



wwPDB X-ray Structure Validation Summary Report ⓘ

Aug 5, 2026 – 08:05 AM EDT

PDB ID : 7RQC / pdb_00007rqc
Title : Crystal structure of the Thermus thermophilus 70S ribosome in complex with protein Y, A-site aminoacyl-tRNA analog ACC-PMN, and P-site MFI-tripeptidyl-tRNA analog ACCA-IFM at 2.50Å resolution
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Deposited on : 2021-08-06
Resolution : 2.50 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.015 (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

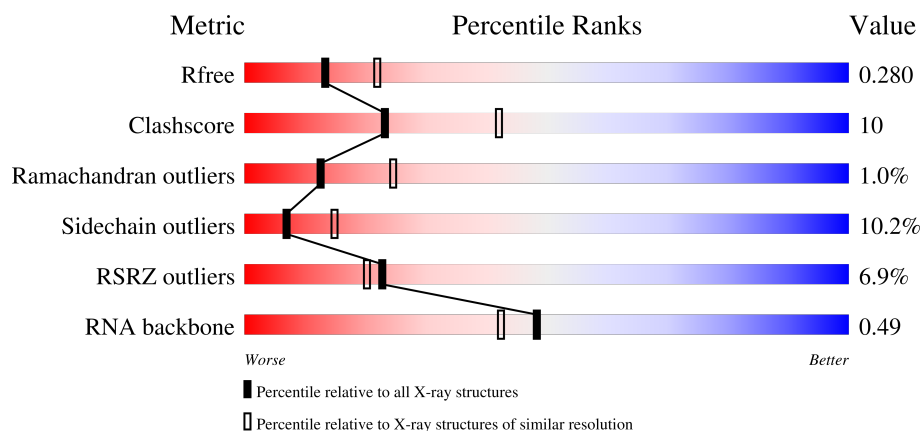
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 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	5829 (2.50-2.50)
Clashscore	190562	6492 (2.50-2.50)
Ramachandran outliers	187476	6378 (2.50-2.50)
Sidechain outliers	187428	6380 (2.50-2.50)
RSRZ outliers	180081	5833 (2.50-2.50)
RNA backbone	3983	1003 (2.78-2.22)

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

Mol	Chain	Length	Quality of chain
1	1A	2915	4% 62% 30% 6% •
1	2A	2915	4% 55% 35% 8% •
2	1B	121	% 63% 31% 5% •

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

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

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

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

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Mol	Chain	Length	Quality of chain
52	2u	27	
53	1y	113	
53	2y	113	
54	1w	4	
54	2w	4	
55	1x	4	
55	2x	4	
56	1v	3	
56	2v	3	

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
57	MG	1A	3638	-	-	-	X
57	MG	1A	4019	-	-	-	X

2 Entry composition

There are 62 unique types of molecules in this entry. The entry contains 297682 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	2872	Total	C	N	O	P	0	0	0
			61869	27540	11574	19884	2871			
1	2A	2867	Total	C	N	O	P	0	0	0
			61758	27491	11552	19850	2865			

- 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
			2572	1145	476	832	119			
2	2B	120	Total	C	N	O	P	0	0	0
			2573	1146	476	832	119			

- 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
			2131	1346	422	360	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
			1426	916	253	253	4			
6	2G	181	Total	C	N	O	S	0	0	0
			1424	912	259	249	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	173	Total	C	N	O	S	0	0	0
			1324	842	247	234	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	1I	147	Total	C	N	O	S	0	0	0
			1094	699	191	203	1			
8	2I	146	Total	C	N	O	S	0	0	0
			1076	687	186	202	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
			1121	722	208	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
			877	553	175	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
			775	498	141	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
			810	520	153	131	6			
20	2Y	107	Total	C	N	O	S	0	0	0
			810	519	153	132	6			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
21	1Z	203	Total	C	N	O	S	0	0	0
			1587	1011	282	292	2			
21	2Z	201	Total	C	N	O	S	0	0	0
			1557	995	274	286	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
			650	401	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
			754	475	148	130	1			
23	21	97	Total	C	N	O	S	0	0	0
			759	478	149	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
			592	368	119	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
			546	346	96	99	5			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
26	24	69	Total	C	N	O	S	0	0	0
			536	342	98	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
			459	288	90	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	1504	Total	C	N	O	P	0	0	0
			32331	14396	5990	10441	1504			

- 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
			1842	1175	330	332	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
			1558	979	305	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
			1665	1043	329	286	7			
35	2d	208	Total	C	N	O	S	0	0	0
			1668	1047	330	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
			1133	716	214	199	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
			814	516	144	151	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
			1235	769	244	216	6			
38	2g	155	Total	C	N	O	S	0	0	0
			1229	766	241	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
			1098	694	210	192	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
			986	625	193	168			
40	2i	126	Total	C	N	O	0	0	0
			966	613	186	167			

- 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
			719	446	142	131			
41	2j	96	Total	C	N	O	0	0	0
			710	442	137	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
			834	520	156	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	116	Total	C	N	O	S	0	0	0
			914	564	189	159	2			
44	2m	114	Total	C	N	O	S	0	0	0
			895	550	186	157	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
			648	415	120	111	2			
50	2s	83	Total	C	N	O	S	0	0	0
			645	410	118	115	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
			732	449	157	124	2			
51	2t	98	Total	C	N	O	S	0	0	0
			733	451	154	126	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 protein called Ribosome-associated inhibitor A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
53	1y	97	Total	C	N	O	S	0	0	0
			764	478	144	139	3			
53	2y	96	Total	C	N	O	S	0	0	0
			749	468	141	137	3			

- Molecule 54 is a RNA chain called A-site Aminoacyl-tRNA Analog.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
54	1w	4	Total	C	N	O	P	0	0	1
			78	40	13	22	3			
54	2w	4	Total	C	N	O	P	0	0	1
			78	40	13	22	3			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
55	1x	4	Total	C	N	O	P	0	0	1
			63	28	12	20	3			
55	2x	4	Total	C	N	O	P	0	0	1
			63	28	12	20	3			

- Molecule 56 is a protein called P-site Peptidyl-tRNA Analog Peptide.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
56	1v	3	Total	C	N	O	S	0	0	0
			27	20	3	3	1			
56	2v	3	Total	C	N	O	S	0	0	0
			27	20	3	3	1			

- Molecule 57 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
57	1A	1022	Total	Mg	0	0
			1022	1022		
57	1B	30	Total	Mg	0	0
			30	30		
57	1D	15	Total	Mg	0	0
			15	15		
57	1E	12	Total	Mg	0	0
			12	12		
57	1F	16	Total	Mg	0	0
			16	16		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
57	1G	4	Total 4	Mg 4	0	0
57	1H	2	Total 2	Mg 2	0	0
57	1N	4	Total 4	Mg 4	0	0
57	1O	1	Total 1	Mg 1	0	0
57	1P	5	Total 5	Mg 5	0	0
57	1Q	7	Total 7	Mg 7	0	0
57	1R	4	Total 4	Mg 4	0	0
57	1S	1	Total 1	Mg 1	0	0
57	1T	5	Total 5	Mg 5	0	0
57	1U	4	Total 4	Mg 4	0	0
57	1V	7	Total 7	Mg 7	0	0
57	1W	3	Total 3	Mg 3	0	0
57	1X	1	Total 1	Mg 1	0	0
57	1Y	1	Total 1	Mg 1	0	0
57	1Z	1	Total 1	Mg 1	0	0
57	10	9	Total 9	Mg 9	0	0
57	11	5	Total 5	Mg 5	0	0
57	13	3	Total 3	Mg 3	0	0
57	15	9	Total 9	Mg 9	0	0
57	17	6	Total 6	Mg 6	0	0
57	18	3	Total 3	Mg 3	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
57	19	2	Total 2	Mg 2	0	0
57	1a	274	Total 274	Mg 274	0	0
57	1b	1	Total 1	Mg 1	0	0
57	1d	6	Total 6	Mg 6	0	0
57	1e	3	Total 3	Mg 3	0	0
57	1f	2	Total 2	Mg 2	0	0
57	1g	1	Total 1	Mg 1	0	0
57	1h	2	Total 2	Mg 2	0	0
57	1i	1	Total 1	Mg 1	0	0
57	1l	3	Total 3	Mg 3	0	0
57	1m	1	Total 1	Mg 1	0	0
57	1n	3	Total 3	Mg 3	0	0
57	1o	2	Total 2	Mg 2	0	0
57	1t	1	Total 1	Mg 1	0	0
57	1u	1	Total 1	Mg 1	0	0
57	1y	4	Total 4	Mg 4	0	0
57	1w	1	Total 1	Mg 1	0	0
57	1x	2	Total 2	Mg 2	0	0
57	2A	733	Total 733	Mg 733	0	0
57	2B	19	Total 19	Mg 19	0	0
57	2D	10	Total 10	Mg 10	0	0

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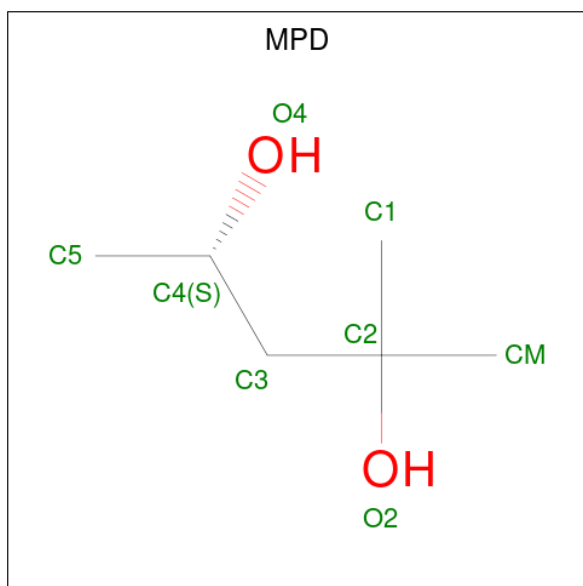
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
57	2E	7	Total 7	Mg 7	0	0
57	2F	4	Total 4	Mg 4	0	0
57	2G	3	Total 3	Mg 3	0	0
57	2I	1	Total 1	Mg 1	0	0
57	2O	2	Total 2	Mg 2	0	0
57	2P	2	Total 2	Mg 2	0	0
57	2Q	4	Total 4	Mg 4	0	0
57	2R	3	Total 3	Mg 3	0	0
57	2T	3	Total 3	Mg 3	0	0
57	2U	1	Total 1	Mg 1	0	0
57	2V	3	Total 3	Mg 3	0	0
57	2W	3	Total 3	Mg 3	0	0
57	2X	1	Total 1	Mg 1	0	0
57	2Y	1	Total 1	Mg 1	0	0
57	20	2	Total 2	Mg 2	0	0
57	21	1	Total 1	Mg 1	0	0
57	25	3	Total 3	Mg 3	0	0
57	27	2	Total 2	Mg 2	0	0
57	28	2	Total 2	Mg 2	0	0
57	2a	190	Total 190	Mg 190	0	0
57	2e	1	Total 1	Mg 1	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
57	2f	1	Total Mg 1 1	0	0
57	2j	1	Total Mg 1 1	0	0
57	2n	1	Total Mg 1 1	0	0
57	2p	1	Total Mg 1 1	0	0
57	2r	1	Total Mg 1 1	0	0
57	2t	1	Total Mg 1 1	0	0
57	2x	1	Total Mg 1 1	0	0

- Molecule 58 is (4S)-2-METHYL-2,4-PENTANEDIOL (CCD ID: MPD) (formula: C₆H₁₄O₂).



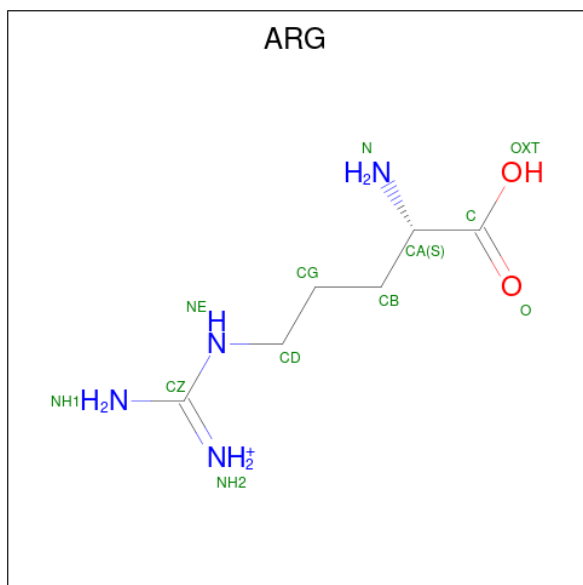
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
58	1A	1	Total C O 8 6 2	0	0
58	18	1	Total C O 8 6 2	0	0
58	1a	1	Total C O 8 6 2	0	0
58	1a	1	Total C O 8 6 2	0	0

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
58	2A	1	Total	C	O	0	0
			8	6	2		
58	2A	1	Total	C	O	0	0
			8	6	2		
58	2B	1	Total	C	O	0	0
			8	6	2		

- Molecule 59 is ARGinine (CCD ID: ARG) (formula: $C_6H_{15}N_4O_2$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
59	1B	1	Total	C	N	O	0	0
			12	6	4	2		
59	1F	1	Total	C	N	O	0	0
			12	6	4	2		

- Molecule 60 is ZINC ION (CCD ID: ZN) (formula: Zn).

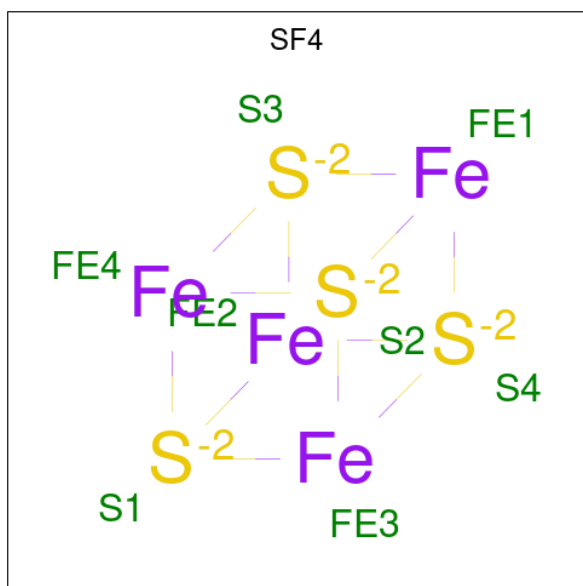
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
60	1Y	1	Total	Zn	0	0
			1	1		
60	14	1	Total	Zn	0	0
			1	1		
60	15	1	Total	Zn	0	0
			1	1		
60	16	1	Total	Zn	0	0
			1	1		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
60	19	1	Total	Zn	0	0
			1	1		
60	1n	1	Total	Zn	0	0
			1	1		
60	2Y	1	Total	Zn	0	0
			1	1		
60	24	1	Total	Zn	0	0
			1	1		
60	25	1	Total	Zn	0	0
			1	1		
60	26	1	Total	Zn	0	0
			1	1		
60	29	1	Total	Zn	0	0
			1	1		
60	2n	1	Total	Zn	0	0
			1	1		

- Molecule 61 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe_4S_4).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
61	1d	1	Total	Fe	S	0	0
			8	4	4		
61	2d	1	Total	Fe	S	0	0
			8	4	4		

- Molecule 62 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
62	1A	3972	Total 3972	O 3972	0	0
62	1B	98	Total 98	O 98	0	0
62	1D	107	Total 107	O 107	0	0
62	1E	75	Total 75	O 75	0	0
62	1F	60	Total 60	O 60	0	0
62	1G	20	Total 20	O 20	0	0
62	1H	15	Total 15	O 15	0	0
62	1I	4	Total 4	O 4	0	0
62	1N	47	Total 47	O 47	0	0
62	1O	26	Total 26	O 26	0	0
62	1P	63	Total 63	O 63	0	0
62	1Q	37	Total 37	O 37	0	0
62	1R	34	Total 34	O 34	0	0
62	1S	15	Total 15	O 15	0	0
62	1T	32	Total 32	O 32	0	0
62	1U	45	Total 45	O 45	0	0
62	1V	36	Total 36	O 36	0	0
62	1W	25	Total 25	O 25	0	0
62	1X	26	Total 26	O 26	0	0
62	1Y	16	Total 16	O 16	0	0
62	1Z	8	Total 8	O 8	0	0
62	10	21	Total 21	O 21	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
62	11	26	Total 26	O 26	0	0
62	12	12	Total 12	O 12	0	0
62	13	21	Total 21	O 21	0	0
62	14	2	Total 2	O 2	0	0
62	15	25	Total 25	O 25	0	0
62	16	18	Total 18	O 18	0	0
62	17	13	Total 13	O 13	0	0
62	18	26	Total 26	O 26	0	0
62	19	5	Total 5	O 5	0	0
62	1a	509	Total 509	O 509	0	0
62	1b	1	Total 1	O 1	0	0
62	1d	10	Total 10	O 10	0	0
62	1e	3	Total 3	O 3	0	0
62	1f	3	Total 3	O 3	0	0
62	1h	1	Total 1	O 1	0	0
62	1j	2	Total 2	O 2	0	0
62	1l	4	Total 4	O 4	0	0
62	1m	1	Total 1	O 1	0	0
62	1o	4	Total 4	O 4	0	0
62	1p	3	Total 3	O 3	0	0
62	1t	1	Total 1	O 1	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
62	1u	1	Total 1	O 1	0	0
62	1y	8	Total 8	O 8	0	0
62	1w	3	Total 3	O 3	0	0
62	1x	3	Total 3	O 3	0	0
62	2A	2105	Total 2105	O 2105	0	0
62	2B	46	Total 46	O 46	0	0
62	2D	48	Total 48	O 48	0	0
62	2E	26	Total 26	O 26	0	0
62	2F	24	Total 24	O 24	0	0
62	2G	4	Total 4	O 4	0	0
62	2H	2	Total 2	O 2	0	0
62	2I	4	Total 4	O 4	0	0
62	2N	5	Total 5	O 5	0	0
62	2O	18	Total 18	O 18	0	0
62	2P	19	Total 19	O 19	0	0
62	2Q	18	Total 18	O 18	0	0
62	2R	22	Total 22	O 22	0	0
62	2S	3	Total 3	O 3	0	0
62	2T	7	Total 7	O 7	0	0
62	2U	10	Total 10	O 10	0	0
62	2V	7	Total 7	O 7	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
62	2W	17	Total 17	O 17	0	0
62	2X	8	Total 8	O 8	0	0
62	2Y	5	Total 5	O 5	0	0
62	2Z	11	Total 11	O 11	0	0
62	20	12	Total 12	O 12	0	0
62	21	20	Total 20	O 20	0	0
62	22	1	Total 1	O 1	0	0
62	23	4	Total 4	O 4	0	0
62	25	10	Total 10	O 10	0	0
62	26	5	Total 5	O 5	0	0
62	27	8	Total 8	O 8	0	0
62	28	12	Total 12	O 12	0	0
62	29	2	Total 2	O 2	0	0
62	2a	291	Total 291	O 291	0	0
62	2d	3	Total 3	O 3	0	0
62	2f	3	Total 3	O 3	0	0
62	2j	2	Total 2	O 2	0	0
62	2l	2	Total 2	O 2	0	0
62	2m	2	Total 2	O 2	0	0
62	2o	4	Total 4	O 4	0	0
62	2p	2	Total 2	O 2	0	0

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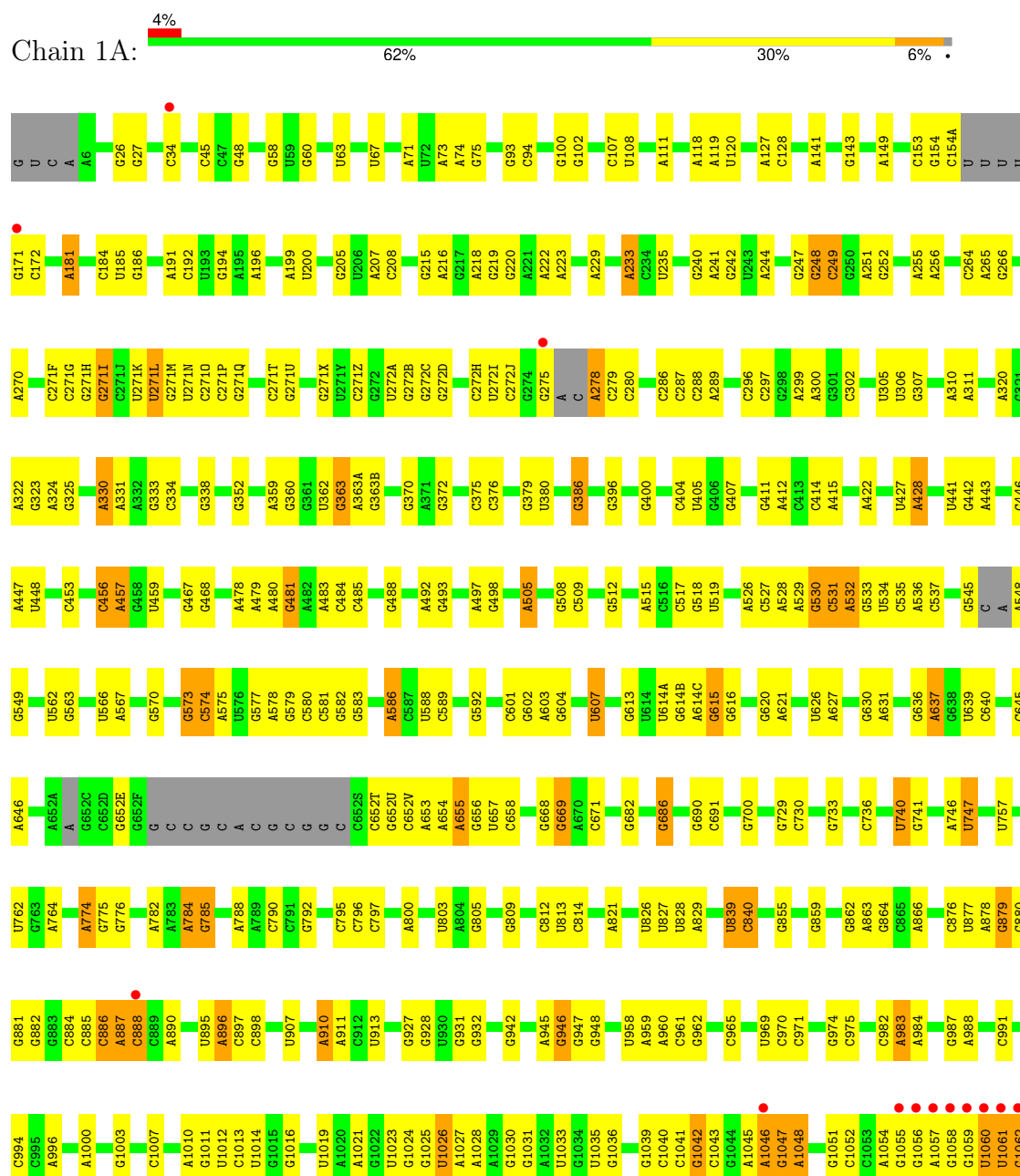
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
62	2q	1	Total 1	O 1	0	0
62	2r	3	Total 3	O 3	0	0
62	2t	2	Total 2	O 2	0	0
62	2y	3	Total 3	O 3	0	0
62	2w	3	Total 3	O 3	0	0
62	2x	1	Total 1	O 1	0	0

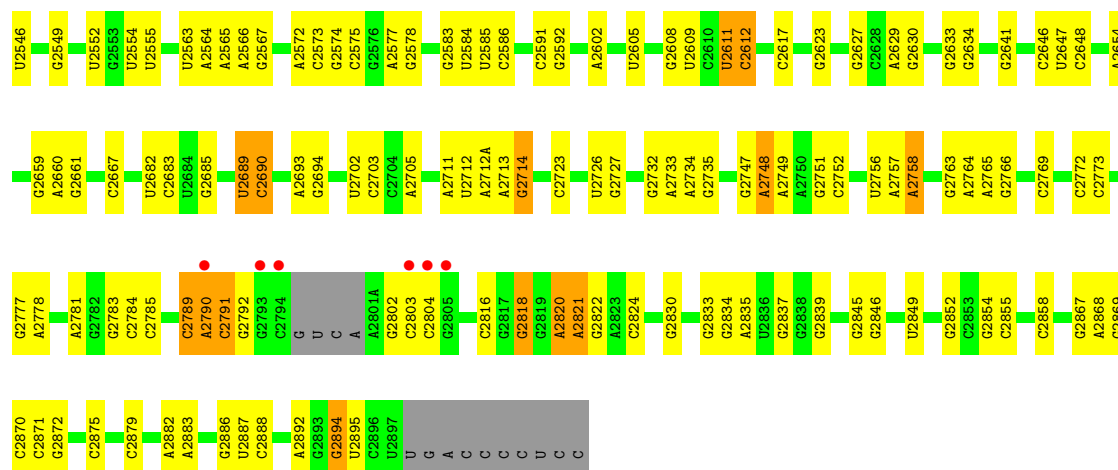
3 Residue-property plots

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.

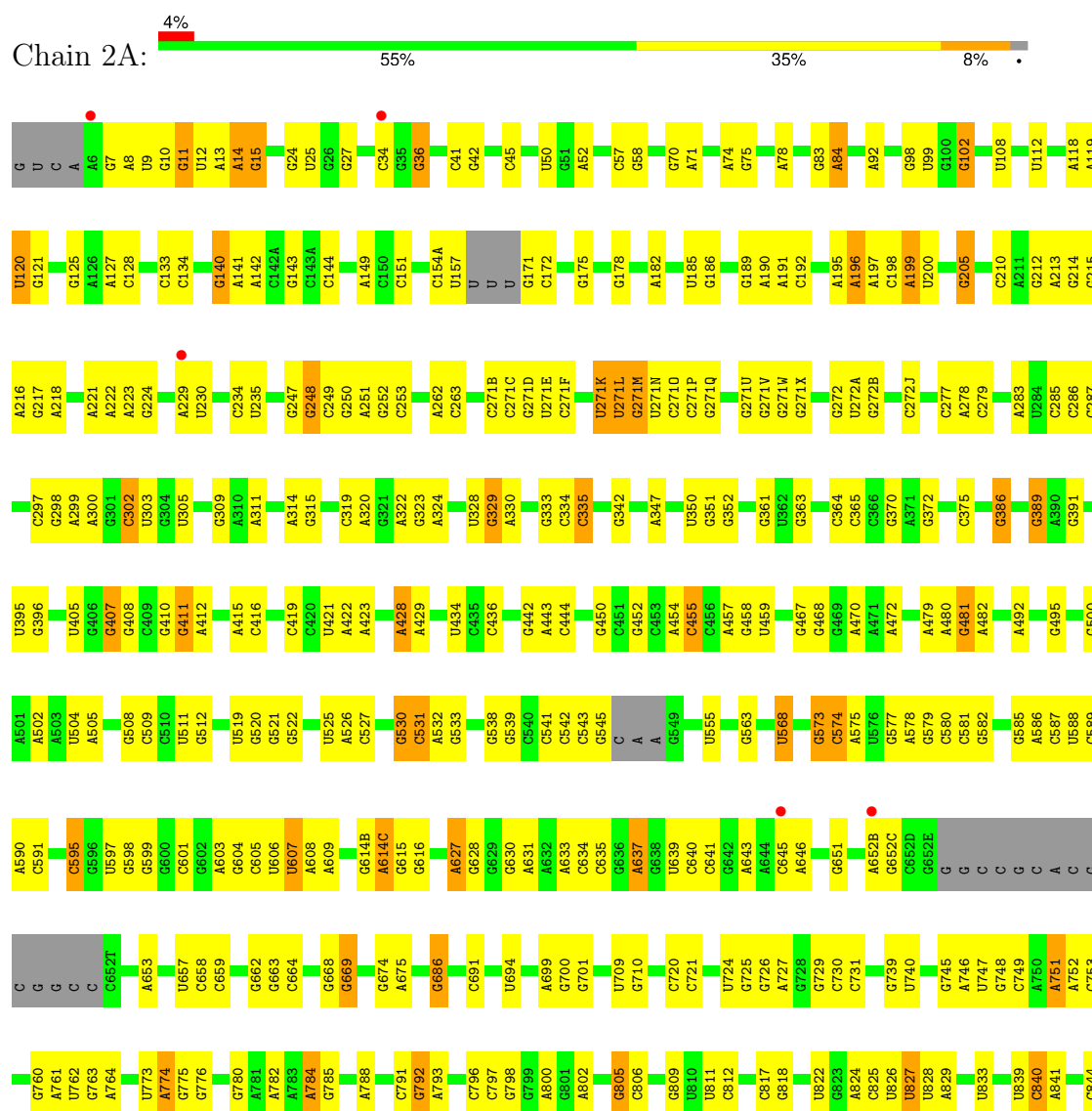
• Molecule 1: 23S Ribosomal RNA



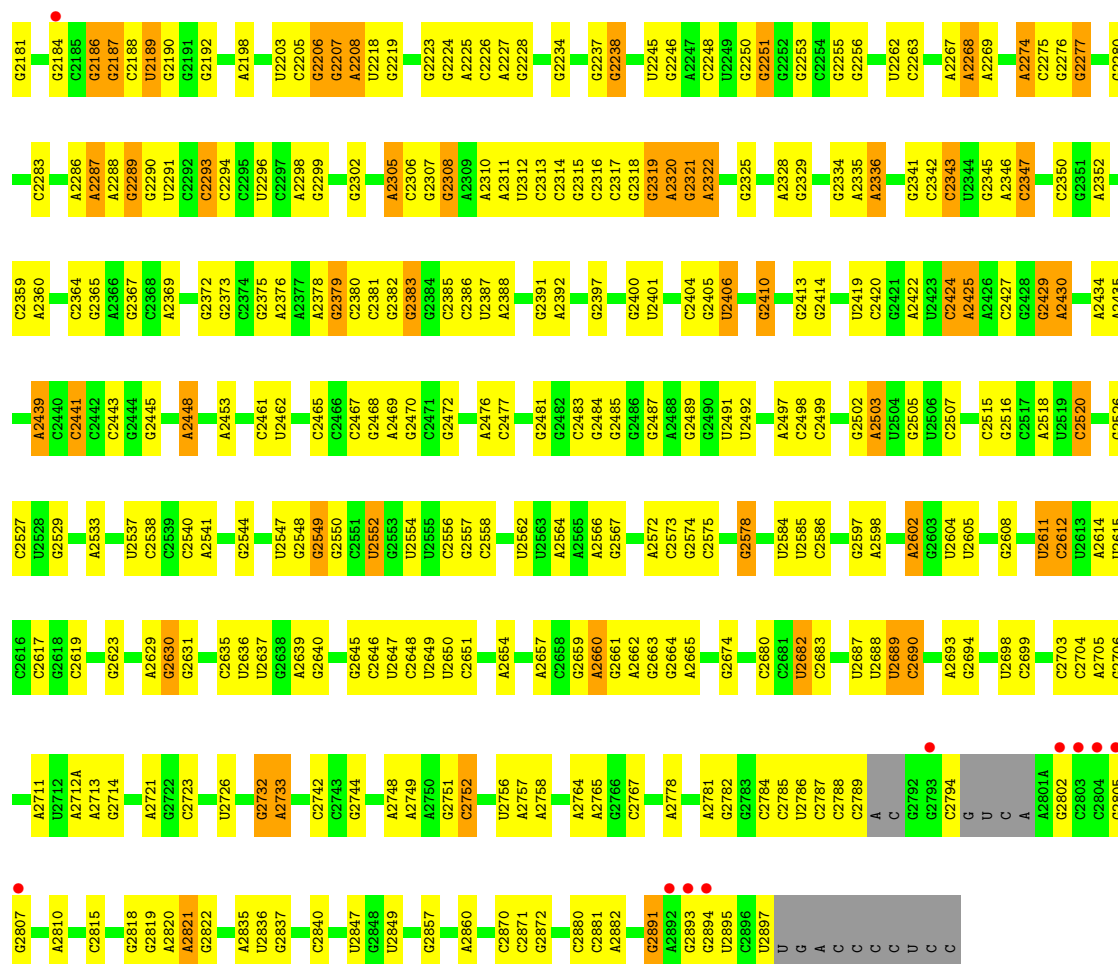
C2441	G2340	G2242	U2150	U2074	A1960	U1820	U1713	C1598	U1503	C1387	G1250	C1135	G1063
G2445	G2341	U2243	G2151	U2075	C1961	A1825	G1721	C1607	C1504	U1405	C1251	G1136	C1064
G2446	G2345	U2244	G2152	U2086	U1962	A1826	A1722	A1608	A1508	U1406	G1252	U1136	U1065
G2447	A2346	G2245	G2153	G2087	U1963	G1828	U1739	A1609	C1509A	C1407	A1253	U1141	U1066
A2448	G2347	C2248	G2154	G2090	C1967	A1829	G1740	A1610	A1509B	G1416	G1256	A1142A	A1067
G2454	U2348	G2251	G2155	G2099	A1970	G1840	A1741	A1616	G1509	G1417	G1257	A1143	A1069
G2455	G2349	G2252	G2156	G2093	A1971	G1844	G1742	G1622	G1511	G1418	C1258	C1153	A1070
G2456	G2350	G2253	A2158	G2094	A1972	G1845	C1745A	G1623	U1512	U1419	G1266	A1155	G1072
G2468	G2351	G2254	G2160	G2099	A1981	G1846	G1746	G1624	U1513	U1420	U1267	A1155	A1073
A2469	A2361	G2259	G2161	U2099	G1980	A1847	G1747	G1624	U1514	G1421	A1268	G1163	C1074
G2470	C2364	G2268	G2162	G2100	C1982	A1848	C1754	A1632	U1518	C1428	A1269	G1163	C1075
C2475	G2365	A2269	G2163	G2101	C1983	A1849	A1755	A1633	G1519	G1429	C1270	G1184	C1076
A2476	A2366	G2270	C2165	U2102	U1984	G1850	G1756	A1634	G1520	C1430	G1271	C1185	C1077
C2477	G2367	G2271	G2166	G2104	U1993	G1851	U1757	A1635	G1521	U1431	A1272	C1186	A1077
A2478	C2368	A2273	G2167	G2107	C1996	A1877	G1758	A1637	G1526	C1432	U1288	G1171	C1079
G2482	A2369	A2274	G2168	C2108	G1997	G1878	A1759	C1638	G1527	G1441	U1300	G1173	U1081
G2486	G2370	G2277	A2169	U2109	C2006	A1889	A1762	U1639	G1529	G1442	A1301	A1174	U1082
U2492	G2371	G2280	G2170	G2110	G2006	A1890	G1763	A1640	C1530	A1302	A1302	G1175	U1083
U2493	A2377	C2283	G2171	G2111	G2010	C1894	G1764	A1641	C1531	A1445	G1303	A1177	A1085
G2494	A2378	G2284	G2172	G2112	G2011	G1899	G1772	G1643	C1532	C1446	U1312	C1178	A1086
U2497	A2379	A2286	G2173	G2113	A2014	A1900	A1773	G1644	G	G1447	C1315	C1179	C1087
C2498	G2380	A2287	C2174	G2114	G2018	G1906	A1773	G1645	U	G1448	C1315	C1180	A1088
C2499	G2381	A2288	G2175	G2115	G2019	G1907	A1773	G1646	C	G1449	C1315	C1181	G1089
G2502	C2382	G2289	A2176	G2116	G2020	A1911	U1777	G1650	A1542	A1449	C1320	C1185	U1090
A2503	C2383	G2290	G2177	G2117	A2020	U1912	U1778	A1652	C1543	G1450	G1329	G1186	G1091
G2504	G2384	G2291	G2178	G2118	G2021	A1913	U1779	A1653	G1544	A1452	G1328	G1187	C1092
U2505	C2385	C2292	G2179	G2119	G2022	A1914	A1780	A1654	C1545	G1453	U1329	U1188	G1093
U2506	G2386	G2293	G2180	G2120	G2023	A1915	A1781	A1665	C1546	G1454	U1332	A1189	U1094
C2507	G2387	C2294	G2181	G2121	A2030	A1916	A1782	A1666	C1547	G1455	G1332	A1197	A1095
G2512	A2404	A2305	G2182	G2122	A2031	U1917	A1783	A1667	C1548	A1460	U1340	U1198	A1096
G2515	G2405	G2306	G2183	G2123	A2032	A1918	A1784	A1670	C1549	C1464	C1345	G1201	A1097
G2516	U2406	A2307	G2184	G2124	A2033	A1919	A1785	U1671	C1550	C1467	U1352	G1202	A1098
C2517	G2407	A2308	G2185	G2125	U2034	U1920	A1786	G1674	C1557	G1470	U1352	G1203	G1099
A2518	C2420	G2315	G2186	G2126	G2038	U1923	A1791	C1675	C1558	A1471	G1358	A1210	C1100
G2526	G2421	C2317	G2187	G2127	G2039	C1924	G1792	A1676	A1557	G1475	G1359	U1211	C1101
G2529	U2422	G2318	G2188	G2128	C2043	U1925	U1794	A1677	A1558	G1476	A1359	G1212	A1103
G2532	U2423	G2319	G2189	G2129	A2051	A1926	C1795	U1693	A1559	C1477	G1364	G1216	C1109
G2533	A2424	U2203	G2190	U2130	G2051	U1927	U1796	G1696	G1568	G1482	A1365	A1220	G1110
G2534	A2425	G2204	G2191	G2131	G2052	A1928	U1797	G1697	A1569	G1486	C1370	A1226	A1111
G2535	G2426	G2205	G2192	G2132	G2053	G1930	U1798	A1698	A1570	A1486	U1372	G1227	G1112
U2537	C2427	G2206	G2193	G2133	A2059	C1934	G1800	G1699	U1578	G1487	G1371	G1228	G1115
C2538	G2428	G2207	G2194	G2134	A2060	G1935	A1801	A1700	A1579	G1487	U1372	G1229	C1116
G2543	G2429	A2208	G2195	U2135	A2061	A1936	A1802	A1701	A1580	A1490	A1378	G1230	G1117
G2544	A2430	G2328	G2196	A2136	G2061	A1937	C1804	U1706	G1581	A1491	A1379	G1231	C1118
G2545	U2431	G2329	G2197	G2137	G2062	A1938	U1804	G1708	A1582	C1493	G1380	G1231	A1126
G2546	G2432	G2330	G2198	G2138	G2063	U1939	A1815	C1709	C1583	C1494	G1381	G1236	A1127
G2547	A2433	G2331	G2199	G2139	G2064	C1942	G1816	U1709	G1584	A1495	G1382	G1236	A1128
G2548	G2434	G2332	G2200	G2140	G2065	U1955	G1817	C1710	C1585	A1496	A1384	A1241	U1129
G2549	A2435	A2333	G2201	G2141	G2066	C2072	U1818	C1711	A1587	U1497	G1385	A1246	U1130
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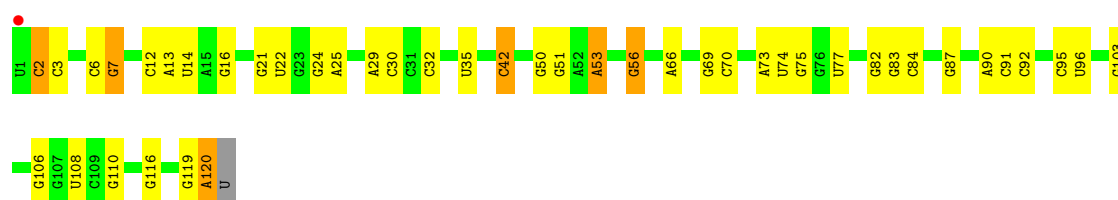
• Molecule 1: 23S Ribosomal RNA



G2023	A1918	G1666	G1559	C1451	A1359	U1255	C1166	U1081	G1015	G928	G845
G2028	A1919	G1667	C1566	A1452	A1360	G1256	U1167	U1082	G1016	G932	G848
G2029	G1920	A1668	C1566	G1455	G1364	G1264	G1168	U1084	G1017		
A2030	G1921	A1669	A1566	G1455	A1365	A1265	G1170	A1085	A1021	G940	U851
A2031	G1922	C1670	A1569	G1459	A1366	G1266	G1171	A1086	G1022	G941	G852
G2032	U1926	C1671	A1569	G1459	A1367	U1267	G	G1087	U1023	G942	G853
A2033	A1927	G1674	U1576	G1466	A1368	A1268	A	U1088	U1026	A945	G854
C2036	U1928	C1577	C1577	C1467	G1371	G1271	U	G1089	A1027	G946	G855
G2037	G1929	U1688	U1578	G1470	U1372	A1272	G	U1090	A1028	G947	C856
G2038	G1930	G1696	A1579	A1471	U1373	U1273	A	G1091		G948	U858
C2039	A1938	G1696	A1580	A1471	A1373		C1178	G1092	A1032	G949	G859
C2040	U1939	A1700	C1581	G1479	A1378	A1278	C1180	G1093	U1033		
C2043	G1942	A1701	C1582	G1479	A1379	G1279	C1181	U1094	U1033	G952	G864
C2043	C1942	G1702	A1583	G1482	G1380	G1280	C1181	A1095	G1034	G953	G865
A2051	A1952	G1703	A1586	A1494	A1395	G1281	G1184	U1096	U1035	G954	A866
C2055	G1955	G1714	A1587	U1489	A1384	U1292	G1185	U1097	G1036		A867
G2056	U1955	G1717	G1591	A1490	G1385	C1293	G1186	U1098	G1037	U958	
A2060	G1959	G1718	C1592	G1491	C1386	C1293	U1188	C1104	C1038	U959	G875
G2061	C1827	U1720	G1593	A1494	A1399	U1300	A1189	U1105	C1041	A960	C876
C2064	U1963	G1721	G1594	A1497	A1400	U1292	G1195	G1107	G1042	G961	U877
C2065	C1967	G1717	U1602	C1503	G1401	C1306	C1201	G1110	G1043	G962	G879
U2068	G1968	G1718	A1603	U1503	U1405	C1306	C1202	A1111	A1045	G963	G880
A1970	A1969	G1719	A1603	C1504	U1405	C1306	G1203	G1112	A1046	G966	G881
A1971	A1970	U1720	A1608	C1505	G1410	C1314	U1204	U1113	A1047	G967	G882
A1972	A1971	C1827	A1609	U1506	G1411	U1316	U1205	U1114	A1048	G968	
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G2083	A1877	G1750	A1614	A1509A	G1416	C1320	U1212	C1124	A1054	G979	C889
U2086	G1878	G1754	G1623	G1515	C1417	A1322	G1216	G1125	G1056	A981	A890
C2097	C1881	A1755	G1624	C1516	A1419	U1393	G1217	A1129	A1057	G982	C893
U2098	C1882	G1756	A1631	A1528A	U1420	G1324	C1218	U1130	G1058	A983	U895
U2099	G1883	A1762	A1632A	G1529	G1421	G1325	G1219	G1131	G1059	A988	A896
G2100	G1889	G1763	A1633	G1530	G1422	G1328	A1220	C1135	U	G989	C898
G2101	A1889	G1764	A1634	C1531	A1427	G1328	G1221	G1136	G1062	A990	A900
U2102	A1890	C1771	A1637	U1532	C1428	G1332	C1221A	G1137	G1063	C991	A901
C2103	G1899	A1772	A1637	G1533	G1429	G1332	G1235	G1138	U1065	G992	C902
G2104	A1900	A1773	C1638	A	C1430	U1340	G1236	C1147	U1066	G993	C903
G2105	C1901	U1779	U1639	C1536	G1436	G1341	C1230	A1142A	A1067	C994	
G2106	A1902	A1780	A1641	G1537	C1437	A1342	G1231	A1143	G1068	A996	A910
C2107	G1906	C1781	A1642	G1538	G1437	G1343	G1235	G1144	A1069	G997	A911
U2108	G2004	C1782	G1642	G1539	G1442	G1345	G1236	G1147	A1070		
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C2110	G1910	A1783	C1648	C1543	A1445A	A1349	U1241	C1153	A1072	G1002	A917
A2014	U1911	A1786	A1787	G1546	A1446	U1352	A1247	G1154	G1073	C1006	G921
U2113	A1912	C1788	C1657	C1547	G1447	A1353	G1248	C1161	C1075	A1010	U922
G2018	A1913	U1789	C1658	G1547	G1448	A1354	G1248	A1077	G1076	G1011	C923
A2019	C1914	A1789	C1658	G1547	A1449	A1354	A1253	U1078	A1077	U1012	C924
A2020	U1915	C1790	A1664	C1557	G1450	A1354	A1253	C1162	C1079	C1013	
C2021	A1916	G1790	A1664	A1558	C1450A	G1358	A1254	U1165	C1080	U1014	G927
U2022	U1917	A1791	A1665								



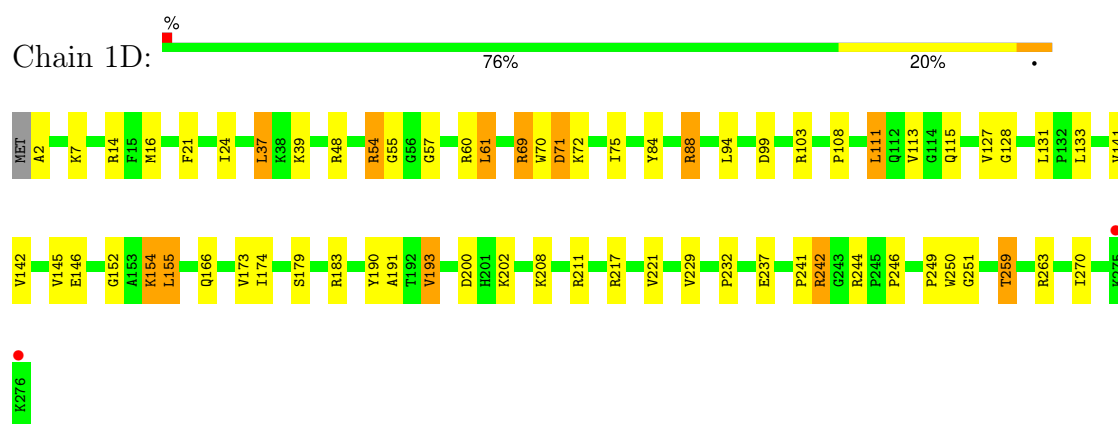
• Molecule 2: 5S Ribosomal RNA



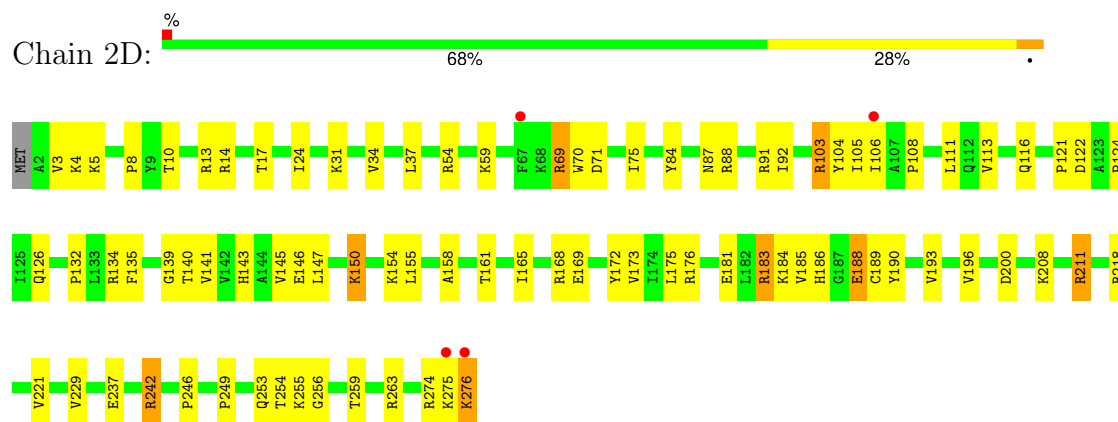
• Molecule 2: 5S Ribosomal RNA



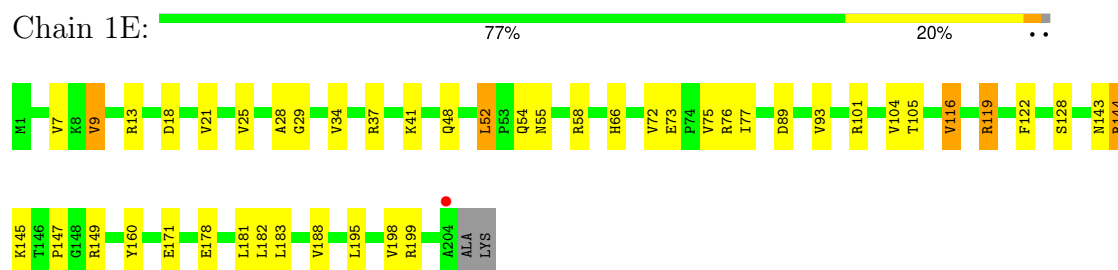
• Molecule 3: 50S ribosomal protein L2



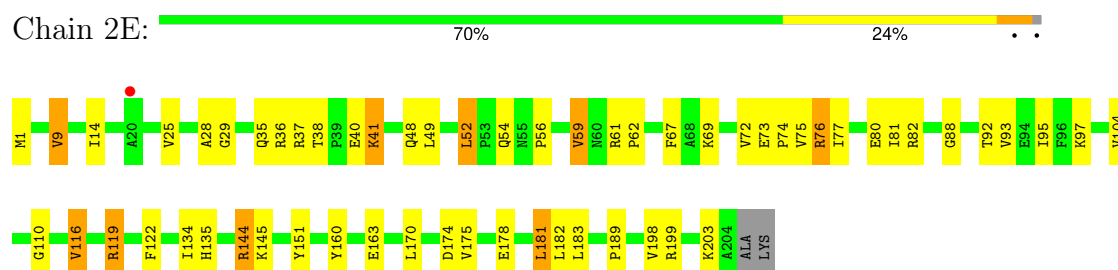
- Molecule 3: 50S ribosomal protein L2



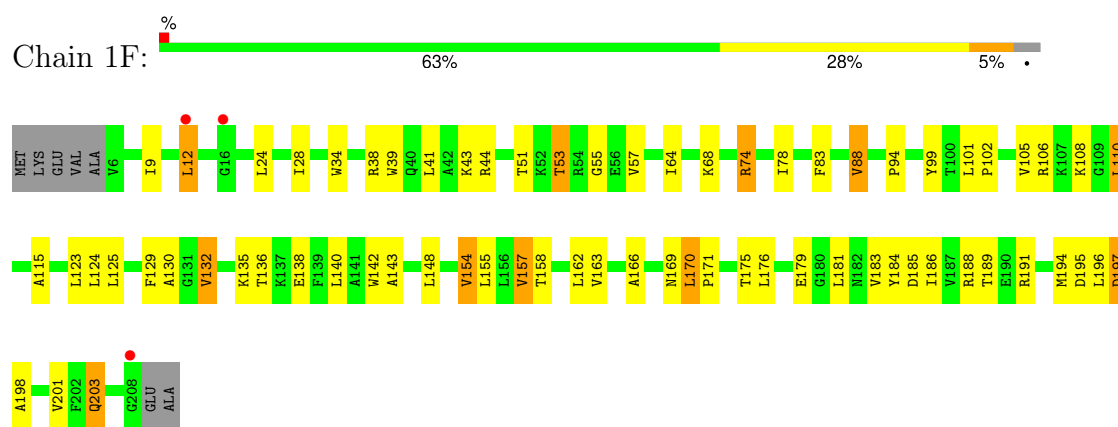
- Molecule 4: 50S ribosomal protein L3



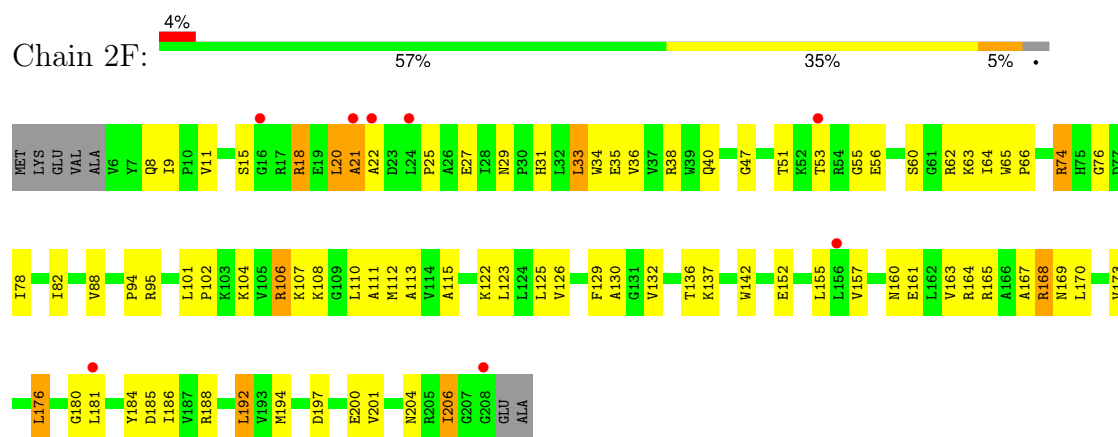
- Molecule 4: 50S ribosomal protein L3



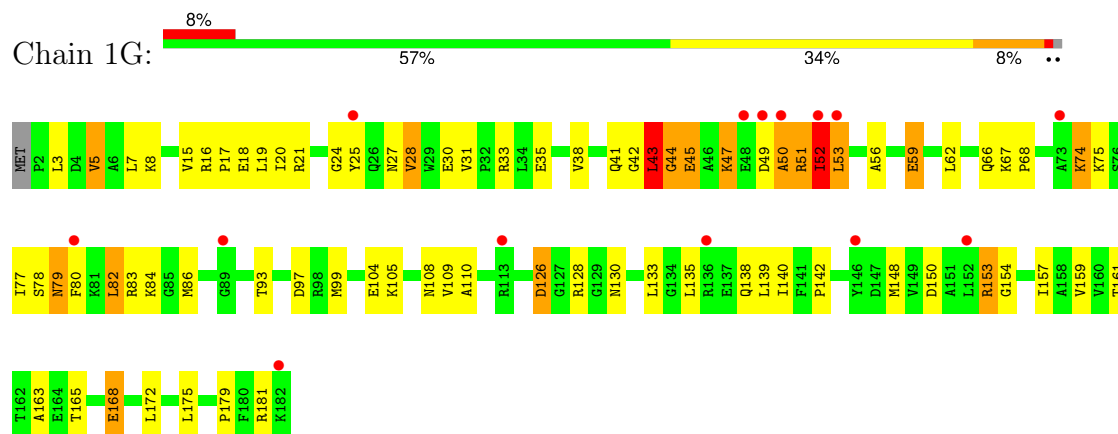
- Molecule 5: 50S ribosomal protein L4



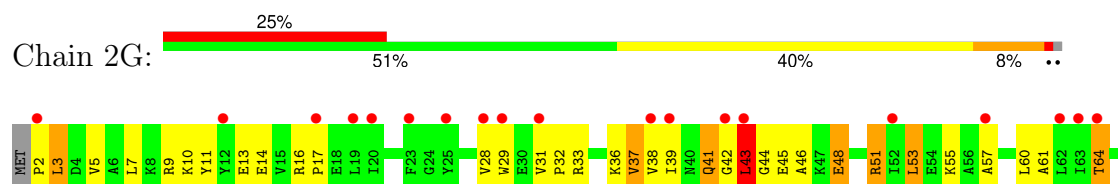
• Molecule 5: 50S ribosomal protein L4

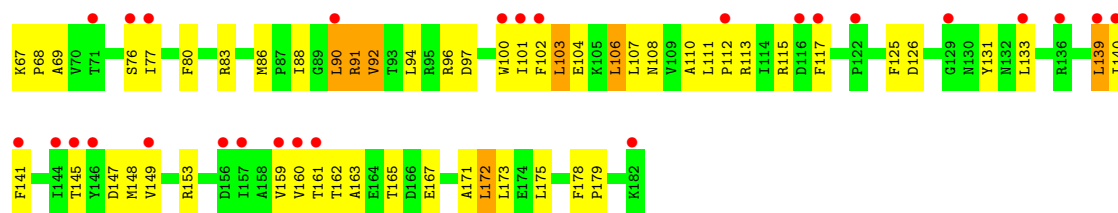


• Molecule 6: 50S ribosomal protein L5

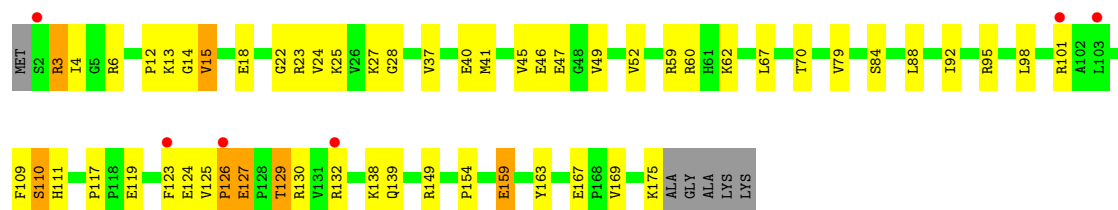


• Molecule 6: 50S ribosomal protein L5

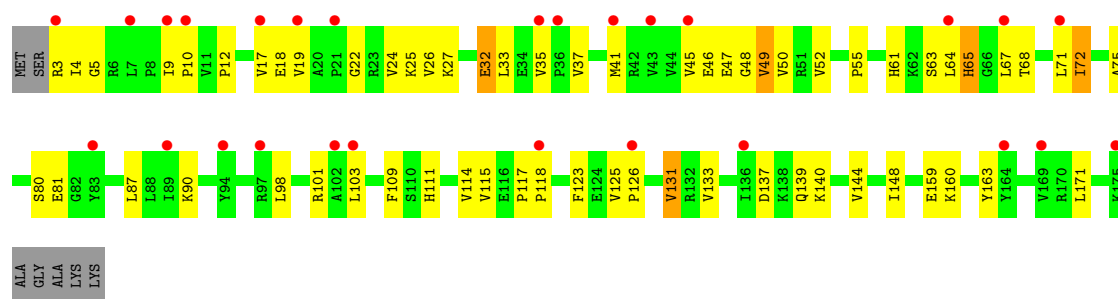




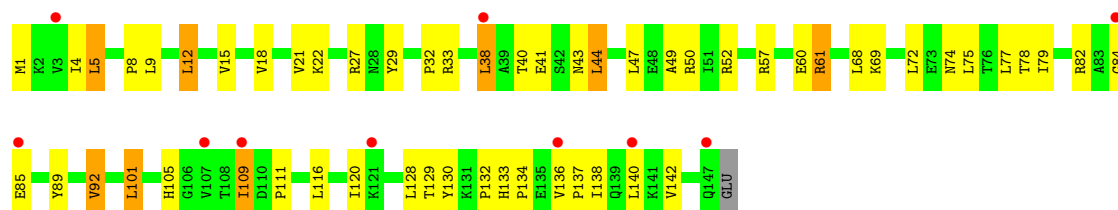
• Molecule 7: 50S ribosomal protein L6



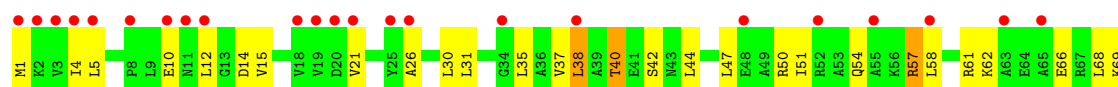
• Molecule 7: 50S ribosomal protein L6

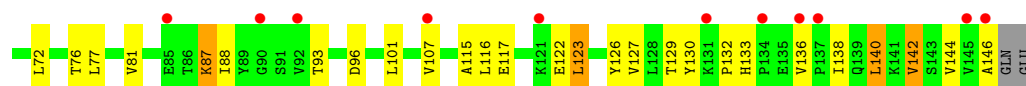


• Molecule 8: 50S ribosomal protein L9

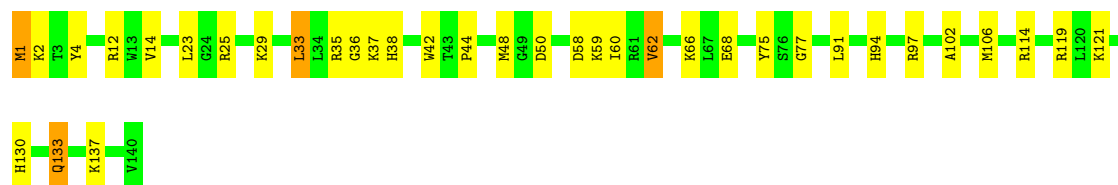


• Molecule 8: 50S ribosomal protein L9

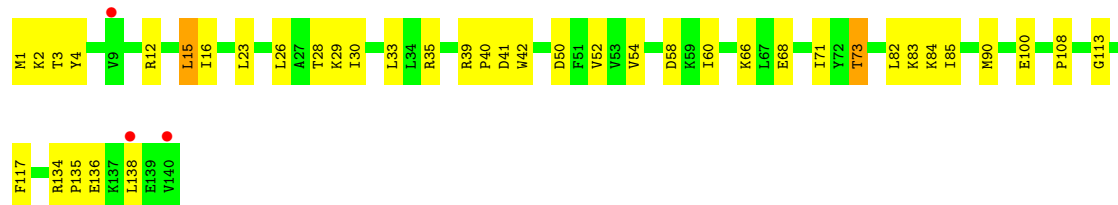
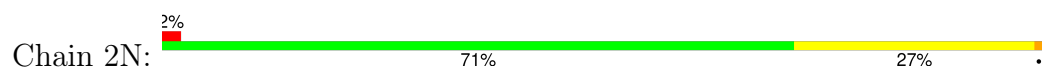




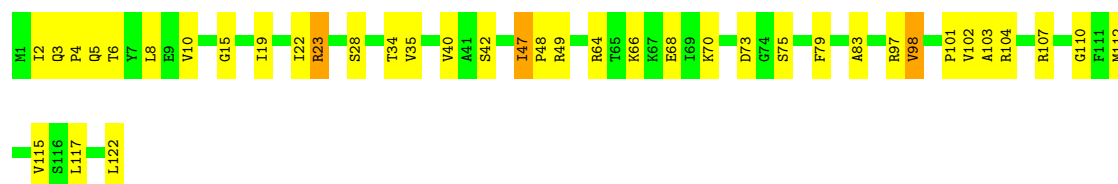
• Molecule 9: 50S ribosomal protein L13



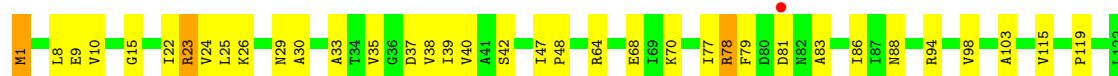
• Molecule 9: 50S ribosomal protein L13



• Molecule 10: 50S ribosomal protein L14



• Molecule 10: 50S ribosomal protein L14

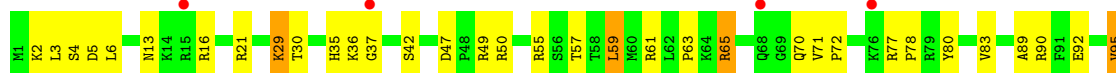


• Molecule 11: 50S ribosomal protein L15

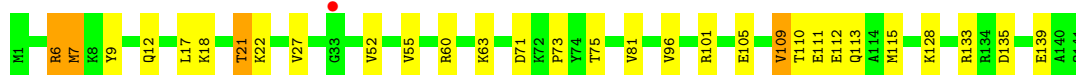
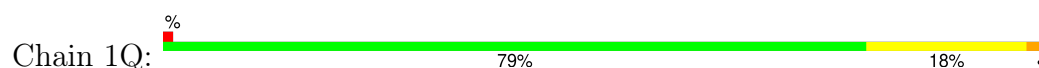




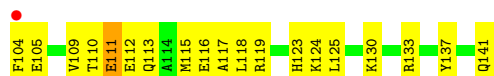
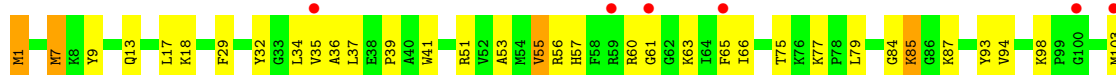
- Molecule 11: 50S ribosomal protein L15



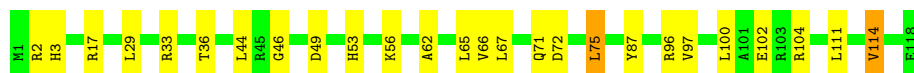
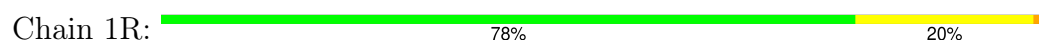
- Molecule 12: 50S ribosomal protein L16



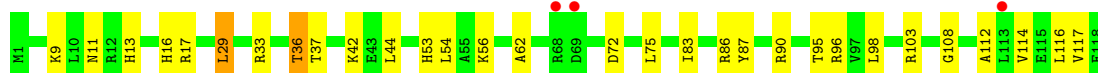
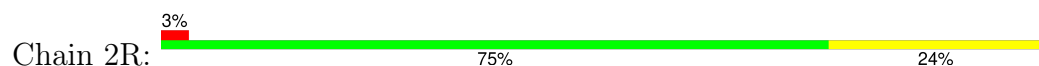
- Molecule 12: 50S ribosomal protein L16



- Molecule 13: 50S ribosomal protein L17



- Molecule 13: 50S ribosomal protein L17

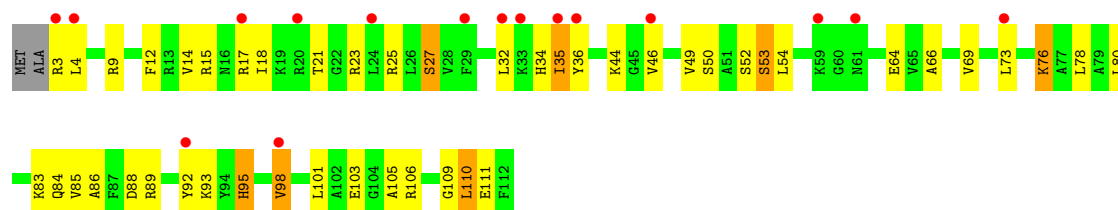


- Molecule 14: 50S ribosomal protein L18

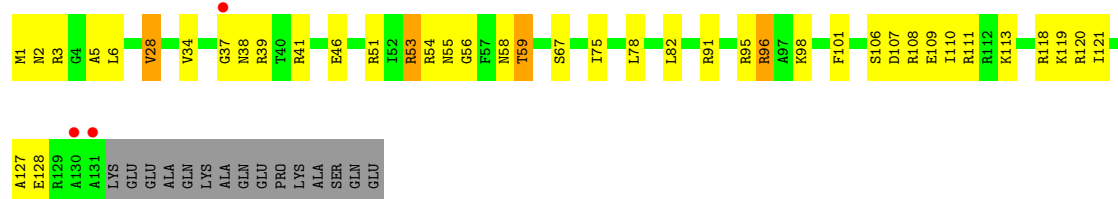




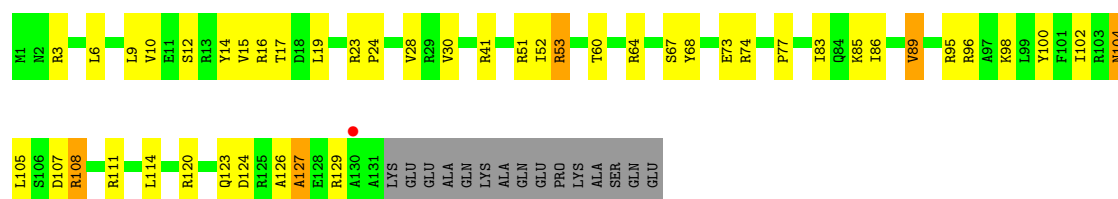
- Molecule 14: 50S ribosomal protein L18



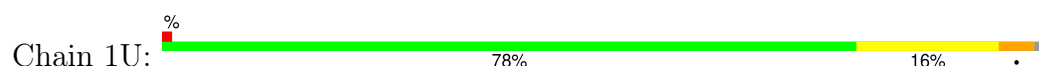
- Molecule 15: 50S ribosomal protein L19



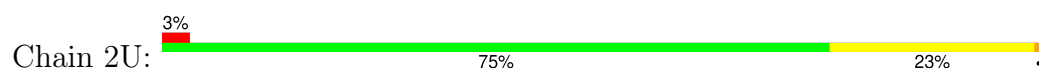
- Molecule 15: 50S ribosomal protein L19



- Molecule 16: 50S ribosomal protein L20

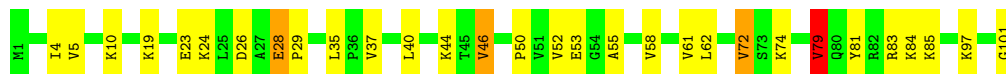


- Molecule 16: 50S ribosomal protein L20



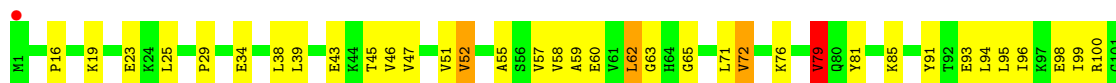
- Molecule 17: 50S ribosomal protein L21

Chain 1V:  70% 26% ..



- Molecule 17: 50S ribosomal protein L21

Chain 2V:  64% 32% ..



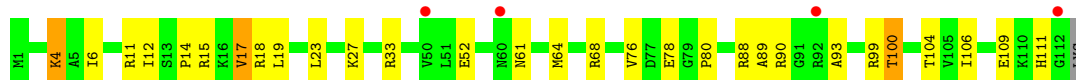
- Molecule 18: 50S ribosomal protein L22

Chain 1W:  75% 22% ..



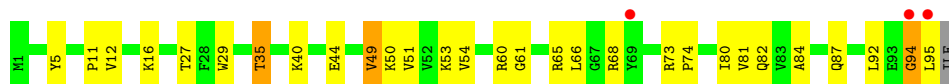
- Molecule 18: 50S ribosomal protein L22

Chain 2W:  73% 23% ..



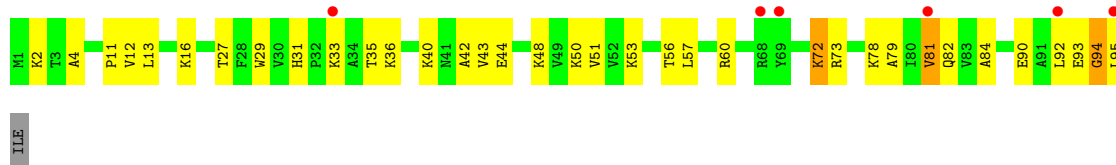
- Molecule 19: 50S ribosomal protein L23

Chain 1X:  69% 27% ..



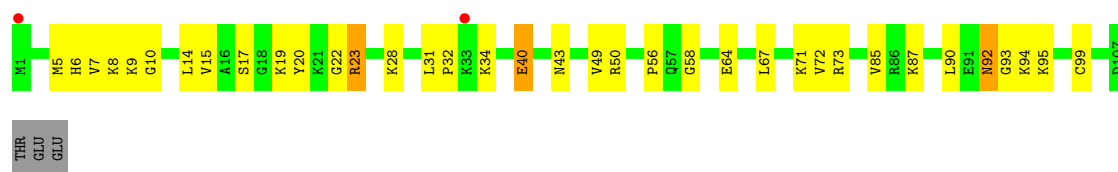
- Molecule 19: 50S ribosomal protein L23

Chain 2X:  63% 33% ..

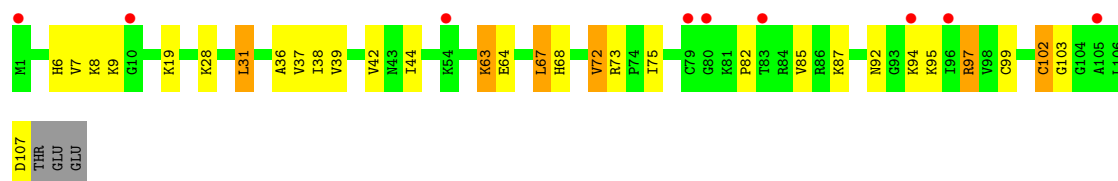


- Molecule 20: 50S ribosomal protein L24

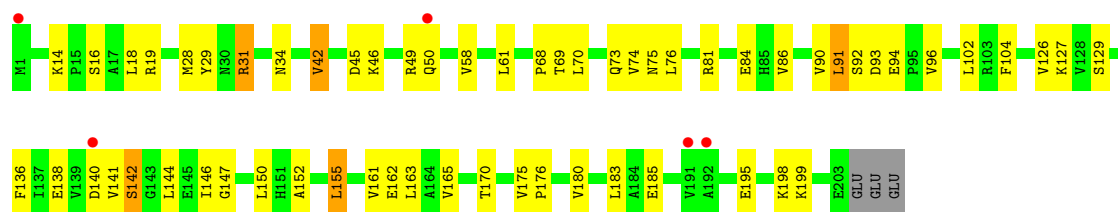
Chain 1Y:  65% 30% ..



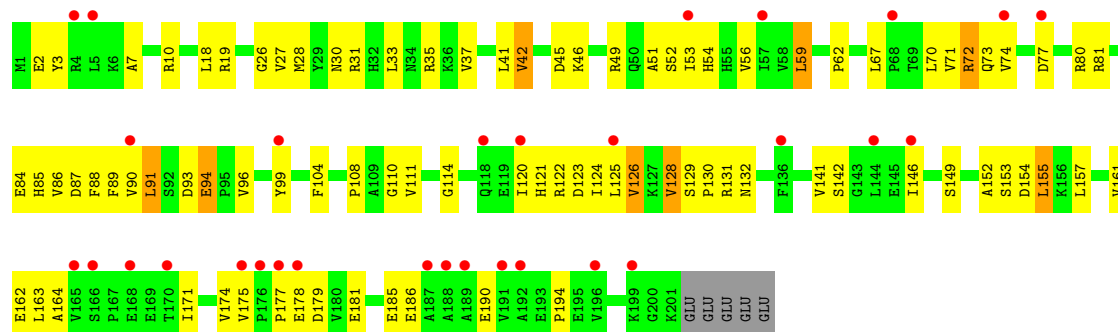
- Molecule 20: 50S ribosomal protein L24



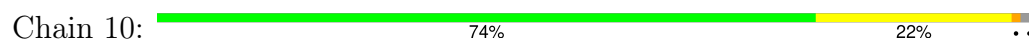
- Molecule 21: 50S ribosomal protein L25



- Molecule 21: 50S ribosomal protein L25



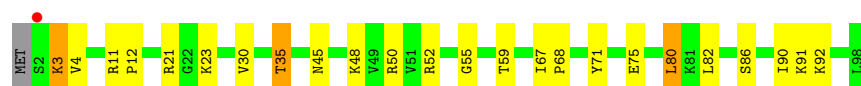
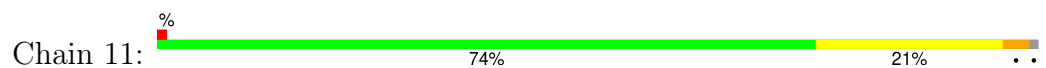
- Molecule 22: 50S ribosomal protein L27



- Molecule 22: 50S ribosomal protein L27



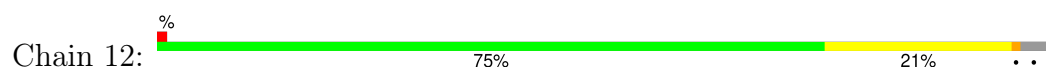
• Molecule 23: 50S ribosomal protein L28



• Molecule 23: 50S ribosomal protein L28



• Molecule 24: 50S ribosomal protein L29



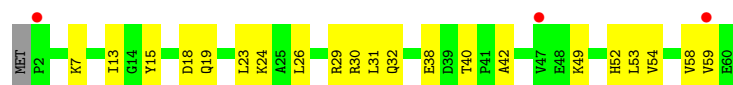
• Molecule 24: 50S ribosomal protein L29



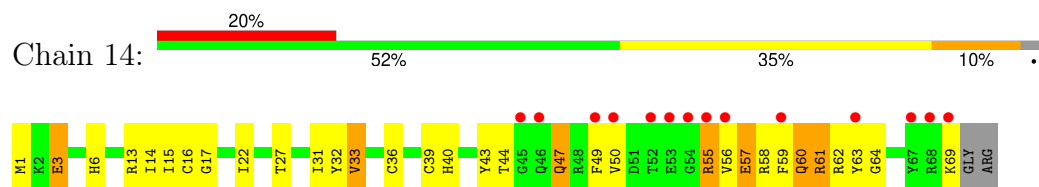
• Molecule 25: 50S ribosomal protein L30



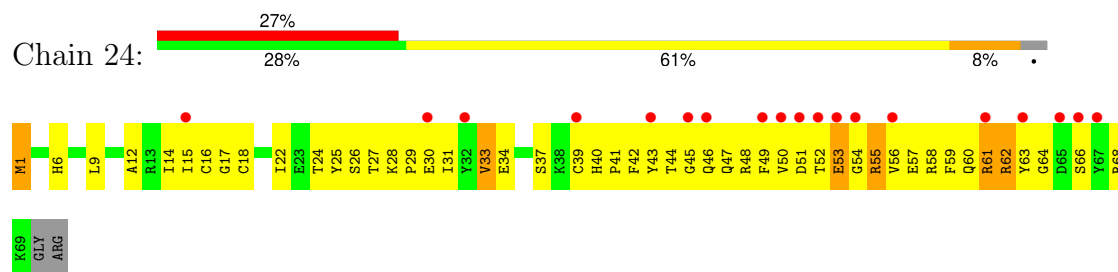
• Molecule 25: 50S ribosomal protein L30



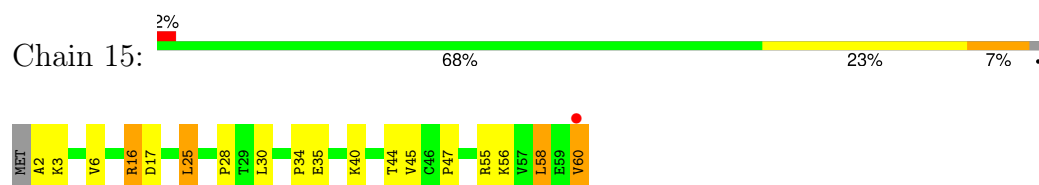
- Molecule 26: 50S ribosomal protein L31



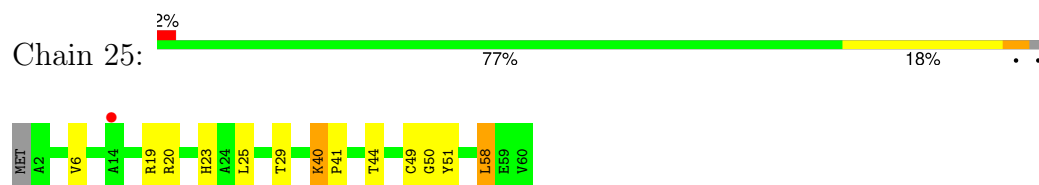
- Molecule 26: 50S ribosomal protein L31



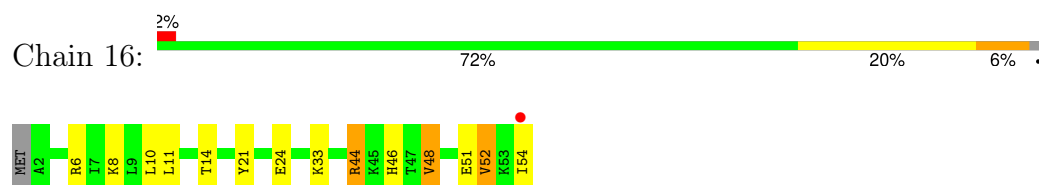
- Molecule 27: 50S ribosomal protein L32



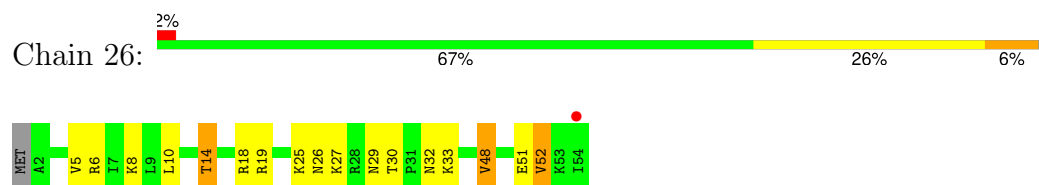
- Molecule 27: 50S ribosomal protein L32



- Molecule 28: 50S ribosomal protein L33

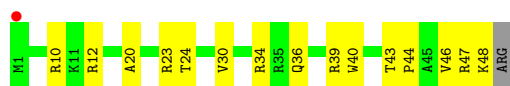


- Molecule 28: 50S ribosomal protein L33

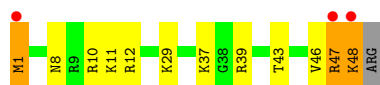
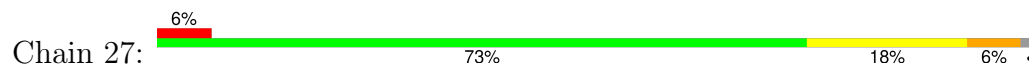


- Molecule 29: 50S ribosomal protein L34





- Molecule 29: 50S ribosomal protein L34



- Molecule 30: 50S ribosomal protein L35



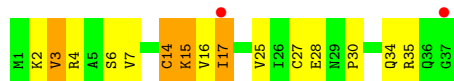
- Molecule 30: 50S ribosomal protein L35



- Molecule 31: 50S ribosomal protein L36



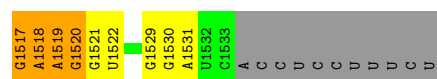
- Molecule 31: 50S ribosomal protein L36



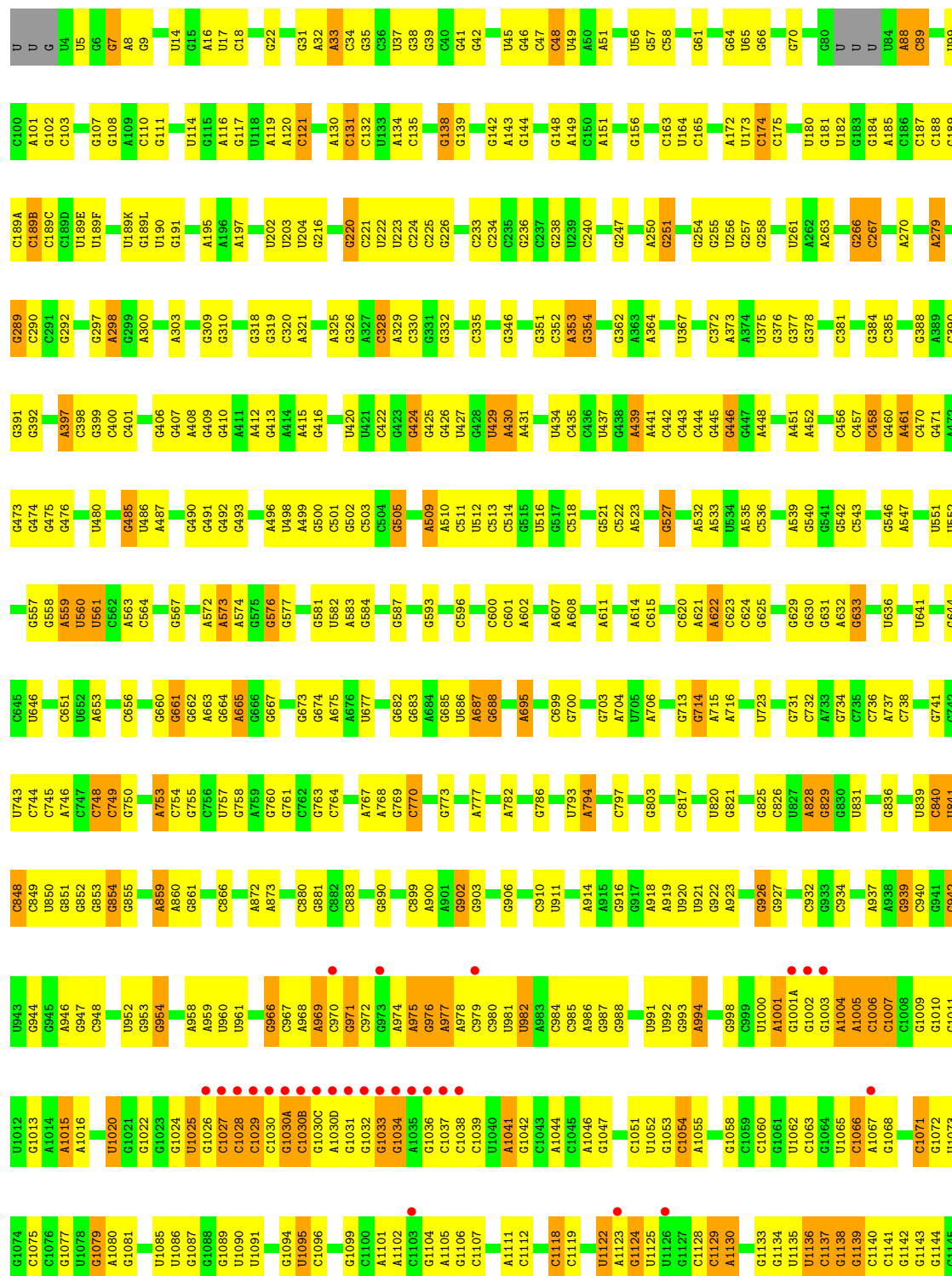
- Molecule 32: 16S Ribosomal RNA

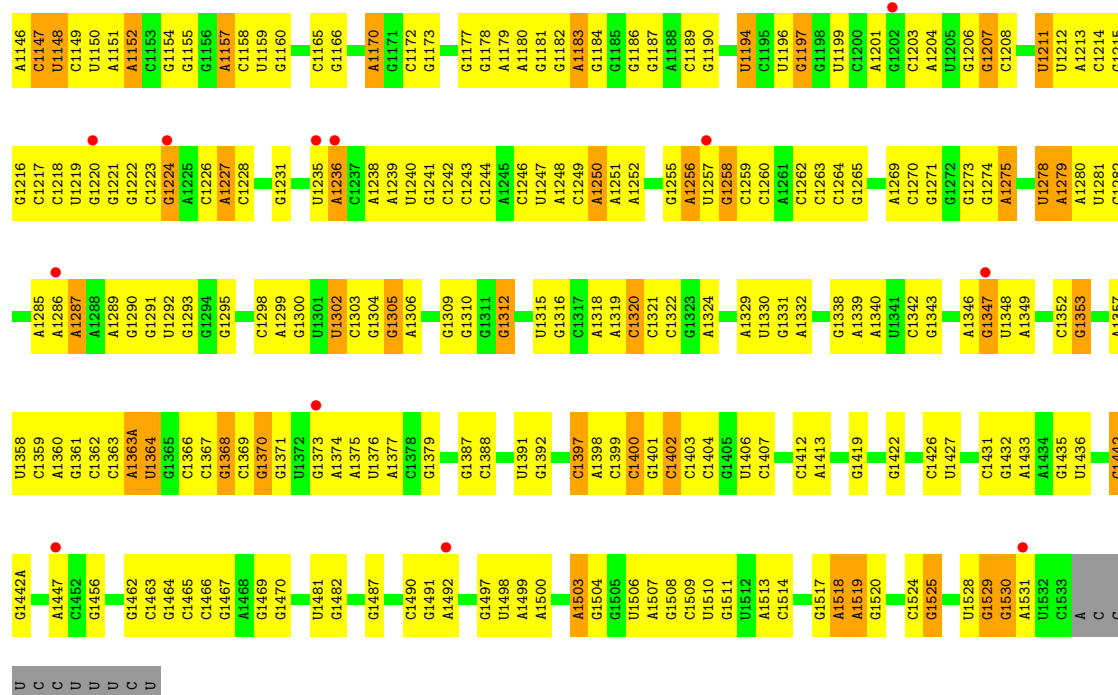


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C1411	C1325	G1233	A1055	G987	G890	G756	A563	C479	C385	G289	U189D	C1411
C1412	C1326	G1234	G1058	G988	G891	G757	C564	G485	U387	G292	U189E	C1412
U1413	A1329	A1238	C1059	G991	G902	G758	G567	U486	G388	G293	U189F	U1413
U1414	A1333	G1239	C1060	U991	G906	A759	A572	A487	A389	C294	G189G	U1414
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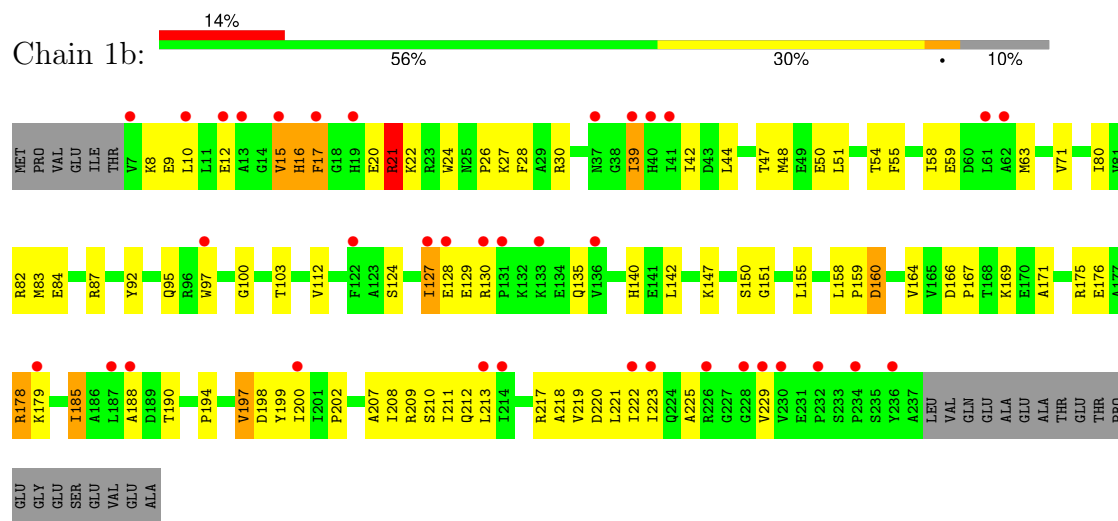


Molecule 32: 16S Ribosomal RNA

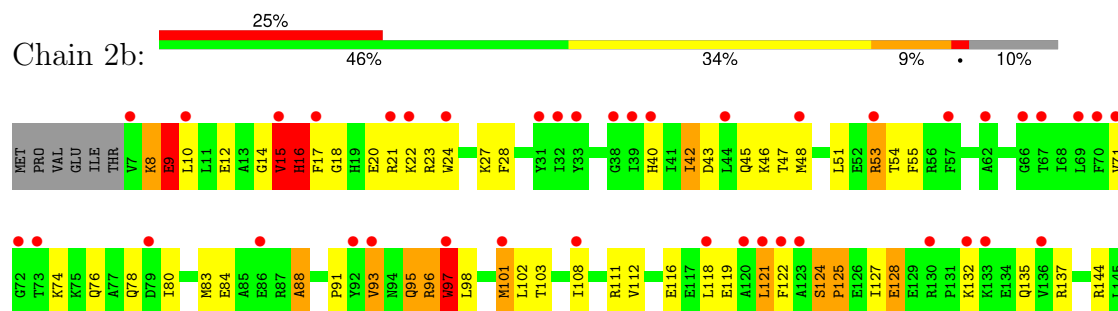


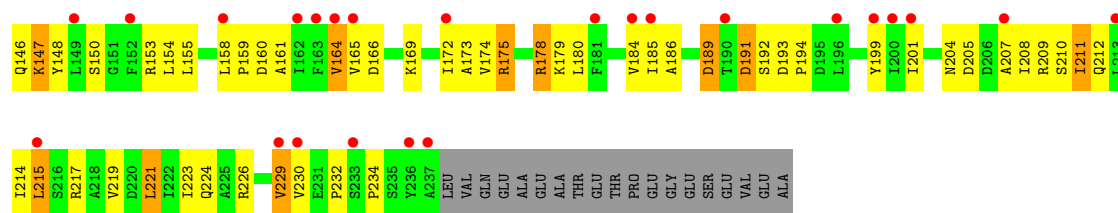


• Molecule 33: 30S ribosomal protein S2

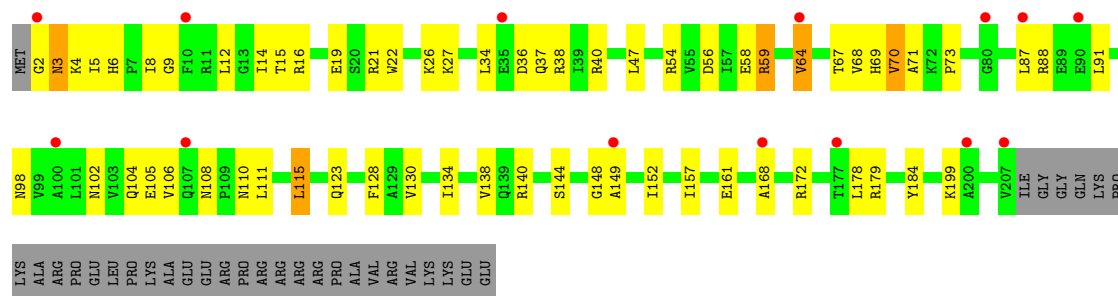


• Molecule 33: 30S ribosomal protein S2

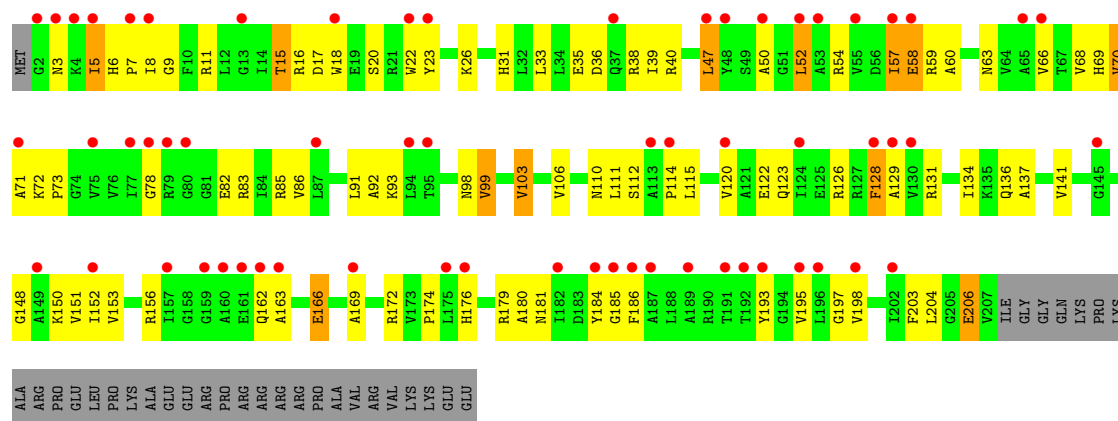




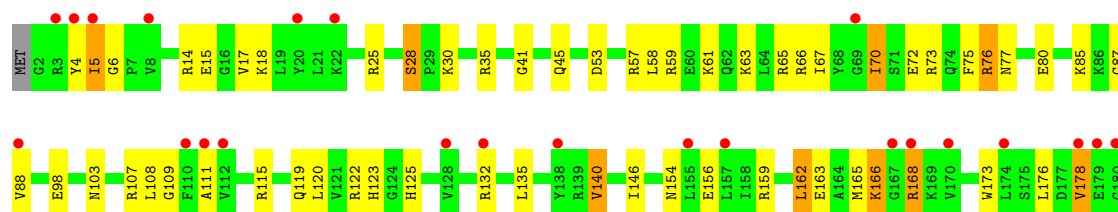
• Molecule 34: 30S ribosomal protein S3

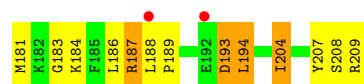


• Molecule 34: 30S ribosomal protein S3

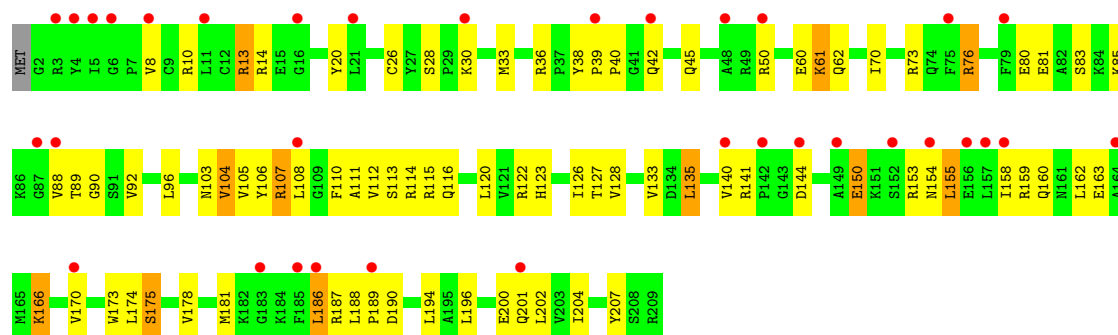


• Molecule 35: 30S ribosomal protein S4

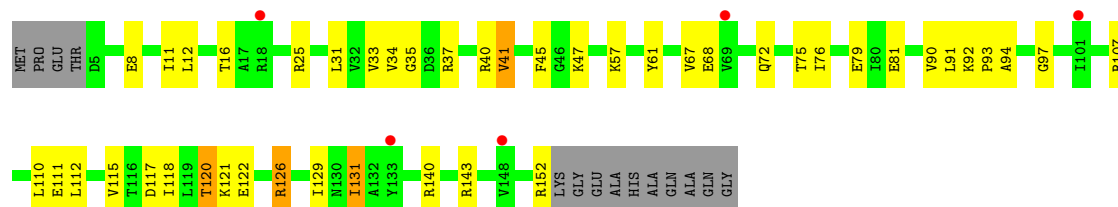




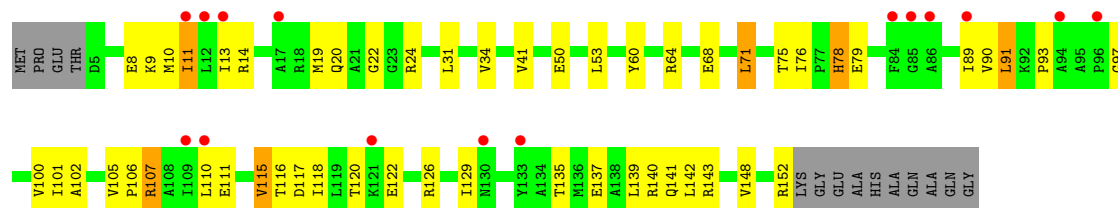
- Molecule 35: 30S ribosomal protein S4



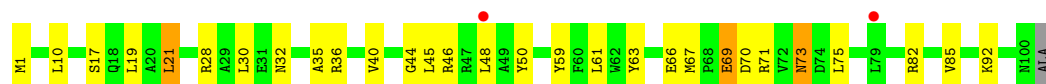
- Molecule 36: 30S ribosomal protein S5



- Molecule 36: 30S ribosomal protein S5

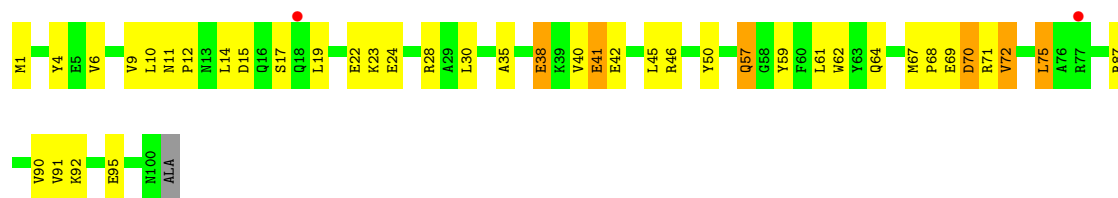


- Molecule 37: 30S ribosomal protein S6

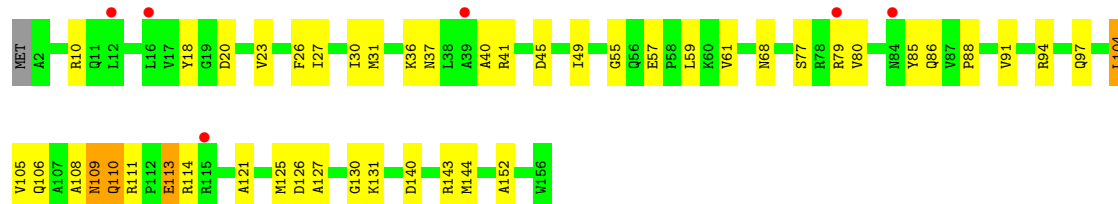


- Molecule 37: 30S ribosomal protein S6

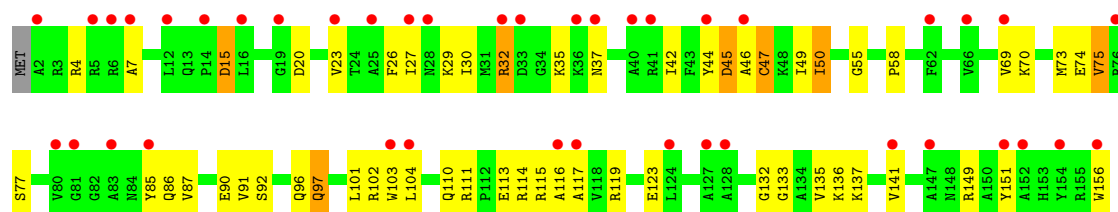




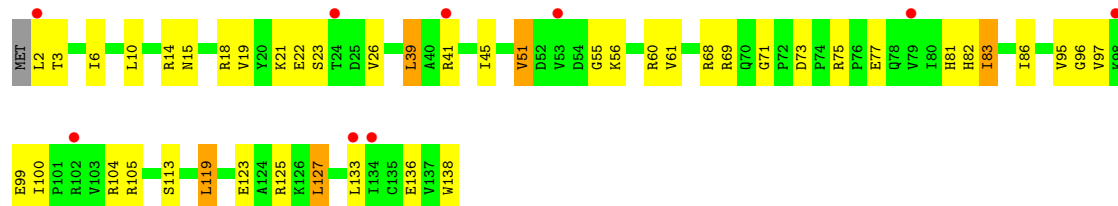
• Molecule 38: 30S ribosomal protein S7



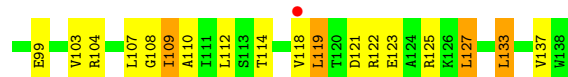
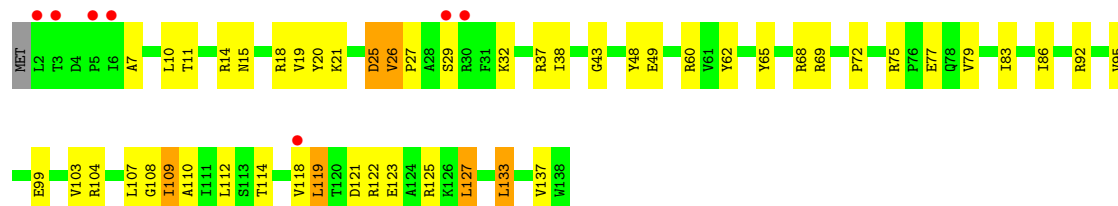
• Molecule 38: 30S ribosomal protein S7



• Molecule 39: 30S ribosomal protein S8

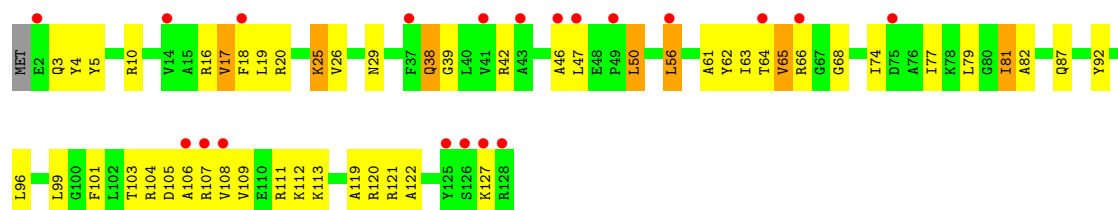


• Molecule 39: 30S ribosomal protein S8

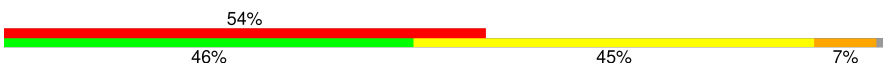


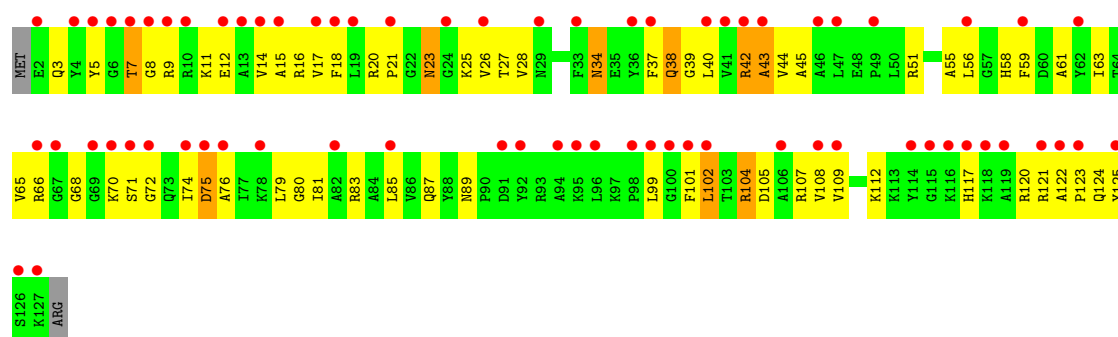
- Molecule 40: 30S ribosomal protein S9

Chain 1i: 



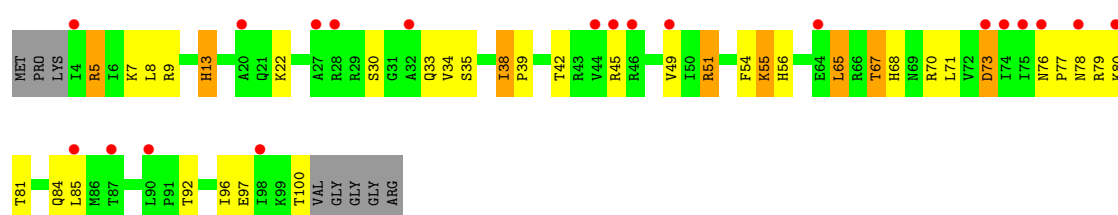
- Molecule 40: 30S ribosomal protein S9

Chain 2i: 



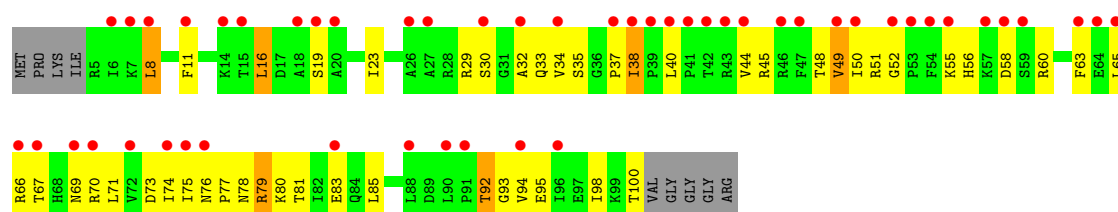
- Molecule 41: 30S ribosomal protein S10

Chain 1j: 

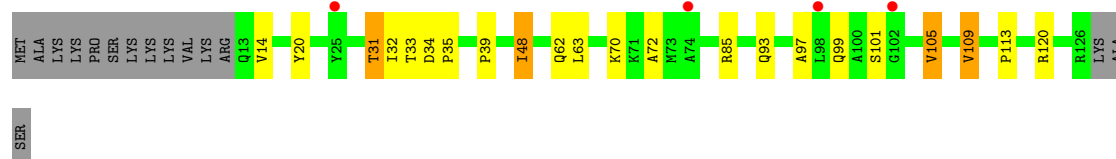
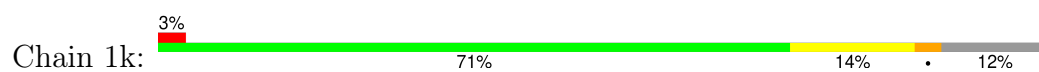


- Molecule 41: 30S ribosomal protein S10

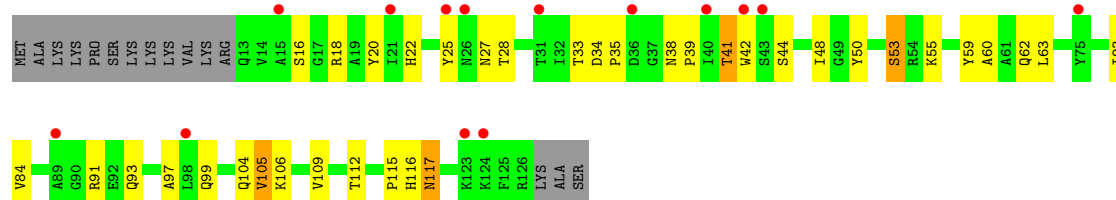
Chain 2j: 



- Molecule 42: 30S ribosomal protein S11



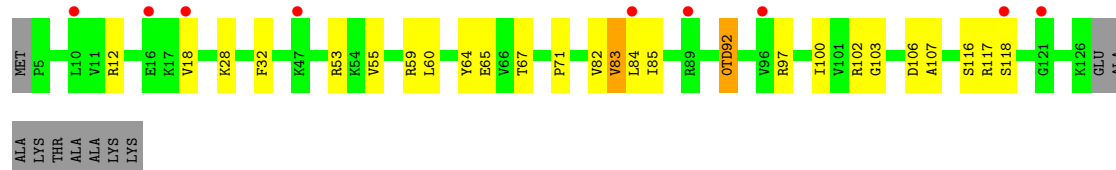
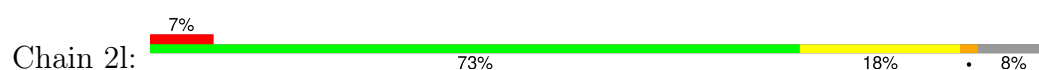
- Molecule 42: 30S ribosomal protein S11



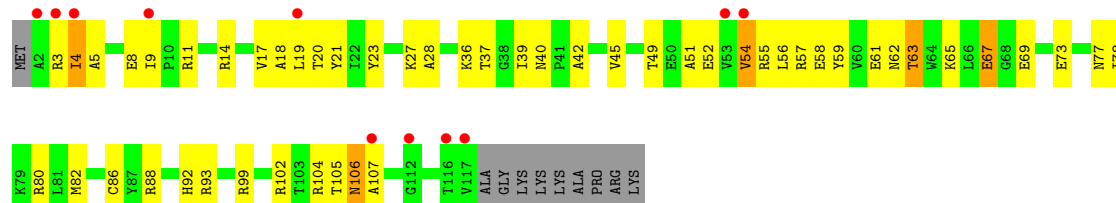
- Molecule 43: 30S ribosomal protein S12



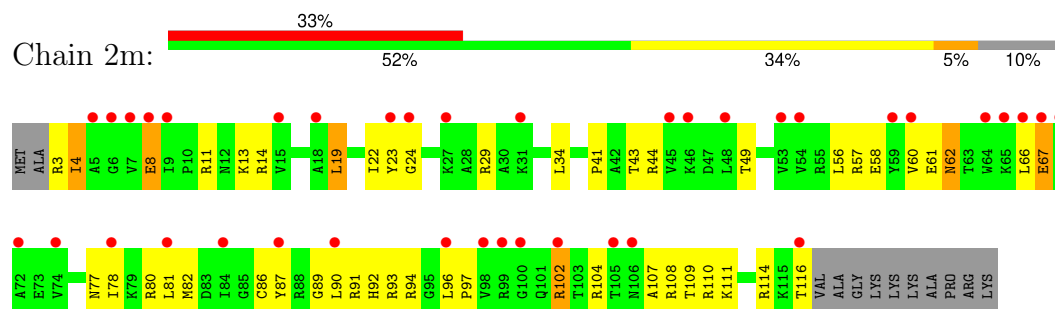
- Molecule 43: 30S ribosomal protein S12



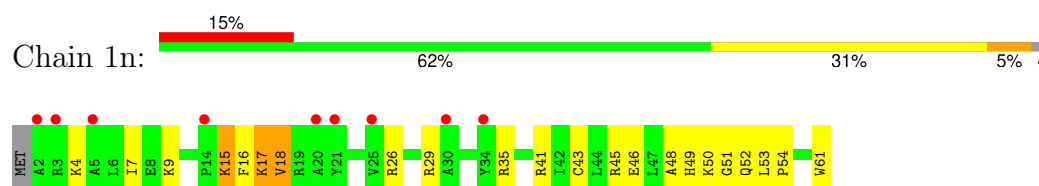
- Molecule 44: 30S ribosomal protein S13



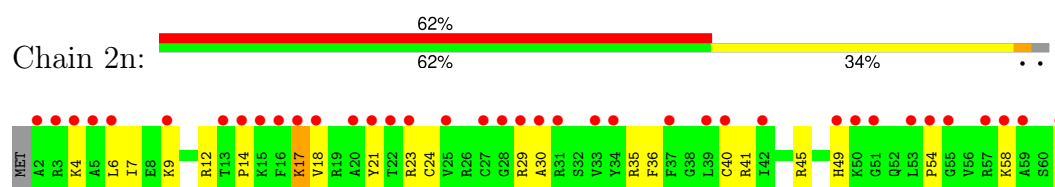
- Molecule 44: 30S ribosomal protein S13



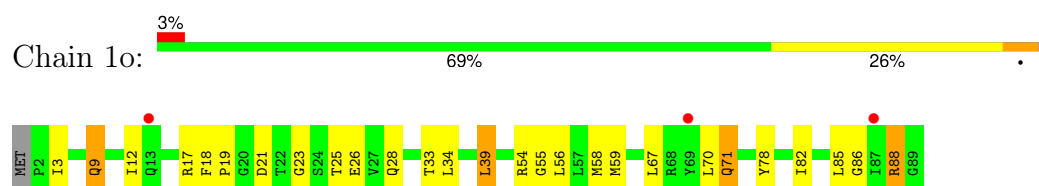
- Molecule 45: 30S ribosomal protein S14 type Z



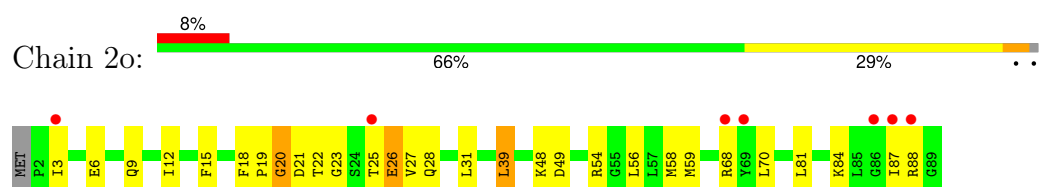
- Molecule 45: 30S ribosomal protein S14 type Z



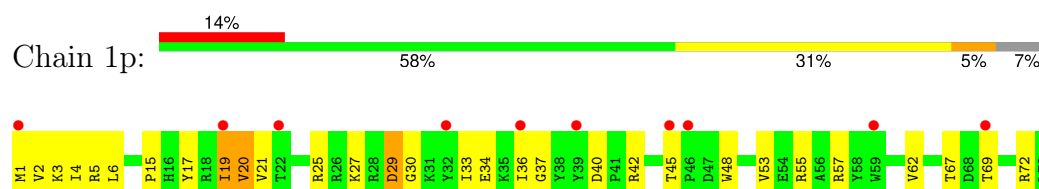
- Molecule 46: 30S ribosomal protein S15

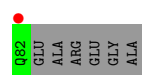


- Molecule 46: 30S ribosomal protein S15

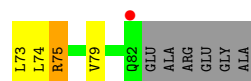
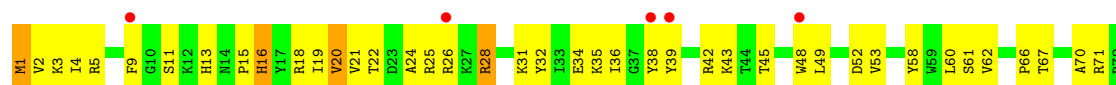
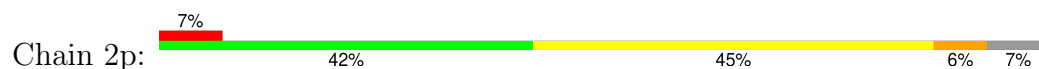


- Molecule 47: 30S ribosomal protein S16

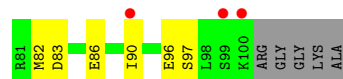




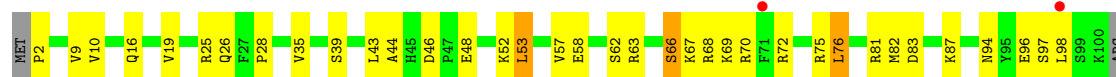
- Molecule 47: 30S ribosomal protein S16



- Molecule 48: 30S ribosomal protein S17



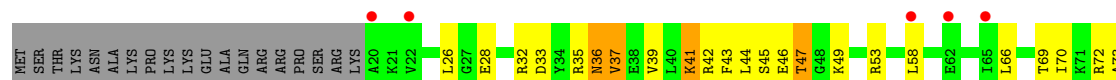
- Molecule 48: 30S ribosomal protein S17



- Molecule 49: 30S ribosomal protein S18

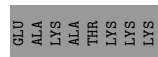


- Molecule 49: 30S ribosomal protein S18

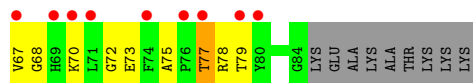
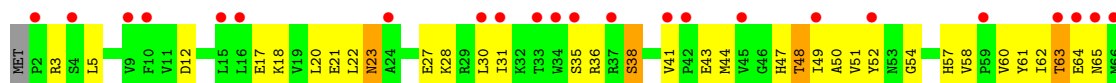




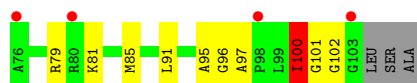
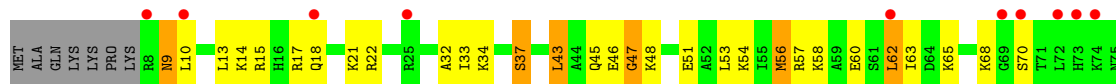
- Molecule 50: 30S ribosomal protein S19



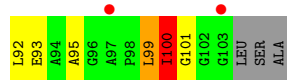
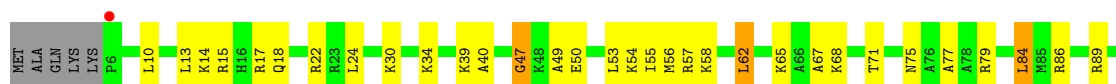
- Molecule 50: 30S ribosomal protein S19



- Molecule 51: 30S ribosomal protein S20

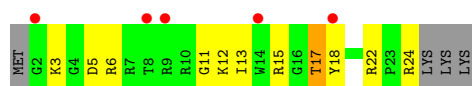


- Molecule 51: 30S ribosomal protein S20

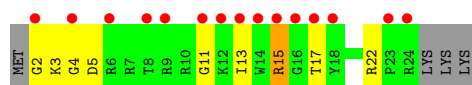


- Molecule 52: 30S ribosomal protein Thx

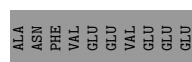
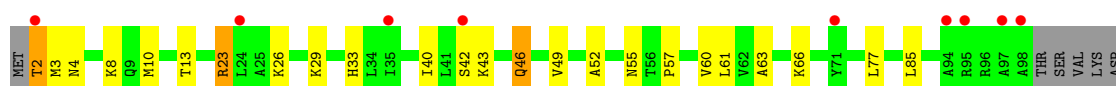




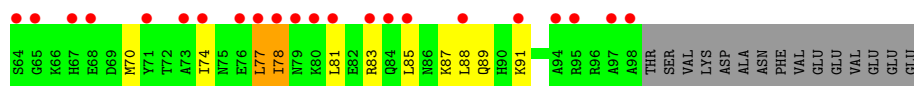
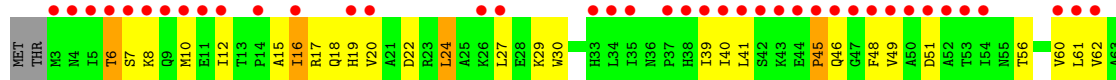
- Molecule 52: 30S ribosomal protein Thx



- Molecule 53: Ribosome-associated inhibitor A



- Molecule 53: Ribosome-associated inhibitor A



- Molecule 54: A-site Aminoacyl-tRNA Analog



- Molecule 54: A-site Aminoacyl-tRNA Analog



- Molecule 55: P-site Peptidyl-tRNA Analog RNA





- Molecule 55: P-site Peptidyl-tRNA Analog RNA



- Molecule 56: P-site Peptidyl-tRNA Analog Peptide



There are no outlier residues recorded for this chain.

- Molecule 56: P-site Peptidyl-tRNA Analog Peptide



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	209.32Å 449.63Å 620.21Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	155.05 – 2.50 155.05 – 2.50	Depositor EDS
% Data completeness (in resolution range)	99.9 (155.05-2.50) 99.9 (155.05-2.50)	Depositor EDS
R_{merge}	0.25	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.29 (at 2.52Å)	Xtriage
Refinement program	PHENIX 1.8.2	Depositor
R, R_{free}	0.230 , 0.278 0.233 , 0.280	Depositor DCC
R_{free} test set	99670 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å ²)	48.3	Xtriage
Anisotropy	0.142	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 62.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.35$, $\langle L^2 \rangle = 0.18$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	297682	wwPDB-VP
Average B, all atoms (Å ²)	56.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.62% 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: SF4, 0TD, 2MA, PPU, MPD, OMC, 5MU, MG, 5MC, OMU, 2MG, 4OC, G7M, M2G, MA6, OMG, ZN, UR3, PSU, 8AN

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	0.28	0/69031	0.49	2/107754 (0.0%)
1	2A	0.23	1/68903 (0.0%)	0.42	1/107552 (0.0%)
2	1B	0.25	0/2876	0.45	0/4486
2	2B	0.19	0/2878	0.38	0/4490
3	1D	0.29	0/2181	0.54	1/2940 (0.0%)
3	2D	0.24	0/2186	0.50	0/2944
4	1E	0.27	0/1592	0.47	0/2149
4	2E	0.23	0/1592	0.44	0/2149
5	1F	0.25	0/1619	0.46	0/2193
5	2F	0.20	0/1615	0.47	2/2188 (0.1%)
6	1G	0.22	0/1451	0.43	0/1961
6	2G	0.21	0/1449	0.46	0/1957
7	1H	0.23	0/1356	0.46	1/1834 (0.1%)
7	2H	0.20	0/1350	0.45	0/1826
8	1I	0.20	0/1109	0.45	0/1512
8	2I	0.21	0/1091	0.44	0/1490
9	1N	0.25	0/1148	0.49	0/1547
9	2N	0.21	0/1144	0.40	0/1543
10	1O	0.27	0/943	0.48	0/1269
10	2O	0.21	0/943	0.45	0/1269
11	1P	0.26	0/1152	0.49	0/1533
11	2P	0.21	0/1152	0.46	0/1533
12	1Q	0.27	0/1143	0.49	0/1527
12	2Q	0.21	0/1143	0.42	0/1527
13	1R	0.29	0/982	0.52	0/1312
13	2R	0.22	0/982	0.48	0/1312
14	1S	0.25	0/887	0.51	0/1180
14	2S	0.21	0/880	0.46	0/1172
15	1T	0.25	0/1105	0.52	0/1477
15	2T	0.22	0/1097	0.48	1/1468 (0.1%)
16	1U	0.28	0/977	0.51	0/1301

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
16	2U	0.19	0/977	0.44	0/1301
17	1V	0.28	0/786	0.49	0/1053
17	2V	0.20	0/782	0.44	0/1049
18	1W	0.26	0/897	0.46	0/1205
18	2W	0.21	0/897	0.42	0/1205
19	1X	0.27	0/764	0.50	0/1025
19	2X	0.20	0/764	0.44	0/1025
20	1Y	0.26	0/823	0.54	0/1099
20	2Y	0.20	0/823	0.44	0/1100
21	1Z	0.23	0/1620	0.45	0/2200
21	2Z	0.20	0/1590	0.42	0/2162
22	10	0.29	0/662	0.51	0/881
22	20	0.21	0/659	0.49	0/877
23	11	0.25	0/761	0.47	0/1013
23	21	0.21	0/766	0.43	0/1018
24	12	0.23	0/590	0.43	0/781
24	22	0.22	0/594	0.42	0/785
25	13	0.28	0/474	0.50	0/635
25	23	0.19	0/469	0.42	0/630
26	14	0.23	0/559	0.57	0/754
26	24	0.27	0/549	0.68	0/741
27	15	0.28	0/473	0.50	0/639
27	25	0.24	0/469	0.46	0/635
28	16	0.25	0/460	0.47	0/613
28	26	0.21	0/456	0.43	0/608
29	17	0.31	0/426	0.54	0/561
29	27	0.26	0/426	0.53	0/561
30	18	0.28	0/525	0.50	0/691
30	28	0.21	0/525	0.39	0/691
31	19	0.30	0/310	0.51	0/407
31	29	0.24	0/310	0.50	0/407
32	1a	0.21	0/35795	0.40	1/55864 (0.0%)
32	2a	0.20	0/35890	0.39	0/56012
33	1b	0.23	0/1876	0.48	0/2533
33	2b	0.23	0/1860	0.54	2/2518 (0.1%)
34	1c	0.20	0/1582	0.43	0/2137
34	2c	0.21	0/1566	0.44	0/2119
35	1d	0.21	0/1695	0.45	0/2274
35	2d	0.21	0/1698	0.45	0/2277
36	1e	0.20	0/1149	0.44	0/1548
36	2e	0.20	0/1149	0.43	0/1548
37	1f	0.21	0/827	0.39	0/1120
37	2f	0.19	0/829	0.40	0/1123

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
38	1g	0.18	0/1254	0.41	0/1683
38	2g	0.20	0/1248	0.39	0/1676
39	1h	0.20	0/1118	0.45	0/1506
39	2h	0.18	0/1108	0.42	0/1494
40	1i	0.20	0/1005	0.44	0/1351
40	2i	0.22	0/985	0.48	0/1329
41	1j	0.18	0/732	0.41	0/993
41	2j	0.24	0/723	0.50	0/984
42	1k	0.20	0/849	0.40	0/1150
42	2k	0.20	0/848	0.47	0/1149
43	1l	0.22	0/937	0.45	0/1260
43	2l	0.18	0/937	0.41	0/1260
44	1m	0.20	0/924	0.47	0/1242
44	2m	0.22	0/905	0.49	0/1217
45	1n	0.22	0/501	0.47	0/664
45	2n	0.22	0/501	0.46	0/664
46	1o	0.20	0/739	0.42	0/985
46	2o	0.19	0/739	0.36	0/985
47	1p	0.19	0/697	0.48	0/939
47	2p	0.19	0/693	0.46	0/935
48	1q	0.20	0/836	0.41	0/1117
48	2q	0.19	0/836	0.37	0/1117
49	1r	0.20	0/560	0.42	0/746
49	2r	0.20	0/560	0.42	0/746
50	1s	0.19	0/663	0.44	0/895
50	2s	0.22	0/660	0.43	0/893
51	1t	0.20	0/734	0.50	0/969
51	2t	0.21	0/736	0.49	1/976 (0.1%)
52	1u	0.17	0/203	0.43	0/266
52	2u	0.20	0/203	0.43	0/266
53	1y	0.20	0/776	0.42	0/1048
53	2y	0.19	0/761	0.39	0/1030
54	1w	0.26	0/44	0.43	0/67
54	2w	0.22	0/44	0.23	0/67
55	1x	0.23	0/44	0.52	0/67
55	2x	0.31	0/44	0.51	0/67
56	1v	0.25	0/27	0.28	0/34
56	2v	0.16	0/27	0.38	0/34
All	All	0.24	1/310260 (0.0%)	0.44	12/463691 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a

sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
11	1P	0	1
11	2P	0	1
17	2V	0	1
41	2j	0	1
47	1p	0	1
All	All	0	5

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	2A	2552	OMU	O3'-P	5.02	1.61	1.56

The worst 5 of 12 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1A	1042	G	OP1-P-O3'	-9.75	78.76	108.00
1	1A	1042	G	OP2-P-O3'	-6.63	88.09	108.00
33	2b	232	PRO	CA-C-N	6.14	132.42	122.48
33	2b	232	PRO	C-N-CA	6.14	132.42	122.48
51	2t	101	GLY	N-CA-C	6.04	120.15	110.90

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
11	1P	35	HIS	Peptide
47	1p	19	ILE	Peptide
11	2P	35	HIS	Peptide
17	2V	52	VAL	Peptide
41	2j	35	SER	Peptide

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	1A	61869	0	31204	725	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	2A	61758	0	31152	875	0
2	1B	2572	0	1305	35	0
2	2B	2573	0	1306	40	0
3	1D	2131	0	2206	45	0
3	2D	2136	0	2218	58	0
4	1E	1559	0	1618	31	0
4	2E	1559	0	1618	41	0
5	1F	1584	0	1625	53	0
5	2F	1580	0	1619	56	0
6	1G	1426	0	1445	60	0
6	2G	1424	0	1441	72	0
7	1H	1330	0	1407	37	0
7	2H	1324	0	1402	37	0
8	1I	1094	0	1127	28	0
8	2I	1076	0	1094	29	0
9	1N	1121	0	1195	22	0
9	2N	1117	0	1184	23	0
10	1O	933	0	996	25	0
10	2O	933	0	996	24	0
11	1P	1135	0	1212	29	0
11	2P	1135	0	1212	36	0
12	1Q	1122	0	1179	21	0
12	2Q	1122	0	1179	35	0
13	1R	968	0	1033	16	0
13	2R	968	0	1033	24	0
14	1S	877	0	938	25	0
14	2S	870	0	923	38	0
15	1T	1091	0	1151	29	0
15	2T	1083	0	1136	34	0
16	1U	959	0	1019	17	0
16	2U	959	0	1019	21	0
17	1V	775	0	841	17	0
17	2V	771	0	829	22	0
18	1W	886	0	940	14	0
18	2W	886	0	940	20	0
19	1X	750	0	814	22	0
19	2X	750	0	814	22	0
20	1Y	810	0	892	22	0
20	2Y	810	0	887	20	0
21	1Z	1587	0	1598	35	0
21	2Z	1557	0	1564	61	0
22	10	653	0	673	16	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
22	20	650	0	665	19	0
23	11	754	0	823	19	0
23	21	759	0	837	20	0
24	12	588	0	643	13	0
24	22	592	0	654	15	0
25	13	469	0	518	9	0
25	23	464	0	514	15	0
26	14	546	0	522	26	0
26	24	536	0	514	40	0
27	15	459	0	476	11	0
27	25	455	0	465	9	0
28	16	453	0	473	10	0
28	26	449	0	469	11	0
29	17	418	0	467	13	0
29	27	418	0	467	13	0
30	18	517	0	582	16	0
30	28	517	0	582	15	0
31	19	307	0	335	7	0
31	29	307	0	335	11	0
32	1a	32246	0	16295	440	0
32	2a	32331	0	16338	562	0
33	1b	1842	0	1862	51	0
33	2b	1825	0	1828	77	0
34	1c	1558	0	1557	43	0
34	2c	1542	0	1517	68	0
35	1d	1665	0	1687	57	0
35	2d	1668	0	1703	61	0
36	1e	1133	0	1191	31	0
36	2e	1133	0	1191	38	0
37	1f	814	0	808	16	0
37	2f	816	0	808	24	0
38	1g	1235	0	1249	26	0
38	2g	1229	0	1238	35	0
39	1h	1098	0	1143	32	0
39	2h	1088	0	1126	36	0
40	1i	986	0	990	39	0
40	2i	966	0	953	55	0
41	1j	719	0	672	22	0
41	2j	710	0	661	32	0
42	1k	834	0	838	12	0
42	2k	833	0	836	25	0
43	1l	932	0	981	29	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
43	2l	932	0	981	14	0
44	1m	914	0	954	37	0
44	2m	895	0	920	40	0
45	1n	492	0	528	20	0
45	2n	492	0	529	23	0
46	1o	728	0	760	18	0
46	2o	728	0	760	15	0
47	1p	681	0	697	19	0
47	2p	677	0	686	29	0
48	1q	823	0	891	28	0
48	2q	823	0	891	27	0
49	1r	555	0	618	10	0
49	2r	555	0	618	15	0
50	1s	648	0	658	33	0
50	2s	645	0	635	44	0
51	1t	732	0	809	29	0
51	2t	733	0	795	25	0
52	1u	199	0	208	10	0
52	2u	199	0	208	5	0
53	1y	764	0	786	19	0
53	2y	749	0	757	31	0
54	1w	78	0	50	4	0
54	2w	78	0	50	1	0
55	1x	63	0	33	1	0
55	2x	63	0	33	2	0
56	1v	27	0	31	0	0
56	2v	27	0	31	1	0
57	10	9	0	0	0	0
57	11	5	0	0	0	0
57	13	3	0	0	0	0
57	15	9	0	0	0	0
57	17	6	0	0	0	0
57	18	3	0	0	0	0
57	19	2	0	0	0	0
57	1A	1022	0	0	0	0
57	1B	30	0	0	0	0
57	1D	15	0	0	0	0
57	1E	12	0	0	0	0
57	1F	16	0	0	0	0
57	1G	4	0	0	0	0
57	1H	2	0	0	0	0
57	1N	4	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
57	1O	1	0	0	0	0
57	1P	5	0	0	0	0
57	1Q	7	0	0	0	0
57	1R	4	0	0	0	0
57	1S	1	0	0	0	0
57	1T	5	0	0	0	0
57	1U	4	0	0	0	0
57	1V	7	0	0	0	0
57	1W	3	0	0	0	0
57	1X	1	0	0	0	0
57	1Y	1	0	0	0	0
57	1Z	1	0	0	0	0
57	1a	274	0	0	0	0
57	1b	1	0	0	0	0
57	1d	6	0	0	0	0
57	1e	3	0	0	0	0
57	1f	2	0	0	0	0
57	1g	1	0	0	0	0
57	1h	2	0	0	0	0
57	1i	1	0	0	0	0
57	1l	3	0	0	0	0
57	1m	1	0	0	0	0
57	1n	3	0	0	0	0
57	1o	2	0	0	0	0
57	1t	1	0	0	0	0
57	1u	1	0	0	0	0
57	1w	1	0	0	0	0
57	1x	2	0	0	0	0
57	1y	4	0	0	0	0
57	20	2	0	0	0	0
57	21	1	0	0	0	0
57	25	3	0	0	0	0
57	27	2	0	0	0	0
57	28	2	0	0	0	0
57	2A	733	0	0	0	0
57	2B	19	0	0	0	0
57	2D	10	0	0	0	0
57	2E	7	0	0	0	0
57	2F	4	0	0	0	0
57	2G	3	0	0	0	0
57	2I	1	0	0	0	0
57	2O	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
57	2P	2	0	0	0	0
57	2Q	4	0	0	0	0
57	2R	3	0	0	0	0
57	2T	3	0	0	0	0
57	2U	1	0	0	0	0
57	2V	3	0	0	0	0
57	2W	3	0	0	0	0
57	2X	1	0	0	0	0
57	2Y	1	0	0	0	0
57	2a	190	0	0	0	0
57	2e	1	0	0	0	0
57	2f	1	0	0	0	0
57	2j	1	0	0	0	0
57	2n	1	0	0	0	0
57	2p	1	0	0	0	0
57	2r	1	0	0	0	0
57	2t	1	0	0	0	0
57	2x	1	0	0	0	0
58	18	8	0	14	2	0
58	1A	8	0	14	0	0
58	1a	16	0	28	5	0
58	2A	16	0	28	1	0
58	2B	8	0	14	1	0
59	1B	12	0	12	1	0
59	1F	12	0	12	2	0
60	14	1	0	0	0	0
60	15	1	0	0	0	0
60	16	1	0	0	0	0
60	19	1	0	0	0	0
60	1Y	1	0	0	0	0
60	1n	1	0	0	0	0
60	24	1	0	0	0	0
60	25	1	0	0	0	0
60	26	1	0	0	0	0
60	29	1	0	0	0	0
60	2Y	1	0	0	0	0
60	2n	1	0	0	0	0
61	1d	8	0	0	1	0
61	2d	8	0	0	0	0
62	10	21	0	0	2	0
62	11	26	0	0	0	0
62	12	12	0	0	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
62	13	21	0	0	1	0
62	14	2	0	0	1	0
62	15	25	0	0	2	0
62	16	18	0	0	0	0
62	17	13	0	0	1	0
62	18	26	0	0	3	0
62	19	5	0	0	0	0
62	1A	3972	0	0	161	0
62	1B	98	0	0	5	0
62	1D	107	0	0	5	0
62	1E	75	0	0	9	0
62	1F	60	0	0	3	0
62	1G	20	0	0	0	0
62	1H	15	0	0	0	0
62	1I	4	0	0	0	0
62	1N	47	0	0	1	0
62	1O	26	0	0	1	0
62	1P	63	0	0	0	0
62	1Q	37	0	0	1	0
62	1R	34	0	0	3	0
62	1S	15	0	0	2	0
62	1T	32	0	0	1	0
62	1U	45	0	0	3	0
62	1V	36	0	0	1	0
62	1W	25	0	0	0	0
62	1X	26	0	0	3	0
62	1Y	16	0	0	2	0
62	1Z	8	0	0	1	0
62	1a	509	0	0	28	0
62	1b	1	0	0	0	0
62	1d	10	0	0	1	0
62	1e	3	0	0	0	0
62	1f	3	0	0	0	0
62	1h	1	0	0	0	0
62	1j	2	0	0	0	0
62	1l	4	0	0	0	0
62	1m	1	0	0	0	0
62	1o	4	0	0	1	0
62	1p	3	0	0	0	0
62	1t	1	0	0	0	0
62	1u	1	0	0	1	0
62	1w	3	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
62	1x	3	0	0	1	0
62	1y	8	0	0	1	0
62	20	12	0	0	1	0
62	21	20	0	0	1	0
62	22	1	0	0	0	0
62	23	4	0	0	1	0
62	25	10	0	0	0	0
62	26	5	0	0	1	0
62	27	8	0	0	0	0
62	28	12	0	0	0	0
62	29	2	0	0	1	0
62	2A	2105	0	0	158	0
62	2B	46	0	0	2	0
62	2D	48	0	0	4	0
62	2E	26	0	0	2	0
62	2F	24	0	0	0	0
62	2G	4	0	0	0	0
62	2H	2	0	0	0	0
62	2I	4	0	0	1	0
62	2N	5	0	0	0	0
62	2O	18	0	0	2	0
62	2P	19	0	0	2	0
62	2Q	18	0	0	2	0
62	2R	22	0	0	5	0
62	2S	3	0	0	0	0
62	2T	7	0	0	0	0
62	2U	10	0	0	2	0
62	2V	7	0	0	0	0
62	2W	17	0	0	1	0
62	2X	8	0	0	1	0
62	2Y	5	0	0	1	0
62	2Z	11	0	0	1	0
62	2a	291	0	0	37	0
62	2d	3	0	0	0	0
62	2f	3	0	0	0	0
62	2j	2	0	0	0	0
62	2l	2	0	0	0	0
62	2m	2	0	0	0	0
62	2o	4	0	0	0	0
62	2p	2	0	0	0	0
62	2q	1	0	0	0	0
62	2r	3	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
62	2t	2	0	0	0	0
62	2w	3	0	0	0	0
62	2x	1	0	0	0	0
62	2y	3	0	0	0	0
All	All	297682	0	194836	4809	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 4809 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1A:1082:U:H3	1:1A:1086:A:N6	1.28	1.30
1:2A:2139:C:N4	1:2A:2152:G:H1	1.45	1.11
1:1A:2137:C:N4	1:1A:2154:G:H1	1.48	1.10
1:1A:2319:G:H22	14:1S:3:ARG:HD3	1.15	1.09
1:1A:1082:U:O4	1:1A:1086:A:N1	1.92	1.02

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%)	262 (96%)	11 (4%)	0	100	100
3	2D	273/276 (99%)	251 (92%)	22 (8%)	0	100	100
4	1E	202/206 (98%)	194 (96%)	7 (4%)	1 (0%)	24	43
4	2E	202/206 (98%)	188 (93%)	13 (6%)	1 (0%)	24	43
5	1F	201/210 (96%)	196 (98%)	4 (2%)	1 (0%)	24	43
5	2F	201/210 (96%)	196 (98%)	4 (2%)	1 (0%)	24	43

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
6	1G	179/182 (98%)	157 (88%)	14 (8%)	8 (4%)	2	2
6	2G	179/182 (98%)	145 (81%)	28 (16%)	6 (3%)	3	4
7	1H	172/180 (96%)	161 (94%)	8 (5%)	3 (2%)	7	13
7	2H	171/180 (95%)	148 (86%)	20 (12%)	3 (2%)	6	12
8	1I	145/148 (98%)	122 (84%)	21 (14%)	2 (1%)	9	17
8	2I	144/148 (97%)	130 (90%)	12 (8%)	2 (1%)	9	17
9	1N	138/140 (99%)	132 (96%)	6 (4%)	0	100	100
9	2N	138/140 (99%)	129 (94%)	9 (6%)	0	100	100
10	1O	120/122 (98%)	112 (93%)	8 (7%)	0	100	100
10	2O	120/122 (98%)	111 (92%)	9 (8%)	0	100	100
11	1P	147/150 (98%)	140 (95%)	7 (5%)	0	100	100
11	2P	147/150 (98%)	136 (92%)	10 (7%)	1 (1%)	18	34
12	1Q	139/141 (99%)	130 (94%)	9 (6%)	0	100	100
12	2Q	139/141 (99%)	129 (93%)	10 (7%)	0	100	100
13	1R	116/118 (98%)	112 (97%)	4 (3%)	0	100	100
13	2R	116/118 (98%)	111 (96%)	5 (4%)	0	100	100
14	1S	108/112 (96%)	100 (93%)	6 (6%)	2 (2%)	6	11
14	2S	108/112 (96%)	100 (93%)	8 (7%)	0	100	100
15	1T	129/146 (88%)	123 (95%)	5 (4%)	1 (1%)	16	31
15	2T	129/146 (88%)	123 (95%)	5 (4%)	1 (1%)	16	31
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%)	92 (93%)	4 (4%)	3 (3%)	3	5
17	2V	99/101 (98%)	91 (92%)	7 (7%)	1 (1%)	12	24
18	1W	110/113 (97%)	108 (98%)	2 (2%)	0	100	100
18	2W	110/113 (97%)	109 (99%)	1 (1%)	0	100	100
19	1X	93/96 (97%)	91 (98%)	1 (1%)	1 (1%)	11	22
19	2X	93/96 (97%)	90 (97%)	2 (2%)	1 (1%)	11	22
20	1Y	105/110 (96%)	94 (90%)	11 (10%)	0	100	100
20	2Y	105/110 (96%)	95 (90%)	9 (9%)	1 (1%)	12	24
21	1Z	201/206 (98%)	183 (91%)	18 (9%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
21	2Z	199/206 (97%)	167 (84%)	31 (16%)	1 (0%)	24	43
22	10	81/85 (95%)	76 (94%)	5 (6%)	0	100	100
22	20	81/85 (95%)	74 (91%)	6 (7%)	1 (1%)	10	20
23	11	95/98 (97%)	90 (95%)	4 (4%)	1 (1%)	11	22
23	21	95/98 (97%)	92 (97%)	3 (3%)	0	100	100
24	12	68/72 (94%)	66 (97%)	2 (3%)	0	100	100
24	22	68/72 (94%)	63 (93%)	5 (7%)	0	100	100
25	13	57/60 (95%)	55 (96%)	2 (4%)	0	100	100
25	23	57/60 (95%)	54 (95%)	3 (5%)	0	100	100
26	14	67/71 (94%)	53 (79%)	10 (15%)	4 (6%)	1	1
26	24	67/71 (94%)	47 (70%)	14 (21%)	6 (9%)	0	0
27	15	57/60 (95%)	55 (96%)	2 (4%)	0	100	100
27	25	57/60 (95%)	56 (98%)	1 (2%)	0	100	100
28	16	51/54 (94%)	49 (96%)	2 (4%)	0	100	100
28	26	51/54 (94%)	47 (92%)	4 (8%)	0	100	100
29	17	46/49 (94%)	44 (96%)	2 (4%)	0	100	100
29	27	46/49 (94%)	46 (100%)	0	0	100	100
30	18	62/65 (95%)	62 (100%)	0	0	100	100
30	28	62/65 (95%)	60 (97%)	2 (3%)	0	100	100
31	19	35/37 (95%)	34 (97%)	1 (3%)	0	100	100
31	29	35/37 (95%)	33 (94%)	2 (6%)	0	100	100
33	1b	229/256 (90%)	192 (84%)	28 (12%)	9 (4%)	2	3
33	2b	229/256 (90%)	187 (82%)	30 (13%)	12 (5%)	1	1
34	1c	204/239 (85%)	187 (92%)	17 (8%)	0	100	100
34	2c	204/239 (85%)	174 (85%)	28 (14%)	2 (1%)	12	24
35	1d	206/209 (99%)	191 (93%)	14 (7%)	1 (0%)	24	43
35	2d	206/209 (99%)	188 (91%)	18 (9%)	0	100	100
36	1e	146/162 (90%)	138 (94%)	8 (6%)	0	100	100
36	2e	146/162 (90%)	136 (93%)	10 (7%)	0	100	100
37	1f	98/101 (97%)	92 (94%)	6 (6%)	0	100	100
37	2f	98/101 (97%)	93 (95%)	3 (3%)	2 (2%)	6	10

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
38	1g	153/156 (98%)	144 (94%)	7 (5%)	2 (1%)	9	18
38	2g	153/156 (98%)	137 (90%)	14 (9%)	2 (1%)	9	18
39	1h	135/138 (98%)	128 (95%)	6 (4%)	1 (1%)	18	34
39	2h	135/138 (98%)	123 (91%)	12 (9%)	0	100	100
40	1i	125/128 (98%)	112 (90%)	13 (10%)	0	100	100
40	2i	124/128 (97%)	108 (87%)	14 (11%)	2 (2%)	7	14
41	1j	95/105 (90%)	84 (88%)	8 (8%)	3 (3%)	3	4
41	2j	94/105 (90%)	79 (84%)	13 (14%)	2 (2%)	5	9
42	1k	112/129 (87%)	101 (90%)	11 (10%)	0	100	100
42	2k	112/129 (87%)	101 (90%)	9 (8%)	2 (2%)	6	12
43	1l	119/132 (90%)	109 (92%)	10 (8%)	0	100	100
43	2l	119/132 (90%)	109 (92%)	10 (8%)	0	100	100
44	1m	114/126 (90%)	101 (89%)	11 (10%)	2 (2%)	6	12
44	2m	112/126 (89%)	96 (86%)	14 (12%)	2 (2%)	6	12
45	1n	58/61 (95%)	56 (97%)	2 (3%)	0	100	100
45	2n	58/61 (95%)	53 (91%)	3 (5%)	2 (3%)	3	4
46	1o	86/89 (97%)	81 (94%)	5 (6%)	0	100	100
46	2o	86/89 (97%)	78 (91%)	6 (7%)	2 (2%)	5	8
47	1p	80/88 (91%)	72 (90%)	8 (10%)	0	100	100
47	2p	80/88 (91%)	67 (84%)	12 (15%)	1 (1%)	9	18
48	1q	97/105 (92%)	90 (93%)	7 (7%)	0	100	100
48	2q	97/105 (92%)	85 (88%)	12 (12%)	0	100	100
49	1r	66/88 (75%)	63 (96%)	2 (3%)	1 (2%)	8	16
49	2r	66/88 (75%)	63 (96%)	2 (3%)	1 (2%)	8	16
50	1s	81/93 (87%)	68 (84%)	13 (16%)	0	100	100
50	2s	81/93 (87%)	65 (80%)	16 (20%)	0	100	100
51	1t	94/106 (89%)	83 (88%)	8 (8%)	3 (3%)	3	4
51	2t	96/106 (91%)	86 (90%)	7 (7%)	3 (3%)	3	5
52	1u	21/27 (78%)	20 (95%)	1 (5%)	0	100	100
52	2u	21/27 (78%)	17 (81%)	3 (14%)	1 (5%)	2	2
53	1y	95/113 (84%)	92 (97%)	3 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
53	2y	94/113 (83%)	88 (94%)	5 (5%)	1 (1%)	11	22
56	1v	1/3 (33%)	1 (100%)	0	0	100	100
56	2v	1/3 (33%)	1 (100%)	0	0	100	100
All	All	11643/12360 (94%)	10680 (92%)	851 (7%)	112 (1%)	12	24

5 of 112 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
6	1G	47	LYS
33	1b	17	PHE
33	1b	124	SER
33	1b	127	ILE
41	1j	55	LYS

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	1D	214/218 (98%)	191 (89%)	23 (11%)	6	13
3	2D	215/218 (99%)	191 (89%)	24 (11%)	6	12
4	1E	164/166 (99%)	151 (92%)	13 (8%)	11	24
4	2E	164/166 (99%)	148 (90%)	16 (10%)	7	16
5	1F	160/166 (96%)	142 (89%)	18 (11%)	5	12
5	2F	159/166 (96%)	137 (86%)	22 (14%)	3	7
6	1G	144/156 (92%)	123 (85%)	21 (15%)	3	6
6	2G	142/156 (91%)	119 (84%)	23 (16%)	2	4
7	1H	144/148 (97%)	131 (91%)	13 (9%)	9	19
7	2H	143/148 (97%)	130 (91%)	13 (9%)	9	19
8	1I	111/124 (90%)	93 (84%)	18 (16%)	2	4
8	2I	108/124 (87%)	91 (84%)	17 (16%)	2	5
9	1N	119/119 (100%)	109 (92%)	10 (8%)	10	22

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
9	2N	118/119 (99%)	113 (96%)	5 (4%)	26	52
10	1O	100/100 (100%)	93 (93%)	7 (7%)	14	29
10	2O	100/100 (100%)	92 (92%)	8 (8%)	11	24
11	1P	115/116 (99%)	104 (90%)	11 (10%)	8	17
11	2P	115/116 (99%)	105 (91%)	10 (9%)	9	21
12	1Q	111/111 (100%)	102 (92%)	9 (8%)	11	23
12	2Q	111/111 (100%)	100 (90%)	11 (10%)	7	16
13	1R	101/101 (100%)	92 (91%)	9 (9%)	9	20
13	2R	101/101 (100%)	96 (95%)	5 (5%)	22	44
14	1S	87/88 (99%)	79 (91%)	8 (9%)	8	19
14	2S	85/88 (97%)	68 (80%)	17 (20%)	1	2
15	1T	115/127 (91%)	105 (91%)	10 (9%)	9	21
15	2T	113/127 (89%)	102 (90%)	11 (10%)	8	17
16	1U	93/94 (99%)	83 (89%)	10 (11%)	6	13
16	2U	93/94 (99%)	88 (95%)	5 (5%)	20	41
17	1V	81/82 (99%)	72 (89%)	9 (11%)	6	12
17	2V	80/82 (98%)	73 (91%)	7 (9%)	9	20
18	1W	90/92 (98%)	81 (90%)	9 (10%)	7	15
18	2W	90/92 (98%)	84 (93%)	6 (7%)	15	31
19	1X	77/78 (99%)	73 (95%)	4 (5%)	21	42
19	2X	77/78 (99%)	75 (97%)	2 (3%)	40	68
20	1Y	86/91 (94%)	73 (85%)	13 (15%)	3	5
20	2Y	86/91 (94%)	78 (91%)	8 (9%)	8	18
21	1Z	169/179 (94%)	147 (87%)	22 (13%)	4	8
21	2Z	165/179 (92%)	144 (87%)	21 (13%)	4	9
22	10	65/67 (97%)	62 (95%)	3 (5%)	24	48
22	20	64/67 (96%)	60 (94%)	4 (6%)	16	34
23	11	79/83 (95%)	75 (95%)	4 (5%)	21	43
23	21	81/83 (98%)	73 (90%)	8 (10%)	7	16
24	12	65/67 (97%)	63 (97%)	2 (3%)	35	62
24	22	66/67 (98%)	56 (85%)	10 (15%)	3	5

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
25	13	51/52 (98%)	47 (92%)	4 (8%)	11	24
25	23	50/52 (96%)	44 (88%)	6 (12%)	5	10
26	14	58/63 (92%)	49 (84%)	9 (16%)	2	5
26	24	54/63 (86%)	47 (87%)	7 (13%)	4	8
27	15	51/52 (98%)	45 (88%)	6 (12%)	5	11
27	25	50/52 (96%)	47 (94%)	3 (6%)	17	36
28	16	51/52 (98%)	48 (94%)	3 (6%)	18	37
28	26	50/52 (96%)	45 (90%)	5 (10%)	7	15
29	17	41/42 (98%)	39 (95%)	2 (5%)	22	45
29	27	41/42 (98%)	37 (90%)	4 (10%)	7	16
30	18	54/55 (98%)	51 (94%)	3 (6%)	19	39
30	28	54/55 (98%)	52 (96%)	2 (4%)	30	57
31	19	34/34 (100%)	31 (91%)	3 (9%)	9	20
31	29	34/34 (100%)	28 (82%)	6 (18%)	2	3
33	1b	191/220 (87%)	171 (90%)	20 (10%)	6	14
33	2b	187/220 (85%)	156 (83%)	31 (17%)	2	4
34	1c	144/188 (77%)	134 (93%)	10 (7%)	14	30
34	2c	140/188 (74%)	122 (87%)	18 (13%)	4	9
35	1d	171/181 (94%)	150 (88%)	21 (12%)	4	10
35	2d	172/181 (95%)	146 (85%)	26 (15%)	3	5
36	1e	114/123 (93%)	103 (90%)	11 (10%)	8	17
36	2e	114/123 (93%)	103 (90%)	11 (10%)	8	17
37	1f	85/90 (94%)	76 (89%)	9 (11%)	6	14
37	2f	85/90 (94%)	76 (89%)	9 (11%)	6	14
38	1g	120/127 (94%)	111 (92%)	9 (8%)	12	26
38	2g	119/127 (94%)	108 (91%)	11 (9%)	8	19
39	1h	116/119 (98%)	109 (94%)	7 (6%)	17	36
39	2h	114/119 (96%)	103 (90%)	11 (10%)	8	17
40	1i	91/99 (92%)	81 (89%)	10 (11%)	6	13
40	2i	88/99 (89%)	74 (84%)	14 (16%)	2	5
41	1j	68/92 (74%)	56 (82%)	12 (18%)	2	3

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
41	2j	68/92 (74%)	54 (79%)	14 (21%)	1	2
42	1k	83/99 (84%)	78 (94%)	5 (6%)	17	36
42	2k	83/99 (84%)	77 (93%)	6 (7%)	13	28
43	1l	96/108 (89%)	90 (94%)	6 (6%)	16	34
43	2l	96/108 (89%)	90 (94%)	6 (6%)	16	34
44	1m	90/101 (89%)	82 (91%)	8 (9%)	9	20
44	2m	87/101 (86%)	79 (91%)	8 (9%)	8	19
45	1n	49/50 (98%)	45 (92%)	4 (8%)	10	23
45	2n	49/50 (98%)	46 (94%)	3 (6%)	17	35
46	1o	78/80 (98%)	73 (94%)	5 (6%)	16	33
46	2o	78/80 (98%)	70 (90%)	8 (10%)	7	14
47	1p	69/74 (93%)	61 (88%)	8 (12%)	5	11
47	2p	68/74 (92%)	54 (79%)	14 (21%)	1	2
48	1q	94/97 (97%)	83 (88%)	11 (12%)	5	11
48	2q	94/97 (97%)	87 (93%)	7 (7%)	13	27
49	1r	59/77 (77%)	55 (93%)	4 (7%)	14	31
49	2r	59/77 (77%)	53 (90%)	6 (10%)	7	15
50	1s	68/80 (85%)	64 (94%)	4 (6%)	18	37
50	2s	67/80 (84%)	59 (88%)	8 (12%)	5	11
51	1t	71/82 (87%)	62 (87%)	9 (13%)	4	9
51	2t	70/82 (85%)	62 (89%)	8 (11%)	5	12
52	1u	18/22 (82%)	17 (94%)	1 (6%)	19	39
52	2u	18/22 (82%)	16 (89%)	2 (11%)	6	12
53	1y	82/98 (84%)	75 (92%)	7 (8%)	10	22
53	2y	79/98 (81%)	69 (87%)	10 (13%)	4	9
56	1v	3/3 (100%)	3 (100%)	0	100	100
56	2v	3/3 (100%)	3 (100%)	0	100	100
All	All	9537/10266 (93%)	8563 (90%)	974 (10%)	7	15

5 of 974 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	2D	111	LEU

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Mol	Chain	Res	Type
41	2j	98	ILE
9	2N	28	THR
41	2j	30	SER
50	2s	5	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 155 such sidechains are listed below:

Mol	Chain	Res	Type
33	2b	204	ASN
44	2m	106	ASN
34	2c	102	ASN
38	2g	64	GLN
46	2o	71	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	1A	2865/2915 (98%)	414 (14%)	27 (0%)
1	2A	2858/2915 (98%)	486 (17%)	30 (1%)
2	1B	119/121 (98%)	13 (10%)	0
2	2B	119/121 (98%)	17 (14%)	0
32	1a	1497/1521 (98%)	267 (17%)	0
32	2a	1501/1521 (98%)	278 (18%)	0
54	1w	1/4 (25%)	0	0
54	2w	1/4 (25%)	0	0
55	1x	1/4 (25%)	0	0
55	2x	1/4 (25%)	0	0
All	All	8963/9130 (98%)	1475 (16%)	57 (0%)

5 of 1475 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	1A	34	C
1	1A	45	C
1	1A	63	U
1	1A	71	A
1	1A	74	A

5 of 57 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	2A	271(M)	G
1	2A	2689	U
1	2A	856	C
1	2A	2406	U
1	2A	1992	G

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

52 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	4OC	2a	1402	32	20,23,24	0.77	0	25,32,35	0.94	1 (4%)
32	G7M	2a	527	32,57	23,26,27	1.49	3 (13%)	34,39,42	1.62	4 (11%)
54	PPU	2w	76	54,1	37,40,41	1.33	4 (10%)	47,57,60	1.95	12 (25%)
1	5MU	1A	1939	57,1	19,22,23	1.41	5 (26%)	27,32,35	2.27	6 (22%)
32	5MC	2a	967	32	19,22,23	1.83	2 (10%)	26,32,35	1.02	2 (7%)
1	5MU	2A	1915	1	19,22,23	1.35	4 (21%)	27,32,35	2.13	7 (25%)
1	PSU	2A	1911	1	18,21,22	1.39	2 (11%)	21,30,33	2.03	3 (14%)
32	G7M	1a	527	32,57	23,26,27	1.53	3 (13%)	34,39,42	1.63	4 (11%)
1	5MC	2A	1962	57,1	19,22,23	1.46	3 (15%)	26,32,35	1.20	4 (15%)
32	2MG	1a	1207	32	23,26,27	1.27	3 (13%)	33,38,41	2.21	7 (21%)
1	5MU	2A	1939	57,1	19,22,23	1.53	5 (26%)	27,32,35	2.24	8 (29%)
1	5MU	1A	1915	1	19,22,23	1.43	4 (21%)	27,32,35	2.29	9 (33%)
1	OMU	1A	2552	57,1	19,22,23	1.32	3 (15%)	25,31,34	1.79	6 (24%)
43	0TD	1l	92	43	8,9,10	4.46	1 (12%)	6,11,13	3.17	2 (33%)
1	PSU	2A	2605	1	18,21,22	1.38	3 (16%)	21,30,33	1.95	4 (19%)
32	MA6	2a	1519	32	23,26,27	0.42	0	33,38,41	2.11	9 (27%)
1	OMC	1A	1920	1	19,22,23	0.85	0	25,31,34	1.15	2 (8%)
32	5MC	2a	1407	32	19,22,23	1.75	2 (10%)	26,32,35	1.13	3 (11%)
32	PSU	1a	516	32,57	18,21,22	1.36	2 (11%)	21,30,33	1.94	5 (23%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
55	8AN	2x	76	56,55,57	21,24,25	1.38	3 (14%)	26,35,38	2.45	11 (42%)
1	2MA	2A	2503	57,1	22,25,26	1.45	3 (13%)	32,37,40	2.36	9 (28%)
43	0TD	2l	92	43	8,9,10	4.45	1 (12%)	6,11,13	6.67	3 (50%)
32	M2G	1a	966	32	24,27,28	1.34	3 (12%)	33,40,43	1.87	5 (15%)
1	5MC	1A	1942	57,1	19,22,23	1.57	3 (15%)	26,32,35	1.13	2 (7%)
32	M2G	2a	966	32,57	24,27,28	1.29	3 (12%)	33,40,43	1.80	5 (15%)
1	5MC	1A	1962	57,1	19,22,23	1.59	3 (15%)	26,32,35	1.12	3 (11%)
1	PSU	1A	1911	1	18,21,22	1.36	2 (11%)	21,30,33	2.05	4 (19%)
1	OMC	2A	1920	1	19,22,23	0.81	0	25,31,34	1.03	1 (4%)
32	MA6	2a	1518	32	23,26,27	0.39	0	33,38,41	2.05	9 (27%)
32	5MC	2a	1404	32	19,22,23	1.79	3 (15%)	26,32,35	1.15	2 (7%)
32	5MC	1a	967	32	19,22,23	1.59	3 (15%)	26,32,35	1.14	3 (11%)
1	PSU	1A	1917	1	18,21,22	1.34	2 (11%)	21,30,33	1.95	3 (14%)
1	2MA	1A	2503	57,1	22,25,26	1.48	6 (27%)	32,37,40	2.43	9 (28%)
32	5MC	2a	1400	32	19,22,23	1.67	3 (15%)	26,32,35	1.24	3 (11%)
32	UR3	1a	1498	32	19,22,23	0.97	1 (5%)	26,32,35	1.85	3 (11%)
1	OMU	2A	2552	57,1	19,22,23	1.22	2 (10%)	25,31,34	1.83	6 (24%)
32	UR3	2a	1498	32	19,22,23	1.02	2 (10%)	26,32,35	1.64	3 (11%)
32	2MG	2a	1207	32	23,26,27	1.22	3 (13%)	33,38,41	2.13	8 (24%)
1	OMG	2A	2251	57,55,1	23,26,27	1.17	3 (13%)	32,38,41	2.01	6 (18%)
1	PSU	2A	1917	1	18,21,22	1.34	3 (16%)	21,30,33	2.00	4 (19%)
1	PSU	1A	2605	1	18,21,22	1.43	4 (22%)	21,30,33	2.15	5 (23%)
32	MA6	1a	1519	32	23,26,27	0.41	0	33,38,41	2.09	10 (30%)
1	5MC	2A	1942	1	19,22,23	1.80	3 (15%)	26,32,35	1.30	2 (7%)
32	4OC	1a	1402	32	20,23,24	0.76	0	25,32,35	0.90	1 (4%)
32	5MC	1a	1404	32	19,22,23	1.71	3 (15%)	26,32,35	1.14	3 (11%)
32	5MC	1a	1407	32	19,22,23	1.69	2 (10%)	26,32,35	1.16	3 (11%)
54	PPU	1w	76	54,1	37,40,41	1.23	3 (8%)	47,57,60	2.11	14 (29%)
32	5MC	1a	1400	32	19,22,23	1.75	3 (15%)	26,32,35	1.23	2 (7%)
55	8AN	1x	76	56,55,57	21,24,25	1.42	3 (14%)	26,35,38	2.97	10 (38%)
32	MA6	1a	1518	32	23,26,27	0.41	0	33,38,41	1.93	9 (27%)
32	PSU	2a	516	32,57	18,21,22	1.37	2 (11%)	21,30,33	2.06	5 (23%)
1	OMG	1A	2251	57,55,1	23,26,27	1.22	3 (13%)	32,38,41	2.02	6 (18%)

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	4OC	2a	1402	32	-	0/9/29/30	0/2/2/2
32	G7M	2a	527	32,57	-	2/7/25/26	0/3/3/3
54	PPU	2w	76	54,1	-	2/25/43/44	0/4/4/4
1	5MU	1A	1939	57,1	-	0/7/25/26	0/2/2/2
32	5MC	2a	967	32	-	0/7/25/26	0/2/2/2
1	5MU	2A	1915	1	-	2/7/25/26	0/2/2/2
1	PSU	2A	1911	1	-	0/7/25/26	0/2/2/2
32	G7M	1a	527	32,57	-	1/7/25/26	0/3/3/3
1	5MC	2A	1962	57,1	-	0/7/25/26	0/2/2/2
32	2MG	1a	1207	32	-	1/9/27/28	0/3/3/3
1	5MU	2A	1939	57,1	-	0/7/25/26	0/2/2/2
1	5MU	1A	1915	1	-	2/7/25/26	0/2/2/2
1	OMU	1A	2552	57,1	-	0/9/27/28	0/2/2/2
43	0TD	1l	92	43	-	1/7/12/14	-
1	PSU	2A	2605	1	-	0/7/25/26	0/2/2/2
32	MA6	2a	1519	32	-	3/11/29/30	0/3/3/3
1	OMC	1A	1920	1	-	2/9/27/28	0/2/2/2
32	5MC	2a	1407	32	-	0/7/25/26	0/2/2/2
32	PSU	1a	516	32,57	-	1/7/25/26	0/2/2/2
55	8AN	2x	76	56,55,57	-	3/7/25/26	0/3/3/3
1	2MA	2A	2503	57,1	-	0/7/25/26	0/3/3/3
43	0TD	2l	92	43	-	1/7/12/14	-
32	M2G	1a	966	32	-	0/11/29/30	0/3/3/3
1	5MC	1A	1942	57,1	-	0/7/25/26	0/2/2/2
32	M2G	2a	966	32,57	-	0/11/29/30	0/3/3/3
1	5MC	1A	1962	57,1	-	0/7/25/26	0/2/2/2
1	PSU	1A	1911	1	-	2/7/25/26	0/2/2/2
1	OMC	2A	1920	1	-	1/9/27/28	0/2/2/2
32	MA6	2a	1518	32	-	0/11/29/30	0/3/3/3
32	5MC	2a	1404	32	-	0/7/25/26	0/2/2/2
32	5MC	1a	967	32	-	0/7/25/26	0/2/2/2
1	PSU	1A	1917	1	-	0/7/25/26	0/2/2/2
1	2MA	1A	2503	57,1	-	1/7/25/26	0/3/3/3
32	5MC	2a	1400	32	-	6/7/25/26	0/2/2/2
32	UR3	1a	1498	32	-	0/7/25/26	0/2/2/2
1	OMU	2A	2552	57,1	-	0/9/27/28	0/2/2/2
32	UR3	2a	1498	32	-	0/7/25/26	0/2/2/2
32	2MG	2a	1207	32	-	0/9/27/28	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	OMG	2A	2251	57,55,1	-	1/9/27/28	0/3/3/3
1	PSU	2A	1917	1	-	0/7/25/26	0/2/2/2
1	PSU	1A	2605	1	-	0/7/25/26	0/2/2/2
32	MA6	1a	1519	32	-	2/11/29/30	0/3/3/3
1	5MC	2A	1942	1	-	0/7/25/26	0/2/2/2
32	4OC	1a	1402	32	-	3/9/29/30	0/2/2/2
32	5MC	1a	1404	32	-	0/7/25/26	0/2/2/2
32	5MC	1a	1407	32	-	0/7/25/26	0/2/2/2
54	PPU	1w	76	54,1	-	2/25/43/44	0/4/4/4
32	5MC	1a	1400	32	-	0/7/25/26	0/2/2/2
55	8AN	1x	76	56,55,57	-	3/7/25/26	0/3/3/3
32	MA6	1a	1518	32	-	0/11/29/30	0/3/3/3
32	PSU	2a	516	32,57	-	0/7/25/26	0/2/2/2
1	OMG	1A	2251	57,55,1	-	0/9/27/28	0/3/3/3

The worst 5 of 127 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
43	2l	92	0TD	CB-SB	-12.23	1.69	1.82
43	1l	92	0TD	CB-SB	-12.15	1.70	1.82
32	2a	967	5MC	C5-C4	6.83	1.49	1.44
1	2A	1942	5MC	C5-C4	6.67	1.49	1.44
32	2a	1404	5MC	C5-C4	6.66	1.49	1.44

The worst 5 of 270 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
43	2l	92	0TD	CSB-SB-CB	-15.74	74.08	102.36
55	1x	76	8AN	O4'-C1'-N9	10.22	127.73	108.09
1	2A	2503	2MA	C5-C4-N3	-8.00	118.75	127.18
1	1A	2503	2MA	C5-C4-N3	-7.97	118.78	127.18
32	1a	1498	UR3	C4-N3-C2	-7.43	118.60	124.58

There are no chirality outliers.

5 of 42 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	1A	1915	5MU	O4'-C1'-N1-C2
1	1A	1915	5MU	O4'-C1'-N1-C6
1	2A	1915	5MU	O4'-C1'-N1-C2
1	2A	1915	5MU	O4'-C1'-N1-C6

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Mol	Chain	Res	Type	Atoms
32	2a	1400	5MC	C2'-C1'-N1-C6

There are no ring outliers.

24 monomers are involved in 32 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
32	2a	1402	4OC	1	0
54	2w	76	PPU	1	0
1	2A	1911	PSU	1	0
32	1a	1207	2MG	1	0
1	2A	1939	5MU	2	0
43	1l	92	0TD	1	0
32	2a	1519	MA6	1	0
55	2x	76	8AN	1	0
1	2A	2503	2MA	1	0
43	2l	92	0TD	2	0
1	2A	1920	OMC	2	0
32	2a	1518	MA6	1	0
1	1A	2503	2MA	1	0
1	2A	2552	OMU	1	0
32	2a	1207	2MG	4	0
1	2A	2251	OMG	1	0
1	2A	1917	PSU	1	0
32	1a	1519	MA6	1	0
32	1a	1402	4OC	2	0
54	1w	76	PPU	2	0
32	1a	1400	5MC	2	0
55	1x	76	8AN	1	0
32	1a	1518	MA6	1	0
1	1A	2251	OMG	2	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 2521 ligands modelled in this entry, 2510 are monoatomic - leaving 11 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
58	MPD	1A	4023	-	7,7,7	0.29	0	9,10,10	0.38	0
58	MPD	2A	3735	-	7,7,7	0.31	0	9,10,10	0.24	0
58	MPD	1a	3276	-	7,7,7	0.39	0	9,10,10	0.43	0
58	MPD	2A	3734	-	7,7,7	0.33	0	9,10,10	0.36	0
61	SF4	2d	501	35	0,12,12	-	-	-	-	-
58	MPD	18	104	-	7,7,7	0.33	0	9,10,10	0.55	0
59	ARG	1F	317	57	10,11,11	0.75	1 (10%)	9,13,13	1.06	1 (11%)
58	MPD	2B	220	-	7,7,7	0.35	0	9,10,10	0.32	0
59	ARG	1B	231	57	10,11,11	0.82	1 (10%)	9,13,13	1.05	1 (11%)
61	SF4	1d	307	35	0,12,12	-	-	-	-	-
58	MPD	1a	3275	-	7,7,7	0.30	0	9,10,10	0.40	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
58	MPD	1A	4023	-	-	1/5/5/5	-
58	MPD	2A	3735	-	-	3/5/5/5	-
58	MPD	1a	3276	-	-	5/5/5/5	-
58	MPD	2A	3734	-	-	0/5/5/5	-
61	SF4	2d	501	35	-	-	0/6/5/5
58	MPD	18	104	-	-	1/5/5/5	-
59	ARG	1F	317	57	-	2/11/11/11	-
58	MPD	2B	220	-	-	0/5/5/5	-
59	ARG	1B	231	57	-	2/11/11/11	-
61	SF4	1d	307	35	-	-	0/6/5/5
58	MPD	1a	3275	-	-	0/5/5/5	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
59	1B	231	ARG	OXT-C	-2.44	1.22	1.30
59	1F	317	ARG	OXT-C	-2.11	1.23	1.30

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
59	1F	317	ARG	OXT-C-O	-3.10	117.04	124.08
59	1B	231	ARG	OXT-C-O	-2.84	117.63	124.08

There are no chirality outliers.

5 of 14 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
58	18	104	MPD	C2-C3-C4-C5
58	1a	3276	MPD	C2-C3-C4-O4
58	1a	3276	MPD	C2-C3-C4-C5
59	1F	317	ARG	O-C-CA-N
59	1F	317	ARG	OXT-C-CA-N

There are no ring outliers.

8 monomers are involved in 13 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
58	1a	3276	MPD	4	0
58	2A	3734	MPD	1	0
58	18	104	MPD	2	0
59	1F	317	ARG	2	0
58	2B	220	MPD	1	0
59	1B	231	ARG	1	0
61	1d	307	SF4	1	0
58	1a	3275	MPD	1	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	1A	2861/2915 (98%)	-0.48	110 (3%) 44 39	19, 36, 84, 98	0
1	2A	2856/2915 (97%)	0.03	111 (3%) 43 38	33, 55, 87, 99	0
2	1B	120/121 (99%)	-0.27	1 (0%) 82 80	29, 47, 61, 78	0
2	2B	120/121 (99%)	0.65	2 (1%) 69 65	57, 71, 79, 84	0
3	1D	275/276 (99%)	-0.04	2 (0%) 84 81	22, 36, 51, 61	0
3	2D	275/276 (99%)	0.44	4 (1%) 72 68	29, 50, 61, 74	0
4	1E	204/206 (99%)	0.07	1 (0%) 87 85	20, 40, 58, 70	0
4	2E	204/206 (99%)	0.39	1 (0%) 87 85	31, 53, 68, 76	0
5	1F	203/210 (96%)	0.10	3 (1%) 72 68	19, 41, 64, 77	0
5	2F	203/210 (96%)	0.72	8 (3%) 43 38	33, 62, 74, 79	0
6	1G	181/182 (99%)	0.89	14 (7%) 19 17	43, 59, 71, 78	0
6	2G	181/182 (99%)	1.55	46 (25%) 1 1	64, 74, 79, 83	0
7	1H	174/180 (96%)	0.45	6 (3%) 48 43	38, 51, 62, 66	0
7	2H	173/180 (96%)	1.37	27 (15%) 5 4	65, 72, 77, 84	0
8	1I	147/148 (99%)	0.96	10 (6%) 23 20	43, 67, 74, 77	0
8	2I	146/148 (98%)	1.49	34 (23%) 2 1	57, 70, 78, 80	0
9	1N	140/140 (100%)	0.02	0 100 100	23, 38, 56, 67	0
9	2N	140/140 (100%)	0.74	3 (2%) 63 59	43, 60, 71, 75	0
10	1O	122/122 (100%)	0.00	0 100 100	29, 40, 58, 68	0
10	2O	122/122 (100%)	0.42	1 (0%) 82 80	41, 53, 65, 68	0
11	1P	149/150 (99%)	0.23	0 100 100	19, 45, 64, 71	0
11	2P	149/150 (99%)	0.86	9 (6%) 27 24	37, 61, 74, 82	0
12	1Q	141/141 (100%)	0.04	1 (0%) 84 81	25, 39, 52, 60	0
12	2Q	141/141 (100%)	0.92	7 (4%) 34 30	45, 60, 68, 72	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
13	1R	118/118 (100%)	-0.03	0 100 100	25, 35, 47, 60	0
13	2R	118/118 (100%)	0.51	3 (2%) 58 54	38, 50, 60, 67	0
14	1S	110/112 (98%)	0.54	1 (0%) 81 78	35, 48, 58, 63	0
14	2S	110/112 (98%)	1.37	16 (14%) 6 5	60, 67, 73, 74	0
15	1T	131/146 (89%)	0.17	3 (2%) 61 57	31, 45, 62, 73	0
15	2T	131/146 (89%)	0.48	1 (0%) 82 80	45, 55, 69, 75	0
16	1U	116/118 (98%)	-0.18	1 (0%) 81 78	21, 29, 46, 59	0
16	2U	116/118 (98%)	0.74	3 (2%) 57 52	38, 56, 68, 71	0
17	1V	101/101 (100%)	0.06	0 100 100	20, 42, 56, 64	0
17	2V	101/101 (100%)	0.84	1 (0%) 79 76	40, 63, 70, 74	0
18	1W	112/113 (99%)	-0.14	0 100 100	23, 33, 50, 74	0
18	2W	112/113 (99%)	0.39	4 (3%) 46 41	37, 48, 62, 80	0
19	1X	95/96 (98%)	0.10	3 (3%) 50 46	25, 36, 57, 71	0
19	2X	95/96 (98%)	0.87	6 (6%) 26 23	48, 57, 68, 75	0
20	1Y	107/110 (97%)	0.44	2 (1%) 66 62	36, 47, 61, 71	0
20	2Y	107/110 (97%)	1.12	9 (8%) 17 15	56, 65, 72, 73	0
21	1Z	203/206 (98%)	0.59	5 (2%) 58 54	37, 55, 67, 76	0
21	2Z	201/206 (97%)	1.33	30 (14%) 5 4	60, 70, 76, 81	0
22	10	83/85 (97%)	0.06	0 100 100	26, 35, 50, 56	0
22	20	83/85 (97%)	1.09	7 (8%) 17 15	41, 57, 66, 70	0
23	11	97/98 (98%)	0.35	1 (1%) 79 76	28, 43, 61, 68	0
23	21	97/98 (98%)	0.68	2 (2%) 63 59	38, 54, 69, 73	0
24	12	70/72 (97%)	0.44	1 (1%) 73 70	36, 47, 57, 73	0
24	22	70/72 (97%)	0.88	4 (5%) 29 26	56, 63, 68, 70	0
25	13	59/60 (98%)	0.06	0 100 100	26, 36, 59, 65	0
25	23	59/60 (98%)	0.84	3 (5%) 33 29	48, 58, 69, 75	0
26	14	69/71 (97%)	1.21	14 (20%) 3 2	50, 70, 81, 84	0
26	24	69/71 (97%)	1.76	19 (27%) 1 1	73, 79, 86, 89	0
27	15	59/60 (98%)	-0.12	1 (1%) 69 65	20, 34, 49, 59	0
27	25	59/60 (98%)	0.23	1 (1%) 69 65	34, 49, 63, 69	0
28	16	53/54 (98%)	0.10	1 (1%) 66 62	31, 41, 52, 61	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
28	26	53/54 (98%)	0.62	1 (1%) 66 62	48, 56, 65, 66	0
29	17	48/49 (97%)	-0.14	1 (2%) 63 59	20, 28, 47, 52	0
29	27	48/49 (97%)	0.18	3 (6%) 26 23	32, 41, 57, 65	0
30	18	64/65 (98%)	-0.13	0 100 100	25, 34, 40, 51	0
30	28	64/65 (98%)	0.72	1 (1%) 70 67	45, 51, 58, 64	0
31	19	37/37 (100%)	-0.01	0 100 100	28, 39, 54, 59	0
31	29	37/37 (100%)	1.06	2 (5%) 31 27	51, 61, 68, 71	0
32	1a	1488/1521 (97%)	0.25	28 (1%) 66 62	35, 64, 84, 98	0
32	2a	1492/1521 (98%)	0.53	39 (2%) 57 52	48, 71, 86, 97	0
33	1b	231/256 (90%)	1.16	36 (15%) 5 4	60, 71, 79, 84	0
33	2b	231/256 (90%)	1.61	65 (28%) 1 1	64, 76, 81, 84	0
34	1c	206/239 (86%)	1.01	14 (6%) 23 20	56, 67, 74, 82	0
34	2c	206/239 (86%)	1.57	62 (30%) 1 1	66, 76, 81, 84	0
35	1d	208/209 (99%)	1.05	25 (12%) 9 7	52, 65, 74, 82	0
35	2d	208/209 (99%)	1.29	34 (16%) 4 3	56, 67, 73, 78	0
36	1e	148/162 (91%)	0.79	5 (3%) 48 43	48, 62, 69, 76	0
36	2e	148/162 (91%)	1.09	15 (10%) 12 10	55, 68, 74, 82	0
37	1f	100/101 (99%)	0.68	2 (2%) 65 61	50, 60, 70, 72	0
37	2f	100/101 (99%)	0.76	2 (2%) 65 61	56, 66, 72, 78	0
38	1g	155/156 (99%)	0.78	6 (3%) 43 38	55, 66, 71, 76	0
38	2g	155/156 (99%)	1.55	41 (26%) 1 1	66, 74, 79, 81	0
39	1h	137/138 (99%)	0.84	9 (6%) 24 21	50, 63, 69, 71	0
39	2h	137/138 (99%)	1.14	7 (5%) 33 29	62, 68, 74, 77	0
40	1i	127/128 (99%)	1.44	20 (15%) 5 4	55, 70, 76, 79	0
40	2i	126/128 (98%)	2.21	69 (54%) 0 0	69, 77, 82, 87	0
41	1j	97/105 (92%)	1.37	20 (20%) 2 2	56, 69, 79, 81	0
41	2j	96/105 (91%)	2.20	50 (52%) 0 0	68, 77, 81, 85	0
42	1k	114/129 (88%)	0.62	4 (3%) 47 42	44, 60, 68, 73	0
42	2k	114/129 (88%)	1.08	14 (12%) 8 7	57, 68, 75, 77	0
43	1l	121/132 (91%)	0.85	7 (5%) 29 25	48, 57, 68, 72	0
43	2l	121/132 (91%)	0.99	9 (7%) 20 18	54, 62, 68, 73	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
44	1m	116/126 (92%)	1.07	11 (9%) 14 12	56, 67, 74, 79	0
44	2m	114/126 (90%)	1.76	41 (35%) 1 1	69, 76, 80, 81	0
45	1n	60/61 (98%)	1.28	9 (15%) 5 4	56, 65, 71, 72	0
45	2n	60/61 (98%)	2.19	38 (63%) 0 0	69, 75, 80, 85	0
46	1o	88/89 (98%)	0.84	3 (3%) 48 43	45, 60, 70, 75	0
46	2o	88/89 (98%)	1.12	7 (7%) 18 16	56, 66, 74, 77	0
47	1p	82/88 (93%)	1.31	12 (14%) 6 4	60, 66, 75, 83	0
47	2p	82/88 (93%)	1.19	6 (7%) 21 19	57, 66, 72, 79	0
48	1q	99/105 (94%)	1.02	8 (8%) 18 15	51, 62, 69, 74	0
48	2q	99/105 (94%)	0.87	2 (2%) 65 61	57, 65, 73, 75	0
49	1r	68/88 (77%)	0.61	1 (1%) 72 68	52, 59, 72, 76	0
49	2r	68/88 (77%)	1.10	6 (8%) 15 14	62, 70, 76, 80	0
50	1s	83/93 (89%)	1.03	6 (7%) 21 19	57, 68, 75, 79	0
50	2s	83/93 (89%)	1.86	32 (38%) 1 0	70, 77, 82, 84	0
51	1t	96/106 (90%)	1.11	14 (14%) 6 4	57, 65, 73, 74	0
51	2t	98/106 (92%)	0.92	3 (3%) 51 47	54, 65, 74, 78	0
52	1u	23/27 (85%)	1.52	5 (21%) 2 2	61, 67, 71, 73	0
52	2u	23/27 (85%)	2.63	15 (65%) 0 0	72, 75, 79, 80	0
53	1y	97/113 (85%)	1.01	9 (9%) 14 12	46, 59, 68, 79	0
53	2y	96/113 (84%)	2.44	62 (64%) 0 0	69, 78, 83, 91	0
54	1w	3/4 (75%)	-0.10	0 100 100	36, 36, 42, 43	0
54	2w	3/4 (75%)	-0.20	0 100 100	49, 49, 52, 64	0
55	1x	3/4 (75%)	-0.09	0 100 100	36, 36, 37, 48	0
55	2x	3/4 (75%)	1.05	1 (33%) 1 1	49, 49, 54, 65	0
56	1v	3/3 (100%)	0.20	0 100 100	32, 32, 32, 38	0
56	2v	3/3 (100%)	1.47	1 (33%) 1 1	48, 48, 54, 60	0
All	All	20796/21490 (96%)	0.47	1426 (6%) 23 20	19, 60, 80, 99	0

The worst 5 of 1426 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
53	1y	98	ALA	9.2
1	1A	1087	G	6.4

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Mol	Chain	Res	Type	RSRZ
44	1m	2	ALA	6.1
45	2n	2	ALA	6.1
32	2a	1030(A)	G	6.0

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
1	PSU	2A	1917	20/21	0.82	0.11	64,74,85,92	0
1	5MU	2A	1915	21/22	0.83	0.12	73,80,85,96	0
32	2MG	2a	1207	24/25	0.84	0.13	72,77,87,90	0
1	5MU	1A	1915	21/22	0.86	0.11	62,71,74,87	0
32	PSU	2a	516	20/21	0.88	0.11	68,70,79,81	0
32	M2G	2a	966	25/26	0.88	0.16	58,71,83,94	0
1	PSU	2A	1911	20/21	0.88	0.11	63,68,81,82	0
1	PSU	1A	1917	20/21	0.89	0.10	62,67,70,75	0
32	5MC	2a	967	21/22	0.90	0.14	65,69,74,76	0
32	2MG	1a	1207	24/25	0.90	0.13	59,68,73,75	0
1	OMC	2A	1920	21/22	0.91	0.12	57,65,69,72	0
1	PSU	1A	1911	20/21	0.92	0.10	59,61,66,67	0
43	0TD	1l	92	10/11	0.92	0.11	54,59,62,71	0
43	0TD	2l	92	10/11	0.92	0.13	63,65,69,72	0
32	G7M	2a	527	24/25	0.93	0.12	60,63,67,71	0
32	MA6	1a	1519	24/25	0.94	0.11	41,49,53,55	0
32	5MC	1a	967	21/22	0.94	0.11	56,64,70,75	0
32	5MC	2a	1400	21/22	0.94	0.14	61,70,75,78	0
32	4OC	2a	1402	22/23	0.94	0.11	60,66,69,73	0
32	5MC	2a	1404	21/22	0.94	0.11	51,61,66,72	0
32	5MC	2a	1407	21/22	0.94	0.11	54,65,68,69	0
32	UR3	2a	1498	21/22	0.94	0.11	57,61,66,69	0
1	5MC	2A	1942	21/22	0.94	0.10	43,52,58,58	0
32	G7M	1a	527	24/25	0.95	0.10	43,55,60,61	0
32	UR3	1a	1498	21/22	0.95	0.11	43,49,52,55	0
32	M2G	1a	966	25/26	0.95	0.10	53,57,62,65	0
32	MA6	2a	1518	24/25	0.95	0.10	58,63,66,69	0
32	MA6	2a	1519	24/25	0.95	0.11	57,65,69,74	0
32	PSU	1a	516	20/21	0.95	0.09	53,62,66,70	0
55	8AN	2x	76	22/23	0.95	0.09	41,45,53,58	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
32	5MC	1a	1404	21/22	0.96	0.10	44,50,54,56	0
1	5MU	2A	1939	21/22	0.96	0.09	33,39,43,43	0
32	5MC	1a	1407	21/22	0.96	0.10	38,51,57,60	0
1	5MC	2A	1962	21/22	0.96	0.09	41,47,54,57	0
1	OMC	1A	1920	21/22	0.96	0.10	38,54,60,63	0
54	PPU	2w	76	37/38	0.96	0.09	30,41,45,51	0
32	4OC	1a	1402	22/23	0.96	0.09	43,50,52,68	0
1	PSU	2A	2605	20/21	0.97	0.08	29,38,42,44	0
32	5MC	1a	1400	21/22	0.97	0.10	48,52,57,60	0
1	PSU	1A	2605	20/21	0.97	0.08	24,28,32,35	0
32	MA6	1a	1518	24/25	0.97	0.09	42,47,50,50	0
1	5MC	1A	1942	21/22	0.97	0.07	30,36,42,46	0
1	OMG	2A	2251	24/25	0.97	0.08	30,38,42,45	0
1	2MA	2A	2503	23/24	0.97	0.08	30,35,39,41	0
55	8AN	1x	76	22/23	0.97	0.08	28,35,41,48	0
1	OMU	2A	2552	21/22	0.97	0.08	33,40,44,45	0
1	5MC	1A	1962	21/22	0.98	0.06	33,38,43,44	0
1	OMG	1A	2251	24/25	0.98	0.07	20,25,29,30	0
54	PPU	1w	76	37/38	0.98	0.07	23,28,32,33	0
1	2MA	1A	2503	23/24	0.98	0.06	17,21,24,28	0
1	OMU	1A	2552	21/22	0.98	0.07	21,27,33,33	0
1	5MU	1A	1939	21/22	0.98	0.07	23,28,31,34	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
57	MG	1A	4019	1/1	0.48	0.42	80,80,80,80	0
57	MG	2A	3677	1/1	0.59	0.21	63,63,63,63	0
57	MG	2A	3530	1/1	0.63	0.30	75,75,75,75	0
57	MG	1a	3135	1/1	0.67	0.22	79,79,79,79	0
57	MG	1a	3153	1/1	0.67	0.19	71,71,71,71	0
57	MG	1B	227	1/1	0.67	0.21	74,74,74,74	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	1P	203	1/1	0.67	0.22	51,51,51,51	0
57	MG	2a	3132	1/1	0.67	0.25	81,81,81,81	0
58	MPD	2B	220	8/8	0.67	0.29	53,65,71,77	0
57	MG	1A	3658	1/1	0.68	0.15	44,44,44,44	0
57	MG	1A	3885	1/1	0.69	0.27	53,53,53,53	0
57	MG	2A	3619	1/1	0.70	0.24	60,60,60,60	0
57	MG	2A	3728	1/1	0.71	0.15	76,76,76,76	0
57	MG	2A	3666	1/1	0.71	0.16	75,75,75,75	0
57	MG	1a	3273	1/1	0.71	0.19	63,63,63,63	0
57	MG	2A	3091	1/1	0.72	0.20	84,84,84,84	0
57	MG	2A	3457	1/1	0.72	0.20	71,71,71,71	0
57	MG	2a	3184	1/1	0.72	0.21	67,67,67,67	0
57	MG	1A	3507	1/1	0.72	0.19	76,76,76,76	0
57	MG	2a	3164	1/1	0.73	0.15	71,71,71,71	0
57	MG	2a	3010	1/1	0.73	0.26	81,81,81,81	0
57	MG	2B	206	1/1	0.73	0.21	74,74,74,74	0
57	MG	1a	3199	1/1	0.74	0.18	59,59,59,59	0
57	MG	1a	3145	1/1	0.74	0.19	67,67,67,67	0
57	MG	2j	201	1/1	0.74	0.12	71,71,71,71	0
57	MG	1A	3866	1/1	0.74	0.22	70,70,70,70	0
57	MG	2A	3731	1/1	0.75	0.20	64,64,64,64	0
57	MG	1a	3228	1/1	0.75	0.18	72,72,72,72	0
57	MG	1A	3746	1/1	0.75	0.23	63,63,63,63	0
57	MG	1A	3694	1/1	0.75	0.20	63,63,63,63	0
57	MG	1a	3133	1/1	0.76	0.16	63,63,63,63	0
57	MG	1A	3621	1/1	0.76	0.19	37,37,37,37	0
57	MG	1A	3868	1/1	0.76	0.12	40,40,40,40	0
57	MG	2A	3174	1/1	0.76	0.16	63,63,63,63	0
57	MG	2B	207	1/1	0.76	0.20	70,70,70,70	0
57	MG	2A	3301	1/1	0.76	0.38	64,64,64,64	0
57	MG	2a	3064	1/1	0.76	0.29	75,75,75,75	0
57	MG	1A	3812	1/1	0.76	0.18	55,55,55,55	0
57	MG	1a	3156	1/1	0.76	0.13	64,64,64,64	0
57	MG	2A	3534	1/1	0.76	0.20	70,70,70,70	0
57	MG	1a	3189	1/1	0.76	0.12	77,77,77,77	0
57	MG	1a	3052	1/1	0.76	0.16	76,76,76,76	0
57	MG	1B	222	1/1	0.77	0.22	74,74,74,74	0
57	MG	1A	3638	1/1	0.77	0.45	38,38,38,38	0
57	MG	2B	203	1/1	0.77	0.22	71,71,71,71	0
57	MG	1a	3176	1/1	0.78	0.16	74,74,74,74	0
57	MG	2a	3068	1/1	0.78	0.19	75,75,75,75	0
57	MG	1A	3968	1/1	0.78	0.23	56,56,56,56	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	1A	3994	1/1	0.78	0.16	72,72,72,72	0
57	MG	2A	3216	1/1	0.78	0.14	56,56,56,56	0
57	MG	2A	3287	1/1	0.78	0.22	67,67,67,67	0
57	MG	1A	3865	1/1	0.78	0.24	46,46,46,46	0
57	MG	1A	3850	1/1	0.79	0.13	63,63,63,63	0
57	MG	1A	3671	1/1	0.79	0.18	52,52,52,52	0
57	MG	2A	3313	1/1	0.79	0.24	68,68,68,68	0
57	MG	2U	201	1/1	0.79	0.12	64,64,64,64	0
57	MG	1a	3209	1/1	0.79	0.17	68,68,68,68	0
57	MG	2a	3062	1/1	0.79	0.35	69,69,69,69	0
57	MG	1A	3779	1/1	0.79	0.12	34,34,34,34	0
57	MG	1A	4004	1/1	0.79	0.17	51,51,51,51	0
57	MG	1a	3164	1/1	0.79	0.29	79,79,79,79	0
57	MG	2A	3114	1/1	0.79	0.19	70,70,70,70	0
57	MG	2A	3157	1/1	0.79	0.20	63,63,63,63	0
57	MG	1a	3175	1/1	0.79	0.13	63,63,63,63	0
57	MG	1A	3483	1/1	0.79	0.14	31,31,31,31	0
57	MG	1A	3768	1/1	0.80	0.16	55,55,55,55	0
57	MG	1A	3461	1/1	0.80	0.09	16,16,16,16	0
57	MG	1a	3081	1/1	0.80	0.27	72,72,72,72	0
57	MG	2A	3533	1/1	0.80	0.19	71,71,71,71	0
57	MG	1a	3100	1/1	0.80	0.23	78,78,78,78	0
57	MG	2A	3541	1/1	0.80	0.17	60,60,60,60	0
57	MG	2A	3581	1/1	0.80	0.17	62,62,62,62	0
57	MG	2A	3613	1/1	0.80	0.11	43,43,43,43	0
57	MG	1A	3933	1/1	0.80	0.11	51,51,51,51	0
57	MG	1A	3687	1/1	0.80	0.14	56,56,56,56	0
57	MG	1a	3141	1/1	0.80	0.13	60,60,60,60	0
57	MG	1a	3205	1/1	0.80	0.18	77,77,77,77	0
57	MG	1A	3979	1/1	0.80	0.12	29,29,29,29	0
57	MG	2A	3326	1/1	0.81	0.16	63,63,63,63	0
57	MG	1a	3040	1/1	0.81	0.20	66,66,66,66	0
57	MG	1a	3263	1/1	0.81	0.16	55,55,55,55	0
57	MG	1A	3608	1/1	0.81	0.22	70,70,70,70	0
57	MG	1A	3951	1/1	0.81	0.10	60,60,60,60	0
57	MG	1a	3099	1/1	0.81	0.19	59,59,59,59	0
57	MG	1A	4020	1/1	0.81	0.22	59,59,59,59	0
57	MG	2A	3599	1/1	0.81	0.15	49,49,49,49	0
57	MG	1a	3108	1/1	0.81	0.17	56,56,56,56	0
57	MG	1a	3119	1/1	0.81	0.17	69,69,69,69	0
57	MG	1A	3502	1/1	0.81	0.13	50,50,50,50	0
57	MG	1A	3433	1/1	0.81	0.13	32,32,32,32	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	2A	3718	1/1	0.81	0.16	71,71,71,71	0
57	MG	1A	3605	1/1	0.81	0.11	52,52,52,52	0
57	MG	1A	3378	1/1	0.82	0.15	60,60,60,60	0
57	MG	1a	3010	1/1	0.82	0.26	58,58,58,58	0
57	MG	2A	3386	1/1	0.82	0.15	62,62,62,62	0
57	MG	1a	3218	1/1	0.82	0.27	71,71,71,71	0
57	MG	2A	3476	1/1	0.82	0.20	63,63,63,63	0
57	MG	2A	3508	1/1	0.82	0.16	72,72,72,72	0
57	MG	1a	3178	1/1	0.82	0.19	70,70,70,70	0
57	MG	1a	3104	1/1	0.82	0.19	61,61,61,61	0
57	MG	1a	3011	1/1	0.82	0.14	69,69,69,69	0
57	MG	2A	3043	1/1	0.82	0.23	71,71,71,71	0
57	MG	2A	3575	1/1	0.82	0.12	62,62,62,62	0
57	MG	2A	3327	1/1	0.83	0.19	65,65,65,65	0
57	MG	2A	3368	1/1	0.83	0.15	60,60,60,60	0
57	MG	1B	228	1/1	0.83	0.12	52,52,52,52	0
57	MG	1G	203	1/1	0.83	0.13	67,67,67,67	0
57	MG	2A	3001	1/1	0.83	0.23	55,55,55,55	0
57	MG	2A	3503	1/1	0.83	0.14	63,63,63,63	0
57	MG	1A	3196	1/1	0.83	0.14	66,66,66,66	0
57	MG	2G	203	1/1	0.83	0.25	72,72,72,72	0
57	MG	2A	3090	1/1	0.83	0.20	70,70,70,70	0
57	MG	1T	203	1/1	0.83	0.14	65,65,65,65	0
57	MG	2a	3015	1/1	0.83	0.20	61,61,61,61	0
57	MG	1A	3513	1/1	0.83	0.14	31,31,31,31	0
57	MG	1a	3123	1/1	0.83	0.22	78,78,78,78	0
57	MG	1A	3572	1/1	0.83	0.13	42,42,42,42	0
57	MG	1a	3203	1/1	0.83	0.27	75,75,75,75	0
57	MG	2a	3134	1/1	0.83	0.12	63,63,63,63	0
57	MG	1A	3468	1/1	0.83	0.14	50,50,50,50	0
57	MG	1A	3389	1/1	0.83	0.08	31,31,31,31	0
57	MG	1a	3067	1/1	0.83	0.12	54,54,54,54	0
57	MG	1A	3221	1/1	0.83	0.12	65,65,65,65	0
57	MG	1A	3218	1/1	0.84	0.20	64,64,64,64	0
57	MG	1A	3518	1/1	0.84	0.12	50,50,50,50	0
57	MG	2A	3611	1/1	0.84	0.16	43,43,43,43	0
57	MG	2A	3246	1/1	0.84	0.34	62,62,62,62	0
57	MG	1G	204	1/1	0.84	0.13	50,50,50,50	0
57	MG	1A	3969	1/1	0.84	0.21	59,59,59,59	0
57	MG	1A	3976	1/1	0.84	0.17	55,55,55,55	0
57	MG	2A	3314	1/1	0.84	0.14	37,37,37,37	0
57	MG	1W	201	1/1	0.84	0.20	59,59,59,59	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	1A	3627	1/1	0.84	0.11	22,22,22,22	0
57	MG	1a	3140	1/1	0.84	0.26	58,58,58,58	0
57	MG	2A	3376	1/1	0.84	0.15	69,69,69,69	0
57	MG	2A	3377	1/1	0.84	0.10	39,39,39,39	0
57	MG	2B	211	1/1	0.84	0.10	59,59,59,59	0
57	MG	1a	3256	1/1	0.84	0.20	61,61,61,61	0
57	MG	2A	3398	1/1	0.84	0.17	59,59,59,59	0
57	MG	2a	3009	1/1	0.84	0.33	70,70,70,70	0
57	MG	1A	3530	1/1	0.84	0.11	56,56,56,56	0
57	MG	2A	3462	1/1	0.84	0.18	53,53,53,53	0
57	MG	2a	3023	1/1	0.84	0.19	69,69,69,69	0
57	MG	2a	3059	1/1	0.84	0.25	71,71,71,71	0
57	MG	1A	3547	1/1	0.84	0.11	44,44,44,44	0
57	MG	1A	3571	1/1	0.84	0.11	65,65,65,65	0
57	MG	1A	3419	1/1	0.84	0.12	25,25,25,25	0
57	MG	2a	3120	1/1	0.84	0.15	71,71,71,71	0
57	MG	2A	3522	1/1	0.84	0.14	35,35,35,35	0
57	MG	1a	3159	1/1	0.84	0.11	56,56,56,56	0
57	MG	2a	3148	1/1	0.84	0.12	67,67,67,67	0
57	MG	1a	3070	1/1	0.84	0.22	73,73,73,73	0
57	MG	1A	3578	1/1	0.84	0.12	40,40,40,40	0
57	MG	2A	3137	1/1	0.84	0.27	67,67,67,67	0
57	MG	1A	3425	1/1	0.84	0.11	35,35,35,35	0
57	MG	1A	3306	1/1	0.85	0.24	70,70,70,70	0
57	MG	2A	3322	1/1	0.85	0.12	52,52,52,52	0
57	MG	1l	201	1/1	0.85	0.19	68,68,68,68	0
57	MG	1a	3191	1/1	0.85	0.12	69,69,69,69	0
57	MG	1a	3195	1/1	0.85	0.14	63,63,63,63	0
57	MG	2A	3699	1/1	0.85	0.11	71,71,71,71	0
57	MG	2A	3717	1/1	0.85	0.20	63,63,63,63	0
57	MG	2A	3062	1/1	0.85	0.21	70,70,70,70	0
57	MG	2A	3724	1/1	0.85	0.20	66,66,66,66	0
57	MG	1A	3990	1/1	0.85	0.11	47,47,47,47	0
57	MG	2A	3730	1/1	0.85	0.12	52,52,52,52	0
57	MG	1A	3792	1/1	0.85	0.11	49,49,49,49	0
57	MG	2A	3104	1/1	0.85	0.23	63,63,63,63	0
57	MG	2A	3442	1/1	0.85	0.13	56,56,56,56	0
57	MG	2A	3447	1/1	0.85	0.18	64,64,64,64	0
57	MG	1A	3959	1/1	0.85	0.12	65,65,65,65	0
57	MG	2B	212	1/1	0.85	0.16	67,67,67,67	0
57	MG	1A	3330	1/1	0.85	0.16	61,61,61,61	0
57	MG	2A	3468	1/1	0.85	0.19	40,40,40,40	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	2A	3469	1/1	0.85	0.09	67,67,67,67	0
57	MG	1A	3222	1/1	0.85	0.10	59,59,59,59	0
57	MG	2A	3160	1/1	0.85	0.23	63,63,63,63	0
57	MG	2A	3167	1/1	0.85	0.21	56,56,56,56	0
57	MG	1a	3220	1/1	0.85	0.15	76,76,76,76	0
57	MG	2A	3523	1/1	0.85	0.10	48,48,48,48	0
57	MG	2A	3528	1/1	0.85	0.15	65,65,65,65	0
57	MG	2A	3175	1/1	0.85	0.20	70,70,70,70	0
57	MG	2A	3181	1/1	0.85	0.31	74,74,74,74	0
57	MG	1A	3893	1/1	0.85	0.13	54,54,54,54	0
57	MG	1a	3229	1/1	0.85	0.14	66,66,66,66	0
57	MG	2a	3143	1/1	0.85	0.21	64,64,64,64	0
57	MG	2A	3561	1/1	0.85	0.13	58,58,58,58	0
57	MG	2A	3568	1/1	0.85	0.14	43,43,43,43	0
57	MG	1a	3242	1/1	0.85	0.19	64,64,64,64	0
57	MG	1a	3094	1/1	0.85	0.24	69,69,69,69	0
57	MG	1a	3096	1/1	0.85	0.27	69,69,69,69	0
59	ARG	1F	317	12/12	0.85	0.15	48,60,72,73	0
57	MG	2A	3588	1/1	0.86	0.11	54,54,54,54	0
57	MG	2A	3363	1/1	0.86	0.09	48,48,48,48	0
57	MG	1A	3808	1/1	0.86	0.14	70,70,70,70	0
57	MG	1A	3643	1/1	0.86	0.23	58,58,58,58	0
57	MG	1a	3109	1/1	0.86	0.26	72,72,72,72	0
57	MG	1A	3843	1/1	0.86	0.12	56,56,56,56	0
57	MG	2A	3668	1/1	0.86	0.09	51,51,51,51	0
57	MG	2A	3397	1/1	0.86	0.10	37,37,37,37	0
57	MG	1A	3292	1/1	0.86	0.15	67,67,67,67	0
57	MG	2A	3700	1/1	0.86	0.12	80,80,80,80	0
57	MG	2A	3408	1/1	0.86	0.15	52,52,52,52	0
57	MG	2A	3437	1/1	0.86	0.36	49,49,49,49	0
57	MG	2A	3723	1/1	0.86	0.15	65,65,65,65	0
57	MG	1A	3582	1/1	0.86	0.37	40,40,40,40	0
57	MG	2A	3726	1/1	0.86	0.12	69,69,69,69	0
57	MG	2A	3443	1/1	0.86	0.15	51,51,51,51	0
57	MG	2A	3131	1/1	0.86	0.27	63,63,63,63	0
57	MG	2A	3451	1/1	0.86	0.14	53,53,53,53	0
57	MG	2A	3732	1/1	0.86	0.27	66,66,66,66	0
57	MG	1A	3675	1/1	0.86	0.10	71,71,71,71	0
57	MG	1A	3475	1/1	0.86	0.10	20,20,20,20	0
57	MG	2A	3465	1/1	0.86	0.13	63,63,63,63	0
57	MG	1A	3477	1/1	0.86	0.08	18,18,18,18	0
57	MG	1a	3069	1/1	0.86	0.10	61,61,61,61	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	1A	3707	1/1	0.86	0.14	65,65,65,65	0
57	MG	2O	202	1/1	0.86	0.11	69,69,69,69	0
57	MG	1A	3393	1/1	0.86	0.09	29,29,29,29	0
57	MG	1a	3232	1/1	0.86	0.16	47,47,47,47	0
57	MG	2A	3510	1/1	0.86	0.13	58,58,58,58	0
57	MG	2a	3011	1/1	0.86	0.22	58,58,58,58	0
57	MG	2A	3511	1/1	0.86	0.17	73,73,73,73	0
57	MG	2A	3198	1/1	0.86	0.31	61,61,61,61	0
57	MG	2a	3047	1/1	0.86	0.24	69,69,69,69	0
57	MG	2a	3056	1/1	0.86	0.16	74,74,74,74	0
57	MG	1A	3624	1/1	0.86	0.12	29,29,29,29	0
57	MG	2a	3060	1/1	0.86	0.25	76,76,76,76	0
57	MG	2A	3526	1/1	0.86	0.35	52,52,52,52	0
57	MG	1a	3253	1/1	0.86	0.10	51,51,51,51	0
57	MG	1G	202	1/1	0.86	0.09	42,42,42,42	0
57	MG	2A	3291	1/1	0.86	0.19	62,62,62,62	0
57	MG	1a	3167	1/1	0.86	0.09	39,39,39,39	0
57	MG	2A	3535	1/1	0.86	0.17	60,60,60,60	0
57	MG	2A	3539	1/1	0.86	0.15	67,67,67,67	0
57	MG	1a	3168	1/1	0.86	0.20	60,60,60,60	0
57	MG	1a	3274	1/1	0.86	0.19	68,68,68,68	0
57	MG	2A	3564	1/1	0.86	0.12	66,66,66,66	0
57	MG	1b	301	1/1	0.86	0.09	75,75,75,75	0
57	MG	1A	3444	1/1	0.86	0.11	55,55,55,55	0
57	MG	1A	3275	1/1	0.86	0.28	62,62,62,62	0
57	MG	1A	3697	1/1	0.87	0.18	39,39,39,39	0
57	MG	1A	3705	1/1	0.87	0.18	57,57,57,57	0
57	MG	1a	3219	1/1	0.87	0.15	63,63,63,63	0
57	MG	2A	3189	1/1	0.87	0.17	59,59,59,59	0
57	MG	2A	3196	1/1	0.87	0.17	55,55,55,55	0
57	MG	1a	3032	1/1	0.87	0.16	60,60,60,60	0
57	MG	1A	3595	1/1	0.87	0.17	69,69,69,69	0
57	MG	1a	3144	1/1	0.87	0.11	61,61,61,61	0
57	MG	2A	3733	1/1	0.87	0.11	59,59,59,59	0
57	MG	2A	3283	1/1	0.87	0.10	75,75,75,75	0
57	MG	1A	3597	1/1	0.87	0.13	41,41,41,41	0
57	MG	1a	3150	1/1	0.87	0.14	56,56,56,56	0
57	MG	1a	3251	1/1	0.87	0.13	61,61,61,61	0
57	MG	1a	3059	1/1	0.87	0.30	60,60,60,60	0
57	MG	1A	4013	1/1	0.87	0.10	47,47,47,47	0
57	MG	1A	3747	1/1	0.87	0.08	61,61,61,61	0
57	MG	2R	203	1/1	0.87	0.13	54,54,54,54	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	1A	3883	1/1	0.87	0.07	46,46,46,46	0
57	MG	2V	201	1/1	0.87	0.10	62,62,62,62	0
57	MG	1a	3165	1/1	0.87	0.21	70,70,70,70	0
57	MG	2A	3335	1/1	0.87	0.13	63,63,63,63	0
57	MG	2A	3553	1/1	0.87	0.13	53,53,53,53	0
57	MG	1A	3766	1/1	0.87	0.13	41,41,41,41	0
57	MG	1A	3123	1/1	0.87	0.22	49,49,49,49	0
57	MG	2a	3031	1/1	0.87	0.22	65,65,65,65	0
57	MG	2a	3040	1/1	0.87	0.25	66,66,66,66	0
57	MG	2A	3373	1/1	0.87	0.13	74,74,74,74	0
57	MG	1A	3776	1/1	0.87	0.08	22,22,22,22	0
57	MG	1D	309	1/1	0.87	0.45	48,48,48,48	0
57	MG	1A	3942	1/1	0.87	0.11	67,67,67,67	0
57	MG	1a	3188	1/1	0.87	0.10	80,80,80,80	0
57	MG	1A	3462	1/1	0.87	0.08	35,35,35,35	0
57	MG	2a	3066	1/1	0.87	0.15	68,68,68,68	0
57	MG	1A	3480	1/1	0.87	0.11	27,27,27,27	0
57	MG	2a	3069	1/1	0.87	0.17	57,57,57,57	0
57	MG	2a	3073	1/1	0.87	0.26	69,69,69,69	0
57	MG	2A	3614	1/1	0.87	0.14	62,62,62,62	0
57	MG	2a	3131	1/1	0.87	0.15	72,72,72,72	0
57	MG	1a	3193	1/1	0.87	0.13	59,59,59,59	0
57	MG	2A	3640	1/1	0.87	0.10	59,59,59,59	0
57	MG	2A	3646	1/1	0.87	0.12	55,55,55,55	0
57	MG	1A	3197	1/1	0.87	0.26	64,64,64,64	0
57	MG	2a	3153	1/1	0.87	0.13	63,63,63,63	0
57	MG	1A	3494	1/1	0.87	0.11	32,32,32,32	0
57	MG	1a	3201	1/1	0.87	0.20	72,72,72,72	0
57	MG	2a	3190	1/1	0.87	0.33	64,64,64,64	0
57	MG	1A	3814	1/1	0.87	0.12	43,43,43,43	0
58	MPD	1a	3275	8/8	0.87	0.20	57,66,67,71	0
57	MG	2A	3165	1/1	0.87	0.23	59,59,59,59	0
57	MG	1a	3128	1/1	0.87	0.17	64,64,64,64	0
57	MG	2A	3411	1/1	0.88	0.19	41,41,41,41	0
57	MG	2A	3430	1/1	0.88	0.17	64,64,64,64	0
57	MG	2A	3722	1/1	0.88	0.10	54,54,54,54	0
57	MG	2A	3149	1/1	0.88	0.23	56,56,56,56	0
57	MG	1B	217	1/1	0.88	0.10	54,54,54,54	0
57	MG	2A	3158	1/1	0.88	0.10	63,63,63,63	0
57	MG	2A	3727	1/1	0.88	0.14	56,56,56,56	0
57	MG	1a	3147	1/1	0.88	0.18	64,64,64,64	0
57	MG	1B	219	1/1	0.88	0.09	43,43,43,43	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	1a	3225	1/1	0.88	0.26	71,71,71,71	0
57	MG	1A	3769	1/1	0.88	0.13	51,51,51,51	0
57	MG	2A	3463	1/1	0.88	0.13	61,61,61,61	0
57	MG	2B	201	1/1	0.88	0.08	64,64,64,64	0
57	MG	1A	3271	1/1	0.88	0.15	49,49,49,49	0
57	MG	2A	3178	1/1	0.88	0.16	46,46,46,46	0
57	MG	1A	3588	1/1	0.88	0.11	40,40,40,40	0
57	MG	2A	3183	1/1	0.88	0.15	61,61,61,61	0
57	MG	2A	3478	1/1	0.88	0.16	64,64,64,64	0
57	MG	2B	218	1/1	0.88	0.09	70,70,70,70	0
57	MG	2E	304	1/1	0.88	0.11	38,38,38,38	0
57	MG	2E	307	1/1	0.88	0.15	63,63,63,63	0
57	MG	2A	3481	1/1	0.88	0.16	67,67,67,67	0
57	MG	1a	3087	1/1	0.88	0.21	57,57,57,57	0
57	MG	2A	3191	1/1	0.88	0.09	72,72,72,72	0
57	MG	1A	3203	1/1	0.88	0.20	44,44,44,44	0
57	MG	1E	304	1/1	0.88	0.09	26,26,26,26	0
57	MG	1A	3463	1/1	0.88	0.21	59,59,59,59	0
57	MG	2A	3219	1/1	0.88	0.20	63,63,63,63	0
57	MG	2A	3231	1/1	0.88	0.18	59,59,59,59	0
57	MG	2A	3233	1/1	0.88	0.28	63,63,63,63	0
57	MG	1A	3600	1/1	0.88	0.08	33,33,33,33	0
57	MG	2a	3028	1/1	0.88	0.13	56,56,56,56	0
57	MG	2A	3248	1/1	0.88	0.18	67,67,67,67	0
57	MG	2a	3033	1/1	0.88	0.13	57,57,57,57	0
57	MG	2a	3037	1/1	0.88	0.14	66,66,66,66	0
57	MG	2a	3038	1/1	0.88	0.16	61,61,61,61	0
57	MG	2A	3277	1/1	0.88	0.29	73,73,73,73	0
57	MG	2a	3042	1/1	0.88	0.23	63,63,63,63	0
57	MG	1A	3516	1/1	0.88	0.11	52,52,52,52	0
57	MG	2a	3049	1/1	0.88	0.26	57,57,57,57	0
57	MG	1N	203	1/1	0.88	0.12	58,58,58,58	0
57	MG	2a	3057	1/1	0.88	0.23	68,68,68,68	0
57	MG	1A	3193	1/1	0.88	0.22	61,61,61,61	0
57	MG	1A	3298	1/1	0.88	0.13	63,63,63,63	0
57	MG	2A	3304	1/1	0.88	0.22	54,54,54,54	0
57	MG	2A	3307	1/1	0.88	0.43	70,70,70,70	0
57	MG	1w	101	1/1	0.88	0.12	52,52,52,52	0
57	MG	1a	3121	1/1	0.88	0.11	52,52,52,52	0
57	MG	2A	3003	1/1	0.88	0.15	62,62,62,62	0
57	MG	2A	3037	1/1	0.88	0.20	62,62,62,62	0
57	MG	1A	3736	1/1	0.88	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
57	MG	1A	3086	1/1	0.88	0.11	44,44,44,44	0
57	MG	2A	3075	1/1	0.88	0.18	64,64,64,64	0
57	MG	2A	3084	1/1	0.88	0.18	63,63,63,63	0
57	MG	1A	3027	1/1	0.88	0.07	65,65,65,65	0
57	MG	2a	3147	1/1	0.88	0.13	53,53,53,53	0
57	MG	2A	3620	1/1	0.88	0.12	54,54,54,54	0
57	MG	1A	3353	1/1	0.88	0.10	31,31,31,31	0
57	MG	1A	3449	1/1	0.88	0.14	58,58,58,58	0
57	MG	2a	3170	1/1	0.88	0.16	82,82,82,82	0
57	MG	1a	3204	1/1	0.88	0.09	63,63,63,63	0
57	MG	2A	3395	1/1	0.88	0.14	60,60,60,60	0
57	MG	1a	3048	1/1	0.88	0.23	61,61,61,61	0
57	MG	2A	3689	1/1	0.88	0.12	55,55,55,55	0
58	MPD	2A	3734	8/8	0.88	0.22	38,49,52,57	0
57	MG	1A	3886	1/1	0.88	0.13	48,48,48,48	0
57	MG	2A	3143	1/1	0.88	0.12	53,53,53,53	0
57	MG	2A	3225	1/1	0.89	0.10	55,55,55,55	0
57	MG	1A	3974	1/1	0.89	0.08	44,44,44,44	0
57	MG	1A	3439	1/1	0.89	0.15	57,57,57,57	0
57	MG	2A	3237	1/1	0.89	0.17	57,57,57,57	0
57	MG	1a	3068	1/1	0.89	0.24	67,67,67,67	0
57	MG	1a	3211	1/1	0.89	0.24	68,68,68,68	0
57	MG	2A	3268	1/1	0.89	0.17	55,55,55,55	0
57	MG	1A	3506	1/1	0.89	0.07	29,29,29,29	0
57	MG	1A	3988	1/1	0.89	0.28	48,48,48,48	0
57	MG	1a	3077	1/1	0.89	0.13	60,60,60,60	0
57	MG	1A	3372	1/1	0.89	0.16	65,65,65,65	0
57	MG	2A	3300	1/1	0.89	0.34	64,64,64,64	0
57	MG	1A	3010	1/1	0.89	0.12	50,50,50,50	0
57	MG	1A	3995	1/1	0.89	0.11	57,57,57,57	0
57	MG	1a	3095	1/1	0.89	0.12	63,63,63,63	0
57	MG	2A	3312	1/1	0.89	0.16	55,55,55,55	0
57	MG	1A	4002	1/1	0.89	0.12	54,54,54,54	0
57	MG	1a	3097	1/1	0.89	0.34	60,60,60,60	0
57	MG	1A	3625	1/1	0.89	0.15	52,52,52,52	0
57	MG	1A	3457	1/1	0.89	0.08	44,44,44,44	0
57	MG	1A	3381	1/1	0.89	0.10	44,44,44,44	0
57	MG	1a	3266	1/1	0.89	0.10	61,61,61,61	0
57	MG	2A	3340	1/1	0.89	0.15	68,68,68,68	0
57	MG	2A	3361	1/1	0.89	0.12	55,55,55,55	0
57	MG	1A	3816	1/1	0.89	0.11	56,56,56,56	0
57	MG	1B	203	1/1	0.89	0.18	64,64,64,64	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	1B	207	1/1	0.89	0.16	53,53,53,53	0
57	MG	1d	303	1/1	0.89	0.17	64,64,64,64	0
57	MG	1d	306	1/1	0.89	0.10	78,78,78,78	0
57	MG	2B	210	1/1	0.89	0.30	66,66,66,66	0
57	MG	1h	202	1/1	0.89	0.19	66,66,66,66	0
57	MG	1A	3842	1/1	0.89	0.12	45,45,45,45	0
57	MG	1l	202	1/1	0.89	0.11	56,56,56,56	0
57	MG	1y	203	1/1	0.89	0.14	73,73,73,73	0
57	MG	2A	3404	1/1	0.89	0.09	32,32,32,32	0
57	MG	2G	202	1/1	0.89	0.14	66,66,66,66	0
57	MG	2A	3407	1/1	0.89	0.13	45,45,45,45	0
57	MG	1B	218	1/1	0.89	0.11	46,46,46,46	0
57	MG	2R	201	1/1	0.89	0.15	59,59,59,59	0
57	MG	1a	3126	1/1	0.89	0.14	61,61,61,61	0
57	MG	1A	3210	1/1	0.89	0.11	52,52,52,52	0
57	MG	1A	3531	1/1	0.89	0.09	52,52,52,52	0
57	MG	2W	202	1/1	0.89	0.18	52,52,52,52	0
57	MG	28	102	1/1	0.89	0.13	52,52,52,52	0
57	MG	1A	3857	1/1	0.89	0.08	51,51,51,51	0
57	MG	2A	3048	1/1	0.89	0.19	53,53,53,53	0
57	MG	2A	3049	1/1	0.89	0.17	57,57,57,57	0
57	MG	1A	3860	1/1	0.89	0.10	50,50,50,50	0
57	MG	2a	3021	1/1	0.89	0.16	62,62,62,62	0
57	MG	1A	3533	1/1	0.89	0.10	44,44,44,44	0
57	MG	2a	3024	1/1	0.89	0.25	70,70,70,70	0
57	MG	2a	3026	1/1	0.89	0.30	69,69,69,69	0
57	MG	1A	3537	1/1	0.89	0.22	61,61,61,61	0
57	MG	1A	3680	1/1	0.89	0.14	58,58,58,58	0
57	MG	1A	3313	1/1	0.89	0.18	39,39,39,39	0
57	MG	1A	3466	1/1	0.89	0.10	62,62,62,62	0
57	MG	2A	3112	1/1	0.89	0.11	57,57,57,57	0
57	MG	1a	3151	1/1	0.89	0.17	64,64,64,64	0
57	MG	2A	3120	1/1	0.89	0.27	55,55,55,55	0
57	MG	2A	3126	1/1	0.89	0.26	65,65,65,65	0
57	MG	2A	3484	1/1	0.89	0.10	28,28,28,28	0
57	MG	2A	3490	1/1	0.89	0.14	56,56,56,56	0
57	MG	2A	3499	1/1	0.89	0.11	44,44,44,44	0
57	MG	1A	3401	1/1	0.89	0.08	19,19,19,19	0
57	MG	1A	3418	1/1	0.89	0.11	26,26,26,26	0
57	MG	1A	3917	1/1	0.89	0.09	21,21,21,21	0
57	MG	1A	3041	1/1	0.89	0.23	58,58,58,58	0
57	MG	10	104	1/1	0.89	0.12	60,60,60,60	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	10	107	1/1	0.89	0.10	55,55,55,55	0
57	MG	10	109	1/1	0.89	0.16	58,58,58,58	0
57	MG	1a	3002	1/1	0.89	0.12	60,60,60,60	0
57	MG	2a	3078	1/1	0.89	0.27	69,69,69,69	0
57	MG	2a	3086	1/1	0.89	0.19	54,54,54,54	0
57	MG	2a	3090	1/1	0.89	0.12	66,66,66,66	0
57	MG	2a	3101	1/1	0.89	0.39	64,64,64,64	0
57	MG	2a	3112	1/1	0.89	0.33	65,65,65,65	0
57	MG	2a	3115	1/1	0.89	0.23	65,65,65,65	0
57	MG	2a	3119	1/1	0.89	0.12	50,50,50,50	0
57	MG	1a	3006	1/1	0.89	0.10	63,63,63,63	0
57	MG	1A	3585	1/1	0.89	0.09	36,36,36,36	0
57	MG	1a	3181	1/1	0.89	0.16	63,63,63,63	0
57	MG	1A	3189	1/1	0.89	0.16	66,66,66,66	0
57	MG	1a	3020	1/1	0.89	0.14	57,57,57,57	0
57	MG	1a	3022	1/1	0.89	0.11	73,73,73,73	0
57	MG	2A	3552	1/1	0.89	0.08	50,50,50,50	0
57	MG	1a	3023	1/1	0.89	0.23	61,61,61,61	0
57	MG	1A	3952	1/1	0.89	0.12	58,58,58,58	0
57	MG	2a	3168	1/1	0.89	0.10	66,66,66,66	0
57	MG	2A	3193	1/1	0.89	0.12	58,58,58,58	0
57	MG	1A	3358	1/1	0.89	0.06	22,22,22,22	0
57	MG	1a	3200	1/1	0.89	0.13	66,66,66,66	0
57	MG	2A	3576	1/1	0.89	0.11	50,50,50,50	0
57	MG	1A	3486	1/1	0.89	0.09	18,18,18,18	0
57	MG	2A	3218	1/1	0.89	0.12	53,53,53,53	0
58	MPD	2A	3735	8/8	0.89	0.19	53,57,64,68	0
57	MG	2A	3596	1/1	0.89	0.09	39,39,39,39	0
57	MG	1A	3438	1/1	0.89	0.10	51,51,51,51	0
57	MG	2A	3130	1/1	0.90	0.20	47,47,47,47	0
57	MG	1A	3441	1/1	0.90	0.14	48,48,48,48	0
57	MG	2A	3132	1/1	0.90	0.17	60,60,60,60	0
57	MG	2A	3412	1/1	0.90	0.09	59,59,59,59	0
57	MG	1A	3601	1/1	0.90	0.11	50,50,50,50	0
57	MG	1A	3604	1/1	0.90	0.18	54,54,54,54	0
57	MG	2A	3438	1/1	0.90	0.19	60,60,60,60	0
57	MG	1a	3089	1/1	0.90	0.14	55,55,55,55	0
57	MG	1A	3398	1/1	0.90	0.08	44,44,44,44	0
57	MG	2B	208	1/1	0.90	0.25	55,55,55,55	0
57	MG	1A	3322	1/1	0.90	0.31	59,59,59,59	0
57	MG	1A	3753	1/1	0.90	0.10	52,52,52,52	0
57	MG	1A	3924	1/1	0.90	0.12	56,56,56,56	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	1A	3932	1/1	0.90	0.12	51,51,51,51	0
57	MG	2D	302	1/1	0.90	0.13	49,49,49,49	0
57	MG	2E	301	1/1	0.90	0.16	47,47,47,47	0
57	MG	1A	3374	1/1	0.90	0.13	46,46,46,46	0
57	MG	1E	311	1/1	0.90	0.10	38,38,38,38	0
57	MG	1F	315	1/1	0.90	0.11	53,53,53,53	0
57	MG	1A	3940	1/1	0.90	0.09	39,39,39,39	0
57	MG	2I	201	1/1	0.90	0.15	64,64,64,64	0
57	MG	1A	3460	1/1	0.90	0.16	43,43,43,43	0
57	MG	2Q	202	1/1	0.90	0.19	53,53,53,53	0
57	MG	2A	3187	1/1	0.90	0.16	63,63,63,63	0
57	MG	2A	3188	1/1	0.90	0.15	60,60,60,60	0
57	MG	2T	201	1/1	0.90	0.15	66,66,66,66	0
57	MG	1a	3231	1/1	0.90	0.10	53,53,53,53	0
57	MG	1A	3949	1/1	0.90	0.12	38,38,38,38	0
57	MG	1a	3236	1/1	0.90	0.09	65,65,65,65	0
57	MG	1A	3558	1/1	0.90	0.18	51,51,51,51	0
57	MG	2a	3005	1/1	0.90	0.25	66,66,66,66	0
57	MG	2a	3008	1/1	0.90	0.11	64,64,64,64	0
57	MG	1A	3129	1/1	0.90	0.15	47,47,47,47	0
57	MG	2A	3214	1/1	0.90	0.15	60,60,60,60	0
57	MG	1A	3955	1/1	0.90	0.09	40,40,40,40	0
57	MG	1A	3635	1/1	0.90	0.15	44,44,44,44	0
57	MG	2a	3019	1/1	0.90	0.06	86,86,86,86	0
57	MG	1X	101	1/1	0.90	0.22	48,48,48,48	0
57	MG	1a	3139	1/1	0.90	0.18	66,66,66,66	0
57	MG	1Z	301	1/1	0.90	0.13	61,61,61,61	0
57	MG	2a	3025	1/1	0.90	0.18	52,52,52,52	0
57	MG	1A	3207	1/1	0.90	0.15	58,58,58,58	0
57	MG	1A	3642	1/1	0.90	0.19	63,63,63,63	0
57	MG	1A	3973	1/1	0.90	0.12	55,55,55,55	0
57	MG	15	3108	1/1	0.90	0.08	48,48,48,48	0
57	MG	2a	3035	1/1	0.90	0.21	59,59,59,59	0
57	MG	2A	3253	1/1	0.90	0.23	55,55,55,55	0
57	MG	2A	3254	1/1	0.90	0.24	57,57,57,57	0
57	MG	2a	3039	1/1	0.90	0.30	82,82,82,82	0
57	MG	2A	3551	1/1	0.90	0.09	60,60,60,60	0
57	MG	1f	202	1/1	0.90	0.06	40,40,40,40	0
57	MG	1A	3575	1/1	0.90	0.12	61,61,61,61	0
57	MG	2A	3281	1/1	0.90	0.19	66,66,66,66	0
57	MG	1a	3004	1/1	0.90	0.12	55,55,55,55	0
57	MG	2A	3566	1/1	0.90	0.12	68,68,68,68	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	2a	3058	1/1	0.90	0.25	64,64,64,64	0
57	MG	1A	3975	1/1	0.90	0.13	52,52,52,52	0
57	MG	1n	102	1/1	0.90	0.08	53,53,53,53	0
57	MG	1A	3650	1/1	0.90	0.09	49,49,49,49	0
57	MG	1a	3158	1/1	0.90	0.11	55,55,55,55	0
57	MG	2A	3584	1/1	0.90	0.07	55,55,55,55	0
57	MG	1x	102	1/1	0.90	0.09	41,41,41,41	0
57	MG	1A	3977	1/1	0.90	0.09	64,64,64,64	0
57	MG	2A	3597	1/1	0.90	0.11	64,64,64,64	0
57	MG	1a	3161	1/1	0.90	0.19	65,65,65,65	0
57	MG	1A	3270	1/1	0.90	0.26	65,65,65,65	0
57	MG	1A	3824	1/1	0.90	0.23	26,26,26,26	0
57	MG	1A	3989	1/1	0.90	0.14	32,32,32,32	0
57	MG	2A	3618	1/1	0.90	0.11	44,44,44,44	0
57	MG	1A	3436	1/1	0.90	0.09	51,51,51,51	0
57	MG	2A	3055	1/1	0.90	0.13	56,56,56,56	0
57	MG	2A	3057	1/1	0.90	0.11	51,51,51,51	0
57	MG	2a	3122	1/1	0.90	0.14	62,62,62,62	0
57	MG	2a	3124	1/1	0.90	0.09	56,56,56,56	0
57	MG	2a	3129	1/1	0.90	0.10	62,62,62,62	0
57	MG	2A	3336	1/1	0.90	0.17	54,54,54,54	0
57	MG	2A	3657	1/1	0.90	0.09	58,58,58,58	0
57	MG	1a	3174	1/1	0.90	0.09	76,76,76,76	0
57	MG	2A	3347	1/1	0.90	0.13	47,47,47,47	0
57	MG	2a	3145	1/1	0.90	0.22	66,66,66,66	0
57	MG	1A	3583	1/1	0.90	0.19	48,48,48,48	0
57	MG	1A	3847	1/1	0.90	0.11	36,36,36,36	0
57	MG	1A	3679	1/1	0.90	0.16	66,66,66,66	0
57	MG	2a	3154	1/1	0.90	0.08	69,69,69,69	0
57	MG	1a	3053	1/1	0.90	0.22	71,71,71,71	0
57	MG	2A	3704	1/1	0.90	0.09	40,40,40,40	0
57	MG	2A	3716	1/1	0.90	0.15	55,55,55,55	0
57	MG	2a	3173	1/1	0.90	0.09	71,71,71,71	0
57	MG	2A	3095	1/1	0.90	0.11	73,73,73,73	0
57	MG	2A	3103	1/1	0.90	0.16	56,56,56,56	0
57	MG	2A	3721	1/1	0.90	0.14	49,49,49,49	0
57	MG	1A	3853	1/1	0.90	0.10	27,27,27,27	0
57	MG	1A	3365	1/1	0.90	0.09	22,22,22,22	0
57	MG	1A	3397	1/1	0.90	0.08	35,35,35,35	0
57	MG	1A	3519	1/1	0.90	0.10	25,25,25,25	0
57	MG	1A	3523	1/1	0.90	0.11	54,54,54,54	0
57	MG	1A	3340	1/1	0.91	0.10	53,53,53,53	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	1A	3848	1/1	0.91	0.14	43,43,43,43	0
57	MG	1a	3041	1/1	0.91	0.09	64,64,64,64	0
57	MG	1a	3044	1/1	0.91	0.16	57,57,57,57	0
57	MG	2A	3094	1/1	0.91	0.18	52,52,52,52	0
57	MG	1A	3849	1/1	0.91	0.11	40,40,40,40	0
57	MG	2A	3096	1/1	0.91	0.17	54,54,54,54	0
57	MG	1A	3274	1/1	0.91	0.15	49,49,49,49	0
57	MG	2A	3381	1/1	0.91	0.13	48,48,48,48	0
57	MG	1A	3696	1/1	0.91	0.20	39,39,39,39	0
57	MG	2A	3105	1/1	0.91	0.18	56,56,56,56	0
57	MG	1A	3854	1/1	0.91	0.07	50,50,50,50	0
57	MG	1A	3527	1/1	0.91	0.14	59,59,59,59	0
57	MG	2A	3403	1/1	0.91	0.10	34,34,34,34	0
57	MG	1A	3145	1/1	0.91	0.15	50,50,50,50	0
57	MG	2A	3121	1/1	0.91	0.17	60,60,60,60	0
57	MG	1A	3362	1/1	0.91	0.09	37,37,37,37	0
57	MG	1A	3728	1/1	0.91	0.11	50,50,50,50	0
57	MG	1A	3421	1/1	0.91	0.07	33,33,33,33	0
57	MG	2A	3413	1/1	0.91	0.13	55,55,55,55	0
57	MG	1a	3078	1/1	0.91	0.15	65,65,65,65	0
57	MG	2A	3136	1/1	0.91	0.18	59,59,59,59	0
57	MG	1A	3869	1/1	0.91	0.11	52,52,52,52	0
57	MG	2B	213	1/1	0.91	0.08	69,69,69,69	0
57	MG	2A	3142	1/1	0.91	0.13	46,46,46,46	0
57	MG	1a	3082	1/1	0.91	0.14	80,80,80,80	0
57	MG	2D	306	1/1	0.91	0.15	44,44,44,44	0
57	MG	2D	308	1/1	0.91	0.13	59,59,59,59	0
57	MG	1a	3083	1/1	0.91	0.14	76,76,76,76	0
57	MG	1a	3210	1/1	0.91	0.21	65,65,65,65	0
57	MG	1A	3875	1/1	0.91	0.10	39,39,39,39	0
57	MG	1a	3215	1/1	0.91	0.12	62,62,62,62	0
57	MG	1A	3741	1/1	0.91	0.08	48,48,48,48	0
57	MG	1A	3744	1/1	0.91	0.18	51,51,51,51	0
57	MG	1A	3164	1/1	0.91	0.14	51,51,51,51	0
57	MG	1A	3889	1/1	0.91	0.11	56,56,56,56	0
57	MG	2A	3470	1/1	0.91	0.14	61,61,61,61	0
57	MG	2A	3475	1/1	0.91	0.10	58,58,58,58	0
57	MG	1A	3368	1/1	0.91	0.08	39,39,39,39	0
57	MG	2T	203	1/1	0.91	0.12	60,60,60,60	0
57	MG	2A	3477	1/1	0.91	0.09	39,39,39,39	0
57	MG	1A	3898	1/1	0.91	0.09	56,56,56,56	0
57	MG	1A	3901	1/1	0.91	0.09	26,26,26,26	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	20	102	1/1	0.91	0.09	56,56,56,56	0
57	MG	1E	310	1/1	0.91	0.10	58,58,58,58	0
57	MG	2a	3002	1/1	0.91	0.17	57,57,57,57	0
57	MG	2a	3004	1/1	0.91	0.17	59,59,59,59	0
57	MG	1a	3106	1/1	0.91	0.16	59,59,59,59	0
57	MG	2A	3491	1/1	0.91	0.15	56,56,56,56	0
57	MG	1a	3238	1/1	0.91	0.12	56,56,56,56	0
57	MG	1A	3557	1/1	0.91	0.09	46,46,46,46	0
57	MG	2A	3192	1/1	0.91	0.31	55,55,55,55	0
57	MG	1A	3758	1/1	0.91	0.15	70,70,70,70	0
57	MG	2a	3016	1/1	0.91	0.18	62,62,62,62	0
57	MG	2A	3195	1/1	0.91	0.17	58,58,58,58	0
57	MG	2A	3512	1/1	0.91	0.14	67,67,67,67	0
57	MG	2A	3518	1/1	0.91	0.16	59,59,59,59	0
57	MG	1a	3116	1/1	0.91	0.10	61,61,61,61	0
57	MG	1A	3761	1/1	0.91	0.13	49,49,49,49	0
57	MG	2A	3524	1/1	0.91	0.07	35,35,35,35	0
57	MG	2a	3027	1/1	0.91	0.08	68,68,68,68	0
57	MG	2A	3209	1/1	0.91	0.13	53,53,53,53	0
57	MG	2A	3527	1/1	0.91	0.12	59,59,59,59	0
57	MG	1a	3120	1/1	0.91	0.11	63,63,63,63	0
57	MG	1A	3171	1/1	0.91	0.14	45,45,45,45	0
57	MG	1A	3243	1/1	0.91	0.16	57,57,57,57	0
57	MG	1A	3264	1/1	0.91	0.12	34,34,34,34	0
57	MG	1N	204	1/1	0.91	0.13	51,51,51,51	0
57	MG	1A	3321	1/1	0.91	0.29	66,66,66,66	0
57	MG	2a	3041	1/1	0.91	0.24	56,56,56,56	0
57	MG	1A	3577	1/1	0.91	0.08	27,27,27,27	0
57	MG	2A	3543	1/1	0.91	0.10	67,67,67,67	0
57	MG	1T	204	1/1	0.91	0.12	64,64,64,64	0
57	MG	2a	3054	1/1	0.91	0.10	60,60,60,60	0
57	MG	2A	3238	1/1	0.91	0.09	58,58,58,58	0
57	MG	1g	201	1/1	0.91	0.23	62,62,62,62	0
57	MG	2A	3555	1/1	0.91	0.20	48,48,48,48	0
57	MG	1A	3646	1/1	0.91	0.23	52,52,52,52	0
57	MG	2A	3251	1/1	0.91	0.11	53,53,53,53	0
57	MG	1A	3802	1/1	0.91	0.07	26,26,26,26	0
57	MG	1A	3059	1/1	0.91	0.17	47,47,47,47	0
57	MG	2A	3569	1/1	0.91	0.10	45,45,45,45	0
57	MG	2A	3570	1/1	0.91	0.11	63,63,63,63	0
57	MG	2A	3571	1/1	0.91	0.10	44,44,44,44	0
57	MG	2a	3071	1/1	0.91	0.16	64,64,64,64	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	2a	3072	1/1	0.91	0.15	59,59,59,59	0
57	MG	2A	3255	1/1	0.91	0.09	49,49,49,49	0
57	MG	1l	203	1/1	0.91	0.10	63,63,63,63	0
57	MG	2a	3083	1/1	0.91	0.21	64,64,64,64	0
57	MG	1A	3965	1/1	0.91	0.07	35,35,35,35	0
57	MG	2A	3582	1/1	0.91	0.10	50,50,50,50	0
57	MG	2a	3094	1/1	0.91	0.21	55,55,55,55	0
57	MG	1A	3447	1/1	0.91	0.13	55,55,55,55	0
57	MG	1A	3666	1/1	0.91	0.13	21,21,21,21	0
57	MG	2a	3113	1/1	0.91	0.29	53,53,53,53	0
57	MG	2a	3114	1/1	0.91	0.33	62,62,62,62	0
57	MG	1A	3972	1/1	0.91	0.10	56,56,56,56	0
57	MG	17	105	1/1	0.91	0.23	62,62,62,62	0
57	MG	1A	3448	1/1	0.91	0.12	61,61,61,61	0
57	MG	2A	3600	1/1	0.91	0.07	47,47,47,47	0
57	MG	2A	3033	1/1	0.91	0.23	52,52,52,52	0
57	MG	2a	3127	1/1	0.91	0.10	71,71,71,71	0
57	MG	1A	3817	1/1	0.91	0.08	21,21,21,21	0
57	MG	2A	3306	1/1	0.91	0.12	43,43,43,43	0
57	MG	1A	3392	1/1	0.91	0.09	35,35,35,35	0
57	MG	2A	3310	1/1	0.91	0.13	58,58,58,58	0
57	MG	2a	3137	1/1	0.91	0.14	55,55,55,55	0
57	MG	2A	3044	1/1	0.91	0.14	53,53,53,53	0
57	MG	1A	3835	1/1	0.91	0.08	44,44,44,44	0
57	MG	1A	3328	1/1	0.91	0.13	51,51,51,51	0
57	MG	2A	3317	1/1	0.91	0.07	50,50,50,50	0
57	MG	1A	3034	1/1	0.91	0.15	51,51,51,51	0
57	MG	1A	3983	1/1	0.91	0.08	55,55,55,55	0
57	MG	2a	3160	1/1	0.91	0.15	74,74,74,74	0
57	MG	2A	3669	1/1	0.91	0.21	75,75,75,75	0
57	MG	2a	3166	1/1	0.91	0.12	58,58,58,58	0
57	MG	2A	3671	1/1	0.91	0.09	53,53,53,53	0
57	MG	2A	3675	1/1	0.91	0.11	45,45,45,45	0
57	MG	1A	3987	1/1	0.91	0.12	32,32,32,32	0
57	MG	2a	3179	1/1	0.91	0.13	60,60,60,60	0
57	MG	2A	3678	1/1	0.91	0.09	54,54,54,54	0
57	MG	2a	3189	1/1	0.91	0.25	55,55,55,55	0
57	MG	2A	3685	1/1	0.91	0.14	55,55,55,55	0
57	MG	2f	201	1/1	0.91	0.13	60,60,60,60	0
57	MG	2A	3688	1/1	0.91	0.09	59,59,59,59	0
57	MG	2A	3334	1/1	0.91	0.12	52,52,52,52	0
57	MG	2A	3693	1/1	0.91	0.10	58,58,58,58	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	2A	3064	1/1	0.91	0.14	49,49,49,49	0
57	MG	2A	3067	1/1	0.91	0.09	47,47,47,47	0
57	MG	2A	3702	1/1	0.91	0.08	62,62,62,62	0
57	MG	2A	3698	1/1	0.92	0.08	72,72,72,72	0
57	MG	1D	311	1/1	0.92	0.13	52,52,52,52	0
57	MG	1D	314	1/1	0.92	0.07	67,67,67,67	0
57	MG	1a	3107	1/1	0.92	0.21	52,52,52,52	0
57	MG	1D	315	1/1	0.92	0.11	48,48,48,48	0
57	MG	1n	103	1/1	0.92	0.17	60,60,60,60	0
57	MG	1y	201	1/1	0.92	0.15	66,66,66,66	0
57	MG	1y	202	1/1	0.92	0.14	56,56,56,56	0
57	MG	1A	3751	1/1	0.92	0.08	25,25,25,25	0
57	MG	1a	3110	1/1	0.92	0.17	53,53,53,53	0
57	MG	1E	308	1/1	0.92	0.14	44,44,44,44	0
57	MG	1A	3545	1/1	0.92	0.12	41,41,41,41	0
57	MG	1A	3130	1/1	0.92	0.29	37,37,37,37	0
57	MG	1F	314	1/1	0.92	0.10	41,41,41,41	0
57	MG	1A	3908	1/1	0.92	0.24	55,55,55,55	0
57	MG	2A	3729	1/1	0.92	0.19	53,53,53,53	0
57	MG	2A	3039	1/1	0.92	0.27	58,58,58,58	0
57	MG	1A	3911	1/1	0.92	0.06	20,20,20,20	0
57	MG	1A	3555	1/1	0.92	0.11	45,45,45,45	0
57	MG	2A	3375	1/1	0.92	0.10	40,40,40,40	0
57	MG	1a	3129	1/1	0.92	0.12	64,64,64,64	0
57	MG	1A	3326	1/1	0.92	0.11	41,41,41,41	0
57	MG	2A	3050	1/1	0.92	0.17	66,66,66,66	0
57	MG	2A	3053	1/1	0.92	0.08	48,48,48,48	0
57	MG	1A	3384	1/1	0.92	0.13	56,56,56,56	0
57	MG	1A	3562	1/1	0.92	0.10	57,57,57,57	0
57	MG	2A	3060	1/1	0.92	0.09	43,43,43,43	0
57	MG	2A	3400	1/1	0.92	0.16	55,55,55,55	0
57	MG	1A	3935	1/1	0.92	0.14	58,58,58,58	0
57	MG	2B	215	1/1	0.92	0.07	72,72,72,72	0
57	MG	1Q	206	1/1	0.92	0.10	41,41,41,41	0
57	MG	1a	3142	1/1	0.92	0.09	58,58,58,58	0
57	MG	1R	204	1/1	0.92	0.16	50,50,50,50	0
57	MG	2A	3409	1/1	0.92	0.10	40,40,40,40	0
57	MG	2A	3083	1/1	0.92	0.13	55,55,55,55	0
57	MG	1A	3487	1/1	0.92	0.08	53,53,53,53	0
57	MG	2A	3085	1/1	0.92	0.11	41,41,41,41	0
57	MG	2G	201	1/1	0.92	0.10	70,70,70,70	0
57	MG	1A	3388	1/1	0.92	0.07	27,27,27,27	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	2A	3435	1/1	0.92	0.18	56,56,56,56	0
57	MG	1V	206	1/1	0.92	0.20	48,48,48,48	0
57	MG	1A	3948	1/1	0.92	0.12	39,39,39,39	0
57	MG	1a	3152	1/1	0.92	0.08	65,65,65,65	0
57	MG	2Q	203	1/1	0.92	0.10	62,62,62,62	0
57	MG	1A	3785	1/1	0.92	0.12	48,48,48,48	0
57	MG	1A	3787	1/1	0.92	0.07	28,28,28,28	0
57	MG	1A	3573	1/1	0.92	0.08	43,43,43,43	0
57	MG	2A	3455	1/1	0.92	0.11	57,57,57,57	0
57	MG	1A	3794	1/1	0.92	0.10	59,59,59,59	0
57	MG	2A	3111	1/1	0.92	0.11	55,55,55,55	0
57	MG	1A	3956	1/1	0.92	0.10	51,51,51,51	0
57	MG	1A	3796	1/1	0.92	0.07	70,70,70,70	0
57	MG	25	102	1/1	0.92	0.21	45,45,45,45	0
57	MG	2A	3116	1/1	0.92	0.17	51,51,51,51	0
57	MG	2A	3119	1/1	0.92	0.09	54,54,54,54	0
57	MG	1A	3138	1/1	0.92	0.07	43,43,43,43	0
57	MG	1A	3659	1/1	0.92	0.05	19,19,19,19	0
57	MG	1a	3003	1/1	0.92	0.13	53,53,53,53	0
57	MG	1A	3064	1/1	0.92	0.11	59,59,59,59	0
57	MG	1A	3069	1/1	0.92	0.29	29,29,29,29	0
57	MG	1A	3512	1/1	0.92	0.09	17,17,17,17	0
57	MG	2a	3013	1/1	0.92	0.18	66,66,66,66	0
57	MG	1a	3177	1/1	0.92	0.07	59,59,59,59	0
57	MG	2A	3489	1/1	0.92	0.18	67,67,67,67	0
57	MG	1A	3678	1/1	0.92	0.08	55,55,55,55	0
57	MG	2A	3138	1/1	0.92	0.11	44,44,44,44	0
57	MG	2A	3494	1/1	0.92	0.11	42,42,42,42	0
57	MG	1a	3019	1/1	0.92	0.15	58,58,58,58	0
57	MG	2A	3502	1/1	0.92	0.10	60,60,60,60	0
57	MG	1a	3184	1/1	0.92	0.09	69,69,69,69	0
57	MG	2A	3148	1/1	0.92	0.09	55,55,55,55	0
57	MG	1a	3185	1/1	0.92	0.19	72,72,72,72	0
57	MG	2A	3153	1/1	0.92	0.27	58,58,58,58	0
57	MG	2a	3032	1/1	0.92	0.25	57,57,57,57	0
57	MG	1A	3822	1/1	0.92	0.15	55,55,55,55	0
57	MG	1A	3347	1/1	0.92	0.09	46,46,46,46	0
57	MG	1a	3190	1/1	0.92	0.10	55,55,55,55	0
57	MG	1A	3832	1/1	0.92	0.08	36,36,36,36	0
57	MG	1a	3025	1/1	0.92	0.14	60,60,60,60	0
57	MG	2A	3525	1/1	0.92	0.14	50,50,50,50	0
57	MG	2A	3169	1/1	0.92	0.12	62,62,62,62	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	1A	3046	1/1	0.92	0.22	54,54,54,54	0
57	MG	2a	3043	1/1	0.92	0.18	70,70,70,70	0
57	MG	2a	3045	1/1	0.92	0.09	54,54,54,54	0
57	MG	1a	3035	1/1	0.92	0.18	52,52,52,52	0
57	MG	1a	3038	1/1	0.92	0.18	64,64,64,64	0
57	MG	2A	3531	1/1	0.92	0.12	63,63,63,63	0
57	MG	1A	3682	1/1	0.92	0.08	68,68,68,68	0
57	MG	1A	3683	1/1	0.92	0.09	66,66,66,66	0
57	MG	1a	3042	1/1	0.92	0.20	71,71,71,71	0
57	MG	1A	3088	1/1	0.92	0.09	46,46,46,46	0
57	MG	1A	3590	1/1	0.92	0.12	54,54,54,54	0
57	MG	1A	3695	1/1	0.92	0.10	49,49,49,49	0
57	MG	2A	3547	1/1	0.92	0.10	32,32,32,32	0
57	MG	2A	3550	1/1	0.92	0.07	62,62,62,62	0
57	MG	1A	3991	1/1	0.92	0.09	50,50,50,50	0
57	MG	1a	3214	1/1	0.92	0.16	71,71,71,71	0
57	MG	1A	3011	1/1	0.92	0.09	50,50,50,50	0
57	MG	1a	3060	1/1	0.92	0.21	65,65,65,65	0
57	MG	2A	3557	1/1	0.92	0.09	60,60,60,60	0
57	MG	2a	3077	1/1	0.92	0.32	60,60,60,60	0
57	MG	1a	3062	1/1	0.92	0.11	57,57,57,57	0
57	MG	2a	3082	1/1	0.92	0.15	58,58,58,58	0
57	MG	1a	3064	1/1	0.92	0.14	58,58,58,58	0
57	MG	2a	3084	1/1	0.92	0.17	79,79,79,79	0
57	MG	2a	3085	1/1	0.92	0.14	60,60,60,60	0
57	MG	2A	3213	1/1	0.92	0.14	56,56,56,56	0
57	MG	1A	3851	1/1	0.92	0.11	61,61,61,61	0
57	MG	1A	3060	1/1	0.92	0.12	36,36,36,36	0
57	MG	1A	3309	1/1	0.92	0.20	25,25,25,25	0
57	MG	2a	3102	1/1	0.92	0.18	51,51,51,51	0
57	MG	1A	4009	1/1	0.92	0.12	45,45,45,45	0
57	MG	2A	3221	1/1	0.92	0.07	53,53,53,53	0
57	MG	1a	3074	1/1	0.92	0.18	60,60,60,60	0
57	MG	2A	3226	1/1	0.92	0.18	59,59,59,59	0
57	MG	1a	3234	1/1	0.92	0.11	63,63,63,63	0
57	MG	1A	3249	1/1	0.92	0.15	42,42,42,42	0
57	MG	1A	3711	1/1	0.92	0.09	33,33,33,33	0
57	MG	1a	3241	1/1	0.92	0.28	62,62,62,62	0
57	MG	1A	3714	1/1	0.92	0.21	30,30,30,30	0
57	MG	2A	3247	1/1	0.92	0.08	54,54,54,54	0
57	MG	2a	3130	1/1	0.92	0.11	65,65,65,65	0
57	MG	1A	3720	1/1	0.92	0.09	35,35,35,35	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	2A	3602	1/1	0.92	0.09	54,54,54,54	0
57	MG	1A	3603	1/1	0.92	0.09	30,30,30,30	0
57	MG	2A	3252	1/1	0.92	0.24	66,66,66,66	0
57	MG	2a	3138	1/1	0.92	0.07	67,67,67,67	0
57	MG	1a	3086	1/1	0.92	0.22	61,61,61,61	0
57	MG	1A	3474	1/1	0.92	0.10	59,59,59,59	0
57	MG	1a	3265	1/1	0.92	0.20	64,64,64,64	0
57	MG	2A	3266	1/1	0.92	0.13	63,63,63,63	0
57	MG	1a	3088	1/1	0.92	0.07	58,58,58,58	0
57	MG	2A	3644	1/1	0.92	0.08	48,48,48,48	0
57	MG	2a	3155	1/1	0.92	0.15	61,61,61,61	0
57	MG	2a	3156	1/1	0.92	0.10	72,72,72,72	0
57	MG	2a	3157	1/1	0.92	0.09	68,68,68,68	0
57	MG	1a	3267	1/1	0.92	0.13	55,55,55,55	0
57	MG	2A	3654	1/1	0.92	0.07	23,23,23,23	0
57	MG	2A	3278	1/1	0.92	0.20	45,45,45,45	0
57	MG	2a	3167	1/1	0.92	0.11	67,67,67,67	0
57	MG	1A	3263	1/1	0.92	0.11	59,59,59,59	0
57	MG	2A	3667	1/1	0.92	0.09	50,50,50,50	0
57	MG	1A	3534	1/1	0.92	0.08	38,38,38,38	0
57	MG	2a	3177	1/1	0.92	0.12	59,59,59,59	0
57	MG	1A	3884	1/1	0.92	0.09	42,42,42,42	0
57	MG	2a	3183	1/1	0.92	0.21	66,66,66,66	0
57	MG	1A	3614	1/1	0.92	0.11	43,43,43,43	0
57	MG	2A	3299	1/1	0.92	0.20	53,53,53,53	0
57	MG	1d	304	1/1	0.92	0.10	63,63,63,63	0
57	MG	2e	201	1/1	0.92	0.25	61,61,61,61	0
57	MG	1A	3377	1/1	0.92	0.08	66,66,66,66	0
57	MG	1B	230	1/1	0.92	0.08	61,61,61,61	0
57	MG	2n	101	1/1	0.92	0.22	58,58,58,58	0
57	MG	2A	3686	1/1	0.92	0.10	47,47,47,47	0
57	MG	1A	3748	1/1	0.92	0.09	49,49,49,49	0
57	MG	1a	3103	1/1	0.92	0.13	67,67,67,67	0
57	MG	2A	3309	1/1	0.92	0.10	55,55,55,55	0
59	ARG	1B	231	12/12	0.92	0.10	29,44,51,55	0
57	MG	2A	3695	1/1	0.92	0.12	61,61,61,61	0
57	MG	1B	210	1/1	0.93	0.09	49,49,49,49	0
57	MG	2A	3651	1/1	0.93	0.08	37,37,37,37	0
57	MG	2A	3263	1/1	0.93	0.16	51,51,51,51	0
57	MG	2A	3265	1/1	0.93	0.27	50,50,50,50	0
57	MG	2A	3663	1/1	0.93	0.09	70,70,70,70	0
57	MG	1B	211	1/1	0.93	0.19	71,71,71,71	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	1A	3718	1/1	0.93	0.35	38,38,38,38	0
57	MG	1A	3619	1/1	0.93	0.12	57,57,57,57	0
57	MG	1A	3726	1/1	0.93	0.10	42,42,42,42	0
57	MG	2A	3279	1/1	0.93	0.26	44,44,44,44	0
57	MG	1e	201	1/1	0.93	0.18	63,63,63,63	0
57	MG	2A	3282	1/1	0.93	0.14	55,55,55,55	0
57	MG	1B	220	1/1	0.93	0.07	28,28,28,28	0
57	MG	2A	3286	1/1	0.93	0.28	44,44,44,44	0
57	MG	1A	3867	1/1	0.93	0.08	38,38,38,38	0
57	MG	1A	3727	1/1	0.93	0.09	42,42,42,42	0
57	MG	2A	3292	1/1	0.93	0.31	64,64,64,64	0
57	MG	2A	3298	1/1	0.93	0.34	56,56,56,56	0
57	MG	1A	3556	1/1	0.93	0.09	39,39,39,39	0
57	MG	2A	3696	1/1	0.93	0.11	62,62,62,62	0
57	MG	1B	229	1/1	0.93	0.13	56,56,56,56	0
57	MG	1A	3730	1/1	0.93	0.10	52,52,52,52	0
57	MG	1n	101	1/1	0.93	0.25	66,66,66,66	0
57	MG	1A	3879	1/1	0.93	0.07	28,28,28,28	0
57	MG	1A	3880	1/1	0.93	0.12	54,54,54,54	0
57	MG	2A	3707	1/1	0.93	0.09	46,46,46,46	0
57	MG	2A	3709	1/1	0.93	0.07	44,44,44,44	0
57	MG	1o	101	1/1	0.93	0.20	58,58,58,58	0
57	MG	1o	102	1/1	0.93	0.10	56,56,56,56	0
57	MG	1A	3881	1/1	0.93	0.07	29,29,29,29	0
57	MG	2A	3719	1/1	0.93	0.09	47,47,47,47	0
57	MG	1A	3357	1/1	0.93	0.07	25,25,25,25	0
57	MG	1a	3111	1/1	0.93	0.10	56,56,56,56	0
57	MG	1a	3113	1/1	0.93	0.10	41,41,41,41	0
57	MG	2A	3320	1/1	0.93	0.12	45,45,45,45	0
57	MG	1A	3740	1/1	0.93	0.06	24,24,24,24	0
57	MG	2A	3323	1/1	0.93	0.10	57,57,57,57	0
57	MG	1E	305	1/1	0.93	0.18	47,47,47,47	0
57	MG	1E	306	1/1	0.93	0.09	42,42,42,42	0
57	MG	2A	3332	1/1	0.93	0.06	35,35,35,35	0
57	MG	2A	3023	1/1	0.93	0.16	54,54,54,54	0
57	MG	2A	3028	1/1	0.93	0.09	59,59,59,59	0
57	MG	2A	3032	1/1	0.93	0.09	50,50,50,50	0
57	MG	1A	3496	1/1	0.93	0.10	53,53,53,53	0
57	MG	2B	202	1/1	0.93	0.20	62,62,62,62	0
57	MG	2A	3342	1/1	0.93	0.12	45,45,45,45	0
57	MG	1E	309	1/1	0.93	0.08	25,25,25,25	0
57	MG	2A	3348	1/1	0.93	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
57	MG	2A	3358	1/1	0.93	0.07	31,31,31,31	0
57	MG	1A	3626	1/1	0.93	0.13	49,49,49,49	0
57	MG	2A	3041	1/1	0.93	0.14	44,44,44,44	0
57	MG	2A	3366	1/1	0.93	0.09	40,40,40,40	0
57	MG	2A	3367	1/1	0.93	0.12	63,63,63,63	0
57	MG	1A	3559	1/1	0.93	0.17	61,61,61,61	0
57	MG	1F	312	1/1	0.93	0.15	52,52,52,52	0
57	MG	1A	3391	1/1	0.93	0.08	43,43,43,43	0
57	MG	1A	3636	1/1	0.93	0.10	43,43,43,43	0
57	MG	1G	201	1/1	0.93	0.10	62,62,62,62	0
57	MG	1A	3563	1/1	0.93	0.07	51,51,51,51	0
57	MG	2A	3054	1/1	0.93	0.10	60,60,60,60	0
57	MG	2A	3388	1/1	0.93	0.16	63,63,63,63	0
57	MG	2F	303	1/1	0.93	0.16	57,57,57,57	0
57	MG	2A	3394	1/1	0.93	0.07	58,58,58,58	0
57	MG	1A	3902	1/1	0.93	0.10	20,20,20,20	0
57	MG	1A	3639	1/1	0.93	0.24	30,30,30,30	0
57	MG	1A	3503	1/1	0.93	0.08	37,37,37,37	0
57	MG	1A	3505	1/1	0.93	0.06	42,42,42,42	0
57	MG	1A	3921	1/1	0.93	0.10	50,50,50,50	0
57	MG	1A	3644	1/1	0.93	0.15	60,60,60,60	0
57	MG	2A	3406	1/1	0.93	0.10	63,63,63,63	0
57	MG	1A	3930	1/1	0.93	0.09	55,55,55,55	0
57	MG	2A	3078	1/1	0.93	0.14	53,53,53,53	0
57	MG	1T	201	1/1	0.93	0.08	42,42,42,42	0
57	MG	1A	3767	1/1	0.93	0.07	31,31,31,31	0
57	MG	1A	3014	1/1	0.93	0.09	39,39,39,39	0
57	MG	1a	3157	1/1	0.93	0.12	58,58,58,58	0
57	MG	2A	3429	1/1	0.93	0.08	44,44,44,44	0
57	MG	1A	3317	1/1	0.93	0.15	37,37,37,37	0
57	MG	27	101	1/1	0.93	0.20	49,49,49,49	0
57	MG	2A	3431	1/1	0.93	0.08	48,48,48,48	0
57	MG	2A	3432	1/1	0.93	0.14	56,56,56,56	0
57	MG	1A	3938	1/1	0.93	0.09	52,52,52,52	0
57	MG	1A	3652	1/1	0.93	0.08	35,35,35,35	0
57	MG	2a	3007	1/1	0.93	0.21	60,60,60,60	0
57	MG	1A	3395	1/1	0.93	0.07	18,18,18,18	0
57	MG	2A	3439	1/1	0.93	0.14	52,52,52,52	0
57	MG	2A	3098	1/1	0.93	0.12	54,54,54,54	0
57	MG	1A	3782	1/1	0.93	0.11	44,44,44,44	0
57	MG	1A	3039	1/1	0.93	0.10	38,38,38,38	0
57	MG	2A	3448	1/1	0.93	0.16	54,54,54,54	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	1A	3090	1/1	0.93	0.13	43,43,43,43	0
57	MG	2a	3018	1/1	0.93	0.21	54,54,54,54	0
57	MG	1a	3173	1/1	0.93	0.13	68,68,68,68	0
57	MG	11	102	1/1	0.93	0.18	48,48,48,48	0
57	MG	2A	3459	1/1	0.93	0.07	47,47,47,47	0
57	MG	2A	3461	1/1	0.93	0.10	61,61,61,61	0
57	MG	1A	3667	1/1	0.93	0.07	46,46,46,46	0
57	MG	1A	3370	1/1	0.93	0.07	23,23,23,23	0
57	MG	2A	3464	1/1	0.93	0.12	58,58,58,58	0
57	MG	2A	3117	1/1	0.93	0.17	58,58,58,58	0
57	MG	18	103	1/1	0.93	0.08	50,50,50,50	0
57	MG	1A	3674	1/1	0.93	0.14	31,31,31,31	0
57	MG	1A	3957	1/1	0.93	0.11	49,49,49,49	0
57	MG	2A	3473	1/1	0.93	0.06	52,52,52,52	0
57	MG	2a	3036	1/1	0.93	0.07	66,66,66,66	0
57	MG	1A	3800	1/1	0.93	0.12	48,48,48,48	0
57	MG	2A	3129	1/1	0.93	0.11	46,46,46,46	0
57	MG	1A	3402	1/1	0.93	0.10	14,14,14,14	0
57	MG	1A	3805	1/1	0.93	0.08	34,34,34,34	0
57	MG	2A	3479	1/1	0.93	0.09	45,45,45,45	0
57	MG	1A	3406	1/1	0.93	0.17	57,57,57,57	0
57	MG	1A	3809	1/1	0.93	0.12	24,24,24,24	0
57	MG	1A	3589	1/1	0.93	0.09	43,43,43,43	0
57	MG	1a	3192	1/1	0.93	0.09	63,63,63,63	0
57	MG	2a	3048	1/1	0.93	0.27	63,63,63,63	0
57	MG	1A	3228	1/1	0.93	0.09	38,38,38,38	0
57	MG	2a	3053	1/1	0.93	0.10	56,56,56,56	0
57	MG	1a	3194	1/1	0.93	0.10	51,51,51,51	0
57	MG	2A	3495	1/1	0.93	0.16	57,57,57,57	0
57	MG	1A	3591	1/1	0.93	0.11	56,56,56,56	0
57	MG	2A	3500	1/1	0.93	0.09	42,42,42,42	0
57	MG	1a	3197	1/1	0.93	0.10	64,64,64,64	0
57	MG	1a	3198	1/1	0.93	0.07	46,46,46,46	0
57	MG	2A	3154	1/1	0.93	0.07	47,47,47,47	0
57	MG	2A	3509	1/1	0.93	0.12	64,64,64,64	0
57	MG	2a	3065	1/1	0.93	0.12	76,76,76,76	0
57	MG	2A	3156	1/1	0.93	0.10	55,55,55,55	0
57	MG	2a	3067	1/1	0.93	0.21	69,69,69,69	0
57	MG	1A	3184	1/1	0.93	0.09	43,43,43,43	0
57	MG	1A	3685	1/1	0.93	0.09	28,28,28,28	0
57	MG	2a	3070	1/1	0.93	0.07	51,51,51,51	0
57	MG	1A	3296	1/1	0.93	0.18	46,46,46,46	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	1A	3981	1/1	0.93	0.07	66,66,66,66	0
57	MG	1a	3039	1/1	0.93	0.34	64,64,64,64	0
57	MG	1A	3827	1/1	0.93	0.08	45,45,45,45	0
57	MG	1a	3206	1/1	0.93	0.12	56,56,56,56	0
57	MG	2a	3079	1/1	0.93	0.11	59,59,59,59	0
57	MG	1A	3986	1/1	0.93	0.26	46,46,46,46	0
57	MG	2A	3176	1/1	0.93	0.09	57,57,57,57	0
57	MG	1A	3830	1/1	0.93	0.07	45,45,45,45	0
57	MG	2A	3529	1/1	0.93	0.20	62,62,62,62	0
57	MG	2A	3179	1/1	0.93	0.12	52,52,52,52	0
57	MG	2a	3088	1/1	0.93	0.12	67,67,67,67	0
57	MG	1A	3691	1/1	0.93	0.13	53,53,53,53	0
57	MG	2a	3093	1/1	0.93	0.22	65,65,65,65	0
57	MG	1A	3834	1/1	0.93	0.10	26,26,26,26	0
57	MG	2a	3095	1/1	0.93	0.13	53,53,53,53	0
57	MG	1a	3051	1/1	0.93	0.19	56,56,56,56	0
57	MG	1A	3599	1/1	0.93	0.12	48,48,48,48	0
57	MG	2A	3536	1/1	0.93	0.15	69,69,69,69	0
57	MG	1A	3331	1/1	0.93	0.07	21,21,21,21	0
57	MG	2A	3190	1/1	0.93	0.15	58,58,58,58	0
57	MG	1a	3056	1/1	0.93	0.12	52,52,52,52	0
57	MG	2A	3544	1/1	0.93	0.08	29,29,29,29	0
57	MG	1a	3221	1/1	0.93	0.20	62,62,62,62	0
57	MG	1a	3223	1/1	0.93	0.13	61,61,61,61	0
57	MG	2a	3123	1/1	0.93	0.08	55,55,55,55	0
57	MG	1A	3992	1/1	0.93	0.23	37,37,37,37	0
57	MG	1a	3226	1/1	0.93	0.08	60,60,60,60	0
57	MG	1A	3188	1/1	0.93	0.18	42,42,42,42	0
57	MG	2A	3199	1/1	0.93	0.12	51,51,51,51	0
57	MG	2A	3202	1/1	0.93	0.11	46,46,46,46	0
57	MG	2A	3204	1/1	0.93	0.18	64,64,64,64	0
57	MG	1A	3536	1/1	0.93	0.12	50,50,50,50	0
57	MG	2A	3210	1/1	0.93	0.21	59,59,59,59	0
57	MG	1A	3996	1/1	0.93	0.12	56,56,56,56	0
57	MG	1A	3997	1/1	0.93	0.19	55,55,55,55	0
57	MG	2a	3144	1/1	0.93	0.24	68,68,68,68	0
57	MG	1A	3703	1/1	0.93	0.17	40,40,40,40	0
57	MG	1A	3382	1/1	0.93	0.08	43,43,43,43	0
57	MG	2A	3572	1/1	0.93	0.08	47,47,47,47	0
57	MG	1a	3237	1/1	0.93	0.17	48,48,48,48	0
57	MG	1A	3437	1/1	0.93	0.11	44,44,44,44	0
57	MG	2A	3579	1/1	0.93	0.12	55,55,55,55	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	2A	3580	1/1	0.93	0.06	43,43,43,43	0
57	MG	2A	3223	1/1	0.93	0.18	57,57,57,57	0
57	MG	1a	3071	1/1	0.93	0.10	62,62,62,62	0
57	MG	2a	3161	1/1	0.93	0.07	65,65,65,65	0
57	MG	2a	3163	1/1	0.93	0.11	64,64,64,64	0
57	MG	2A	3583	1/1	0.93	0.07	52,52,52,52	0
57	MG	1a	3073	1/1	0.93	0.19	59,59,59,59	0
57	MG	1A	3709	1/1	0.93	0.08	53,53,53,53	0
57	MG	2A	3591	1/1	0.93	0.09	50,50,50,50	0
57	MG	2a	3169	1/1	0.93	0.07	56,56,56,56	0
57	MG	1A	3095	1/1	0.93	0.09	45,45,45,45	0
57	MG	2A	3234	1/1	0.93	0.15	46,46,46,46	0
57	MG	2A	3236	1/1	0.93	0.09	55,55,55,55	0
57	MG	1A	3713	1/1	0.93	0.09	36,36,36,36	0
57	MG	2A	3601	1/1	0.93	0.10	62,62,62,62	0
57	MG	1B	201	1/1	0.93	0.08	43,43,43,43	0
57	MG	2A	3606	1/1	0.93	0.08	56,56,56,56	0
57	MG	2A	3245	1/1	0.93	0.10	55,55,55,55	0
57	MG	1a	3264	1/1	0.93	0.11	77,77,77,77	0
57	MG	1A	3216	1/1	0.93	0.16	48,48,48,48	0
57	MG	1B	205	1/1	0.93	0.31	39,39,39,39	0
57	MG	1B	206	1/1	0.93	0.08	47,47,47,47	0
57	MG	2p	101	1/1	0.93	0.25	60,60,60,60	0
58	MPD	1A	4023	8/8	0.93	0.16	41,51,57,57	0
57	MG	1a	3269	1/1	0.93	0.15	75,75,75,75	0
58	MPD	1a	3276	8/8	0.93	0.11	54,57,61,63	0
57	MG	2A	3623	1/1	0.93	0.07	71,71,71,71	0
57	MG	2A	3626	1/1	0.93	0.14	61,61,61,61	0
57	MG	2A	3630	1/1	0.93	0.08	55,55,55,55	0
57	MG	1a	3271	1/1	0.93	0.11	52,52,52,52	0
57	MG	1A	3858	1/1	0.93	0.09	40,40,40,40	0
57	MG	2A	3270	1/1	0.94	0.21	56,56,56,56	0
57	MG	2A	3271	1/1	0.94	0.10	50,50,50,50	0
57	MG	1A	3361	1/1	0.94	0.18	60,60,60,60	0
57	MG	1B	223	1/1	0.94	0.07	44,44,44,44	0
57	MG	1B	226	1/1	0.94	0.06	32,32,32,32	0
57	MG	2A	3280	1/1	0.94	0.23	56,56,56,56	0
57	MG	1A	3283	1/1	0.94	0.16	51,51,51,51	0
57	MG	2A	3645	1/1	0.94	0.08	70,70,70,70	0
57	MG	1a	3098	1/1	0.94	0.17	57,57,57,57	0
57	MG	2A	3647	1/1	0.94	0.07	46,46,46,46	0
57	MG	2A	3650	1/1	0.94	0.08	30,30,30,30	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	1A	3743	1/1	0.94	0.07	41,41,41,41	0
57	MG	1A	3290	1/1	0.94	0.15	67,67,67,67	0
57	MG	1a	3101	1/1	0.94	0.24	57,57,57,57	0
57	MG	2A	3662	1/1	0.94	0.07	61,61,61,61	0
57	MG	2A	3288	1/1	0.94	0.15	57,57,57,57	0
57	MG	2A	3665	1/1	0.94	0.07	37,37,37,37	0
57	MG	2A	3290	1/1	0.94	0.16	49,49,49,49	0
57	MG	1A	3022	1/1	0.94	0.08	47,47,47,47	0
57	MG	1A	3293	1/1	0.94	0.12	62,62,62,62	0
57	MG	2A	3293	1/1	0.94	0.20	57,57,57,57	0
57	MG	2A	3296	1/1	0.94	0.07	40,40,40,40	0
57	MG	2A	3672	1/1	0.94	0.07	33,33,33,33	0
57	MG	2A	3297	1/1	0.94	0.11	52,52,52,52	0
57	MG	1a	3105	1/1	0.94	0.11	46,46,46,46	0
57	MG	1t	201	1/1	0.94	0.15	65,65,65,65	0
57	MG	1A	3629	1/1	0.94	0.14	42,42,42,42	0
57	MG	1A	3633	1/1	0.94	0.14	57,57,57,57	0
57	MG	2A	3687	1/1	0.94	0.08	43,43,43,43	0
57	MG	1A	3194	1/1	0.94	0.08	45,45,45,45	0
57	MG	1y	204	1/1	0.94	0.08	63,63,63,63	0
57	MG	2A	3691	1/1	0.94	0.14	51,51,51,51	0
57	MG	1A	3755	1/1	0.94	0.13	48,48,48,48	0
57	MG	2A	3308	1/1	0.94	0.21	51,51,51,51	0
57	MG	1A	3195	1/1	0.94	0.15	51,51,51,51	0
57	MG	1A	3759	1/1	0.94	0.07	35,35,35,35	0
57	MG	2A	3311	1/1	0.94	0.07	43,43,43,43	0
57	MG	1a	3112	1/1	0.94	0.11	72,72,72,72	0
57	MG	1A	3224	1/1	0.94	0.07	41,41,41,41	0
57	MG	2A	3026	1/1	0.94	0.11	55,55,55,55	0
57	MG	2A	3316	1/1	0.94	0.08	40,40,40,40	0
57	MG	2A	3708	1/1	0.94	0.12	59,59,59,59	0
57	MG	1A	3023	1/1	0.94	0.09	28,28,28,28	0
57	MG	2A	3711	1/1	0.94	0.09	49,49,49,49	0
57	MG	2A	3713	1/1	0.94	0.09	24,24,24,24	0
57	MG	2A	3714	1/1	0.94	0.15	49,49,49,49	0
57	MG	2A	3030	1/1	0.94	0.08	26,26,26,26	0
57	MG	1A	3918	1/1	0.94	0.10	34,34,34,34	0
57	MG	1A	3553	1/1	0.94	0.16	59,59,59,59	0
57	MG	2A	3036	1/1	0.94	0.10	46,46,46,46	0
57	MG	1E	312	1/1	0.94	0.10	59,59,59,59	0
57	MG	2A	3330	1/1	0.94	0.08	38,38,38,38	0
57	MG	1A	3312	1/1	0.94	0.18	26,26,26,26	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	1a	3124	1/1	0.94	0.10	73,73,73,73	0
57	MG	1A	3926	1/1	0.94	0.06	51,51,51,51	0
57	MG	1A	3231	1/1	0.94	0.13	32,32,32,32	0
57	MG	1A	3770	1/1	0.94	0.06	26,26,26,26	0
57	MG	1a	3132	1/1	0.94	0.07	57,57,57,57	0
57	MG	2A	3343	1/1	0.94	0.10	56,56,56,56	0
57	MG	2A	3345	1/1	0.94	0.10	63,63,63,63	0
57	MG	1A	3772	1/1	0.94	0.05	37,37,37,37	0
57	MG	1A	3773	1/1	0.94	0.08	26,26,26,26	0
57	MG	2A	3351	1/1	0.94	0.10	38,38,38,38	0
57	MG	2A	3354	1/1	0.94	0.08	38,38,38,38	0
57	MG	2A	3355	1/1	0.94	0.13	65,65,65,65	0
57	MG	2B	204	1/1	0.94	0.20	56,56,56,56	0
57	MG	1a	3137	1/1	0.94	0.09	51,51,51,51	0
57	MG	1A	3775	1/1	0.94	0.05	32,32,32,32	0
57	MG	1A	3234	1/1	0.94	0.12	34,34,34,34	0
57	MG	2B	209	1/1	0.94	0.14	61,61,61,61	0
57	MG	2A	3059	1/1	0.94	0.28	46,46,46,46	0
57	MG	1A	3941	1/1	0.94	0.07	47,47,47,47	0
57	MG	1O	201	1/1	0.94	0.17	48,48,48,48	0
57	MG	2A	3369	1/1	0.94	0.06	36,36,36,36	0
57	MG	2B	214	1/1	0.94	0.09	52,52,52,52	0
57	MG	2A	3372	1/1	0.94	0.08	35,35,35,35	0
57	MG	2B	217	1/1	0.94	0.10	62,62,62,62	0
57	MG	1a	3143	1/1	0.94	0.18	65,65,65,65	0
57	MG	1A	3647	1/1	0.94	0.13	36,36,36,36	0
57	MG	2D	305	1/1	0.94	0.12	44,44,44,44	0
57	MG	2A	3072	1/1	0.94	0.15	49,49,49,49	0
57	MG	1A	3943	1/1	0.94	0.09	23,23,23,23	0
57	MG	2D	309	1/1	0.94	0.10	46,46,46,46	0
57	MG	2D	310	1/1	0.94	0.12	47,47,47,47	0
57	MG	1R	202	1/1	0.94	0.12	35,35,35,35	0
57	MG	2E	303	1/1	0.94	0.07	49,49,49,49	0
57	MG	2A	3382	1/1	0.94	0.09	58,58,58,58	0
57	MG	2A	3079	1/1	0.94	0.07	43,43,43,43	0
57	MG	2F	302	1/1	0.94	0.12	51,51,51,51	0
57	MG	2A	3080	1/1	0.94	0.17	56,56,56,56	0
57	MG	2A	3082	1/1	0.94	0.09	53,53,53,53	0
57	MG	1A	3387	1/1	0.94	0.09	24,24,24,24	0
57	MG	1A	3108	1/1	0.94	0.11	51,51,51,51	0
57	MG	1A	3786	1/1	0.94	0.11	45,45,45,45	0
57	MG	2A	3399	1/1	0.94	0.18	56,56,56,56	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	2P	201	1/1	0.94	0.10	60,60,60,60	0
57	MG	2A	3086	1/1	0.94	0.35	42,42,42,42	0
57	MG	2A	3087	1/1	0.94	0.13	45,45,45,45	0
57	MG	2Q	204	1/1	0.94	0.08	67,67,67,67	0
57	MG	1A	3200	1/1	0.94	0.09	38,38,38,38	0
57	MG	1U	201	1/1	0.94	0.22	33,33,33,33	0
57	MG	1V	204	1/1	0.94	0.08	43,43,43,43	0
57	MG	1A	3473	1/1	0.94	0.12	47,47,47,47	0
57	MG	1A	3663	1/1	0.94	0.08	24,24,24,24	0
57	MG	1W	203	1/1	0.94	0.10	58,58,58,58	0
57	MG	1a	3162	1/1	0.94	0.25	57,57,57,57	0
57	MG	1a	3163	1/1	0.94	0.10	57,57,57,57	0
57	MG	2A	3420	1/1	0.94	0.08	30,30,30,30	0
57	MG	2A	3422	1/1	0.94	0.08	31,31,31,31	0
57	MG	2A	3426	1/1	0.94	0.09	65,65,65,65	0
57	MG	2A	3428	1/1	0.94	0.07	42,42,42,42	0
57	MG	1A	3795	1/1	0.94	0.10	47,47,47,47	0
57	MG	2A	3108	1/1	0.94	0.09	51,51,51,51	0
57	MG	2A	3110	1/1	0.94	0.12	56,56,56,56	0
57	MG	1A	3567	1/1	0.94	0.12	55,55,55,55	0
57	MG	2A	3433	1/1	0.94	0.13	49,49,49,49	0
57	MG	10	101	1/1	0.94	0.20	45,45,45,45	0
57	MG	1A	3962	1/1	0.94	0.10	46,46,46,46	0
57	MG	1A	3260	1/1	0.94	0.13	39,39,39,39	0
57	MG	10	108	1/1	0.94	0.10	47,47,47,47	0
57	MG	2A	3440	1/1	0.94	0.10	75,75,75,75	0
57	MG	1A	3966	1/1	0.94	0.09	52,52,52,52	0
57	MG	1A	3202	1/1	0.94	0.05	40,40,40,40	0
57	MG	2A	3444	1/1	0.94	0.09	41,41,41,41	0
57	MG	11	103	1/1	0.94	0.08	36,36,36,36	0
57	MG	2A	3122	1/1	0.94	0.07	48,48,48,48	0
57	MG	1A	3329	1/1	0.94	0.12	29,29,29,29	0
57	MG	1A	3082	1/1	0.94	0.13	47,47,47,47	0
57	MG	2A	3456	1/1	0.94	0.08	39,39,39,39	0
57	MG	1a	3183	1/1	0.94	0.08	66,66,66,66	0
57	MG	2a	3030	1/1	0.94	0.10	57,57,57,57	0
57	MG	2A	3458	1/1	0.94	0.08	49,49,49,49	0
57	MG	1A	3676	1/1	0.94	0.10	48,48,48,48	0
57	MG	2A	3460	1/1	0.94	0.11	63,63,63,63	0
57	MG	19	102	1/1	0.94	0.09	60,60,60,60	0
57	MG	2A	3133	1/1	0.94	0.15	64,64,64,64	0
57	MG	2A	3134	1/1	0.94	0.21	56,56,56,56	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	2A	3135	1/1	0.94	0.08	27,27,27,27	0
57	MG	1a	3187	1/1	0.94	0.11	60,60,60,60	0
57	MG	1A	3204	1/1	0.94	0.09	50,50,50,50	0
57	MG	1A	3333	1/1	0.94	0.23	48,48,48,48	0
57	MG	1A	3339	1/1	0.94	0.08	36,36,36,36	0
57	MG	1A	3681	1/1	0.94	0.07	58,58,58,58	0
57	MG	1A	3818	1/1	0.94	0.12	37,37,37,37	0
57	MG	1A	3491	1/1	0.94	0.07	59,59,59,59	0
57	MG	1a	3015	1/1	0.94	0.17	64,64,64,64	0
57	MG	1A	3126	1/1	0.94	0.11	62,62,62,62	0
57	MG	2a	3050	1/1	0.94	0.17	54,54,54,54	0
57	MG	2a	3052	1/1	0.94	0.11	59,59,59,59	0
57	MG	1A	3587	1/1	0.94	0.07	48,48,48,48	0
57	MG	1A	3405	1/1	0.94	0.07	34,34,34,34	0
57	MG	2A	3483	1/1	0.94	0.07	64,64,64,64	0
57	MG	1A	3342	1/1	0.94	0.07	48,48,48,48	0
57	MG	2A	3485	1/1	0.94	0.07	61,61,61,61	0
57	MG	2A	3487	1/1	0.94	0.11	62,62,62,62	0
57	MG	2A	3488	1/1	0.94	0.07	64,64,64,64	0
57	MG	1A	3415	1/1	0.94	0.06	35,35,35,35	0
57	MG	2a	3063	1/1	0.94	0.25	66,66,66,66	0
57	MG	2A	3164	1/1	0.94	0.09	48,48,48,48	0
57	MG	1a	3027	1/1	0.94	0.16	56,56,56,56	0
57	MG	1a	3029	1/1	0.94	0.09	49,49,49,49	0
57	MG	2A	3168	1/1	0.94	0.08	48,48,48,48	0
57	MG	2A	3498	1/1	0.94	0.08	64,64,64,64	0
57	MG	1A	3346	1/1	0.94	0.07	41,41,41,41	0
57	MG	1A	3021	1/1	0.94	0.15	39,39,39,39	0
57	MG	1a	3036	1/1	0.94	0.29	52,52,52,52	0
57	MG	1a	3207	1/1	0.94	0.08	69,69,69,69	0
57	MG	2A	3507	1/1	0.94	0.09	56,56,56,56	0
57	MG	1a	3208	1/1	0.94	0.14	58,58,58,58	0
57	MG	1A	3420	1/1	0.94	0.10	53,53,53,53	0
57	MG	2A	3180	1/1	0.94	0.16	56,56,56,56	0
57	MG	1A	3845	1/1	0.94	0.07	42,42,42,42	0
57	MG	1A	3846	1/1	0.94	0.13	31,31,31,31	0
57	MG	2A	3513	1/1	0.94	0.07	42,42,42,42	0
57	MG	2A	3514	1/1	0.94	0.07	62,62,62,62	0
57	MG	2A	3517	1/1	0.94	0.09	49,49,49,49	0
57	MG	2a	3087	1/1	0.94	0.13	54,54,54,54	0
57	MG	2A	3185	1/1	0.94	0.10	55,55,55,55	0
57	MG	2A	3519	1/1	0.94	0.09	50,50,50,50	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	1A	3699	1/1	0.94	0.17	45,45,45,45	0
57	MG	1A	3348	1/1	0.94	0.16	52,52,52,52	0
57	MG	1a	3217	1/1	0.94	0.09	66,66,66,66	0
57	MG	2a	3098	1/1	0.94	0.31	66,66,66,66	0
57	MG	2a	3099	1/1	0.94	0.27	45,45,45,45	0
57	MG	1A	3999	1/1	0.94	0.13	30,30,30,30	0
57	MG	1a	3047	1/1	0.94	0.15	56,56,56,56	0
57	MG	2a	3103	1/1	0.94	0.22	49,49,49,49	0
57	MG	2a	3108	1/1	0.94	0.20	51,51,51,51	0
57	MG	2a	3109	1/1	0.94	0.15	62,62,62,62	0
57	MG	2a	3111	1/1	0.94	0.28	64,64,64,64	0
57	MG	1A	4000	1/1	0.94	0.11	15,15,15,15	0
57	MG	1A	4001	1/1	0.94	0.11	47,47,47,47	0
57	MG	1A	3063	1/1	0.94	0.07	35,35,35,35	0
57	MG	1A	3706	1/1	0.94	0.10	57,57,57,57	0
57	MG	2a	3116	1/1	0.94	0.23	49,49,49,49	0
57	MG	1A	3515	1/1	0.94	0.09	21,21,21,21	0
57	MG	2A	3532	1/1	0.94	0.08	62,62,62,62	0
57	MG	1a	3057	1/1	0.94	0.08	58,58,58,58	0
57	MG	2A	3200	1/1	0.94	0.07	41,41,41,41	0
57	MG	1A	4010	1/1	0.94	0.09	36,36,36,36	0
57	MG	2a	3126	1/1	0.94	0.17	61,61,61,61	0
57	MG	1A	4012	1/1	0.94	0.17	33,33,33,33	0
57	MG	2a	3128	1/1	0.94	0.15	71,71,71,71	0
57	MG	2A	3205	1/1	0.94	0.07	50,50,50,50	0
57	MG	2A	3207	1/1	0.94	0.15	52,52,52,52	0
57	MG	2A	3208	1/1	0.94	0.19	54,54,54,54	0
57	MG	1A	3426	1/1	0.94	0.09	37,37,37,37	0
57	MG	2a	3133	1/1	0.94	0.12	66,66,66,66	0
57	MG	1A	3276	1/1	0.94	0.10	43,43,43,43	0
57	MG	2a	3136	1/1	0.94	0.09	71,71,71,71	0
57	MG	1a	3065	1/1	0.94	0.08	58,58,58,58	0
57	MG	1a	3066	1/1	0.94	0.10	63,63,63,63	0
57	MG	2a	3140	1/1	0.94	0.10	69,69,69,69	0
57	MG	1A	3435	1/1	0.94	0.09	44,44,44,44	0
57	MG	2A	3217	1/1	0.94	0.31	65,65,65,65	0
57	MG	1A	3606	1/1	0.94	0.08	27,27,27,27	0
57	MG	1B	202	1/1	0.94	0.13	52,52,52,52	0
57	MG	2A	3558	1/1	0.94	0.08	40,40,40,40	0
57	MG	1a	3245	1/1	0.94	0.08	46,46,46,46	0
57	MG	2A	3222	1/1	0.94	0.07	43,43,43,43	0
57	MG	1A	3520	1/1	0.94	0.27	47,47,47,47	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	1a	3252	1/1	0.94	0.17	54,54,54,54	0
57	MG	1A	3861	1/1	0.94	0.10	49,49,49,49	0
57	MG	1A	3862	1/1	0.94	0.06	54,54,54,54	0
57	MG	1a	3260	1/1	0.94	0.10	55,55,55,55	0
57	MG	1A	3610	1/1	0.94	0.16	32,32,32,32	0
57	MG	1a	3076	1/1	0.94	0.15	47,47,47,47	0
57	MG	1B	208	1/1	0.94	0.18	50,50,50,50	0
57	MG	1B	209	1/1	0.94	0.07	38,38,38,38	0
57	MG	2A	3239	1/1	0.94	0.17	52,52,52,52	0
57	MG	2A	3240	1/1	0.94	0.34	59,59,59,59	0
57	MG	2A	3241	1/1	0.94	0.07	54,54,54,54	0
57	MG	2a	3172	1/1	0.94	0.12	55,55,55,55	0
57	MG	1A	3521	1/1	0.94	0.09	46,46,46,46	0
57	MG	1A	3616	1/1	0.94	0.24	38,38,38,38	0
57	MG	2A	3585	1/1	0.94	0.18	55,55,55,55	0
57	MG	1B	216	1/1	0.94	0.16	43,43,43,43	0
57	MG	1a	3084	1/1	0.94	0.07	50,50,50,50	0
57	MG	2a	3185	1/1	0.94	0.10	77,77,77,77	0
57	MG	2a	3186	1/1	0.94	0.10	67,67,67,67	0
57	MG	2a	3188	1/1	0.94	0.09	58,58,58,58	0
57	MG	2A	3249	1/1	0.94	0.23	49,49,49,49	0
57	MG	1a	3085	1/1	0.94	0.27	64,64,64,64	0
57	MG	1A	3617	1/1	0.94	0.16	34,34,34,34	0
57	MG	1d	302	1/1	0.94	0.19	63,63,63,63	0
57	MG	1A	3618	1/1	0.94	0.07	30,30,30,30	0
57	MG	1A	3734	1/1	0.94	0.08	41,41,41,41	0
57	MG	2A	3603	1/1	0.94	0.06	51,51,51,51	0
57	MG	2A	3604	1/1	0.94	0.08	41,41,41,41	0
57	MG	2A	3258	1/1	0.94	0.10	48,48,48,48	0
57	MG	1d	305	1/1	0.94	0.12	55,55,55,55	0
57	MG	1A	3278	1/1	0.94	0.07	47,47,47,47	0
57	MG	1a	3092	1/1	0.94	0.09	52,52,52,52	0
57	MG	2A	3616	1/1	0.94	0.10	49,49,49,49	0
57	MG	2A	3617	1/1	0.94	0.07	75,75,75,75	0
57	MG	1e	203	1/1	0.94	0.24	59,59,59,59	0
60	ZN	24	501	1/1	0.94	0.14	119,119,119,119	0
57	MG	1A	3971	1/1	0.95	0.04	27,27,27,27	0
57	MG	2A	3344	1/1	0.95	0.12	53,53,53,53	0
57	MG	11	104	1/1	0.95	0.17	48,48,48,48	0
57	MG	13	102	1/1	0.95	0.08	51,51,51,51	0
57	MG	15	3107	1/1	0.95	0.17	25,25,25,25	0
57	MG	2A	3350	1/1	0.95	0.07	46,46,46,46	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	1A	3478	1/1	0.95	0.08	29,29,29,29	0
57	MG	2A	3352	1/1	0.95	0.09	44,44,44,44	0
57	MG	1A	3806	1/1	0.95	0.06	48,48,48,48	0
57	MG	1a	3169	1/1	0.95	0.08	66,66,66,66	0
57	MG	2A	3356	1/1	0.95	0.06	40,40,40,40	0
57	MG	2A	3697	1/1	0.95	0.33	39,39,39,39	0
57	MG	1a	3171	1/1	0.95	0.14	61,61,61,61	0
57	MG	18	101	1/1	0.95	0.07	43,43,43,43	0
57	MG	1A	3161	1/1	0.95	0.15	35,35,35,35	0
57	MG	2A	3364	1/1	0.95	0.08	44,44,44,44	0
57	MG	1A	3481	1/1	0.95	0.07	25,25,25,25	0
57	MG	2A	3705	1/1	0.95	0.10	56,56,56,56	0
57	MG	2A	3706	1/1	0.95	0.08	39,39,39,39	0
57	MG	2A	3099	1/1	0.95	0.05	48,48,48,48	0
57	MG	2A	3101	1/1	0.95	0.09	43,43,43,43	0
57	MG	1a	3001	1/1	0.95	0.14	68,68,68,68	0
57	MG	1A	3581	1/1	0.95	0.11	47,47,47,47	0
57	MG	2A	3712	1/1	0.95	0.06	47,47,47,47	0
57	MG	1A	3813	1/1	0.95	0.06	37,37,37,37	0
57	MG	2A	3106	1/1	0.95	0.07	39,39,39,39	0
57	MG	1a	3180	1/1	0.95	0.07	49,49,49,49	0
57	MG	1A	3482	1/1	0.95	0.07	45,45,45,45	0
57	MG	2A	3378	1/1	0.95	0.10	66,66,66,66	0
57	MG	1a	3182	1/1	0.95	0.12	59,59,59,59	0
57	MG	1A	3265	1/1	0.95	0.09	46,46,46,46	0
57	MG	2A	3383	1/1	0.95	0.11	53,53,53,53	0
57	MG	2A	3384	1/1	0.95	0.14	57,57,57,57	0
57	MG	1A	3584	1/1	0.95	0.10	39,39,39,39	0
57	MG	2A	3115	1/1	0.95	0.24	54,54,54,54	0
57	MG	2A	3393	1/1	0.95	0.08	59,59,59,59	0
57	MG	1A	3485	1/1	0.95	0.08	29,29,29,29	0
57	MG	1A	3267	1/1	0.95	0.09	28,28,28,28	0
57	MG	2A	3396	1/1	0.95	0.08	59,59,59,59	0
57	MG	1a	3016	1/1	0.95	0.10	60,60,60,60	0
57	MG	1a	3017	1/1	0.95	0.14	57,57,57,57	0
57	MG	1A	3688	1/1	0.95	0.09	53,53,53,53	0
57	MG	1A	3689	1/1	0.95	0.11	56,56,56,56	0
57	MG	2A	3123	1/1	0.95	0.14	38,38,38,38	0
57	MG	2A	3125	1/1	0.95	0.13	48,48,48,48	0
57	MG	2A	3405	1/1	0.95	0.07	49,49,49,49	0
57	MG	1A	3828	1/1	0.95	0.09	34,34,34,34	0
57	MG	1A	3829	1/1	0.95	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
57	MG	1a	3024	1/1	0.95	0.07	50,50,50,50	0
57	MG	1A	3690	1/1	0.95	0.07	37,37,37,37	0
57	MG	1A	3993	1/1	0.95	0.11	24,24,24,24	0
57	MG	1a	3028	1/1	0.95	0.14	59,59,59,59	0
57	MG	1A	3163	1/1	0.95	0.13	50,50,50,50	0
57	MG	2A	3414	1/1	0.95	0.09	47,47,47,47	0
57	MG	2A	3416	1/1	0.95	0.19	50,50,50,50	0
57	MG	1a	3030	1/1	0.95	0.08	46,46,46,46	0
57	MG	2A	3421	1/1	0.95	0.12	49,49,49,49	0
57	MG	1A	3332	1/1	0.95	0.12	20,20,20,20	0
57	MG	2D	301	1/1	0.95	0.47	46,46,46,46	0
57	MG	1a	3034	1/1	0.95	0.12	48,48,48,48	0
57	MG	2A	3427	1/1	0.95	0.07	40,40,40,40	0
57	MG	1A	3206	1/1	0.95	0.22	41,41,41,41	0
57	MG	2A	3140	1/1	0.95	0.14	53,53,53,53	0
57	MG	2A	3141	1/1	0.95	0.09	60,60,60,60	0
57	MG	1A	3028	1/1	0.95	0.25	26,26,26,26	0
57	MG	1A	3594	1/1	0.95	0.09	50,50,50,50	0
57	MG	2A	3145	1/1	0.95	0.20	46,46,46,46	0
57	MG	2A	3434	1/1	0.95	0.09	50,50,50,50	0
57	MG	1A	3698	1/1	0.95	0.12	48,48,48,48	0
57	MG	1A	3500	1/1	0.95	0.10	47,47,47,47	0
57	MG	2A	3150	1/1	0.95	0.05	41,41,41,41	0
57	MG	2A	3152	1/1	0.95	0.17	46,46,46,46	0
57	MG	1A	3700	1/1	0.95	0.22	53,53,53,53	0
57	MG	2A	3441	1/1	0.95	0.07	43,43,43,43	0
57	MG	1A	3168	1/1	0.95	0.07	45,45,45,45	0
57	MG	1A	4005	1/1	0.95	0.09	47,47,47,47	0
57	MG	1A	3031	1/1	0.95	0.04	14,14,14,14	0
57	MG	2P	202	1/1	0.95	0.15	64,64,64,64	0
57	MG	2Q	201	1/1	0.95	0.08	56,56,56,56	0
57	MG	1A	3408	1/1	0.95	0.08	28,28,28,28	0
57	MG	1a	3216	1/1	0.95	0.08	74,74,74,74	0
57	MG	2A	3450	1/1	0.95	0.07	51,51,51,51	0
57	MG	2A	3162	1/1	0.95	0.20	41,41,41,41	0
57	MG	2A	3453	1/1	0.95	0.07	58,58,58,58	0
57	MG	1A	3345	1/1	0.95	0.10	48,48,48,48	0
57	MG	1A	3033	1/1	0.95	0.08	36,36,36,36	0
57	MG	1A	4016	1/1	0.95	0.08	47,47,47,47	0
57	MG	1a	3055	1/1	0.95	0.13	44,44,44,44	0
57	MG	2V	202	1/1	0.95	0.14	54,54,54,54	0
57	MG	2V	203	1/1	0.95	0.09	59,59,59,59	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	1A	4017	1/1	0.95	0.10	58,58,58,58	0
57	MG	2W	203	1/1	0.95	0.11	61,61,61,61	0
57	MG	2Y	201	1/1	0.95	0.13	53,53,53,53	0
57	MG	20	101	1/1	0.95	0.11	54,54,54,54	0
57	MG	2A	3170	1/1	0.95	0.19	44,44,44,44	0
57	MG	2A	3171	1/1	0.95	0.08	42,42,42,42	0
57	MG	2A	3172	1/1	0.95	0.06	39,39,39,39	0
57	MG	1a	3222	1/1	0.95	0.09	49,49,49,49	0
57	MG	1A	3186	1/1	0.95	0.23	38,38,38,38	0
57	MG	1A	3112	1/1	0.95	0.14	32,32,32,32	0
57	MG	2A	3467	1/1	0.95	0.08	53,53,53,53	0
57	MG	1A	3071	1/1	0.95	0.11	40,40,40,40	0
57	MG	1a	3061	1/1	0.95	0.11	60,60,60,60	0
57	MG	1A	3607	1/1	0.95	0.23	30,30,30,30	0
57	MG	1a	3063	1/1	0.95	0.18	68,68,68,68	0
57	MG	2A	3182	1/1	0.95	0.09	64,64,64,64	0
57	MG	1A	3423	1/1	0.95	0.11	20,20,20,20	0
57	MG	1B	204	1/1	0.95	0.07	45,45,45,45	0
57	MG	2A	3186	1/1	0.95	0.09	49,49,49,49	0
57	MG	1A	3722	1/1	0.95	0.10	43,43,43,43	0
57	MG	2A	3480	1/1	0.95	0.09	48,48,48,48	0
57	MG	1A	3723	1/1	0.95	0.07	39,39,39,39	0
57	MG	2A	3482	1/1	0.95	0.09	45,45,45,45	0
57	MG	1A	3424	1/1	0.95	0.09	32,32,32,32	0
57	MG	1A	3354	1/1	0.95	0.12	55,55,55,55	0
57	MG	1A	3355	1/1	0.95	0.08	23,23,23,23	0
57	MG	2A	3486	1/1	0.95	0.06	64,64,64,64	0
57	MG	1a	3243	1/1	0.95	0.07	47,47,47,47	0
57	MG	1A	3075	1/1	0.95	0.20	40,40,40,40	0
57	MG	1a	3248	1/1	0.95	0.09	54,54,54,54	0
57	MG	1A	3874	1/1	0.95	0.09	46,46,46,46	0
57	MG	1B	212	1/1	0.95	0.06	48,48,48,48	0
57	MG	1a	3075	1/1	0.95	0.17	66,66,66,66	0
57	MG	1a	3254	1/1	0.95	0.07	49,49,49,49	0
57	MG	1B	215	1/1	0.95	0.10	56,56,56,56	0
57	MG	2A	3203	1/1	0.95	0.08	52,52,52,52	0
57	MG	1a	3258	1/1	0.95	0.10	68,68,68,68	0
57	MG	1A	3020	1/1	0.95	0.33	28,28,28,28	0
57	MG	1a	3262	1/1	0.95	0.08	57,57,57,57	0
57	MG	1A	3876	1/1	0.95	0.05	27,27,27,27	0
57	MG	1a	3080	1/1	0.95	0.14	65,65,65,65	0
57	MG	1A	3877	1/1	0.95	0.09	62,62,62,62	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	2a	3046	1/1	0.95	0.34	62,62,62,62	0
57	MG	2A	3211	1/1	0.95	0.18	52,52,52,52	0
57	MG	1A	3359	1/1	0.95	0.09	32,32,32,32	0
57	MG	1A	3739	1/1	0.95	0.09	42,42,42,42	0
57	MG	1a	3268	1/1	0.95	0.09	62,62,62,62	0
57	MG	2a	3051	1/1	0.95	0.21	54,54,54,54	0
57	MG	1B	221	1/1	0.95	0.10	34,34,34,34	0
57	MG	2A	3515	1/1	0.95	0.07	59,59,59,59	0
57	MG	1A	3083	1/1	0.95	0.22	28,28,28,28	0
57	MG	1A	3882	1/1	0.95	0.06	27,27,27,27	0
57	MG	1B	225	1/1	0.95	0.12	54,54,54,54	0
57	MG	2A	3520	1/1	0.95	0.14	57,57,57,57	0
57	MG	1A	3300	1/1	0.95	0.08	31,31,31,31	0
57	MG	1d	301	1/1	0.95	0.24	67,67,67,67	0
57	MG	2a	3061	1/1	0.95	0.30	67,67,67,67	0
57	MG	2A	3224	1/1	0.95	0.10	42,42,42,42	0
57	MG	1A	3742	1/1	0.95	0.10	41,41,41,41	0
57	MG	1a	3090	1/1	0.95	0.13	47,47,47,47	0
57	MG	1A	3532	1/1	0.95	0.07	25,25,25,25	0
57	MG	1A	3304	1/1	0.95	0.10	33,33,33,33	0
57	MG	1A	3887	1/1	0.95	0.13	27,27,27,27	0
57	MG	2A	3235	1/1	0.95	0.10	58,58,58,58	0
57	MG	1D	308	1/1	0.95	0.16	35,35,35,35	0
57	MG	1A	3745	1/1	0.95	0.06	58,58,58,58	0
57	MG	1A	3240	1/1	0.95	0.16	32,32,32,32	0
57	MG	1A	3896	1/1	0.95	0.07	45,45,45,45	0
57	MG	1h	201	1/1	0.95	0.20	49,49,49,49	0
57	MG	2a	3074	1/1	0.95	0.24	50,50,50,50	0
57	MG	1A	3628	1/1	0.95	0.08	46,46,46,46	0
57	MG	2A	3243	1/1	0.95	0.34	47,47,47,47	0
57	MG	2A	3540	1/1	0.95	0.08	53,53,53,53	0
57	MG	1A	3900	1/1	0.95	0.08	48,48,48,48	0
57	MG	2A	3542	1/1	0.95	0.09	64,64,64,64	0
57	MG	1A	3535	1/1	0.95	0.10	49,49,49,49	0
57	MG	1A	3631	1/1	0.95	0.07	30,30,30,30	0
57	MG	1m	201	1/1	0.95	0.06	62,62,62,62	0
57	MG	1A	3905	1/1	0.95	0.06	27,27,27,27	0
57	MG	1A	3443	1/1	0.95	0.08	42,42,42,42	0
57	MG	2a	3089	1/1	0.95	0.16	60,60,60,60	0
57	MG	1A	3909	1/1	0.95	0.09	28,28,28,28	0
57	MG	1A	3754	1/1	0.95	0.14	56,56,56,56	0
57	MG	1A	3307	1/1	0.95	0.06	42,42,42,42	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	2A	3556	1/1	0.95	0.06	53,53,53,53	0
57	MG	2a	3096	1/1	0.95	0.20	51,51,51,51	0
57	MG	1F	310	1/1	0.95	0.06	41,41,41,41	0
57	MG	1u	101	1/1	0.95	0.10	64,64,64,64	0
57	MG	1A	3038	1/1	0.95	0.06	26,26,26,26	0
57	MG	1A	3373	1/1	0.95	0.09	44,44,44,44	0
57	MG	1A	3548	1/1	0.95	0.11	41,41,41,41	0
57	MG	2a	3107	1/1	0.95	0.23	50,50,50,50	0
57	MG	1A	3310	1/1	0.95	0.07	32,32,32,32	0
57	MG	1A	3554	1/1	0.95	0.08	37,37,37,37	0
57	MG	1A	3375	1/1	0.95	0.09	36,36,36,36	0
57	MG	2A	3272	1/1	0.95	0.10	38,38,38,38	0
57	MG	2A	3273	1/1	0.95	0.08	42,42,42,42	0
57	MG	2A	3275	1/1	0.95	0.26	38,38,38,38	0
57	MG	1A	3244	1/1	0.95	0.23	51,51,51,51	0
57	MG	1a	3122	1/1	0.95	0.11	58,58,58,58	0
57	MG	2A	3007	1/1	0.95	0.09	42,42,42,42	0
57	MG	2A	3015	1/1	0.95	0.21	50,50,50,50	0
57	MG	2A	3018	1/1	0.95	0.23	37,37,37,37	0
57	MG	2A	3019	1/1	0.95	0.25	53,53,53,53	0
57	MG	1H	201	1/1	0.95	0.11	40,40,40,40	0
57	MG	2a	3125	1/1	0.95	0.13	56,56,56,56	0
57	MG	2A	3284	1/1	0.95	0.08	51,51,51,51	0
57	MG	2A	3587	1/1	0.95	0.11	54,54,54,54	0
57	MG	2A	3024	1/1	0.95	0.14	50,50,50,50	0
57	MG	1A	3245	1/1	0.95	0.16	49,49,49,49	0
57	MG	2A	3594	1/1	0.95	0.06	67,67,67,67	0
57	MG	1A	3936	1/1	0.95	0.05	20,20,20,20	0
57	MG	1A	3062	1/1	0.95	0.08	46,46,46,46	0
57	MG	2A	3031	1/1	0.95	0.13	59,59,59,59	0
57	MG	1A	3651	1/1	0.95	0.07	34,34,34,34	0
57	MG	1a	3130	1/1	0.95	0.08	55,55,55,55	0
57	MG	2A	3035	1/1	0.95	0.08	45,45,45,45	0
57	MG	1Q	204	1/1	0.95	0.06	30,30,30,30	0
57	MG	1A	3259	1/1	0.95	0.19	57,57,57,57	0
57	MG	2a	3141	1/1	0.95	0.08	68,68,68,68	0
57	MG	2A	3605	1/1	0.95	0.10	34,34,34,34	0
57	MG	1A	3653	1/1	0.95	0.36	44,44,44,44	0
57	MG	2A	3607	1/1	0.95	0.08	43,43,43,43	0
57	MG	2a	3146	1/1	0.95	0.10	49,49,49,49	0
57	MG	2A	3609	1/1	0.95	0.09	48,48,48,48	0
57	MG	1A	3654	1/1	0.95	0.05	37,37,37,37	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	2a	3151	1/1	0.95	0.10	60,60,60,60	0
57	MG	2a	3152	1/1	0.95	0.08	65,65,65,65	0
57	MG	2A	3612	1/1	0.95	0.07	59,59,59,59	0
57	MG	1A	3944	1/1	0.95	0.05	35,35,35,35	0
57	MG	2A	3303	1/1	0.95	0.18	45,45,45,45	0
57	MG	2A	3615	1/1	0.95	0.06	71,71,71,71	0
57	MG	1A	3946	1/1	0.95	0.07	23,23,23,23	0
57	MG	2a	3159	1/1	0.95	0.10	62,62,62,62	0
57	MG	1A	3781	1/1	0.95	0.31	49,49,49,49	0
57	MG	1A	3656	1/1	0.95	0.28	48,48,48,48	0
57	MG	1A	3152	1/1	0.95	0.21	31,31,31,31	0
57	MG	1A	3385	1/1	0.95	0.11	32,32,32,32	0
57	MG	2a	3165	1/1	0.95	0.10	49,49,49,49	0
57	MG	2A	3621	1/1	0.95	0.09	62,62,62,62	0
57	MG	1A	3953	1/1	0.95	0.12	50,50,50,50	0
57	MG	2A	3625	1/1	0.95	0.07	44,44,44,44	0
57	MG	1A	3661	1/1	0.95	0.07	21,21,21,21	0
57	MG	2A	3627	1/1	0.95	0.08	38,38,38,38	0
57	MG	2a	3171	1/1	0.95	0.07	66,66,66,66	0
57	MG	1a	3149	1/1	0.95	0.11	48,48,48,48	0
57	MG	2A	3633	1/1	0.95	0.12	61,61,61,61	0
57	MG	2a	3174	1/1	0.95	0.06	54,54,54,54	0
57	MG	2A	3636	1/1	0.95	0.07	53,53,53,53	0
57	MG	1A	3789	1/1	0.95	0.08	20,20,20,20	0
57	MG	2A	3642	1/1	0.95	0.09	45,45,45,45	0
57	MG	1Y	201	1/1	0.95	0.10	53,53,53,53	0
57	MG	2A	3315	1/1	0.95	0.14	53,53,53,53	0
57	MG	2A	3061	1/1	0.95	0.08	43,43,43,43	0
57	MG	1A	3564	1/1	0.95	0.08	45,45,45,45	0
57	MG	2A	3648	1/1	0.95	0.12	53,53,53,53	0
57	MG	2A	3063	1/1	0.95	0.09	46,46,46,46	0
57	MG	1A	3565	1/1	0.95	0.10	49,49,49,49	0
57	MG	2A	3065	1/1	0.95	0.10	54,54,54,54	0
57	MG	2A	3325	1/1	0.95	0.14	50,50,50,50	0
57	MG	2A	3661	1/1	0.95	0.07	57,57,57,57	0
57	MG	1a	3154	1/1	0.95	0.13	60,60,60,60	0
57	MG	2r	101	1/1	0.95	0.12	63,63,63,63	0
57	MG	2x	101	1/1	0.95	0.10	50,50,50,50	0
57	MG	2A	3069	1/1	0.95	0.20	50,50,50,50	0
58	MPD	18	104	8/8	0.95	0.14	31,40,43,44	0
57	MG	1A	3323	1/1	0.95	0.08	27,27,27,27	0
57	MG	1A	3324	1/1	0.95	0.06	35,35,35,35	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	2A	3333	1/1	0.95	0.06	31,31,31,31	0
57	MG	1A	3158	1/1	0.95	0.14	27,27,27,27	0
57	MG	1A	3327	1/1	0.95	0.09	41,41,41,41	0
57	MG	1a	3160	1/1	0.95	0.08	60,60,60,60	0
57	MG	2A	3081	1/1	0.95	0.10	73,73,73,73	0
57	MG	1A	3803	1/1	0.95	0.06	52,52,52,52	0
57	MG	1a	3014	1/1	0.96	0.05	47,47,47,47	0
57	MG	1A	3156	1/1	0.96	0.15	39,39,39,39	0
57	MG	1A	3793	1/1	0.96	0.07	45,45,45,45	0
57	MG	1A	3549	1/1	0.96	0.05	43,43,43,43	0
57	MG	1A	3551	1/1	0.96	0.17	29,29,29,29	0
57	MG	1A	3552	1/1	0.96	0.06	40,40,40,40	0
57	MG	1A	3978	1/1	0.96	0.07	46,46,46,46	0
57	MG	2A	3144	1/1	0.96	0.14	28,28,28,28	0
57	MG	1a	3213	1/1	0.96	0.06	54,54,54,54	0
57	MG	1A	3797	1/1	0.96	0.08	39,39,39,39	0
57	MG	1A	3798	1/1	0.96	0.06	31,31,31,31	0
57	MG	1A	3081	1/1	0.96	0.11	31,31,31,31	0
57	MG	2A	3419	1/1	0.96	0.08	51,51,51,51	0
57	MG	2A	3151	1/1	0.96	0.05	56,56,56,56	0
57	MG	1A	3801	1/1	0.96	0.07	35,35,35,35	0
57	MG	1A	3349	1/1	0.96	0.09	31,31,31,31	0
57	MG	2A	3424	1/1	0.96	0.11	54,54,54,54	0
57	MG	1A	3660	1/1	0.96	0.07	52,52,52,52	0
57	MG	1A	3350	1/1	0.96	0.05	36,36,36,36	0
57	MG	1A	3662	1/1	0.96	0.08	49,49,49,49	0
57	MG	1A	3807	1/1	0.96	0.18	40,40,40,40	0
57	MG	2A	3159	1/1	0.96	0.07	38,38,38,38	0
57	MG	1A	3352	1/1	0.96	0.07	26,26,26,26	0
57	MG	1A	3002	1/1	0.96	0.06	44,44,44,44	0
57	MG	2A	3163	1/1	0.96	0.09	47,47,47,47	0
57	MG	1A	3277	1/1	0.96	0.13	34,34,34,34	0
57	MG	1a	3227	1/1	0.96	0.11	45,45,45,45	0
57	MG	2A	3166	1/1	0.96	0.12	70,70,70,70	0
57	MG	1A	3016	1/1	0.96	0.17	28,28,28,28	0
57	MG	1A	3672	1/1	0.96	0.08	44,44,44,44	0
57	MG	1A	3673	1/1	0.96	0.12	56,56,56,56	0
57	MG	1A	3998	1/1	0.96	0.13	47,47,47,47	0
57	MG	1A	3560	1/1	0.96	0.06	38,38,38,38	0
57	MG	1a	3235	1/1	0.96	0.12	61,61,61,61	0
57	MG	2B	216	1/1	0.96	0.07	63,63,63,63	0
57	MG	1a	3045	1/1	0.96	0.19	50,50,50,50	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	2A	3445	1/1	0.96	0.24	71,71,71,71	0
57	MG	1A	3280	1/1	0.96	0.06	33,33,33,33	0
57	MG	1A	3819	1/1	0.96	0.10	33,33,33,33	0
57	MG	2A	3449	1/1	0.96	0.08	43,43,43,43	0
57	MG	1A	3125	1/1	0.96	0.12	45,45,45,45	0
57	MG	2D	307	1/1	0.96	0.07	40,40,40,40	0
57	MG	1A	3823	1/1	0.96	0.06	12,12,12,12	0
57	MG	1A	3677	1/1	0.96	0.11	55,55,55,55	0
57	MG	1a	3244	1/1	0.96	0.08	50,50,50,50	0
57	MG	1A	4006	1/1	0.96	0.14	42,42,42,42	0
57	MG	1A	3456	1/1	0.96	0.09	41,41,41,41	0
57	MG	1a	3249	1/1	0.96	0.13	68,68,68,68	0
57	MG	1A	3286	1/1	0.96	0.17	32,32,32,32	0
57	MG	1A	3566	1/1	0.96	0.17	49,49,49,49	0
57	MG	1A	3458	1/1	0.96	0.07	46,46,46,46	0
57	MG	1A	4014	1/1	0.96	0.13	37,37,37,37	0
57	MG	1a	3255	1/1	0.96	0.06	48,48,48,48	0
57	MG	1A	4015	1/1	0.96	0.09	36,36,36,36	0
57	MG	1A	3288	1/1	0.96	0.09	50,50,50,50	0
57	MG	2O	201	1/1	0.96	0.05	52,52,52,52	0
57	MG	2A	3466	1/1	0.96	0.12	42,42,42,42	0
57	MG	1A	3004	1/1	0.96	0.08	37,37,37,37	0
57	MG	2A	3194	1/1	0.96	0.15	40,40,40,40	0
57	MG	1A	3291	1/1	0.96	0.08	31,31,31,31	0
57	MG	1A	3837	1/1	0.96	0.08	38,38,38,38	0
57	MG	2A	3471	1/1	0.96	0.07	36,36,36,36	0
57	MG	2A	3197	1/1	0.96	0.30	59,59,59,59	0
57	MG	1A	4021	1/1	0.96	0.07	57,57,57,57	0
57	MG	2R	202	1/1	0.96	0.17	51,51,51,51	0
57	MG	1A	3839	1/1	0.96	0.24	42,42,42,42	0
57	MG	1A	3128	1/1	0.96	0.06	54,54,54,54	0
57	MG	2A	3201	1/1	0.96	0.08	61,61,61,61	0
57	MG	1A	3576	1/1	0.96	0.05	57,57,57,57	0
57	MG	1A	3844	1/1	0.96	0.06	38,38,38,38	0
57	MG	1A	3464	1/1	0.96	0.09	52,52,52,52	0
57	MG	1A	3173	1/1	0.96	0.09	22,22,22,22	0
57	MG	1A	3579	1/1	0.96	0.06	21,21,21,21	0
57	MG	1A	3692	1/1	0.96	0.07	47,47,47,47	0
57	MG	1A	3177	1/1	0.96	0.18	47,47,47,47	0
57	MG	1A	3472	1/1	0.96	0.13	49,49,49,49	0
57	MG	1A	3225	1/1	0.96	0.14	28,28,28,28	0
57	MG	2I	101	1/1	0.96	0.08	66,66,66,66	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	2A	3212	1/1	0.96	0.05	47,47,47,47	0
57	MG	25	103	1/1	0.96	0.12	57,57,57,57	0
57	MG	1A	3299	1/1	0.96	0.08	44,44,44,44	0
57	MG	27	102	1/1	0.96	0.21	32,32,32,32	0
57	MG	1A	3183	1/1	0.96	0.33	32,32,32,32	0
57	MG	2a	3001	1/1	0.96	0.07	50,50,50,50	0
57	MG	2A	3215	1/1	0.96	0.21	53,53,53,53	0
57	MG	1A	3855	1/1	0.96	0.08	35,35,35,35	0
57	MG	1A	3229	1/1	0.96	0.32	39,39,39,39	0
57	MG	2a	3006	1/1	0.96	0.09	50,50,50,50	0
57	MG	2A	3497	1/1	0.96	0.06	63,63,63,63	0
57	MG	1A	3051	1/1	0.96	0.19	42,42,42,42	0
57	MG	1A	3379	1/1	0.96	0.06	33,33,33,33	0
57	MG	2A	3220	1/1	0.96	0.06	44,44,44,44	0
57	MG	2A	3501	1/1	0.96	0.12	50,50,50,50	0
57	MG	1A	3380	1/1	0.96	0.07	50,50,50,50	0
57	MG	1A	3233	1/1	0.96	0.09	44,44,44,44	0
57	MG	2A	3505	1/1	0.96	0.09	59,59,59,59	0
57	MG	1A	3308	1/1	0.96	0.09	49,49,49,49	0
57	MG	1A	3035	1/1	0.96	0.15	42,42,42,42	0
57	MG	1A	3235	1/1	0.96	0.25	34,34,34,34	0
57	MG	1A	3598	1/1	0.96	0.09	50,50,50,50	0
57	MG	1A	3236	1/1	0.96	0.08	35,35,35,35	0
57	MG	1A	3870	1/1	0.96	0.09	25,25,25,25	0
57	MG	1A	3871	1/1	0.96	0.06	50,50,50,50	0
57	MG	1A	3716	1/1	0.96	0.08	33,33,33,33	0
57	MG	1D	301	1/1	0.96	0.24	33,33,33,33	0
57	MG	2a	3029	1/1	0.96	0.14	53,53,53,53	0
57	MG	1D	303	1/1	0.96	0.08	36,36,36,36	0
57	MG	1A	3490	1/1	0.96	0.06	40,40,40,40	0
57	MG	1a	3102	1/1	0.96	0.30	57,57,57,57	0
57	MG	1A	3719	1/1	0.96	0.17	33,33,33,33	0
57	MG	1A	3238	1/1	0.96	0.14	33,33,33,33	0
57	MG	1D	312	1/1	0.96	0.21	40,40,40,40	0
57	MG	2A	3244	1/1	0.96	0.11	53,53,53,53	0
57	MG	1D	313	1/1	0.96	0.07	50,50,50,50	0
57	MG	1A	3314	1/1	0.96	0.11	26,26,26,26	0
57	MG	1A	3187	1/1	0.96	0.06	42,42,42,42	0
57	MG	1A	3319	1/1	0.96	0.07	35,35,35,35	0
57	MG	1A	3501	1/1	0.96	0.09	45,45,45,45	0
57	MG	1A	3320	1/1	0.96	0.42	59,59,59,59	0
57	MG	2a	3044	1/1	0.96	0.14	57,57,57,57	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	2A	3006	1/1	0.96	0.07	38,38,38,38	0
57	MG	1A	3132	1/1	0.96	0.17	33,33,33,33	0
57	MG	1A	3731	1/1	0.96	0.09	26,26,26,26	0
57	MG	2A	3016	1/1	0.96	0.10	38,38,38,38	0
57	MG	2A	3017	1/1	0.96	0.11	47,47,47,47	0
57	MG	2A	3260	1/1	0.96	0.24	40,40,40,40	0
57	MG	2A	3537	1/1	0.96	0.14	47,47,47,47	0
57	MG	2A	3538	1/1	0.96	0.12	59,59,59,59	0
57	MG	1a	3114	1/1	0.96	0.06	30,30,30,30	0
57	MG	2A	3264	1/1	0.96	0.20	50,50,50,50	0
57	MG	1a	3115	1/1	0.96	0.10	47,47,47,47	0
57	MG	2A	3020	1/1	0.96	0.22	42,42,42,42	0
57	MG	2A	3022	1/1	0.96	0.14	51,51,51,51	0
57	MG	1A	3732	1/1	0.96	0.10	25,25,25,25	0
57	MG	2A	3546	1/1	0.96	0.10	36,36,36,36	0
57	MG	1a	3117	1/1	0.96	0.08	55,55,55,55	0
57	MG	1A	3733	1/1	0.96	0.07	46,46,46,46	0
57	MG	1A	3609	1/1	0.96	0.08	45,45,45,45	0
57	MG	2A	3274	1/1	0.96	0.26	55,55,55,55	0
57	MG	1F	305	1/1	0.96	0.12	23,23,23,23	0
57	MG	1F	307	1/1	0.96	0.07	28,28,28,28	0
57	MG	1F	308	1/1	0.96	0.11	24,24,24,24	0
57	MG	1A	3137	1/1	0.96	0.09	45,45,45,45	0
57	MG	2A	3034	1/1	0.96	0.12	63,63,63,63	0
57	MG	2A	3559	1/1	0.96	0.09	57,57,57,57	0
57	MG	2A	3560	1/1	0.96	0.06	30,30,30,30	0
57	MG	1A	3737	1/1	0.96	0.18	44,44,44,44	0
57	MG	1A	3738	1/1	0.96	0.05	32,32,32,32	0
57	MG	1A	3613	1/1	0.96	0.14	29,29,29,29	0
57	MG	2A	3567	1/1	0.96	0.07	50,50,50,50	0
57	MG	2A	3038	1/1	0.96	0.08	43,43,43,43	0
57	MG	1F	316	1/1	0.96	0.10	50,50,50,50	0
57	MG	2a	3080	1/1	0.96	0.12	55,55,55,55	0
57	MG	1a	3131	1/1	0.96	0.14	57,57,57,57	0
57	MG	2A	3042	1/1	0.96	0.06	27,27,27,27	0
57	MG	1A	3190	1/1	0.96	0.05	28,28,28,28	0
57	MG	1A	3615	1/1	0.96	0.16	35,35,35,35	0
57	MG	2A	3045	1/1	0.96	0.10	52,52,52,52	0
57	MG	2A	3046	1/1	0.96	0.22	63,63,63,63	0
57	MG	2A	3294	1/1	0.96	0.13	50,50,50,50	0
57	MG	2A	3295	1/1	0.96	0.07	42,42,42,42	0
57	MG	2A	3047	1/1	0.96	0.12	44,44,44,44	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	2a	3091	1/1	0.96	0.15	64,64,64,64	0
57	MG	1A	3092	1/1	0.96	0.16	26,26,26,26	0
57	MG	1A	3508	1/1	0.96	0.07	46,46,46,46	0
57	MG	1A	3510	1/1	0.96	0.04	16,16,16,16	0
57	MG	2A	3586	1/1	0.96	0.06	54,54,54,54	0
57	MG	2A	3051	1/1	0.96	0.12	53,53,53,53	0
57	MG	1H	202	1/1	0.96	0.07	49,49,49,49	0
57	MG	2A	3302	1/1	0.96	0.14	44,44,44,44	0
57	MG	2A	3593	1/1	0.96	0.09	54,54,54,54	0
57	MG	1A	3910	1/1	0.96	0.06	37,37,37,37	0
57	MG	2a	3105	1/1	0.96	0.09	48,48,48,48	0
57	MG	2a	3106	1/1	0.96	0.26	54,54,54,54	0
57	MG	1A	3325	1/1	0.96	0.08	29,29,29,29	0
57	MG	2A	3056	1/1	0.96	0.19	60,60,60,60	0
57	MG	1A	3914	1/1	0.96	0.21	39,39,39,39	0
57	MG	2a	3110	1/1	0.96	0.33	51,51,51,51	0
57	MG	1A	3916	1/1	0.96	0.05	47,47,47,47	0
57	MG	1P	204	1/1	0.96	0.06	69,69,69,69	0
57	MG	1Q	201	1/1	0.96	0.23	35,35,35,35	0
57	MG	1A	3250	1/1	0.96	0.26	30,30,30,30	0
57	MG	1A	3622	1/1	0.96	0.07	23,23,23,23	0
57	MG	1A	3255	1/1	0.96	0.14	36,36,36,36	0
57	MG	1R	203	1/1	0.96	0.07	45,45,45,45	0
57	MG	2A	3066	1/1	0.96	0.08	44,44,44,44	0
57	MG	2a	3121	1/1	0.96	0.09	58,58,58,58	0
57	MG	1A	3922	1/1	0.96	0.11	52,52,52,52	0
57	MG	2A	3068	1/1	0.96	0.09	48,48,48,48	0
57	MG	1A	3407	1/1	0.96	0.13	45,45,45,45	0
57	MG	2A	3070	1/1	0.96	0.11	47,47,47,47	0
57	MG	1A	3257	1/1	0.96	0.08	39,39,39,39	0
57	MG	2A	3074	1/1	0.96	0.07	48,48,48,48	0
57	MG	1A	3412	1/1	0.96	0.13	48,48,48,48	0
57	MG	2A	3077	1/1	0.96	0.08	57,57,57,57	0
57	MG	2A	3329	1/1	0.96	0.05	38,38,38,38	0
57	MG	1A	3012	1/1	0.96	0.10	30,30,30,30	0
57	MG	2A	3331	1/1	0.96	0.05	41,41,41,41	0
57	MG	1U	202	1/1	0.96	0.17	43,43,43,43	0
57	MG	2A	3622	1/1	0.96	0.07	53,53,53,53	0
57	MG	1A	3146	1/1	0.96	0.06	31,31,31,31	0
57	MG	1A	3934	1/1	0.96	0.06	38,38,38,38	0
57	MG	1V	207	1/1	0.96	0.06	45,45,45,45	0
57	MG	2a	3139	1/1	0.96	0.19	76,76,76,76	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	1A	3148	1/1	0.96	0.08	40,40,40,40	0
57	MG	1A	3760	1/1	0.96	0.09	35,35,35,35	0
57	MG	2a	3142	1/1	0.96	0.09	60,60,60,60	0
57	MG	1A	3150	1/1	0.96	0.07	61,61,61,61	0
57	MG	1a	3166	1/1	0.96	0.10	51,51,51,51	0
57	MG	2A	3639	1/1	0.96	0.10	55,55,55,55	0
57	MG	1A	3762	1/1	0.96	0.10	48,48,48,48	0
57	MG	2A	3641	1/1	0.96	0.06	43,43,43,43	0
57	MG	2A	3089	1/1	0.96	0.10	45,45,45,45	0
57	MG	1A	3099	1/1	0.96	0.22	38,38,38,38	0
57	MG	1A	3266	1/1	0.96	0.12	37,37,37,37	0
57	MG	1A	3637	1/1	0.96	0.14	41,41,41,41	0
57	MG	1a	3172	1/1	0.96	0.15	58,58,58,58	0
57	MG	10	106	1/1	0.96	0.08	47,47,47,47	0
57	MG	2A	3649	1/1	0.96	0.08	46,46,46,46	0
57	MG	1A	3201	1/1	0.96	0.09	41,41,41,41	0
57	MG	2a	3158	1/1	0.96	0.06	67,67,67,67	0
57	MG	1A	3269	1/1	0.96	0.09	48,48,48,48	0
57	MG	1A	3771	1/1	0.96	0.04	36,36,36,36	0
57	MG	2A	3357	1/1	0.96	0.06	47,47,47,47	0
57	MG	2a	3162	1/1	0.96	0.07	57,57,57,57	0
57	MG	2A	3658	1/1	0.96	0.07	66,66,66,66	0
57	MG	2A	3659	1/1	0.96	0.05	50,50,50,50	0
57	MG	1A	3640	1/1	0.96	0.14	34,34,34,34	0
57	MG	1A	3641	1/1	0.96	0.11	32,32,32,32	0
57	MG	1a	3179	1/1	0.96	0.05	65,65,65,65	0
57	MG	1A	3344	1/1	0.96	0.06	25,25,25,25	0
57	MG	2A	3365	1/1	0.96	0.06	34,34,34,34	0
57	MG	11	105	1/1	0.96	0.06	26,26,26,26	0
57	MG	1A	3428	1/1	0.96	0.06	20,20,20,20	0
57	MG	15	3102	1/1	0.96	0.12	34,34,34,34	0
57	MG	1A	3430	1/1	0.96	0.05	15,15,15,15	0
57	MG	2A	3113	1/1	0.96	0.14	52,52,52,52	0
57	MG	1A	3432	1/1	0.96	0.14	46,46,46,46	0
57	MG	2A	3374	1/1	0.96	0.09	46,46,46,46	0
57	MG	2a	3182	1/1	0.96	0.05	71,71,71,71	0
57	MG	1a	3186	1/1	0.96	0.08	50,50,50,50	0
57	MG	2A	3679	1/1	0.96	0.09	48,48,48,48	0
57	MG	2A	3683	1/1	0.96	0.06	38,38,38,38	0
57	MG	1A	3544	1/1	0.96	0.05	36,36,36,36	0
57	MG	1A	3783	1/1	0.96	0.14	35,35,35,35	0
57	MG	18	102	1/1	0.96	0.17	36,36,36,36	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	2A	3379	1/1	0.96	0.09	42,42,42,42	0
57	MG	1A	3960	1/1	0.96	0.08	38,38,38,38	0
57	MG	19	101	1/1	0.96	0.14	46,46,46,46	0
57	MG	1A	3961	1/1	0.96	0.10	47,47,47,47	0
57	MG	1A	3784	1/1	0.96	0.09	29,29,29,29	0
57	MG	2A	3124	1/1	0.96	0.06	38,38,38,38	0
57	MG	1A	3648	1/1	0.96	0.08	32,32,32,32	0
57	MG	2A	3391	1/1	0.96	0.07	53,53,53,53	0
57	MG	2A	3392	1/1	0.96	0.08	40,40,40,40	0
57	MG	1A	3649	1/1	0.96	0.10	49,49,49,49	0
57	MG	1A	3153	1/1	0.96	0.04	31,31,31,31	0
57	MG	2A	3703	1/1	0.96	0.11	55,55,55,55	0
57	MG	1A	3788	1/1	0.96	0.15	39,39,39,39	0
57	MG	1a	3007	1/1	0.96	0.08	47,47,47,47	0
57	MG	1a	3008	1/1	0.96	0.07	55,55,55,55	0
57	MG	1A	3154	1/1	0.96	0.06	48,48,48,48	0
57	MG	1A	3790	1/1	0.96	0.10	47,47,47,47	0
57	MG	1a	3013	1/1	0.96	0.08	54,54,54,54	0
57	MG	1A	3939	1/1	0.97	0.08	44,44,44,44	0
57	MG	10	103	1/1	0.97	0.06	38,38,38,38	0
57	MG	2A	3701	1/1	0.97	0.06	50,50,50,50	0
57	MG	2A	3385	1/1	0.97	0.06	37,37,37,37	0
57	MG	2A	3118	1/1	0.97	0.20	57,57,57,57	0
57	MG	2A	3387	1/1	0.97	0.10	41,41,41,41	0
57	MG	1A	3756	1/1	0.97	0.05	40,40,40,40	0
57	MG	10	105	1/1	0.97	0.07	43,43,43,43	0
57	MG	1A	3757	1/1	0.97	0.05	31,31,31,31	0
57	MG	1A	3611	1/1	0.97	0.17	31,31,31,31	0
57	MG	1A	3208	1/1	0.97	0.16	39,39,39,39	0
57	MG	2A	3710	1/1	0.97	0.07	53,53,53,53	0
57	MG	1A	3289	1/1	0.97	0.05	45,45,45,45	0
57	MG	11	101	1/1	0.97	0.10	39,39,39,39	0
57	MG	1A	3484	1/1	0.97	0.07	29,29,29,29	0
57	MG	2A	3128	1/1	0.97	0.08	33,33,33,33	0
57	MG	1A	3209	1/1	0.97	0.17	42,42,42,42	0
57	MG	1A	3764	1/1	0.97	0.05	30,30,30,30	0
57	MG	2A	3401	1/1	0.97	0.05	56,56,56,56	0
57	MG	2A	3402	1/1	0.97	0.05	45,45,45,45	0
57	MG	1A	3950	1/1	0.97	0.05	43,43,43,43	0
57	MG	13	101	1/1	0.97	0.11	43,43,43,43	0
57	MG	1A	3765	1/1	0.97	0.05	38,38,38,38	0
57	MG	15	3101	1/1	0.97	0.10	26,26,26,26	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	1A	3151	1/1	0.97	0.08	43,43,43,43	0
57	MG	1A	3213	1/1	0.97	0.21	37,37,37,37	0
57	MG	1A	3954	1/1	0.97	0.06	55,55,55,55	0
57	MG	15	3109	1/1	0.97	0.08	51,51,51,51	0
57	MG	17	104	1/1	0.97	0.14	30,30,30,30	0
57	MG	1A	3488	1/1	0.97	0.08	27,27,27,27	0
57	MG	17	106	1/1	0.97	0.07	40,40,40,40	0
57	MG	1A	3489	1/1	0.97	0.06	23,23,23,23	0
57	MG	1A	3215	1/1	0.97	0.45	35,35,35,35	0
57	MG	1A	3295	1/1	0.97	0.06	15,15,15,15	0
57	MG	1A	3065	1/1	0.97	0.04	38,38,38,38	0
57	MG	1a	3212	1/1	0.97	0.05	69,69,69,69	0
57	MG	2B	205	1/1	0.97	0.18	54,54,54,54	0
57	MG	1A	3495	1/1	0.97	0.06	48,48,48,48	0
57	MG	1A	3217	1/1	0.97	0.18	31,31,31,31	0
57	MG	1A	3497	1/1	0.97	0.12	22,22,22,22	0
57	MG	1A	3777	1/1	0.97	0.06	41,41,41,41	0
57	MG	1A	3498	1/1	0.97	0.05	52,52,52,52	0
57	MG	2A	3155	1/1	0.97	0.12	52,52,52,52	0
57	MG	1a	3005	1/1	0.97	0.23	54,54,54,54	0
57	MG	1A	3780	1/1	0.97	0.13	43,43,43,43	0
57	MG	1A	3499	1/1	0.97	0.05	32,32,32,32	0
57	MG	1A	3632	1/1	0.97	0.08	24,24,24,24	0
57	MG	1A	3066	1/1	0.97	0.08	42,42,42,42	0
57	MG	2A	3436	1/1	0.97	0.06	48,48,48,48	0
57	MG	1A	3634	1/1	0.97	0.07	35,35,35,35	0
57	MG	2B	219	1/1	0.97	0.08	66,66,66,66	0
57	MG	1a	3224	1/1	0.97	0.04	46,46,46,46	0
57	MG	1A	3096	1/1	0.97	0.08	50,50,50,50	0
57	MG	2D	303	1/1	0.97	0.34	39,39,39,39	0
57	MG	2D	304	1/1	0.97	0.09	34,34,34,34	0
57	MG	1A	3386	1/1	0.97	0.06	31,31,31,31	0
57	MG	1A	3302	1/1	0.97	0.05	46,46,46,46	0
57	MG	1A	3504	1/1	0.97	0.07	42,42,42,42	0
57	MG	1A	3098	1/1	0.97	0.10	49,49,49,49	0
57	MG	1a	3230	1/1	0.97	0.08	64,64,64,64	0
57	MG	1A	3980	1/1	0.97	0.06	48,48,48,48	0
57	MG	2A	3446	1/1	0.97	0.11	57,57,57,57	0
57	MG	1A	3305	1/1	0.97	0.12	45,45,45,45	0
57	MG	1a	3233	1/1	0.97	0.14	52,52,52,52	0
57	MG	2A	3173	1/1	0.97	0.09	40,40,40,40	0
57	MG	1A	3390	1/1	0.97	0.04	29,29,29,29	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	1A	3984	1/1	0.97	0.05	47,47,47,47	0
57	MG	2A	3452	1/1	0.97	0.04	36,36,36,36	0
57	MG	1A	3157	1/1	0.97	0.09	44,44,44,44	0
57	MG	2A	3454	1/1	0.97	0.04	45,45,45,45	0
57	MG	1A	3025	1/1	0.97	0.12	33,33,33,33	0
57	MG	1a	3026	1/1	0.97	0.05	49,49,49,49	0
57	MG	1a	3239	1/1	0.97	0.08	58,58,58,58	0
57	MG	1A	3159	1/1	0.97	0.12	22,22,22,22	0
57	MG	1A	3645	1/1	0.97	0.11	37,37,37,37	0
57	MG	1A	3394	1/1	0.97	0.08	22,22,22,22	0
57	MG	1A	3105	1/1	0.97	0.06	31,31,31,31	0
57	MG	1A	3396	1/1	0.97	0.10	27,27,27,27	0
57	MG	1a	3246	1/1	0.97	0.04	50,50,50,50	0
57	MG	1A	3517	1/1	0.97	0.05	36,36,36,36	0
57	MG	1A	3230	1/1	0.97	0.12	33,33,33,33	0
57	MG	1a	3250	1/1	0.97	0.05	57,57,57,57	0
57	MG	1A	3311	1/1	0.97	0.06	19,19,19,19	0
57	MG	2T	202	1/1	0.97	0.07	51,51,51,51	0
57	MG	1A	3106	1/1	0.97	0.06	43,43,43,43	0
57	MG	1A	3232	1/1	0.97	0.09	31,31,31,31	0
57	MG	1A	3522	1/1	0.97	0.08	24,24,24,24	0
57	MG	1A	3404	1/1	0.97	0.04	22,22,22,22	0
57	MG	2A	3472	1/1	0.97	0.05	66,66,66,66	0
57	MG	1A	3657	1/1	0.97	0.10	38,38,38,38	0
57	MG	1a	3043	1/1	0.97	0.05	54,54,54,54	0
57	MG	2X	101	1/1	0.97	0.08	51,51,51,51	0
57	MG	1A	3811	1/1	0.97	0.16	42,42,42,42	0
57	MG	1A	3525	1/1	0.97	0.04	25,25,25,25	0
57	MG	1a	3046	1/1	0.97	0.23	49,49,49,49	0
57	MG	1A	4003	1/1	0.97	0.34	44,44,44,44	0
57	MG	1A	3048	1/1	0.97	0.10	37,37,37,37	0
57	MG	1a	3049	1/1	0.97	0.16	41,41,41,41	0
57	MG	1A	3528	1/1	0.97	0.05	39,39,39,39	0
57	MG	1A	3529	1/1	0.97	0.04	23,23,23,23	0
57	MG	28	101	1/1	0.97	0.06	51,51,51,51	0
57	MG	2A	3206	1/1	0.97	0.18	41,41,41,41	0
57	MG	1A	4007	1/1	0.97	0.05	54,54,54,54	0
57	MG	1A	4008	1/1	0.97	0.13	43,43,43,43	0
57	MG	1a	3272	1/1	0.97	0.13	58,58,58,58	0
57	MG	1A	3165	1/1	0.97	0.09	24,24,24,24	0
57	MG	1A	3318	1/1	0.97	0.06	21,21,21,21	0
57	MG	1A	4011	1/1	0.97	0.07	53,53,53,53	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	1A	3664	1/1	0.97	0.04	46,46,46,46	0
57	MG	1A	3665	1/1	0.97	0.11	45,45,45,45	0
57	MG	1A	3166	1/1	0.97	0.07	42,42,42,42	0
57	MG	1A	3409	1/1	0.97	0.06	54,54,54,54	0
57	MG	1A	3825	1/1	0.97	0.04	26,26,26,26	0
57	MG	2a	3014	1/1	0.97	0.17	55,55,55,55	0
57	MG	1A	3668	1/1	0.97	0.06	49,49,49,49	0
57	MG	1A	4018	1/1	0.97	0.06	39,39,39,39	0
57	MG	1e	202	1/1	0.97	0.06	51,51,51,51	0
57	MG	1A	3669	1/1	0.97	0.06	46,46,46,46	0
57	MG	2a	3020	1/1	0.97	0.08	59,59,59,59	0
57	MG	1A	3410	1/1	0.97	0.06	18,18,18,18	0
57	MG	2A	3504	1/1	0.97	0.05	35,35,35,35	0
57	MG	1A	3167	1/1	0.97	0.04	27,27,27,27	0
57	MG	1A	4022	1/1	0.97	0.05	36,36,36,36	0
57	MG	1A	3414	1/1	0.97	0.09	46,46,46,46	0
57	MG	1i	201	1/1	0.97	0.04	51,51,51,51	0
57	MG	2A	3227	1/1	0.97	0.11	44,44,44,44	0
57	MG	2A	3228	1/1	0.97	0.10	33,33,33,33	0
57	MG	1a	3072	1/1	0.97	0.14	44,44,44,44	0
57	MG	2A	3232	1/1	0.97	0.10	52,52,52,52	0
57	MG	1A	3237	1/1	0.97	0.14	26,26,26,26	0
57	MG	1A	3538	1/1	0.97	0.21	31,31,31,31	0
57	MG	2a	3034	1/1	0.97	0.06	45,45,45,45	0
57	MG	2A	3516	1/1	0.97	0.08	74,74,74,74	0
57	MG	1A	3836	1/1	0.97	0.05	36,36,36,36	0
57	MG	1A	3539	1/1	0.97	0.07	41,41,41,41	0
57	MG	1A	3838	1/1	0.97	0.05	42,42,42,42	0
57	MG	1A	3540	1/1	0.97	0.05	22,22,22,22	0
57	MG	2A	3521	1/1	0.97	0.06	53,53,53,53	0
57	MG	1A	3840	1/1	0.97	0.06	44,44,44,44	0
57	MG	1A	3541	1/1	0.97	0.04	23,23,23,23	0
57	MG	1A	3416	1/1	0.97	0.05	38,38,38,38	0
57	MG	2A	3242	1/1	0.97	0.20	37,37,37,37	0
57	MG	1A	3417	1/1	0.97	0.04	21,21,21,21	0
57	MG	1A	3072	1/1	0.97	0.11	31,31,31,31	0
57	MG	1A	3169	1/1	0.97	0.33	35,35,35,35	0
57	MG	1A	3114	1/1	0.97	0.10	39,39,39,39	0
57	MG	1A	3172	1/1	0.97	0.12	46,46,46,46	0
57	MG	1A	3422	1/1	0.97	0.05	44,44,44,44	0
57	MG	1A	3120	1/1	0.97	0.06	31,31,31,31	0
57	MG	2A	3250	1/1	0.97	0.08	57,57,57,57	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	1A	3248	1/1	0.97	0.20	39,39,39,39	0
57	MG	2A	3002	1/1	0.97	0.07	41,41,41,41	0
57	MG	2a	3055	1/1	0.97	0.09	51,51,51,51	0
57	MG	1a	3091	1/1	0.97	0.10	51,51,51,51	0
57	MG	1A	3852	1/1	0.97	0.09	36,36,36,36	0
57	MG	1a	3093	1/1	0.97	0.09	47,47,47,47	0
57	MG	2A	3257	1/1	0.97	0.07	36,36,36,36	0
57	MG	2A	3009	1/1	0.97	0.07	45,45,45,45	0
57	MG	2A	3259	1/1	0.97	0.10	24,24,24,24	0
57	MG	2A	3011	1/1	0.97	0.05	34,34,34,34	0
57	MG	2A	3261	1/1	0.97	0.11	55,55,55,55	0
57	MG	2A	3262	1/1	0.97	0.14	33,33,33,33	0
57	MG	2A	3013	1/1	0.97	0.06	31,31,31,31	0
57	MG	2A	3014	1/1	0.97	0.06	49,49,49,49	0
57	MG	2A	3549	1/1	0.97	0.05	45,45,45,45	0
57	MG	1A	3121	1/1	0.97	0.10	31,31,31,31	0
57	MG	1A	3179	1/1	0.97	0.12	42,42,42,42	0
57	MG	2A	3267	1/1	0.97	0.04	25,25,25,25	0
57	MG	1B	224	1/1	0.97	0.04	38,38,38,38	0
57	MG	2A	3269	1/1	0.97	0.06	45,45,45,45	0
57	MG	1A	3427	1/1	0.97	0.09	16,16,16,16	0
57	MG	1A	3856	1/1	0.97	0.06	40,40,40,40	0
57	MG	2a	3075	1/1	0.97	0.13	53,53,53,53	0
57	MG	2a	3076	1/1	0.97	0.06	61,61,61,61	0
57	MG	1A	3693	1/1	0.97	0.16	40,40,40,40	0
57	MG	1A	3251	1/1	0.97	0.05	37,37,37,37	0
57	MG	1A	3429	1/1	0.97	0.11	27,27,27,27	0
57	MG	1A	3253	1/1	0.97	0.14	37,37,37,37	0
57	MG	2a	3081	1/1	0.97	0.30	51,51,51,51	0
57	MG	2A	3025	1/1	0.97	0.07	34,34,34,34	0
57	MG	1A	3431	1/1	0.97	0.07	32,32,32,32	0
57	MG	2A	3027	1/1	0.97	0.08	38,38,38,38	0
57	MG	1A	3863	1/1	0.97	0.04	28,28,28,28	0
57	MG	1D	304	1/1	0.97	0.06	34,34,34,34	0
57	MG	1D	307	1/1	0.97	0.08	47,47,47,47	0
57	MG	1A	3182	1/1	0.97	0.12	30,30,30,30	0
57	MG	1A	3074	1/1	0.97	0.09	29,29,29,29	0
57	MG	2A	3573	1/1	0.97	0.05	49,49,49,49	0
57	MG	1A	3334	1/1	0.97	0.06	25,25,25,25	0
57	MG	2a	3092	1/1	0.97	0.29	52,52,52,52	0
57	MG	1A	3702	1/1	0.97	0.09	54,54,54,54	0
57	MG	2A	3577	1/1	0.97	0.07	61,61,61,61	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	1A	3335	1/1	0.97	0.07	20,20,20,20	0
57	MG	2A	3289	1/1	0.97	0.10	42,42,42,42	0
57	MG	2a	3097	1/1	0.97	0.29	55,55,55,55	0
57	MG	1A	3337	1/1	0.97	0.10	14,14,14,14	0
57	MG	1A	3258	1/1	0.97	0.09	47,47,47,47	0
57	MG	2a	3100	1/1	0.97	0.18	41,41,41,41	0
57	MG	1E	302	1/1	0.97	0.18	35,35,35,35	0
57	MG	2A	3040	1/1	0.97	0.06	44,44,44,44	0
57	MG	1A	3872	1/1	0.97	0.11	27,27,27,27	0
57	MG	1A	3037	1/1	0.97	0.07	44,44,44,44	0
57	MG	1A	3440	1/1	0.97	0.03	14,14,14,14	0
57	MG	1a	3118	1/1	0.97	0.06	42,42,42,42	0
57	MG	2A	3589	1/1	0.97	0.06	42,42,42,42	0
57	MG	1E	307	1/1	0.97	0.06	45,45,45,45	0
57	MG	1A	3710	1/1	0.97	0.05	37,37,37,37	0
57	MG	1A	3574	1/1	0.97	0.10	34,34,34,34	0
57	MG	1A	3878	1/1	0.97	0.07	39,39,39,39	0
57	MG	1A	3712	1/1	0.97	0.03	32,32,32,32	0
57	MG	1A	3341	1/1	0.97	0.06	34,34,34,34	0
57	MG	1a	3125	1/1	0.97	0.05	50,50,50,50	0
57	MG	2A	3305	1/1	0.97	0.18	46,46,46,46	0
57	MG	2a	3118	1/1	0.97	0.07	67,67,67,67	0
57	MG	2A	3052	1/1	0.97	0.04	32,32,32,32	0
57	MG	1F	303	1/1	0.97	0.15	28,28,28,28	0
57	MG	1A	3077	1/1	0.97	0.07	27,27,27,27	0
57	MG	1A	3715	1/1	0.97	0.07	35,35,35,35	0
57	MG	1A	3262	1/1	0.97	0.06	44,44,44,44	0
57	MG	1A	3078	1/1	0.97	0.06	44,44,44,44	0
57	MG	2A	3058	1/1	0.97	0.05	32,32,32,32	0
57	MG	1F	311	1/1	0.97	0.05	33,33,33,33	0
57	MG	1A	3056	1/1	0.97	0.08	38,38,38,38	0
57	MG	1A	3032	1/1	0.97	0.08	40,40,40,40	0
57	MG	1A	3450	1/1	0.97	0.08	40,40,40,40	0
57	MG	1a	3138	1/1	0.97	0.08	48,48,48,48	0
57	MG	1A	3454	1/1	0.97	0.09	56,56,56,56	0
57	MG	1A	3009	1/1	0.97	0.04	26,26,26,26	0
57	MG	1A	3133	1/1	0.97	0.08	32,32,32,32	0
57	MG	2A	3324	1/1	0.97	0.10	26,26,26,26	0
57	MG	1A	3268	1/1	0.97	0.12	31,31,31,31	0
57	MG	1A	3459	1/1	0.97	0.05	53,53,53,53	0
57	MG	1A	3134	1/1	0.97	0.07	37,37,37,37	0
57	MG	1A	3084	1/1	0.97	0.15	40,40,40,40	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	1A	3903	1/1	0.97	0.04	30,30,30,30	0
57	MG	2A	3073	1/1	0.97	0.05	24,24,24,24	0
57	MG	1A	3040	1/1	0.97	0.05	37,37,37,37	0
57	MG	2A	3628	1/1	0.97	0.05	49,49,49,49	0
57	MG	2A	3629	1/1	0.97	0.05	69,69,69,69	0
57	MG	1A	3592	1/1	0.97	0.15	52,52,52,52	0
57	MG	2A	3632	1/1	0.97	0.07	70,70,70,70	0
57	MG	1P	201	1/1	0.97	0.22	31,31,31,31	0
57	MG	2A	3634	1/1	0.97	0.04	40,40,40,40	0
57	MG	2a	3149	1/1	0.97	0.11	54,54,54,54	0
57	MG	2a	3150	1/1	0.97	0.07	49,49,49,49	0
57	MG	2A	3635	1/1	0.97	0.05	68,68,68,68	0
57	MG	1A	3593	1/1	0.97	0.03	18,18,18,18	0
57	MG	1A	3139	1/1	0.97	0.12	38,38,38,38	0
57	MG	2A	3337	1/1	0.97	0.07	42,42,42,42	0
57	MG	2A	3339	1/1	0.97	0.10	53,53,53,53	0
57	MG	1A	3140	1/1	0.97	0.08	32,32,32,32	0
57	MG	2A	3341	1/1	0.97	0.10	38,38,38,38	0
57	MG	1Q	203	1/1	0.97	0.16	29,29,29,29	0
57	MG	1A	3913	1/1	0.97	0.12	28,28,28,28	0
57	MG	1Q	205	1/1	0.97	0.06	47,47,47,47	0
57	MG	1A	3465	1/1	0.97	0.07	55,55,55,55	0
57	MG	2A	3346	1/1	0.97	0.09	49,49,49,49	0
57	MG	1A	3087	1/1	0.97	0.10	41,41,41,41	0
57	MG	1A	3008	1/1	0.97	0.06	27,27,27,27	0
57	MG	2A	3349	1/1	0.97	0.07	52,52,52,52	0
57	MG	1A	3471	1/1	0.97	0.04	26,26,26,26	0
57	MG	2A	3088	1/1	0.97	0.14	60,60,60,60	0
57	MG	1S	201	1/1	0.97	0.10	48,48,48,48	0
57	MG	1A	3920	1/1	0.97	0.08	49,49,49,49	0
57	MG	1T	202	1/1	0.97	0.09	41,41,41,41	0
57	MG	2A	3092	1/1	0.97	0.08	42,42,42,42	0
57	MG	2A	3664	1/1	0.97	0.04	47,47,47,47	0
57	MG	2A	3093	1/1	0.97	0.06	45,45,45,45	0
57	MG	1A	3147	1/1	0.97	0.13	29,29,29,29	0
57	MG	2a	3175	1/1	0.97	0.09	55,55,55,55	0
57	MG	2a	3176	1/1	0.97	0.12	63,63,63,63	0
57	MG	2A	3359	1/1	0.97	0.11	35,35,35,35	0
57	MG	2a	3178	1/1	0.97	0.09	74,74,74,74	0
57	MG	2A	3360	1/1	0.97	0.12	33,33,33,33	0
57	MG	2a	3180	1/1	0.97	0.05	61,61,61,61	0
57	MG	2a	3181	1/1	0.97	0.04	57,57,57,57	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	1A	3602	1/1	0.97	0.04	33,33,33,33	0
57	MG	2A	3670	1/1	0.97	0.09	50,50,50,50	0
57	MG	1A	3042	1/1	0.97	0.07	28,28,28,28	0
57	MG	2A	3097	1/1	0.97	0.08	48,48,48,48	0
57	MG	2A	3673	1/1	0.97	0.06	49,49,49,49	0
57	MG	2a	3187	1/1	0.97	0.28	57,57,57,57	0
57	MG	1A	3364	1/1	0.97	0.05	42,42,42,42	0
57	MG	2A	3676	1/1	0.97	0.05	40,40,40,40	0
57	MG	1a	3170	1/1	0.97	0.07	57,57,57,57	0
57	MG	1U	203	1/1	0.97	0.11	36,36,36,36	0
57	MG	1V	202	1/1	0.97	0.16	23,23,23,23	0
57	MG	2A	3680	1/1	0.97	0.07	63,63,63,63	0
57	MG	2A	3682	1/1	0.97	0.07	53,53,53,53	0
57	MG	1A	3928	1/1	0.97	0.08	32,32,32,32	0
57	MG	2A	3684	1/1	0.97	0.07	45,45,45,45	0
57	MG	2t	201	1/1	0.97	0.07	35,35,35,35	0
57	MG	1V	205	1/1	0.97	0.04	44,44,44,44	0
57	MG	1A	3282	1/1	0.97	0.08	33,33,33,33	0
57	MG	1A	3149	1/1	0.97	0.06	32,32,32,32	0
57	MG	2A	3109	1/1	0.97	0.07	50,50,50,50	0
57	MG	1A	3369	1/1	0.97	0.04	25,25,25,25	0
57	MG	1W	202	1/1	0.97	0.05	38,38,38,38	0
57	MG	1A	3752	1/1	0.97	0.12	34,34,34,34	0
57	MG	1A	3479	1/1	0.97	0.04	28,28,28,28	0
57	MG	2A	3380	1/1	0.97	0.09	42,42,42,42	0
57	MG	1A	3091	1/1	0.97	0.19	31,31,31,31	0
57	MG	1A	3287	1/1	0.97	0.26	44,44,44,44	0
60	ZN	29	501	1/1	0.97	0.05	78,78,78,78	0
57	MG	2A	3076	1/1	0.98	0.09	35,35,35,35	0
57	MG	2E	305	1/1	0.98	0.04	38,38,38,38	0
57	MG	2E	306	1/1	0.98	0.07	30,30,30,30	0
57	MG	1A	3729	1/1	0.98	0.09	23,23,23,23	0
57	MG	2F	301	1/1	0.98	0.23	40,40,40,40	0
57	MG	1A	3135	1/1	0.98	0.22	24,24,24,24	0
57	MG	1A	3036	1/1	0.98	0.05	27,27,27,27	0
57	MG	2F	304	1/1	0.98	0.19	41,41,41,41	0
57	MG	1A	3067	1/1	0.98	0.05	27,27,27,27	0
57	MG	1A	3338	1/1	0.98	0.08	44,44,44,44	0
57	MG	1A	3859	1/1	0.98	0.05	38,38,38,38	0
57	MG	1A	3620	1/1	0.98	0.05	37,37,37,37	0
57	MG	1A	3735	1/1	0.98	0.07	27,27,27,27	0
57	MG	1a	3009	1/1	0.98	0.27	51,51,51,51	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	1A	3191	1/1	0.98	0.18	34,34,34,34	0
57	MG	1A	3192	1/1	0.98	0.15	45,45,45,45	0
57	MG	1A	3864	1/1	0.98	0.04	31,31,31,31	0
57	MG	1A	3094	1/1	0.98	0.04	14,14,14,14	0
57	MG	1A	3049	1/1	0.98	0.06	35,35,35,35	0
57	MG	1A	3343	1/1	0.98	0.05	31,31,31,31	0
57	MG	1a	3202	1/1	0.98	0.04	70,70,70,70	0
57	MG	1A	3524	1/1	0.98	0.05	36,36,36,36	0
57	MG	1a	3018	1/1	0.98	0.06	46,46,46,46	0
57	MG	1A	3142	1/1	0.98	0.03	31,31,31,31	0
57	MG	1A	3526	1/1	0.98	0.24	26,26,26,26	0
57	MG	1a	3021	1/1	0.98	0.04	48,48,48,48	0
57	MG	1A	3630	1/1	0.98	0.04	22,22,22,22	0
57	MG	1A	3143	1/1	0.98	0.05	34,34,34,34	0
57	MG	2A	3100	1/1	0.98	0.10	45,45,45,45	0
57	MG	1A	3144	1/1	0.98	0.05	34,34,34,34	0
57	MG	2W	201	1/1	0.98	0.14	42,42,42,42	0
57	MG	1A	3199	1/1	0.98	0.10	27,27,27,27	0
57	MG	1A	3070	1/1	0.98	0.16	28,28,28,28	0
57	MG	1A	3097	1/1	0.98	0.05	34,34,34,34	0
57	MG	1A	3434	1/1	0.98	0.03	19,19,19,19	0
57	MG	1A	3273	1/1	0.98	0.22	37,37,37,37	0
57	MG	2A	3545	1/1	0.98	0.07	41,41,41,41	0
57	MG	1A	3351	1/1	0.98	0.06	51,51,51,51	0
57	MG	25	101	1/1	0.98	0.20	39,39,39,39	0
57	MG	1a	3031	1/1	0.98	0.15	52,52,52,52	0
57	MG	2A	3548	1/1	0.98	0.05	51,51,51,51	0
57	MG	2A	3321	1/1	0.98	0.05	37,37,37,37	0
57	MG	1A	3050	1/1	0.98	0.19	39,39,39,39	0
57	MG	1a	3033	1/1	0.98	0.03	28,28,28,28	0
57	MG	1A	3029	1/1	0.98	0.07	32,32,32,32	0
57	MG	1B	214	1/1	0.98	0.05	37,37,37,37	0
57	MG	2A	3554	1/1	0.98	0.04	69,69,69,69	0
57	MG	2a	3003	1/1	0.98	0.03	46,46,46,46	0
57	MG	1A	3100	1/1	0.98	0.15	27,27,27,27	0
57	MG	1a	3037	1/1	0.98	0.08	36,36,36,36	0
57	MG	2A	3328	1/1	0.98	0.07	50,50,50,50	0
57	MG	1A	3205	1/1	0.98	0.10	40,40,40,40	0
57	MG	1A	3356	1/1	0.98	0.07	18,18,18,18	0
57	MG	1A	3102	1/1	0.98	0.05	30,30,30,30	0
57	MG	1A	3279	1/1	0.98	0.06	41,41,41,41	0
57	MG	2A	3562	1/1	0.98	0.04	45,45,45,45	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	2a	3012	1/1	0.98	0.05	48,48,48,48	0
57	MG	1A	3888	1/1	0.98	0.08	27,27,27,27	0
57	MG	2A	3565	1/1	0.98	0.05	51,51,51,51	0
57	MG	1A	3542	1/1	0.98	0.05	29,29,29,29	0
57	MG	1A	3891	1/1	0.98	0.04	46,46,46,46	0
57	MG	2a	3017	1/1	0.98	0.04	55,55,55,55	0
57	MG	1A	3892	1/1	0.98	0.05	32,32,32,32	0
57	MG	1A	3446	1/1	0.98	0.17	31,31,31,31	0
57	MG	2A	3338	1/1	0.98	0.05	33,33,33,33	0
57	MG	1A	3895	1/1	0.98	0.04	28,28,28,28	0
57	MG	2a	3022	1/1	0.98	0.06	50,50,50,50	0
57	MG	2A	3127	1/1	0.98	0.15	34,34,34,34	0
57	MG	1A	3103	1/1	0.98	0.25	27,27,27,27	0
57	MG	1A	3546	1/1	0.98	0.09	27,27,27,27	0
57	MG	1A	3052	1/1	0.98	0.08	27,27,27,27	0
57	MG	1A	3054	1/1	0.98	0.05	23,23,23,23	0
57	MG	2A	3578	1/1	0.98	0.03	50,50,50,50	0
57	MG	1A	3363	1/1	0.98	0.05	10,10,10,10	0
57	MG	1a	3054	1/1	0.98	0.05	40,40,40,40	0
57	MG	1a	3240	1/1	0.98	0.08	51,51,51,51	0
57	MG	1A	3550	1/1	0.98	0.18	46,46,46,46	0
57	MG	1D	302	1/1	0.98	0.05	42,42,42,42	0
57	MG	1A	3451	1/1	0.98	0.06	35,35,35,35	0
57	MG	1a	3058	1/1	0.98	0.21	47,47,47,47	0
57	MG	2A	3139	1/1	0.98	0.17	36,36,36,36	0
57	MG	2A	3353	1/1	0.98	0.05	41,41,41,41	0
57	MG	1A	3906	1/1	0.98	0.06	30,30,30,30	0
57	MG	1D	305	1/1	0.98	0.19	42,42,42,42	0
57	MG	1a	3247	1/1	0.98	0.04	51,51,51,51	0
57	MG	1D	306	1/1	0.98	0.07	20,20,20,20	0
57	MG	1A	3907	1/1	0.98	0.04	14,14,14,14	0
57	MG	2A	3595	1/1	0.98	0.05	40,40,40,40	0
57	MG	1A	3655	1/1	0.98	0.11	44,44,44,44	0
57	MG	2A	3146	1/1	0.98	0.09	61,61,61,61	0
57	MG	2A	3598	1/1	0.98	0.08	39,39,39,39	0
57	MG	2A	3147	1/1	0.98	0.09	54,54,54,54	0
57	MG	1A	3453	1/1	0.98	0.06	21,21,21,21	0
57	MG	1D	310	1/1	0.98	0.11	26,26,26,26	0
57	MG	1A	3774	1/1	0.98	0.04	34,34,34,34	0
57	MG	1A	3076	1/1	0.98	0.23	30,30,30,30	0
57	MG	1A	3912	1/1	0.98	0.06	42,42,42,42	0
57	MG	1A	3455	1/1	0.98	0.06	51,51,51,51	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	1a	3257	1/1	0.98	0.06	51,51,51,51	0
57	MG	2A	3371	1/1	0.98	0.04	43,43,43,43	0
57	MG	1A	3211	1/1	0.98	0.12	40,40,40,40	0
57	MG	1E	301	1/1	0.98	0.09	28,28,28,28	0
57	MG	1a	3261	1/1	0.98	0.04	51,51,51,51	0
57	MG	1A	3915	1/1	0.98	0.04	47,47,47,47	0
57	MG	1E	303	1/1	0.98	0.05	28,28,28,28	0
57	MG	1A	3778	1/1	0.98	0.04	22,22,22,22	0
57	MG	2A	3161	1/1	0.98	0.17	43,43,43,43	0
57	MG	1A	3366	1/1	0.98	0.06	19,19,19,19	0
57	MG	1A	3367	1/1	0.98	0.13	45,45,45,45	0
57	MG	1A	3919	1/1	0.98	0.05	47,47,47,47	0
57	MG	1A	3155	1/1	0.98	0.24	40,40,40,40	0
57	MG	1A	3214	1/1	0.98	0.05	29,29,29,29	0
57	MG	1A	3110	1/1	0.98	0.10	26,26,26,26	0
57	MG	1A	3561	1/1	0.98	0.10	38,38,38,38	0
57	MG	2A	3624	1/1	0.98	0.04	41,41,41,41	0
57	MG	1A	3925	1/1	0.98	0.05	27,27,27,27	0
57	MG	1F	301	1/1	0.98	0.12	28,28,28,28	0
57	MG	1F	302	1/1	0.98	0.07	25,25,25,25	0
57	MG	2A	3389	1/1	0.98	0.04	37,37,37,37	0
57	MG	1A	3371	1/1	0.98	0.11	58,58,58,58	0
57	MG	1A	3927	1/1	0.98	0.06	47,47,47,47	0
57	MG	2A	3631	1/1	0.98	0.08	58,58,58,58	0
57	MG	1A	3111	1/1	0.98	0.11	37,37,37,37	0
57	MG	1A	3929	1/1	0.98	0.04	42,42,42,42	0
57	MG	1A	3055	1/1	0.98	0.10	38,38,38,38	0
57	MG	2A	3177	1/1	0.98	0.10	32,32,32,32	0
57	MG	1A	3931	1/1	0.98	0.09	60,60,60,60	0
57	MG	1A	3113	1/1	0.98	0.08	21,21,21,21	0
57	MG	1F	313	1/1	0.98	0.07	31,31,31,31	0
57	MG	1A	3670	1/1	0.98	0.07	38,38,38,38	0
57	MG	1f	201	1/1	0.98	0.28	62,62,62,62	0
57	MG	2A	3643	1/1	0.98	0.07	55,55,55,55	0
57	MG	1A	3219	1/1	0.98	0.11	26,26,26,26	0
57	MG	1A	3791	1/1	0.98	0.06	27,27,27,27	0
57	MG	1A	3220	1/1	0.98	0.09	17,17,17,17	0
57	MG	1A	3568	1/1	0.98	0.11	34,34,34,34	0
57	MG	1A	3569	1/1	0.98	0.03	19,19,19,19	0
57	MG	1A	3570	1/1	0.98	0.05	34,34,34,34	0
57	MG	1A	3470	1/1	0.98	0.05	31,31,31,31	0
57	MG	1A	3297	1/1	0.98	0.13	34,34,34,34	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	2A	3652	1/1	0.98	0.04	36,36,36,36	0
57	MG	2A	3410	1/1	0.98	0.04	38,38,38,38	0
57	MG	2A	3656	1/1	0.98	0.04	38,38,38,38	0
57	MG	1N	201	1/1	0.98	0.05	38,38,38,38	0
57	MG	1N	202	1/1	0.98	0.10	38,38,38,38	0
57	MG	1A	3160	1/1	0.98	0.19	29,29,29,29	0
57	MG	2A	3660	1/1	0.98	0.06	36,36,36,36	0
57	MG	1A	3799	1/1	0.98	0.10	45,45,45,45	0
57	MG	2A	3415	1/1	0.98	0.08	49,49,49,49	0
57	MG	1A	3030	1/1	0.98	0.04	26,26,26,26	0
57	MG	2A	3417	1/1	0.98	0.07	41,41,41,41	0
57	MG	2A	3418	1/1	0.98	0.08	35,35,35,35	0
57	MG	1A	3223	1/1	0.98	0.15	34,34,34,34	0
57	MG	1A	3301	1/1	0.98	0.10	32,32,32,32	0
57	MG	1A	3162	1/1	0.98	0.08	33,33,33,33	0
57	MG	1P	205	1/1	0.98	0.07	27,27,27,27	0
57	MG	1A	3804	1/1	0.98	0.05	39,39,39,39	0
57	MG	2A	3425	1/1	0.98	0.07	35,35,35,35	0
57	MG	1Q	202	1/1	0.98	0.03	29,29,29,29	0
57	MG	1A	3117	1/1	0.98	0.19	27,27,27,27	0
57	MG	2a	3117	1/1	0.98	0.06	68,68,68,68	0
57	MG	2A	3674	1/1	0.98	0.07	61,61,61,61	0
57	MG	1A	3226	1/1	0.98	0.06	37,37,37,37	0
57	MG	1x	101	1/1	0.98	0.04	46,46,46,46	0
57	MG	1A	3686	1/1	0.98	0.04	39,39,39,39	0
57	MG	1A	3580	1/1	0.98	0.08	34,34,34,34	0
57	MG	1R	201	1/1	0.98	0.07	30,30,30,30	0
57	MG	1A	3118	1/1	0.98	0.07	21,21,21,21	0
57	MG	2A	3681	1/1	0.98	0.06	36,36,36,36	0
57	MG	2A	3004	1/1	0.98	0.04	35,35,35,35	0
57	MG	1A	3810	1/1	0.98	0.08	38,38,38,38	0
57	MG	1A	3080	1/1	0.98	0.06	33,33,33,33	0
57	MG	2A	3008	1/1	0.98	0.06	29,29,29,29	0
57	MG	1A	3057	1/1	0.98	0.04	26,26,26,26	0
57	MG	2A	3010	1/1	0.98	0.07	61,61,61,61	0
57	MG	1A	3122	1/1	0.98	0.14	37,37,37,37	0
57	MG	2A	3012	1/1	0.98	0.25	57,57,57,57	0
57	MG	2A	3690	1/1	0.98	0.06	56,56,56,56	0
57	MG	2a	3135	1/1	0.98	0.05	46,46,46,46	0
57	MG	1A	3018	1/1	0.98	0.14	23,23,23,23	0
57	MG	2A	3692	1/1	0.98	0.06	50,50,50,50	0
57	MG	1A	3963	1/1	0.98	0.06	44,44,44,44	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	1A	3964	1/1	0.98	0.06	28,28,28,28	0
57	MG	1T	205	1/1	0.98	0.05	40,40,40,40	0
57	MG	1A	3815	1/1	0.98	0.04	38,38,38,38	0
57	MG	1A	3586	1/1	0.98	0.07	38,38,38,38	0
57	MG	1A	3967	1/1	0.98	0.08	39,39,39,39	0
57	MG	1A	3124	1/1	0.98	0.08	40,40,40,40	0
57	MG	2A	3021	1/1	0.98	0.04	34,34,34,34	0
57	MG	1V	203	1/1	0.98	0.09	34,34,34,34	0
57	MG	1a	3134	1/1	0.98	0.04	43,43,43,43	0
57	MG	2A	3229	1/1	0.98	0.06	50,50,50,50	0
57	MG	2A	3230	1/1	0.98	0.13	45,45,45,45	0
57	MG	1A	3170	1/1	0.98	0.09	41,41,41,41	0
57	MG	1a	3136	1/1	0.98	0.08	34,34,34,34	0
57	MG	1A	3970	1/1	0.98	0.06	22,22,22,22	0
57	MG	1A	3024	1/1	0.98	0.04	15,15,15,15	0
57	MG	1A	3820	1/1	0.98	0.16	28,28,28,28	0
57	MG	2A	3029	1/1	0.98	0.04	39,39,39,39	0
57	MG	1A	3821	1/1	0.98	0.23	26,26,26,26	0
57	MG	1A	3061	1/1	0.98	0.04	30,30,30,30	0
57	MG	1A	3316	1/1	0.98	0.04	21,21,21,21	0
57	MG	2A	3715	1/1	0.98	0.07	40,40,40,40	0
57	MG	1A	3127	1/1	0.98	0.03	24,24,24,24	0
57	MG	1A	3174	1/1	0.98	0.18	30,30,30,30	0
57	MG	1A	3826	1/1	0.98	0.05	24,24,24,24	0
57	MG	1A	3701	1/1	0.98	0.12	34,34,34,34	0
57	MG	2A	3720	1/1	0.98	0.08	46,46,46,46	0
57	MG	1a	3148	1/1	0.98	0.05	56,56,56,56	0
57	MG	10	102	1/1	0.98	0.04	27,27,27,27	0
57	MG	1A	3400	1/1	0.98	0.07	25,25,25,25	0
57	MG	1A	3239	1/1	0.98	0.09	33,33,33,33	0
57	MG	2A	3725	1/1	0.98	0.11	45,45,45,45	0
57	MG	1A	3982	1/1	0.98	0.08	39,39,39,39	0
57	MG	1A	3175	1/1	0.98	0.14	32,32,32,32	0
57	MG	2A	3474	1/1	0.98	0.06	40,40,40,40	0
57	MG	1A	3403	1/1	0.98	0.08	21,21,21,21	0
57	MG	1a	3155	1/1	0.98	0.06	46,46,46,46	0
57	MG	1A	3985	1/1	0.98	0.05	20,20,20,20	0
57	MG	1A	3833	1/1	0.98	0.04	41,41,41,41	0
57	MG	1A	3241	1/1	0.98	0.16	31,31,31,31	0
57	MG	1A	3176	1/1	0.98	0.12	24,24,24,24	0
57	MG	2A	3256	1/1	0.98	0.19	44,44,44,44	0
57	MG	1A	3085	1/1	0.98	0.33	38,38,38,38	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	1A	3013	1/1	0.98	0.05	22,22,22,22	0
57	MG	1A	3246	1/1	0.98	0.20	32,32,32,32	0
57	MG	1A	3180	1/1	0.98	0.15	29,29,29,29	0
57	MG	1A	3006	1/1	0.98	0.07	25,25,25,25	0
57	MG	13	103	1/1	0.98	0.10	34,34,34,34	0
57	MG	1A	3841	1/1	0.98	0.03	22,22,22,22	0
57	MG	1A	3411	1/1	0.98	0.03	33,33,33,33	0
57	MG	15	3103	1/1	0.98	0.14	22,22,22,22	0
57	MG	15	3104	1/1	0.98	0.16	30,30,30,30	0
57	MG	2A	3493	1/1	0.98	0.06	49,49,49,49	0
57	MG	15	3105	1/1	0.98	0.11	33,33,33,33	0
57	MG	15	3106	1/1	0.98	0.04	40,40,40,40	0
57	MG	1A	3131	1/1	0.98	0.15	30,30,30,30	0
57	MG	1A	3717	1/1	0.98	0.08	58,58,58,58	0
57	MG	1A	3044	1/1	0.98	0.09	25,25,25,25	0
57	MG	17	101	1/1	0.98	0.04	32,32,32,32	0
57	MG	17	102	1/1	0.98	0.10	28,28,28,28	0
57	MG	17	103	1/1	0.98	0.14	32,32,32,32	0
57	MG	1A	3252	1/1	0.98	0.41	38,38,38,38	0
57	MG	1A	3509	1/1	0.98	0.04	44,44,44,44	0
57	MG	1A	3185	1/1	0.98	0.12	38,38,38,38	0
57	MG	1A	3612	1/1	0.98	0.21	35,35,35,35	0
57	MG	2A	3071	1/1	0.98	0.11	39,39,39,39	0
57	MG	1A	3725	1/1	0.98	0.07	36,36,36,36	0
57	MG	1A	3089	1/1	0.98	0.09	36,36,36,36	0
57	MG	1A	3001	1/1	0.98	0.04	26,26,26,26	0
57	MG	1A	3514	1/1	0.98	0.04	36,36,36,36	0
60	ZN	14	501	1/1	0.98	0.08	105,105,105,105	0
60	ZN	2Y	202	1/1	0.98	0.04	82,82,82,82	0
57	MG	2E	302	1/1	0.98	0.07	39,39,39,39	0
57	MG	2A	3285	1/1	0.98	0.11	37,37,37,37	0
60	ZN	2n	102	1/1	0.98	0.06	76,76,76,76	0
61	SF4	2d	501	8/8	0.98	0.04	64,74,77,79	0
57	MG	2A	3563	1/1	0.99	0.06	53,53,53,53	0
57	MG	1A	3256	1/1	0.99	0.07	38,38,38,38	0
57	MG	1A	3079	1/1	0.99	0.14	37,37,37,37	0
57	MG	1A	3053	1/1	0.99	0.17	23,23,23,23	0
57	MG	1A	3119	1/1	0.99	0.07	32,32,32,32	0
57	MG	1A	3043	1/1	0.99	0.09	21,21,21,21	0
57	MG	2a	3104	1/1	0.99	0.34	50,50,50,50	0
57	MG	1A	3945	1/1	0.99	0.13	23,23,23,23	0
57	MG	1a	3012	1/1	0.99	0.12	27,27,27,27	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	2A	3362	1/1	0.99	0.07	27,27,27,27	0
57	MG	1P	202	1/1	0.99	0.17	23,23,23,23	0
57	MG	1A	3492	1/1	0.99	0.04	25,25,25,25	0
57	MG	2A	3574	1/1	0.99	0.07	31,31,31,31	0
57	MG	1A	3947	1/1	0.99	0.07	45,45,45,45	0
57	MG	1A	3493	1/1	0.99	0.06	24,24,24,24	0
57	MG	1A	3261	1/1	0.99	0.12	26,26,26,26	0
57	MG	1A	3227	1/1	0.99	0.09	30,30,30,30	0
57	MG	2A	3694	1/1	0.99	0.05	49,49,49,49	0
57	MG	1A	3873	1/1	0.99	0.05	30,30,30,30	0
57	MG	2A	3370	1/1	0.99	0.03	35,35,35,35	0
57	MG	1A	3303	1/1	0.99	0.12	30,30,30,30	0
57	MG	1A	3198	1/1	0.99	0.16	36,36,36,36	0
57	MG	1A	3442	1/1	0.99	0.08	27,27,27,27	0
57	MG	1Q	207	1/1	0.99	0.11	45,45,45,45	0
57	MG	1A	3003	1/1	0.99	0.03	28,28,28,28	0
57	MG	1B	213	1/1	0.99	0.06	34,34,34,34	0
57	MG	2A	3276	1/1	0.99	0.18	29,29,29,29	0
57	MG	1A	3068	1/1	0.99	0.18	29,29,29,29	0
57	MG	1A	3445	1/1	0.99	0.03	22,22,22,22	0
57	MG	1A	3958	1/1	0.99	0.03	37,37,37,37	0
57	MG	2A	3592	1/1	0.99	0.07	57,57,57,57	0
57	MG	1A	3045	1/1	0.99	0.10	8,8,8,8	0
57	MG	2A	3184	1/1	0.99	0.02	41,41,41,41	0
57	MG	1A	3101	1/1	0.99	0.03	45,45,45,45	0
57	MG	1A	3017	1/1	0.99	0.19	27,27,27,27	0
57	MG	1A	3399	1/1	0.99	0.08	15,15,15,15	0
57	MG	1A	3623	1/1	0.99	0.06	30,30,30,30	0
57	MG	1A	3749	1/1	0.99	0.06	26,26,26,26	0
57	MG	1A	3750	1/1	0.99	0.09	29,29,29,29	0
57	MG	2A	3492	1/1	0.99	0.05	35,35,35,35	0
57	MG	1A	3684	1/1	0.99	0.06	34,34,34,34	0
57	MG	1U	204	1/1	0.99	0.17	32,32,32,32	0
57	MG	1a	3127	1/1	0.99	0.04	32,32,32,32	0
57	MG	2A	3496	1/1	0.99	0.06	47,47,47,47	0
57	MG	2A	3005	1/1	0.99	0.05	62,62,62,62	0
57	MG	1V	201	1/1	0.99	0.14	27,27,27,27	0
57	MG	2A	3608	1/1	0.99	0.03	40,40,40,40	0
57	MG	1A	3058	1/1	0.99	0.17	42,42,42,42	0
57	MG	2A	3610	1/1	0.99	0.04	25,25,25,25	0
57	MG	1A	3104	1/1	0.99	0.08	35,35,35,35	0
57	MG	2A	3102	1/1	0.99	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
57	MG	1A	3890	1/1	0.99	0.03	21,21,21,21	0
57	MG	1A	3452	1/1	0.99	0.07	22,22,22,22	0
57	MG	1A	3178	1/1	0.99	0.23	28,28,28,28	0
57	MG	1A	3272	1/1	0.99	0.17	31,31,31,31	0
57	MG	2A	3506	1/1	0.99	0.04	44,44,44,44	0
57	MG	2A	3107	1/1	0.99	0.04	30,30,30,30	0
57	MG	1A	3894	1/1	0.99	0.03	36,36,36,36	0
57	MG	1A	3511	1/1	0.99	0.07	18,18,18,18	0
57	MG	1A	3047	1/1	0.99	0.04	24,24,24,24	0
57	MG	1A	3897	1/1	0.99	0.03	48,48,48,48	0
57	MG	1A	3315	1/1	0.99	0.09	29,29,29,29	0
57	MG	1a	3050	1/1	0.99	0.07	46,46,46,46	0
57	MG	1A	3899	1/1	0.99	0.07	49,49,49,49	0
57	MG	1A	3073	1/1	0.99	0.04	33,33,33,33	0
57	MG	1A	3360	1/1	0.99	0.03	19,19,19,19	0
57	MG	1A	3181	1/1	0.99	0.11	26,26,26,26	0
57	MG	1A	3763	1/1	0.99	0.04	31,31,31,31	0
57	MG	1a	3146	1/1	0.99	0.05	52,52,52,52	0
57	MG	1A	3904	1/1	0.99	0.03	49,49,49,49	0
57	MG	1A	3831	1/1	0.99	0.05	46,46,46,46	0
57	MG	1A	3107	1/1	0.99	0.08	35,35,35,35	0
57	MG	1A	3007	1/1	0.99	0.06	33,33,33,33	0
57	MG	1A	3242	1/1	0.99	0.17	21,21,21,21	0
57	MG	2A	3318	1/1	0.99	0.08	17,17,17,17	0
57	MG	2A	3637	1/1	0.99	0.08	33,33,33,33	0
57	MG	2A	3638	1/1	0.99	0.07	30,30,30,30	0
57	MG	2A	3319	1/1	0.99	0.05	57,57,57,57	0
57	MG	1A	3212	1/1	0.99	0.05	39,39,39,39	0
57	MG	2A	3423	1/1	0.99	0.05	37,37,37,37	0
57	MG	1A	3413	1/1	0.99	0.02	26,26,26,26	0
57	MG	1A	3109	1/1	0.99	0.18	27,27,27,27	0
57	MG	1A	3281	1/1	0.99	0.06	32,32,32,32	0
57	MG	1A	3467	1/1	0.99	0.04	32,32,32,32	0
57	MG	1A	3019	1/1	0.99	0.15	23,23,23,23	0
57	MG	1A	3469	1/1	0.99	0.05	40,40,40,40	0
57	MG	1A	3026	1/1	0.99	0.11	29,29,29,29	0
57	MG	1A	3708	1/1	0.99	0.05	21,21,21,21	0
57	MG	1A	3284	1/1	0.99	0.04	23,23,23,23	0
57	MG	1A	3285	1/1	0.99	0.09	31,31,31,31	0
57	MG	1A	3247	1/1	0.99	0.14	28,28,28,28	0
57	MG	2A	3653	1/1	0.99	0.04	34,34,34,34	0
57	MG	1A	3005	1/1	0.99	0.09	22,22,22,22	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	2A	3655	1/1	0.99	0.04	69,69,69,69	0
57	MG	1A	3136	1/1	0.99	0.12	24,24,24,24	0
57	MG	1A	3923	1/1	0.99	0.03	46,46,46,46	0
57	MG	1a	3259	1/1	0.99	0.06	33,33,33,33	0
57	MG	1F	304	1/1	0.99	0.10	28,28,28,28	0
57	MG	1A	3476	1/1	0.99	0.08	42,42,42,42	0
57	MG	1F	306	1/1	0.99	0.06	35,35,35,35	0
57	MG	1a	3079	1/1	0.99	0.16	43,43,43,43	0
57	MG	1A	3093	1/1	0.99	0.03	31,31,31,31	0
57	MG	1A	3376	1/1	0.99	0.04	30,30,30,30	0
57	MG	1A	3015	1/1	0.99	0.04	26,26,26,26	0
57	MG	1A	3115	1/1	0.99	0.04	28,28,28,28	0
57	MG	1A	3596	1/1	0.99	0.06	41,41,41,41	0
57	MG	1A	3116	1/1	0.99	0.14	31,31,31,31	0
57	MG	1A	3721	1/1	0.99	0.05	22,22,22,22	0
57	MG	1A	3254	1/1	0.99	0.11	34,34,34,34	0
57	MG	1A	3336	1/1	0.99	0.04	30,30,30,30	0
60	ZN	1Y	202	1/1	0.99	0.03	53,53,53,53	0
57	MG	1A	3724	1/1	0.99	0.03	35,35,35,35	0
60	ZN	15	3110	1/1	0.99	0.02	43,43,43,43	0
60	ZN	16	501	1/1	0.99	0.05	40,40,40,40	0
60	ZN	19	103	1/1	0.99	0.04	41,41,41,41	0
60	ZN	1n	104	1/1	0.99	0.03	65,65,65,65	0
57	MG	1A	3294	1/1	0.99	0.04	20,20,20,20	0
57	MG	1A	3383	1/1	0.99	0.09	42,42,42,42	0
60	ZN	25	104	1/1	0.99	0.02	49,49,49,49	0
57	MG	1A	3937	1/1	0.99	0.06	35,35,35,35	0
57	MG	1A	3543	1/1	0.99	0.03	30,30,30,30	0
61	SF4	1d	307	8/8	0.99	0.04	54,58,64,66	0
57	MG	1A	3141	1/1	0.99	0.08	21,21,21,21	0
57	MG	1A	3704	1/1	1.00	0.03	31,31,31,31	0
57	MG	1a	3196	1/1	1.00	0.06	52,52,52,52	0
60	ZN	26	501	1/1	1.00	0.04	59,59,59,59	0
57	MG	1F	309	1/1	1.00	0.04	33,33,33,33	0
57	MG	2A	3590	1/1	1.00	0.03	32,32,32,32	0
57	MG	2A	3390	1/1	1.00	0.04	44,44,44,44	0
57	MG	1a	3270	1/1	1.00	0.03	56,56,56,56	0

6.5 Other polymers ⓘ

There are no such residues in this entry.