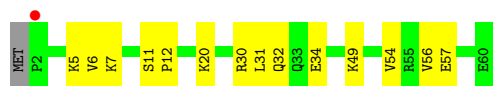
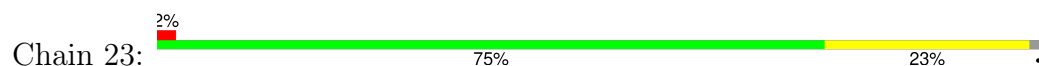
- Molecule 24: 50S ribosomal protein L29



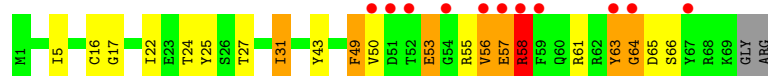
- Molecule 25: 50S ribosomal protein L30



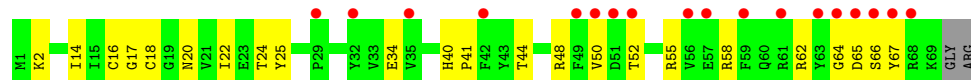
- Molecule 25: 50S ribosomal protein L30



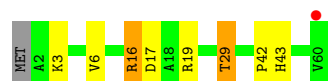
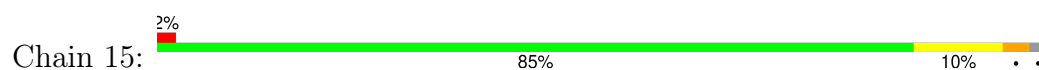
- Molecule 26: 50S ribosomal protein L31



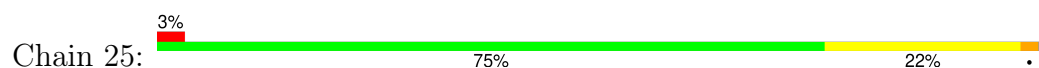
- Molecule 26: 50S ribosomal protein L31



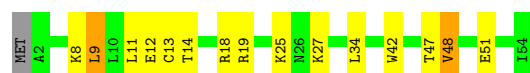
- Molecule 27: 50S ribosomal protein L32



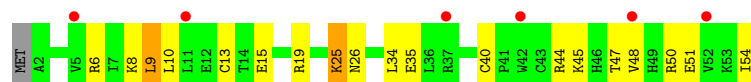
- Molecule 27: 50S ribosomal protein L32



- Molecule 28: 50S ribosomal protein L33



- Molecule 28: 50S ribosomal protein L33



- Molecule 29: 50S ribosomal protein L34



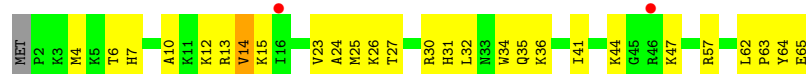
- Molecule 29: 50S ribosomal protein L34



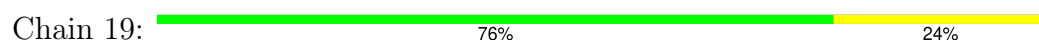
- Molecule 30: 50S ribosomal protein L35



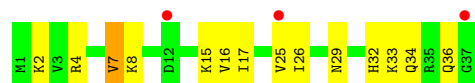
- Molecule 30: 50S ribosomal protein L35



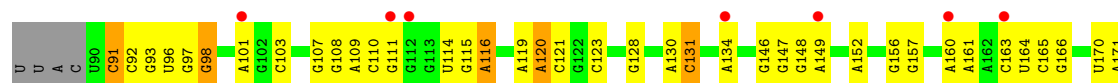
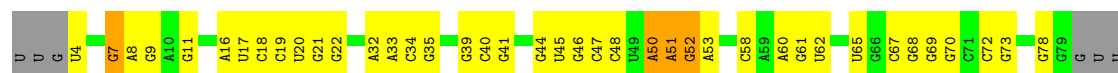
- Molecule 31: 50S ribosomal protein L36

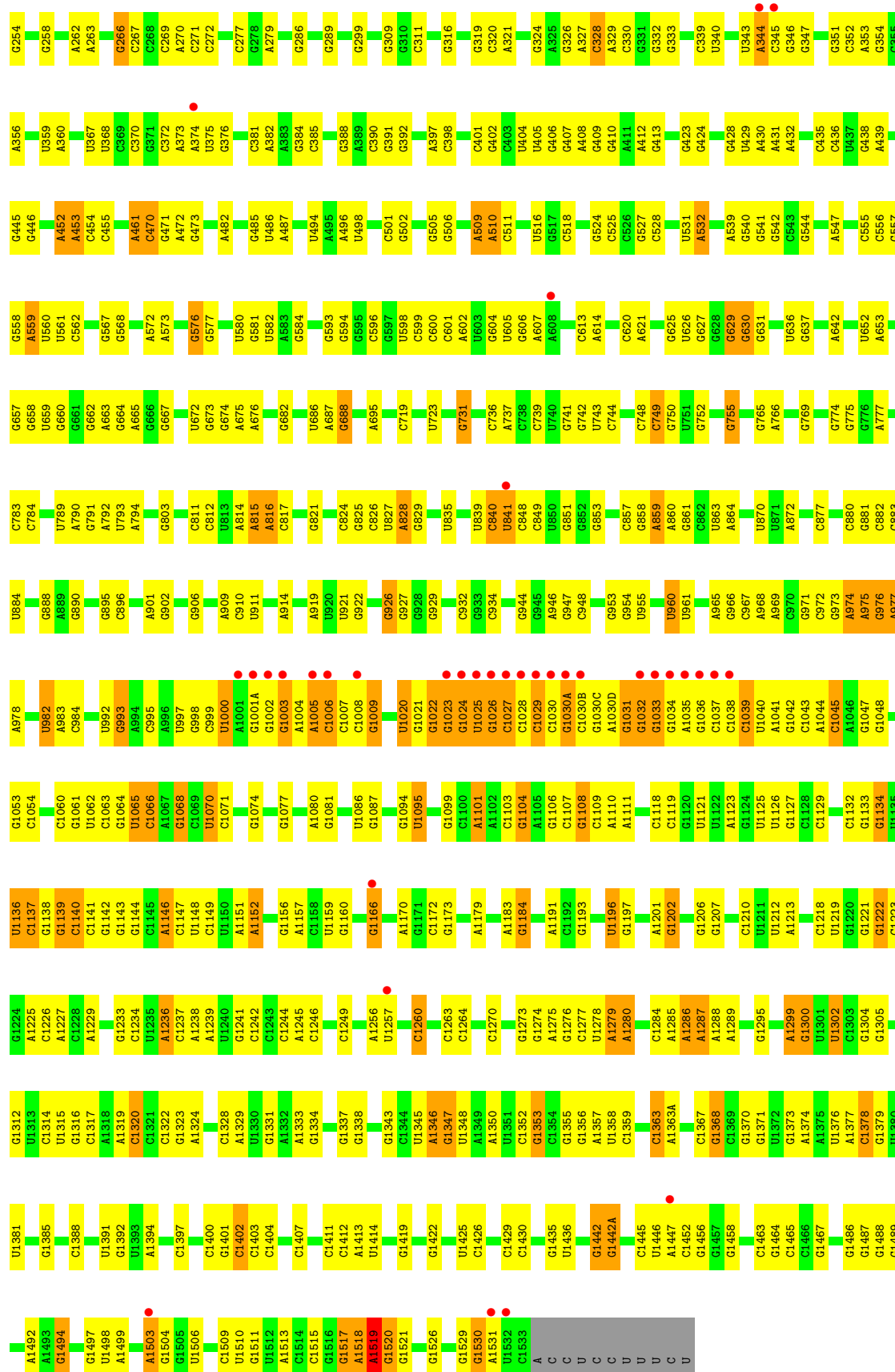


- Molecule 31: 50S ribosomal protein L36



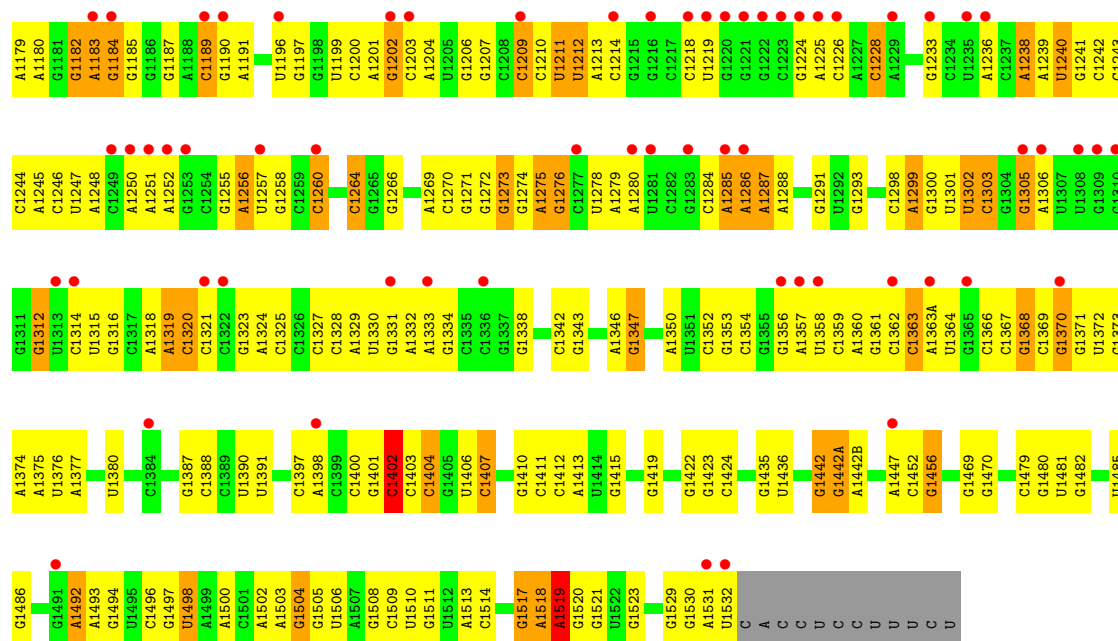
- Molecule 32: 16S Ribosomal RNA



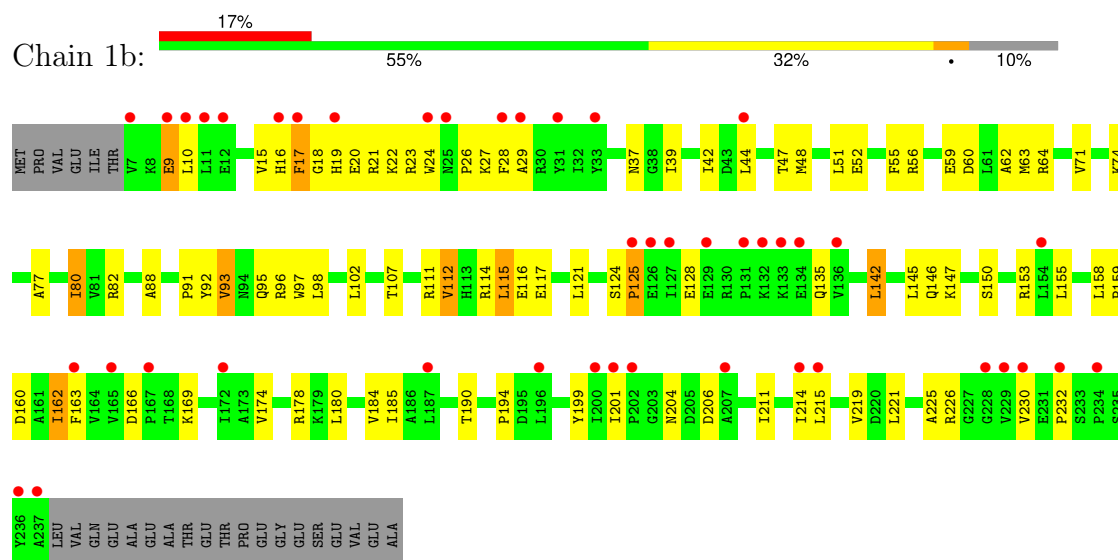


• Molecule 32: 16S Ribosomal RNA

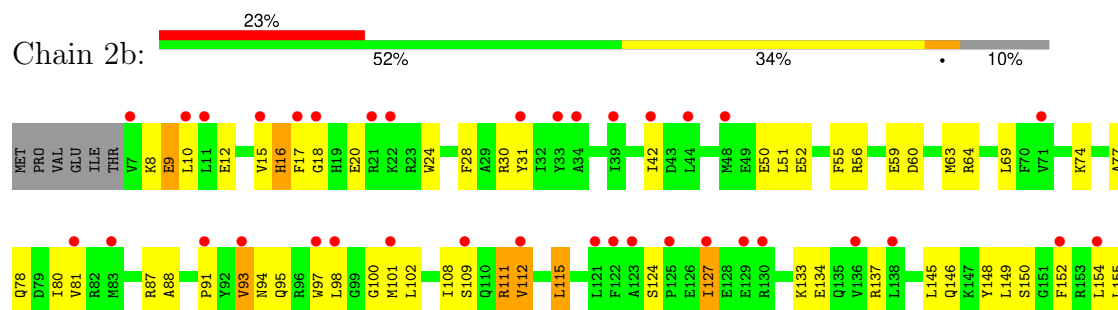


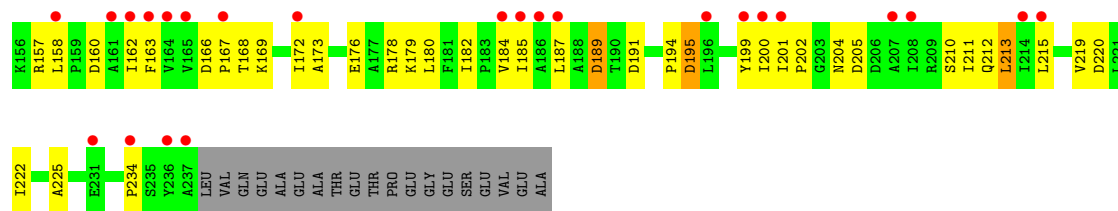


• Molecule 33: 30S ribosomal protein S2

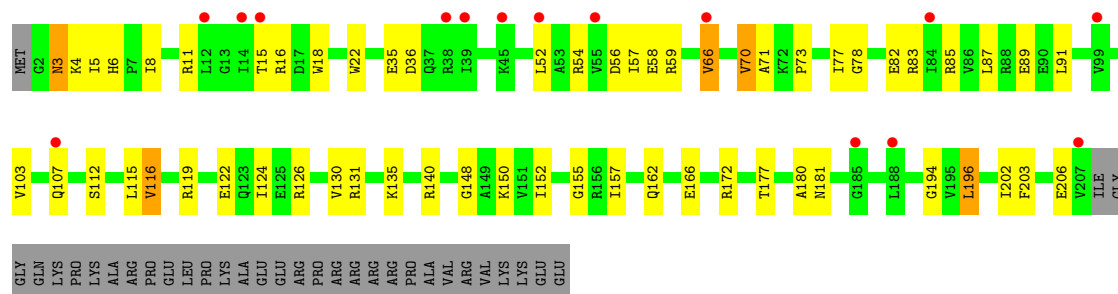


• Molecule 33: 30S ribosomal protein S2

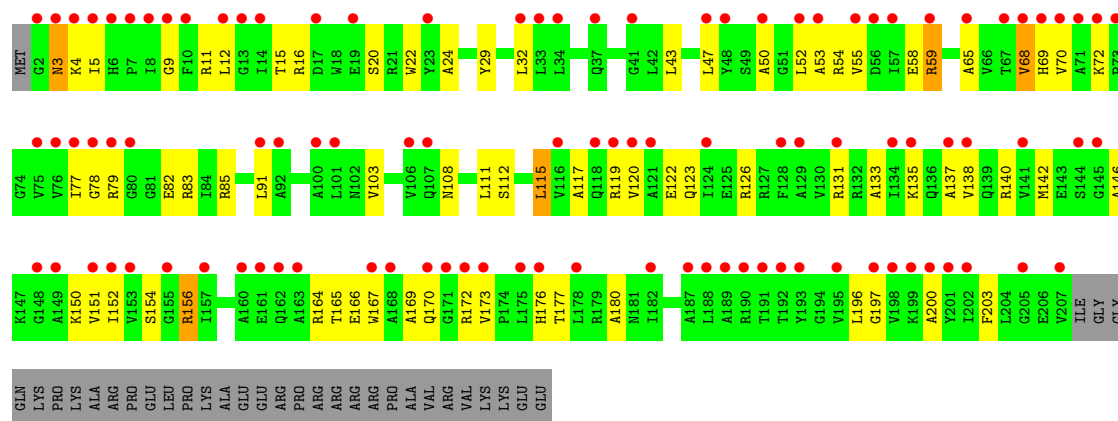
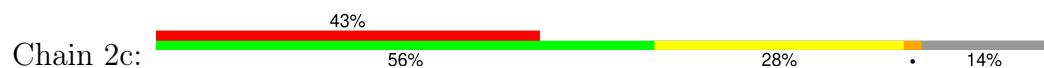




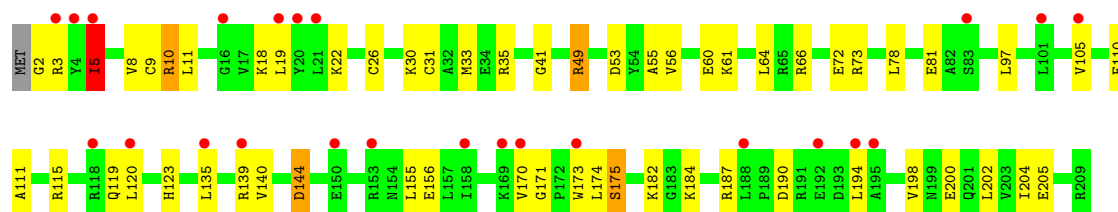
• Molecule 34: 30S ribosomal protein S3



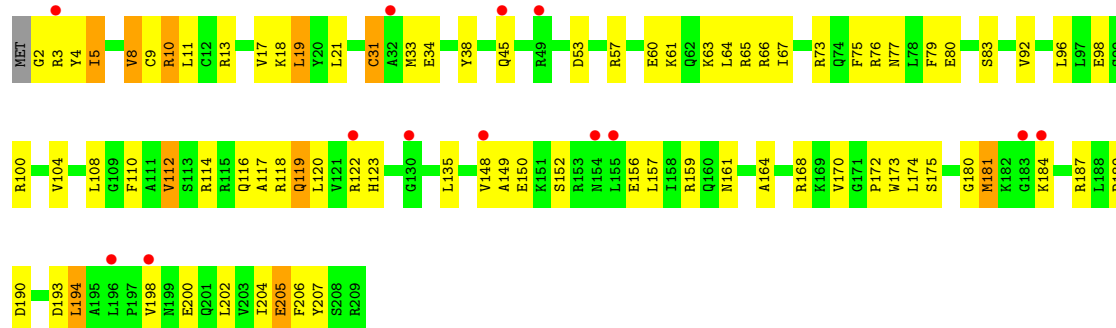
• Molecule 34: 30S ribosomal protein S3



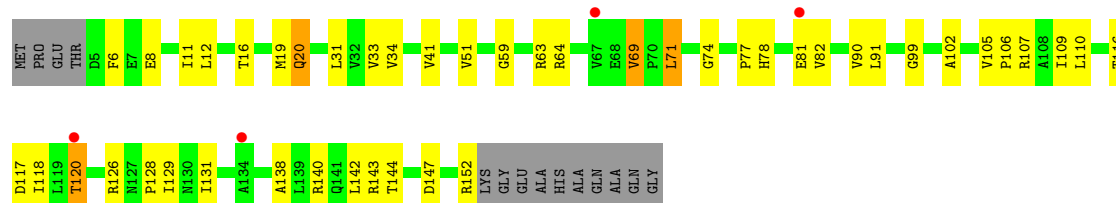
• Molecule 35: 30S ribosomal protein S4



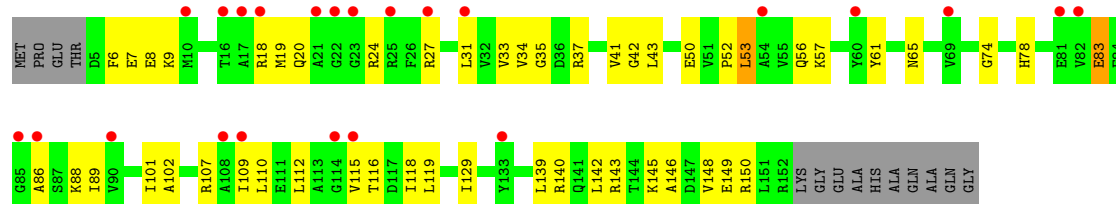
• Molecule 35: 30S ribosomal protein S4



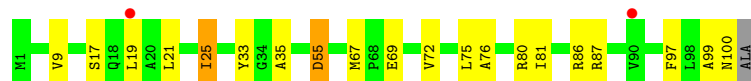
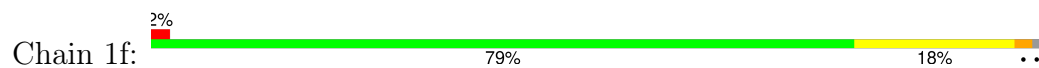
• Molecule 36: 30S ribosomal protein S5



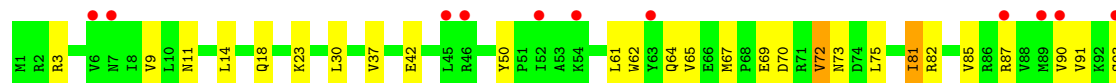
• Molecule 36: 30S ribosomal protein S5

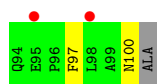


• Molecule 37: 30S ribosomal protein S6

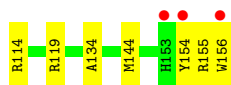
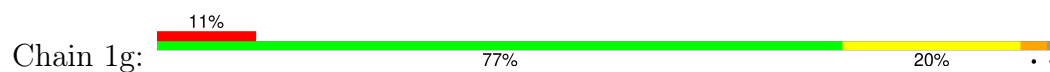


• Molecule 37: 30S ribosomal protein S6

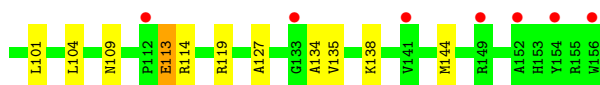
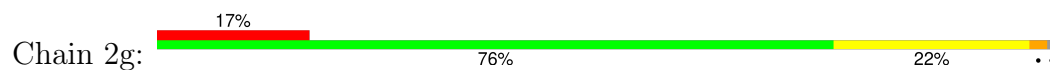




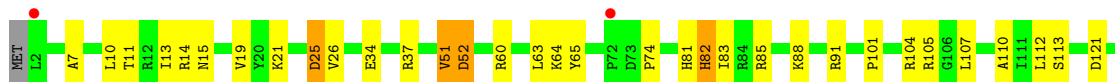
• Molecule 38: 30S ribosomal protein S7



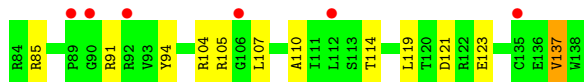
• Molecule 38: 30S ribosomal protein S7



• Molecule 39: 30S ribosomal protein S8

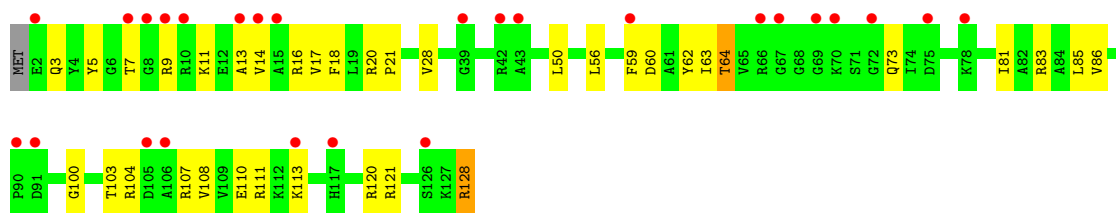


• Molecule 39: 30S ribosomal protein S8

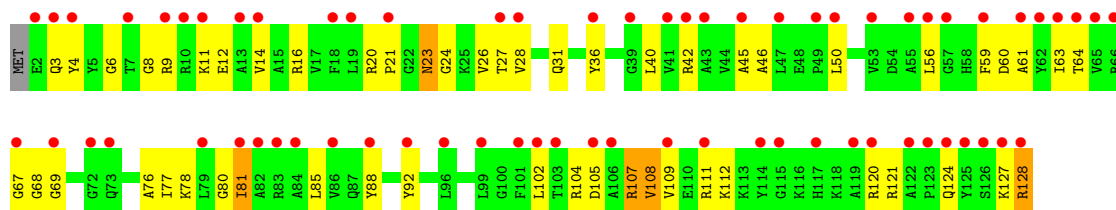


• Molecule 40: 30S ribosomal protein S9

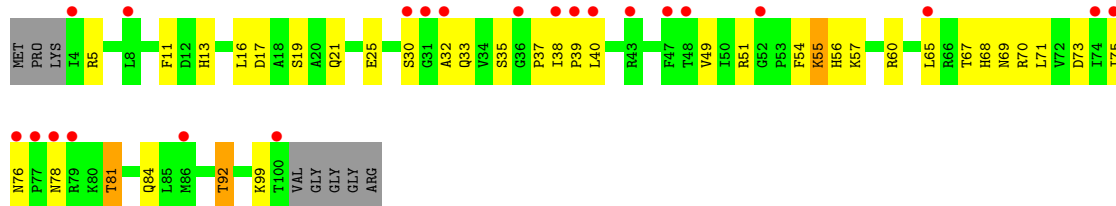




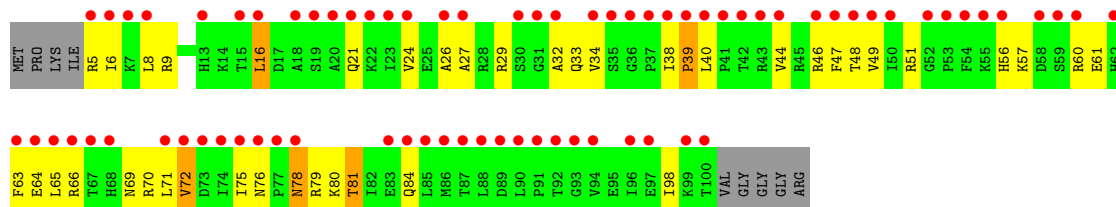
• Molecule 40: 30S ribosomal protein S9



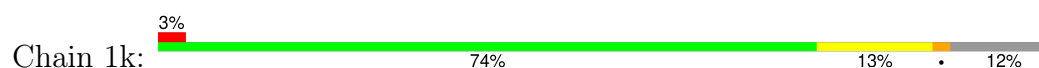
• Molecule 41: 30S ribosomal protein S10



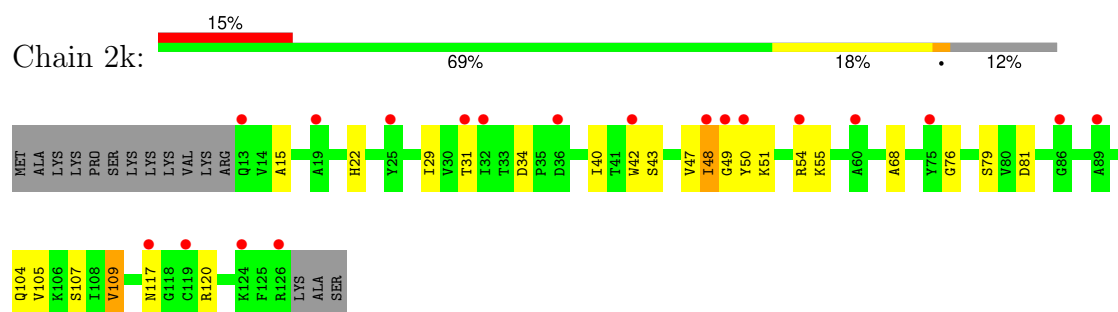
• Molecule 41: 30S ribosomal protein S10



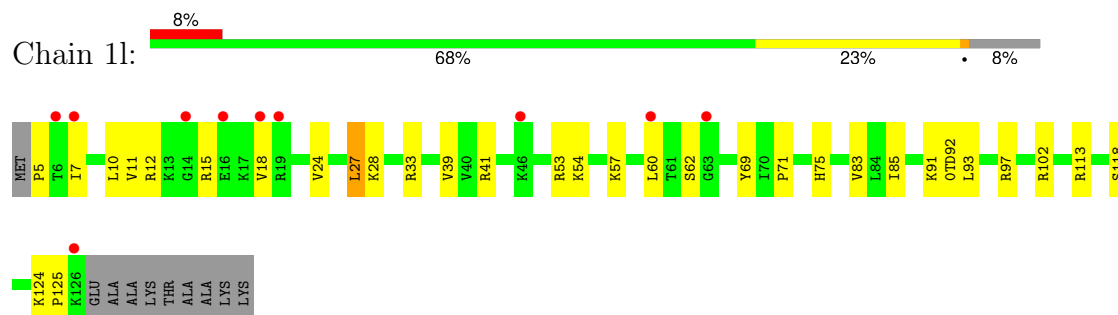
• Molecule 42: 30S ribosomal protein S11



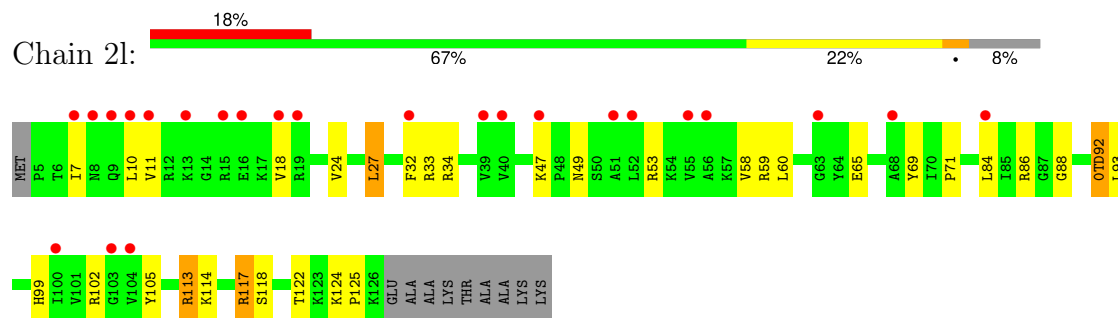
• Molecule 42: 30S ribosomal protein S11



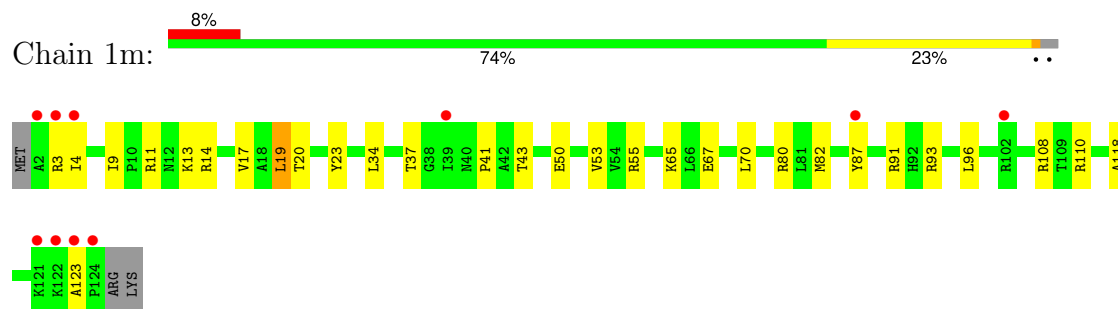
- Molecule 43: 30S ribosomal protein S12



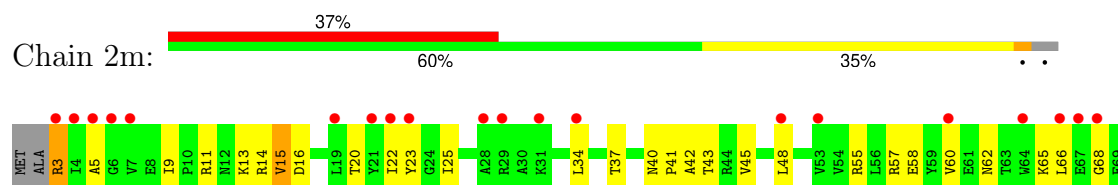
- Molecule 43: 30S ribosomal protein S12

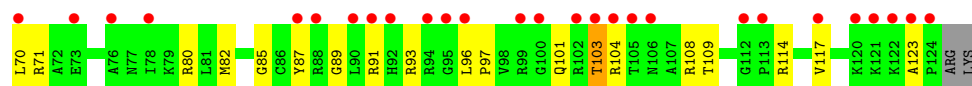


- Molecule 44: 30S ribosomal protein S13

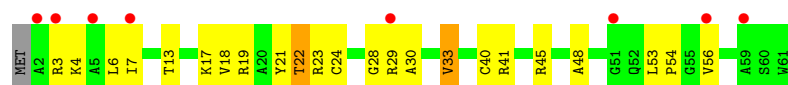


- Molecule 44: 30S ribosomal protein S13

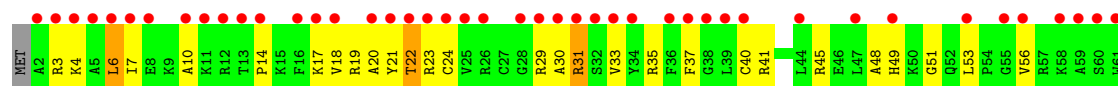
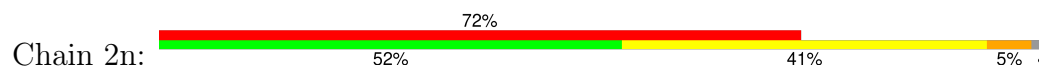




- Molecule 45: 30S ribosomal protein S14 type Z



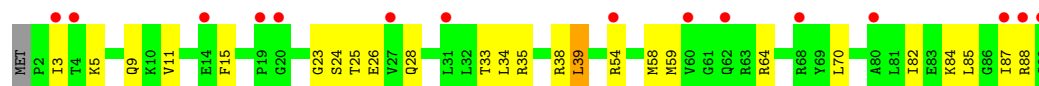
- Molecule 45: 30S ribosomal protein S14 type Z



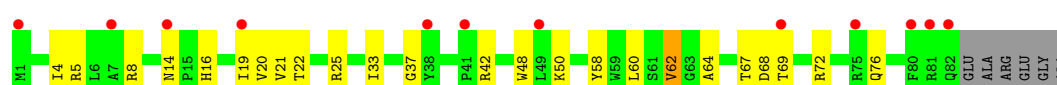
- Molecule 46: 30S ribosomal protein S15



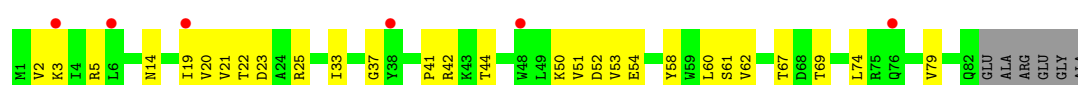
- Molecule 46: 30S ribosomal protein S15



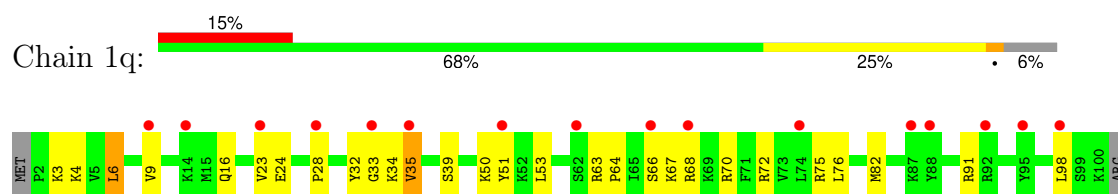
- Molecule 47: 30S ribosomal protein S16



- Molecule 47: 30S ribosomal protein S16

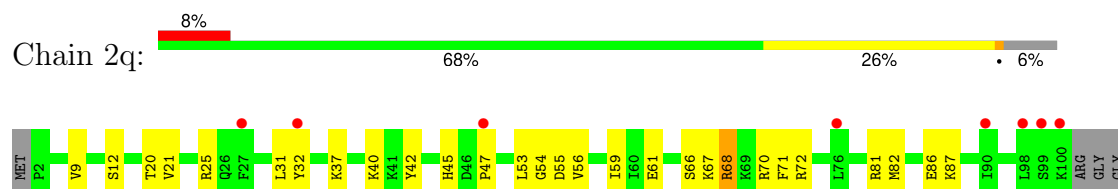


- Molecule 48: 30S ribosomal protein S17



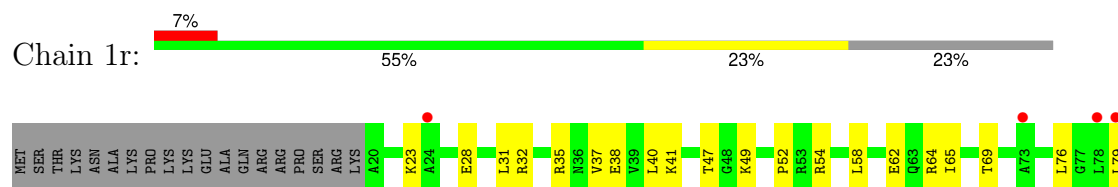
GLY
GLY
LYS
ALA

- Molecule 48: 30S ribosomal protein S17



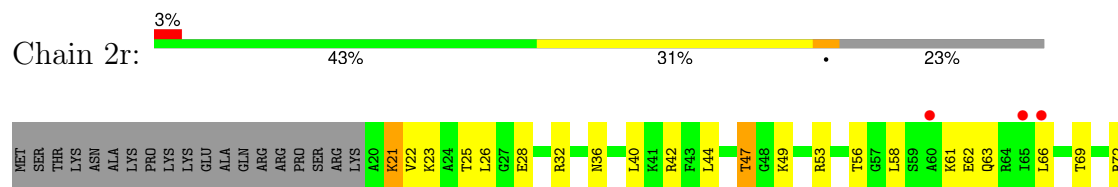
LYS
ALA

- Molecule 49: 30S ribosomal protein S18



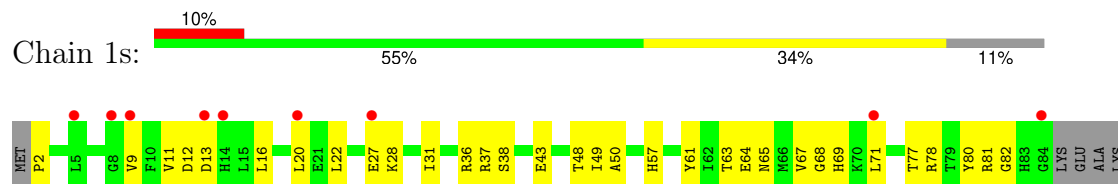
V86
R57
LYS

- Molecule 49: 30S ribosomal protein S18



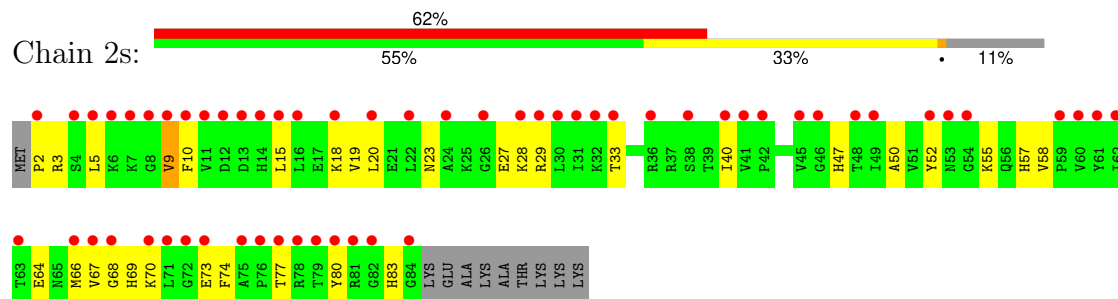
A73
R74
I75
G77
L78
L79
K84
L85
V86
R87
LYS

- Molecule 50: 30S ribosomal protein S19

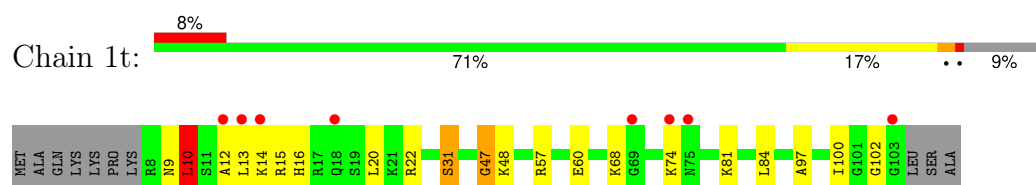


ALA
THR
LYS
LYS
LYS

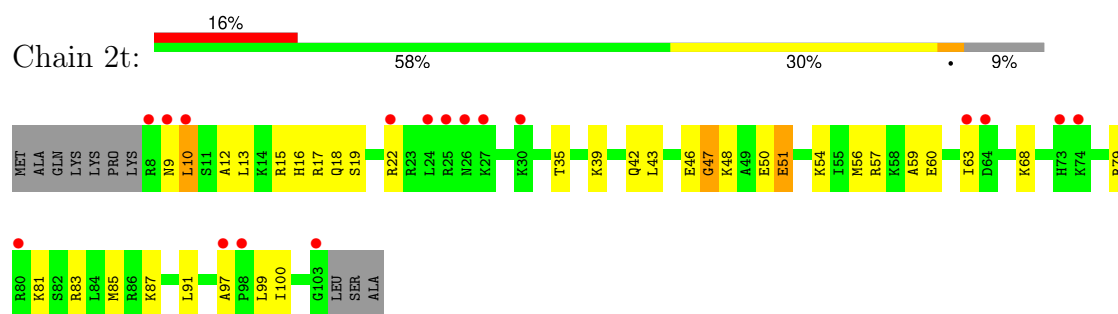
- Molecule 50: 30S ribosomal protein S19



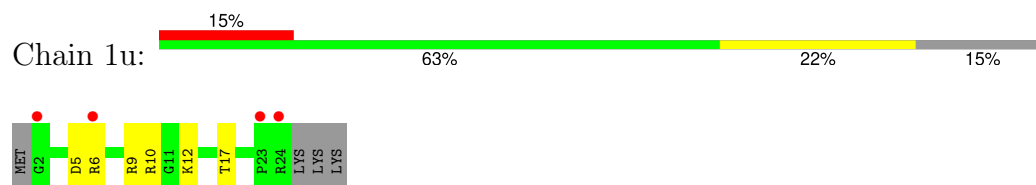
- Molecule 51: 30S ribosomal protein S20



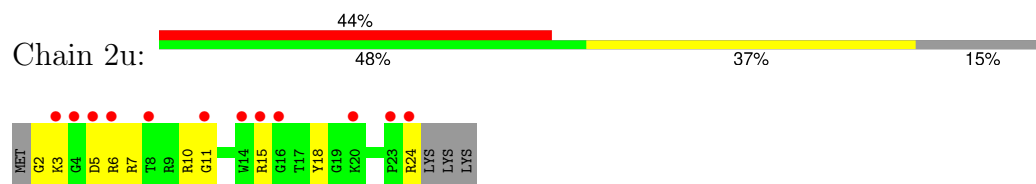
- Molecule 51: 30S ribosomal protein S20



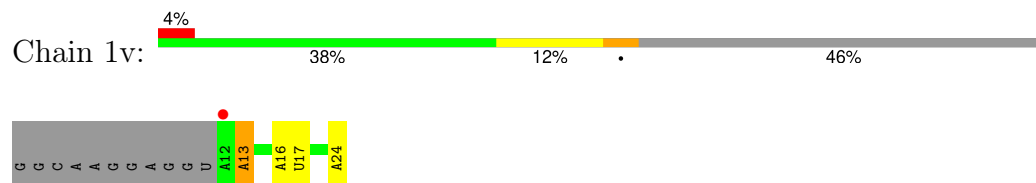
- Molecule 52: 30S ribosomal protein Thx



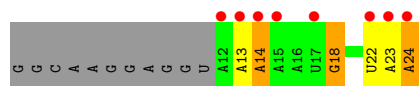
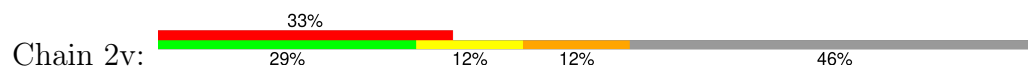
- Molecule 52: 30S ribosomal protein Thx



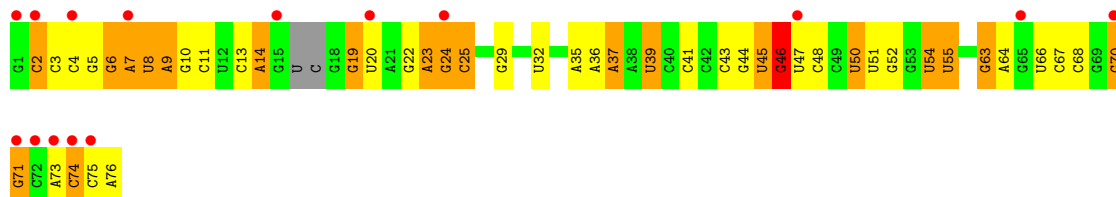
- Molecule 53: mRNA



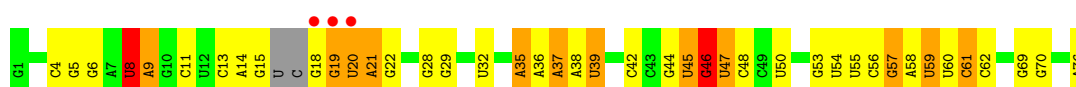
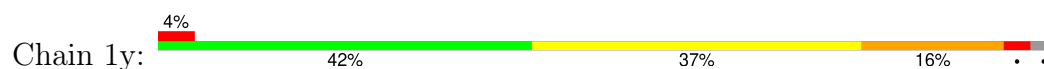
- Molecule 53: mRNA



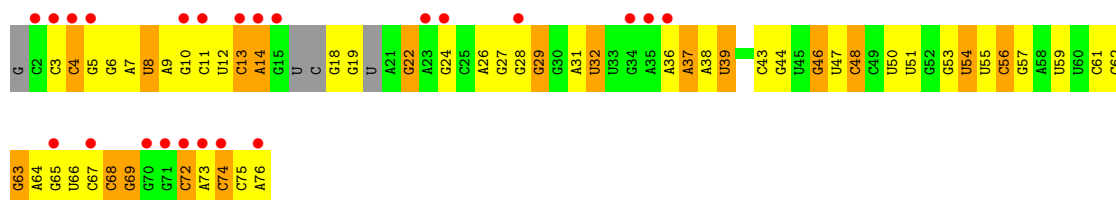
- Molecule 54: A-site and E-site tRNAs



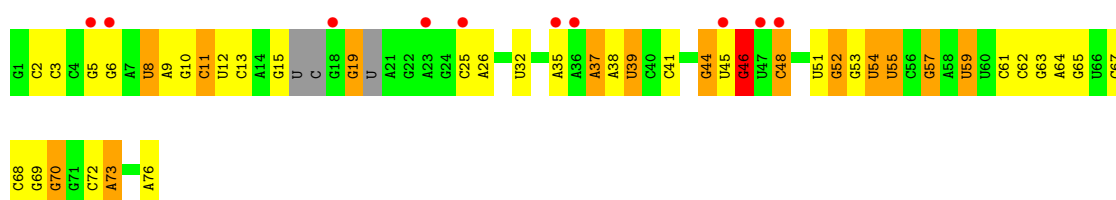
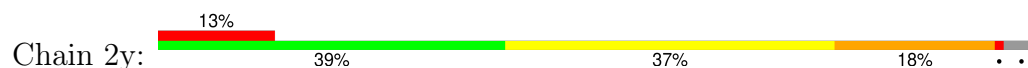
- Molecule 54: A-site and E-site tRNAs



- Molecule 54: A-site and E-site tRNAs

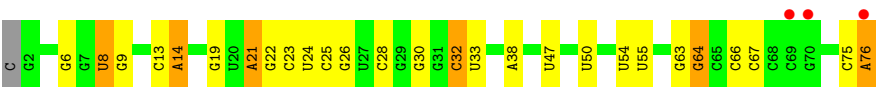


- Molecule 54: A-site and E-site tRNAs

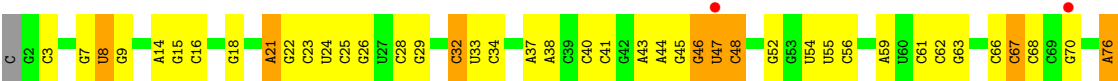


- Molecule 55: P-site tRNA





• Molecule 55: P-site tRNA



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	208.99Å 448.29Å 618.52Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	127.28 – 2.60 127.28 – 2.60	Depositor EDS
% Data completeness (in resolution range)	98.7 (127.28-2.60) 98.7 (127.28-2.60)	Depositor EDS
R_{merge}	0.20	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.19 (at 2.62Å)	Xtriage
Refinement program	PHENIX 1.8.2	Depositor
R, R_{free}	0.229 , 0.276 0.234 , 0.278	Depositor DCC
R_{free} test set	86986 reflections (4.96%)	wwPDB-VP
Wilson B-factor (Å ²)	52.3	Xtriage
Anisotropy	0.172	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 50.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.38$, $\langle L^2 \rangle = 0.21$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	300833	wwPDB-VP
Average B, all atoms (Å ²)	58.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.59% 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: 5MC, PSU, 4SU, MA6, SF4, 4OC, 2MA, 7MG, 5MU, 2MU, MG, MIA, UR3, 2MG, ZN, CLM, OMG, K, M2G, 0TD

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	0.19	0/69009	0.37	0/107712
1	2A	0.14	0/67293	0.32	0/105034
2	1B	0.14	0/2882	0.31	0/4494
2	2B	0.13	0/2879	0.32	0/4487
3	1D	0.25	0/2186	0.46	0/2944
3	2D	0.17	0/2186	0.41	0/2944
4	1E	0.18	0/1592	0.43	0/2149
4	2E	0.15	0/1592	0.39	0/2149
5	1F	0.17	0/1619	0.42	0/2193
5	2F	0.14	0/1615	0.35	0/2188
6	1G	0.16	0/1448	0.37	0/1957
6	2G	0.13	0/1453	0.39	0/1963
7	1H	0.16	0/1356	0.35	0/1834
7	2H	0.13	0/1356	0.33	0/1834
8	1I	0.13	0/1112	0.33	0/1514
8	2I	0.14	0/1079	0.36	0/1475
9	1N	0.18	0/1144	0.39	0/1543
9	2N	0.13	0/1144	0.36	0/1543
10	1O	0.19	0/943	0.38	0/1269
10	2O	0.15	0/943	0.35	0/1269
11	1P	0.19	0/1152	0.41	0/1533
11	2P	0.15	0/1152	0.39	0/1533
12	1Q	0.18	0/1143	0.38	0/1527
12	2Q	0.14	0/1143	0.37	0/1527
13	1R	0.18	0/982	0.41	0/1312
13	2R	0.14	0/982	0.37	0/1312
14	1S	0.15	0/883	0.41	0/1176
14	2S	0.13	0/880	0.37	0/1172
15	1T	0.17	0/1105	0.39	0/1477
15	2T	0.14	0/1097	0.37	0/1468
16	1U	0.19	0/977	0.38	0/1301

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
16	2U	0.14	0/977	0.34	0/1301
17	1V	0.19	0/782	0.39	0/1049
17	2V	0.15	0/782	0.37	0/1049
18	1W	0.19	0/897	0.40	0/1205
18	2W	0.14	0/897	0.34	0/1205
19	1X	0.18	0/764	0.44	0/1025
19	2X	0.13	0/764	0.35	0/1025
20	1Y	0.17	0/819	0.41	0/1095
20	2Y	0.14	0/819	0.38	0/1095
21	1Z	0.16	0/1267	0.39	0/1717
21	2Z	0.15	0/1299	0.39	0/1763
22	10	0.18	0/662	0.43	0/881
22	20	0.15	0/662	0.43	0/881
23	11	0.16	0/762	0.36	0/1014
23	21	0.15	0/762	0.34	0/1014
24	12	0.16	0/590	0.36	0/781
24	22	0.14	0/590	0.31	0/781
25	13	0.18	0/474	0.38	0/635
25	23	0.15	0/469	0.36	0/630
26	14	0.20	0/565	0.53	0/761
26	24	0.19	0/545	0.46	0/737
27	15	0.20	0/469	0.48	0/635
27	25	0.16	0/469	0.38	0/635
28	16	0.18	0/460	0.42	0/613
28	26	0.15	0/456	0.41	0/608
29	17	0.19	0/426	0.42	0/561
29	27	0.17	0/426	0.42	0/561
30	18	0.18	0/525	0.38	0/691
30	28	0.14	0/525	0.32	0/691
31	19	0.18	0/310	0.38	0/407
31	29	0.15	0/310	0.40	0/407
32	1a	0.14	1/35795 (0.0%)	0.32	0/55864
32	2a	0.14	0/35886	0.32	0/56005
33	1b	0.15	0/1881	0.42	0/2542
33	2b	0.17	0/1860	0.42	0/2518
34	1c	0.14	0/1572	0.34	0/2126
34	2c	0.14	0/1566	0.37	0/2119
35	1d	0.15	0/1685	0.37	0/2262
35	2d	0.14	0/1704	0.38	0/2284
36	1e	0.14	0/1145	0.40	0/1543
36	2e	0.15	0/1149	0.43	0/1548
37	1f	0.14	0/823	0.35	0/1115
37	2f	0.14	0/829	0.34	0/1123

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
38	1g	0.14	0/1250	0.35	0/1679
38	2g	0.14	0/1254	0.38	0/1683
39	1h	0.13	0/1108	0.34	0/1494
39	2h	0.12	0/1108	0.36	0/1494
40	1i	0.16	0/1002	0.42	0/1346
40	2i	0.15	0/997	0.42	0/1343
41	1j	0.14	0/722	0.41	0/982
41	2j	0.15	0/727	0.43	0/988
42	1k	0.12	0/844	0.32	0/1145
42	2k	0.12	0/848	0.31	0/1149
43	1l	0.14	0/937	0.38	0/1260
43	2l	0.14	0/937	0.37	0/1260
44	1m	0.16	0/969	0.37	0/1302
44	2m	0.16	0/961	0.39	0/1291
45	1n	0.13	0/501	0.36	0/664
45	2n	0.14	0/501	0.35	0/664
46	1o	0.13	0/739	0.33	0/985
46	2o	0.12	0/739	0.33	0/985
47	1p	0.14	0/697	0.39	0/939
47	2p	0.18	0/693	0.43	0/935
48	1q	0.14	0/836	0.34	0/1117
48	2q	0.14	0/836	0.36	0/1117
49	1r	0.13	0/560	0.33	0/746
49	2r	0.12	0/560	0.33	0/746
50	1s	0.17	0/667	0.46	0/900
50	2s	0.20	0/661	0.55	0/893
51	1t	0.14	0/730	0.41	0/965
51	2t	0.16	0/729	0.43	0/965
52	1u	0.15	0/203	0.42	0/266
52	2u	0.17	0/203	0.43	0/266
53	1v	0.16	0/310	0.29	0/480
53	2v	0.19	0/310	0.34	0/480
54	1w	0.21	1/1606 (0.1%)	0.37	0/2497
54	1y	0.20	1/1606 (0.1%)	0.35	0/2497
54	2w	0.21	0/1556	0.35	0/2418
54	2y	0.20	0/1583	0.35	0/2459
55	1x	0.21	0/1725	0.36	0/2689
55	2x	0.19	0/1725	0.31	0/2689
All	All	0.16	3/316686 (0.0%)	0.35	0/474113

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
26	14	0	1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
54	1w	8	4SU	O3'-P	5.09	1.61	1.56
54	1y	8	4SU	O3'-P	5.07	1.61	1.56
32	1a	1498	UR3	O3'-P	5.03	1.61	1.56

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
26	14	57	GLU	Peptide

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	1A	61852	0	31191	679	0
1	2A	60322	0	30425	778	0
2	1B	2577	0	1305	23	0
2	2B	2575	0	1303	45	0
3	1D	2136	0	2218	45	0
3	2D	2136	0	2218	61	0
4	1E	1559	0	1618	31	0
4	2E	1559	0	1618	38	0
5	1F	1584	0	1625	44	0
5	2F	1580	0	1619	40	0
6	1G	1423	0	1436	34	0
6	2G	1428	0	1438	46	0
7	1H	1330	0	1407	24	0
7	2H	1330	0	1407	41	0
8	1I	1097	0	1140	17	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
8	2I	1064	0	1082	20	0
9	1N	1117	0	1184	18	0
9	2N	1117	0	1184	26	0
10	1O	933	0	996	18	0
10	2O	933	0	996	31	0
11	1P	1135	0	1212	38	0
11	2P	1135	0	1212	28	0
12	1Q	1122	0	1179	27	0
12	2Q	1122	0	1179	28	0
13	1R	968	0	1033	27	0
13	2R	968	0	1033	26	0
14	1S	873	0	927	18	0
14	2S	870	0	923	18	0
15	1T	1091	0	1151	26	0
15	2T	1083	0	1136	34	0
16	1U	959	0	1019	22	0
16	2U	959	0	1018	20	0
17	1V	771	0	829	10	0
17	2V	771	0	830	15	0
18	1W	886	0	940	24	0
18	2W	886	0	940	11	0
19	1X	750	0	814	9	0
19	2X	750	0	814	16	0
20	1Y	806	0	881	22	0
20	2Y	806	0	881	24	0
21	1Z	1240	0	1240	27	0
21	2Z	1271	0	1273	30	0
22	10	653	0	674	18	0
22	20	653	0	674	20	0
23	11	755	0	826	13	0
23	21	755	0	826	19	0
24	12	588	0	643	12	0
24	22	588	0	643	13	0
25	13	469	0	518	15	0
25	23	464	0	514	9	0
26	14	552	0	533	24	0
26	24	532	0	503	16	0
27	15	455	0	465	6	0
27	25	455	0	465	13	0
28	16	453	0	473	10	0
28	26	449	0	469	13	0
29	17	418	0	467	9	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
29	27	418	0	467	14	0
30	18	517	0	582	22	0
30	28	517	0	582	23	0
31	19	307	0	335	5	0
31	29	307	0	335	10	0
32	1a	32246	0	16295	479	0
32	2a	32327	0	16340	586	0
33	1b	1846	0	1867	67	0
33	2b	1825	0	1828	76	0
34	1c	1548	0	1535	39	0
34	2c	1542	0	1517	57	0
35	1d	1655	0	1675	50	0
35	2d	1674	0	1714	61	0
36	1e	1129	0	1184	31	0
36	2e	1133	0	1191	39	0
37	1f	810	0	804	13	0
37	2f	816	0	808	24	0
38	1g	1231	0	1238	21	0
38	2g	1235	0	1249	28	0
39	1h	1088	0	1126	29	0
39	2h	1088	0	1126	33	0
40	1i	983	0	986	24	0
40	2i	978	0	966	44	0
41	1j	709	0	650	24	0
41	2j	714	0	672	31	0
42	1k	829	0	825	10	0
42	2k	833	0	836	16	0
43	1l	932	0	981	19	0
43	2l	932	0	981	25	0
44	1m	958	0	1002	22	0
44	2m	950	0	988	35	0
45	1n	492	0	529	20	0
45	2n	492	0	529	24	0
46	1o	728	0	760	20	0
46	2o	728	0	760	19	0
47	1p	681	0	697	19	0
47	2p	677	0	686	16	0
48	1q	823	0	891	19	0
48	2q	823	0	891	22	0
49	1r	555	0	618	12	0
49	2r	555	0	618	21	0
50	1s	652	0	662	31	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
50	2s	646	0	644	27	0
51	1t	728	0	798	17	0
51	2t	727	0	796	25	0
52	1u	199	0	208	4	0
52	2u	199	0	208	9	0
53	1v	277	0	140	3	0
53	2v	277	0	140	5	0
54	1w	1592	0	819	42	0
54	1y	1585	0	804	30	0
54	2w	1544	0	788	45	0
54	2y	1565	0	795	26	0
55	1x	1625	0	829	14	0
55	2x	1625	0	829	28	0
56	10	6	0	0	0	0
56	11	5	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	16	3	0	0	0	0
56	17	8	0	0	0	0
56	18	7	0	0	0	0
56	19	1	0	0	0	0
56	1A	1101	0	0	0	0
56	1B	39	0	0	0	0
56	1D	13	0	0	0	0
56	1E	15	0	0	0	0
56	1F	10	0	0	0	0
56	1G	4	0	0	0	0
56	1I	1	0	0	0	0
56	1N	6	0	0	0	0
56	1O	5	0	0	0	0
56	1P	9	0	0	0	0
56	1Q	8	0	0	0	0
56	1R	3	0	0	0	0
56	1S	3	0	0	0	0
56	1T	4	0	0	0	0
56	1U	12	0	0	0	0
56	1V	7	0	0	0	0
56	1W	5	0	0	0	0
56	1X	5	0	0	0	0
56	1Y	3	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
56	1Z	3	0	0	0	0
56	1a	233	0	0	0	0
56	1b	2	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	2	0	0	0	0
56	1m	2	0	0	0	0
56	1n	1	0	0	0	0
56	1s	1	0	0	0	0
56	1t	1	0	0	0	0
56	1v	1	0	0	0	0
56	1w	12	0	0	0	0
56	1x	18	0	0	0	0
56	20	3	0	0	0	0
56	21	1	0	0	0	0
56	23	3	0	0	0	0
56	25	5	0	0	0	0
56	27	2	0	0	0	0
56	28	3	0	0	0	0
56	2A	887	0	0	0	0
56	2B	20	0	0	0	0
56	2D	10	0	0	0	0
56	2E	4	0	0	0	0
56	2F	6	0	0	0	0
56	2G	1	0	0	0	0
56	2N	1	0	0	0	0
56	2O	1	0	0	0	0
56	2P	4	0	0	0	0
56	2Q	4	0	0	0	0
56	2R	2	0	0	0	0
56	2T	4	0	0	0	0
56	2U	3	0	0	0	0
56	2V	3	0	0	0	0
56	2W	3	0	0	0	0
56	2X	1	0	0	0	0
56	2Z	1	0	0	0	0
56	2a	241	0	0	0	0
56	2d	1	0	0	0	0
56	2e	1	0	0	0	0
56	2f	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
56	2g	1	0	0	0	0
56	2i	1	0	0	0	0
56	2j	1	0	0	0	0
56	2k	1	0	0	0	0
56	2l	4	0	0	0	0
56	2m	1	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	1	0	0	0	0
56	2w	4	0	0	0	0
56	2x	5	0	0	0	0
56	2y	6	0	0	0	0
57	1A	20	0	11	0	0
57	2A	20	0	11	1	0
58	1A	1	0	0	0	0
58	2A	1	0	0	0	0
59	14	1	0	0	0	0
59	15	1	0	0	0	0
59	16	1	0	0	0	0
59	19	1	0	0	0	0
59	1Y	1	0	0	0	0
59	1n	1	0	0	0	0
59	24	1	0	0	0	0
59	25	1	0	0	0	0
59	26	1	0	0	0	0
59	29	1	0	0	0	0
59	2Y	1	0	0	0	0
59	2n	1	0	0	0	0
60	1d	8	0	0	11	0
60	2d	8	0	0	3	0
61	10	12	0	0	1	0
61	11	10	0	0	0	0
61	12	4	0	0	0	0
61	13	4	0	0	0	0
61	14	2	0	0	0	0
61	15	7	0	0	0	0
61	16	1	0	0	1	0
61	17	7	0	0	0	0
61	18	19	0	0	2	0
61	1A	2246	0	0	71	0
61	1B	73	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
61	1D	24	0	0	1	0
61	1E	27	0	0	0	0
61	1F	9	0	0	0	0
61	1G	5	0	0	0	0
61	1H	1	0	0	0	0
61	1I	2	0	0	0	0
61	1N	4	0	0	0	0
61	1O	7	0	0	0	0
61	1P	21	0	0	0	0
61	1Q	11	0	0	0	0
61	1R	8	0	0	1	0
61	1S	4	0	0	0	0
61	1T	6	0	0	0	0
61	1U	9	0	0	0	0
61	1V	7	0	0	0	0
61	1W	9	0	0	2	0
61	1X	7	0	0	0	0
61	1Y	3	0	0	0	0
61	1Z	1	0	0	0	0
61	1a	430	0	0	26	0
61	1b	1	0	0	0	0
61	1d	1	0	0	0	0
61	1f	1	0	0	0	0
61	1l	7	0	0	0	0
61	1q	4	0	0	0	0
61	1w	16	0	0	0	0
61	1x	15	0	0	0	0
61	1y	1	0	0	0	0
61	20	10	0	0	1	0
61	21	6	0	0	0	0
61	22	1	0	0	0	0
61	25	4	0	0	0	0
61	27	2	0	0	1	0
61	28	6	0	0	0	0
61	29	1	0	0	0	0
61	2A	1405	0	0	57	0
61	2B	25	0	0	1	0
61	2D	17	0	0	0	0
61	2E	3	0	0	0	0
61	2F	6	0	0	0	0
61	2I	3	0	0	0	0
61	2N	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
61	2O	1	0	0	0	0
61	2P	11	0	0	1	0
61	2Q	2	0	0	0	0
61	2R	3	0	0	0	0
61	2T	5	0	0	0	0
61	2U	2	0	0	0	0
61	2W	3	0	0	0	0
61	2Z	1	0	0	0	0
61	2a	380	0	0	22	0
61	2d	1	0	0	0	0
61	2g	1	0	0	0	0
61	2i	1	0	0	0	0
61	2j	3	0	0	2	0
61	2l	2	0	0	1	0
61	2p	1	0	0	0	0
61	2r	1	0	0	0	0
61	2t	2	0	0	0	0
61	2x	7	0	0	1	0
61	2y	13	0	0	0	0
All	All	300833	0	196713	4469	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 10.

The worst 5 of 4469 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)
1:2A:2138:C:N4	1:2A:2153:G:H1	1.53	1.07
35:1d:22:LYS:HB2	35:1d:26:CYS:SG	1.95	1.05
54:1w:7:A:N6	54:1w:66:U:H3	1.54	1.05
1:2A:2129:C:N4	1:2A:2159:G:H1	1.55	1.03
1:1A:1058:G:H1	1:1A:1080:C:N4	1.56	1.01

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%)	261 (96%)	11 (4%)	1 (0%)	30	51
3	2D	273/276 (99%)	261 (96%)	11 (4%)	1 (0%)	30	51
4	1E	202/206 (98%)	194 (96%)	7 (4%)	1 (0%)	24	46
4	2E	202/206 (98%)	195 (96%)	6 (3%)	1 (0%)	24	46
5	1F	201/210 (96%)	193 (96%)	7 (4%)	1 (0%)	24	46
5	2F	201/210 (96%)	197 (98%)	1 (0%)	3 (2%)	8	18
6	1G	179/182 (98%)	168 (94%)	10 (6%)	1 (1%)	21	42
6	2G	179/182 (98%)	159 (89%)	18 (10%)	2 (1%)	11	25
7	1H	172/180 (96%)	163 (95%)	8 (5%)	1 (1%)	21	42
7	2H	172/180 (96%)	160 (93%)	10 (6%)	2 (1%)	10	23
8	1I	144/148 (97%)	137 (95%)	7 (5%)	0	100	100
8	2I	144/148 (97%)	134 (93%)	10 (7%)	0	100	100
9	1N	138/140 (99%)	135 (98%)	3 (2%)	0	100	100
9	2N	138/140 (99%)	133 (96%)	5 (4%)	0	100	100
10	1O	120/122 (98%)	116 (97%)	4 (3%)	0	100	100
10	2O	120/122 (98%)	114 (95%)	6 (5%)	0	100	100
11	1P	147/150 (98%)	139 (95%)	8 (5%)	0	100	100
11	2P	147/150 (98%)	141 (96%)	6 (4%)	0	100	100
12	1Q	139/141 (99%)	129 (93%)	10 (7%)	0	100	100
12	2Q	139/141 (99%)	132 (95%)	7 (5%)	0	100	100
13	1R	116/118 (98%)	111 (96%)	5 (4%)	0	100	100
13	2R	116/118 (98%)	112 (97%)	4 (3%)	0	100	100
14	1S	108/112 (96%)	103 (95%)	5 (5%)	0	100	100
14	2S	108/112 (96%)	102 (94%)	6 (6%)	0	100	100
15	1T	129/146 (88%)	122 (95%)	7 (5%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
15	2T	129/146 (88%)	124 (96%)	5 (4%)	0	100	100
16	1U	114/118 (97%)	114 (100%)	0	0	100	100
16	2U	114/118 (97%)	113 (99%)	1 (1%)	0	100	100
17	1V	99/101 (98%)	93 (94%)	5 (5%)	1 (1%)	12	28
17	2V	99/101 (98%)	94 (95%)	4 (4%)	1 (1%)	12	28
18	1W	110/113 (97%)	108 (98%)	2 (2%)	0	100	100
18	2W	110/113 (97%)	108 (98%)	2 (2%)	0	100	100
19	1X	93/96 (97%)	90 (97%)	3 (3%)	0	100	100
19	2X	93/96 (97%)	89 (96%)	4 (4%)	0	100	100
20	1Y	105/110 (96%)	101 (96%)	4 (4%)	0	100	100
20	2Y	105/110 (96%)	102 (97%)	3 (3%)	0	100	100
21	1Z	148/206 (72%)	140 (95%)	8 (5%)	0	100	100
21	2Z	156/206 (76%)	142 (91%)	14 (9%)	0	100	100
22	10	81/85 (95%)	80 (99%)	1 (1%)	0	100	100
22	20	81/85 (95%)	77 (95%)	4 (5%)	0	100	100
23	11	95/98 (97%)	93 (98%)	1 (1%)	1 (1%)	11	25
23	21	95/98 (97%)	93 (98%)	2 (2%)	0	100	100
24	12	68/72 (94%)	67 (98%)	1 (2%)	0	100	100
24	22	68/72 (94%)	67 (98%)	1 (2%)	0	100	100
25	13	57/60 (95%)	55 (96%)	2 (4%)	0	100	100
25	23	57/60 (95%)	55 (96%)	2 (4%)	0	100	100
26	14	67/71 (94%)	57 (85%)	7 (10%)	3 (4%)	2	2
26	24	67/71 (94%)	54 (81%)	11 (16%)	2 (3%)	3	6
27	15	57/60 (95%)	56 (98%)	1 (2%)	0	100	100
27	25	57/60 (95%)	54 (95%)	3 (5%)	0	100	100
28	16	51/54 (94%)	50 (98%)	1 (2%)	0	100	100
28	26	51/54 (94%)	51 (100%)	0	0	100	100
29	17	46/49 (94%)	46 (100%)	0	0	100	100
29	27	46/49 (94%)	44 (96%)	2 (4%)	0	100	100
30	18	62/65 (95%)	62 (100%)	0	0	100	100
30	28	62/65 (95%)	61 (98%)	1 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
31	19	35/37 (95%)	35 (100%)	0	0	100	100
31	29	35/37 (95%)	34 (97%)	1 (3%)	0	100	100
33	1b	229/256 (90%)	202 (88%)	20 (9%)	7 (3%)	3	5
33	2b	229/256 (90%)	203 (89%)	20 (9%)	6 (3%)	4	7
34	1c	204/239 (85%)	187 (92%)	15 (7%)	2 (1%)	12	28
34	2c	204/239 (85%)	187 (92%)	15 (7%)	2 (1%)	12	28
35	1d	206/209 (99%)	198 (96%)	7 (3%)	1 (0%)	24	46
35	2d	206/209 (99%)	193 (94%)	11 (5%)	2 (1%)	12	28
36	1e	146/162 (90%)	140 (96%)	5 (3%)	1 (1%)	18	38
36	2e	146/162 (90%)	141 (97%)	5 (3%)	0	100	100
37	1f	98/101 (97%)	95 (97%)	3 (3%)	0	100	100
37	2f	98/101 (97%)	96 (98%)	2 (2%)	0	100	100
38	1g	153/156 (98%)	144 (94%)	7 (5%)	2 (1%)	9	21
38	2g	153/156 (98%)	140 (92%)	11 (7%)	2 (1%)	9	21
39	1h	135/138 (98%)	132 (98%)	3 (2%)	0	100	100
39	2h	135/138 (98%)	130 (96%)	5 (4%)	0	100	100
40	1i	125/128 (98%)	112 (90%)	13 (10%)	0	100	100
40	2i	125/128 (98%)	109 (87%)	16 (13%)	0	100	100
41	1j	95/105 (90%)	85 (90%)	6 (6%)	4 (4%)	2	3
41	2j	94/105 (90%)	81 (86%)	6 (6%)	7 (7%)	1	1
42	1k	112/129 (87%)	104 (93%)	6 (5%)	2 (2%)	6	14
42	2k	112/129 (87%)	104 (93%)	6 (5%)	2 (2%)	6	14
43	1l	119/132 (90%)	112 (94%)	6 (5%)	1 (1%)	16	34
43	2l	119/132 (90%)	112 (94%)	7 (6%)	0	100	100
44	1m	121/126 (96%)	112 (93%)	9 (7%)	0	100	100
44	2m	120/126 (95%)	111 (92%)	9 (8%)	0	100	100
45	1n	58/61 (95%)	56 (97%)	2 (3%)	0	100	100
45	2n	58/61 (95%)	54 (93%)	4 (7%)	0	100	100
46	1o	86/89 (97%)	84 (98%)	2 (2%)	0	100	100
46	2o	86/89 (97%)	84 (98%)	2 (2%)	0	100	100
47	1p	80/88 (91%)	74 (92%)	6 (8%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
47	2p	80/88 (91%)	77 (96%)	3 (4%)	0	100	100
48	1q	97/105 (92%)	94 (97%)	2 (2%)	1 (1%)	12	28
48	2q	97/105 (92%)	93 (96%)	3 (3%)	1 (1%)	12	28
49	1r	66/88 (75%)	64 (97%)	2 (3%)	0	100	100
49	2r	66/88 (75%)	64 (97%)	2 (3%)	0	100	100
50	1s	81/93 (87%)	72 (89%)	9 (11%)	0	100	100
50	2s	81/93 (87%)	72 (89%)	8 (10%)	1 (1%)	10	23
51	1t	94/106 (89%)	86 (92%)	5 (5%)	3 (3%)	3	5
51	2t	94/106 (89%)	85 (90%)	6 (6%)	3 (3%)	3	5
52	1u	21/27 (78%)	20 (95%)	1 (5%)	0	100	100
52	2u	21/27 (78%)	20 (95%)	1 (5%)	0	100	100
All	All	11370/12128 (94%)	10749 (94%)	549 (5%)	72 (1%)	21	42

5 of 72 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
5	1F	130	ALA
7	1H	126	PRO
23	11	3	LYS
26	14	58	ARG
33	1b	10	LEU

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%)	198 (92%)	17 (8%)	11	26
3	2D	215/218 (99%)	201 (94%)	14 (6%)	15	35
4	1E	164/166 (99%)	148 (90%)	16 (10%)	7	17
4	2E	164/166 (99%)	155 (94%)	9 (6%)	19	41
5	1F	160/166 (96%)	146 (91%)	14 (9%)	9	21

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
5	2F	159/166 (96%)	148 (93%)	11 (7%)	14	32
6	1G	143/156 (92%)	134 (94%)	9 (6%)	16	36
6	2G	143/156 (92%)	129 (90%)	14 (10%)	7	17
7	1H	144/148 (97%)	136 (94%)	8 (6%)	19	40
7	2H	144/148 (97%)	138 (96%)	6 (4%)	26	52
8	1I	113/124 (91%)	107 (95%)	6 (5%)	20	43
8	2I	105/124 (85%)	95 (90%)	10 (10%)	8	18
9	1N	118/119 (99%)	108 (92%)	10 (8%)	10	22
9	2N	118/119 (99%)	110 (93%)	8 (7%)	14	32
10	1O	100/100 (100%)	96 (96%)	4 (4%)	28	55
10	2O	100/100 (100%)	97 (97%)	3 (3%)	36	64
11	1P	115/116 (99%)	109 (95%)	6 (5%)	21	44
11	2P	115/116 (99%)	110 (96%)	5 (4%)	26	51
12	1Q	111/111 (100%)	106 (96%)	5 (4%)	24	50
12	2Q	111/111 (100%)	107 (96%)	4 (4%)	31	58
13	1R	101/101 (100%)	88 (87%)	13 (13%)	4	8
13	2R	101/101 (100%)	90 (89%)	11 (11%)	6	13
14	1S	86/88 (98%)	82 (95%)	4 (5%)	23	48
14	2S	85/88 (97%)	83 (98%)	2 (2%)	43	70
15	1T	115/127 (91%)	111 (96%)	4 (4%)	32	59
15	2T	113/127 (89%)	112 (99%)	1 (1%)	70	87
16	1U	93/94 (99%)	90 (97%)	3 (3%)	34	62
16	2U	93/94 (99%)	89 (96%)	4 (4%)	26	51
17	1V	80/82 (98%)	70 (88%)	10 (12%)	4	9
17	2V	80/82 (98%)	70 (88%)	10 (12%)	4	9
18	1W	90/92 (98%)	81 (90%)	9 (10%)	7	16
18	2W	90/92 (98%)	84 (93%)	6 (7%)	15	33
19	1X	77/78 (99%)	73 (95%)	4 (5%)	21	44
19	2X	77/78 (99%)	75 (97%)	2 (3%)	40	68
20	1Y	85/91 (93%)	78 (92%)	7 (8%)	10	24
20	2Y	85/91 (93%)	76 (89%)	9 (11%)	6	14

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
21	1Z	135/179 (75%)	124 (92%)	11 (8%)	11	24
21	2Z	137/179 (76%)	131 (96%)	6 (4%)	25	50
22	10	65/67 (97%)	63 (97%)	2 (3%)	35	63
22	20	65/67 (97%)	64 (98%)	1 (2%)	57	80
23	11	80/83 (96%)	76 (95%)	4 (5%)	22	46
23	21	80/83 (96%)	77 (96%)	3 (4%)	29	56
24	12	65/67 (97%)	62 (95%)	3 (5%)	24	49
24	22	65/67 (97%)	65 (100%)	0	100	100
25	13	51/52 (98%)	48 (94%)	3 (6%)	18	38
25	23	50/52 (96%)	48 (96%)	2 (4%)	28	55
26	14	59/63 (94%)	53 (90%)	6 (10%)	7	15
26	24	53/63 (84%)	52 (98%)	1 (2%)	50	75
27	15	50/52 (96%)	47 (94%)	3 (6%)	17	37
27	25	50/52 (96%)	47 (94%)	3 (6%)	17	37
28	16	51/52 (98%)	49 (96%)	2 (4%)	28	55
28	26	50/52 (96%)	47 (94%)	3 (6%)	17	37
29	17	41/42 (98%)	36 (88%)	5 (12%)	5	10
29	27	41/42 (98%)	36 (88%)	5 (12%)	5	10
30	18	54/55 (98%)	49 (91%)	5 (9%)	8	18
30	28	54/55 (98%)	52 (96%)	2 (4%)	30	57
31	19	34/34 (100%)	33 (97%)	1 (3%)	37	65
31	29	34/34 (100%)	30 (88%)	4 (12%)	5	10
33	1b	192/220 (87%)	183 (95%)	9 (5%)	23	48
33	2b	187/220 (85%)	177 (95%)	10 (5%)	20	43
34	1c	142/188 (76%)	135 (95%)	7 (5%)	22	47
34	2c	140/188 (74%)	133 (95%)	7 (5%)	22	46
35	1d	169/181 (93%)	157 (93%)	12 (7%)	13	31
35	2d	173/181 (96%)	159 (92%)	14 (8%)	11	24
36	1e	113/123 (92%)	103 (91%)	10 (9%)	9	21
36	2e	114/123 (93%)	110 (96%)	4 (4%)	32	59
37	1f	84/90 (93%)	79 (94%)	5 (6%)	17	37

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
37	2f	85/90 (94%)	82 (96%)	3 (4%)	32	59
38	1g	119/127 (94%)	113 (95%)	6 (5%)	22	46
38	2g	120/127 (94%)	116 (97%)	4 (3%)	33	61
39	1h	114/119 (96%)	104 (91%)	10 (9%)	9	21
39	2h	114/119 (96%)	107 (94%)	7 (6%)	17	37
40	1i	90/99 (91%)	86 (96%)	4 (4%)	25	50
40	2i	89/99 (90%)	81 (91%)	8 (9%)	9	20
41	1j	66/92 (72%)	63 (96%)	3 (4%)	24	50
41	2j	69/92 (75%)	66 (96%)	3 (4%)	26	51
42	1k	82/99 (83%)	80 (98%)	2 (2%)	43	70
42	2k	83/99 (84%)	81 (98%)	2 (2%)	43	70
43	1l	96/108 (89%)	91 (95%)	5 (5%)	21	44
43	2l	96/108 (89%)	92 (96%)	4 (4%)	26	52
44	1m	93/101 (92%)	90 (97%)	3 (3%)	34	62
44	2m	92/101 (91%)	87 (95%)	5 (5%)	20	42
45	1n	49/50 (98%)	44 (90%)	5 (10%)	7	15
45	2n	49/50 (98%)	42 (86%)	7 (14%)	3	6
46	1o	78/80 (98%)	76 (97%)	2 (3%)	40	68
46	2o	78/80 (98%)	77 (99%)	1 (1%)	61	82
47	1p	69/74 (93%)	66 (96%)	3 (4%)	26	51
47	2p	68/74 (92%)	61 (90%)	7 (10%)	7	15
48	1q	94/97 (97%)	90 (96%)	4 (4%)	26	51
48	2q	94/97 (97%)	94 (100%)	0	100	100
49	1r	59/77 (77%)	55 (93%)	4 (7%)	14	32
49	2r	59/77 (77%)	55 (93%)	4 (7%)	14	32
50	1s	69/80 (86%)	68 (99%)	1 (1%)	59	81
50	2s	67/80 (84%)	63 (94%)	4 (6%)	17	37
51	1t	70/82 (85%)	65 (93%)	5 (7%)	13	31
51	2t	70/82 (85%)	69 (99%)	1 (1%)	59	81
52	1u	18/22 (82%)	17 (94%)	1 (6%)	19	40
52	2u	18/22 (82%)	18 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
All	All	9303/10064 (92%)	8754 (94%)	549 (6%)	18	38

5 of 549 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
33	2b	213	LEU
35	2d	34	GLU
33	2b	195	ASP
44	2m	3	ARG
33	1b	80	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 115 such sidechains are listed below:

Mol	Chain	Res	Type
8	2I	104	GLN
50	2s	47	HIS
18	2W	62	HIS
50	2s	23	ASN
40	2i	58	HIS

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	1A	2864/2915 (98%)	431 (15%)	29 (1%)
1	2A	2791/2915 (95%)	482 (17%)	24 (0%)
2	1B	120/121 (99%)	11 (9%)	1 (0%)
2	2B	118/121 (97%)	33 (27%)	0
32	1a	1497/1521 (98%)	240 (16%)	0
32	2a	1501/1521 (98%)	286 (19%)	0
53	1v	12/24 (50%)	2 (16%)	0
53	2v	12/24 (50%)	4 (33%)	0
54	1w	72/76 (94%)	23 (31%)	0
54	1y	72/76 (94%)	19 (26%)	0
54	2w	69/76 (90%)	22 (31%)	0
54	2y	70/76 (92%)	21 (30%)	0
55	1x	75/77 (97%)	10 (13%)	0
55	2x	75/77 (97%)	13 (17%)	0
All	All	9348/9620 (97%)	1597 (17%)	54 (0%)

5 of 1597 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	1A	9	U
1	1A	12	U
1	1A	13	A
1	1A	27	G
1	1A	34	C

5 of 54 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	1A	2756	U
1	2A	277	C
1	2A	1992	G
2	1B	1	U
1	2A	266	G

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

84 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	5MC	1a	967	32	19,22,23	1.62	3 (15%)	26,32,35	1.14	2 (7%)
1	OMG	2A	2251	1,56,55	23,26,27	1.21	3 (13%)	32,38,41	1.97	6 (18%)
1	PSU	2A	1917	1	18,21,22	1.36	2 (11%)	21,30,33	2.05	4 (19%)
43	0TD	2l	92	43	8,9,10	4.51	1 (12%)	6,11,13	3.45	3 (50%)
1	5MU	2A	1915	1	19,22,23	1.44	5 (26%)	27,32,35	2.06	6 (22%)
54	MIA	2y	37	54	21,24,32	1.59	4 (19%)	30,35,47	2.05	7 (23%)
54	4SU	1y	8	54	18,21,22	1.76	4 (22%)	25,30,33	2.01	4 (16%)
32	5MC	1a	1400	32	19,22,23	1.68	3 (15%)	26,32,35	1.13	3 (11%)
55	5MU	2x	54	55	19,22,23	1.41	6 (31%)	27,32,35	2.03	6 (22%)
54	PSU	2w	39	54	18,21,22	1.37	2 (11%)	21,30,33	1.84	3 (14%)
32	MA6	2a	1519	32	23,26,27	1.59	4 (17%)	33,38,41	2.28	11 (33%)
1	5MC	2A	1962	1,56	19,22,23	1.65	3 (15%)	26,32,35	1.11	2 (7%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	PSU	1A	1911	1	18,21,22	1.39	2 (11%)	21,30,33	2.07	4 (19%)
54	4SU	2y	8	54	18,21,22	1.87	5 (27%)	25,30,33	2.03	5 (20%)
55	PSU	1x	55	56,55	18,21,22	1.37	2 (11%)	21,30,33	2.02	4 (19%)
1	5MU	1A	1939	1,56	19,22,23	1.40	6 (31%)	27,32,35	2.15	6 (22%)
32	5MC	2a	1400	32	19,22,23	1.64	3 (15%)	26,32,35	1.10	2 (7%)
54	PSU	1y	32	54	18,21,22	1.37	2 (11%)	21,30,33	1.99	3 (14%)
1	4OC	1A	1920	1	19,22,24	0.80	0	25,31,35	0.95	1 (4%)
54	MIA	2w	37	54	24,27,32	2.05	5 (20%)	32,39,47	2.42	10 (31%)
1	2MU	1A	2552	1,56	19,22,24	1.19	2 (10%)	25,31,36	2.00	6 (24%)
1	2MA	1A	2503	1,56	22,25,26	1.49	5 (22%)	32,37,40	2.26	9 (28%)
32	5MC	2a	1407	32	19,22,23	1.56	3 (15%)	26,32,35	1.11	3 (11%)
55	PSU	2x	55	55	18,21,22	1.38	2 (11%)	21,30,33	2.03	4 (19%)
54	7MG	2w	46	54	23,26,27	1.36	4 (17%)	27,39,42	2.56	7 (25%)
54	PSU	2y	39	54	18,21,22	1.34	2 (11%)	21,30,33	2.00	4 (19%)
55	5MC	2x	32	55	19,22,23	1.69	3 (15%)	26,32,35	1.16	3 (11%)
54	PSU	2y	32	54	18,21,22	1.37	2 (11%)	21,30,33	2.02	4 (19%)
32	7MG	1a	527	32,56	23,26,27	1.36	4 (17%)	27,39,42	2.61	7 (25%)
54	PSU	1y	55	54	18,21,22	1.35	2 (11%)	21,30,33	2.03	3 (14%)
32	5MC	2a	967	32	19,22,23	1.71	3 (15%)	26,32,35	1.13	3 (11%)
54	7MG	1y	46	54	23,26,27	1.34	4 (17%)	27,39,42	2.62	7 (25%)
32	2MG	1a	1207	32	23,26,27	1.25	4 (17%)	33,38,41	2.15	6 (18%)
54	4SU	1w	8	54	18,21,22	1.81	5 (27%)	25,30,33	1.89	5 (20%)
32	MA6	2a	1518	32	23,26,27	1.57	5 (21%)	33,38,41	2.28	12 (36%)
1	5MU	2A	1939	1,56	19,22,23	1.42	6 (31%)	27,32,35	2.23	6 (22%)
1	2MU	2A	2552	1,56	19,22,24	1.30	3 (15%)	25,31,36	1.88	6 (24%)
55	4SU	2x	8	56,55	18,21,22	2.04	5 (27%)	25,30,33	1.79	7 (28%)
1	5MC	1A	1962	1,56	19,22,23	1.63	3 (15%)	26,32,35	1.10	2 (7%)
54	4SU	2w	8	54	18,21,22	1.80	4 (22%)	25,30,33	2.67	6 (24%)
54	PSU	1y	39	54	18,21,22	1.33	2 (11%)	21,30,33	2.07	4 (19%)
32	4OC	2a	1402	32,56	20,23,24	0.77	0	25,32,35	0.97	1 (4%)
32	UR3	2a	1498	32	19,22,23	1.04	2 (10%)	26,32,35	1.78	3 (11%)
54	PSU	1w	32	54	18,21,22	1.37	2 (11%)	21,30,33	1.94	3 (14%)
54	5MU	1w	54	54	19,22,23	1.37	6 (31%)	27,32,35	2.17	7 (25%)
1	2MA	2A	2503	1,56	22,25,26	1.50	4 (18%)	32,37,40	2.27	7 (21%)
32	PSU	1a	516	32	18,21,22	1.37	2 (11%)	21,30,33	1.96	3 (14%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
55	4SU	1x	8	55	18,21,22	2.15	6 (33%)	25,30,33	1.61	5 (20%)
55	5MC	1x	32	55	19,22,23	1.72	3 (15%)	26,32,35	1.22	2 (7%)
54	PSU	2w	55	54	18,21,22	1.39	2 (11%)	21,30,33	2.02	3 (14%)
54	5MU	2y	54	54	19,22,23	1.44	6 (31%)	27,32,35	1.85	7 (25%)
1	5MU	1A	1915	1	19,22,23	1.44	5 (26%)	27,32,35	2.08	6 (22%)
54	PSU	1w	55	54	18,21,22	1.43	2 (11%)	21,30,33	2.11	3 (14%)
32	UR3	1a	1498	32	19,22,23	1.02	1 (5%)	26,32,35	1.73	3 (11%)
32	5MC	2a	1404	32	19,22,23	1.74	3 (15%)	26,32,35	1.19	3 (11%)
1	5MC	2A	1942	1	19,22,23	1.65	3 (15%)	26,32,35	1.11	2 (7%)
32	5MC	1a	1407	32	19,22,23	1.65	3 (15%)	26,32,35	1.14	2 (7%)
32	2MG	2a	1207	32	23,26,27	1.24	3 (13%)	33,38,41	2.18	7 (21%)
32	M2G	1a	966	32	24,27,28	1.30	3 (12%)	33,40,43	1.82	5 (15%)
32	PSU	2a	516	32	18,21,22	1.38	2 (11%)	21,30,33	1.91	3 (14%)
1	PSU	1A	1917	1	18,21,22	1.36	2 (11%)	21,30,33	2.02	4 (19%)
1	PSU	2A	1911	1	18,21,22	1.36	2 (11%)	21,30,33	2.00	3 (14%)
55	5MU	1x	54	56,55	19,22,23	1.42	5 (26%)	27,32,35	1.98	6 (22%)
32	MA6	1a	1519	32	23,26,27	1.56	4 (17%)	33,38,41	2.31	13 (39%)
1	4OC	2A	1920	1	19,22,24	0.78	0	25,31,35	0.90	1 (4%)
32	7MG	2a	527	32,56	23,26,27	1.33	3 (13%)	27,39,42	2.62	7 (25%)
32	M2G	2a	966	32	24,27,28	1.31	4 (16%)	33,40,43	1.87	6 (18%)
54	PSU	2y	55	54	18,21,22	1.34	2 (11%)	21,30,33	2.03	4 (19%)
54	7MG	1w	46	54	23,26,27	1.42	4 (17%)	27,39,42	2.55	8 (29%)
54	PSU	2w	32	54	18,21,22	1.35	2 (11%)	21,30,33	1.99	3 (14%)
54	5MU	2w	54	54	19,22,23	1.37	5 (26%)	27,32,35	1.86	7 (25%)
1	PSU	2A	2605	1	18,21,22	1.38	3 (16%)	21,30,33	2.03	4 (19%)
54	7MG	2y	46	54	23,26,27	1.34	3 (13%)	27,39,42	2.74	6 (22%)
32	5MC	1a	1404	32	19,22,23	1.71	3 (15%)	26,32,35	1.14	3 (11%)
54	MIA	1w	37	54	28,31,32	2.33	6 (21%)	38,44,47	2.73	13 (34%)
54	5MU	1y	54	54	19,22,23	1.41	5 (26%)	27,32,35	2.13	6 (22%)
32	4OC	1a	1402	32	20,23,24	0.77	0	25,32,35	0.95	1 (4%)
54	PSU	1w	39	54	18,21,22	1.37	2 (11%)	21,30,33	2.01	4 (19%)
1	PSU	1A	2605	1,56	18,21,22	1.37	2 (11%)	21,30,33	1.92	3 (14%)
1	5MC	1A	1942	1	19,22,23	1.60	3 (15%)	26,32,35	1.12	2 (7%)
1	OMG	1A	2251	1,56,55	23,26,27	1.17	3 (13%)	32,38,41	1.98	6 (18%)
54	MIA	1y	37	54	21,24,32	1.59	4 (19%)	30,35,47	2.00	8 (26%)

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	1.51	4 (17%)	33,38,41	2.31	13 (39%)
43	0TD	1l	92	43	8,9,10	4.56	1 (12%)	6,11,13	4.80	3 (50%)

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	5MC	1a	967	32	-	1/7/25/26	0/2/2/2
1	OMG	2A	2251	1,56,55	-	1/9/27/28	0/3/3/3
1	PSU	2A	1917	1	-	0/7/25/26	0/2/2/2
43	0TD	2l	92	43	-	2/7/12/14	-
1	5MU	2A	1915	1	-	0/7/25/26	0/2/2/2
54	MIA	2y	37	54	-	0/7/25/34	0/3/3/3
54	4SU	1y	8	54	-	3/7/25/26	0/2/2/2
32	5MC	1a	1400	32	-	2/7/25/26	0/2/2/2
55	5MU	2x	54	55	-	0/7/25/26	0/2/2/2
54	PSU	2w	39	54	-	2/7/25/26	0/2/2/2
32	MA6	2a	1519	32	-	6/11/29/30	0/3/3/3
1	5MC	2A	1962	1,56	-	0/7/25/26	0/2/2/2
1	PSU	1A	1911	1	-	0/7/25/26	0/2/2/2
54	4SU	2y	8	54	-	2/7/25/26	0/2/2/2
55	PSU	1x	55	56,55	-	0/7/25/26	0/2/2/2
1	5MU	1A	1939	1,56	-	0/7/25/26	0/2/2/2
32	5MC	2a	1400	32	-	1/7/25/26	0/2/2/2
54	PSU	1y	32	54	-	0/7/25/26	0/2/2/2
1	4OC	1A	1920	1	-	1/9/27/30	0/2/2/2
54	MIA	2w	37	54	-	0/11/29/34	0/3/3/3
1	2MU	1A	2552	1,56	-	0/9/27/28	0/2/2/2
1	2MA	1A	2503	1,56	-	1/7/25/26	0/3/3/3
32	5MC	2a	1407	32	-	0/7/25/26	0/2/2/2
55	PSU	2x	55	55	-	0/7/25/26	0/2/2/2
54	7MG	2w	46	54	-	2/7/37/38	0/3/3/3
54	PSU	2y	39	54	-	0/7/25/26	0/2/2/2
55	5MC	2x	32	55	-	0/7/25/26	0/2/2/2
54	PSU	2y	32	54	-	0/7/25/26	0/2/2/2
32	7MG	1a	527	32,56	-	3/7/37/38	0/3/3/3
54	PSU	1y	55	54	-	0/7/25/26	0/2/2/2
32	5MC	2a	967	32	-	0/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
54	7MG	1y	46	54	-	3/7/37/38	0/3/3/3
32	2MG	1a	1207	32	-	0/9/27/28	0/3/3/3
54	4SU	1w	8	54	-	0/7/25/26	0/2/2/2
32	MA6	2a	1518	32	-	2/11/29/30	0/3/3/3
1	5MU	2A	1939	1,56	-	0/7/25/26	0/2/2/2
1	2MU	2A	2552	1,56	-	0/9/27/28	0/2/2/2
55	4SU	2x	8	56,55	-	1/7/25/26	0/2/2/2
1	5MC	1A	1962	1,56	-	0/7/25/26	0/2/2/2
54	4SU	2w	8	54	-	0/7/25/26	0/2/2/2
54	PSU	1y	39	54	-	0/7/25/26	0/2/2/2
32	4OC	2a	1402	32,56	-	2/9/29/30	0/2/2/2
32	UR3	2a	1498	32	-	0/7/25/26	0/2/2/2
54	PSU	1w	32	54	-	0/7/25/26	0/2/2/2
54	5MU	1w	54	54	-	0/7/25/26	0/2/2/2
1	2MA	2A	2503	1,56	-	0/7/25/26	0/3/3/3
32	PSU	1a	516	32	-	0/7/25/26	0/2/2/2
55	4SU	1x	8	55	-	0/7/25/26	0/2/2/2
55	5MC	1x	32	55	-	0/7/25/26	0/2/2/2
54	PSU	2w	55	54	-	0/7/25/26	0/2/2/2
54	5MU	2y	54	54	-	0/7/25/26	0/2/2/2
1	5MU	1A	1915	1	-	2/7/25/26	0/2/2/2
54	PSU	1w	55	54	-	0/7/25/26	0/2/2/2
32	UR3	1a	1498	32	-	0/7/25/26	0/2/2/2
32	5MC	2a	1404	32	-	0/7/25/26	0/2/2/2
1	5MC	2A	1942	1	-	0/7/25/26	0/2/2/2
32	5MC	1a	1407	32	-	0/7/25/26	0/2/2/2
32	2MG	2a	1207	32	-	0/9/27/28	0/3/3/3
32	M2G	1a	966	32	-	0/11/29/30	0/3/3/3
32	PSU	2a	516	32	-	0/7/25/26	0/2/2/2
1	PSU	1A	1917	1	-	0/7/25/26	0/2/2/2
1	PSU	2A	1911	1	-	0/7/25/26	0/2/2/2
55	5MU	1x	54	56,55	-	0/7/25/26	0/2/2/2
32	MA6	1a	1519	32	-	4/11/29/30	0/3/3/3
1	4OC	2A	1920	1	-	0/9/27/30	0/2/2/2
32	7MG	2a	527	32,56	-	1/7/37/38	0/3/3/3
32	M2G	2a	966	32	-	0/11/29/30	0/3/3/3
54	PSU	2y	55	54	-	0/7/25/26	0/2/2/2
54	7MG	1w	46	54	-	2/7/37/38	0/3/3/3
54	PSU	2w	32	54	-	0/7/25/26	0/2/2/2
54	5MU	2w	54	54	-	0/7/25/26	0/2/2/2
1	PSU	2A	2605	1	-	0/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
54	7MG	2y	46	54	-	3/7/37/38	0/3/3/3
32	5MC	1a	1404	32	-	0/7/25/26	0/2/2/2
54	MIA	1w	37	54	-	1/15/33/34	0/3/3/3
54	5MU	1y	54	54	-	1/7/25/26	0/2/2/2
32	4OC	1a	1402	32	-	2/9/29/30	0/2/2/2
54	PSU	1w	39	54	-	0/7/25/26	0/2/2/2
1	PSU	1A	2605	1,56	-	0/7/25/26	0/2/2/2
1	5MC	1A	1942	1	-	0/7/25/26	0/2/2/2
1	OMG	1A	2251	1,56,55	-	0/9/27/28	0/3/3/3
54	MIA	1y	37	54	-	0/7/25/34	0/3/3/3
32	MA6	1a	1518	32	-	2/11/29/30	0/3/3/3
43	0TD	1l	92	43	-	1/7/12/14	-

The worst 5 of 268 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
43	1l	92	0TD	CB-SB	-12.49	1.69	1.82
43	2l	92	0TD	CB-SB	-12.35	1.69	1.82
54	1w	37	MIA	C13-C14	6.84	1.52	1.32
54	1w	37	MIA	C2-S10	-6.74	1.70	1.75
54	2w	37	MIA	C2-S10	-6.47	1.70	1.75

The worst 5 of 415 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
43	1l	92	0TD	CSB-SB-CB	-11.01	82.57	102.36
54	2y	46	7MG	N9-C4-N3	9.82	139.84	125.46
54	1y	46	7MG	N9-C4-N3	9.20	138.94	125.46
32	2a	527	7MG	N9-C4-N3	9.09	138.78	125.46
54	1w	37	MIA	C12-C13-C14	-9.05	110.76	127.01

There are no chirality outliers.

5 of 54 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
32	1a	1519	MA6	O4'-C4'-C5'-O5'
32	2a	1402	4OC	O4'-C4'-C5'-O5'
32	2a	1518	MA6	C5-C6-N6-C9
32	2a	1519	MA6	O4'-C4'-C5'-O5'
43	2l	92	0TD	O-C-CA-CB

There are no ring outliers.

46 monomers are involved in 63 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	2A	2251	OMG	2	0
1	2A	1917	PSU	1	0
43	2l	92	0TD	1	0
1	2A	1915	5MU	1	0
54	2y	37	MIA	1	0
54	1y	8	4SU	1	0
54	2w	39	PSU	1	0
32	2a	1519	MA6	2	0
1	1A	1939	5MU	2	0
1	1A	1920	4OC	1	0
54	2w	37	MIA	1	0
1	1A	2552	2MU	1	0
32	2a	1407	5MC	1	0
54	2y	39	PSU	1	0
55	2x	32	5MC	1	0
32	2a	967	5MC	2	0
54	1y	46	7MG	1	0
32	2a	1518	MA6	3	0
1	2A	1939	5MU	1	0
1	2A	2552	2MU	1	0
55	2x	8	4SU	2	0
54	2w	8	4SU	5	0
54	1y	39	PSU	1	0
32	2a	1402	4OC	2	0
32	2a	1498	UR3	2	0
54	1w	54	5MU	1	0
1	2A	2503	2MA	1	0
55	1x	8	4SU	2	0
55	1x	32	5MC	1	0
54	2y	54	5MU	1	0
54	1w	55	PSU	1	0
32	2a	1404	5MC	1	0
32	2a	516	PSU	1	0
32	1a	1519	MA6	3	0
1	2A	1920	4OC	2	0
32	2a	966	M2G	2	0
54	2y	55	PSU	2	0
54	1w	46	7MG	1	0
54	2w	32	PSU	1	0
54	2w	54	5MU	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
54	2y	46	7MG	2	0
54	1w	37	MIA	1	0
32	1a	1402	4OC	2	0
54	1w	39	PSU	1	0
54	1y	37	MIA	1	0
32	1a	1518	MA6	3	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 2840 ligands modelled in this entry, 2836 are monoatomic - leaving 4 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	$\# Z > 2$
60	SF4	2d	302	35	0,12,12	-	-	-		
57	CLM	2A	3888	-	20,20,20	0.93	2 (10%)	23,27,27	1.00	1 (4%)
60	SF4	1d	302	35	0,12,12	-	-	-		
57	CLM	1A	4102	-	20,20,20	0.91	2 (10%)	23,27,27	0.74	0

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
60	SF4	2d	302	35	-	-	0/6/5/5
57	CLM	2A	3888	-	-	6/20/22/22	0/1/1/1
60	SF4	1d	302	35	-	-	0/6/5/5
57	CLM	1A	4102	-	-	7/20/22/22	0/1/1/1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
57	2A	3888	CLM	C6-C5	-2.44	1.48	1.51
57	2A	3888	CLM	C9-N9	-2.15	1.40	1.45
57	1A	4102	CLM	C6-C5	-2.12	1.48	1.51
57	1A	4102	CLM	C9-N9	-2.02	1.40	1.45

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
57	2A	3888	CLM	C6-C5-C3	-2.82	106.66	111.72

There are no chirality outliers.

5 of 13 torsion outliers are listed below:

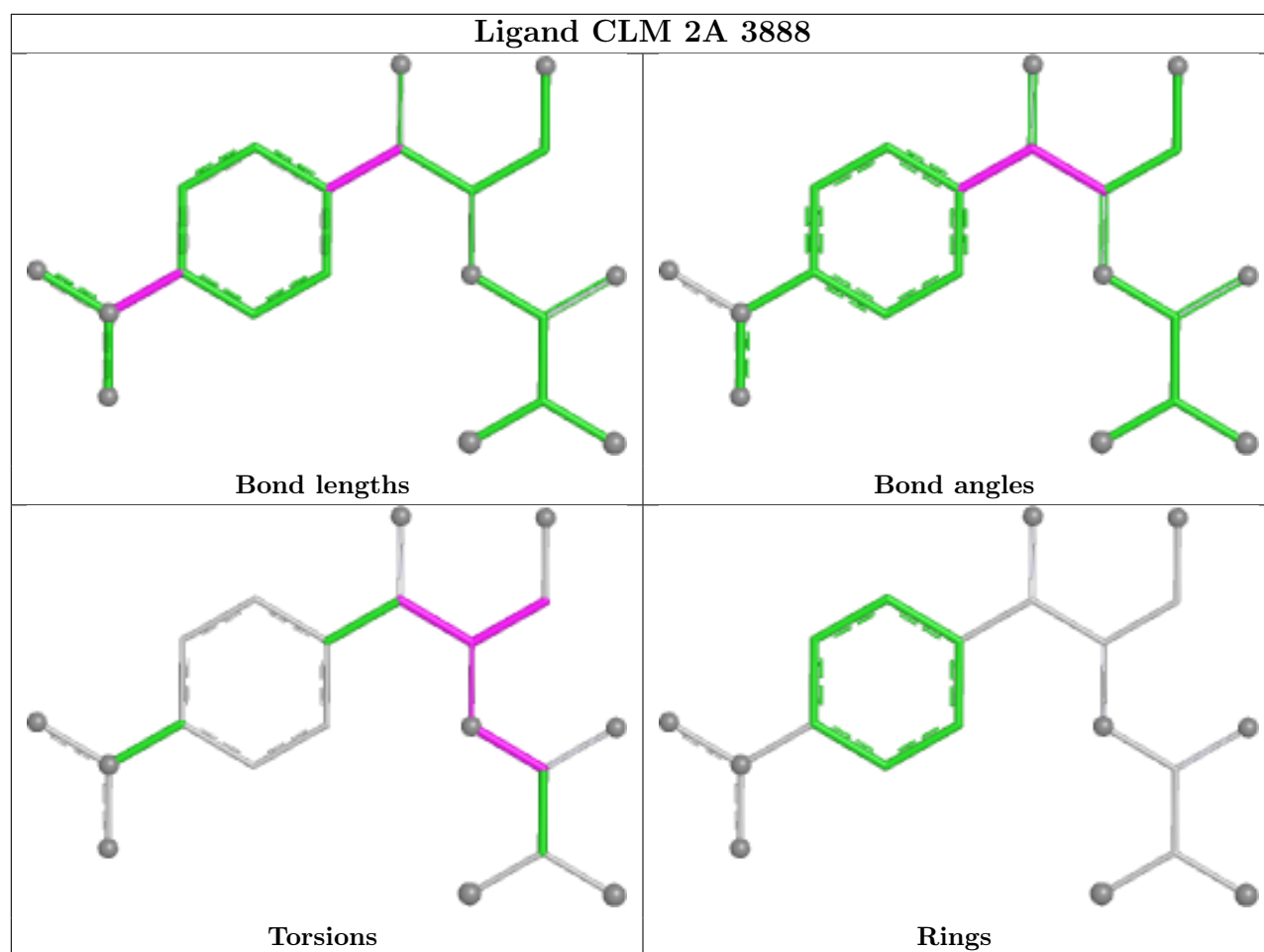
Mol	Chain	Res	Type	Atoms
57	2A	3888	CLM	C1-C2-N2-C3
57	2A	3888	CLM	O2-C2-N2-C3
57	2A	3888	CLM	C4-C3-N2-C2
57	2A	3888	CLM	N2-C3-C4-O4
57	2A	3888	CLM	C5-C3-C4-O4

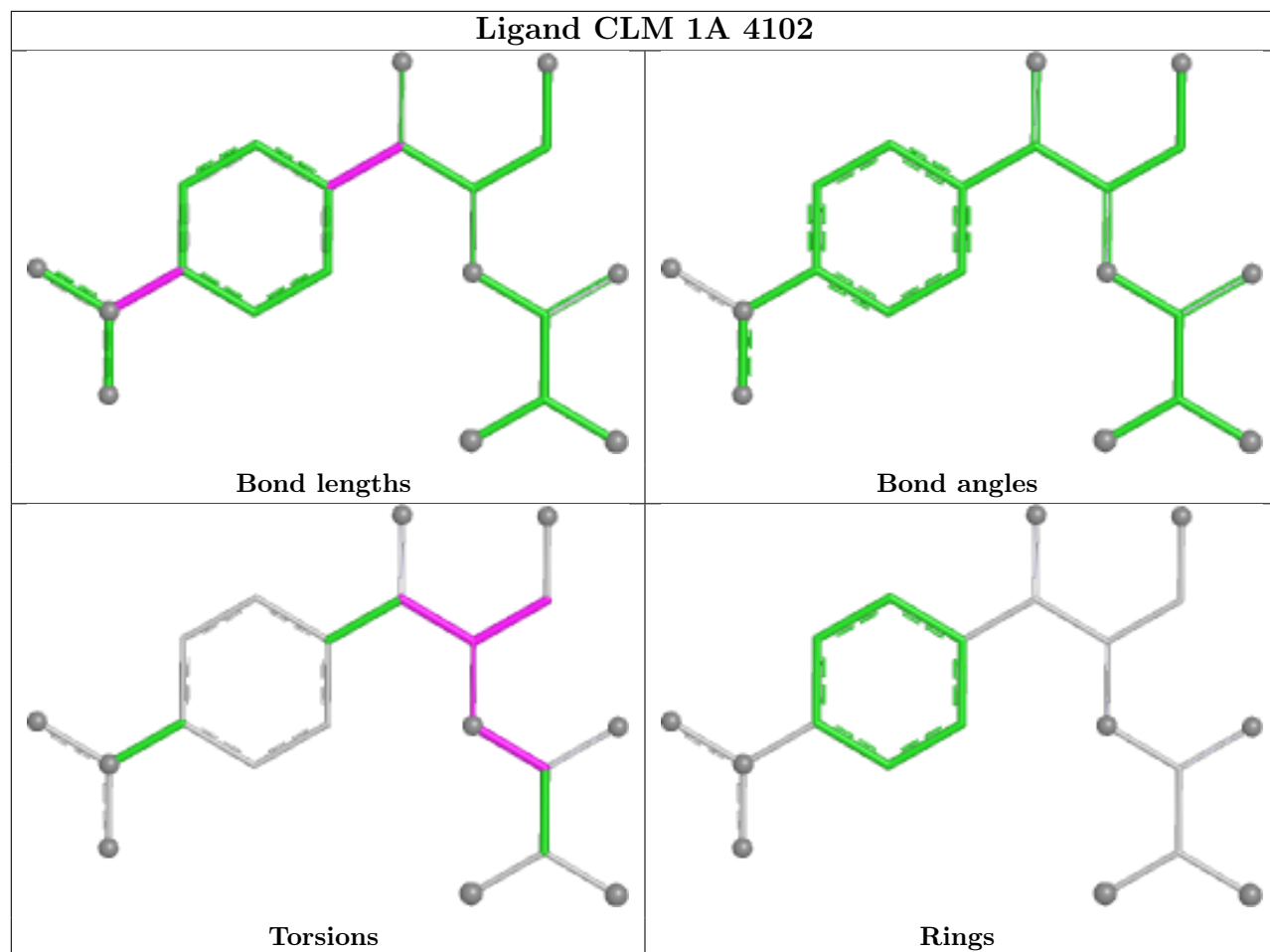
There are no ring outliers.

3 monomers are involved in 15 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
60	2d	302	SF4	3	0
57	2A	3888	CLM	1	0
60	1d	302	SF4	11	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.





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%)	-0.41	102 (3%)	46	40	17, 34, 87, 101	0
1	2A	2789/2915 (95%)	0.13	94 (3%)	48	42	34, 57, 87, 102	0
2	1B	120/121 (99%)	-0.29	0	100	100	27, 48, 58, 79	0
2	2B	120/121 (99%)	1.04	9 (7%)	20	16	58, 78, 85, 87	0
3	1D	275/276 (99%)	-0.01	4 (1%)	72	68	20, 35, 50, 73	0
3	2D	275/276 (99%)	0.44	2 (0%)	84	82	33, 51, 62, 73	0
4	1E	204/206 (99%)	-0.04	1 (0%)	87	85	18, 40, 57, 73	0
4	2E	204/206 (99%)	0.55	9 (4%)	39	33	35, 58, 69, 79	0
5	1F	203/210 (96%)	-0.01	2 (0%)	79	76	16, 41, 63, 80	0
5	2F	203/210 (96%)	0.64	6 (2%)	52	47	37, 64, 77, 83	0
6	1G	181/182 (99%)	0.55	8 (4%)	39	33	39, 56, 69, 78	0
6	2G	181/182 (99%)	1.21	23 (12%)	8	6	68, 77, 85, 93	0
7	1H	174/180 (96%)	0.30	3 (1%)	69	64	37, 50, 62, 71	0
7	2H	174/180 (96%)	1.38	39 (22%)	2	2	67, 78, 84, 91	0
8	1I	146/148 (98%)	0.89	4 (2%)	56	50	45, 70, 77, 81	0
8	2I	146/148 (98%)	1.13	16 (10%)	10	8	53, 70, 80, 85	0
9	1N	140/140 (100%)	0.01	1 (0%)	84	82	26, 38, 54, 72	0
9	2N	140/140 (100%)	0.64	4 (2%)	53	48	46, 64, 75, 80	0
10	1O	122/122 (100%)	-0.03	0	100	100	26, 40, 55, 61	0
10	2O	122/122 (100%)	0.58	1 (0%)	82	80	44, 57, 68, 73	0
11	1P	149/150 (99%)	0.10	0	100	100	17, 44, 64, 72	0
11	2P	149/150 (99%)	0.66	1 (0%)	84	82	38, 64, 77, 83	0
12	1Q	141/141 (100%)	0.10	1 (0%)	84	82	27, 41, 54, 74	0
12	2Q	141/141 (100%)	1.01	12 (8%)	16	13	52, 65, 74, 80	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2		OWAB(Å ²)	Q<0.9
13	1R	118/118 (100%)	-0.23	0	100 100	22, 34, 47, 55	0
13	2R	118/118 (100%)	0.29	0	100 100	38, 51, 59, 67	0
14	1S	110/112 (98%)	0.25	0	100 100	37, 49, 61, 65	0
14	2S	110/112 (98%)	1.56	35 (31%)	1 1	63, 73, 80, 84	0
15	1T	131/146 (89%)	0.18	2 (1%)	72 68	33, 43, 64, 70	0
15	2T	131/146 (89%)	0.65	4 (3%)	51 45	49, 59, 74, 79	0
16	1U	116/118 (98%)	-0.21	1 (0%)	81 78	20, 29, 47, 60	0
16	2U	116/118 (98%)	0.84	5 (4%)	40 34	47, 61, 74, 80	0
17	1V	101/101 (100%)	-0.19	0	100 100	20, 39, 56, 69	0
17	2V	101/101 (100%)	0.75	1 (0%)	79 76	42, 68, 76, 82	0
18	1W	112/113 (99%)	-0.23	2 (1%)	67 63	21, 30, 46, 75	0
18	2W	112/113 (99%)	0.55	1 (0%)	81 78	38, 50, 66, 88	0
19	1X	95/96 (98%)	-0.04	2 (2%)	63 58	24, 36, 55, 72	0
19	2X	95/96 (98%)	0.80	4 (4%)	40 35	44, 58, 70, 81	0
20	1Y	107/110 (97%)	0.41	1 (0%)	81 78	33, 48, 66, 74	0
20	2Y	107/110 (97%)	0.92	5 (4%)	36 30	59, 68, 75, 84	0
21	1Z	154/206 (74%)	0.67	9 (5%)	29 23	41, 60, 77, 85	0
21	2Z	160/206 (77%)	1.71	51 (31%)	1 1	66, 78, 86, 88	0
22	10	83/85 (97%)	0.40	7 (8%)	17 13	27, 37, 60, 72	0
22	20	83/85 (97%)	1.32	12 (14%)	6 4	53, 64, 74, 83	0
23	11	97/98 (98%)	0.22	2 (2%)	63 58	24, 43, 63, 68	0
23	21	97/98 (98%)	0.71	5 (5%)	33 27	40, 56, 71, 73	0
24	12	70/72 (97%)	0.19	2 (2%)	53 48	32, 46, 57, 65	0
24	22	70/72 (97%)	0.97	5 (7%)	22 17	54, 68, 73, 76	0
25	13	59/60 (98%)	-0.04	1 (1%)	69 64	25, 36, 58, 78	0
25	23	59/60 (98%)	0.64	1 (1%)	69 64	53, 64, 77, 79	0
26	14	69/71 (97%)	1.04	11 (15%)	5 4	49, 71, 81, 85	0
26	24	69/71 (97%)	1.50	18 (26%)	1 1	76, 82, 88, 91	0
27	15	59/60 (98%)	-0.32	1 (1%)	69 64	18, 29, 45, 63	0
27	25	59/60 (98%)	0.32	2 (3%)	48 42	38, 50, 63, 67	0
28	16	53/54 (98%)	0.07	0	100 100	30, 41, 55, 61	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
28	26	53/54 (98%)	1.17	6 (11%) 10 8	49, 61, 68, 75	0
29	17	48/49 (97%)	-0.12	0 100 100	18, 24, 52, 58	0
29	27	48/49 (97%)	0.23	4 (8%) 17 13	32, 41, 60, 68	0
30	18	64/65 (98%)	-0.03	1 (1%) 70 66	26, 31, 38, 54	0
30	28	64/65 (98%)	0.67	2 (3%) 51 45	45, 54, 60, 71	0
31	19	37/37 (100%)	-0.13	0 100 100	27, 38, 54, 57	0
31	29	37/37 (100%)	1.15	3 (8%) 18 14	59, 66, 73, 76	0
32	1a	1488/1521 (97%)	0.39	45 (3%) 52 47	33, 65, 87, 100	0
32	2a	1491/1521 (98%)	0.90	157 (10%) 11 9	50, 75, 91, 99	0
33	1b	231/256 (90%)	1.35	44 (19%) 3 2	63, 74, 82, 87	0
33	2b	231/256 (90%)	1.53	60 (25%) 1 1	71, 83, 88, 92	0
34	1c	206/239 (86%)	0.91	15 (7%) 21 17	59, 70, 78, 83	0
34	2c	206/239 (86%)	2.08	102 (49%) 0 0	72, 82, 87, 91	0
35	1d	208/209 (99%)	1.10	24 (11%) 9 7	56, 69, 80, 84	0
35	2d	208/209 (99%)	0.97	13 (6%) 26 20	57, 67, 75, 82	0
36	1e	148/162 (91%)	0.66	4 (2%) 56 50	49, 63, 70, 76	0
36	2e	148/162 (91%)	1.30	23 (15%) 5 4	67, 76, 81, 88	0
37	1f	100/101 (99%)	0.64	2 (2%) 65 60	50, 64, 70, 73	0
37	2f	100/101 (99%)	1.19	13 (13%) 7 5	60, 70, 77, 81	0
38	1g	155/156 (99%)	1.01	17 (10%) 10 8	50, 67, 76, 87	0
38	2g	155/156 (99%)	1.31	27 (17%) 4 3	66, 75, 82, 88	0
39	1h	137/138 (99%)	0.50	2 (1%) 72 68	56, 64, 71, 75	0
39	2h	137/138 (99%)	1.20	17 (12%) 8 6	67, 75, 80, 86	0
40	1i	127/128 (99%)	1.32	26 (20%) 2 2	52, 72, 77, 79	0
40	2i	127/128 (99%)	2.05	67 (52%) 0 0	68, 80, 86, 89	0
41	1j	97/105 (92%)	1.29	22 (22%) 2 1	58, 76, 83, 89	0
41	2j	96/105 (91%)	2.67	74 (77%) 0 0	71, 82, 88, 96	0
42	1k	114/129 (88%)	0.69	4 (3%) 47 41	38, 61, 70, 74	0
42	2k	114/129 (88%)	1.17	19 (16%) 4 3	56, 72, 77, 82	0
43	1l	121/132 (91%)	0.70	10 (8%) 17 13	42, 56, 66, 69	0
43	2l	121/132 (91%)	1.44	24 (19%) 3 2	58, 69, 76, 80	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
44	1m	123/126 (97%)	0.98	10 (8%) 18 14	55, 67, 75, 81	0
44	2m	122/126 (96%)	1.94	47 (38%) 1 0	71, 79, 85, 88	0
45	1n	60/61 (98%)	1.28	8 (13%) 7 5	60, 68, 73, 76	0
45	2n	60/61 (98%)	2.55	44 (73%) 0 0	74, 82, 86, 90	0
46	1o	88/89 (98%)	0.81	5 (5%) 29 24	48, 60, 70, 74	0
46	2o	88/89 (98%)	1.14	15 (17%) 4 3	60, 70, 78, 82	0
47	1p	82/88 (93%)	1.33	12 (14%) 6 4	56, 70, 76, 79	0
47	2p	82/88 (93%)	1.11	6 (7%) 21 17	58, 65, 74, 80	0
48	1q	99/105 (94%)	1.23	16 (16%) 4 3	50, 63, 71, 73	0
48	2q	99/105 (94%)	0.99	8 (8%) 18 14	62, 69, 77, 81	0
49	1r	68/88 (77%)	0.75	6 (8%) 15 12	55, 64, 73, 75	0
49	2r	68/88 (77%)	1.04	3 (4%) 39 33	62, 71, 78, 82	0
50	1s	83/93 (89%)	1.06	9 (10%) 11 8	60, 70, 77, 80	0
50	2s	83/93 (89%)	2.47	58 (69%) 0 0	75, 82, 87, 91	0
51	1t	96/106 (90%)	1.06	8 (8%) 17 13	58, 68, 76, 81	0
51	2t	96/106 (90%)	1.28	17 (17%) 4 3	57, 69, 76, 79	0
52	1u	23/27 (85%)	1.42	4 (17%) 4 3	59, 64, 69, 71	0
52	2u	23/27 (85%)	2.10	12 (52%) 0 0	74, 77, 81, 85	0
53	1v	13/24 (54%)	0.80	1 (7%) 19 15	47, 66, 80, 86	0
53	2v	13/24 (54%)	2.51	8 (61%) 0 0	69, 82, 92, 92	0
54	1w	67/76 (88%)	1.56	15 (22%) 2 2	59, 87, 94, 98	0
54	1y	67/76 (88%)	0.83	3 (4%) 38 32	38, 86, 93, 96	0
54	2w	65/76 (85%)	1.76	23 (35%) 1 1	74, 91, 96, 101	0
54	2y	66/76 (86%)	1.41	10 (15%) 5 4	57, 92, 96, 99	0
55	1x	72/77 (93%)	0.42	3 (4%) 40 35	37, 62, 77, 85	0
55	2x	72/77 (93%)	0.84	2 (2%) 55 49	55, 78, 86, 89	0
All	All	20875/21748 (95%)	0.53	1712 (8%) 17 14	16, 62, 85, 102	0

The worst 5 of 1712 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
44	2m	124	PRO	8.5
45	1n	2	ALA	8.0

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Mol	Chain	Res	Type	RSRZ
38	2g	80	VAL	7.6
34	2c	2	GLY	7.4
38	1g	80	VAL	7.0

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	7MG	2w	46	24/25	0.51	0.16	80,93,101,121	0
54	7MG	1w	46	24/25	0.58	0.16	77,89,99,107	0
54	4SU	2w	8	20/21	0.60	0.15	83,93,104,117	0
54	7MG	2y	46	24/25	0.60	0.17	86,95,102,123	0
54	PSU	2w	55	20/21	0.67	0.13	81,91,96,98	0
54	PSU	2y	55	20/21	0.67	0.18	90,96,107,107	0
54	4SU	2y	8	20/21	0.69	0.13	88,93,99,104	0
54	7MG	1y	46	24/25	0.69	0.14	79,90,98,101	0
54	MIA	2y	37	22/30	0.72	0.14	75,87,99,109	0
54	5MU	2y	54	21/22	0.72	0.15	84,91,99,112	0
54	5MU	1y	54	21/22	0.73	0.13	79,85,91,97	0
54	PSU	2y	32	20/21	0.75	0.14	79,85,93,102	0
54	4SU	1w	8	20/21	0.75	0.14	80,85,93,94	0
54	4SU	1y	8	20/21	0.79	0.12	81,89,98,99	0
54	PSU	1y	55	20/21	0.79	0.12	80,89,98,103	0
32	2MG	2a	1207	24/25	0.80	0.14	63,83,92,95	0
1	5MU	2A	1915	21/22	0.80	0.16	74,78,84,94	0
54	PSU	2w	39	20/21	0.81	0.14	81,86,88,92	0
54	MIA	2w	37	25/30	0.81	0.17	75,82,88,103	0
54	PSU	1y	32	20/21	0.81	0.12	78,82,87,88	0
54	5MU	2w	54	21/22	0.81	0.11	67,82,87,93	0
54	PSU	1w	55	20/21	0.82	0.11	74,83,92,95	0
54	PSU	2y	39	20/21	0.82	0.13	79,84,92,96	0
55	4SU	2x	8	20/21	0.83	0.14	73,79,87,90	0
55	PSU	2x	55	20/21	0.83	0.11	72,80,82,85	0
55	5MU	2x	54	21/22	0.84	0.12	68,77,82,94	0
32	PSU	2a	516	20/21	0.86	0.12	70,77,83,85	0
1	PSU	2A	1917	20/21	0.86	0.12	62,71,81,87	0
54	MIA	1y	37	22/30	0.86	0.11	74,78,84,85	0
32	M2G	2a	966	25/26	0.87	0.20	60,69,84,86	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	PSU	1y	39	20/21	0.87	0.09	74,76,80,80	0
43	0TD	2l	92	10/11	0.87	0.14	67,71,72,79	0
55	5MU	1x	54	21/22	0.88	0.11	51,64,70,76	0
54	PSU	2w	32	20/21	0.89	0.13	78,85,93,97	0
54	PSU	1w	32	20/21	0.89	0.13	65,76,82,84	0
54	MIA	1w	37	29/30	0.89	0.16	56,65,72,74	0
1	4OC	2A	1920	21/23	0.90	0.13	61,65,67,71	0
43	0TD	1l	92	10/11	0.90	0.12	47,55,60,75	0
1	PSU	2A	1911	20/21	0.90	0.11	60,66,73,75	0
32	5MC	2a	967	21/22	0.90	0.16	61,70,78,82	0
55	4SU	1x	8	20/21	0.92	0.11	51,59,65,71	0
54	5MU	1w	54	21/22	0.92	0.09	64,72,79,82	0
55	5MC	2x	32	21/22	0.92	0.13	60,73,78,82	0
32	5MC	2a	1400	21/22	0.92	0.16	60,69,76,83	0
54	PSU	1w	39	20/21	0.92	0.11	67,74,85,85	0
55	PSU	1x	55	20/21	0.92	0.10	49,63,70,73	0
32	5MC	2a	1404	21/22	0.92	0.13	56,60,65,68	0
1	5MU	1A	1915	21/22	0.93	0.10	56,61,68,71	0
55	5MC	1x	32	21/22	0.93	0.13	46,54,60,74	0
32	4OC	2a	1402	22/23	0.93	0.13	53,65,69,70	0
32	PSU	1a	516	20/21	0.93	0.10	60,66,71,71	0
32	UR3	2a	1498	21/22	0.93	0.13	55,61,65,66	0
32	MA6	2a	1518	24/25	0.93	0.12	55,65,68,71	0
32	7MG	2a	527	24/25	0.93	0.12	63,66,72,76	0
32	MA6	2a	1519	24/25	0.94	0.12	52,63,67,69	0
32	2MG	1a	1207	24/25	0.94	0.10	59,67,73,75	0
32	5MC	1a	967	21/22	0.94	0.11	52,59,63,64	0
1	PSU	1A	1917	20/21	0.94	0.10	48,57,62,63	0
1	5MC	2A	1962	21/22	0.95	0.10	40,52,59,68	0
1	2MA	2A	2503	23/24	0.95	0.11	32,36,43,45	0
32	5MC	2a	1407	21/22	0.95	0.13	53,59,63,64	0
1	5MU	2A	1939	21/22	0.95	0.11	36,44,49,51	0
1	5MC	2A	1942	21/22	0.95	0.10	54,60,66,68	0
32	5MC	1a	1404	21/22	0.96	0.08	35,41,44,44	0
32	5MC	1a	1407	21/22	0.96	0.09	36,41,43,45	0
32	MA6	1a	1519	24/25	0.96	0.10	38,42,47,50	0
1	PSU	1A	1911	20/21	0.96	0.09	40,49,57,57	0
32	7MG	1a	527	24/25	0.96	0.09	42,49,57,58	0
1	OMG	2A	2251	24/25	0.96	0.09	42,45,51,56	0
1	5MC	1A	1942	21/22	0.96	0.09	31,40,43,49	0
1	2MU	2A	2552	21/23	0.96	0.09	35,42,46,62	0
32	M2G	1a	966	25/26	0.96	0.09	49,55,59,66	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
32	5MC	1a	1400	21/22	0.96	0.09	39,50,54,59	0
32	4OC	1a	1402	22/23	0.96	0.09	37,45,51,57	0
32	MA6	1a	1518	24/25	0.97	0.08	34,41,45,49	0
1	5MC	1A	1962	21/22	0.97	0.07	29,36,41,44	0
1	2MU	1A	2552	21/23	0.97	0.08	21,29,33,39	0
1	PSU	2A	2605	20/21	0.97	0.07	34,42,47,47	0
1	4OC	1A	1920	21/23	0.97	0.07	37,44,48,53	0
1	2MA	1A	2503	23/24	0.98	0.06	14,21,24,31	0
32	UR3	1a	1498	21/22	0.98	0.07	39,43,46,48	0
1	5MU	1A	1939	21/22	0.98	0.06	23,29,33,40	0
1	PSU	1A	2605	20/21	0.98	0.07	19,26,35,35	0
1	OMG	1A	2251	24/25	0.98	0.06	19,25,28,29	0

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	1A	3982	1/1	0.54	0.32	77,77,77,77	0
56	MG	1P	206	1/1	0.57	0.20	62,62,62,62	0
56	MG	2a	3225	1/1	0.57	0.40	73,73,73,73	0
56	MG	2A	3698	1/1	0.63	0.16	56,56,56,56	0
56	MG	2A	3762	1/1	0.64	0.20	59,59,59,59	0
56	MG	2A	3650	1/1	0.66	0.18	67,67,67,67	0
56	MG	2a	3199	1/1	0.66	0.27	70,70,70,70	0
56	MG	1A	3402	1/1	0.66	0.16	85,85,85,85	0
56	MG	1a	1784	1/1	0.67	0.21	56,56,56,56	0
56	MG	2a	3227	1/1	0.67	0.16	78,78,78,78	0
56	MG	2a	3209	1/1	0.68	0.31	73,73,73,73	0
56	MG	2A	3516	1/1	0.68	0.26	74,74,74,74	0
56	MG	2A	3636	1/1	0.68	0.28	55,55,55,55	0
56	MG	1A	3771	1/1	0.69	0.13	19,19,19,19	0
56	MG	1A	4083	1/1	0.70	0.14	51,51,51,51	0
56	MG	1a	1755	1/1	0.70	0.21	88,88,88,88	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	2A	3687	1/1	0.70	0.17	71,71,71,71	0
56	MG	2a	3239	1/1	0.70	0.24	66,66,66,66	0
56	MG	2A	3817	1/1	0.71	0.21	75,75,75,75	0
56	MG	2B	216	1/1	0.71	0.17	65,65,65,65	0
56	MG	2a	3193	1/1	0.71	0.40	82,82,82,82	0
56	MG	2A	3405	1/1	0.71	0.28	64,64,64,64	0
56	MG	2A	3048	1/1	0.72	0.16	65,65,65,65	0
56	MG	2A	3809	1/1	0.72	0.21	60,60,60,60	0
56	MG	2A	3674	1/1	0.72	0.20	63,63,63,63	0
56	MG	2A	3620	1/1	0.72	0.15	64,64,64,64	0
56	MG	1a	1790	1/1	0.72	0.14	74,74,74,74	0
56	MG	2A	3678	1/1	0.73	0.28	76,76,76,76	0
56	MG	1a	1772	1/1	0.73	0.31	60,60,60,60	0
56	MG	1A	3800	1/1	0.73	0.12	60,60,60,60	0
56	MG	2A	3731	1/1	0.73	0.25	60,60,60,60	0
56	MG	2a	3031	1/1	0.73	0.23	69,69,69,69	0
56	MG	2a	3107	1/1	0.73	0.39	74,74,74,74	0
56	MG	2v	101	1/1	0.73	0.25	78,78,78,78	0
56	MG	2A	3688	1/1	0.74	0.23	57,57,57,57	0
56	MG	1x	111	1/1	0.74	0.27	71,71,71,71	0
56	MG	2a	3003	1/1	0.74	0.21	63,63,63,63	0
56	MG	1A	3341	1/1	0.74	0.18	50,50,50,50	0
56	MG	2A	3285	1/1	0.74	0.14	62,62,62,62	0
56	MG	2A	3334	1/1	0.74	0.19	74,74,74,74	0
56	MG	2A	3773	1/1	0.75	0.13	73,73,73,73	0
56	MG	2A	3396	1/1	0.75	0.20	63,63,63,63	0
56	MG	2A	3709	1/1	0.75	0.17	48,48,48,48	0
56	MG	2A	3712	1/1	0.75	0.20	70,70,70,70	0
56	MG	2A	3713	1/1	0.75	0.17	48,48,48,48	0
56	MG	2A	3040	1/1	0.75	0.26	88,88,88,88	0
56	MG	2j	201	1/1	0.75	0.20	76,76,76,76	0
56	MG	2A	3623	1/1	0.75	0.19	60,60,60,60	0
56	MG	2A	3069	1/1	0.76	0.15	54,54,54,54	0
56	MG	1A	4006	1/1	0.76	0.15	29,29,29,29	0
56	MG	2A	3665	1/1	0.76	0.12	61,61,61,61	0
56	MG	1a	1655	1/1	0.76	0.23	76,76,76,76	0
56	MG	2a	3070	1/1	0.76	0.21	68,68,68,68	0
56	MG	2A	3796	1/1	0.76	0.16	77,77,77,77	0
56	MG	1w	104	1/1	0.76	0.23	72,72,72,72	0
56	MG	2A	3602	1/1	0.77	0.20	55,55,55,55	0
56	MG	1A	3667	1/1	0.77	0.14	28,28,28,28	0
56	MG	2A	3333	1/1	0.77	0.15	65,65,65,65	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	1A	3852	1/1	0.77	0.21	39,39,39,39	0
56	MG	2A	3828	1/1	0.77	0.14	59,59,59,59	0
56	MG	1A	3930	1/1	0.77	0.13	30,30,30,30	0
56	MG	1A	3425	1/1	0.77	0.20	60,60,60,60	0
56	MG	1s	101	1/1	0.77	0.17	71,71,71,71	0
56	MG	2A	3585	1/1	0.77	0.18	77,77,77,77	0
56	MG	1A	3968	1/1	0.78	0.26	43,43,43,43	0
56	MG	1A	3979	1/1	0.78	0.15	69,69,69,69	0
56	MG	2a	3053	1/1	0.78	0.31	70,70,70,70	0
56	MG	2a	3057	1/1	0.78	0.19	65,65,65,65	0
56	MG	18	105	1/1	0.78	0.23	45,45,45,45	0
56	MG	2A	3715	1/1	0.78	0.21	68,68,68,68	0
56	MG	1A	3801	1/1	0.78	0.11	53,53,53,53	0
56	MG	2a	3196	1/1	0.78	0.20	76,76,76,76	0
56	MG	2A	3350	1/1	0.78	0.31	68,68,68,68	0
56	MG	1a	1700	1/1	0.78	0.23	68,68,68,68	0
56	MG	1x	117	1/1	0.78	0.12	71,71,71,71	0
56	MG	2A	3452	1/1	0.78	0.37	70,70,70,70	0
56	MG	1A	3948	1/1	0.78	0.14	36,36,36,36	0
56	MG	2A	3532	1/1	0.78	0.27	61,61,61,61	0
56	MG	1A	4043	1/1	0.78	0.20	66,66,66,66	0
56	MG	2A	3171	1/1	0.79	0.32	74,74,74,74	0
56	MG	2a	3036	1/1	0.79	0.24	72,72,72,72	0
56	MG	2A	3661	1/1	0.79	0.15	59,59,59,59	0
56	MG	1A	3626	1/1	0.79	0.15	47,47,47,47	0
56	MG	2A	3750	1/1	0.79	0.16	55,55,55,55	0
56	MG	2A	3671	1/1	0.79	0.13	59,59,59,59	0
56	MG	2a	3170	1/1	0.79	0.14	73,73,73,73	0
56	MG	1a	1693	1/1	0.79	0.28	69,69,69,69	0
56	MG	2A	3543	1/1	0.79	0.13	45,45,45,45	0
56	MG	1A	3791	1/1	0.79	0.20	63,63,63,63	0
56	MG	1a	1739	1/1	0.79	0.14	77,77,77,77	0
56	MG	2A	3823	1/1	0.79	0.11	50,50,50,50	0
56	MG	1A	4060	1/1	0.79	0.27	52,52,52,52	0
56	MG	2A	3402	1/1	0.79	0.15	65,65,65,65	0
56	MG	2G	201	1/1	0.79	0.19	65,65,65,65	0
56	MG	2A	3088	1/1	0.79	0.30	78,78,78,78	0
56	MG	2B	220	1/1	0.80	0.20	65,65,65,65	0
56	MG	1a	1767	1/1	0.80	0.20	67,67,67,67	0
56	MG	14	101	1/1	0.80	0.16	69,69,69,69	0
56	MG	1A	3661	1/1	0.80	0.12	29,29,29,29	0
56	MG	2A	3736	1/1	0.80	0.11	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	2a	3049	1/1	0.80	0.29	64,64,64,64	0
56	MG	1a	1642	1/1	0.80	0.13	57,57,57,57	0
56	MG	2A	3754	1/1	0.80	0.21	67,67,67,67	0
56	MG	2a	3064	1/1	0.80	0.15	64,64,64,64	0
56	MG	2a	3068	1/1	0.80	0.14	74,74,74,74	0
56	MG	1A	4032	1/1	0.80	0.20	57,57,57,57	0
56	MG	1A	4058	1/1	0.81	0.14	28,28,28,28	0
56	MG	2A	3595	1/1	0.81	0.22	65,65,65,65	0
56	MG	2A	3152	1/1	0.81	0.20	71,71,71,71	0
56	MG	1A	3699	1/1	0.81	0.13	37,37,37,37	0
56	MG	2A	3734	1/1	0.81	0.09	52,52,52,52	0
56	MG	2A	3261	1/1	0.81	0.14	59,59,59,59	0
56	MG	2a	3060	1/1	0.81	0.10	71,71,71,71	0
56	MG	1A	4067	1/1	0.81	0.14	55,55,55,55	0
56	MG	1A	3767	1/1	0.81	0.12	30,30,30,30	0
56	MG	1A	3061	1/1	0.81	0.20	67,67,67,67	0
56	MG	1A	3103	1/1	0.81	0.17	60,60,60,60	0
56	MG	1A	3317	1/1	0.81	0.28	65,65,65,65	0
56	MG	2A	3804	1/1	0.81	0.14	53,53,53,53	0
56	MG	1A	4000	1/1	0.81	0.18	62,62,62,62	0
56	MG	2A	3676	1/1	0.81	0.13	61,61,61,61	0
56	MG	2A	3819	1/1	0.81	0.19	69,69,69,69	0
56	MG	1A	3693	1/1	0.81	0.20	42,42,42,42	0
56	MG	1A	3808	1/1	0.81	0.25	65,65,65,65	0
56	MG	1A	3697	1/1	0.81	0.15	38,38,38,38	0
56	MG	1a	1721	1/1	0.81	0.34	54,54,54,54	0
56	MG	1a	1731	1/1	0.81	0.40	69,69,69,69	0
56	MG	1A	3263	1/1	0.82	0.22	64,64,64,64	0
56	MG	2D	309	1/1	0.82	0.15	35,35,35,35	0
56	MG	1a	1606	1/1	0.82	0.24	71,71,71,71	0
56	MG	2Q	204	1/1	0.82	0.18	62,62,62,62	0
56	MG	2A	3094	1/1	0.82	0.12	62,62,62,62	0
56	MG	2a	3027	1/1	0.82	0.21	70,70,70,70	0
56	MG	1A	3991	1/1	0.82	0.10	22,22,22,22	0
56	MG	1A	3498	1/1	0.82	0.29	59,59,59,59	0
56	MG	2A	3198	1/1	0.82	0.34	68,68,68,68	0
56	MG	2A	3228	1/1	0.82	0.16	72,72,72,72	0
56	MG	2A	3247	1/1	0.82	0.23	70,70,70,70	0
56	MG	2A	3748	1/1	0.82	0.19	68,68,68,68	0
56	MG	1a	1659	1/1	0.82	0.18	55,55,55,55	0
56	MG	2A	3637	1/1	0.82	0.16	47,47,47,47	0
56	MG	2A	3759	1/1	0.82	0.16	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	3100	1/1	0.82	0.20	77,77,77,77	0
56	MG	2A	3640	1/1	0.82	0.11	64,64,64,64	0
56	MG	1b	302	1/1	0.82	0.20	71,71,71,71	0
56	MG	2A	3315	1/1	0.82	0.16	62,62,62,62	0
56	MG	1A	3551	1/1	0.82	0.18	50,50,50,50	0
56	MG	2A	3805	1/1	0.82	0.10	67,67,67,67	0
56	MG	1w	102	1/1	0.82	0.09	75,75,75,75	0
56	MG	1A	4100	1/1	0.82	0.19	85,85,85,85	0
56	MG	1B	237	1/1	0.82	0.16	68,68,68,68	0
56	MG	2a	3233	1/1	0.82	0.21	67,67,67,67	0
56	MG	1A	3605	1/1	0.82	0.12	37,37,37,37	0
56	MG	2a	3240	1/1	0.82	0.17	67,67,67,67	0
56	MG	1A	3845	1/1	0.82	0.23	57,57,57,57	0
56	MG	1a	1753	1/1	0.82	0.17	53,53,53,53	0
56	MG	2w	102	1/1	0.82	0.20	72,72,72,72	0
56	MG	1A	3686	1/1	0.83	0.12	54,54,54,54	0
56	MG	1a	1779	1/1	0.83	0.12	88,88,88,88	0
56	MG	2A	3493	1/1	0.83	0.11	61,61,61,61	0
56	MG	1A	3532	1/1	0.83	0.20	52,52,52,52	0
56	MG	1a	1666	1/1	0.83	0.22	63,63,63,63	0
56	MG	2a	3017	1/1	0.83	0.21	71,71,71,71	0
56	MG	2a	3021	1/1	0.83	0.23	69,69,69,69	0
56	MG	2a	3023	1/1	0.83	0.24	76,76,76,76	0
56	MG	2A	3173	1/1	0.83	0.21	72,72,72,72	0
56	MG	2A	3729	1/1	0.83	0.20	68,68,68,68	0
56	MG	1a	1800	1/1	0.83	0.11	50,50,50,50	0
56	MG	2a	3041	1/1	0.83	0.28	66,66,66,66	0
56	MG	2a	3046	1/1	0.83	0.24	66,66,66,66	0
56	MG	2A	3214	1/1	0.83	0.13	62,62,62,62	0
56	MG	2A	3599	1/1	0.83	0.23	68,68,68,68	0
56	MG	2a	3054	1/1	0.83	0.19	71,71,71,71	0
56	MG	2A	3739	1/1	0.83	0.20	59,59,59,59	0
56	MG	1a	1692	1/1	0.83	0.23	70,70,70,70	0
56	MG	2A	3609	1/1	0.83	0.12	29,29,29,29	0
56	MG	1E	313	1/1	0.83	0.15	54,54,54,54	0
56	MG	1A	3838	1/1	0.83	0.22	60,60,60,60	0
56	MG	2a	3077	1/1	0.83	0.22	59,59,59,59	0
56	MG	1S	201	1/1	0.83	0.26	40,40,40,40	0
56	MG	2a	3101	1/1	0.83	0.27	68,68,68,68	0
56	MG	2A	3302	1/1	0.83	0.19	61,61,61,61	0
56	MG	2A	3310	1/1	0.83	0.28	65,65,65,65	0
56	MG	2a	3173	1/1	0.83	0.17	70,70,70,70	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	2a	3174	1/1	0.83	0.14	75,75,75,75	0
56	MG	1x	110	1/1	0.83	0.28	61,61,61,61	0
56	MG	1A	3459	1/1	0.83	0.13	49,49,49,49	0
56	MG	2a	3197	1/1	0.83	0.14	73,73,73,73	0
56	MG	1A	3306	1/1	0.83	0.17	41,41,41,41	0
56	MG	2A	3816	1/1	0.83	0.18	68,68,68,68	0
56	MG	2A	3339	1/1	0.83	0.17	64,64,64,64	0
56	MG	1A	3876	1/1	0.83	0.16	34,34,34,34	0
56	MG	2A	3391	1/1	0.83	0.13	68,68,68,68	0
56	MG	2a	3238	1/1	0.83	0.18	72,72,72,72	0
56	MG	1A	3897	1/1	0.83	0.19	56,56,56,56	0
56	MG	2A	3830	1/1	0.83	0.11	77,77,77,77	0
56	MG	2d	301	1/1	0.83	0.13	65,65,65,65	0
56	MG	2A	3869	1/1	0.83	0.13	45,45,45,45	0
56	MG	1a	1654	1/1	0.83	0.25	71,71,71,71	0
56	MG	2B	218	1/1	0.83	0.22	67,67,67,67	0
56	MG	1A	3224	1/1	0.84	0.14	45,45,45,45	0
56	MG	1a	1609	1/1	0.84	0.17	65,65,65,65	0
56	MG	1a	1611	1/1	0.84	0.13	68,68,68,68	0
56	MG	1B	233	1/1	0.84	0.13	63,63,63,63	0
56	MG	2A	3257	1/1	0.84	0.17	62,62,62,62	0
56	MG	2A	3538	1/1	0.84	0.10	38,38,38,38	0
56	MG	2A	3702	1/1	0.84	0.13	31,31,31,31	0
56	MG	2a	3092	1/1	0.84	0.18	77,77,77,77	0
56	MG	1A	3195	1/1	0.84	0.10	55,55,55,55	0
56	MG	2A	3570	1/1	0.84	0.13	48,48,48,48	0
56	MG	2A	3873	1/1	0.84	0.17	75,75,75,75	0
56	MG	2a	3162	1/1	0.84	0.10	82,82,82,82	0
56	MG	2a	3163	1/1	0.84	0.14	68,68,68,68	0
56	MG	2A	3027	1/1	0.84	0.17	71,71,71,71	0
56	MG	2A	3297	1/1	0.84	0.29	72,72,72,72	0
56	MG	2A	3029	1/1	0.84	0.28	62,62,62,62	0
56	MG	2a	3178	1/1	0.84	0.12	91,91,91,91	0
56	MG	1A	3411	1/1	0.84	0.20	57,57,57,57	0
56	MG	1A	3329	1/1	0.84	0.17	51,51,51,51	0
56	MG	2A	3612	1/1	0.84	0.11	41,41,41,41	0
56	MG	1A	3689	1/1	0.84	0.14	26,26,26,26	0
56	MG	2a	3201	1/1	0.84	0.16	60,60,60,60	0
56	MG	1Y	202	1/1	0.84	0.09	68,68,68,68	0
56	MG	2a	3220	1/1	0.84	0.15	63,63,63,63	0
56	MG	2a	3020	1/1	0.84	0.27	71,71,71,71	0
56	MG	1A	3797	1/1	0.84	0.14	27,27,27,27	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	2A	3120	1/1	0.84	0.14	62,62,62,62	0
56	MG	2A	3757	1/1	0.84	0.15	66,66,66,66	0
56	MG	2A	3352	1/1	0.84	0.26	72,72,72,72	0
56	MG	2A	3368	1/1	0.84	0.16	65,65,65,65	0
56	MG	2A	3770	1/1	0.84	0.12	54,54,54,54	0
56	MG	1A	3458	1/1	0.84	0.22	62,62,62,62	0
56	MG	2l	203	1/1	0.84	0.21	61,61,61,61	0
56	MG	1e	201	1/1	0.84	0.10	73,73,73,73	0
56	MG	1a	1604	1/1	0.84	0.11	55,55,55,55	0
56	MG	2x	105	1/1	0.84	0.20	67,67,67,67	0
56	MG	2A	3191	1/1	0.85	0.18	70,70,70,70	0
56	MG	2A	3353	1/1	0.85	0.10	71,71,71,71	0
56	MG	2A	3624	1/1	0.85	0.17	40,40,40,40	0
56	MG	2A	3364	1/1	0.85	0.33	66,66,66,66	0
56	MG	1A	3665	1/1	0.85	0.09	30,30,30,30	0
56	MG	2A	3210	1/1	0.85	0.12	61,61,61,61	0
56	MG	1a	1818	1/1	0.85	0.11	71,71,71,71	0
56	MG	1a	1827	1/1	0.85	0.21	52,52,52,52	0
56	MG	2A	3234	1/1	0.85	0.21	60,60,60,60	0
56	MG	2A	3433	1/1	0.85	0.36	49,49,49,49	0
56	MG	2a	3080	1/1	0.85	0.23	62,62,62,62	0
56	MG	2A	3444	1/1	0.85	0.28	57,57,57,57	0
56	MG	2a	3096	1/1	0.85	0.20	67,67,67,67	0
56	MG	1B	207	1/1	0.85	0.31	70,70,70,70	0
56	MG	2A	3467	1/1	0.85	0.22	74,74,74,74	0
56	MG	2A	3679	1/1	0.85	0.11	52,52,52,52	0
56	MG	2a	3135	1/1	0.85	0.18	59,59,59,59	0
56	MG	2A	3686	1/1	0.85	0.14	53,53,53,53	0
56	MG	2A	3853	1/1	0.85	0.13	49,49,49,49	0
56	MG	2A	3858	1/1	0.85	0.12	64,64,64,64	0
56	MG	2A	3484	1/1	0.85	0.12	58,58,58,58	0
56	MG	2A	3491	1/1	0.85	0.18	50,50,50,50	0
56	MG	2A	3881	1/1	0.85	0.16	62,62,62,62	0
56	MG	2a	3188	1/1	0.85	0.15	59,59,59,59	0
56	MG	2A	3058	1/1	0.85	0.13	52,52,52,52	0
56	MG	2B	217	1/1	0.85	0.14	84,84,84,84	0
56	MG	2A	3059	1/1	0.85	0.13	58,58,58,58	0
56	MG	2A	3531	1/1	0.85	0.20	55,55,55,55	0
56	MG	2A	3711	1/1	0.85	0.12	54,54,54,54	0
56	MG	2A	3062	1/1	0.85	0.14	66,66,66,66	0
56	MG	2A	3065	1/1	0.85	0.25	68,68,68,68	0
56	MG	20	101	1/1	0.85	0.24	67,67,67,67	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	1A	3739	1/1	0.85	0.13	51,51,51,51	0
56	MG	2a	3228	1/1	0.85	0.29	62,62,62,62	0
56	MG	2a	3005	1/1	0.85	0.25	66,66,66,66	0
56	MG	2a	3012	1/1	0.85	0.25	70,70,70,70	0
56	MG	1A	3766	1/1	0.85	0.10	26,26,26,26	0
56	MG	1A	3512	1/1	0.85	0.17	60,60,60,60	0
56	MG	1A	3270	1/1	0.85	0.12	55,55,55,55	0
56	MG	1a	1780	1/1	0.85	0.10	58,58,58,58	0
56	MG	2A	3601	1/1	0.85	0.17	58,58,58,58	0
56	MG	2q	202	1/1	0.85	0.16	72,72,72,72	0
56	MG	1A	3913	1/1	0.85	0.29	34,34,34,34	0
56	MG	2A	3341	1/1	0.85	0.11	66,66,66,66	0
56	MG	2w	104	1/1	0.85	0.10	69,69,69,69	0
56	MG	1A	3921	1/1	0.85	0.12	41,41,41,41	0
56	MG	2A	3718	1/1	0.86	0.09	41,41,41,41	0
56	MG	1B	222	1/1	0.86	0.16	55,55,55,55	0
56	MG	2A	3502	1/1	0.86	0.12	55,55,55,55	0
56	MG	2A	3514	1/1	0.86	0.18	67,67,67,67	0
56	MG	2a	3043	1/1	0.86	0.28	66,66,66,66	0
56	MG	1B	230	1/1	0.86	0.08	61,61,61,61	0
56	MG	2A	3225	1/1	0.86	0.28	62,62,62,62	0
56	MG	1a	1691	1/1	0.86	0.26	64,64,64,64	0
56	MG	1A	3131	1/1	0.86	0.09	63,63,63,63	0
56	MG	1A	3428	1/1	0.86	0.09	56,56,56,56	0
56	MG	1a	1698	1/1	0.86	0.30	62,62,62,62	0
56	MG	1A	3577	1/1	0.86	0.22	47,47,47,47	0
56	MG	2A	3761	1/1	0.86	0.16	62,62,62,62	0
56	MG	1x	112	1/1	0.86	0.16	58,58,58,58	0
56	MG	2A	3596	1/1	0.86	0.09	40,40,40,40	0
56	MG	2A	3287	1/1	0.86	0.24	67,67,67,67	0
56	MG	2a	3082	1/1	0.86	0.20	65,65,65,65	0
56	MG	2a	3085	1/1	0.86	0.32	73,73,73,73	0
56	MG	1x	113	1/1	0.86	0.23	65,65,65,65	0
56	MG	2a	3095	1/1	0.86	0.16	79,79,79,79	0
56	MG	2A	3299	1/1	0.86	0.12	49,49,49,49	0
56	MG	1a	1715	1/1	0.86	0.11	53,53,53,53	0
56	MG	2A	3308	1/1	0.86	0.16	56,56,56,56	0
56	MG	2a	3106	1/1	0.86	0.19	65,65,65,65	0
56	MG	2A	3008	1/1	0.86	0.10	60,60,60,60	0
56	MG	2a	3121	1/1	0.86	0.17	54,54,54,54	0
56	MG	1A	3901	1/1	0.86	0.10	53,53,53,53	0
56	MG	2a	3147	1/1	0.86	0.11	80,80,80,80	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	2a	3160	1/1	0.86	0.13	84,84,84,84	0
56	MG	2A	3321	1/1	0.86	0.14	65,65,65,65	0
56	MG	1A	3911	1/1	0.86	0.18	55,55,55,55	0
56	MG	2a	3165	1/1	0.86	0.09	78,78,78,78	0
56	MG	1U	201	1/1	0.86	0.18	51,51,51,51	0
56	MG	1A	4039	1/1	0.86	0.11	61,61,61,61	0
56	MG	2A	3831	1/1	0.86	0.15	56,56,56,56	0
56	MG	2A	3645	1/1	0.86	0.10	37,37,37,37	0
56	MG	1A	3798	1/1	0.86	0.10	39,39,39,39	0
56	MG	2A	3347	1/1	0.86	0.13	66,66,66,66	0
56	MG	1a	1763	1/1	0.86	0.18	62,62,62,62	0
56	MG	1A	4047	1/1	0.86	0.12	47,47,47,47	0
56	MG	2B	211	1/1	0.86	0.26	75,75,75,75	0
56	MG	1A	4056	1/1	0.86	0.10	45,45,45,45	0
56	MG	1A	3917	1/1	0.86	0.13	34,34,34,34	0
56	MG	2a	3216	1/1	0.86	0.13	72,72,72,72	0
56	MG	2A	3086	1/1	0.86	0.23	66,66,66,66	0
56	MG	2A	3377	1/1	0.86	0.10	65,65,65,65	0
56	MG	1A	3446	1/1	0.86	0.11	52,52,52,52	0
56	MG	1A	3004	1/1	0.86	0.10	22,22,22,22	0
56	MG	1a	1634	1/1	0.86	0.29	66,66,66,66	0
56	MG	2a	3235	1/1	0.86	0.12	66,66,66,66	0
56	MG	2a	3236	1/1	0.86	0.28	73,73,73,73	0
56	MG	2R	201	1/1	0.86	0.14	65,65,65,65	0
56	MG	2Z	301	1/1	0.86	0.12	72,72,72,72	0
56	MG	2A	3123	1/1	0.86	0.33	59,59,59,59	0
56	MG	27	101	1/1	0.86	0.11	46,46,46,46	0
56	MG	2f	202	1/1	0.86	0.18	65,65,65,65	0
56	MG	2g	201	1/1	0.86	0.11	81,81,81,81	0
56	MG	2A	3124	1/1	0.86	0.09	66,66,66,66	0
56	MG	1a	1793	1/1	0.86	0.10	78,78,78,78	0
56	MG	1A	3214	1/1	0.86	0.15	57,57,57,57	0
56	MG	1A	3121	1/1	0.86	0.13	46,46,46,46	0
56	MG	1a	1826	1/1	0.86	0.19	58,58,58,58	0
56	MG	2A	3714	1/1	0.86	0.11	57,57,57,57	0
56	MG	2x	103	1/1	0.86	0.10	60,60,60,60	0
56	MG	2x	104	1/1	0.86	0.17	62,62,62,62	0
56	MG	1A	3422	1/1	0.86	0.12	58,58,58,58	0
56	MG	2y	106	1/1	0.86	0.16	83,83,83,83	0
56	MG	1A	3302	1/1	0.87	0.26	52,52,52,52	0
56	MG	2A	3330	1/1	0.87	0.20	60,60,60,60	0
56	MG	2a	3013	1/1	0.87	0.18	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	1A	3928	1/1	0.87	0.15	69,69,69,69	0
56	MG	1A	3417	1/1	0.87	0.14	48,48,48,48	0
56	MG	1A	3932	1/1	0.87	0.12	48,48,48,48	0
56	MG	1A	3165	1/1	0.87	0.15	39,39,39,39	0
56	MG	2A	3346	1/1	0.87	0.13	67,67,67,67	0
56	MG	1B	234	1/1	0.87	0.16	56,56,56,56	0
56	MG	2A	3349	1/1	0.87	0.19	59,59,59,59	0
56	MG	2a	3039	1/1	0.87	0.22	55,55,55,55	0
56	MG	1A	3817	1/1	0.87	0.46	39,39,39,39	0
56	MG	1D	312	1/1	0.87	0.16	37,37,37,37	0
56	MG	1A	3822	1/1	0.87	0.14	25,25,25,25	0
56	MG	2A	3361	1/1	0.87	0.19	61,61,61,61	0
56	MG	1N	205	1/1	0.87	0.10	57,57,57,57	0
56	MG	1O	205	1/1	0.87	0.14	72,72,72,72	0
56	MG	1A	3471	1/1	0.87	0.17	51,51,51,51	0
56	MG	2A	3380	1/1	0.87	0.14	75,75,75,75	0
56	MG	2a	3062	1/1	0.87	0.23	71,71,71,71	0
56	MG	2A	3089	1/1	0.87	0.27	61,61,61,61	0
56	MG	1Q	208	1/1	0.87	0.16	47,47,47,47	0
56	MG	2A	3397	1/1	0.87	0.16	72,72,72,72	0
56	MG	2A	3099	1/1	0.87	0.28	68,68,68,68	0
56	MG	2A	3721	1/1	0.87	0.13	62,62,62,62	0
56	MG	1A	3483	1/1	0.87	0.18	59,59,59,59	0
56	MG	2A	3416	1/1	0.87	0.16	64,64,64,64	0
56	MG	2A	3418	1/1	0.87	0.10	66,66,66,66	0
56	MG	1A	3993	1/1	0.87	0.09	27,27,27,27	0
56	MG	2A	3737	1/1	0.87	0.08	70,70,70,70	0
56	MG	2A	3440	1/1	0.87	0.21	61,61,61,61	0
56	MG	2A	3443	1/1	0.87	0.22	59,59,59,59	0
56	MG	1A	3643	1/1	0.87	0.14	56,56,56,56	0
56	MG	2A	3753	1/1	0.87	0.12	42,42,42,42	0
56	MG	2a	3112	1/1	0.87	0.20	62,62,62,62	0
56	MG	2a	3117	1/1	0.87	0.19	65,65,65,65	0
56	MG	1A	3866	1/1	0.87	0.09	22,22,22,22	0
56	MG	2A	3155	1/1	0.87	0.16	55,55,55,55	0
56	MG	2a	3136	1/1	0.87	0.15	78,78,78,78	0
56	MG	2A	3474	1/1	0.87	0.07	61,61,61,61	0
56	MG	2a	3150	1/1	0.87	0.10	76,76,76,76	0
56	MG	1A	4028	1/1	0.87	0.09	61,61,61,61	0
56	MG	1A	3869	1/1	0.87	0.17	45,45,45,45	0
56	MG	1A	3360	1/1	0.87	0.17	65,65,65,65	0
56	MG	1A	3888	1/1	0.87	0.18	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	2A	3205	1/1	0.87	0.09	63,63,63,63	0
56	MG	2A	3802	1/1	0.87	0.11	57,57,57,57	0
56	MG	2A	3207	1/1	0.87	0.19	64,64,64,64	0
56	MG	1a	1832	1/1	0.87	0.15	55,55,55,55	0
56	MG	2a	3186	1/1	0.87	0.16	54,54,54,54	0
56	MG	1a	1833	1/1	0.87	0.19	43,43,43,43	0
56	MG	2A	3533	1/1	0.87	0.10	60,60,60,60	0
56	MG	1A	3894	1/1	0.87	0.07	21,21,21,21	0
56	MG	1d	301	1/1	0.87	0.17	48,48,48,48	0
56	MG	2A	3562	1/1	0.87	0.13	35,35,35,35	0
56	MG	2A	3563	1/1	0.87	0.10	36,36,36,36	0
56	MG	2a	3202	1/1	0.87	0.26	75,75,75,75	0
56	MG	2A	3568	1/1	0.87	0.10	47,47,47,47	0
56	MG	1A	4049	1/1	0.87	0.11	54,54,54,54	0
56	MG	2A	3838	1/1	0.87	0.17	43,43,43,43	0
56	MG	1A	3143	1/1	0.87	0.10	37,37,37,37	0
56	MG	2A	3586	1/1	0.87	0.11	60,60,60,60	0
56	MG	2A	3860	1/1	0.87	0.11	73,73,73,73	0
56	MG	2A	3254	1/1	0.87	0.28	63,63,63,63	0
56	MG	1A	3514	1/1	0.87	0.21	64,64,64,64	0
56	MG	1A	3793	1/1	0.87	0.14	56,56,56,56	0
56	MG	2A	3884	1/1	0.87	0.38	61,61,61,61	0
56	MG	2A	3886	1/1	0.87	0.17	71,71,71,71	0
56	MG	2A	3280	1/1	0.87	0.15	57,57,57,57	0
56	MG	2B	215	1/1	0.87	0.19	69,69,69,69	0
56	MG	1w	106	1/1	0.87	0.12	61,61,61,61	0
56	MG	1x	104	1/1	0.87	0.34	56,56,56,56	0
56	MG	1x	109	1/1	0.87	0.17	61,61,61,61	0
56	MG	2A	3614	1/1	0.87	0.14	45,45,45,45	0
56	MG	2m	201	1/1	0.87	0.27	73,73,73,73	0
56	MG	2A	3618	1/1	0.87	0.10	49,49,49,49	0
56	MG	1A	3682	1/1	0.87	0.14	61,61,61,61	0
56	MG	2A	3300	1/1	0.87	0.17	52,52,52,52	0
56	MG	1a	1662	1/1	0.87	0.20	60,60,60,60	0
56	MG	1A	3531	1/1	0.87	0.15	47,47,47,47	0
56	MG	1A	4084	1/1	0.87	0.14	14,14,14,14	0
56	MG	1A	4093	1/1	0.87	0.10	38,38,38,38	0
56	MG	2A	3643	1/1	0.87	0.12	62,62,62,62	0
56	MG	1A	4081	1/1	0.88	0.10	44,44,44,44	0
56	MG	1A	3784	1/1	0.88	0.08	66,66,66,66	0
56	MG	2T	202	1/1	0.88	0.14	61,61,61,61	0
56	MG	2U	201	1/1	0.88	0.12	54,54,54,54	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	2A	3615	1/1	0.88	0.16	60,60,60,60	0
56	MG	2A	3303	1/1	0.88	0.25	71,71,71,71	0
56	MG	1A	3650	1/1	0.88	0.09	49,49,49,49	0
56	MG	1a	1667	1/1	0.88	0.26	58,58,58,58	0
56	MG	1a	1669	1/1	0.88	0.11	75,75,75,75	0
56	MG	2a	3007	1/1	0.88	0.19	63,63,63,63	0
56	MG	1a	1674	1/1	0.88	0.10	53,53,53,53	0
56	MG	2A	3323	1/1	0.88	0.10	57,57,57,57	0
56	MG	2A	3324	1/1	0.88	0.16	49,49,49,49	0
56	MG	2A	3329	1/1	0.88	0.20	60,60,60,60	0
56	MG	1x	115	1/1	0.88	0.24	64,64,64,64	0
56	MG	1a	1688	1/1	0.88	0.27	63,63,63,63	0
56	MG	1A	3399	1/1	0.88	0.09	48,48,48,48	0
56	MG	1A	3513	1/1	0.88	0.23	63,63,63,63	0
56	MG	2a	3032	1/1	0.88	0.43	65,65,65,65	0
56	MG	2a	3034	1/1	0.88	0.12	72,72,72,72	0
56	MG	1A	3124	1/1	0.88	0.13	46,46,46,46	0
56	MG	2A	3343	1/1	0.88	0.20	57,57,57,57	0
56	MG	2A	3039	1/1	0.88	0.33	65,65,65,65	0
56	MG	1A	3675	1/1	0.88	0.09	24,24,24,24	0
56	MG	2a	3045	1/1	0.88	0.33	72,72,72,72	0
56	MG	1A	3339	1/1	0.88	0.12	42,42,42,42	0
56	MG	2A	3684	1/1	0.88	0.22	56,56,56,56	0
56	MG	1a	1707	1/1	0.88	0.14	57,57,57,57	0
56	MG	1A	3955	1/1	0.88	0.09	65,65,65,65	0
56	MG	1A	3208	1/1	0.88	0.11	61,61,61,61	0
56	MG	1a	1730	1/1	0.88	0.22	65,65,65,65	0
56	MG	2A	3066	1/1	0.88	0.08	51,51,51,51	0
56	MG	2A	3703	1/1	0.88	0.12	59,59,59,59	0
56	MG	1A	3533	1/1	0.88	0.12	55,55,55,55	0
56	MG	2A	3373	1/1	0.88	0.17	67,67,67,67	0
56	MG	1A	3548	1/1	0.88	0.24	46,46,46,46	0
56	MG	1A	3823	1/1	0.88	0.17	50,50,50,50	0
56	MG	2A	3387	1/1	0.88	0.27	62,62,62,62	0
56	MG	1A	3461	1/1	0.88	0.14	61,61,61,61	0
56	MG	1a	1759	1/1	0.88	0.14	61,61,61,61	0
56	MG	1A	3563	1/1	0.88	0.12	53,53,53,53	0
56	MG	1A	3709	1/1	0.88	0.09	41,41,41,41	0
56	MG	2A	3121	1/1	0.88	0.14	48,48,48,48	0
56	MG	1A	4016	1/1	0.88	0.09	25,25,25,25	0
56	MG	2a	3102	1/1	0.88	0.12	54,54,54,54	0
56	MG	1a	1774	1/1	0.88	0.16	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	1A	4018	1/1	0.88	0.10	35,35,35,35	0
56	MG	1T	201	1/1	0.88	0.09	47,47,47,47	0
56	MG	2a	3113	1/1	0.88	0.10	56,56,56,56	0
56	MG	1A	3855	1/1	0.88	0.10	20,20,20,20	0
56	MG	2a	3120	1/1	0.88	0.25	66,66,66,66	0
56	MG	1X	104	1/1	0.88	0.19	61,61,61,61	0
56	MG	2a	3124	1/1	0.88	0.20	55,55,55,55	0
56	MG	2A	3751	1/1	0.88	0.10	67,67,67,67	0
56	MG	1A	3722	1/1	0.88	0.15	59,59,59,59	0
56	MG	2A	3455	1/1	0.88	0.29	61,61,61,61	0
56	MG	2A	3457	1/1	0.88	0.13	50,50,50,50	0
56	MG	2a	3151	1/1	0.88	0.08	91,91,91,91	0
56	MG	2a	3153	1/1	0.88	0.13	73,73,73,73	0
56	MG	2A	3460	1/1	0.88	0.19	57,57,57,57	0
56	MG	10	102	1/1	0.88	0.08	41,41,41,41	0
56	MG	2A	3204	1/1	0.88	0.12	47,47,47,47	0
56	MG	2A	3475	1/1	0.88	0.18	56,56,56,56	0
56	MG	10	104	1/1	0.88	0.14	59,59,59,59	0
56	MG	2A	3490	1/1	0.88	0.28	53,53,53,53	0
56	MG	1A	3725	1/1	0.88	0.15	66,66,66,66	0
56	MG	16	102	1/1	0.88	0.22	40,40,40,40	0
56	MG	2a	3183	1/1	0.88	0.14	60,60,60,60	0
56	MG	2A	3498	1/1	0.88	0.16	58,58,58,58	0
56	MG	1a	1831	1/1	0.88	0.21	43,43,43,43	0
56	MG	2a	3190	1/1	0.88	0.18	77,77,77,77	0
56	MG	2A	3812	1/1	0.88	0.22	76,76,76,76	0
56	MG	2A	3216	1/1	0.88	0.21	65,65,65,65	0
56	MG	2A	3222	1/1	0.88	0.10	61,61,61,61	0
56	MG	2A	3525	1/1	0.88	0.15	60,60,60,60	0
56	MG	2a	3200	1/1	0.88	0.16	77,77,77,77	0
56	MG	1A	3726	1/1	0.88	0.09	53,53,53,53	0
56	MG	2A	3826	1/1	0.88	0.16	55,55,55,55	0
56	MG	1A	3420	1/1	0.88	0.20	51,51,51,51	0
56	MG	1A	3892	1/1	0.88	0.11	30,30,30,30	0
56	MG	2A	3237	1/1	0.88	0.21	44,44,44,44	0
56	MG	2A	3239	1/1	0.88	0.17	56,56,56,56	0
56	MG	1A	4053	1/1	0.88	0.09	34,34,34,34	0
56	MG	2A	3251	1/1	0.88	0.19	62,62,62,62	0
56	MG	2A	3566	1/1	0.88	0.11	44,44,44,44	0
56	MG	2A	3253	1/1	0.88	0.16	64,64,64,64	0
56	MG	1A	3053	1/1	0.88	0.15	62,62,62,62	0
56	MG	2A	3875	1/1	0.88	0.18	74,74,74,74	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	2A	3878	1/1	0.88	0.16	38,38,38,38	0
56	MG	2A	3575	1/1	0.88	0.20	65,65,65,65	0
56	MG	2a	3241	1/1	0.88	0.24	63,63,63,63	0
56	MG	1f	202	1/1	0.88	0.21	70,70,70,70	0
56	MG	2A	3259	1/1	0.88	0.09	60,60,60,60	0
56	MG	2B	203	1/1	0.88	0.19	60,60,60,60	0
56	MG	2A	3587	1/1	0.88	0.22	56,56,56,56	0
56	MG	2B	212	1/1	0.88	0.14	57,57,57,57	0
56	MG	2B	213	1/1	0.88	0.18	56,56,56,56	0
56	MG	2q	201	1/1	0.88	0.16	68,68,68,68	0
56	MG	1A	3494	1/1	0.88	0.13	56,56,56,56	0
56	MG	1A	4059	1/1	0.88	0.12	27,27,27,27	0
56	MG	1A	3372	1/1	0.88	0.14	43,43,43,43	0
56	MG	2w	103	1/1	0.88	0.10	64,64,64,64	0
56	MG	2A	3600	1/1	0.88	0.11	56,56,56,56	0
56	MG	1w	105	1/1	0.88	0.15	62,62,62,62	0
56	MG	2D	308	1/1	0.88	0.08	39,39,39,39	0
56	MG	1A	3772	1/1	0.88	0.09	28,28,28,28	0
56	MG	1w	110	1/1	0.88	0.20	74,74,74,74	0
56	MG	2A	3250	1/1	0.89	0.12	64,64,64,64	0
56	MG	1a	1625	1/1	0.89	0.12	55,55,55,55	0
56	MG	2A	3252	1/1	0.89	0.13	48,48,48,48	0
56	MG	1a	1626	1/1	0.89	0.18	52,52,52,52	0
56	MG	2A	3572	1/1	0.89	0.18	51,51,51,51	0
56	MG	1A	3676	1/1	0.89	0.09	16,16,16,16	0
56	MG	1a	1640	1/1	0.89	0.26	69,69,69,69	0
56	MG	1A	3789	1/1	0.89	0.10	43,43,43,43	0
56	MG	1A	3561	1/1	0.89	0.29	62,62,62,62	0
56	MG	2R	202	1/1	0.89	0.12	47,47,47,47	0
56	MG	2A	3594	1/1	0.89	0.18	66,66,66,66	0
56	MG	2A	3262	1/1	0.89	0.11	60,60,60,60	0
56	MG	2W	201	1/1	0.89	0.07	57,57,57,57	0
56	MG	1A	4068	1/1	0.89	0.10	61,61,61,61	0
56	MG	2A	3281	1/1	0.89	0.13	70,70,70,70	0
56	MG	1A	4076	1/1	0.89	0.15	36,36,36,36	0
56	MG	2a	3002	1/1	0.89	0.07	63,63,63,63	0
56	MG	1A	3292	1/1	0.89	0.13	57,57,57,57	0
56	MG	2A	3295	1/1	0.89	0.09	58,58,58,58	0
56	MG	2a	3006	1/1	0.89	0.17	61,61,61,61	0
56	MG	2A	3605	1/1	0.89	0.10	51,51,51,51	0
56	MG	2a	3009	1/1	0.89	0.13	72,72,72,72	0
56	MG	2a	3010	1/1	0.89	0.18	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	3011	1/1	0.89	0.23	66,66,66,66	0
56	MG	2A	3608	1/1	0.89	0.10	34,34,34,34	0
56	MG	1w	109	1/1	0.89	0.24	77,77,77,77	0
56	MG	2a	3015	1/1	0.89	0.32	69,69,69,69	0
56	MG	1A	3796	1/1	0.89	0.15	20,20,20,20	0
56	MG	1w	112	1/1	0.89	0.13	53,53,53,53	0
56	MG	1A	3924	1/1	0.89	0.11	71,71,71,71	0
56	MG	1A	3574	1/1	0.89	0.22	40,40,40,40	0
56	MG	1a	1673	1/1	0.89	0.14	63,63,63,63	0
56	MG	1A	3691	1/1	0.89	0.12	24,24,24,24	0
56	MG	1a	1675	1/1	0.89	0.23	64,64,64,64	0
56	MG	1B	202	1/1	0.89	0.18	47,47,47,47	0
56	MG	1A	3331	1/1	0.89	0.10	43,43,43,43	0
56	MG	1B	208	1/1	0.89	0.16	57,57,57,57	0
56	MG	2A	3002	1/1	0.89	0.23	53,53,53,53	0
56	MG	1A	3602	1/1	0.89	0.13	47,47,47,47	0
56	MG	2a	3044	1/1	0.89	0.22	56,56,56,56	0
56	MG	1A	3251	1/1	0.89	0.17	69,69,69,69	0
56	MG	2A	3652	1/1	0.89	0.13	50,50,50,50	0
56	MG	2A	3657	1/1	0.89	0.12	84,84,84,84	0
56	MG	1A	3966	1/1	0.89	0.12	36,36,36,36	0
56	MG	2A	3337	1/1	0.89	0.10	49,49,49,49	0
56	MG	2A	3034	1/1	0.89	0.11	56,56,56,56	0
56	MG	1A	3703	1/1	0.89	0.14	48,48,48,48	0
56	MG	1a	1709	1/1	0.89	0.20	50,50,50,50	0
56	MG	1A	3971	1/1	0.89	0.15	32,32,32,32	0
56	MG	2A	3054	1/1	0.89	0.19	63,63,63,63	0
56	MG	2A	3680	1/1	0.89	0.12	54,54,54,54	0
56	MG	2A	3348	1/1	0.89	0.08	65,65,65,65	0
56	MG	1A	3706	1/1	0.89	0.12	53,53,53,53	0
56	MG	1A	3708	1/1	0.89	0.09	45,45,45,45	0
56	MG	1F	308	1/1	0.89	0.13	49,49,49,49	0
56	MG	2a	3086	1/1	0.89	0.20	63,63,63,63	0
56	MG	2A	3693	1/1	0.89	0.21	62,62,62,62	0
56	MG	1a	1734	1/1	0.89	0.16	53,53,53,53	0
56	MG	1F	309	1/1	0.89	0.12	53,53,53,53	0
56	MG	1a	1746	1/1	0.89	0.11	59,59,59,59	0
56	MG	2A	3704	1/1	0.89	0.13	44,44,44,44	0
56	MG	2A	3365	1/1	0.89	0.11	54,54,54,54	0
56	MG	2A	3710	1/1	0.89	0.13	42,42,42,42	0
56	MG	2A	3367	1/1	0.89	0.15	54,54,54,54	0
56	MG	2a	3108	1/1	0.89	0.30	65,65,65,65	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	2A	3085	1/1	0.89	0.18	55,55,55,55	0
56	MG	1a	1751	1/1	0.89	0.15	52,52,52,52	0
56	MG	2a	3116	1/1	0.89	0.23	53,53,53,53	0
56	MG	2A	3087	1/1	0.89	0.13	48,48,48,48	0
56	MG	1A	3988	1/1	0.89	0.15	21,21,21,21	0
56	MG	2A	3383	1/1	0.89	0.16	66,66,66,66	0
56	MG	1A	3989	1/1	0.89	0.12	31,31,31,31	0
56	MG	2a	3127	1/1	0.89	0.19	63,63,63,63	0
56	MG	2a	3132	1/1	0.89	0.10	54,54,54,54	0
56	MG	2a	3133	1/1	0.89	0.20	66,66,66,66	0
56	MG	1A	3826	1/1	0.89	0.11	45,45,45,45	0
56	MG	1A	3835	1/1	0.89	0.09	33,33,33,33	0
56	MG	2A	3108	1/1	0.89	0.29	65,65,65,65	0
56	MG	1a	1766	1/1	0.89	0.08	61,61,61,61	0
56	MG	1A	3098	1/1	0.89	0.09	44,44,44,44	0
56	MG	2A	3408	1/1	0.89	0.27	52,52,52,52	0
56	MG	2A	3746	1/1	0.89	0.19	57,57,57,57	0
56	MG	2A	3414	1/1	0.89	0.09	59,59,59,59	0
56	MG	1A	3712	1/1	0.89	0.08	54,54,54,54	0
56	MG	2a	3164	1/1	0.89	0.10	58,58,58,58	0
56	MG	1A	3359	1/1	0.89	0.22	58,58,58,58	0
56	MG	2A	3424	1/1	0.89	0.21	49,49,49,49	0
56	MG	2A	3431	1/1	0.89	0.21	49,49,49,49	0
56	MG	2A	3138	1/1	0.89	0.20	70,70,70,70	0
56	MG	2A	3437	1/1	0.89	0.17	56,56,56,56	0
56	MG	2A	3140	1/1	0.89	0.16	57,57,57,57	0
56	MG	1A	4017	1/1	0.89	0.09	39,39,39,39	0
56	MG	1A	3644	1/1	0.89	0.09	58,58,58,58	0
56	MG	2A	3169	1/1	0.89	0.09	57,57,57,57	0
56	MG	2A	3781	1/1	0.89	0.09	57,57,57,57	0
56	MG	1A	3534	1/1	0.89	0.17	63,63,63,63	0
56	MG	2A	3799	1/1	0.89	0.12	75,75,75,75	0
56	MG	2A	3801	1/1	0.89	0.09	80,80,80,80	0
56	MG	1a	1785	1/1	0.89	0.08	65,65,65,65	0
56	MG	2A	3189	1/1	0.89	0.11	60,60,60,60	0
56	MG	2A	3463	1/1	0.89	0.23	55,55,55,55	0
56	MG	2A	3466	1/1	0.89	0.10	47,47,47,47	0
56	MG	2A	3810	1/1	0.89	0.11	78,78,78,78	0
56	MG	1a	1786	1/1	0.89	0.09	73,73,73,73	0
56	MG	2A	3815	1/1	0.89	0.10	73,73,73,73	0
56	MG	2A	3196	1/1	0.89	0.16	62,62,62,62	0
56	MG	1a	1787	1/1	0.89	0.12	66,66,66,66	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	1A	3654	1/1	0.89	0.10	37,37,37,37	0
56	MG	2A	3821	1/1	0.89	0.09	55,55,55,55	0
56	MG	2A	3485	1/1	0.89	0.26	44,44,44,44	0
56	MG	1A	3547	1/1	0.89	0.09	42,42,42,42	0
56	MG	1a	1795	1/1	0.89	0.11	64,64,64,64	0
56	MG	1A	3877	1/1	0.89	0.18	30,30,30,30	0
56	MG	2A	3497	1/1	0.89	0.13	51,51,51,51	0
56	MG	2A	3212	1/1	0.89	0.24	66,66,66,66	0
56	MG	1a	1807	1/1	0.89	0.10	66,66,66,66	0
56	MG	2A	3503	1/1	0.89	0.16	39,39,39,39	0
56	MG	2A	3509	1/1	0.89	0.11	41,41,41,41	0
56	MG	1a	1809	1/1	0.89	0.11	72,72,72,72	0
56	MG	1a	1812	1/1	0.89	0.10	62,62,62,62	0
56	MG	1A	3503	1/1	0.89	0.15	57,57,57,57	0
56	MG	1A	3891	1/1	0.89	0.12	21,21,21,21	0
56	MG	1A	3240	1/1	0.89	0.12	34,34,34,34	0
56	MG	1A	3559	1/1	0.89	0.21	54,54,54,54	0
56	MG	1A	3774	1/1	0.89	0.10	19,19,19,19	0
56	MG	2A	3540	1/1	0.89	0.10	35,35,35,35	0
56	MG	2A	3541	1/1	0.89	0.12	49,49,49,49	0
56	MG	1a	1617	1/1	0.89	0.09	53,53,53,53	0
56	MG	2A	3556	1/1	0.89	0.22	50,50,50,50	0
56	MG	2A	3248	1/1	0.89	0.23	65,65,65,65	0
56	MG	1a	1799	1/1	0.90	0.15	46,46,46,46	0
56	MG	2B	201	1/1	0.90	0.18	66,66,66,66	0
56	MG	2A	3227	1/1	0.90	0.15	56,56,56,56	0
56	MG	2B	204	1/1	0.90	0.10	61,61,61,61	0
56	MG	1A	3238	1/1	0.90	0.29	56,56,56,56	0
56	MG	1Z	301	1/1	0.90	0.11	48,48,48,48	0
56	MG	1Z	302	1/1	0.90	0.08	60,60,60,60	0
56	MG	2B	214	1/1	0.90	0.21	62,62,62,62	0
56	MG	1A	3809	1/1	0.90	0.12	39,39,39,39	0
56	MG	2A	3240	1/1	0.90	0.12	51,51,51,51	0
56	MG	2A	3551	1/1	0.90	0.12	43,43,43,43	0
56	MG	1A	3990	1/1	0.90	0.09	33,33,33,33	0
56	MG	1A	3816	1/1	0.90	0.15	54,54,54,54	0
56	MG	1A	3189	1/1	0.90	0.25	47,47,47,47	0
56	MG	2A	3564	1/1	0.90	0.13	53,53,53,53	0
56	MG	1A	3819	1/1	0.90	0.08	44,44,44,44	0
56	MG	1A	3136	1/1	0.90	0.09	41,41,41,41	0
56	MG	1A	3467	1/1	0.90	0.12	46,46,46,46	0
56	MG	1A	3253	1/1	0.90	0.12	54,54,54,54	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	1A	3700	1/1	0.90	0.10	25,25,25,25	0
56	MG	1A	3836	1/1	0.90	0.10	50,50,50,50	0
56	MG	1A	3473	1/1	0.90	0.16	65,65,65,65	0
56	MG	1A	3705	1/1	0.90	0.12	28,28,28,28	0
56	MG	2A	3264	1/1	0.90	0.15	56,56,56,56	0
56	MG	25	104	1/1	0.90	0.14	54,54,54,54	0
56	MG	25	105	1/1	0.90	0.12	49,49,49,49	0
56	MG	2A	3265	1/1	0.90	0.17	57,57,57,57	0
56	MG	2a	3001	1/1	0.90	0.14	57,57,57,57	0
56	MG	2A	3274	1/1	0.90	0.15	59,59,59,59	0
56	MG	2A	3276	1/1	0.90	0.09	51,51,51,51	0
56	MG	2A	3278	1/1	0.90	0.18	65,65,65,65	0
56	MG	1a	1630	1/1	0.90	0.15	60,60,60,60	0
56	MG	1A	3847	1/1	0.90	0.14	51,51,51,51	0
56	MG	1A	3481	1/1	0.90	0.12	40,40,40,40	0
56	MG	2A	3606	1/1	0.90	0.10	62,62,62,62	0
56	MG	1A	3575	1/1	0.90	0.24	55,55,55,55	0
56	MG	2A	3291	1/1	0.90	0.15	57,57,57,57	0
56	MG	2A	3610	1/1	0.90	0.09	41,41,41,41	0
56	MG	2a	3014	1/1	0.90	0.19	63,63,63,63	0
56	MG	2A	3294	1/1	0.90	0.09	67,67,67,67	0
56	MG	1A	3858	1/1	0.90	0.09	43,43,43,43	0
56	MG	1A	3083	1/1	0.90	0.23	37,37,37,37	0
56	MG	1a	1657	1/1	0.90	0.09	68,68,68,68	0
56	MG	1A	3867	1/1	0.90	0.13	55,55,55,55	0
56	MG	1a	1660	1/1	0.90	0.20	72,72,72,72	0
56	MG	2a	3030	1/1	0.90	0.38	63,63,63,63	0
56	MG	1A	3404	1/1	0.90	0.25	60,60,60,60	0
56	MG	2A	3630	1/1	0.90	0.20	42,42,42,42	0
56	MG	1A	3018	1/1	0.90	0.09	30,30,30,30	0
56	MG	1A	4061	1/1	0.90	0.17	68,68,68,68	0
56	MG	2A	3314	1/1	0.90	0.08	60,60,60,60	0
56	MG	1A	3724	1/1	0.90	0.14	53,53,53,53	0
56	MG	2a	3042	1/1	0.90	0.20	60,60,60,60	0
56	MG	1A	3885	1/1	0.90	0.07	25,25,25,25	0
56	MG	1A	4075	1/1	0.90	0.15	48,48,48,48	0
56	MG	1A	3609	1/1	0.90	0.14	25,25,25,25	0
56	MG	2A	3003	1/1	0.90	0.24	44,44,44,44	0
56	MG	2A	3006	1/1	0.90	0.27	54,54,54,54	0
56	MG	2A	3662	1/1	0.90	0.08	59,59,59,59	0
56	MG	2A	3664	1/1	0.90	0.15	57,57,57,57	0
56	MG	1a	1687	1/1	0.90	0.14	50,50,50,50	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	1A	3611	1/1	0.90	0.12	36,36,36,36	0
56	MG	2A	3673	1/1	0.90	0.12	57,57,57,57	0
56	MG	1A	3624	1/1	0.90	0.17	46,46,46,46	0
56	MG	2a	3066	1/1	0.90	0.17	60,60,60,60	0
56	MG	1A	3741	1/1	0.90	0.12	37,37,37,37	0
56	MG	1A	4088	1/1	0.90	0.12	21,21,21,21	0
56	MG	1a	1694	1/1	0.90	0.06	56,56,56,56	0
56	MG	1a	1697	1/1	0.90	0.25	49,49,49,49	0
56	MG	2A	3681	1/1	0.90	0.10	54,54,54,54	0
56	MG	2A	3049	1/1	0.90	0.13	54,54,54,54	0
56	MG	2A	3052	1/1	0.90	0.21	63,63,63,63	0
56	MG	2A	3053	1/1	0.90	0.36	64,64,64,64	0
56	MG	2a	3094	1/1	0.90	0.26	62,62,62,62	0
56	MG	1A	3748	1/1	0.90	0.10	47,47,47,47	0
56	MG	1A	3756	1/1	0.90	0.14	45,45,45,45	0
56	MG	2A	3697	1/1	0.90	0.16	72,72,72,72	0
56	MG	1A	3762	1/1	0.90	0.14	21,21,21,21	0
56	MG	2A	3356	1/1	0.90	0.10	62,62,62,62	0
56	MG	2a	3104	1/1	0.90	0.15	54,54,54,54	0
56	MG	2A	3357	1/1	0.90	0.09	50,50,50,50	0
56	MG	1A	3340	1/1	0.90	0.14	50,50,50,50	0
56	MG	1a	1714	1/1	0.90	0.16	62,62,62,62	0
56	MG	1A	3916	1/1	0.90	0.10	22,22,22,22	0
56	MG	1a	1716	1/1	0.90	0.08	49,49,49,49	0
56	MG	2A	3074	1/1	0.90	0.13	41,41,41,41	0
56	MG	2A	3083	1/1	0.90	0.13	57,57,57,57	0
56	MG	1a	1720	1/1	0.90	0.28	51,51,51,51	0
56	MG	2A	3378	1/1	0.90	0.15	55,55,55,55	0
56	MG	1B	221	1/1	0.90	0.12	56,56,56,56	0
56	MG	2A	3381	1/1	0.90	0.10	57,57,57,57	0
56	MG	2A	3722	1/1	0.90	0.11	40,40,40,40	0
56	MG	1a	1728	1/1	0.90	0.26	51,51,51,51	0
56	MG	2A	3730	1/1	0.90	0.07	41,41,41,41	0
56	MG	1A	3632	1/1	0.90	0.08	34,34,34,34	0
56	MG	1A	3188	1/1	0.90	0.06	37,37,37,37	0
56	MG	2A	3735	1/1	0.90	0.09	62,62,62,62	0
56	MG	1a	1732	1/1	0.90	0.25	64,64,64,64	0
56	MG	1A	3344	1/1	0.90	0.13	53,53,53,53	0
56	MG	2a	3154	1/1	0.90	0.09	69,69,69,69	0
56	MG	2A	3107	1/1	0.90	0.09	65,65,65,65	0
56	MG	2A	3742	1/1	0.90	0.08	72,72,72,72	0
56	MG	2A	3743	1/1	0.90	0.11	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	3349	1/1	0.90	0.15	56,56,56,56	0
56	MG	2A	3406	1/1	0.90	0.11	66,66,66,66	0
56	MG	2A	3112	1/1	0.90	0.16	51,51,51,51	0
56	MG	1a	1743	1/1	0.90	0.14	61,61,61,61	0
56	MG	1A	3515	1/1	0.90	0.09	47,47,47,47	0
56	MG	2a	3175	1/1	0.90	0.08	73,73,73,73	0
56	MG	2a	3176	1/1	0.90	0.09	72,72,72,72	0
56	MG	1A	3522	1/1	0.90	0.18	53,53,53,53	0
56	MG	2A	3421	1/1	0.90	0.29	69,69,69,69	0
56	MG	1A	3937	1/1	0.90	0.10	60,60,60,60	0
56	MG	2A	3131	1/1	0.90	0.21	75,75,75,75	0
56	MG	1A	3942	1/1	0.90	0.09	51,51,51,51	0
56	MG	1A	3524	1/1	0.90	0.12	51,51,51,51	0
56	MG	2A	3771	1/1	0.90	0.11	62,62,62,62	0
56	MG	2A	3439	1/1	0.90	0.32	55,55,55,55	0
56	MG	2A	3149	1/1	0.90	0.17	63,63,63,63	0
56	MG	2A	3442	1/1	0.90	0.13	57,57,57,57	0
56	MG	2A	3150	1/1	0.90	0.13	53,53,53,53	0
56	MG	2A	3151	1/1	0.90	0.27	60,60,60,60	0
56	MG	2a	3204	1/1	0.90	0.29	65,65,65,65	0
56	MG	2a	3208	1/1	0.90	0.19	69,69,69,69	0
56	MG	2A	3448	1/1	0.90	0.38	64,64,64,64	0
56	MG	1G	203	1/1	0.90	0.07	63,63,63,63	0
56	MG	1A	3526	1/1	0.90	0.32	42,42,42,42	0
56	MG	2a	3224	1/1	0.90	0.16	61,61,61,61	0
56	MG	2A	3808	1/1	0.90	0.15	63,63,63,63	0
56	MG	1A	3962	1/1	0.90	0.11	48,48,48,48	0
56	MG	1A	3964	1/1	0.90	0.09	33,33,33,33	0
56	MG	2a	3229	1/1	0.90	0.10	61,61,61,61	0
56	MG	2A	3462	1/1	0.90	0.33	60,60,60,60	0
56	MG	1A	3353	1/1	0.90	0.16	33,33,33,33	0
56	MG	2A	3176	1/1	0.90	0.11	59,59,59,59	0
56	MG	2a	3237	1/1	0.90	0.23	61,61,61,61	0
56	MG	2A	3179	1/1	0.90	0.18	65,65,65,65	0
56	MG	2A	3469	1/1	0.90	0.28	64,64,64,64	0
56	MG	2A	3472	1/1	0.90	0.10	64,64,64,64	0
56	MG	1a	1775	1/1	0.90	0.12	65,65,65,65	0
56	MG	2A	3190	1/1	0.90	0.37	67,67,67,67	0
56	MG	1A	3438	1/1	0.90	0.10	50,50,50,50	0
56	MG	2A	3194	1/1	0.90	0.09	60,60,60,60	0
56	MG	1S	202	1/1	0.90	0.16	51,51,51,51	0
56	MG	2k	201	1/1	0.90	0.16	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	1782	1/1	0.90	0.07	79,79,79,79	0
56	MG	2A	3839	1/1	0.90	0.10	35,35,35,35	0
56	MG	1S	203	1/1	0.90	0.09	66,66,66,66	0
56	MG	1A	3356	1/1	0.90	0.09	53,53,53,53	0
56	MG	1T	204	1/1	0.90	0.13	59,59,59,59	0
56	MG	2A	3868	1/1	0.90	0.16	70,70,70,70	0
56	MG	1A	3685	1/1	0.90	0.17	31,31,31,31	0
56	MG	1a	1789	1/1	0.90	0.16	77,77,77,77	0
56	MG	2x	102	1/1	0.90	0.19	70,70,70,70	0
56	MG	1V	202	1/1	0.90	0.14	39,39,39,39	0
56	MG	1A	3450	1/1	0.90	0.14	50,50,50,50	0
56	MG	2A	3217	1/1	0.90	0.28	67,67,67,67	0
56	MG	2y	102	1/1	0.90	0.10	74,74,74,74	0
56	MG	2y	103	1/1	0.90	0.11	76,76,76,76	0
56	MG	1Y	201	1/1	0.90	0.09	32,32,32,32	0
56	MG	2A	3293	1/1	0.91	0.07	52,52,52,52	0
56	MG	2A	3046	1/1	0.91	0.12	48,48,48,48	0
56	MG	1A	3039	1/1	0.91	0.14	54,54,54,54	0
56	MG	1A	3380	1/1	0.91	0.09	48,48,48,48	0
56	MG	2A	3051	1/1	0.91	0.30	72,72,72,72	0
56	MG	1A	3844	1/1	0.91	0.08	57,57,57,57	0
56	MG	2A	3301	1/1	0.91	0.08	57,57,57,57	0
56	MG	1A	3394	1/1	0.91	0.11	50,50,50,50	0
56	MG	2P	202	1/1	0.91	0.07	47,47,47,47	0
56	MG	2Q	203	1/1	0.91	0.11	56,56,56,56	0
56	MG	1a	1722	1/1	0.91	0.16	50,50,50,50	0
56	MG	2A	3597	1/1	0.91	0.18	58,58,58,58	0
56	MG	1a	1726	1/1	0.91	0.15	61,61,61,61	0
56	MG	1A	3733	1/1	0.91	0.11	45,45,45,45	0
56	MG	2A	3311	1/1	0.91	0.16	59,59,59,59	0
56	MG	2V	202	1/1	0.91	0.27	48,48,48,48	0
56	MG	1a	1729	1/1	0.91	0.25	54,54,54,54	0
56	MG	1A	3191	1/1	0.91	0.09	43,43,43,43	0
56	MG	1A	3646	1/1	0.91	0.09	30,30,30,30	0
56	MG	1A	3254	1/1	0.91	0.11	36,36,36,36	0
56	MG	2A	3071	1/1	0.91	0.07	40,40,40,40	0
56	MG	1a	1733	1/1	0.91	0.31	53,53,53,53	0
56	MG	2A	3611	1/1	0.91	0.11	51,51,51,51	0
56	MG	1A	3992	1/1	0.91	0.08	25,25,25,25	0
56	MG	1A	3865	1/1	0.91	0.11	65,65,65,65	0
56	MG	1A	3998	1/1	0.91	0.18	67,67,67,67	0
56	MG	1A	3346	1/1	0.91	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	1A	4005	1/1	0.91	0.07	26,26,26,26	0
56	MG	2a	3008	1/1	0.91	0.14	57,57,57,57	0
56	MG	1A	3759	1/1	0.91	0.08	15,15,15,15	0
56	MG	1A	3324	1/1	0.91	0.10	39,39,39,39	0
56	MG	2A	3095	1/1	0.91	0.08	59,59,59,59	0
56	MG	2A	3631	1/1	0.91	0.12	39,39,39,39	0
56	MG	2A	3634	1/1	0.91	0.14	56,56,56,56	0
56	MG	2A	3096	1/1	0.91	0.13	52,52,52,52	0
56	MG	2A	3097	1/1	0.91	0.11	45,45,45,45	0
56	MG	2A	3098	1/1	0.91	0.20	61,61,61,61	0
56	MG	1A	3662	1/1	0.91	0.09	19,19,19,19	0
56	MG	1A	3538	1/1	0.91	0.10	50,50,50,50	0
56	MG	1A	3880	1/1	0.91	0.16	60,60,60,60	0
56	MG	1A	3883	1/1	0.91	0.28	66,66,66,66	0
56	MG	2A	3113	1/1	0.91	0.24	59,59,59,59	0
56	MG	2A	3359	1/1	0.91	0.11	51,51,51,51	0
56	MG	2A	3116	1/1	0.91	0.30	60,60,60,60	0
56	MG	1A	3541	1/1	0.91	0.14	43,43,43,43	0
56	MG	1A	4042	1/1	0.91	0.10	40,40,40,40	0
56	MG	2a	3037	1/1	0.91	0.18	48,48,48,48	0
56	MG	1A	3414	1/1	0.91	0.15	43,43,43,43	0
56	MG	11	104	1/1	0.91	0.14	48,48,48,48	0
56	MG	2A	3372	1/1	0.91	0.12	50,50,50,50	0
56	MG	12	101	1/1	0.91	0.09	54,54,54,54	0
56	MG	2A	3376	1/1	0.91	0.10	53,53,53,53	0
56	MG	1A	3477	1/1	0.91	0.09	53,53,53,53	0
56	MG	15	103	1/1	0.91	0.16	33,33,33,33	0
56	MG	1A	3680	1/1	0.91	0.14	38,38,38,38	0
56	MG	2A	3683	1/1	0.91	0.16	64,64,64,64	0
56	MG	1A	4052	1/1	0.91	0.12	48,48,48,48	0
56	MG	2A	3382	1/1	0.91	0.23	47,47,47,47	0
56	MG	2a	3059	1/1	0.91	0.18	80,80,80,80	0
56	MG	18	107	1/1	0.91	0.14	56,56,56,56	0
56	MG	1A	3480	1/1	0.91	0.12	54,54,54,54	0
56	MG	2a	3063	1/1	0.91	0.10	63,63,63,63	0
56	MG	1A	3232	1/1	0.91	0.25	56,56,56,56	0
56	MG	2a	3065	1/1	0.91	0.10	77,77,77,77	0
56	MG	2A	3395	1/1	0.91	0.24	66,66,66,66	0
56	MG	2A	3156	1/1	0.91	0.28	54,54,54,54	0
56	MG	2A	3699	1/1	0.91	0.11	70,70,70,70	0
56	MG	2A	3160	1/1	0.91	0.15	57,57,57,57	0
56	MG	2A	3399	1/1	0.91	0.18	69,69,69,69	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	2A	3166	1/1	0.91	0.18	50,50,50,50	0
56	MG	2a	3083	1/1	0.91	0.22	65,65,65,65	0
56	MG	1a	1607	1/1	0.91	0.09	55,55,55,55	0
56	MG	2A	3170	1/1	0.91	0.14	52,52,52,52	0
56	MG	2a	3089	1/1	0.91	0.15	69,69,69,69	0
56	MG	1A	4057	1/1	0.91	0.10	23,23,23,23	0
56	MG	2A	3410	1/1	0.91	0.11	70,70,70,70	0
56	MG	2A	3412	1/1	0.91	0.10	53,53,53,53	0
56	MG	1A	3898	1/1	0.91	0.14	32,32,32,32	0
56	MG	1A	3418	1/1	0.91	0.11	55,55,55,55	0
56	MG	1a	1619	1/1	0.91	0.19	52,52,52,52	0
56	MG	2A	3419	1/1	0.91	0.13	62,62,62,62	0
56	MG	2A	3420	1/1	0.91	0.12	60,60,60,60	0
56	MG	2A	3723	1/1	0.91	0.12	51,51,51,51	0
56	MG	2A	3182	1/1	0.91	0.15	49,49,49,49	0
56	MG	2A	3186	1/1	0.91	0.24	53,53,53,53	0
56	MG	2A	3428	1/1	0.91	0.21	50,50,50,50	0
56	MG	1A	3904	1/1	0.91	0.10	32,32,32,32	0
56	MG	2a	3115	1/1	0.91	0.20	61,61,61,61	0
56	MG	2A	3432	1/1	0.91	0.26	40,40,40,40	0
56	MG	1A	3909	1/1	0.91	0.13	49,49,49,49	0
56	MG	1A	3486	1/1	0.91	0.13	44,44,44,44	0
56	MG	2A	3438	1/1	0.91	0.31	56,56,56,56	0
56	MG	2a	3122	1/1	0.91	0.33	73,73,73,73	0
56	MG	2a	3123	1/1	0.91	0.27	68,68,68,68	0
56	MG	2A	3741	1/1	0.91	0.12	42,42,42,42	0
56	MG	1A	3690	1/1	0.91	0.12	19,19,19,19	0
56	MG	1A	3565	1/1	0.91	0.10	58,58,58,58	0
56	MG	2A	3745	1/1	0.91	0.07	50,50,50,50	0
56	MG	2a	3134	1/1	0.91	0.18	58,58,58,58	0
56	MG	2A	3441	1/1	0.91	0.19	60,60,60,60	0
56	MG	1a	1641	1/1	0.91	0.09	57,57,57,57	0
56	MG	2a	3138	1/1	0.91	0.09	67,67,67,67	0
56	MG	2A	3201	1/1	0.91	0.32	70,70,70,70	0
56	MG	1A	3572	1/1	0.91	0.25	39,39,39,39	0
56	MG	2A	3447	1/1	0.91	0.28	55,55,55,55	0
56	MG	1A	4078	1/1	0.91	0.07	24,24,24,24	0
56	MG	1A	3491	1/1	0.91	0.09	38,38,38,38	0
56	MG	2a	3155	1/1	0.91	0.07	70,70,70,70	0
56	MG	1A	3807	1/1	0.91	0.32	27,27,27,27	0
56	MG	1A	3133	1/1	0.91	0.14	35,35,35,35	0
56	MG	2A	3458	1/1	0.91	0.08	53,53,53,53	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	2A	3764	1/1	0.91	0.10	44,44,44,44	0
56	MG	2A	3765	1/1	0.91	0.13	53,53,53,53	0
56	MG	2A	3768	1/1	0.91	0.08	42,42,42,42	0
56	MG	1A	3357	1/1	0.91	0.20	48,48,48,48	0
56	MG	1a	1661	1/1	0.91	0.12	58,58,58,58	0
56	MG	1t	201	1/1	0.91	0.13	59,59,59,59	0
56	MG	2A	3775	1/1	0.91	0.16	66,66,66,66	0
56	MG	1A	4089	1/1	0.91	0.15	65,65,65,65	0
56	MG	2A	3792	1/1	0.91	0.14	63,63,63,63	0
56	MG	2A	3795	1/1	0.91	0.09	55,55,55,55	0
56	MG	1w	103	1/1	0.91	0.24	64,64,64,64	0
56	MG	1A	3815	1/1	0.91	0.08	28,28,28,28	0
56	MG	2a	3192	1/1	0.91	0.11	56,56,56,56	0
56	MG	1A	3933	1/1	0.91	0.08	49,49,49,49	0
56	MG	1A	3585	1/1	0.91	0.16	35,35,35,35	0
56	MG	1w	107	1/1	0.91	0.20	69,69,69,69	0
56	MG	2A	3479	1/1	0.91	0.13	52,52,52,52	0
56	MG	2A	3806	1/1	0.91	0.12	50,50,50,50	0
56	MG	1A	3601	1/1	0.91	0.23	43,43,43,43	0
56	MG	1A	3947	1/1	0.91	0.08	27,27,27,27	0
56	MG	1B	212	1/1	0.91	0.09	40,40,40,40	0
56	MG	1a	1676	1/1	0.91	0.17	72,72,72,72	0
56	MG	1x	108	1/1	0.91	0.26	62,62,62,62	0
56	MG	2A	3495	1/1	0.91	0.10	57,57,57,57	0
56	MG	2a	3217	1/1	0.91	0.13	72,72,72,72	0
56	MG	1a	1685	1/1	0.91	0.28	65,65,65,65	0
56	MG	1a	1686	1/1	0.91	0.14	62,62,62,62	0
56	MG	1A	3358	1/1	0.91	0.08	45,45,45,45	0
56	MG	1A	3336	1/1	0.91	0.12	60,60,60,60	0
56	MG	2A	3255	1/1	0.91	0.13	69,69,69,69	0
56	MG	2A	3513	1/1	0.91	0.10	50,50,50,50	0
56	MG	2a	3231	1/1	0.91	0.10	58,58,58,58	0
56	MG	1a	1690	1/1	0.91	0.08	56,56,56,56	0
56	MG	1B	226	1/1	0.91	0.08	69,69,69,69	0
56	MG	2A	3517	1/1	0.91	0.08	46,46,46,46	0
56	MG	2A	3524	1/1	0.91	0.18	69,69,69,69	0
56	MG	1B	229	1/1	0.91	0.07	38,38,38,38	0
56	MG	2A	3527	1/1	0.91	0.12	44,44,44,44	0
56	MG	2A	3859	1/1	0.91	0.09	60,60,60,60	0
56	MG	1A	3958	1/1	0.91	0.09	50,50,50,50	0
56	MG	2A	3864	1/1	0.91	0.11	69,69,69,69	0
56	MG	1A	3431	1/1	0.91	0.14	54,54,54,54	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	1a	1695	1/1	0.91	0.20	52,52,52,52	0
56	MG	2A	3267	1/1	0.91	0.17	67,67,67,67	0
56	MG	2A	3271	1/1	0.91	0.20	58,58,58,58	0
56	MG	1A	3963	1/1	0.91	0.09	33,33,33,33	0
56	MG	1B	236	1/1	0.91	0.10	49,49,49,49	0
56	MG	2A	3547	1/1	0.91	0.11	34,34,34,34	0
56	MG	2A	3550	1/1	0.91	0.15	57,57,57,57	0
56	MG	2t	201	1/1	0.91	0.14	47,47,47,47	0
56	MG	2A	3887	1/1	0.91	0.11	56,56,56,56	0
56	MG	2w	101	1/1	0.91	0.32	69,69,69,69	0
56	MG	1A	3433	1/1	0.91	0.07	31,31,31,31	0
56	MG	2B	202	1/1	0.91	0.08	63,63,63,63	0
56	MG	2A	3033	1/1	0.91	0.13	36,36,36,36	0
56	MG	1A	3091	1/1	0.91	0.26	50,50,50,50	0
56	MG	2B	205	1/1	0.91	0.11	66,66,66,66	0
56	MG	2B	207	1/1	0.91	0.12	61,61,61,61	0
56	MG	2A	3282	1/1	0.91	0.14	63,63,63,63	0
56	MG	2A	3037	1/1	0.91	0.29	68,68,68,68	0
56	MG	1E	303	1/1	0.91	0.13	38,38,38,38	0
56	MG	1E	309	1/1	0.91	0.13	47,47,47,47	0
56	MG	1a	1710	1/1	0.92	0.15	53,53,53,53	0
56	MG	1A	3123	1/1	0.92	0.12	41,41,41,41	0
56	MG	2D	302	1/1	0.92	0.19	55,55,55,55	0
56	MG	2D	304	1/1	0.92	0.18	57,57,57,57	0
56	MG	2A	3326	1/1	0.92	0.12	61,61,61,61	0
56	MG	1A	3954	1/1	0.92	0.11	75,75,75,75	0
56	MG	1A	3663	1/1	0.92	0.07	21,21,21,21	0
56	MG	1F	304	1/1	0.92	0.07	34,34,34,34	0
56	MG	1A	3002	1/1	0.92	0.13	51,51,51,51	0
56	MG	1A	3342	1/1	0.92	0.25	60,60,60,60	0
56	MG	1A	3089	1/1	0.92	0.10	41,41,41,41	0
56	MG	1G	204	1/1	0.92	0.07	52,52,52,52	0
56	MG	1N	201	1/1	0.92	0.30	51,51,51,51	0
56	MG	2A	3613	1/1	0.92	0.10	46,46,46,46	0
56	MG	2U	203	1/1	0.92	0.14	54,54,54,54	0
56	MG	1A	3530	1/1	0.92	0.09	40,40,40,40	0
56	MG	1O	201	1/1	0.92	0.08	57,57,57,57	0
56	MG	2A	3617	1/1	0.92	0.22	59,59,59,59	0
56	MG	1A	3813	1/1	0.92	0.13	40,40,40,40	0
56	MG	20	103	1/1	0.92	0.14	66,66,66,66	0
56	MG	2A	3619	1/1	0.92	0.08	36,36,36,36	0
56	MG	1A	3814	1/1	0.92	0.16	63,63,63,63	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	2A	3621	1/1	0.92	0.19	63,63,63,63	0
56	MG	2A	3622	1/1	0.92	0.08	38,38,38,38	0
56	MG	1P	209	1/1	0.92	0.09	40,40,40,40	0
56	MG	1a	1736	1/1	0.92	0.20	46,46,46,46	0
56	MG	1a	1737	1/1	0.92	0.31	62,62,62,62	0
56	MG	2A	3110	1/1	0.92	0.21	61,61,61,61	0
56	MG	1A	3345	1/1	0.92	0.08	46,46,46,46	0
56	MG	1A	3973	1/1	0.92	0.11	50,50,50,50	0
56	MG	1A	3256	1/1	0.92	0.10	53,53,53,53	0
56	MG	1A	3684	1/1	0.92	0.09	36,36,36,36	0
56	MG	1A	3986	1/1	0.92	0.16	70,70,70,70	0
56	MG	1A	3261	1/1	0.92	0.15	52,52,52,52	0
56	MG	2A	3648	1/1	0.92	0.21	47,47,47,47	0
56	MG	1A	3444	1/1	0.92	0.14	43,43,43,43	0
56	MG	2A	3371	1/1	0.92	0.16	64,64,64,64	0
56	MG	1a	1760	1/1	0.92	0.11	56,56,56,56	0
56	MG	2A	3658	1/1	0.92	0.19	69,69,69,69	0
56	MG	2A	3135	1/1	0.92	0.19	51,51,51,51	0
56	MG	1A	3535	1/1	0.92	0.15	57,57,57,57	0
56	MG	1W	204	1/1	0.92	0.11	34,34,34,34	0
56	MG	2a	3028	1/1	0.92	0.13	62,62,62,62	0
56	MG	1A	3536	1/1	0.92	0.13	69,69,69,69	0
56	MG	1A	3832	1/1	0.92	0.21	59,59,59,59	0
56	MG	1A	3834	1/1	0.92	0.18	32,32,32,32	0
56	MG	1A	3048	1/1	0.92	0.08	20,20,20,20	0
56	MG	1A	3205	1/1	0.92	0.10	46,46,46,46	0
56	MG	1A	3696	1/1	0.92	0.06	20,20,20,20	0
56	MG	2A	3390	1/1	0.92	0.18	54,54,54,54	0
56	MG	2a	3040	1/1	0.92	0.12	77,77,77,77	0
56	MG	2A	3159	1/1	0.92	0.17	66,66,66,66	0
56	MG	1A	3840	1/1	0.92	0.07	22,22,22,22	0
56	MG	2A	3164	1/1	0.92	0.13	48,48,48,48	0
56	MG	1A	3283	1/1	0.92	0.21	33,33,33,33	0
56	MG	1A	3207	1/1	0.92	0.10	47,47,47,47	0
56	MG	1A	3062	1/1	0.92	0.25	51,51,51,51	0
56	MG	2a	3048	1/1	0.92	0.19	58,58,58,58	0
56	MG	2A	3404	1/1	0.92	0.15	45,45,45,45	0
56	MG	2a	3050	1/1	0.92	0.10	47,47,47,47	0
56	MG	2a	3052	1/1	0.92	0.17	56,56,56,56	0
56	MG	15	102	1/1	0.92	0.14	42,42,42,42	0
56	MG	2A	3172	1/1	0.92	0.12	50,50,50,50	0
56	MG	1A	3848	1/1	0.92	0.15	54,54,54,54	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	2a	3058	1/1	0.92	0.12	74,74,74,74	0
56	MG	2A	3175	1/1	0.92	0.13	50,50,50,50	0
56	MG	15	105	1/1	0.92	0.11	49,49,49,49	0
56	MG	1A	4030	1/1	0.92	0.10	61,61,61,61	0
56	MG	2A	3181	1/1	0.92	0.15	44,44,44,44	0
56	MG	2A	3417	1/1	0.92	0.20	68,68,68,68	0
56	MG	18	103	1/1	0.92	0.07	22,22,22,22	0
56	MG	1A	3463	1/1	0.92	0.12	47,47,47,47	0
56	MG	1A	4033	1/1	0.92	0.14	55,55,55,55	0
56	MG	1a	1602	1/1	0.92	0.16	61,61,61,61	0
56	MG	2a	3071	1/1	0.92	0.21	62,62,62,62	0
56	MG	2a	3072	1/1	0.92	0.17	51,51,51,51	0
56	MG	1A	3464	1/1	0.92	0.07	46,46,46,46	0
56	MG	2A	3425	1/1	0.92	0.20	43,43,43,43	0
56	MG	1a	1605	1/1	0.92	0.10	55,55,55,55	0
56	MG	2A	3429	1/1	0.92	0.29	53,53,53,53	0
56	MG	1A	3065	1/1	0.92	0.10	51,51,51,51	0
56	MG	1A	3468	1/1	0.92	0.17	57,57,57,57	0
56	MG	2A	3724	1/1	0.92	0.20	56,56,56,56	0
56	MG	1A	3367	1/1	0.92	0.16	57,57,57,57	0
56	MG	2a	3093	1/1	0.92	0.18	53,53,53,53	0
56	MG	2A	3202	1/1	0.92	0.12	47,47,47,47	0
56	MG	1A	3711	1/1	0.92	0.15	48,48,48,48	0
56	MG	1a	1616	1/1	0.92	0.07	55,55,55,55	0
56	MG	2a	3098	1/1	0.92	0.22	62,62,62,62	0
56	MG	2A	3206	1/1	0.92	0.15	53,53,53,53	0
56	MG	1A	3162	1/1	0.92	0.38	31,31,31,31	0
56	MG	1b	301	1/1	0.92	0.07	74,74,74,74	0
56	MG	2A	3738	1/1	0.92	0.08	48,48,48,48	0
56	MG	1A	3713	1/1	0.92	0.17	63,63,63,63	0
56	MG	2A	3213	1/1	0.92	0.21	61,61,61,61	0
56	MG	1A	3714	1/1	0.92	0.06	14,14,14,14	0
56	MG	2a	3109	1/1	0.92	0.08	72,72,72,72	0
56	MG	1A	3323	1/1	0.92	0.10	50,50,50,50	0
56	MG	2A	3744	1/1	0.92	0.10	44,44,44,44	0
56	MG	2A	3449	1/1	0.92	0.22	56,56,56,56	0
56	MG	1a	1627	1/1	0.92	0.08	55,55,55,55	0
56	MG	1A	3478	1/1	0.92	0.15	41,41,41,41	0
56	MG	2A	3749	1/1	0.92	0.10	58,58,58,58	0
56	MG	1a	1632	1/1	0.92	0.15	58,58,58,58	0
56	MG	1a	1633	1/1	0.92	0.14	52,52,52,52	0
56	MG	1A	3479	1/1	0.92	0.11	53,53,53,53	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	2A	3461	1/1	0.92	0.18	44,44,44,44	0
56	MG	2a	3126	1/1	0.92	0.26	66,66,66,66	0
56	MG	2A	3755	1/1	0.92	0.19	54,54,54,54	0
56	MG	1A	3592	1/1	0.92	0.10	22,22,22,22	0
56	MG	2A	3758	1/1	0.92	0.18	64,64,64,64	0
56	MG	1A	3382	1/1	0.92	0.12	46,46,46,46	0
56	MG	1A	3163	1/1	0.92	0.27	48,48,48,48	0
56	MG	1a	1651	1/1	0.92	0.12	61,61,61,61	0
56	MG	2A	3243	1/1	0.92	0.15	64,64,64,64	0
56	MG	2a	3145	1/1	0.92	0.09	79,79,79,79	0
56	MG	1A	3893	1/1	0.92	0.10	21,21,21,21	0
56	MG	2A	3766	1/1	0.92	0.13	68,68,68,68	0
56	MG	2A	3767	1/1	0.92	0.15	51,51,51,51	0
56	MG	1A	4073	1/1	0.92	0.15	59,59,59,59	0
56	MG	1a	1656	1/1	0.92	0.15	62,62,62,62	0
56	MG	2A	3476	1/1	0.92	0.10	62,62,62,62	0
56	MG	2A	3478	1/1	0.92	0.08	43,43,43,43	0
56	MG	1A	3482	1/1	0.92	0.08	43,43,43,43	0
56	MG	2A	3483	1/1	0.92	0.12	68,68,68,68	0
56	MG	2A	3788	1/1	0.92	0.07	51,51,51,51	0
56	MG	2A	3789	1/1	0.92	0.10	44,44,44,44	0
56	MG	1A	3895	1/1	0.92	0.08	18,18,18,18	0
56	MG	1A	3742	1/1	0.92	0.10	17,17,17,17	0
56	MG	2A	3486	1/1	0.92	0.13	62,62,62,62	0
56	MG	2A	3489	1/1	0.92	0.34	62,62,62,62	0
56	MG	1A	3397	1/1	0.92	0.20	30,30,30,30	0
56	MG	1A	3398	1/1	0.92	0.22	23,23,23,23	0
56	MG	2a	3179	1/1	0.92	0.07	69,69,69,69	0
56	MG	2A	3492	1/1	0.92	0.34	58,58,58,58	0
56	MG	2A	3256	1/1	0.92	0.21	68,68,68,68	0
56	MG	1a	1664	1/1	0.92	0.08	60,60,60,60	0
56	MG	1A	3613	1/1	0.92	0.14	42,42,42,42	0
56	MG	1A	3905	1/1	0.92	0.23	23,23,23,23	0
56	MG	1A	3623	1/1	0.92	0.09	26,26,26,26	0
56	MG	2a	3194	1/1	0.92	0.09	55,55,55,55	0
56	MG	2A	3811	1/1	0.92	0.09	54,54,54,54	0
56	MG	1a	1671	1/1	0.92	0.08	49,49,49,49	0
56	MG	2a	3198	1/1	0.92	0.12	62,62,62,62	0
56	MG	1A	3074	1/1	0.92	0.25	55,55,55,55	0
56	MG	2A	3511	1/1	0.92	0.10	58,58,58,58	0
56	MG	1A	4099	1/1	0.92	0.10	40,40,40,40	0
56	MG	2A	3269	1/1	0.92	0.12	53,53,53,53	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	2A	3515	1/1	0.92	0.10	36,36,36,36	0
56	MG	1A	3493	1/1	0.92	0.10	48,48,48,48	0
56	MG	2A	3011	1/1	0.92	0.10	53,53,53,53	0
56	MG	2a	3215	1/1	0.92	0.12	59,59,59,59	0
56	MG	2A	3016	1/1	0.92	0.29	57,57,57,57	0
56	MG	1A	3770	1/1	0.92	0.06	32,32,32,32	0
56	MG	2a	3218	1/1	0.92	0.20	74,74,74,74	0
56	MG	1a	1678	1/1	0.92	0.08	59,59,59,59	0
56	MG	2A	3833	1/1	0.92	0.11	53,53,53,53	0
56	MG	1A	3184	1/1	0.92	0.15	64,64,64,64	0
56	MG	1A	3918	1/1	0.92	0.11	28,28,28,28	0
56	MG	2A	3844	1/1	0.92	0.09	72,72,72,72	0
56	MG	1A	3640	1/1	0.92	0.15	49,49,49,49	0
56	MG	2A	3855	1/1	0.92	0.11	74,74,74,74	0
56	MG	2A	3536	1/1	0.92	0.09	57,57,57,57	0
56	MG	1B	215	1/1	0.92	0.10	55,55,55,55	0
56	MG	1A	3332	1/1	0.92	0.09	57,57,57,57	0
56	MG	1A	3775	1/1	0.92	0.09	21,21,21,21	0
56	MG	2A	3867	1/1	0.92	0.10	35,35,35,35	0
56	MG	2A	3047	1/1	0.92	0.06	24,24,24,24	0
56	MG	1B	224	1/1	0.92	0.13	52,52,52,52	0
56	MG	1A	3929	1/1	0.92	0.09	39,39,39,39	0
56	MG	2A	3050	1/1	0.92	0.14	57,57,57,57	0
56	MG	2e	201	1/1	0.92	0.12	64,64,64,64	0
56	MG	1A	3333	1/1	0.92	0.27	56,56,56,56	0
56	MG	1A	3504	1/1	0.92	0.12	54,54,54,54	0
56	MG	1A	3647	1/1	0.92	0.09	30,30,30,30	0
56	MG	2A	3885	1/1	0.92	0.08	59,59,59,59	0
56	MG	1A	3934	1/1	0.92	0.09	55,55,55,55	0
56	MG	2l	204	1/1	0.92	0.16	72,72,72,72	0
56	MG	2A	3304	1/1	0.92	0.11	44,44,44,44	0
56	MG	2A	3306	1/1	0.92	0.14	50,50,50,50	0
56	MG	2A	3569	1/1	0.92	0.09	46,46,46,46	0
56	MG	1A	3245	1/1	0.92	0.09	43,43,43,43	0
56	MG	1a	1701	1/1	0.92	0.29	53,53,53,53	0
56	MG	1a	1703	1/1	0.92	0.28	60,60,60,60	0
56	MG	2B	206	1/1	0.92	0.17	60,60,60,60	0
56	MG	2A	3583	1/1	0.92	0.08	61,61,61,61	0
56	MG	2B	210	1/1	0.92	0.14	67,67,67,67	0
56	MG	2A	3313	1/1	0.92	0.09	57,57,57,57	0
56	MG	2A	3063	1/1	0.92	0.15	58,58,58,58	0
56	MG	1A	3338	1/1	0.92	0.17	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	3317	1/1	0.92	0.24	49,49,49,49	0
56	MG	2A	3318	1/1	0.92	0.15	50,50,50,50	0
56	MG	2A	3319	1/1	0.92	0.16	53,53,53,53	0
56	MG	1A	3247	1/1	0.92	0.12	53,53,53,53	0
56	MG	2A	3529	1/1	0.93	0.20	52,52,52,52	0
56	MG	1a	1646	1/1	0.93	0.14	56,56,56,56	0
56	MG	1A	3499	1/1	0.93	0.07	44,44,44,44	0
56	MG	2A	3268	1/1	0.93	0.27	57,57,57,57	0
56	MG	1A	3116	1/1	0.93	0.08	36,36,36,36	0
56	MG	1A	3289	1/1	0.93	0.06	49,49,49,49	0
56	MG	1A	3506	1/1	0.93	0.08	47,47,47,47	0
56	MG	2A	3275	1/1	0.93	0.08	59,59,59,59	0
56	MG	2A	3542	1/1	0.93	0.07	46,46,46,46	0
56	MG	2B	208	1/1	0.93	0.11	59,59,59,59	0
56	MG	1A	3760	1/1	0.93	0.18	45,45,45,45	0
56	MG	1A	3117	1/1	0.93	0.10	35,35,35,35	0
56	MG	2A	3279	1/1	0.93	0.16	62,62,62,62	0
56	MG	1A	4090	1/1	0.93	0.12	53,53,53,53	0
56	MG	1A	3296	1/1	0.93	0.06	32,32,32,32	0
56	MG	2A	3005	1/1	0.93	0.22	55,55,55,55	0
56	MG	2A	3283	1/1	0.93	0.07	57,57,57,57	0
56	MG	1A	3297	1/1	0.93	0.10	50,50,50,50	0
56	MG	2A	3565	1/1	0.93	0.20	68,68,68,68	0
56	MG	2B	219	1/1	0.93	0.13	62,62,62,62	0
56	MG	2A	3286	1/1	0.93	0.19	56,56,56,56	0
56	MG	2A	3567	1/1	0.93	0.08	54,54,54,54	0
56	MG	1A	3768	1/1	0.93	0.09	38,38,38,38	0
56	MG	2A	3289	1/1	0.93	0.14	61,61,61,61	0
56	MG	1a	1665	1/1	0.93	0.16	51,51,51,51	0
56	MG	2D	310	1/1	0.93	0.09	56,56,56,56	0
56	MG	2F	304	1/1	0.93	0.10	54,54,54,54	0
56	MG	2A	3014	1/1	0.93	0.13	55,55,55,55	0
56	MG	2O	8400	1/1	0.93	0.11	64,64,64,64	0
56	MG	1B	201	1/1	0.93	0.20	48,48,48,48	0
56	MG	2P	203	1/1	0.93	0.08	38,38,38,38	0
56	MG	2P	204	1/1	0.93	0.13	57,57,57,57	0
56	MG	2A	3576	1/1	0.93	0.07	26,26,26,26	0
56	MG	2A	3578	1/1	0.93	0.18	54,54,54,54	0
56	MG	2A	3020	1/1	0.93	0.18	39,39,39,39	0
56	MG	2A	3022	1/1	0.93	0.10	56,56,56,56	0
56	MG	2T	201	1/1	0.93	0.12	54,54,54,54	0
56	MG	1A	3769	1/1	0.93	0.09	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	2T	204	1/1	0.93	0.13	54,54,54,54	0
56	MG	1a	1668	1/1	0.93	0.09	66,66,66,66	0
56	MG	1B	203	1/1	0.93	0.06	33,33,33,33	0
56	MG	2V	201	1/1	0.93	0.21	69,69,69,69	0
56	MG	1a	1670	1/1	0.93	0.20	60,60,60,60	0
56	MG	2V	203	1/1	0.93	0.07	57,57,57,57	0
56	MG	1A	3634	1/1	0.93	0.09	52,52,52,52	0
56	MG	1A	3639	1/1	0.93	0.07	36,36,36,36	0
56	MG	2A	3305	1/1	0.93	0.10	54,54,54,54	0
56	MG	1B	211	1/1	0.93	0.17	51,51,51,51	0
56	MG	25	103	1/1	0.93	0.11	45,45,45,45	0
56	MG	2A	3043	1/1	0.93	0.15	57,57,57,57	0
56	MG	2A	3309	1/1	0.93	0.35	55,55,55,55	0
56	MG	1A	3440	1/1	0.93	0.06	36,36,36,36	0
56	MG	28	101	1/1	0.93	0.13	66,66,66,66	0
56	MG	1B	213	1/1	0.93	0.09	56,56,56,56	0
56	MG	1a	1677	1/1	0.93	0.15	57,57,57,57	0
56	MG	1A	3920	1/1	0.93	0.22	65,65,65,65	0
56	MG	1a	1679	1/1	0.93	0.18	66,66,66,66	0
56	MG	2A	3316	1/1	0.93	0.18	53,53,53,53	0
56	MG	1A	3518	1/1	0.93	0.12	54,54,54,54	0
56	MG	1A	3234	1/1	0.93	0.12	54,54,54,54	0
56	MG	1B	223	1/1	0.93	0.15	51,51,51,51	0
56	MG	1A	3776	1/1	0.93	0.06	31,31,31,31	0
56	MG	1B	225	1/1	0.93	0.10	53,53,53,53	0
56	MG	1A	3783	1/1	0.93	0.07	17,17,17,17	0
56	MG	2A	3325	1/1	0.93	0.11	57,57,57,57	0
56	MG	2A	3060	1/1	0.93	0.10	46,46,46,46	0
56	MG	2A	3327	1/1	0.93	0.07	51,51,51,51	0
56	MG	1A	3303	1/1	0.93	0.29	55,55,55,55	0
56	MG	2a	3018	1/1	0.93	0.30	61,61,61,61	0
56	MG	1A	3931	1/1	0.93	0.07	40,40,40,40	0
56	MG	2A	3331	1/1	0.93	0.14	72,72,72,72	0
56	MG	2A	3628	1/1	0.93	0.14	55,55,55,55	0
56	MG	2a	3024	1/1	0.93	0.19	59,59,59,59	0
56	MG	2a	3025	1/1	0.93	0.12	59,59,59,59	0
56	MG	2a	3026	1/1	0.93	0.15	60,60,60,60	0
56	MG	2A	3332	1/1	0.93	0.07	46,46,46,46	0
56	MG	1B	232	1/1	0.93	0.09	50,50,50,50	0
56	MG	1A	3447	1/1	0.93	0.17	51,51,51,51	0
56	MG	2A	3068	1/1	0.93	0.18	61,61,61,61	0
56	MG	1A	3528	1/1	0.93	0.11	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	2A	3639	1/1	0.93	0.13	42,42,42,42	0
56	MG	1A	3651	1/1	0.93	0.08	37,37,37,37	0
56	MG	2A	3072	1/1	0.93	0.09	61,61,61,61	0
56	MG	2A	3644	1/1	0.93	0.20	43,43,43,43	0
56	MG	1A	3653	1/1	0.93	0.10	35,35,35,35	0
56	MG	2A	3075	1/1	0.93	0.07	48,48,48,48	0
56	MG	2A	3649	1/1	0.93	0.12	68,68,68,68	0
56	MG	2A	3077	1/1	0.93	0.10	57,57,57,57	0
56	MG	2A	3078	1/1	0.93	0.24	59,59,59,59	0
56	MG	2A	3656	1/1	0.93	0.14	59,59,59,59	0
56	MG	1A	3941	1/1	0.93	0.06	35,35,35,35	0
56	MG	1A	3096	1/1	0.93	0.13	57,57,57,57	0
56	MG	1A	3945	1/1	0.93	0.12	56,56,56,56	0
56	MG	1a	1708	1/1	0.93	0.24	58,58,58,58	0
56	MG	1E	310	1/1	0.93	0.21	61,61,61,61	0
56	MG	1A	3309	1/1	0.93	0.11	38,38,38,38	0
56	MG	2A	3093	1/1	0.93	0.08	37,37,37,37	0
56	MG	1A	3312	1/1	0.93	0.07	34,34,34,34	0
56	MG	1A	3361	1/1	0.93	0.12	56,56,56,56	0
56	MG	1A	3802	1/1	0.93	0.10	60,60,60,60	0
56	MG	1a	1718	1/1	0.93	0.16	53,53,53,53	0
56	MG	1A	3365	1/1	0.93	0.16	55,55,55,55	0
56	MG	1A	3366	1/1	0.93	0.09	40,40,40,40	0
56	MG	1A	3674	1/1	0.93	0.08	22,22,22,22	0
56	MG	1A	3314	1/1	0.93	0.17	48,48,48,48	0
56	MG	1A	3537	1/1	0.93	0.08	61,61,61,61	0
56	MG	2a	3067	1/1	0.93	0.12	47,47,47,47	0
56	MG	1A	3678	1/1	0.93	0.08	23,23,23,23	0
56	MG	2a	3069	1/1	0.93	0.09	62,62,62,62	0
56	MG	1A	3969	1/1	0.93	0.10	42,42,42,42	0
56	MG	2A	3114	1/1	0.93	0.37	64,64,64,64	0
56	MG	1P	207	1/1	0.93	0.11	51,51,51,51	0
56	MG	2a	3074	1/1	0.93	0.21	52,52,52,52	0
56	MG	2A	3694	1/1	0.93	0.12	50,50,50,50	0
56	MG	2a	3078	1/1	0.93	0.18	50,50,50,50	0
56	MG	2A	3695	1/1	0.93	0.07	60,60,60,60	0
56	MG	2a	3081	1/1	0.93	0.28	60,60,60,60	0
56	MG	2A	3696	1/1	0.93	0.08	55,55,55,55	0
56	MG	2A	3117	1/1	0.93	0.10	55,55,55,55	0
56	MG	2a	3084	1/1	0.93	0.28	58,58,58,58	0
56	MG	2A	3384	1/1	0.93	0.09	62,62,62,62	0
56	MG	1A	3016	1/1	0.93	0.16	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	2a	3088	1/1	0.93	0.11	55,55,55,55	0
56	MG	2A	3701	1/1	0.93	0.08	58,58,58,58	0
56	MG	1Q	205	1/1	0.93	0.06	55,55,55,55	0
56	MG	1A	3539	1/1	0.93	0.22	45,45,45,45	0
56	MG	2A	3392	1/1	0.93	0.15	58,58,58,58	0
56	MG	1a	1735	1/1	0.93	0.22	53,53,53,53	0
56	MG	1R	203	1/1	0.93	0.23	46,46,46,46	0
56	MG	2a	3097	1/1	0.93	0.29	49,49,49,49	0
56	MG	1A	3320	1/1	0.93	0.18	46,46,46,46	0
56	MG	1A	3544	1/1	0.93	0.14	37,37,37,37	0
56	MG	2A	3400	1/1	0.93	0.13	59,59,59,59	0
56	MG	1A	3984	1/1	0.93	0.08	71,71,71,71	0
56	MG	2A	3148	1/1	0.93	0.13	51,51,51,51	0
56	MG	2a	3105	1/1	0.93	0.12	45,45,45,45	0
56	MG	2A	3717	1/1	0.93	0.07	51,51,51,51	0
56	MG	1A	3546	1/1	0.93	0.17	43,43,43,43	0
56	MG	1a	1748	1/1	0.93	0.06	36,36,36,36	0
56	MG	1A	3194	1/1	0.93	0.25	33,33,33,33	0
56	MG	2a	3110	1/1	0.93	0.15	62,62,62,62	0
56	MG	2a	3111	1/1	0.93	0.13	63,63,63,63	0
56	MG	1a	1752	1/1	0.93	0.10	74,74,74,74	0
56	MG	2A	3154	1/1	0.93	0.17	52,52,52,52	0
56	MG	2a	3114	1/1	0.93	0.12	65,65,65,65	0
56	MG	1A	3026	1/1	0.93	0.07	45,45,45,45	0
56	MG	2A	3415	1/1	0.93	0.15	62,62,62,62	0
56	MG	1a	1754	1/1	0.93	0.11	57,57,57,57	0
56	MG	2a	3118	1/1	0.93	0.28	62,62,62,62	0
56	MG	2A	3732	1/1	0.93	0.19	72,72,72,72	0
56	MG	1A	3202	1/1	0.93	0.08	40,40,40,40	0
56	MG	1V	205	1/1	0.93	0.07	29,29,29,29	0
56	MG	2A	3163	1/1	0.93	0.14	57,57,57,57	0
56	MG	1V	207	1/1	0.93	0.07	52,52,52,52	0
56	MG	1A	3556	1/1	0.93	0.21	41,41,41,41	0
56	MG	2A	3422	1/1	0.93	0.07	42,42,42,42	0
56	MG	2A	3167	1/1	0.93	0.08	39,39,39,39	0
56	MG	1a	1765	1/1	0.93	0.13	51,51,51,51	0
56	MG	2A	3426	1/1	0.93	0.23	42,42,42,42	0
56	MG	2A	3427	1/1	0.93	0.20	42,42,42,42	0
56	MG	1A	3330	1/1	0.93	0.12	46,46,46,46	0
56	MG	1A	3164	1/1	0.93	0.15	52,52,52,52	0
56	MG	2a	3140	1/1	0.93	0.08	57,57,57,57	0
56	MG	1a	1768	1/1	0.93	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	3996	1/1	0.93	0.16	51,51,51,51	0
56	MG	1A	3107	1/1	0.93	0.07	27,27,27,27	0
56	MG	1A	3843	1/1	0.93	0.07	51,51,51,51	0
56	MG	1a	1776	1/1	0.93	0.12	58,58,58,58	0
56	MG	10	101	1/1	0.93	0.07	38,38,38,38	0
56	MG	1A	4001	1/1	0.93	0.12	48,48,48,48	0
56	MG	1A	3180	1/1	0.93	0.12	35,35,35,35	0
56	MG	2A	3187	1/1	0.93	0.19	56,56,56,56	0
56	MG	11	102	1/1	0.93	0.12	42,42,42,42	0
56	MG	1A	3566	1/1	0.93	0.22	52,52,52,52	0
56	MG	2A	3446	1/1	0.93	0.30	63,63,63,63	0
56	MG	2A	3763	1/1	0.93	0.12	60,60,60,60	0
56	MG	11	105	1/1	0.93	0.09	53,53,53,53	0
56	MG	1A	4008	1/1	0.93	0.33	33,33,33,33	0
56	MG	1A	3212	1/1	0.93	0.08	35,35,35,35	0
56	MG	2A	3450	1/1	0.93	0.21	56,56,56,56	0
56	MG	1A	3484	1/1	0.93	0.13	59,59,59,59	0
56	MG	2A	3453	1/1	0.93	0.14	52,52,52,52	0
56	MG	2a	3182	1/1	0.93	0.09	83,83,83,83	0
56	MG	2A	3454	1/1	0.93	0.24	50,50,50,50	0
56	MG	2a	3185	1/1	0.93	0.14	52,52,52,52	0
56	MG	2A	3200	1/1	0.93	0.23	48,48,48,48	0
56	MG	1A	3183	1/1	0.93	0.08	48,48,48,48	0
56	MG	2A	3777	1/1	0.93	0.09	47,47,47,47	0
56	MG	1A	3853	1/1	0.93	0.13	55,55,55,55	0
56	MG	2A	3784	1/1	0.93	0.11	64,64,64,64	0
56	MG	2A	3785	1/1	0.93	0.08	53,53,53,53	0
56	MG	1a	1797	1/1	0.93	0.08	65,65,65,65	0
56	MG	1a	1798	1/1	0.93	0.09	76,76,76,76	0
56	MG	2A	3791	1/1	0.93	0.13	56,56,56,56	0
56	MG	1A	3576	1/1	0.93	0.20	43,43,43,43	0
56	MG	1A	3487	1/1	0.93	0.10	44,44,44,44	0
56	MG	1A	3861	1/1	0.93	0.10	61,61,61,61	0
56	MG	2A	3798	1/1	0.93	0.09	51,51,51,51	0
56	MG	2a	3203	1/1	0.93	0.07	63,63,63,63	0
56	MG	1A	3864	1/1	0.93	0.13	52,52,52,52	0
56	MG	1A	3584	1/1	0.93	0.07	32,32,32,32	0
56	MG	2A	3470	1/1	0.93	0.16	62,62,62,62	0
56	MG	2A	3803	1/1	0.93	0.08	81,81,81,81	0
56	MG	1a	1603	1/1	0.93	0.08	61,61,61,61	0
56	MG	2A	3215	1/1	0.93	0.15	56,56,56,56	0
56	MG	1A	3265	1/1	0.93	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	2a	3219	1/1	0.93	0.14	68,68,68,68	0
56	MG	1A	3587	1/1	0.93	0.23	35,35,35,35	0
56	MG	2a	3223	1/1	0.93	0.15	64,64,64,64	0
56	MG	2A	3221	1/1	0.93	0.10	57,57,57,57	0
56	MG	1a	1830	1/1	0.93	0.17	42,42,42,42	0
56	MG	1A	3589	1/1	0.93	0.10	35,35,35,35	0
56	MG	1A	4051	1/1	0.93	0.13	58,58,58,58	0
56	MG	1A	3871	1/1	0.93	0.07	32,32,32,32	0
56	MG	2a	3230	1/1	0.93	0.09	65,65,65,65	0
56	MG	2A	3230	1/1	0.93	0.16	67,67,67,67	0
56	MG	2a	3232	1/1	0.93	0.07	63,63,63,63	0
56	MG	2A	3487	1/1	0.93	0.27	48,48,48,48	0
56	MG	2A	3818	1/1	0.93	0.08	64,64,64,64	0
56	MG	1A	3221	1/1	0.93	0.09	46,46,46,46	0
56	MG	1a	1613	1/1	0.93	0.15	49,49,49,49	0
56	MG	1A	4054	1/1	0.93	0.17	53,53,53,53	0
56	MG	1A	3594	1/1	0.93	0.15	55,55,55,55	0
56	MG	2A	3241	1/1	0.93	0.23	62,62,62,62	0
56	MG	1a	1618	1/1	0.93	0.10	49,49,49,49	0
56	MG	1A	3271	1/1	0.93	0.23	44,44,44,44	0
56	MG	2A	3832	1/1	0.93	0.09	38,38,38,38	0
56	MG	1A	3881	1/1	0.93	0.13	36,36,36,36	0
56	MG	2A	3834	1/1	0.93	0.12	48,48,48,48	0
56	MG	2i	201	1/1	0.93	0.08	62,62,62,62	0
56	MG	2A	3836	1/1	0.93	0.10	62,62,62,62	0
56	MG	2A	3499	1/1	0.93	0.09	47,47,47,47	0
56	MG	2A	3501	1/1	0.93	0.07	58,58,58,58	0
56	MG	1w	101	1/1	0.93	0.21	65,65,65,65	0
56	MG	1A	3727	1/1	0.93	0.07	39,39,39,39	0
56	MG	2A	3505	1/1	0.93	0.21	57,57,57,57	0
56	MG	1A	3884	1/1	0.93	0.17	28,28,28,28	0
56	MG	1a	1629	1/1	0.93	0.19	54,54,54,54	0
56	MG	2A	3512	1/1	0.93	0.16	58,58,58,58	0
56	MG	1A	3728	1/1	0.93	0.10	44,44,44,44	0
56	MG	1A	3887	1/1	0.93	0.09	31,31,31,31	0
56	MG	1A	3497	1/1	0.93	0.09	50,50,50,50	0
56	MG	1A	3734	1/1	0.93	0.10	49,49,49,49	0
56	MG	2x	101	1/1	0.93	0.10	60,60,60,60	0
56	MG	1a	1638	1/1	0.93	0.19	61,61,61,61	0
56	MG	2A	3518	1/1	0.93	0.11	53,53,53,53	0
56	MG	1A	4074	1/1	0.93	0.08	48,48,48,48	0
56	MG	2A	3880	1/1	0.93	0.11	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	3279	1/1	0.93	0.18	39,39,39,39	0
56	MG	2A	3526	1/1	0.93	0.08	30,30,30,30	0
56	MG	2y	104	1/1	0.93	0.08	50,50,50,50	0
56	MG	1A	3607	1/1	0.93	0.10	27,27,27,27	0
56	MG	1A	3704	1/1	0.94	0.06	21,21,21,21	0
56	MG	1x	118	1/1	0.94	0.09	58,58,58,58	0
56	MG	1A	3558	1/1	0.94	0.21	54,54,54,54	0
56	MG	2A	3292	1/1	0.94	0.22	57,57,57,57	0
56	MG	2A	3571	1/1	0.94	0.09	42,42,42,42	0
56	MG	1A	3868	1/1	0.94	0.08	35,35,35,35	0
56	MG	2A	3573	1/1	0.94	0.10	62,62,62,62	0
56	MG	2D	306	1/1	0.94	0.32	47,47,47,47	0
56	MG	2D	307	1/1	0.94	0.27	47,47,47,47	0
56	MG	2A	3574	1/1	0.94	0.13	46,46,46,46	0
56	MG	1A	3462	1/1	0.94	0.14	54,54,54,54	0
56	MG	1a	1643	1/1	0.94	0.07	51,51,51,51	0
56	MG	2E	301	1/1	0.94	0.10	49,49,49,49	0
56	MG	2E	302	1/1	0.94	0.13	61,61,61,61	0
56	MG	2F	302	1/1	0.94	0.17	64,64,64,64	0
56	MG	1A	3870	1/1	0.94	0.10	30,30,30,30	0
56	MG	2A	3298	1/1	0.94	0.16	57,57,57,57	0
56	MG	1a	1647	1/1	0.94	0.20	55,55,55,55	0
56	MG	1A	3111	1/1	0.94	0.10	37,37,37,37	0
56	MG	1A	3304	1/1	0.94	0.15	21,21,21,21	0
56	MG	2A	3590	1/1	0.94	0.10	64,64,64,64	0
56	MG	2Q	201	1/1	0.94	0.06	49,49,49,49	0
56	MG	2Q	202	1/1	0.94	0.10	53,53,53,53	0
56	MG	2A	3592	1/1	0.94	0.09	46,46,46,46	0
56	MG	1A	3564	1/1	0.94	0.12	49,49,49,49	0
56	MG	2A	3021	1/1	0.94	0.24	55,55,55,55	0
56	MG	1A	3050	1/1	0.94	0.09	21,21,21,21	0
56	MG	2A	3024	1/1	0.94	0.18	48,48,48,48	0
56	MG	2A	3025	1/1	0.94	0.06	44,44,44,44	0
56	MG	2A	3026	1/1	0.94	0.23	53,53,53,53	0
56	MG	1A	3182	1/1	0.94	0.16	49,49,49,49	0
56	MG	2U	202	1/1	0.94	0.28	58,58,58,58	0
56	MG	1a	1658	1/1	0.94	0.10	63,63,63,63	0
56	MG	1A	3470	1/1	0.94	0.18	49,49,49,49	0
56	MG	2A	3312	1/1	0.94	0.10	50,50,50,50	0
56	MG	1A	3717	1/1	0.94	0.08	41,41,41,41	0
56	MG	1A	3310	1/1	0.94	0.24	40,40,40,40	0
56	MG	2W	202	1/1	0.94	0.08	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	2W	203	1/1	0.94	0.08	51,51,51,51	0
56	MG	2X	101	1/1	0.94	0.08	56,56,56,56	0
56	MG	1A	3243	1/1	0.94	0.17	33,33,33,33	0
56	MG	1A	3474	1/1	0.94	0.23	32,32,32,32	0
56	MG	1A	3889	1/1	0.94	0.10	44,44,44,44	0
56	MG	2I	101	1/1	0.94	0.28	55,55,55,55	0
56	MG	23	101	1/1	0.94	0.10	54,54,54,54	0
56	MG	23	102	1/1	0.94	0.09	45,45,45,45	0
56	MG	25	101	1/1	0.94	0.37	58,58,58,58	0
56	MG	1A	3051	1/1	0.94	0.15	31,31,31,31	0
56	MG	1A	3578	1/1	0.94	0.08	43,43,43,43	0
56	MG	2A	3320	1/1	0.94	0.22	54,54,54,54	0
56	MG	1A	4092	1/1	0.94	0.10	54,54,54,54	0
56	MG	27	102	1/1	0.94	0.16	34,34,34,34	0
56	MG	1A	3581	1/1	0.94	0.06	15,15,15,15	0
56	MG	28	102	1/1	0.94	0.10	48,48,48,48	0
56	MG	1A	3378	1/1	0.94	0.10	42,42,42,42	0
56	MG	1A	3379	1/1	0.94	0.13	48,48,48,48	0
56	MG	1a	1672	1/1	0.94	0.07	44,44,44,44	0
56	MG	1A	3896	1/1	0.94	0.08	60,60,60,60	0
56	MG	1A	3737	1/1	0.94	0.06	41,41,41,41	0
56	MG	1A	3084	1/1	0.94	0.11	33,33,33,33	0
56	MG	1B	206	1/1	0.94	0.12	40,40,40,40	0
56	MG	2A	3629	1/1	0.94	0.10	36,36,36,36	0
56	MG	1A	3381	1/1	0.94	0.19	52,52,52,52	0
56	MG	1A	3318	1/1	0.94	0.20	43,43,43,43	0
56	MG	2A	3633	1/1	0.94	0.12	40,40,40,40	0
56	MG	1A	3746	1/1	0.94	0.12	46,46,46,46	0
56	MG	1a	1680	1/1	0.94	0.20	63,63,63,63	0
56	MG	2A	3338	1/1	0.94	0.14	62,62,62,62	0
56	MG	2A	3638	1/1	0.94	0.15	55,55,55,55	0
56	MG	1a	1683	1/1	0.94	0.10	43,43,43,43	0
56	MG	1a	1684	1/1	0.94	0.28	63,63,63,63	0
56	MG	2A	3641	1/1	0.94	0.09	38,38,38,38	0
56	MG	1A	3906	1/1	0.94	0.10	49,49,49,49	0
56	MG	1A	3747	1/1	0.94	0.06	54,54,54,54	0
56	MG	1A	3910	1/1	0.94	0.11	51,51,51,51	0
56	MG	1A	3388	1/1	0.94	0.12	44,44,44,44	0
56	MG	1a	1689	1/1	0.94	0.07	59,59,59,59	0
56	MG	2A	3076	1/1	0.94	0.12	31,31,31,31	0
56	MG	1A	3600	1/1	0.94	0.12	39,39,39,39	0
56	MG	2A	3653	1/1	0.94	0.17	61,61,61,61	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	1A	3757	1/1	0.94	0.11	50,50,50,50	0
56	MG	2A	3079	1/1	0.94	0.12	46,46,46,46	0
56	MG	1A	3390	1/1	0.94	0.13	36,36,36,36	0
56	MG	2A	3358	1/1	0.94	0.17	56,56,56,56	0
56	MG	1A	3391	1/1	0.94	0.07	42,42,42,42	0
56	MG	1A	3392	1/1	0.94	0.08	45,45,45,45	0
56	MG	2A	3363	1/1	0.94	0.11	51,51,51,51	0
56	MG	2A	3668	1/1	0.94	0.15	54,54,54,54	0
56	MG	2A	3670	1/1	0.94	0.16	47,47,47,47	0
56	MG	1A	3763	1/1	0.94	0.08	22,22,22,22	0
56	MG	1a	1696	1/1	0.94	0.23	44,44,44,44	0
56	MG	1A	3923	1/1	0.94	0.11	59,59,59,59	0
56	MG	2a	3047	1/1	0.94	0.14	55,55,55,55	0
56	MG	2A	3675	1/1	0.94	0.12	57,57,57,57	0
56	MG	1A	3490	1/1	0.94	0.09	35,35,35,35	0
56	MG	2A	3369	1/1	0.94	0.12	64,64,64,64	0
56	MG	2a	3051	1/1	0.94	0.13	62,62,62,62	0
56	MG	2A	3370	1/1	0.94	0.16	64,64,64,64	0
56	MG	1a	1699	1/1	0.94	0.29	47,47,47,47	0
56	MG	1A	3052	1/1	0.94	0.08	40,40,40,40	0
56	MG	2A	3682	1/1	0.94	0.15	74,74,74,74	0
56	MG	1A	3034	1/1	0.94	0.20	23,23,23,23	0
56	MG	1A	3130	1/1	0.94	0.09	29,29,29,29	0
56	MG	1a	1706	1/1	0.94	0.23	59,59,59,59	0
56	MG	1A	3621	1/1	0.94	0.09	27,27,27,27	0
56	MG	2A	3379	1/1	0.94	0.15	56,56,56,56	0
56	MG	2A	3690	1/1	0.94	0.07	40,40,40,40	0
56	MG	1B	239	1/1	0.94	0.07	30,30,30,30	0
56	MG	1D	306	1/1	0.94	0.12	33,33,33,33	0
56	MG	1D	310	1/1	0.94	0.09	24,24,24,24	0
56	MG	1a	1712	1/1	0.94	0.09	53,53,53,53	0
56	MG	1A	3328	1/1	0.94	0.15	48,48,48,48	0
56	MG	1D	313	1/1	0.94	0.18	34,34,34,34	0
56	MG	2A	3115	1/1	0.94	0.08	41,41,41,41	0
56	MG	1A	3400	1/1	0.94	0.33	42,42,42,42	0
56	MG	1a	1717	1/1	0.94	0.15	64,64,64,64	0
56	MG	2a	3075	1/1	0.94	0.16	57,57,57,57	0
56	MG	2a	3076	1/1	0.94	0.07	53,53,53,53	0
56	MG	2A	3394	1/1	0.94	0.25	51,51,51,51	0
56	MG	2A	3118	1/1	0.94	0.15	43,43,43,43	0
56	MG	2A	3706	1/1	0.94	0.08	68,68,68,68	0
56	MG	1E	308	1/1	0.94	0.06	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	3401	1/1	0.94	0.20	35,35,35,35	0
56	MG	2A	3122	1/1	0.94	0.24	53,53,53,53	0
56	MG	1A	3627	1/1	0.94	0.08	18,18,18,18	0
56	MG	2A	3401	1/1	0.94	0.10	54,54,54,54	0
56	MG	1A	3095	1/1	0.94	0.18	44,44,44,44	0
56	MG	2A	3403	1/1	0.94	0.09	57,57,57,57	0
56	MG	1a	1724	1/1	0.94	0.21	49,49,49,49	0
56	MG	2a	3090	1/1	0.94	0.15	66,66,66,66	0
56	MG	1A	3780	1/1	0.94	0.09	34,34,34,34	0
56	MG	1F	305	1/1	0.94	0.07	45,45,45,45	0
56	MG	1A	3781	1/1	0.94	0.07	41,41,41,41	0
56	MG	2A	3409	1/1	0.94	0.26	66,66,66,66	0
56	MG	2A	3144	1/1	0.94	0.19	54,54,54,54	0
56	MG	2A	3726	1/1	0.94	0.07	50,50,50,50	0
56	MG	1A	3403	1/1	0.94	0.08	53,53,53,53	0
56	MG	1A	3635	1/1	0.94	0.11	33,33,33,33	0
56	MG	1A	3505	1/1	0.94	0.08	39,39,39,39	0
56	MG	1A	3257	1/1	0.94	0.15	58,58,58,58	0
56	MG	1N	204	1/1	0.94	0.17	42,42,42,42	0
56	MG	1A	3641	1/1	0.94	0.07	22,22,22,22	0
56	MG	1A	3961	1/1	0.94	0.07	56,56,56,56	0
56	MG	1A	3794	1/1	0.94	0.16	48,48,48,48	0
56	MG	2A	3158	1/1	0.94	0.28	56,56,56,56	0
56	MG	1P	202	1/1	0.94	0.14	23,23,23,23	0
56	MG	1P	205	1/1	0.94	0.07	16,16,16,16	0
56	MG	2A	3161	1/1	0.94	0.15	64,64,64,64	0
56	MG	2A	3162	1/1	0.94	0.19	64,64,64,64	0
56	MG	1a	1744	1/1	0.94	0.15	54,54,54,54	0
56	MG	1A	3642	1/1	0.94	0.06	14,14,14,14	0
56	MG	2A	3165	1/1	0.94	0.30	65,65,65,65	0
56	MG	1A	3510	1/1	0.94	0.06	41,41,41,41	0
56	MG	1A	3408	1/1	0.94	0.18	32,32,32,32	0
56	MG	1Q	204	1/1	0.94	0.08	44,44,44,44	0
56	MG	2a	3119	1/1	0.94	0.11	69,69,69,69	0
56	MG	1A	3258	1/1	0.94	0.17	25,25,25,25	0
56	MG	1A	3054	1/1	0.94	0.07	42,42,42,42	0
56	MG	1A	3416	1/1	0.94	0.12	36,36,36,36	0
56	MG	1A	3972	1/1	0.94	0.08	43,43,43,43	0
56	MG	1A	3020	1/1	0.94	0.07	33,33,33,33	0
56	MG	1a	1762	1/1	0.94	0.10	61,61,61,61	0
56	MG	2A	3178	1/1	0.94	0.14	48,48,48,48	0
56	MG	2a	3129	1/1	0.94	0.07	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	3976	1/1	0.94	0.09	47,47,47,47	0
56	MG	1A	3519	1/1	0.94	0.10	45,45,45,45	0
56	MG	1A	3980	1/1	0.94	0.08	62,62,62,62	0
56	MG	1A	3981	1/1	0.94	0.08	60,60,60,60	0
56	MG	1U	209	1/1	0.94	0.30	44,44,44,44	0
56	MG	1A	3100	1/1	0.94	0.15	41,41,41,41	0
56	MG	1A	3660	1/1	0.94	0.06	31,31,31,31	0
56	MG	2a	3144	1/1	0.94	0.09	65,65,65,65	0
56	MG	1A	3985	1/1	0.94	0.11	61,61,61,61	0
56	MG	1A	3523	1/1	0.94	0.11	53,53,53,53	0
56	MG	1a	1777	1/1	0.94	0.11	59,59,59,59	0
56	MG	2A	3772	1/1	0.94	0.12	66,66,66,66	0
56	MG	1A	3268	1/1	0.94	0.15	35,35,35,35	0
56	MG	1A	3147	1/1	0.94	0.11	39,39,39,39	0
56	MG	2A	3459	1/1	0.94	0.13	41,41,41,41	0
56	MG	2A	3779	1/1	0.94	0.07	71,71,71,71	0
56	MG	1A	3664	1/1	0.94	0.07	40,40,40,40	0
56	MG	1A	3424	1/1	0.94	0.09	48,48,48,48	0
56	MG	2A	3203	1/1	0.94	0.20	48,48,48,48	0
56	MG	1A	3148	1/1	0.94	0.16	35,35,35,35	0
56	MG	2a	3167	1/1	0.94	0.06	75,75,75,75	0
56	MG	1A	3668	1/1	0.94	0.06	21,21,21,21	0
56	MG	2a	3172	1/1	0.94	0.08	62,62,62,62	0
56	MG	1A	3825	1/1	0.94	0.12	34,34,34,34	0
56	MG	2A	3468	1/1	0.94	0.32	51,51,51,51	0
56	MG	2A	3793	1/1	0.94	0.15	77,77,77,77	0
56	MG	1a	1788	1/1	0.94	0.07	61,61,61,61	0
56	MG	2a	3177	1/1	0.94	0.14	65,65,65,65	0
56	MG	1A	3997	1/1	0.94	0.15	45,45,45,45	0
56	MG	1A	3276	1/1	0.94	0.09	45,45,45,45	0
56	MG	2a	3180	1/1	0.94	0.08	71,71,71,71	0
56	MG	2a	3181	1/1	0.94	0.12	64,64,64,64	0
56	MG	2A	3473	1/1	0.94	0.21	60,60,60,60	0
56	MG	11	103	1/1	0.94	0.07	36,36,36,36	0
56	MG	1A	3999	1/1	0.94	0.08	39,39,39,39	0
56	MG	1A	3278	1/1	0.94	0.07	41,41,41,41	0
56	MG	1A	3209	1/1	0.94	0.10	38,38,38,38	0
56	MG	12	102	1/1	0.94	0.09	39,39,39,39	0
56	MG	2A	3480	1/1	0.94	0.11	46,46,46,46	0
56	MG	2A	3219	1/1	0.94	0.16	52,52,52,52	0
56	MG	13	103	1/1	0.94	0.06	39,39,39,39	0
56	MG	1a	1803	1/1	0.94	0.09	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	1A	4002	1/1	0.94	0.07	31,31,31,31	0
56	MG	2A	3226	1/1	0.94	0.10	57,57,57,57	0
56	MG	1A	3435	1/1	0.94	0.08	42,42,42,42	0
56	MG	1A	3436	1/1	0.94	0.07	49,49,49,49	0
56	MG	1A	4007	1/1	0.94	0.07	15,15,15,15	0
56	MG	1A	3837	1/1	0.94	0.11	51,51,51,51	0
56	MG	2A	3235	1/1	0.94	0.12	44,44,44,44	0
56	MG	2A	3236	1/1	0.94	0.10	45,45,45,45	0
56	MG	2a	3206	1/1	0.94	0.15	62,62,62,62	0
56	MG	17	104	1/1	0.94	0.07	37,37,37,37	0
56	MG	2A	3824	1/1	0.94	0.11	66,66,66,66	0
56	MG	1a	1829	1/1	0.94	0.14	43,43,43,43	0
56	MG	2A	3827	1/1	0.94	0.07	62,62,62,62	0
56	MG	18	101	1/1	0.94	0.11	37,37,37,37	0
56	MG	1A	4009	1/1	0.94	0.16	23,23,23,23	0
56	MG	2A	3242	1/1	0.94	0.08	64,64,64,64	0
56	MG	18	104	1/1	0.94	0.12	49,49,49,49	0
56	MG	2a	3221	1/1	0.94	0.10	55,55,55,55	0
56	MG	2A	3245	1/1	0.94	0.09	47,47,47,47	0
56	MG	1A	4011	1/1	0.94	0.08	65,65,65,65	0
56	MG	1A	4012	1/1	0.94	0.09	68,68,68,68	0
56	MG	1A	4015	1/1	0.94	0.05	29,29,29,29	0
56	MG	1A	3437	1/1	0.94	0.18	53,53,53,53	0
56	MG	2A	3841	1/1	0.94	0.09	47,47,47,47	0
56	MG	1A	3151	1/1	0.94	0.12	42,42,42,42	0
56	MG	2A	3848	1/1	0.94	0.07	74,74,74,74	0
56	MG	1e	202	1/1	0.94	0.14	59,59,59,59	0
56	MG	1A	3155	1/1	0.94	0.11	43,43,43,43	0
56	MG	2a	3234	1/1	0.94	0.11	60,60,60,60	0
56	MG	1A	4019	1/1	0.94	0.06	22,22,22,22	0
56	MG	1A	4022	1/1	0.94	0.08	31,31,31,31	0
56	MG	1v	101	1/1	0.94	0.12	65,65,65,65	0
56	MG	1A	3291	1/1	0.94	0.09	32,32,32,32	0
56	MG	1A	3350	1/1	0.94	0.23	51,51,51,51	0
56	MG	1A	3846	1/1	0.94	0.07	39,39,39,39	0
56	MG	1A	3351	1/1	0.94	0.30	47,47,47,47	0
56	MG	1A	4037	1/1	0.94	0.07	68,68,68,68	0
56	MG	2A	3874	1/1	0.94	0.12	66,66,66,66	0
56	MG	2f	201	1/1	0.94	0.10	48,48,48,48	0
56	MG	1A	3545	1/1	0.94	0.09	46,46,46,46	0
56	MG	2A	3876	1/1	0.94	0.14	47,47,47,47	0
56	MG	1A	3217	1/1	0.94	0.06	39,39,39,39	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	1a	1621	1/1	0.94	0.13	51,51,51,51	0
56	MG	1a	1622	1/1	0.94	0.07	40,40,40,40	0
56	MG	2A	3883	1/1	0.94	0.11	68,68,68,68	0
56	MG	2A	3272	1/1	0.94	0.12	56,56,56,56	0
56	MG	1a	1623	1/1	0.94	0.17	55,55,55,55	0
56	MG	1x	101	1/1	0.94	0.12	38,38,38,38	0
56	MG	1A	3454	1/1	0.94	0.19	39,39,39,39	0
56	MG	2r	101	1/1	0.94	0.09	65,65,65,65	0
56	MG	2A	3546	1/1	0.94	0.12	65,65,65,65	0
56	MG	1x	107	1/1	0.94	0.15	49,49,49,49	0
56	MG	2A	3549	1/1	0.94	0.17	47,47,47,47	0
56	MG	1A	3854	1/1	0.94	0.07	60,60,60,60	0
56	MG	1A	3101	1/1	0.94	0.18	56,56,56,56	0
56	MG	2A	3552	1/1	0.94	0.10	43,43,43,43	0
56	MG	2A	3555	1/1	0.94	0.09	27,27,27,27	0
56	MG	1A	3857	1/1	0.94	0.15	36,36,36,36	0
56	MG	2B	209	1/1	0.94	0.23	59,59,59,59	0
56	MG	2A	3557	1/1	0.94	0.10	59,59,59,59	0
56	MG	1A	3046	1/1	0.94	0.10	28,28,28,28	0
56	MG	1A	3019	1/1	0.94	0.15	41,41,41,41	0
56	MG	2A	3284	1/1	0.94	0.07	59,59,59,59	0
56	MG	1A	3701	1/1	0.94	0.08	23,23,23,23	0
56	MG	1A	3557	1/1	0.94	0.08	47,47,47,47	0
59	ZN	24	501	1/1	0.94	0.07	117,117,117,117	0
56	MG	2A	3001	1/1	0.95	0.23	55,55,55,55	0
56	MG	1A	4064	1/1	0.95	0.06	34,34,34,34	0
56	MG	2E	304	1/1	0.95	0.09	43,43,43,43	0
56	MG	2A	3581	1/1	0.95	0.10	46,46,46,46	0
56	MG	2F	303	1/1	0.95	0.09	48,48,48,48	0
56	MG	1A	3873	1/1	0.95	0.10	35,35,35,35	0
56	MG	2A	3004	1/1	0.95	0.24	58,58,58,58	0
56	MG	1a	1635	1/1	0.95	0.09	55,55,55,55	0
56	MG	2P	201	1/1	0.95	0.23	58,58,58,58	0
56	MG	1A	3041	1/1	0.95	0.30	34,34,34,34	0
56	MG	2A	3007	1/1	0.95	0.15	49,49,49,49	0
56	MG	1a	1639	1/1	0.95	0.19	56,56,56,56	0
56	MG	1A	4071	1/1	0.95	0.07	51,51,51,51	0
56	MG	2A	3012	1/1	0.95	0.06	40,40,40,40	0
56	MG	1A	3448	1/1	0.95	0.07	36,36,36,36	0
56	MG	2A	3015	1/1	0.95	0.11	39,39,39,39	0
56	MG	2A	3598	1/1	0.95	0.08	42,42,42,42	0
56	MG	1A	3707	1/1	0.95	0.08	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	2A	3018	1/1	0.95	0.11	49,49,49,49	0
56	MG	1A	3449	1/1	0.95	0.15	32,32,32,32	0
56	MG	1A	3882	1/1	0.95	0.12	44,44,44,44	0
56	MG	1A	3262	1/1	0.95	0.18	59,59,59,59	0
56	MG	1a	1650	1/1	0.95	0.07	56,56,56,56	0
56	MG	1A	4079	1/1	0.95	0.08	53,53,53,53	0
56	MG	1A	3710	1/1	0.95	0.10	51,51,51,51	0
56	MG	1A	3348	1/1	0.95	0.14	41,41,41,41	0
56	MG	1A	3456	1/1	0.95	0.09	49,49,49,49	0
56	MG	2A	3030	1/1	0.95	0.07	46,46,46,46	0
56	MG	1A	4087	1/1	0.95	0.10	53,53,53,53	0
56	MG	1A	3192	1/1	0.95	0.11	25,25,25,25	0
56	MG	1A	3193	1/1	0.95	0.27	30,30,30,30	0
56	MG	2A	3616	1/1	0.95	0.07	63,63,63,63	0
56	MG	2A	3038	1/1	0.95	0.06	48,48,48,48	0
56	MG	20	102	1/1	0.95	0.06	65,65,65,65	0
56	MG	1A	3460	1/1	0.95	0.07	40,40,40,40	0
56	MG	1A	3718	1/1	0.95	0.06	31,31,31,31	0
56	MG	2A	3041	1/1	0.95	0.12	70,70,70,70	0
56	MG	1A	3088	1/1	0.95	0.13	37,37,37,37	0
56	MG	1A	4095	1/1	0.95	0.06	38,38,38,38	0
56	MG	1A	4096	1/1	0.95	0.09	46,46,46,46	0
56	MG	1A	4098	1/1	0.95	0.06	50,50,50,50	0
56	MG	2A	3627	1/1	0.95	0.06	44,44,44,44	0
56	MG	1A	3573	1/1	0.95	0.09	34,34,34,34	0
56	MG	1A	3044	1/1	0.95	0.06	29,29,29,29	0
56	MG	1A	3198	1/1	0.95	0.12	35,35,35,35	0
56	MG	1A	3055	1/1	0.95	0.05	23,23,23,23	0
56	MG	28	103	1/1	0.95	0.08	42,42,42,42	0
56	MG	2A	3632	1/1	0.95	0.13	39,39,39,39	0
56	MG	1A	3465	1/1	0.95	0.28	48,48,48,48	0
56	MG	1A	3277	1/1	0.95	0.18	44,44,44,44	0
56	MG	1A	3580	1/1	0.95	0.19	29,29,29,29	0
56	MG	1A	3735	1/1	0.95	0.07	45,45,45,45	0
56	MG	1B	209	1/1	0.95	0.09	47,47,47,47	0
56	MG	1A	3203	1/1	0.95	0.12	24,24,24,24	0
56	MG	1A	3907	1/1	0.95	0.05	48,48,48,48	0
56	MG	2A	3335	1/1	0.95	0.19	47,47,47,47	0
56	MG	2A	3064	1/1	0.95	0.16	48,48,48,48	0
56	MG	1A	3582	1/1	0.95	0.10	30,30,30,30	0
56	MG	1B	214	1/1	0.95	0.08	46,46,46,46	0
56	MG	2A	3646	1/1	0.95	0.07	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	3092	1/1	0.95	0.17	45,45,45,45	0
56	MG	1B	219	1/1	0.95	0.14	34,34,34,34	0
56	MG	2A	3070	1/1	0.95	0.06	56,56,56,56	0
56	MG	2a	3019	1/1	0.95	0.13	54,54,54,54	0
56	MG	1A	3093	1/1	0.95	0.14	51,51,51,51	0
56	MG	1A	3472	1/1	0.95	0.13	33,33,33,33	0
56	MG	2A	3654	1/1	0.95	0.17	57,57,57,57	0
56	MG	2A	3073	1/1	0.95	0.14	52,52,52,52	0
56	MG	1A	3363	1/1	0.95	0.08	51,51,51,51	0
56	MG	2A	3351	1/1	0.95	0.26	59,59,59,59	0
56	MG	1A	3591	1/1	0.95	0.17	35,35,35,35	0
56	MG	1A	3364	1/1	0.95	0.08	37,37,37,37	0
56	MG	2a	3029	1/1	0.95	0.09	40,40,40,40	0
56	MG	2A	3354	1/1	0.95	0.09	62,62,62,62	0
56	MG	1A	3919	1/1	0.95	0.11	30,30,30,30	0
56	MG	1B	227	1/1	0.95	0.07	60,60,60,60	0
56	MG	2a	3033	1/1	0.95	0.09	81,81,81,81	0
56	MG	1A	3475	1/1	0.95	0.10	48,48,48,48	0
56	MG	2a	3035	1/1	0.95	0.08	76,76,76,76	0
56	MG	2A	3081	1/1	0.95	0.16	52,52,52,52	0
56	MG	2A	3360	1/1	0.95	0.06	56,56,56,56	0
56	MG	2a	3038	1/1	0.95	0.23	53,53,53,53	0
56	MG	1A	3596	1/1	0.95	0.06	29,29,29,29	0
56	MG	1A	3597	1/1	0.95	0.07	49,49,49,49	0
56	MG	1A	3284	1/1	0.95	0.39	35,35,35,35	0
56	MG	1A	3926	1/1	0.95	0.05	28,28,28,28	0
56	MG	1B	235	1/1	0.95	0.12	47,47,47,47	0
56	MG	1A	3288	1/1	0.95	0.11	34,34,34,34	0
56	MG	2A	3090	1/1	0.95	0.09	45,45,45,45	0
56	MG	2A	3091	1/1	0.95	0.11	48,48,48,48	0
56	MG	1A	3765	1/1	0.95	0.12	43,43,43,43	0
56	MG	1A	3140	1/1	0.95	0.14	40,40,40,40	0
56	MG	1A	3370	1/1	0.95	0.11	40,40,40,40	0
56	MG	2A	3374	1/1	0.95	0.24	57,57,57,57	0
56	MG	1D	308	1/1	0.95	0.05	36,36,36,36	0
56	MG	1a	1702	1/1	0.95	0.23	53,53,53,53	0
56	MG	2A	3691	1/1	0.95	0.10	71,71,71,71	0
56	MG	1A	3371	1/1	0.95	0.13	46,46,46,46	0
56	MG	2a	3056	1/1	0.95	0.28	57,57,57,57	0
56	MG	1a	1704	1/1	0.95	0.27	60,60,60,60	0
56	MG	2A	3100	1/1	0.95	0.12	53,53,53,53	0
56	MG	2A	3101	1/1	0.95	0.10	35,35,35,35	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	2A	3103	1/1	0.95	0.16	58,58,58,58	0
56	MG	2A	3104	1/1	0.95	0.08	51,51,51,51	0
56	MG	1a	1705	1/1	0.95	0.14	56,56,56,56	0
56	MG	1A	3608	1/1	0.95	0.07	39,39,39,39	0
56	MG	2A	3109	1/1	0.95	0.13	39,39,39,39	0
56	MG	1A	3290	1/1	0.95	0.10	40,40,40,40	0
56	MG	1A	3610	1/1	0.95	0.09	44,44,44,44	0
56	MG	1E	307	1/1	0.95	0.13	57,57,57,57	0
56	MG	1A	3377	1/1	0.95	0.07	47,47,47,47	0
56	MG	1a	1711	1/1	0.95	0.08	39,39,39,39	0
56	MG	1A	3612	1/1	0.95	0.12	51,51,51,51	0
56	MG	2A	3398	1/1	0.95	0.18	58,58,58,58	0
56	MG	1A	3056	1/1	0.95	0.21	45,45,45,45	0
56	MG	1A	3616	1/1	0.95	0.09	19,19,19,19	0
56	MG	1E	314	1/1	0.95	0.14	30,30,30,30	0
56	MG	1A	3485	1/1	0.95	0.09	42,42,42,42	0
56	MG	1A	3950	1/1	0.95	0.08	55,55,55,55	0
56	MG	1a	1719	1/1	0.95	0.09	41,41,41,41	0
56	MG	1A	3058	1/1	0.95	0.06	32,32,32,32	0
56	MG	1A	3213	1/1	0.95	0.09	44,44,44,44	0
56	MG	2A	3132	1/1	0.95	0.06	36,36,36,36	0
56	MG	1F	310	1/1	0.95	0.11	41,41,41,41	0
56	MG	2A	3728	1/1	0.95	0.07	64,64,64,64	0
56	MG	1G	202	1/1	0.95	0.15	51,51,51,51	0
56	MG	2A	3411	1/1	0.95	0.06	46,46,46,46	0
56	MG	1A	3956	1/1	0.95	0.13	45,45,45,45	0
56	MG	2A	3141	1/1	0.95	0.23	39,39,39,39	0
56	MG	2a	3091	1/1	0.95	0.17	62,62,62,62	0
56	MG	1A	3488	1/1	0.95	0.07	33,33,33,33	0
56	MG	2A	3145	1/1	0.95	0.23	66,66,66,66	0
56	MG	2A	3147	1/1	0.95	0.22	31,31,31,31	0
56	MG	1A	3959	1/1	0.95	0.09	46,46,46,46	0
56	MG	1N	203	1/1	0.95	0.06	46,46,46,46	0
56	MG	1A	3787	1/1	0.95	0.06	44,44,44,44	0
56	MG	1A	3489	1/1	0.95	0.25	48,48,48,48	0
56	MG	1A	3060	1/1	0.95	0.09	39,39,39,39	0
56	MG	1A	3300	1/1	0.95	0.08	44,44,44,44	0
56	MG	1A	3965	1/1	0.95	0.06	49,49,49,49	0
56	MG	2a	3103	1/1	0.95	0.16	62,62,62,62	0
56	MG	1A	3387	1/1	0.95	0.12	48,48,48,48	0
56	MG	2A	3157	1/1	0.95	0.34	44,44,44,44	0
56	MG	2A	3747	1/1	0.95	0.11	66,66,66,66	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	1A	3027	1/1	0.95	0.14	71,71,71,71	0
56	MG	1A	3005	1/1	0.95	0.08	37,37,37,37	0
56	MG	1a	1741	1/1	0.95	0.25	60,60,60,60	0
56	MG	1A	3157	1/1	0.95	0.10	40,40,40,40	0
56	MG	2A	3752	1/1	0.95	0.10	54,54,54,54	0
56	MG	1A	3228	1/1	0.95	0.10	32,32,32,32	0
56	MG	1A	3063	1/1	0.95	0.11	43,43,43,43	0
56	MG	1A	3395	1/1	0.95	0.13	40,40,40,40	0
56	MG	1A	3803	1/1	0.95	0.05	26,26,26,26	0
56	MG	1A	3038	1/1	0.95	0.13	30,30,30,30	0
56	MG	1A	3235	1/1	0.95	0.07	59,59,59,59	0
56	MG	2A	3168	1/1	0.95	0.08	53,53,53,53	0
56	MG	1A	3508	1/1	0.95	0.16	23,23,23,23	0
56	MG	1A	3983	1/1	0.95	0.06	64,64,64,64	0
56	MG	1T	202	1/1	0.95	0.10	45,45,45,45	0
56	MG	1T	203	1/1	0.95	0.07	53,53,53,53	0
56	MG	1A	3811	1/1	0.95	0.10	49,49,49,49	0
56	MG	1A	3313	1/1	0.95	0.09	39,39,39,39	0
56	MG	2a	3125	1/1	0.95	0.10	64,64,64,64	0
56	MG	1U	202	1/1	0.95	0.11	27,27,27,27	0
56	MG	2A	3451	1/1	0.95	0.21	37,37,37,37	0
56	MG	1U	206	1/1	0.95	0.07	33,33,33,33	0
56	MG	1A	3652	1/1	0.95	0.09	31,31,31,31	0
56	MG	1U	212	1/1	0.95	0.10	37,37,37,37	0
56	MG	1A	3987	1/1	0.95	0.08	50,50,50,50	0
56	MG	2A	3456	1/1	0.95	0.14	61,61,61,61	0
56	MG	2A	3183	1/1	0.95	0.12	52,52,52,52	0
56	MG	2A	3780	1/1	0.95	0.07	69,69,69,69	0
56	MG	2A	3184	1/1	0.95	0.09	41,41,41,41	0
56	MG	2a	3142	1/1	0.95	0.06	68,68,68,68	0
56	MG	1A	3110	1/1	0.95	0.13	26,26,26,26	0
56	MG	1A	3315	1/1	0.95	0.08	51,51,51,51	0
56	MG	1W	201	1/1	0.95	0.18	49,49,49,49	0
56	MG	2a	3148	1/1	0.95	0.07	63,63,63,63	0
56	MG	1A	3655	1/1	0.95	0.07	58,58,58,58	0
56	MG	1X	103	1/1	0.95	0.13	37,37,37,37	0
56	MG	2A	3464	1/1	0.95	0.23	63,63,63,63	0
56	MG	1A	3239	1/1	0.95	0.14	25,25,25,25	0
56	MG	1A	3821	1/1	0.95	0.06	26,26,26,26	0
56	MG	2a	3157	1/1	0.95	0.08	57,57,57,57	0
56	MG	1A	3069	1/1	0.95	0.11	28,28,28,28	0
56	MG	2A	3797	1/1	0.95	0.05	40,40,40,40	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	1A	3166	1/1	0.95	0.16	34,34,34,34	0
56	MG	1A	3321	1/1	0.95	0.17	48,48,48,48	0
56	MG	1A	3520	1/1	0.95	0.11	56,56,56,56	0
56	MG	1A	3829	1/1	0.95	0.11	32,32,32,32	0
56	MG	10	103	1/1	0.95	0.07	32,32,32,32	0
56	MG	1A	3831	1/1	0.95	0.08	37,37,37,37	0
56	MG	10	105	1/1	0.95	0.09	53,53,53,53	0
56	MG	1A	3322	1/1	0.95	0.05	43,43,43,43	0
56	MG	2A	3208	1/1	0.95	0.08	53,53,53,53	0
56	MG	1A	3833	1/1	0.95	0.07	55,55,55,55	0
56	MG	2A	3481	1/1	0.95	0.22	60,60,60,60	0
56	MG	2A	3482	1/1	0.95	0.22	42,42,42,42	0
56	MG	1A	3168	1/1	0.95	0.24	40,40,40,40	0
56	MG	1A	3415	1/1	0.95	0.07	40,40,40,40	0
56	MG	1A	3670	1/1	0.95	0.09	28,28,28,28	0
56	MG	1A	3671	1/1	0.95	0.06	29,29,29,29	0
56	MG	1a	1806	1/1	0.95	0.09	59,59,59,59	0
56	MG	2A	3488	1/1	0.95	0.08	56,56,56,56	0
56	MG	1A	3246	1/1	0.95	0.16	50,50,50,50	0
56	MG	2A	3218	1/1	0.95	0.23	35,35,35,35	0
56	MG	1A	3326	1/1	0.95	0.06	48,48,48,48	0
56	MG	1A	3841	1/1	0.95	0.09	39,39,39,39	0
56	MG	1a	1817	1/1	0.95	0.07	58,58,58,58	0
56	MG	2A	3224	1/1	0.95	0.13	49,49,49,49	0
56	MG	1A	4014	1/1	0.95	0.06	46,46,46,46	0
56	MG	1a	1819	1/1	0.95	0.09	68,68,68,68	0
56	MG	15	104	1/1	0.95	0.08	42,42,42,42	0
56	MG	2A	3500	1/1	0.95	0.07	55,55,55,55	0
56	MG	1A	3327	1/1	0.95	0.19	36,36,36,36	0
56	MG	2A	3835	1/1	0.95	0.08	34,34,34,34	0
56	MG	1A	3174	1/1	0.95	0.20	27,27,27,27	0
56	MG	16	103	1/1	0.95	0.07	51,51,51,51	0
56	MG	1A	3679	1/1	0.95	0.07	34,34,34,34	0
56	MG	2A	3506	1/1	0.95	0.08	36,36,36,36	0
56	MG	2a	3207	1/1	0.95	0.09	62,62,62,62	0
56	MG	2A	3842	1/1	0.95	0.07	42,42,42,42	0
56	MG	17	107	1/1	0.95	0.16	49,49,49,49	0
56	MG	2a	3213	1/1	0.95	0.13	75,75,75,75	0
56	MG	2a	3214	1/1	0.95	0.16	74,74,74,74	0
56	MG	2A	3846	1/1	0.95	0.09	62,62,62,62	0
56	MG	1A	3248	1/1	0.95	0.19	51,51,51,51	0
56	MG	2A	3850	1/1	0.95	0.11	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	2A	3851	1/1	0.95	0.10	39,39,39,39	0
56	MG	2A	3238	1/1	0.95	0.11	45,45,45,45	0
56	MG	18	102	1/1	0.95	0.19	41,41,41,41	0
56	MG	1A	3681	1/1	0.95	0.10	47,47,47,47	0
56	MG	2a	3222	1/1	0.95	0.19	55,55,55,55	0
56	MG	1A	4021	1/1	0.95	0.06	32,32,32,32	0
56	MG	1A	3249	1/1	0.95	0.19	42,42,42,42	0
56	MG	1A	4024	1/1	0.95	0.11	70,70,70,70	0
56	MG	2A	3244	1/1	0.95	0.10	43,43,43,43	0
56	MG	2A	3519	1/1	0.95	0.09	33,33,33,33	0
56	MG	1f	201	1/1	0.95	0.15	44,44,44,44	0
56	MG	2A	3872	1/1	0.95	0.10	48,48,48,48	0
56	MG	2A	3246	1/1	0.95	0.11	49,49,49,49	0
56	MG	19	101	1/1	0.95	0.06	34,34,34,34	0
56	MG	1h	201	1/1	0.95	0.07	58,58,58,58	0
56	MG	2A	3528	1/1	0.95	0.08	59,59,59,59	0
56	MG	2A	3249	1/1	0.95	0.08	55,55,55,55	0
56	MG	2A	3879	1/1	0.95	0.16	47,47,47,47	0
56	MG	1m	3002	1/1	0.95	0.09	56,56,56,56	0
56	MG	1n	101	1/1	0.95	0.09	54,54,54,54	0
56	MG	1a	1601	1/1	0.95	0.08	42,42,42,42	0
56	MG	2A	3535	1/1	0.95	0.11	51,51,51,51	0
56	MG	1A	3850	1/1	0.95	0.16	47,47,47,47	0
56	MG	1A	3250	1/1	0.95	0.11	36,36,36,36	0
56	MG	1A	3112	1/1	0.95	0.16	35,35,35,35	0
56	MG	1A	3114	1/1	0.95	0.08	32,32,32,32	0
56	MG	1A	3001	1/1	0.95	0.17	39,39,39,39	0
56	MG	2A	3258	1/1	0.95	0.06	67,67,67,67	0
56	MG	1A	4038	1/1	0.95	0.07	52,52,52,52	0
56	MG	1A	3337	1/1	0.95	0.18	37,37,37,37	0
56	MG	1A	3255	1/1	0.95	0.07	29,29,29,29	0
56	MG	2l	201	1/1	0.95	0.09	55,55,55,55	0
56	MG	2l	202	1/1	0.95	0.07	64,64,64,64	0
56	MG	2A	3263	1/1	0.95	0.39	71,71,71,71	0
56	MG	1a	1612	1/1	0.95	0.08	62,62,62,62	0
56	MG	1A	3859	1/1	0.95	0.24	38,38,38,38	0
56	MG	2A	3266	1/1	0.95	0.10	59,59,59,59	0
56	MG	1A	3860	1/1	0.95	0.17	36,36,36,36	0
56	MG	1A	3082	1/1	0.95	0.16	33,33,33,33	0
56	MG	2A	3559	1/1	0.95	0.10	53,53,53,53	0
56	MG	1A	3863	1/1	0.95	0.07	34,34,34,34	0
56	MG	2A	3270	1/1	0.95	0.19	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	3120	1/1	0.95	0.09	36,36,36,36	0
56	MG	1a	1620	1/1	0.95	0.19	55,55,55,55	0
56	MG	1A	3439	1/1	0.95	0.09	44,44,44,44	0
56	MG	1A	3698	1/1	0.95	0.13	28,28,28,28	0
56	MG	1A	4055	1/1	0.95	0.07	41,41,41,41	0
56	MG	2A	3277	1/1	0.95	0.06	58,58,58,58	0
56	MG	2D	303	1/1	0.95	0.18	42,42,42,42	0
56	MG	1A	3040	1/1	0.95	0.05	30,30,30,30	0
56	MG	2y	101	1/1	0.95	0.26	60,60,60,60	0
56	MG	1A	3443	1/1	0.95	0.10	49,49,49,49	0
56	MG	1A	3259	1/1	0.95	0.06	38,38,38,38	0
56	MG	1A	3260	1/1	0.95	0.09	47,47,47,47	0
56	MG	1A	3553	1/1	0.95	0.22	45,45,45,45	0
57	CLM	1A	4102	20/20	0.95	0.09	18,29,44,60	0
57	CLM	2A	3888	20/20	0.95	0.10	38,45,57,61	0
56	MG	1A	3872	1/1	0.95	0.15	33,33,33,33	0
59	ZN	2n	501	1/1	0.95	0.07	107,107,107,107	0
56	MG	1A	3569	1/1	0.96	0.11	42,42,42,42	0
56	MG	1A	3571	1/1	0.96	0.27	29,29,29,29	0
56	MG	1A	3842	1/1	0.96	0.08	31,31,31,31	0
56	MG	1A	3389	1/1	0.96	0.14	23,23,23,23	0
56	MG	1A	3138	1/1	0.96	0.15	28,28,28,28	0
56	MG	1A	3476	1/1	0.96	0.05	40,40,40,40	0
56	MG	1A	3080	1/1	0.96	0.14	47,47,47,47	0
56	MG	1A	3196	1/1	0.96	0.07	38,38,38,38	0
56	MG	1P	208	1/1	0.96	0.17	42,42,42,42	0
56	MG	1A	3393	1/1	0.96	0.07	43,43,43,43	0
56	MG	1Q	201	1/1	0.96	0.29	42,42,42,42	0
56	MG	2A	3082	1/1	0.96	0.06	43,43,43,43	0
56	MG	2A	3336	1/1	0.96	0.14	62,62,62,62	0
56	MG	1A	4003	1/1	0.96	0.08	42,42,42,42	0
56	MG	2A	3084	1/1	0.96	0.06	46,46,46,46	0
56	MG	1a	1713	1/1	0.96	0.07	50,50,50,50	0
56	MG	2A	3340	1/1	0.96	0.09	53,53,53,53	0
56	MG	1A	3849	1/1	0.96	0.07	52,52,52,52	0
56	MG	2A	3625	1/1	0.96	0.12	57,57,57,57	0
56	MG	2A	3626	1/1	0.96	0.10	33,33,33,33	0
56	MG	2A	3342	1/1	0.96	0.17	55,55,55,55	0
56	MG	1Q	206	1/1	0.96	0.06	51,51,51,51	0
56	MG	2A	3344	1/1	0.96	0.12	48,48,48,48	0
56	MG	2A	3345	1/1	0.96	0.07	39,39,39,39	0
56	MG	1A	3197	1/1	0.96	0.22	38,38,38,38	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	1R	201	1/1	0.96	0.15	32,32,32,32	0
56	MG	1A	3579	1/1	0.96	0.10	21,21,21,21	0
56	MG	1A	3325	1/1	0.96	0.22	26,26,26,26	0
56	MG	2A	3635	1/1	0.96	0.07	61,61,61,61	0
56	MG	1A	3105	1/1	0.96	0.18	30,30,30,30	0
56	MG	1A	3029	1/1	0.96	0.09	23,23,23,23	0
56	MG	25	102	1/1	0.96	0.27	50,50,50,50	0
56	MG	1A	3856	1/1	0.96	0.05	16,16,16,16	0
56	MG	1A	3583	1/1	0.96	0.07	44,44,44,44	0
56	MG	1a	1725	1/1	0.96	0.12	42,42,42,42	0
56	MG	1A	3108	1/1	0.96	0.13	36,36,36,36	0
56	MG	1A	3149	1/1	0.96	0.15	29,29,29,29	0
56	MG	1A	3109	1/1	0.96	0.27	31,31,31,31	0
56	MG	1A	3588	1/1	0.96	0.33	36,36,36,36	0
56	MG	2A	3102	1/1	0.96	0.10	59,59,59,59	0
56	MG	1U	205	1/1	0.96	0.40	38,38,38,38	0
56	MG	1A	3059	1/1	0.96	0.16	47,47,47,47	0
56	MG	2A	3105	1/1	0.96	0.10	57,57,57,57	0
56	MG	2a	3004	1/1	0.96	0.24	51,51,51,51	0
56	MG	1A	3715	1/1	0.96	0.09	48,48,48,48	0
56	MG	2A	3366	1/1	0.96	0.19	60,60,60,60	0
56	MG	1A	3590	1/1	0.96	0.10	26,26,26,26	0
56	MG	2A	3655	1/1	0.96	0.15	56,56,56,56	0
56	MG	1A	4023	1/1	0.96	0.05	30,30,30,30	0
56	MG	1A	3030	1/1	0.96	0.25	32,32,32,32	0
56	MG	2A	3111	1/1	0.96	0.11	59,59,59,59	0
56	MG	2A	3660	1/1	0.96	0.06	33,33,33,33	0
56	MG	1A	4027	1/1	0.96	0.18	65,65,65,65	0
56	MG	1a	1738	1/1	0.96	0.07	57,57,57,57	0
56	MG	1A	3720	1/1	0.96	0.15	44,44,44,44	0
56	MG	1a	1740	1/1	0.96	0.15	43,43,43,43	0
56	MG	2A	3667	1/1	0.96	0.13	57,57,57,57	0
56	MG	2A	3375	1/1	0.96	0.09	64,64,64,64	0
56	MG	1W	202	1/1	0.96	0.15	50,50,50,50	0
56	MG	1A	3210	1/1	0.96	0.08	35,35,35,35	0
56	MG	2A	3672	1/1	0.96	0.06	51,51,51,51	0
56	MG	1W	205	1/1	0.96	0.05	39,39,39,39	0
56	MG	1A	3405	1/1	0.96	0.07	52,52,52,52	0
56	MG	1A	3334	1/1	0.96	0.18	43,43,43,43	0
56	MG	1a	1749	1/1	0.96	0.10	33,33,33,33	0
56	MG	2A	3677	1/1	0.96	0.05	51,51,51,51	0
56	MG	1a	1750	1/1	0.96	0.05	39,39,39,39	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	1A	4035	1/1	0.96	0.06	64,64,64,64	0
56	MG	2A	3126	1/1	0.96	0.11	44,44,44,44	0
56	MG	2A	3385	1/1	0.96	0.17	53,53,53,53	0
56	MG	2A	3129	1/1	0.96	0.09	54,54,54,54	0
56	MG	2A	3388	1/1	0.96	0.09	62,62,62,62	0
56	MG	2A	3130	1/1	0.96	0.09	54,54,54,54	0
56	MG	1A	4036	1/1	0.96	0.09	41,41,41,41	0
56	MG	1Y	203	1/1	0.96	0.13	47,47,47,47	0
56	MG	2A	3134	1/1	0.96	0.05	39,39,39,39	0
56	MG	2A	3689	1/1	0.96	0.06	59,59,59,59	0
56	MG	1A	3211	1/1	0.96	0.18	34,34,34,34	0
56	MG	2A	3136	1/1	0.96	0.10	38,38,38,38	0
56	MG	1A	3598	1/1	0.96	0.11	35,35,35,35	0
56	MG	1a	1756	1/1	0.96	0.11	54,54,54,54	0
56	MG	1A	3412	1/1	0.96	0.07	38,38,38,38	0
56	MG	2A	3143	1/1	0.96	0.12	47,47,47,47	0
56	MG	1A	4040	1/1	0.96	0.12	47,47,47,47	0
56	MG	1a	1761	1/1	0.96	0.10	51,51,51,51	0
56	MG	2A	3146	1/1	0.96	0.17	38,38,38,38	0
56	MG	1A	3732	1/1	0.96	0.08	61,61,61,61	0
56	MG	1A	3495	1/1	0.96	0.18	47,47,47,47	0
56	MG	1a	1764	1/1	0.96	0.07	58,58,58,58	0
56	MG	2A	3407	1/1	0.96	0.09	57,57,57,57	0
56	MG	1A	3878	1/1	0.96	0.22	30,30,30,30	0
56	MG	10	106	1/1	0.96	0.06	49,49,49,49	0
56	MG	2a	3055	1/1	0.96	0.07	60,60,60,60	0
56	MG	11	101	1/1	0.96	0.21	33,33,33,33	0
56	MG	1A	3879	1/1	0.96	0.10	36,36,36,36	0
56	MG	1a	1771	1/1	0.96	0.07	40,40,40,40	0
56	MG	2A	3413	1/1	0.96	0.11	55,55,55,55	0
56	MG	1A	3413	1/1	0.96	0.06	37,37,37,37	0
56	MG	2a	3061	1/1	0.96	0.04	53,53,53,53	0
56	MG	1A	3158	1/1	0.96	0.12	60,60,60,60	0
56	MG	1A	3606	1/1	0.96	0.05	36,36,36,36	0
56	MG	1A	3738	1/1	0.96	0.09	45,45,45,45	0
56	MG	2A	3719	1/1	0.96	0.06	60,60,60,60	0
56	MG	1A	3273	1/1	0.96	0.26	35,35,35,35	0
56	MG	13	101	1/1	0.96	0.09	26,26,26,26	0
56	MG	13	102	1/1	0.96	0.07	38,38,38,38	0
56	MG	1A	3500	1/1	0.96	0.17	37,37,37,37	0
56	MG	1A	3502	1/1	0.96	0.07	47,47,47,47	0
56	MG	2A	3727	1/1	0.96	0.16	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	15	101	1/1	0.96	0.18	31,31,31,31	0
56	MG	1A	3743	1/1	0.96	0.07	22,22,22,22	0
56	MG	1A	3744	1/1	0.96	0.07	50,50,50,50	0
56	MG	1A	3745	1/1	0.96	0.05	14,14,14,14	0
56	MG	1A	3043	1/1	0.96	0.13	33,33,33,33	0
56	MG	1A	4062	1/1	0.96	0.06	32,32,32,32	0
56	MG	1a	1791	1/1	0.96	0.06	64,64,64,64	0
56	MG	1A	3113	1/1	0.96	0.10	37,37,37,37	0
56	MG	1a	1794	1/1	0.96	0.07	60,60,60,60	0
56	MG	2A	3436	1/1	0.96	0.06	41,41,41,41	0
56	MG	2A	3174	1/1	0.96	0.25	56,56,56,56	0
56	MG	2A	3740	1/1	0.96	0.05	67,67,67,67	0
56	MG	17	101	1/1	0.96	0.09	31,31,31,31	0
56	MG	17	102	1/1	0.96	0.07	32,32,32,32	0
56	MG	1A	4066	1/1	0.96	0.05	24,24,24,24	0
56	MG	17	105	1/1	0.96	0.12	37,37,37,37	0
56	MG	2A	3180	1/1	0.96	0.19	47,47,47,47	0
56	MG	1A	3024	1/1	0.96	0.08	43,43,43,43	0
56	MG	1A	3749	1/1	0.96	0.05	30,30,30,30	0
56	MG	2A	3445	1/1	0.96	0.32	60,60,60,60	0
56	MG	1A	4069	1/1	0.96	0.05	20,20,20,20	0
56	MG	1A	4070	1/1	0.96	0.05	52,52,52,52	0
56	MG	1a	1808	1/1	0.96	0.06	50,50,50,50	0
56	MG	1A	3750	1/1	0.96	0.07	34,34,34,34	0
56	MG	2a	3099	1/1	0.96	0.09	52,52,52,52	0
56	MG	1a	1810	1/1	0.96	0.06	59,59,59,59	0
56	MG	1A	4072	1/1	0.96	0.07	48,48,48,48	0
56	MG	1a	1815	1/1	0.96	0.11	66,66,66,66	0
56	MG	2A	3193	1/1	0.96	0.31	63,63,63,63	0
56	MG	1A	3751	1/1	0.96	0.10	42,42,42,42	0
56	MG	2A	3195	1/1	0.96	0.05	44,44,44,44	0
56	MG	2A	3760	1/1	0.96	0.13	54,54,54,54	0
56	MG	1A	3219	1/1	0.96	0.11	32,32,32,32	0
56	MG	1A	3507	1/1	0.96	0.15	42,42,42,42	0
56	MG	1a	1821	1/1	0.96	0.05	53,53,53,53	0
56	MG	1A	3903	1/1	0.96	0.10	45,45,45,45	0
56	MG	1A	3617	1/1	0.96	0.05	36,36,36,36	0
56	MG	1A	3619	1/1	0.96	0.11	41,41,41,41	0
56	MG	1A	3620	1/1	0.96	0.08	52,52,52,52	0
56	MG	1A	3343	1/1	0.96	0.14	47,47,47,47	0
56	MG	2A	3769	1/1	0.96	0.10	39,39,39,39	0
56	MG	1A	3423	1/1	0.96	0.14	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	2A	3465	1/1	0.96	0.13	48,48,48,48	0
56	MG	1a	1608	1/1	0.96	0.17	45,45,45,45	0
56	MG	1A	4085	1/1	0.96	0.08	17,17,17,17	0
56	MG	1a	1610	1/1	0.96	0.06	23,23,23,23	0
56	MG	1A	3511	1/1	0.96	0.06	36,36,36,36	0
56	MG	1A	3282	1/1	0.96	0.26	38,38,38,38	0
56	MG	2A	3471	1/1	0.96	0.06	32,32,32,32	0
56	MG	1A	3912	1/1	0.96	0.16	31,31,31,31	0
56	MG	2A	3783	1/1	0.96	0.08	58,58,58,58	0
56	MG	1a	1614	1/1	0.96	0.11	58,58,58,58	0
56	MG	1a	1615	1/1	0.96	0.06	43,43,43,43	0
56	MG	2A	3787	1/1	0.96	0.06	72,72,72,72	0
56	MG	2a	3131	1/1	0.96	0.35	60,60,60,60	0
56	MG	1A	3003	1/1	0.96	0.04	19,19,19,19	0
56	MG	1m	3001	1/1	0.96	0.09	54,54,54,54	0
56	MG	2A	3790	1/1	0.96	0.07	61,61,61,61	0
56	MG	1A	3426	1/1	0.96	0.14	44,44,44,44	0
56	MG	1A	3427	1/1	0.96	0.10	43,43,43,43	0
56	MG	2a	3137	1/1	0.96	0.11	75,75,75,75	0
56	MG	1A	4094	1/1	0.96	0.12	47,47,47,47	0
56	MG	2a	3139	1/1	0.96	0.07	70,70,70,70	0
56	MG	2A	3223	1/1	0.96	0.15	45,45,45,45	0
56	MG	1A	3516	1/1	0.96	0.11	40,40,40,40	0
56	MG	2a	3143	1/1	0.96	0.06	75,75,75,75	0
56	MG	1A	3636	1/1	0.96	0.06	16,16,16,16	0
56	MG	1A	3638	1/1	0.96	0.07	40,40,40,40	0
56	MG	1A	3223	1/1	0.96	0.16	46,46,46,46	0
56	MG	2A	3800	1/1	0.96	0.05	78,78,78,78	0
56	MG	2a	3149	1/1	0.96	0.06	76,76,76,76	0
56	MG	1A	3429	1/1	0.96	0.05	44,44,44,44	0
56	MG	1A	4101	1/1	0.96	0.07	53,53,53,53	0
56	MG	1A	3777	1/1	0.96	0.06	46,46,46,46	0
56	MG	1a	1628	1/1	0.96	0.15	47,47,47,47	0
56	MG	1A	3925	1/1	0.96	0.07	39,39,39,39	0
56	MG	1A	3778	1/1	0.96	0.10	20,20,20,20	0
56	MG	2A	3807	1/1	0.96	0.07	65,65,65,65	0
56	MG	1B	204	1/1	0.96	0.18	42,42,42,42	0
56	MG	1B	205	1/1	0.96	0.05	47,47,47,47	0
56	MG	1A	3286	1/1	0.96	0.15	42,42,42,42	0
56	MG	1x	102	1/1	0.96	0.16	46,46,46,46	0
56	MG	1x	103	1/1	0.96	0.16	48,48,48,48	0
56	MG	2a	3169	1/1	0.96	0.09	77,77,77,77	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	2A	3814	1/1	0.96	0.10	60,60,60,60	0
56	MG	1A	3022	1/1	0.96	0.08	34,34,34,34	0
56	MG	1x	105	1/1	0.96	0.04	49,49,49,49	0
56	MG	1a	1636	1/1	0.96	0.10	49,49,49,49	0
56	MG	1A	3434	1/1	0.96	0.13	40,40,40,40	0
56	MG	1A	3227	1/1	0.96	0.13	37,37,37,37	0
56	MG	2A	3820	1/1	0.96	0.08	73,73,73,73	0
56	MG	2A	3504	1/1	0.96	0.16	49,49,49,49	0
56	MG	1B	210	1/1	0.96	0.23	51,51,51,51	0
56	MG	1A	3786	1/1	0.96	0.06	24,24,24,24	0
56	MG	1A	3167	1/1	0.96	0.07	38,38,38,38	0
56	MG	1A	3352	1/1	0.96	0.35	41,41,41,41	0
56	MG	1a	1645	1/1	0.96	0.17	52,52,52,52	0
56	MG	1A	3790	1/1	0.96	0.08	19,19,19,19	0
56	MG	1A	3648	1/1	0.96	0.07	30,30,30,30	0
56	MG	1B	218	1/1	0.96	0.08	39,39,39,39	0
56	MG	2a	3189	1/1	0.96	0.15	57,57,57,57	0
56	MG	1A	3230	1/1	0.96	0.07	36,36,36,36	0
56	MG	2a	3191	1/1	0.96	0.18	71,71,71,71	0
56	MG	1a	1652	1/1	0.96	0.07	48,48,48,48	0
56	MG	1A	3943	1/1	0.96	0.05	38,38,38,38	0
56	MG	1A	3066	1/1	0.96	0.06	29,29,29,29	0
56	MG	2a	3195	1/1	0.96	0.17	52,52,52,52	0
56	MG	2A	3521	1/1	0.96	0.08	38,38,38,38	0
56	MG	2A	3522	1/1	0.96	0.06	41,41,41,41	0
56	MG	2A	3523	1/1	0.96	0.09	42,42,42,42	0
56	MG	1A	3293	1/1	0.96	0.19	42,42,42,42	0
56	MG	1A	3169	1/1	0.96	0.14	49,49,49,49	0
56	MG	1A	3170	1/1	0.96	0.07	47,47,47,47	0
56	MG	1A	3799	1/1	0.96	0.05	38,38,38,38	0
56	MG	2A	3849	1/1	0.96	0.07	63,63,63,63	0
56	MG	1A	3236	1/1	0.96	0.20	30,30,30,30	0
56	MG	2A	3013	1/1	0.96	0.11	50,50,50,50	0
56	MG	2A	3852	1/1	0.96	0.06	53,53,53,53	0
56	MG	1A	3657	1/1	0.96	0.05	44,44,44,44	0
56	MG	1A	3659	1/1	0.96	0.08	24,24,24,24	0
56	MG	1a	1663	1/1	0.96	0.10	52,52,52,52	0
56	MG	1B	231	1/1	0.96	0.08	39,39,39,39	0
56	MG	1A	3237	1/1	0.96	0.14	30,30,30,30	0
56	MG	2A	3861	1/1	0.96	0.06	62,62,62,62	0
56	MG	1A	3960	1/1	0.96	0.11	50,50,50,50	0
56	MG	2A	3866	1/1	0.96	0.13	38,38,38,38	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	2A	3273	1/1	0.96	0.10	49,49,49,49	0
56	MG	1A	3172	1/1	0.96	0.05	36,36,36,36	0
56	MG	2A	3023	1/1	0.96	0.22	51,51,51,51	0
56	MG	2A	3870	1/1	0.96	0.10	42,42,42,42	0
56	MG	2A	3871	1/1	0.96	0.07	39,39,39,39	0
56	MG	1A	3067	1/1	0.96	0.04	32,32,32,32	0
56	MG	2A	3544	1/1	0.96	0.07	35,35,35,35	0
56	MG	2A	3545	1/1	0.96	0.12	35,35,35,35	0
56	MG	1A	3049	1/1	0.96	0.20	39,39,39,39	0
56	MG	1A	3451	1/1	0.96	0.17	42,42,42,42	0
56	MG	1A	3543	1/1	0.96	0.20	34,34,34,34	0
56	MG	2A	3028	1/1	0.96	0.24	48,48,48,48	0
56	MG	1D	301	1/1	0.96	0.06	34,34,34,34	0
56	MG	1A	3308	1/1	0.96	0.14	32,32,32,32	0
56	MG	2A	3554	1/1	0.96	0.07	49,49,49,49	0
56	MG	2A	3032	1/1	0.96	0.08	47,47,47,47	0
56	MG	1A	3097	1/1	0.96	0.14	35,35,35,35	0
56	MG	1A	3368	1/1	0.96	0.06	37,37,37,37	0
56	MG	2A	3036	1/1	0.96	0.05	28,28,28,28	0
56	MG	2A	3560	1/1	0.96	0.10	38,38,38,38	0
56	MG	1D	311	1/1	0.96	0.06	50,50,50,50	0
56	MG	1A	3970	1/1	0.96	0.07	20,20,20,20	0
56	MG	1A	3369	1/1	0.96	0.10	44,44,44,44	0
56	MG	1E	302	1/1	0.96	0.16	47,47,47,47	0
56	MG	1A	3818	1/1	0.96	0.07	42,42,42,42	0
56	MG	1a	1681	1/1	0.96	0.08	56,56,56,56	0
56	MG	2A	3044	1/1	0.96	0.12	59,59,59,59	0
56	MG	2A	3296	1/1	0.96	0.10	50,50,50,50	0
56	MG	1a	1682	1/1	0.96	0.20	40,40,40,40	0
56	MG	1A	3673	1/1	0.96	0.09	17,17,17,17	0
56	MG	1A	3129	1/1	0.96	0.17	47,47,47,47	0
56	MG	1A	3978	1/1	0.96	0.09	36,36,36,36	0
56	MG	1A	3550	1/1	0.96	0.18	40,40,40,40	0
56	MG	1A	3311	1/1	0.96	0.15	40,40,40,40	0
56	MG	1A	3552	1/1	0.96	0.14	27,27,27,27	0
56	MG	1A	3072	1/1	0.96	0.22	31,31,31,31	0
56	MG	2A	3579	1/1	0.96	0.07	45,45,45,45	0
56	MG	1A	3375	1/1	0.96	0.14	42,42,42,42	0
56	MG	2A	3055	1/1	0.96	0.21	53,53,53,53	0
56	MG	2D	301	1/1	0.96	0.10	47,47,47,47	0
56	MG	2A	3056	1/1	0.96	0.21	59,59,59,59	0
56	MG	2A	3057	1/1	0.96	0.15	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	1A	3185	1/1	0.96	0.06	37,37,37,37	0
56	MG	1A	3057	1/1	0.96	0.06	28,28,28,28	0
56	MG	1A	3078	1/1	0.96	0.08	31,31,31,31	0
56	MG	2A	3593	1/1	0.96	0.09	46,46,46,46	0
56	MG	2A	3061	1/1	0.96	0.08	63,63,63,63	0
56	MG	1A	3316	1/1	0.96	0.06	40,40,40,40	0
56	MG	1A	3134	1/1	0.96	0.07	41,41,41,41	0
56	MG	1A	3102	1/1	0.96	0.07	46,46,46,46	0
56	MG	1I	201	1/1	0.96	0.07	61,61,61,61	0
56	MG	2F	301	1/1	0.96	0.08	46,46,46,46	0
56	MG	1A	3319	1/1	0.96	0.16	51,51,51,51	0
56	MG	2A	3067	1/1	0.96	0.09	30,30,30,30	0
56	MG	1N	202	1/1	0.96	0.07	42,42,42,42	0
56	MG	2F	305	1/1	0.96	0.08	43,43,43,43	0
56	MG	1A	3137	1/1	0.96	0.09	27,27,27,27	0
56	MG	2A	3322	1/1	0.96	0.14	48,48,48,48	0
56	MG	1A	3242	1/1	0.97	0.15	22,22,22,22	0
56	MG	1A	3025	1/1	0.97	0.06	30,30,30,30	0
56	MG	2a	3016	1/1	0.97	0.06	52,52,52,52	0
56	MG	1A	3244	1/1	0.97	0.10	42,42,42,42	0
56	MG	1A	3077	1/1	0.97	0.11	35,35,35,35	0
56	MG	17	106	1/1	0.97	0.13	25,25,25,25	0
56	MG	1A	3492	1/1	0.97	0.05	33,33,33,33	0
56	MG	17	108	1/1	0.97	0.06	45,45,45,45	0
56	MG	1A	3820	1/1	0.97	0.04	18,18,18,18	0
56	MG	1A	3421	1/1	0.97	0.14	32,32,32,32	0
56	MG	2A	3494	1/1	0.97	0.06	67,67,67,67	0
56	MG	2A	3080	1/1	0.97	0.15	56,56,56,56	0
56	MG	1A	3299	1/1	0.97	0.05	30,30,30,30	0
56	MG	2A	3288	1/1	0.97	0.08	36,36,36,36	0
56	MG	1A	3692	1/1	0.97	0.08	55,55,55,55	0
56	MG	2A	3290	1/1	0.97	0.08	36,36,36,36	0
56	MG	1A	3824	1/1	0.97	0.05	30,30,30,30	0
56	MG	1A	3094	1/1	0.97	0.07	20,20,20,20	0
56	MG	1A	3695	1/1	0.97	0.03	25,25,25,25	0
56	MG	1A	3828	1/1	0.97	0.10	45,45,45,45	0
56	MG	1a	1770	1/1	0.97	0.05	49,49,49,49	0
56	MG	1A	3301	1/1	0.97	0.05	24,24,24,24	0
56	MG	1B	220	1/1	0.97	0.05	32,32,32,32	0
56	MG	1a	1773	1/1	0.97	0.09	54,54,54,54	0
56	MG	1A	3135	1/1	0.97	0.09	23,23,23,23	0
56	MG	1A	3206	1/1	0.97	0.10	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	3045	1/1	0.97	0.04	28,28,28,28	0
56	MG	1A	3037	1/1	0.97	0.09	32,32,32,32	0
56	MG	1a	1778	1/1	0.97	0.09	55,55,55,55	0
56	MG	1A	3362	1/1	0.97	0.06	35,35,35,35	0
56	MG	1A	3430	1/1	0.97	0.06	47,47,47,47	0
56	MG	1a	1781	1/1	0.97	0.10	75,75,75,75	0
56	MG	2A	3520	1/1	0.97	0.09	49,49,49,49	0
56	MG	1A	3013	1/1	0.97	0.12	26,26,26,26	0
56	MG	1a	1783	1/1	0.97	0.10	57,57,57,57	0
56	MG	1B	228	1/1	0.97	0.05	42,42,42,42	0
56	MG	1A	3432	1/1	0.97	0.19	36,36,36,36	0
56	MG	1A	3593	1/1	0.97	0.25	27,27,27,27	0
56	MG	1A	3252	1/1	0.97	0.12	37,37,37,37	0
56	MG	1A	3595	1/1	0.97	0.07	34,34,34,34	0
56	MG	1A	3171	1/1	0.97	0.08	44,44,44,44	0
56	MG	1A	3509	1/1	0.97	0.12	31,31,31,31	0
56	MG	2A	3530	1/1	0.97	0.10	49,49,49,49	0
56	MG	2A	3774	1/1	0.97	0.09	64,64,64,64	0
56	MG	1A	3006	1/1	0.97	0.14	47,47,47,47	0
56	MG	1A	3599	1/1	0.97	0.12	42,42,42,42	0
56	MG	2A	3778	1/1	0.97	0.10	58,58,58,58	0
56	MG	1A	3173	1/1	0.97	0.17	34,34,34,34	0
56	MG	1A	3017	1/1	0.97	0.18	50,50,50,50	0
56	MG	1A	3179	1/1	0.97	0.05	29,29,29,29	0
56	MG	2A	3537	1/1	0.97	0.06	56,56,56,56	0
56	MG	1D	302	1/1	0.97	0.08	36,36,36,36	0
56	MG	2A	3539	1/1	0.97	0.06	48,48,48,48	0
56	MG	1a	1624	1/1	0.97	0.13	62,62,62,62	0
56	MG	1D	303	1/1	0.97	0.08	17,17,17,17	0
56	MG	1a	1801	1/1	0.97	0.07	64,64,64,64	0
56	MG	1a	1802	1/1	0.97	0.09	63,63,63,63	0
56	MG	1D	304	1/1	0.97	0.05	35,35,35,35	0
56	MG	2a	3073	1/1	0.97	0.11	50,50,50,50	0
56	MG	2A	3328	1/1	0.97	0.07	41,41,41,41	0
56	MG	1D	305	1/1	0.97	0.16	29,29,29,29	0
56	MG	1A	3603	1/1	0.97	0.09	39,39,39,39	0
56	MG	2A	3548	1/1	0.97	0.13	35,35,35,35	0
56	MG	1A	3994	1/1	0.97	0.05	70,70,70,70	0
56	MG	2a	3079	1/1	0.97	0.15	56,56,56,56	0
56	MG	2A	3125	1/1	0.97	0.05	58,58,58,58	0
56	MG	1D	309	1/1	0.97	0.17	20,20,20,20	0
56	MG	2A	3127	1/1	0.97	0.16	65,65,65,65	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	2A	3553	1/1	0.97	0.11	49,49,49,49	0
56	MG	2A	3128	1/1	0.97	0.04	42,42,42,42	0
56	MG	1a	1631	1/1	0.97	0.05	33,33,33,33	0
56	MG	1A	3851	1/1	0.97	0.06	11,11,11,11	0
56	MG	2a	3087	1/1	0.97	0.13	59,59,59,59	0
56	MG	1a	1813	1/1	0.97	0.06	53,53,53,53	0
56	MG	2A	3558	1/1	0.97	0.08	52,52,52,52	0
56	MG	1A	3604	1/1	0.97	0.08	27,27,27,27	0
56	MG	2A	3133	1/1	0.97	0.07	55,55,55,55	0
56	MG	2A	3561	1/1	0.97	0.07	36,36,36,36	0
56	MG	1a	1816	1/1	0.97	0.09	53,53,53,53	0
56	MG	1A	3215	1/1	0.97	0.08	39,39,39,39	0
56	MG	1A	3146	1/1	0.97	0.18	25,25,25,25	0
56	MG	2A	3813	1/1	0.97	0.07	53,53,53,53	0
56	MG	1E	301	1/1	0.97	0.28	28,28,28,28	0
56	MG	1A	3723	1/1	0.97	0.07	40,40,40,40	0
56	MG	1a	1822	1/1	0.97	0.06	69,69,69,69	0
56	MG	2A	3142	1/1	0.97	0.10	43,43,43,43	0
56	MG	1a	1824	1/1	0.97	0.05	60,60,60,60	0
56	MG	1A	3441	1/1	0.97	0.07	41,41,41,41	0
56	MG	1E	305	1/1	0.97	0.08	32,32,32,32	0
56	MG	1a	1828	1/1	0.97	0.17	42,42,42,42	0
56	MG	2A	3822	1/1	0.97	0.06	61,61,61,61	0
56	MG	1E	306	1/1	0.97	0.13	26,26,26,26	0
56	MG	1A	3442	1/1	0.97	0.08	36,36,36,36	0
56	MG	1A	3218	1/1	0.97	0.13	34,34,34,34	0
56	MG	2A	3355	1/1	0.97	0.07	51,51,51,51	0
56	MG	2A	3577	1/1	0.97	0.15	57,57,57,57	0
56	MG	1A	4004	1/1	0.97	0.05	51,51,51,51	0
56	MG	1A	3181	1/1	0.97	0.08	39,39,39,39	0
56	MG	1E	312	1/1	0.97	0.12	39,39,39,39	0
56	MG	1a	1649	1/1	0.97	0.14	44,44,44,44	0
56	MG	1A	3521	1/1	0.97	0.05	47,47,47,47	0
56	MG	1A	3445	1/1	0.97	0.10	36,36,36,36	0
56	MG	2A	3362	1/1	0.97	0.10	43,43,43,43	0
56	MG	1E	315	1/1	0.97	0.05	40,40,40,40	0
56	MG	1a	1653	1/1	0.97	0.14	56,56,56,56	0
56	MG	2A	3840	1/1	0.97	0.05	51,51,51,51	0
56	MG	1F	302	1/1	0.97	0.08	30,30,30,30	0
56	MG	1A	3376	1/1	0.97	0.10	44,44,44,44	0
56	MG	1l	201	1/1	0.97	0.08	56,56,56,56	0
56	MG	1l	202	1/1	0.97	0.09	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	2A	3847	1/1	0.97	0.06	47,47,47,47	0
56	MG	1A	3614	1/1	0.97	0.12	35,35,35,35	0
56	MG	1F	306	1/1	0.97	0.10	23,23,23,23	0
56	MG	2a	3128	1/1	0.97	0.12	44,44,44,44	0
56	MG	1A	3220	1/1	0.97	0.12	49,49,49,49	0
56	MG	1A	3736	1/1	0.97	0.06	38,38,38,38	0
56	MG	1A	3525	1/1	0.97	0.13	31,31,31,31	0
56	MG	1G	201	1/1	0.97	0.10	43,43,43,43	0
56	MG	1A	3087	1/1	0.97	0.14	35,35,35,35	0
56	MG	2A	3857	1/1	0.97	0.06	66,66,66,66	0
56	MG	1A	3527	1/1	0.97	0.13	32,32,32,32	0
56	MG	2A	3607	1/1	0.97	0.08	57,57,57,57	0
56	MG	1A	3264	1/1	0.97	0.05	36,36,36,36	0
56	MG	1A	3622	1/1	0.97	0.05	22,22,22,22	0
56	MG	2A	3862	1/1	0.97	0.05	57,57,57,57	0
56	MG	2A	3863	1/1	0.97	0.06	28,28,28,28	0
56	MG	1A	3529	1/1	0.97	0.19	28,28,28,28	0
56	MG	2A	3865	1/1	0.97	0.04	51,51,51,51	0
56	MG	1A	3119	1/1	0.97	0.10	23,23,23,23	0
56	MG	1A	3874	1/1	0.97	0.14	27,27,27,27	0
56	MG	1w	108	1/1	0.97	0.06	74,74,74,74	0
56	MG	1A	3625	1/1	0.97	0.11	53,53,53,53	0
56	MG	1A	3266	1/1	0.97	0.15	40,40,40,40	0
56	MG	1N	206	1/1	0.97	0.08	37,37,37,37	0
56	MG	2a	3152	1/1	0.97	0.06	70,70,70,70	0
56	MG	2A	3386	1/1	0.97	0.39	55,55,55,55	0
56	MG	1A	4025	1/1	0.97	0.09	40,40,40,40	0
56	MG	1O	204	1/1	0.97	0.08	46,46,46,46	0
56	MG	2a	3156	1/1	0.97	0.06	72,72,72,72	0
56	MG	2A	3389	1/1	0.97	0.15	36,36,36,36	0
56	MG	1A	3452	1/1	0.97	0.08	38,38,38,38	0
56	MG	2A	3877	1/1	0.97	0.07	49,49,49,49	0
56	MG	1P	201	1/1	0.97	0.14	25,25,25,25	0
56	MG	1A	3629	1/1	0.97	0.04	29,29,29,29	0
56	MG	2A	3393	1/1	0.97	0.17	40,40,40,40	0
56	MG	1x	106	1/1	0.97	0.17	52,52,52,52	0
56	MG	1A	3630	1/1	0.97	0.06	29,29,29,29	0
56	MG	1A	3631	1/1	0.97	0.04	14,14,14,14	0
56	MG	2a	3171	1/1	0.97	0.09	64,64,64,64	0
56	MG	1A	3453	1/1	0.97	0.20	31,31,31,31	0
56	MG	2A	3192	1/1	0.97	0.12	60,60,60,60	0
56	MG	1A	4034	1/1	0.97	0.09	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	1A	3753	1/1	0.97	0.06	34,34,34,34	0
56	MG	1A	3755	1/1	0.97	0.05	46,46,46,46	0
56	MG	1Q	202	1/1	0.97	0.19	34,34,34,34	0
56	MG	2A	3197	1/1	0.97	0.15	55,55,55,55	0
56	MG	1A	3267	1/1	0.97	0.14	40,40,40,40	0
56	MG	1x	116	1/1	0.97	0.12	65,65,65,65	0
56	MG	1A	3455	1/1	0.97	0.11	28,28,28,28	0
56	MG	1A	3758	1/1	0.97	0.06	40,40,40,40	0
56	MG	1A	3384	1/1	0.97	0.08	41,41,41,41	0
56	MG	2a	3184	1/1	0.97	0.15	57,57,57,57	0
56	MG	1A	3637	1/1	0.97	0.09	48,48,48,48	0
56	MG	1R	202	1/1	0.97	0.21	36,36,36,36	0
56	MG	1A	3385	1/1	0.97	0.05	27,27,27,27	0
56	MG	1A	4046	1/1	0.97	0.06	44,44,44,44	0
56	MG	1A	3068	1/1	0.97	0.09	48,48,48,48	0
56	MG	2A	3209	1/1	0.97	0.13	43,43,43,43	0
56	MG	2A	3647	1/1	0.97	0.32	64,64,64,64	0
56	MG	1A	3269	1/1	0.97	0.05	29,29,29,29	0
56	MG	2A	3211	1/1	0.97	0.07	45,45,45,45	0
56	MG	1A	3540	1/1	0.97	0.06	45,45,45,45	0
56	MG	2A	3010	1/1	0.97	0.16	46,46,46,46	0
56	MG	1A	3225	1/1	0.97	0.06	39,39,39,39	0
56	MG	1A	3542	1/1	0.97	0.11	37,37,37,37	0
56	MG	1A	3226	1/1	0.97	0.11	43,43,43,43	0
56	MG	1A	3645	1/1	0.97	0.10	20,20,20,20	0
56	MG	2A	3423	1/1	0.97	0.13	35,35,35,35	0
56	MG	1A	3902	1/1	0.97	0.10	43,43,43,43	0
56	MG	2A	3659	1/1	0.97	0.11	58,58,58,58	0
56	MG	1A	3272	1/1	0.97	0.13	22,22,22,22	0
56	MG	2a	3205	1/1	0.97	0.07	60,60,60,60	0
56	MG	2A	3220	1/1	0.97	0.07	52,52,52,52	0
56	MG	1A	3150	1/1	0.97	0.08	31,31,31,31	0
56	MG	1A	3275	1/1	0.97	0.17	31,31,31,31	0
56	MG	1U	210	1/1	0.97	0.19	25,25,25,25	0
56	MG	2A	3666	1/1	0.97	0.06	44,44,44,44	0
56	MG	2A	3430	1/1	0.97	0.15	31,31,31,31	0
56	MG	1A	3186	1/1	0.97	0.12	37,37,37,37	0
56	MG	2A	3669	1/1	0.97	0.10	59,59,59,59	0
56	MG	1V	201	1/1	0.97	0.25	30,30,30,30	0
56	MG	2F	306	1/1	0.97	0.17	51,51,51,51	0
56	MG	1A	3229	1/1	0.97	0.18	32,32,32,32	0
56	MG	2N	201	1/1	0.97	0.05	35,35,35,35	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	2A	3434	1/1	0.97	0.24	46,46,46,46	0
56	MG	1V	204	1/1	0.97	0.17	32,32,32,32	0
56	MG	1A	3009	1/1	0.97	0.05	17,17,17,17	0
56	MG	1V	206	1/1	0.97	0.06	29,29,29,29	0
56	MG	2A	3231	1/1	0.97	0.20	50,50,50,50	0
56	MG	2a	3226	1/1	0.97	0.12	50,50,50,50	0
56	MG	2A	3232	1/1	0.97	0.07	60,60,60,60	0
56	MG	2A	3233	1/1	0.97	0.07	33,33,33,33	0
56	MG	1A	4063	1/1	0.97	0.07	46,46,46,46	0
56	MG	1A	3335	1/1	0.97	0.07	36,36,36,36	0
56	MG	1A	3231	1/1	0.97	0.16	33,33,33,33	0
56	MG	2A	3031	1/1	0.97	0.05	48,48,48,48	0
56	MG	1A	3281	1/1	0.97	0.21	31,31,31,31	0
56	MG	1A	3782	1/1	0.97	0.07	48,48,48,48	0
56	MG	2T	203	1/1	0.97	0.12	50,50,50,50	0
56	MG	2A	3685	1/1	0.97	0.06	60,60,60,60	0
56	MG	1A	3656	1/1	0.97	0.07	34,34,34,34	0
56	MG	2A	3035	1/1	0.97	0.08	36,36,36,36	0
56	MG	1A	3554	1/1	0.97	0.26	41,41,41,41	0
56	MG	1A	3658	1/1	0.97	0.08	42,42,42,42	0
56	MG	1A	3555	1/1	0.97	0.05	23,23,23,23	0
56	MG	1A	3788	1/1	0.97	0.05	35,35,35,35	0
56	MG	2A	3692	1/1	0.97	0.06	66,66,66,66	0
56	MG	1A	3154	1/1	0.97	0.15	39,39,39,39	0
56	MG	1A	3922	1/1	0.97	0.04	70,70,70,70	0
56	MG	2A	3042	1/1	0.97	0.08	44,44,44,44	0
56	MG	1A	3122	1/1	0.97	0.11	37,37,37,37	0
56	MG	1A	3156	1/1	0.97	0.23	39,39,39,39	0
56	MG	1A	3792	1/1	0.97	0.06	45,45,45,45	0
56	MG	1A	3285	1/1	0.97	0.25	26,26,26,26	0
56	MG	1A	4082	1/1	0.97	0.07	35,35,35,35	0
56	MG	1A	3560	1/1	0.97	0.07	51,51,51,51	0
56	MG	1A	3104	1/1	0.97	0.04	25,25,25,25	0
56	MG	23	103	1/1	0.97	0.06	55,55,55,55	0
56	MG	1A	3562	1/1	0.97	0.06	43,43,43,43	0
56	MG	2A	3705	1/1	0.97	0.15	51,51,51,51	0
56	MG	1A	3406	1/1	0.97	0.13	43,43,43,43	0
56	MG	1A	3407	1/1	0.97	0.07	36,36,36,36	0
56	MG	1A	3287	1/1	0.97	0.06	43,43,43,43	0
56	MG	1A	3672	1/1	0.97	0.04	35,35,35,35	0
56	MG	1A	3410	1/1	0.97	0.06	39,39,39,39	0
56	MG	1A	3940	1/1	0.97	0.04	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	1A	3567	1/1	0.97	0.12	29,29,29,29	0
56	MG	1A	3804	1/1	0.97	0.06	22,22,22,22	0
56	MG	2A	3716	1/1	0.97	0.05	51,51,51,51	0
56	MG	1A	3568	1/1	0.97	0.14	30,30,30,30	0
56	MG	1A	3090	1/1	0.97	0.09	30,30,30,30	0
56	MG	1A	3159	1/1	0.97	0.17	30,30,30,30	0
56	MG	2A	3720	1/1	0.97	0.06	48,48,48,48	0
56	MG	1A	3106	1/1	0.97	0.06	26,26,26,26	0
56	MG	1a	1745	1/1	0.97	0.06	54,54,54,54	0
56	MG	1A	3812	1/1	0.97	0.05	54,54,54,54	0
56	MG	1a	1747	1/1	0.97	0.06	52,52,52,52	0
56	MG	1A	3951	1/1	0.97	0.05	42,42,42,42	0
56	MG	16	101	1/1	0.97	0.06	41,41,41,41	0
59	ZN	14	102	1/1	0.97	0.04	87,87,87,87	0
56	MG	1A	3347	1/1	0.97	0.20	41,41,41,41	0
56	MG	1A	3033	1/1	0.97	0.30	24,24,24,24	0
60	SF4	1d	302	8/8	0.97	0.06	68,78,85,86	0
60	SF4	2d	302	8/8	0.97	0.05	59,73,81,82	0
56	MG	1B	216	1/1	0.98	0.05	47,47,47,47	0
56	MG	2A	3534	1/1	0.98	0.05	41,41,41,41	0
56	MG	1B	217	1/1	0.98	0.13	47,47,47,47	0
56	MG	1A	3729	1/1	0.98	0.04	32,32,32,32	0
56	MG	1A	3731	1/1	0.98	0.05	24,24,24,24	0
56	MG	2A	3707	1/1	0.98	0.07	36,36,36,36	0
56	MG	2A	3229	1/1	0.98	0.16	33,33,33,33	0
56	MG	1A	3419	1/1	0.98	0.10	32,32,32,32	0
56	MG	1W	203	1/1	0.98	0.06	31,31,31,31	0
56	MG	1a	1814	1/1	0.98	0.05	67,67,67,67	0
56	MG	1A	3153	1/1	0.98	0.07	26,26,26,26	0
56	MG	1A	3081	1/1	0.98	0.08	27,27,27,27	0
56	MG	1X	101	1/1	0.98	0.06	32,32,32,32	0
56	MG	1X	102	1/1	0.98	0.10	35,35,35,35	0
56	MG	1A	4013	1/1	0.98	0.06	62,62,62,62	0
56	MG	1A	3015	1/1	0.98	0.05	39,39,39,39	0
56	MG	1A	3023	1/1	0.98	0.03	15,15,15,15	0
56	MG	1a	1823	1/1	0.98	0.04	59,59,59,59	0
56	MG	1A	3035	1/1	0.98	0.03	39,39,39,39	0
56	MG	1a	1825	1/1	0.98	0.14	43,43,43,43	0
56	MG	1A	3280	1/1	0.98	0.06	21,21,21,21	0
56	MG	2A	3092	1/1	0.98	0.15	48,48,48,48	0
56	MG	1A	3373	1/1	0.98	0.12	43,43,43,43	0
56	MG	1A	3125	1/1	0.98	0.18	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	1Z	303	1/1	0.98	0.07	42,42,42,42	0
56	MG	1A	3241	1/1	0.98	0.23	30,30,30,30	0
56	MG	1A	3126	1/1	0.98	0.16	34,34,34,34	0
56	MG	2D	305	1/1	0.98	0.05	33,33,33,33	0
56	MG	1A	3827	1/1	0.98	0.06	39,39,39,39	0
56	MG	1A	3200	1/1	0.98	0.05	33,33,33,33	0
56	MG	2A	3733	1/1	0.98	0.05	51,51,51,51	0
56	MG	1A	3160	1/1	0.98	0.21	26,26,26,26	0
56	MG	1A	3669	1/1	0.98	0.05	19,19,19,19	0
56	MG	1A	3127	1/1	0.98	0.07	42,42,42,42	0
56	MG	1A	3204	1/1	0.98	0.04	29,29,29,29	0
56	MG	1B	238	1/1	0.98	0.06	37,37,37,37	0
56	MG	1A	3128	1/1	0.98	0.15	36,36,36,36	0
56	MG	2A	3106	1/1	0.98	0.07	36,36,36,36	0
56	MG	2a	3130	1/1	0.98	0.05	68,68,68,68	0
56	MG	1A	3383	1/1	0.98	0.17	31,31,31,31	0
56	MG	2A	3260	1/1	0.98	0.06	57,57,57,57	0
56	MG	1A	3927	1/1	0.98	0.06	55,55,55,55	0
56	MG	1A	3549	1/1	0.98	0.12	30,30,30,30	0
56	MG	1A	3752	1/1	0.98	0.04	37,37,37,37	0
56	MG	1A	3085	1/1	0.98	0.07	23,23,23,23	0
56	MG	1A	3086	1/1	0.98	0.15	28,28,28,28	0
56	MG	1D	307	1/1	0.98	0.10	44,44,44,44	0
56	MG	1A	3386	1/1	0.98	0.07	30,30,30,30	0
56	MG	1A	3010	1/1	0.98	0.07	36,36,36,36	0
56	MG	2a	3141	1/1	0.98	0.06	68,68,68,68	0
56	MG	1A	3132	1/1	0.98	0.06	33,33,33,33	0
56	MG	1A	3936	1/1	0.98	0.06	14,14,14,14	0
56	MG	2A	3580	1/1	0.98	0.09	45,45,45,45	0
56	MG	1A	4044	1/1	0.98	0.04	43,43,43,43	0
56	MG	2a	3146	1/1	0.98	0.07	68,68,68,68	0
56	MG	1A	3011	1/1	0.98	0.10	31,31,31,31	0
56	MG	2A	3756	1/1	0.98	0.14	55,55,55,55	0
56	MG	1A	3938	1/1	0.98	0.04	54,54,54,54	0
56	MG	1A	3615	1/1	0.98	0.05	33,33,33,33	0
56	MG	1A	4050	1/1	0.98	0.09	46,46,46,46	0
56	MG	2A	3588	1/1	0.98	0.07	37,37,37,37	0
56	MG	2A	3589	1/1	0.98	0.05	44,44,44,44	0
56	MG	1A	3761	1/1	0.98	0.06	36,36,36,36	0
56	MG	2A	3591	1/1	0.98	0.07	46,46,46,46	0
56	MG	1A	3683	1/1	0.98	0.10	20,20,20,20	0
56	MG	1A	3294	1/1	0.98	0.06	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	2a	3158	1/1	0.98	0.10	54,54,54,54	0
56	MG	1A	3764	1/1	0.98	0.05	14,14,14,14	0
56	MG	2a	3161	1/1	0.98	0.04	67,67,67,67	0
56	MG	1A	3295	1/1	0.98	0.04	22,22,22,22	0
56	MG	1A	3012	1/1	0.98	0.06	28,28,28,28	0
56	MG	1E	311	1/1	0.98	0.06	52,52,52,52	0
56	MG	1A	3949	1/1	0.98	0.07	54,54,54,54	0
56	MG	2a	3166	1/1	0.98	0.04	67,67,67,67	0
56	MG	2A	3435	1/1	0.98	0.07	28,28,28,28	0
56	MG	2a	3168	1/1	0.98	0.06	51,51,51,51	0
56	MG	1A	3688	1/1	0.98	0.07	33,33,33,33	0
56	MG	1a	1723	1/1	0.98	0.23	46,46,46,46	0
56	MG	1A	3007	1/1	0.98	0.05	26,26,26,26	0
56	MG	2A	3603	1/1	0.98	0.04	60,60,60,60	0
56	MG	2A	3604	1/1	0.98	0.10	44,44,44,44	0
56	MG	1A	3298	1/1	0.98	0.06	36,36,36,36	0
56	MG	18	106	1/1	0.98	0.05	26,26,26,26	0
56	MG	1a	1727	1/1	0.98	0.13	36,36,36,36	0
56	MG	1F	301	1/1	0.98	0.04	27,27,27,27	0
56	MG	2A	3782	1/1	0.98	0.06	55,55,55,55	0
56	MG	1A	3028	1/1	0.98	0.13	21,21,21,21	0
56	MG	1F	303	1/1	0.98	0.09	28,28,28,28	0
56	MG	1A	3396	1/1	0.98	0.17	26,26,26,26	0
56	MG	2A	3786	1/1	0.98	0.08	51,51,51,51	0
56	MG	1A	3957	1/1	0.98	0.09	50,50,50,50	0
56	MG	1A	3071	1/1	0.98	0.09	29,29,29,29	0
56	MG	1F	307	1/1	0.98	0.13	30,30,30,30	0
56	MG	1A	4065	1/1	0.98	0.08	36,36,36,36	0
56	MG	2a	3187	1/1	0.98	0.06	70,70,70,70	0
56	MG	1A	3773	1/1	0.98	0.04	46,46,46,46	0
56	MG	1A	3694	1/1	0.98	0.08	41,41,41,41	0
56	MG	1A	3042	1/1	0.98	0.18	22,22,22,22	0
56	MG	2A	3794	1/1	0.98	0.04	65,65,65,65	0
56	MG	1A	3139	1/1	0.98	0.11	36,36,36,36	0
56	MG	1A	3862	1/1	0.98	0.11	36,36,36,36	0
56	MG	2A	3153	1/1	0.98	0.06	41,41,41,41	0
56	MG	1A	3175	1/1	0.98	0.17	30,30,30,30	0
56	MG	1a	1742	1/1	0.98	0.06	55,55,55,55	0
56	MG	1A	3628	1/1	0.98	0.04	51,51,51,51	0
56	MG	2A	3307	1/1	0.98	0.05	54,54,54,54	0
56	MG	2A	3009	1/1	0.98	0.05	38,38,38,38	0
56	MG	1A	3176	1/1	0.98	0.10	27,27,27,27	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	1A	3177	1/1	0.98	0.12	25,25,25,25	0
56	MG	1A	3178	1/1	0.98	0.05	17,17,17,17	0
56	MG	1A	3702	1/1	0.98	0.03	8,8,8,8	0
56	MG	1A	4077	1/1	0.98	0.06	27,27,27,27	0
56	MG	1A	3570	1/1	0.98	0.12	29,29,29,29	0
56	MG	1A	3785	1/1	0.98	0.06	37,37,37,37	0
56	MG	2A	3017	1/1	0.98	0.04	36,36,36,36	0
56	MG	1O	202	1/1	0.98	0.15	47,47,47,47	0
56	MG	1O	203	1/1	0.98	0.09	40,40,40,40	0
56	MG	2a	3210	1/1	0.98	0.09	57,57,57,57	0
56	MG	2a	3211	1/1	0.98	0.07	50,50,50,50	0
56	MG	2a	3212	1/1	0.98	0.10	59,59,59,59	0
56	MG	1A	3633	1/1	0.98	0.05	28,28,28,28	0
56	MG	1A	3975	1/1	0.98	0.06	50,50,50,50	0
56	MG	1A	3014	1/1	0.98	0.06	22,22,22,22	0
56	MG	1A	3977	1/1	0.98	0.13	59,59,59,59	0
56	MG	1a	1758	1/1	0.98	0.05	32,32,32,32	0
56	MG	1P	203	1/1	0.98	0.10	25,25,25,25	0
56	MG	2A	3477	1/1	0.98	0.12	23,23,23,23	0
56	MG	1P	204	1/1	0.98	0.18	23,23,23,23	0
56	MG	1A	3457	1/1	0.98	0.05	25,25,25,25	0
56	MG	1A	3354	1/1	0.98	0.06	34,34,34,34	0
56	MG	2A	3177	1/1	0.98	0.14	35,35,35,35	0
56	MG	1A	3875	1/1	0.98	0.25	35,35,35,35	0
56	MG	2A	3825	1/1	0.98	0.03	43,43,43,43	0
56	MG	1A	3355	1/1	0.98	0.26	25,25,25,25	0
56	MG	2A	3651	1/1	0.98	0.07	44,44,44,44	0
56	MG	1A	3517	1/1	0.98	0.06	44,44,44,44	0
56	MG	1A	4091	1/1	0.98	0.05	31,31,31,31	0
56	MG	1A	3142	1/1	0.98	0.05	14,14,14,14	0
56	MG	1Q	203	1/1	0.98	0.09	24,24,24,24	0
56	MG	1a	1637	1/1	0.98	0.13	54,54,54,54	0
56	MG	2A	3185	1/1	0.98	0.12	47,47,47,47	0
56	MG	1A	3075	1/1	0.98	0.04	21,21,21,21	0
56	MG	1A	3409	1/1	0.98	0.12	41,41,41,41	0
56	MG	2A	3837	1/1	0.98	0.09	66,66,66,66	0
56	MG	2A	3188	1/1	0.98	0.06	43,43,43,43	0
56	MG	1A	3795	1/1	0.98	0.06	19,19,19,19	0
56	MG	1Q	207	1/1	0.98	0.05	44,44,44,44	0
56	MG	2A	3663	1/1	0.98	0.05	54,54,54,54	0
56	MG	1A	3145	1/1	0.98	0.18	21,21,21,21	0
56	MG	2A	3496	1/1	0.98	0.05	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	4097	1/1	0.98	0.06	35,35,35,35	0
56	MG	1a	1644	1/1	0.98	0.09	39,39,39,39	0
56	MG	1A	3115	1/1	0.98	0.04	32,32,32,32	0
56	MG	2A	3045	1/1	0.98	0.20	53,53,53,53	0
56	MG	1A	3021	1/1	0.98	0.04	21,21,21,21	0
56	MG	1A	3716	1/1	0.98	0.06	31,31,31,31	0
56	MG	1a	1648	1/1	0.98	0.05	48,48,48,48	0
56	MG	2A	3199	1/1	0.98	0.18	50,50,50,50	0
56	MG	1A	3886	1/1	0.98	0.04	23,23,23,23	0
56	MG	2A	3856	1/1	0.98	0.05	58,58,58,58	0
56	MG	1A	3466	1/1	0.98	0.07	36,36,36,36	0
56	MG	2A	3507	1/1	0.98	0.10	44,44,44,44	0
56	MG	1A	3031	1/1	0.98	0.16	31,31,31,31	0
56	MG	2A	3510	1/1	0.98	0.06	41,41,41,41	0
56	MG	1A	3118	1/1	0.98	0.14	22,22,22,22	0
56	MG	1A	3995	1/1	0.98	0.05	61,61,61,61	0
56	MG	1A	3890	1/1	0.98	0.03	33,33,33,33	0
56	MG	1A	3721	1/1	0.98	0.07	27,27,27,27	0
56	MG	1A	3469	1/1	0.98	0.05	33,33,33,33	0
56	MG	1U	203	1/1	0.98	0.26	28,28,28,28	0
56	MG	1A	3806	1/1	0.98	0.05	26,26,26,26	0
56	MG	1a	1792	1/1	0.98	0.06	60,60,60,60	0
56	MG	1A	3649	1/1	0.98	0.04	29,29,29,29	0
56	MG	1U	207	1/1	0.98	0.14	29,29,29,29	0
56	MG	1U	208	1/1	0.98	0.19	30,30,30,30	0
56	MG	1a	1796	1/1	0.98	0.06	59,59,59,59	0
56	MG	1A	3586	1/1	0.98	0.17	31,31,31,31	0
56	MG	1A	3032	1/1	0.98	0.12	26,26,26,26	0
56	MG	1U	211	1/1	0.98	0.11	28,28,28,28	0
56	MG	1A	3810	1/1	0.98	0.06	25,25,25,25	0
56	MG	1A	3099	1/1	0.98	0.10	16,16,16,16	0
56	MG	1A	3152	1/1	0.98	0.03	29,29,29,29	0
56	MG	1V	203	1/1	0.98	0.18	26,26,26,26	0
56	MG	1a	1804	1/1	0.98	0.05	53,53,53,53	0
59	ZN	2Y	501	1/1	0.98	0.04	81,81,81,81	0
56	MG	1a	1805	1/1	0.98	0.08	55,55,55,55	0
56	MG	2A	3882	1/1	0.98	0.06	42,42,42,42	0
56	MG	2A	3700	1/1	0.98	0.04	58,58,58,58	0
56	MG	1A	3274	1/1	0.98	0.11	38,38,38,38	0
56	MG	2A	3776	1/1	0.99	0.04	56,56,56,56	0
56	MG	2A	3854	1/1	0.99	0.06	35,35,35,35	0
56	MG	1A	3305	1/1	0.99	0.18	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	3233	1/1	0.99	0.03	30,30,30,30	0
56	MG	2A	3019	1/1	0.99	0.04	30,30,30,30	0
56	MG	1A	3307	1/1	0.99	0.08	26,26,26,26	0
56	MG	1A	3974	1/1	0.99	0.04	54,54,54,54	0
56	MG	1A	4020	1/1	0.99	0.04	33,33,33,33	0
56	MG	1A	3216	1/1	0.99	0.15	32,32,32,32	0
56	MG	1A	3201	1/1	0.99	0.03	22,22,22,22	0
56	MG	1A	3496	1/1	0.99	0.06	25,25,25,25	0
56	MG	1A	3187	1/1	0.99	0.05	31,31,31,31	0
56	MG	1A	3830	1/1	0.99	0.19	48,48,48,48	0
56	MG	1A	4026	1/1	0.99	0.04	35,35,35,35	0
56	MG	2A	3642	1/1	0.99	0.04	41,41,41,41	0
56	MG	1A	3144	1/1	0.99	0.10	42,42,42,42	0
56	MG	1A	4080	1/1	0.99	0.04	39,39,39,39	0
56	MG	1A	3740	1/1	0.99	0.04	49,49,49,49	0
56	MG	1A	4029	1/1	0.99	0.05	50,50,50,50	0
56	MG	1A	3899	1/1	0.99	0.04	38,38,38,38	0
56	MG	1A	4031	1/1	0.99	0.07	60,60,60,60	0
56	MG	2A	3508	1/1	0.99	0.05	64,64,64,64	0
56	MG	1X	105	1/1	0.99	0.06	29,29,29,29	0
56	MG	1A	3939	1/1	0.99	0.08	21,21,21,21	0
56	MG	2A	3725	1/1	0.99	0.06	34,34,34,34	0
56	MG	1A	4086	1/1	0.99	0.08	28,28,28,28	0
56	MG	1A	3900	1/1	0.99	0.03	20,20,20,20	0
56	MG	2A	3582	1/1	0.99	0.06	39,39,39,39	0
56	MG	1A	3079	1/1	0.99	0.15	26,26,26,26	0
56	MG	2A	3584	1/1	0.99	0.05	59,59,59,59	0
56	MG	1A	3687	1/1	0.99	0.08	27,27,27,27	0
56	MG	1A	3190	1/1	0.99	0.15	25,25,25,25	0
56	MG	1A	3944	1/1	0.99	0.05	44,44,44,44	0
56	MG	1A	3501	1/1	0.99	0.07	28,28,28,28	0
56	MG	1A	3946	1/1	0.99	0.03	40,40,40,40	0
56	MG	1A	3805	1/1	0.99	0.03	35,35,35,35	0
56	MG	1w	111	1/1	0.99	0.06	69,69,69,69	0
56	MG	1A	4041	1/1	0.99	0.02	42,42,42,42	0
56	MG	1A	3374	1/1	0.99	0.03	30,30,30,30	0
56	MG	2a	3159	1/1	0.99	0.03	56,56,56,56	0
56	MG	1A	3839	1/1	0.99	0.07	43,43,43,43	0
56	MG	1A	3908	1/1	0.99	0.04	32,32,32,32	0
56	MG	1A	4045	1/1	0.99	0.03	17,17,17,17	0
56	MG	1A	3222	1/1	0.99	0.16	29,29,29,29	0
56	MG	1A	3952	1/1	0.99	0.04	39,39,39,39	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	2A	3119	1/1	0.99	0.11	36,36,36,36	0
56	MG	1A	4048	1/1	0.99	0.05	34,34,34,34	0
56	MG	1E	304	1/1	0.99	0.11	34,34,34,34	0
56	MG	1A	3953	1/1	0.99	0.03	50,50,50,50	0
56	MG	1A	3666	1/1	0.99	0.05	35,35,35,35	0
56	MG	1A	3719	1/1	0.99	0.09	47,47,47,47	0
56	MG	1A	3779	1/1	0.99	0.03	18,18,18,18	0
56	MG	1a	1811	1/1	0.99	0.05	38,38,38,38	0
56	MG	1x	114	1/1	0.99	0.05	51,51,51,51	0
56	MG	1A	3008	1/1	0.99	0.08	26,26,26,26	0
56	MG	2A	3829	1/1	0.99	0.04	45,45,45,45	0
56	MG	1A	3914	1/1	0.99	0.04	19,19,19,19	0
56	MG	1A	3073	1/1	0.99	0.07	14,14,14,14	0
56	MG	1A	3064	1/1	0.99	0.06	32,32,32,32	0
56	MG	1A	3036	1/1	0.99	0.05	15,15,15,15	0
56	MG	1A	3076	1/1	0.99	0.10	20,20,20,20	0
56	MG	1a	1757	1/1	0.99	0.04	35,35,35,35	0
56	MG	1A	3161	1/1	0.99	0.12	22,22,22,22	0
56	MG	2a	3022	1/1	0.99	0.11	43,43,43,43	0
56	MG	1a	1820	1/1	0.99	0.03	68,68,68,68	0
56	MG	2A	3137	1/1	0.99	0.14	40,40,40,40	0
56	MG	1A	3141	1/1	0.99	0.10	26,26,26,26	0
56	MG	2A	3139	1/1	0.99	0.12	34,34,34,34	0
56	MG	1U	204	1/1	0.99	0.04	22,22,22,22	0
56	MG	2E	303	1/1	0.99	0.11	36,36,36,36	0
56	MG	1A	3070	1/1	0.99	0.06	12,12,12,12	0
56	MG	2A	3843	1/1	0.99	0.11	35,35,35,35	0
56	MG	2y	105	1/1	0.99	0.03	76,76,76,76	0
56	MG	17	103	1/1	0.99	0.03	22,22,22,22	0
56	MG	2A	3845	1/1	0.99	0.04	44,44,44,44	0
56	MG	1A	4010	1/1	0.99	0.06	28,28,28,28	0
58	K	1A	4103	1/1	0.99	0.02	21,21,21,21	0
58	K	2A	3889	1/1	0.99	0.02	36,36,36,36	0
59	ZN	1Y	204	1/1	0.99	0.02	53,53,53,53	0
56	MG	1A	3199	1/1	0.99	0.14	20,20,20,20	0
59	ZN	16	104	1/1	0.99	0.04	37,37,37,37	0
59	ZN	1n	102	1/1	0.99	0.03	66,66,66,66	0
56	MG	1A	3967	1/1	0.99	0.04	46,46,46,46	0
56	MG	1A	3047	1/1	0.99	0.07	23,23,23,23	0
59	ZN	25	106	1/1	0.99	0.04	57,57,57,57	0
59	ZN	26	501	1/1	0.99	0.06	64,64,64,64	0
59	ZN	29	501	1/1	0.99	0.04	72,72,72,72	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	1A	3730	1/1	0.99	0.04	19,19,19,19	0
56	MG	1A	3677	1/1	0.99	0.04	23,23,23,23	0
56	MG	1a	1769	1/1	0.99	0.11	52,52,52,52	0
56	MG	1A	3618	1/1	1.00	0.06	26,26,26,26	0
56	MG	1A	3935	1/1	1.00	0.02	40,40,40,40	0
59	ZN	15	106	1/1	1.00	0.03	38,38,38,38	0
56	MG	2A	3708	1/1	1.00	0.04	31,31,31,31	0
59	ZN	19	102	1/1	1.00	0.04	40,40,40,40	0
56	MG	1A	3754	1/1	1.00	0.04	18,18,18,18	0
56	MG	1A	3915	1/1	1.00	0.02	26,26,26,26	0

6.5 Other polymers [i](#)

There are no such residues in this entry.