



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 20, 2026 – 04:56 PM UTC

PDB ID : 4Y4O / pdb_00004y4o
Title : Crystal structure of the Thermus thermophilus 70S ribosome with rRNA modifications and bound to protein Y (YfiA) at 2.3Å resolution
Authors : Polikanov, Y.S.; Melnikov, S.V.; Soll, D.; Steitz, T.A.
Deposited on : 2015-02-10
Resolution : 2.30 Å(reported)

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

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A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

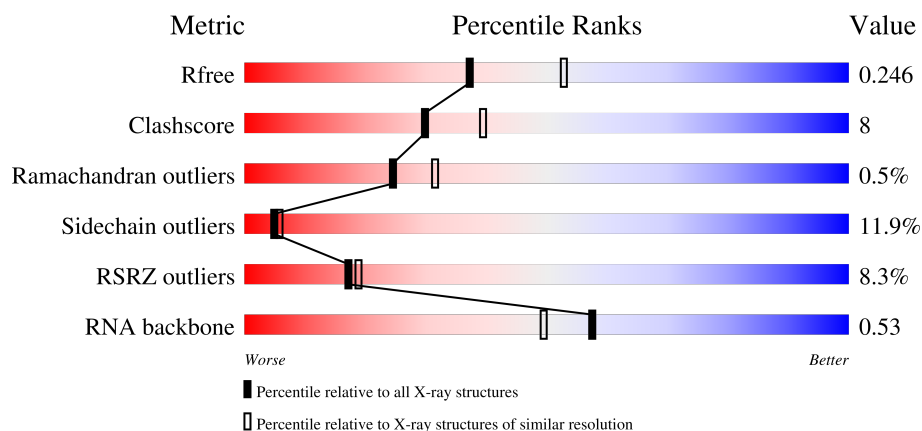
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 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	6319 (2.30-2.30)
Clashscore	190562	6919 (2.30-2.30)
Ramachandran outliers	187476	6854 (2.30-2.30)
Sidechain outliers	187428	6854 (2.30-2.30)
RSRZ outliers	180081	6325 (2.30-2.30)
RNA backbone	3983	1090 (2.60-2.00)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments 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% 69% 24% 6%
1	2A	2915	3% 60% 31% 8%
2	1B	121	% 72% 22% 5%
2	2B	121	% 60% 33% 7%

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

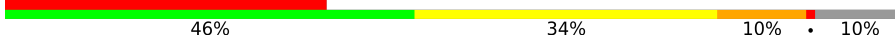
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Mol	Chain	Length	Quality of chain
15	2T	146	
16	1U	118	
16	2U	118	
17	1V	101	
17	2V	101	
18	1W	113	
18	2W	113	
19	1X	96	
19	2X	96	
20	1Y	110	
20	2Y	110	
21	1Z	206	
21	2Z	206	
22	10	85	
22	20	85	
23	11	98	
23	21	98	
24	12	72	
24	22	72	
25	13	60	
25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

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

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

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Mol	Chain	Length	Quality of chain
53	1y	113	
53	2y	113	

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
54	MG	1A	3612	-	-	-	X
55	MPD	1a	1880	-	-	X	-

2 Entry composition

There are 59 unique types of molecules in this entry. The entry contains 298502 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	77	Total	C	N	O	S	0	0	0
			608	375	129	103	1			
22	20	77	Total	C	N	O	S	0	0	0
			608	375	129	103	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 MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
54	1A	1075	Total	Mg	0	0
			1075	1075		
54	1B	30	Total	Mg	0	0
			30	30		
54	1D	14	Total	Mg	0	0
			14	14		
54	1E	6	Total	Mg	0	0
			6	6		
54	1F	10	Total	Mg	0	0
			10	10		
54	1G	4	Total	Mg	0	0
			4	4		
54	1H	2	Total	Mg	0	0
			2	2		
54	1N	3	Total	Mg	0	0
			3	3		
54	1O	1	Total	Mg	0	0
			1	1		
54	1P	2	Total	Mg	0	0
			2	2		
54	1Q	4	Total	Mg	0	0
			4	4		
54	1R	3	Total	Mg	0	0
			3	3		
54	1T	3	Total	Mg	0	0
			3	3		
54	1U	2	Total	Mg	0	0
			2	2		
54	1V	3	Total	Mg	0	0
			3	3		
54	1W	2	Total	Mg	0	0
			2	2		
54	1X	1	Total	Mg	0	0
			1	1		
54	1Z	1	Total	Mg	0	0
			1	1		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
54	10	5	Total 5	Mg 5	0	0
54	11	4	Total 4	Mg 4	0	0
54	13	2	Total 2	Mg 2	0	0
54	14	1	Total 1	Mg 1	0	0
54	15	2	Total 2	Mg 2	0	0
54	17	2	Total 2	Mg 2	0	0
54	18	1	Total 1	Mg 1	0	0
54	19	2	Total 2	Mg 2	0	0
54	1a	280	Total 280	Mg 280	0	0
54	1b	1	Total 1	Mg 1	0	0
54	1d	5	Total 5	Mg 5	0	0
54	1e	4	Total 4	Mg 4	0	0
54	1f	1	Total 1	Mg 1	0	0
54	1g	3	Total 3	Mg 3	0	0
54	1h	2	Total 2	Mg 2	0	0
54	1i	1	Total 1	Mg 1	0	0
54	1l	2	Total 2	Mg 2	0	0
54	1n	2	Total 2	Mg 2	0	0
54	1o	1	Total 1	Mg 1	0	0
54	1q	2	Total 2	Mg 2	0	0
54	1r	1	Total 1	Mg 1	0	0

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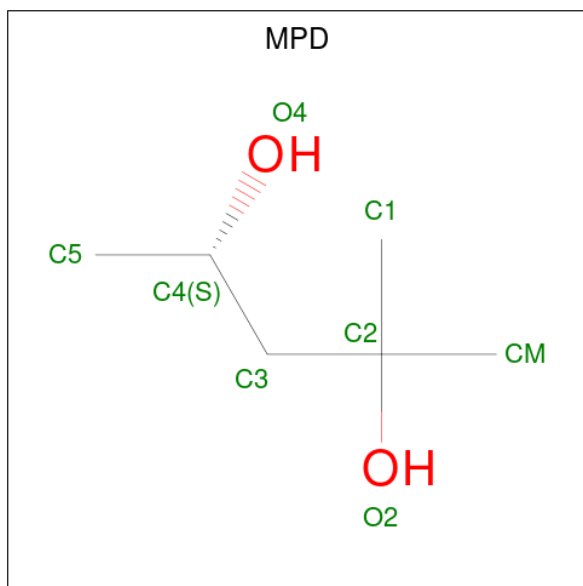
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
54	1t	1	Total 1	Mg 1	0	0
54	1y	4	Total 4	Mg 4	0	0
54	2A	761	Total 761	Mg 761	0	0
54	2B	19	Total 19	Mg 19	0	0
54	2D	9	Total 9	Mg 9	0	0
54	2E	5	Total 5	Mg 5	0	0
54	2F	3	Total 3	Mg 3	0	0
54	2G	3	Total 3	Mg 3	0	0
54	2I	1	Total 1	Mg 1	0	0
54	2N	1	Total 1	Mg 1	0	0
54	2O	2	Total 2	Mg 2	0	0
54	2P	2	Total 2	Mg 2	0	0
54	2Q	2	Total 2	Mg 2	0	0
54	2R	1	Total 1	Mg 1	0	0
54	2T	3	Total 3	Mg 3	0	0
54	2V	1	Total 1	Mg 1	0	0
54	2W	2	Total 2	Mg 2	0	0
54	2X	1	Total 1	Mg 1	0	0
54	20	2	Total 2	Mg 2	0	0
54	21	1	Total 1	Mg 1	0	0
54	26	1	Total 1	Mg 1	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
54	27	1	Total Mg 1 1	0	0
54	28	2	Total Mg 2 2	0	0
54	2a	193	Total Mg 193 193	0	0
54	2e	1	Total Mg 1 1	0	0
54	2f	1	Total Mg 1 1	0	0
54	2j	1	Total Mg 1 1	0	0
54	2l	1	Total Mg 1 1	0	0
54	2r	1	Total Mg 1 1	0	0
54	2t	1	Total Mg 1 1	0	0

- Molecule 55 is (4S)-2-METHYL-2,4-PENTANEDIOL (CCD ID: MPD) (formula: C₆H₁₄O₂).



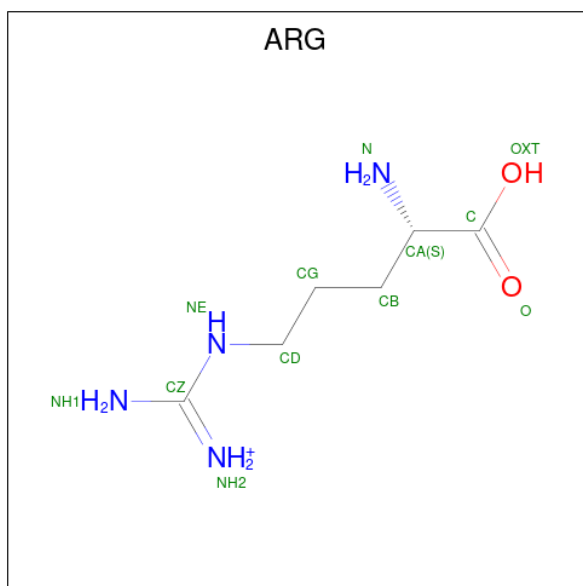
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
55	1A	1	Total C O 8 6 2	0	0
55	1T	1	Total C O 8 6 2	0	0

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
55	18	1	Total	C	O	0	0
			8	6	2		
55	1a	1	Total	C	O	0	0
			8	6	2		
55	2A	1	Total	C	O	0	0
			8	6	2		
55	2A	1	Total	C	O	0	0
			8	6	2		
55	2B	1	Total	C	O	0	0
			8	6	2		

- Molecule 56 is ARGinine (CCD ID: ARG) (formula: $C_6H_{15}N_4O_2$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
56	1B	1	Total	C	N	O	0	0
			12	6	4	2		
56	1F	1	Total	C	N	O	0	0
			12	6	4	2		

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

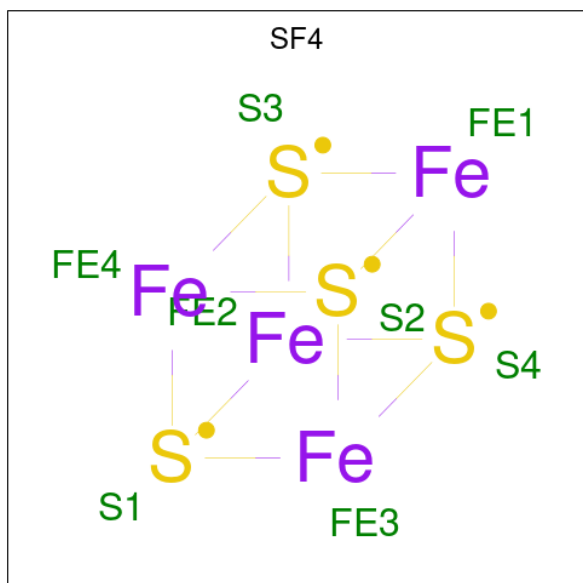
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
57	1Y	1	Total	Zn	0	0
			1	1		
57	14	1	Total	Zn	0	0
			1	1		

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

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



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

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

- Molecule 59 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
59	1A	4154	Total	O	0	0
			4154	4154		
59	1B	109	Total	O	0	0
			109	109		
59	1D	119	Total	O	0	0
			119	119		
59	1E	81	Total	O	0	0
			81	81		
59	1F	66	Total	O	0	0
			66	66		
59	1G	20	Total	O	0	0
			20	20		
59	1H	16	Total	O	0	0
			16	16		
59	1I	9	Total	O	0	0
			9	9		
59	1N	55	Total	O	0	0
			55	55		
59	1O	29	Total	O	0	0
			29	29		
59	1P	56	Total	O	0	0
			56	56		
59	1Q	46	Total	O	0	0
			46	46		
59	1R	37	Total	O	0	0
			37	37		
59	1S	11	Total	O	0	0
			11	11		
59	1T	39	Total	O	0	0
			39	39		
59	1U	49	Total	O	0	0
			49	49		
59	1V	34	Total	O	0	0
			34	34		
59	1W	27	Total	O	0	0
			27	27		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
59	1X	27	Total 27	O 27	0	0
59	1Y	20	Total 20	O 20	0	0
59	1Z	13	Total 13	O 13	0	0
59	10	25	Total 25	O 25	0	0
59	11	25	Total 25	O 25	0	0
59	12	15	Total 15	O 15	0	0
59	13	25	Total 25	O 25	0	0
59	14	4	Total 4	O 4	0	0
59	15	25	Total 25	O 25	0	0
59	16	22	Total 22	O 22	0	0
59	17	19	Total 19	O 19	0	0
59	18	31	Total 31	O 31	0	0
59	19	9	Total 9	O 9	0	0
59	1a	599	Total 599	O 599	0	0
59	1b	1	Total 1	O 1	0	0
59	1c	1	Total 1	O 1	0	0
59	1d	8	Total 8	O 8	0	0
59	1e	5	Total 5	O 5	0	0
59	1f	3	Total 3	O 3	0	0
59	1h	1	Total 1	O 1	0	0
59	1i	1	Total 1	O 1	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
59	1j	1	Total 1	O 1	0	0
59	1k	1	Total 1	O 1	0	0
59	1l	5	Total 5	O 5	0	0
59	1m	2	Total 2	O 2	0	0
59	1o	7	Total 7	O 7	0	0
59	1p	3	Total 3	O 3	0	0
59	1t	1	Total 1	O 1	0	0
59	1y	7	Total 7	O 7	0	0
59	2A	2665	Total 2665	O 2665	0	0
59	2B	69	Total 69	O 69	0	0
59	2D	59	Total 59	O 59	0	0
59	2E	33	Total 33	O 33	0	0
59	2F	26	Total 26	O 26	0	0
59	2G	9	Total 9	O 9	0	0
59	2H	4	Total 4	O 4	0	0
59	2I	4	Total 4	O 4	0	0
59	2N	6	Total 6	O 6	0	0
59	2O	23	Total 23	O 23	0	0
59	2P	30	Total 30	O 30	0	0
59	2Q	28	Total 28	O 28	0	0
59	2R	21	Total 21	O 21	0	0

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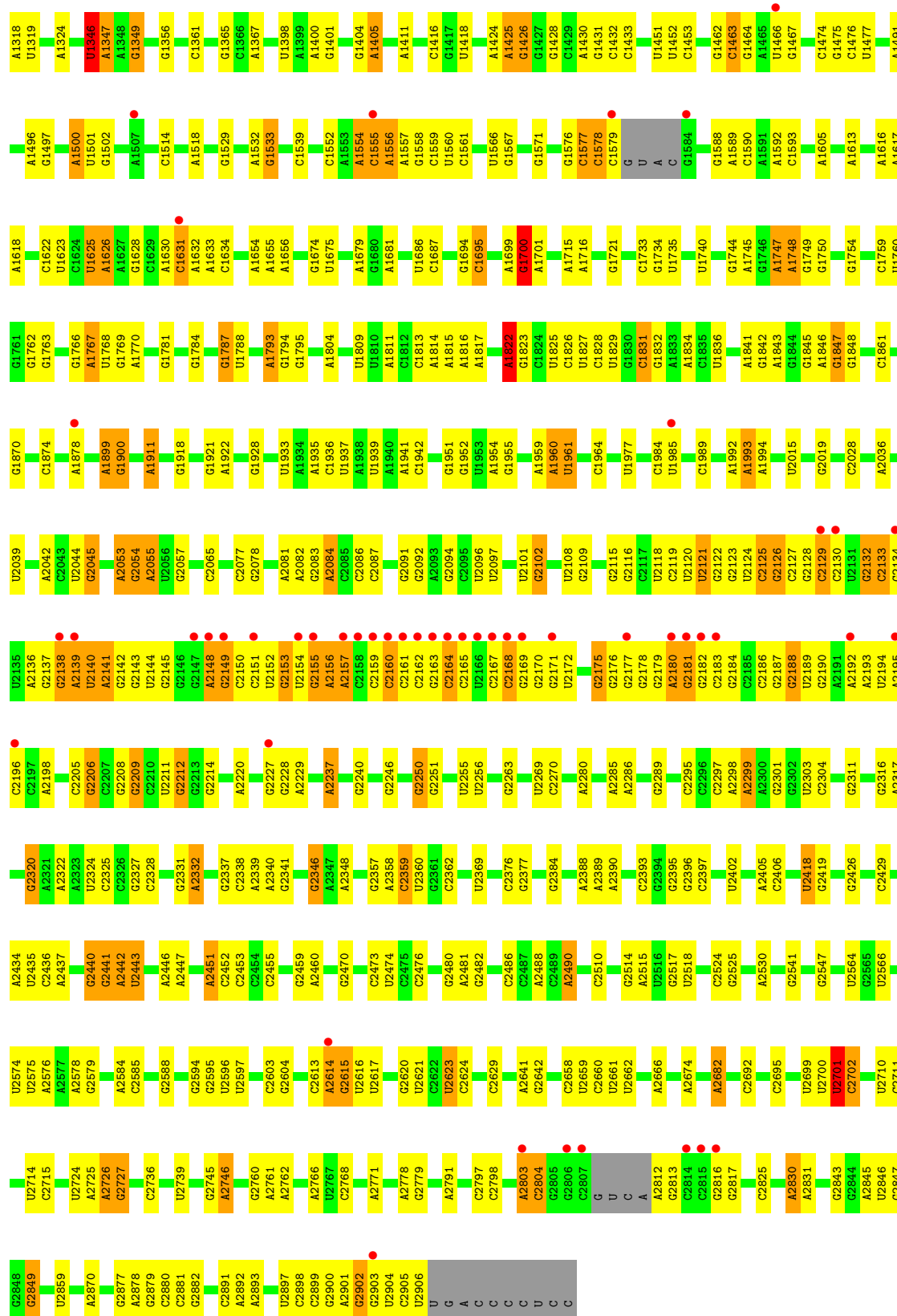
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
59	2S	7	Total 7	O 7	0	0
59	2T	11	Total 11	O 11	0	0
59	2U	20	Total 20	O 20	0	0
59	2V	6	Total 6	O 6	0	0
59	2W	20	Total 20	O 20	0	0
59	2X	10	Total 10	O 10	0	0
59	2Y	4	Total 4	O 4	0	0
59	2Z	16	Total 16	O 16	0	0
59	20	13	Total 13	O 13	0	0
59	21	22	Total 22	O 22	0	0
59	22	4	Total 4	O 4	0	0
59	23	3	Total 3	O 3	0	0
59	24	2	Total 2	O 2	0	0
59	25	10	Total 10	O 10	0	0
59	26	5	Total 5	O 5	0	0
59	27	9	Total 9	O 9	0	0
59	28	16	Total 16	O 16	0	0
59	29	3	Total 3	O 3	0	0
59	2a	459	Total 459	O 459	0	0
59	2d	6	Total 6	O 6	0	0
59	2e	2	Total 2	O 2	0	0

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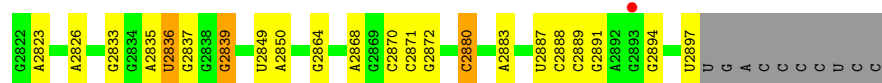
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
59	2f	1	Total	O	0	0
			1	1		
59	2j	2	Total	O	0	0
			2	2		
59	2l	5	Total	O	0	0
			5	5		
59	2m	2	Total	O	0	0
			2	2		
59	2o	2	Total	O	0	0
			2	2		
59	2p	3	Total	O	0	0
			3	3		
59	2q	1	Total	O	0	0
			1	1		
59	2r	5	Total	O	0	0
			5	5		
59	2t	2	Total	O	0	0
			2	2		
59	2y	5	Total	O	0	0
			5	5		

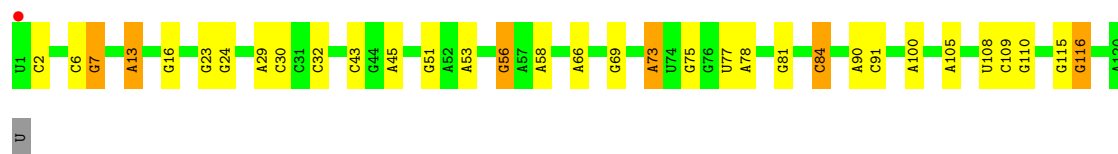
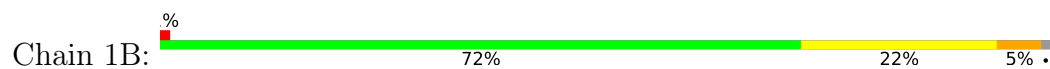




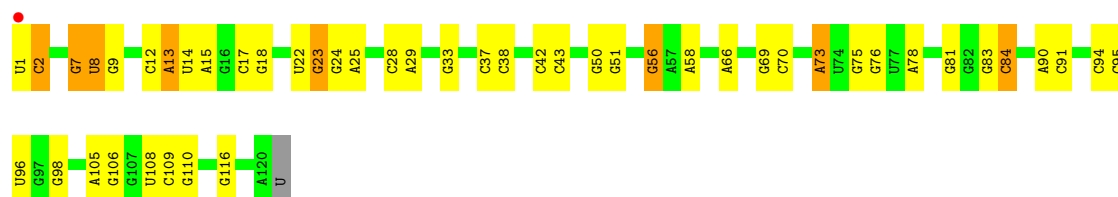
A2734	A2629	G2526	G2391	A2311	U2218	G2139	G1929	U1796	G1666	A1528A	G1529	A1427	G1309
G2735	G2630	C2527	C2394	U2312	A2225	A2069	G1930	C1797	G1667	G1529	G1310	C1428	G1309
C2742	G2640	U2528	G2406	C2314	A2225	A2069	U1931	U1798	A1668	C1530	C1314	C1430	C1314
G2744	G2641	G2529	U2407	C2315	G2234	A2062	G1932	C1800	A1669	C1531	C1315	C1430	C1315
C2745	G2645	A2533	G2410	C2316	G2238	G2069	G1933	A1801	G1674	G1533	A1321	G1442	G1442
G2746	G2646	A2534	G2411	C2317	G2239	U2074	A1937	A1802	C1683	U	A1445	A1445	A1445
U2747	G2647	G2535	G2412	C2318	G2240	U2075	A1938	A1803	C1684	A	G1324	A1449	G1324
C2748	G2648	U2537	G2413	A2320	U2243	U2076	U1939	U1805	U1688	G1536	G1450	A1449	G1450
A2749	U2649	C2538	U2414	G2321	U2244	G2077	U1940	G1814	G1688	G1539	G1328	A1449	G1328
G2750	G2650	G2539	C2417	A2322	U2245	U2078	U1941	G1815	U1689	G1540	G1451	A1450	G1451
G2751	A2654	C2540	A2422	G2323	A2247	G2080	U1942	A1816	U1690	A1542	A1342	A1451	A1342
C2752	A2657	A2542	A2423	G2324	C2248	G2081	U1943	G1817	C1694	C1543	A1452	A1452	A1452
U2753	C2658	G2543	A2424	C2325	G2249	U2082	U1944	U1818	G1695	U1453	C1345	U1453	C1345
G2754	G2659	A2426	A2425	G2326	G2251	G2083	C1962	G1819	A1698	C1547	U1352	G1455	U1352
C2755	U2660	G2544	G2427	A2328	G2252	U2084	U1963	G1820	A1699	C1550	G1356	G1459	G1356
U2756	A2661	G2545	G2428	G2329	G2253	C2087	C1967	G1821	C1551	C1551	G1357	C1467	G1357
A2757	G2662	G2546	G2429	A2330	U2254	U2088	U1968	G1822	A1700	G1552	G1358	C1467	G1358
G2758	U2663	C2547	G2430	A2331	C2255	U2089	A1970	G1823	A1701	G1553	A1359	A1470	A1359
A2759	G2664	U2548	U2431	G2332	G2256	U2090	A1971	G1824	G1702	C1557	A1360	A1471	A1360
G2760	A2665	U2549	A2432	G2333	A2257	G2091	A1972	G1825	U1720	C1558	G1361	A1472	G1361
A2761	G2666	G2550	A2433	G2334	A2258	C2092	U1973	G1826	G1721	A1559	G1362	G1473	G1362
G2762	U2667	U2551	G2434	A2335	U2259	U2092	C1974	G1827	A1722	A1560	G1363	G1474	G1363
A2763	C2668	G2552	A2435	A2336	G2260	U2093	A1974	G1828	U1723	C1561	A1364	A1475	G1364
G2764	U2669	U2553	G2436	A2337	C2261	G2094	A1975	G1829	G1724	G1562	A1365	G1476	A1365
A2765	C2670	A2554	A2437	G2338	A2262	U2095	U1976	G1830	U1725	C1563	G1366	G1477	G1366
G2766	U2671	G2555	G2438	A2339	A2263	C2096	C1975	G1831	A1726	A1564	A1367	G1478	A1367
C2767	G2672	U2556	G2439	A2340	U2264	U2096	U1977	G1832	U1727	C1565	G1368	G1479	G1368
G2768	A2673	G2557	A2440	A2341	G2265	C2097	U1978	G1833	U1728	A1566	G1369	G1480	G1369
A2769	U2674	U2558	C2441	G2342	A2266	U2098	U1979	G1834	G1729	A1567	A1370	G1481	A1370
G2770	C2675	A2559	G2442	A2343	U2267	U2099	U1980	G1835	A1730	C1568	G1371	G1482	G1371
U2771	U2676	G2560	A2443	G2344	A2268	G2100	G1981	G1836	U1731	A1569	G1372	G1483	G1372
A2772	G2677	C2561	A2444	A2345	U2269	G2101	U1982	G1837	G1732	C1570	U1373	G1484	U1373
G2773	U2678	U2562	A2445	G2346	A2270	G2102	U1983	G1838	G1733	A1571	G1374	G1485	G1374
U2774	U2679	U2563	A2446	A2347	A2271	C2103	C1984	G1839	G1734	A1572	G1375	G1486	G1375
A2775	C2680	G2564	G2447	G2348	U2272	G2104	U1985	G1840	A1735	A1573	A1376	G1487	A1376
G2776	U2681	A2565	A2448	A2349	A2273	G2105	G1986	G1841	U1736	A1574	G1377	G1488	G1377
C2777	G2682	U2566	C2449	G2350	U2274	C2106	U1987	G1842	G1737	A1575	A1378	G1489	A1378
A2778	U2683	A2567	G2450	G2351	G2275	G2107	G1988	G1843	G1738	A1576	A1379	G1490	A1379
U2779	U2684	C2568	A2451	A2352	U2276	G2108	U1989	G1844	G1739	C1577	G1380	G1491	G1380
G2780	C2685	U2569	A2452	G2353	A2277	G2109	U1990	G1845	G1740	A1578	G1381	G1492	G1381
A2781	U2686	G2570	A2453	A2354	U2278	G2110	G1991	G1846	A1741	A1579	G1382	G1493	G1382
G2782	C2687	U2571	G2454	G2355	G2279	G2111	U1992	G1847	G1742	A1580	G1383	G1494	A1580
U2783	U2688	A2572	A2455	A2356	U2280	G2112	G1993	G1848	G1743	A1581	G1384	G1495	A1581
A2784	C2689	G2573	G2456	A2357	A2281	G2113	U1994	G1849	G1744	A1582	A1385	G1496	A1582
G2785	U2690	U2574	A2457	U2358	A2282	G2114	G1995	G1850	G1745	C1583	G1386	G1497	A1583
C2786	A2693	G2575	G2458	G2359	G2283	G2115	G2000	G1851	A1761	A1584	G1387	U1498	A1584
G2787	C2694	U2576	A2459	A2360	A2284	G2116	A2001	G1852	A1762	C1585	G1388	G1499	A1585
A2788	U2695	A2577	G2460	A2361	A2285	G2117	G2002	G1853	G1763	G1586	G1389	G1500	G1500
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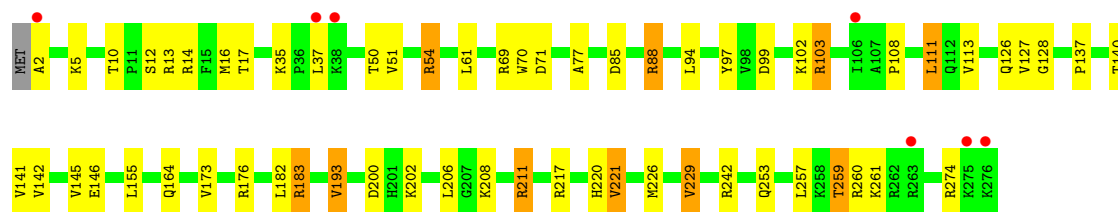
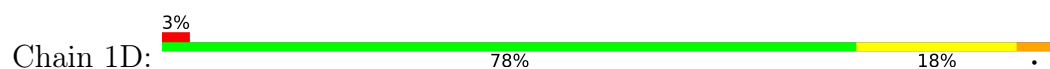
• Molecule 2: 5S Ribosomal RNA



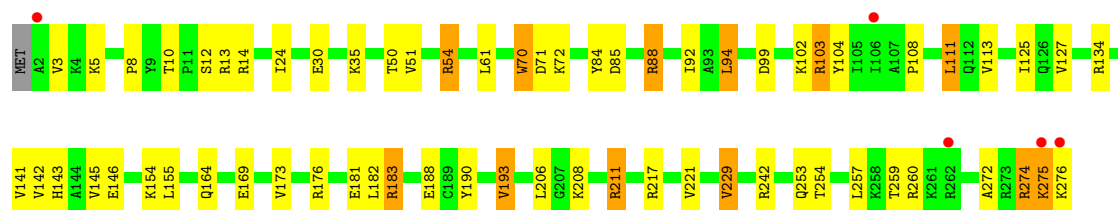
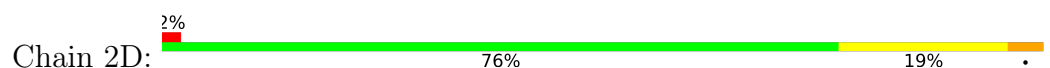
• Molecule 2: 5S Ribosomal RNA



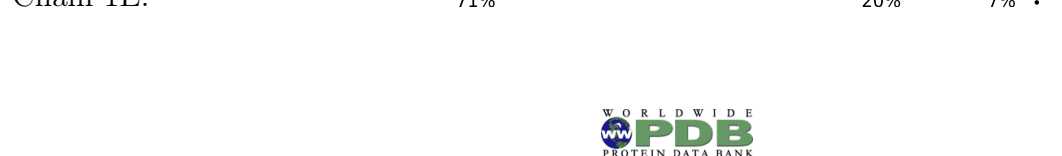
• Molecule 3: 50S ribosomal protein L2



• Molecule 3: 50S ribosomal protein L2

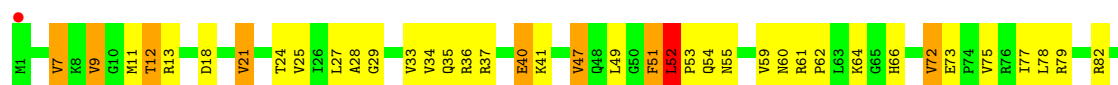


• Molecule 4: 50S ribosomal protein L3

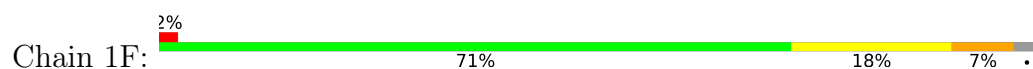




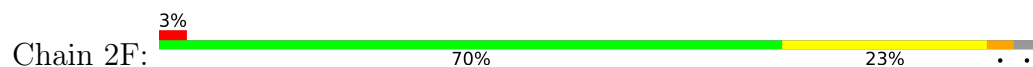
• Molecule 4: 50S ribosomal protein L3



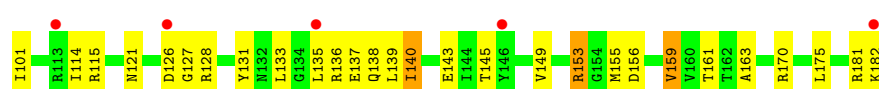
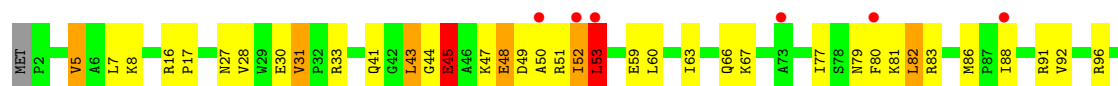
• Molecule 5: 50S ribosomal protein L4



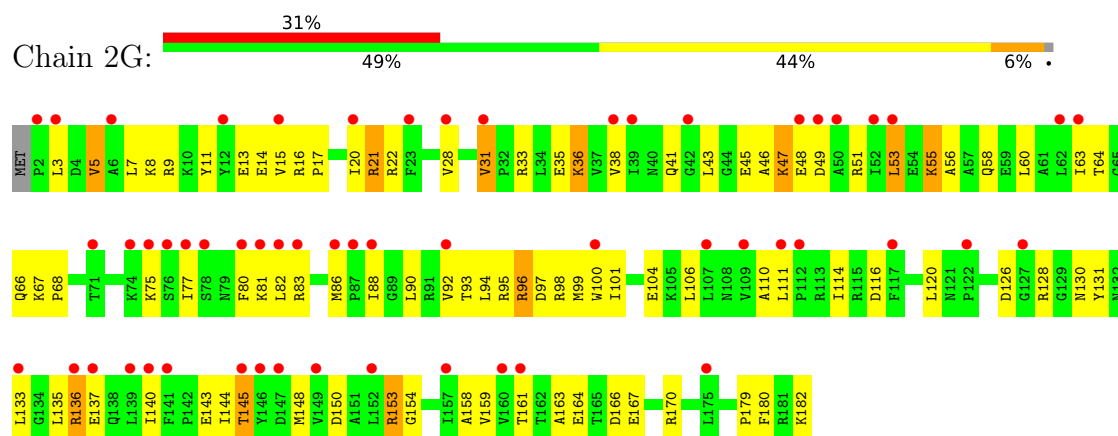
• Molecule 5: 50S ribosomal protein L4



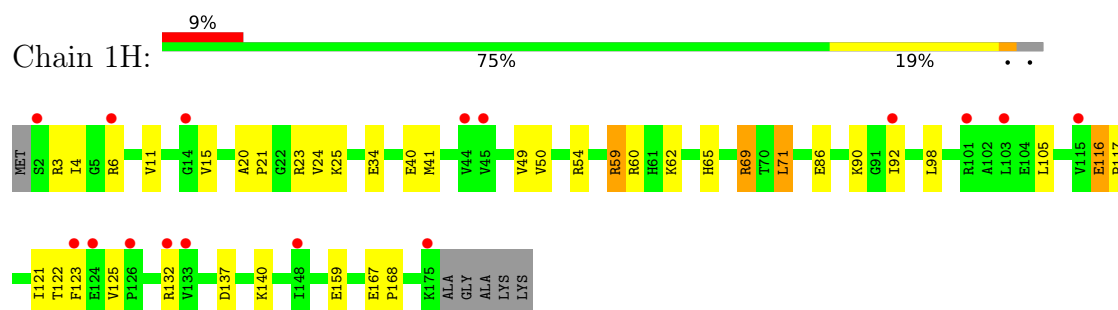
• Molecule 6: 50S ribosomal protein L5



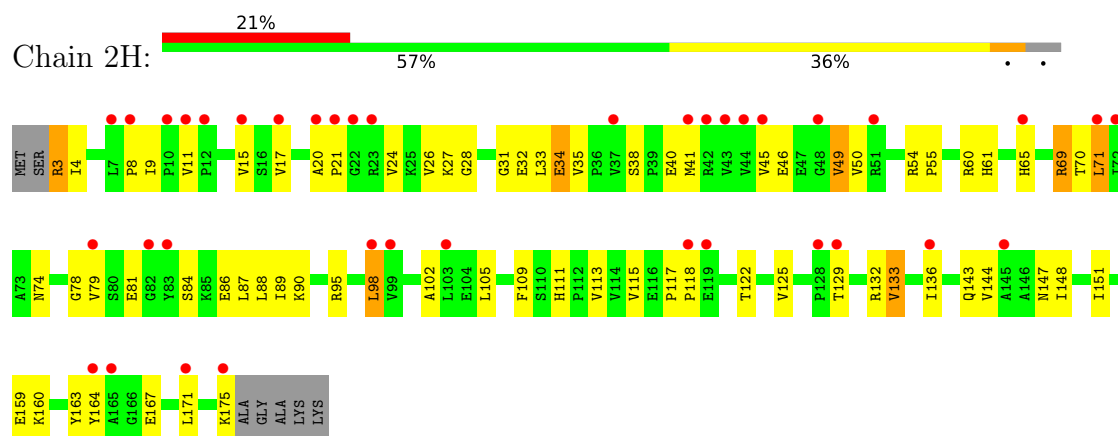
- Molecule 6: 50S ribosomal protein L5



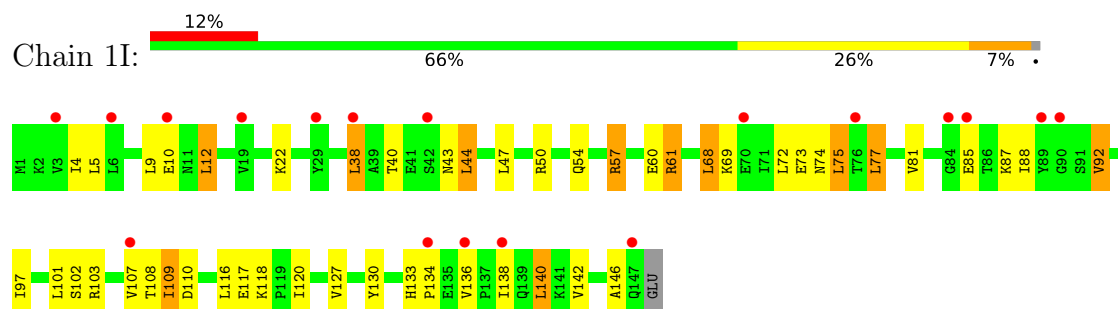
- Molecule 7: 50S ribosomal protein L6



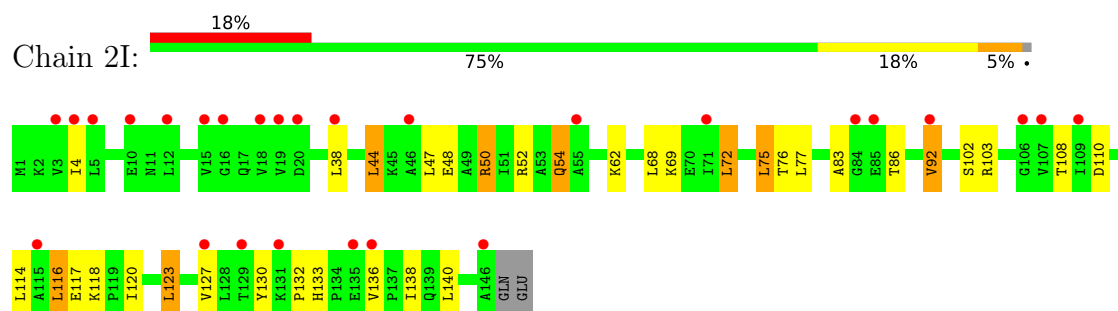
- Molecule 7: 50S ribosomal protein L6



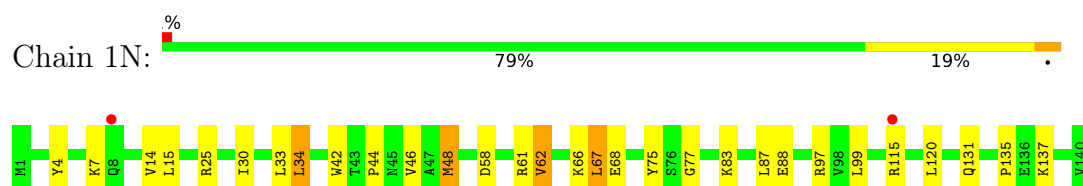
- Molecule 8: 50S ribosomal protein L9



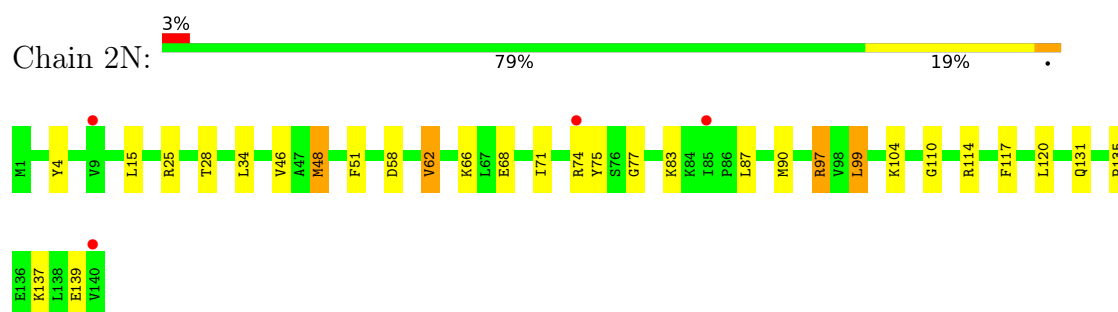
- Molecule 8: 50S ribosomal protein L9



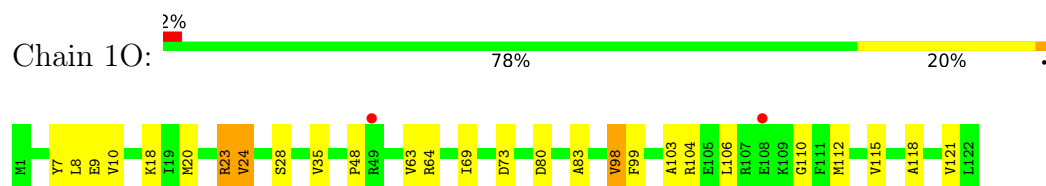
- Molecule 9: 50S ribosomal protein L13



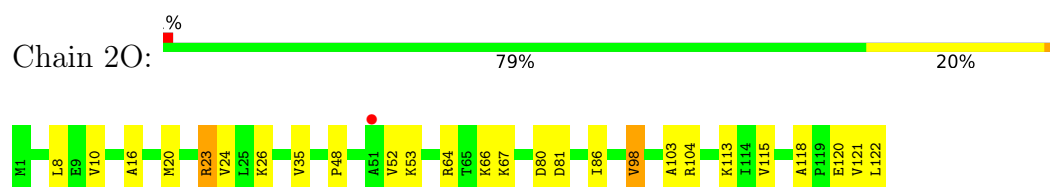
- Molecule 9: 50S ribosomal protein L13



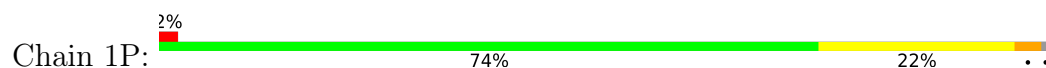
- Molecule 10: 50S ribosomal protein L14

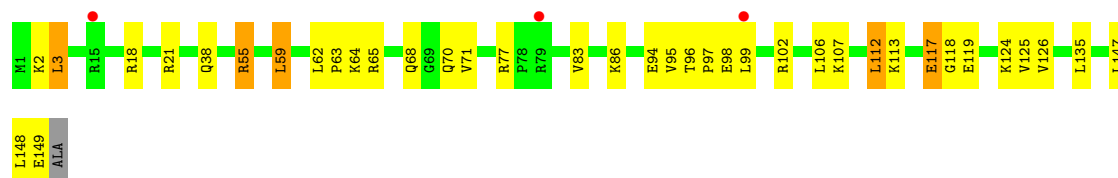


- Molecule 10: 50S ribosomal protein L14

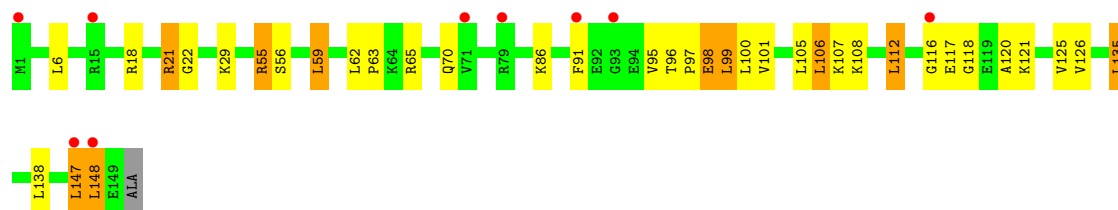
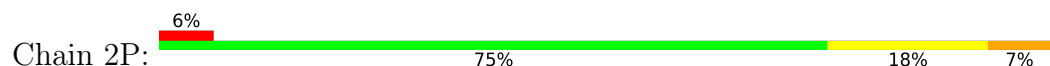


- Molecule 11: 50S ribosomal protein L15

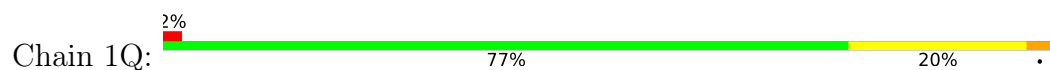




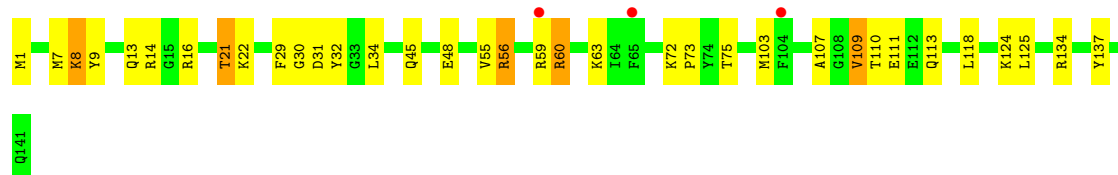
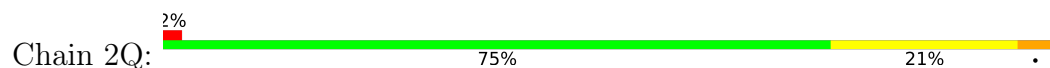
- Molecule 11: 50S ribosomal protein L15



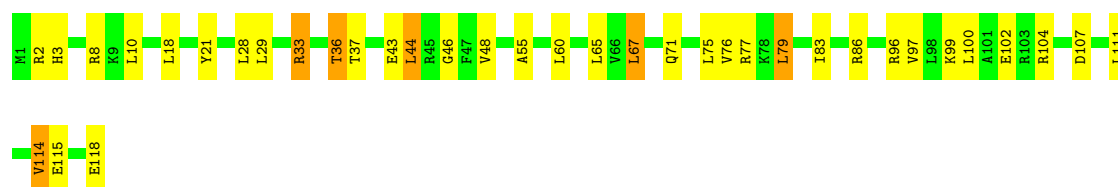
- Molecule 12: 50S ribosomal protein L16



- Molecule 12: 50S ribosomal protein L16



- Molecule 13: 50S ribosomal protein L17

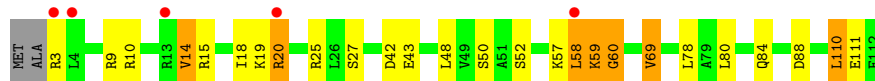
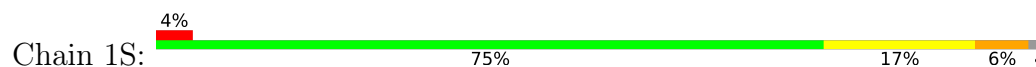


- Molecule 13: 50S ribosomal protein L17

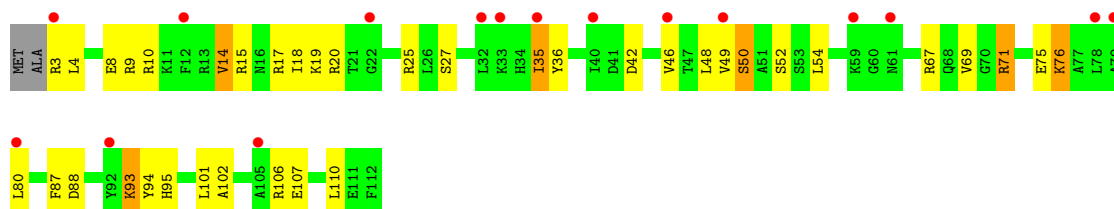




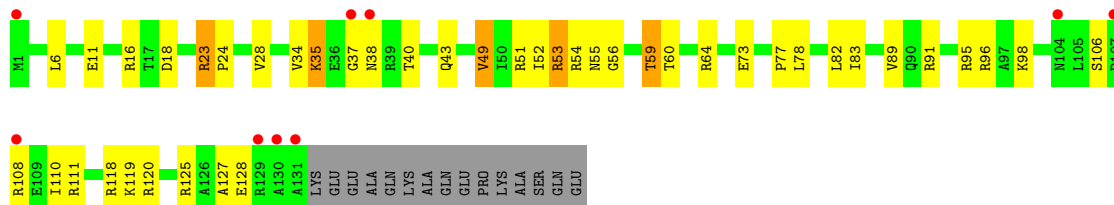
- Molecule 14: 50S ribosomal protein L18



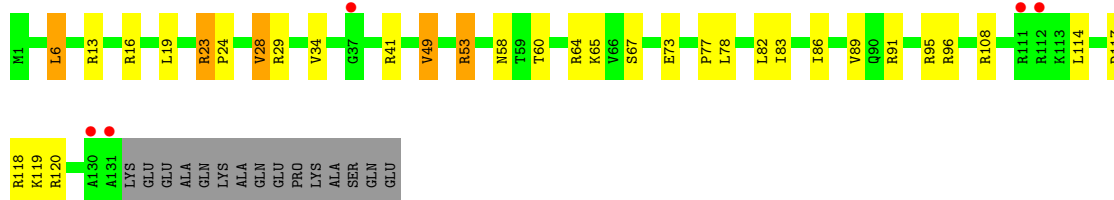
- Molecule 14: 50S ribosomal protein L18



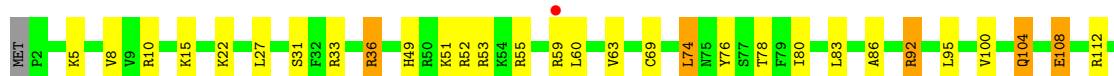
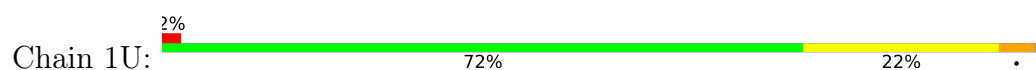
- Molecule 15: 50S ribosomal protein L19



- Molecule 15: 50S ribosomal protein L19

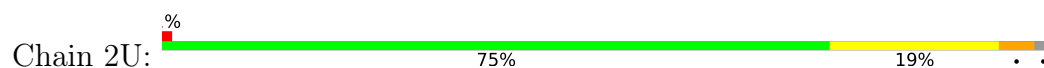


- Molecule 16: 50S ribosomal protein L20

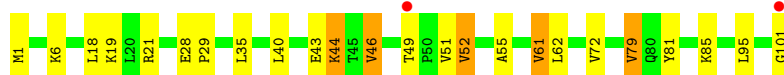
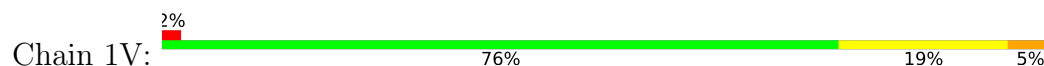




- Molecule 16: 50S ribosomal protein L20



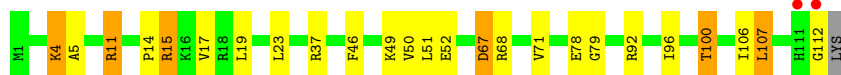
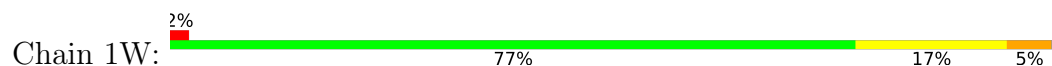
- Molecule 17: 50S ribosomal protein L21



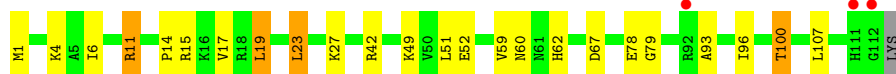
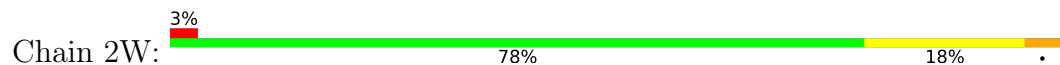
- Molecule 17: 50S ribosomal protein L21



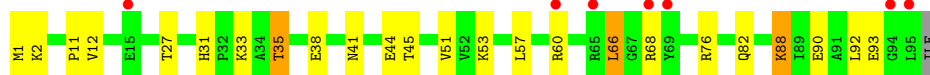
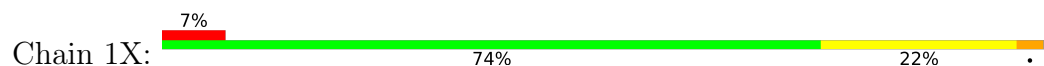
- Molecule 18: 50S ribosomal protein L22



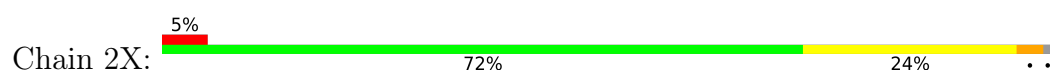
- Molecule 18: 50S ribosomal protein L22



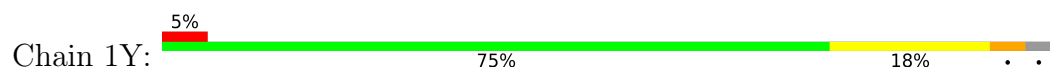
- Molecule 19: 50S ribosomal protein L23



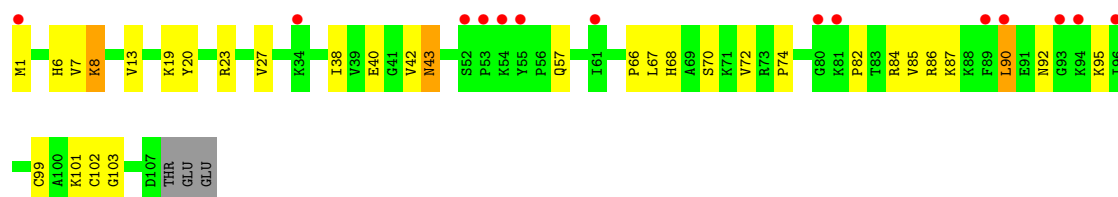
- Molecule 19: 50S ribosomal protein L23



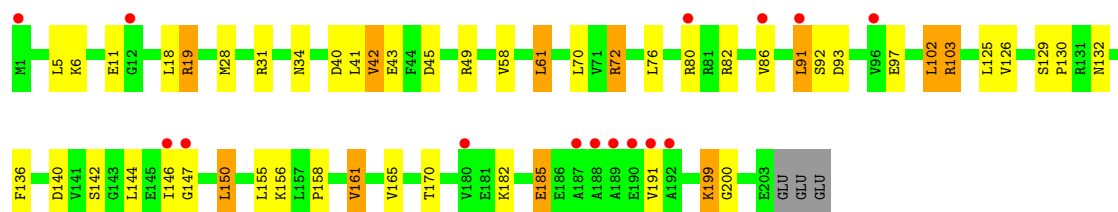
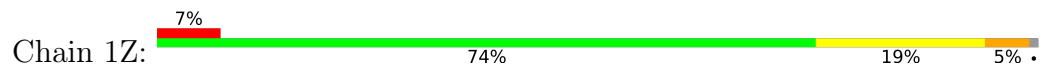
- Molecule 20: 50S ribosomal protein L24



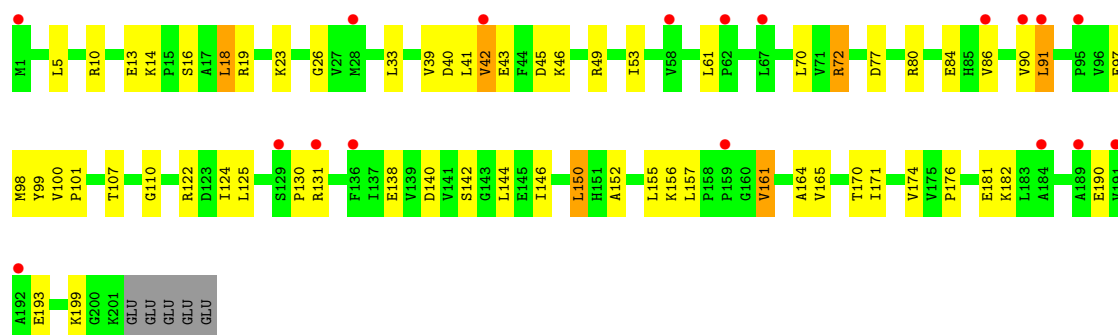
- Molecule 20: 50S ribosomal protein L24



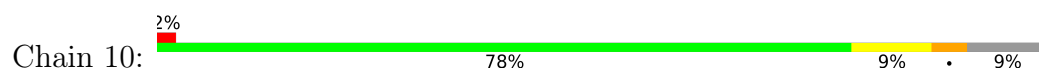
- Molecule 21: 50S ribosomal protein L25



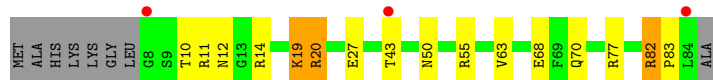
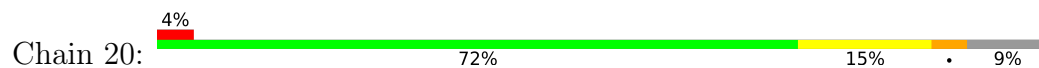
- Molecule 21: 50S ribosomal protein L25



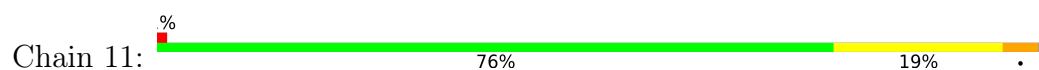
- Molecule 22: 50S ribosomal protein L27



- Molecule 22: 50S ribosomal protein L27



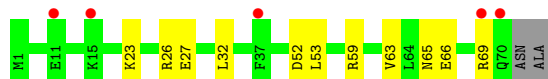
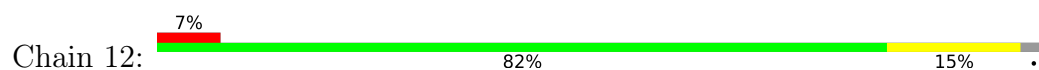
- Molecule 23: 50S ribosomal protein L28



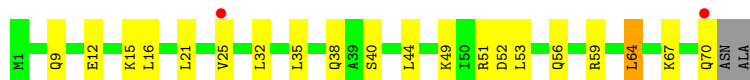
- Molecule 23: 50S ribosomal protein L28



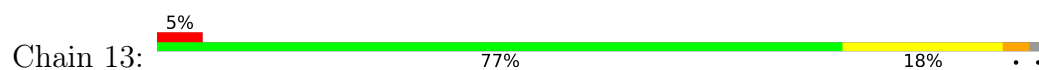
- Molecule 24: 50S ribosomal protein L29



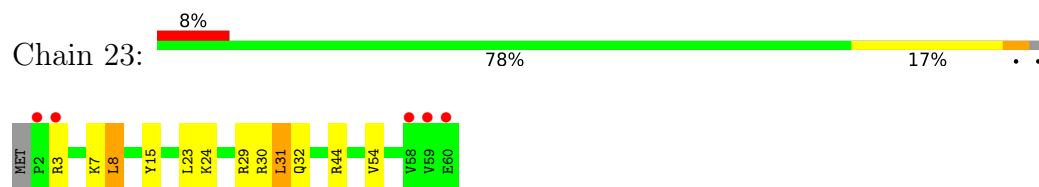
- Molecule 24: 50S ribosomal protein L29



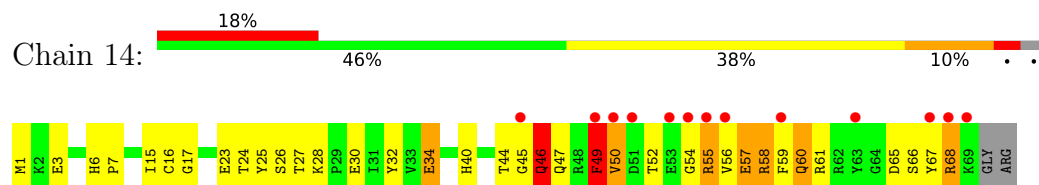
- Molecule 25: 50S ribosomal protein L30



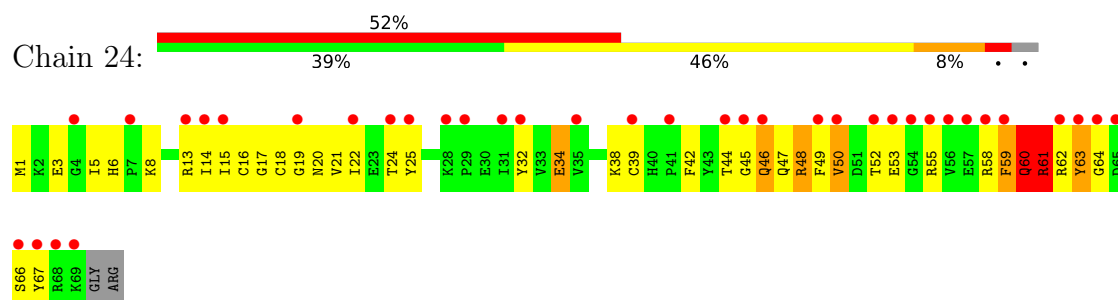
- Molecule 25: 50S ribosomal protein L30



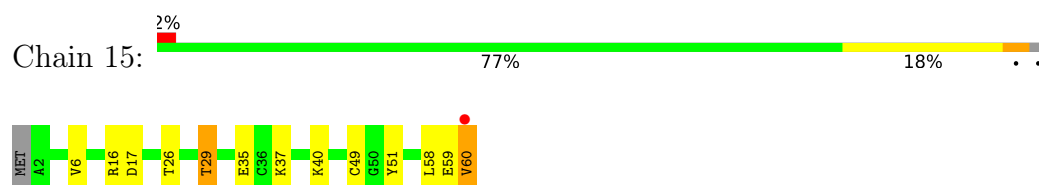
- Molecule 26: 50S ribosomal protein L31



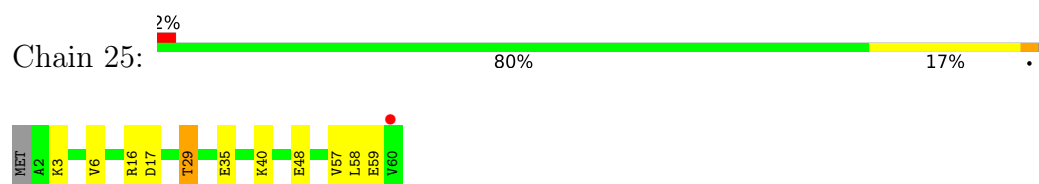
- Molecule 26: 50S ribosomal protein L31



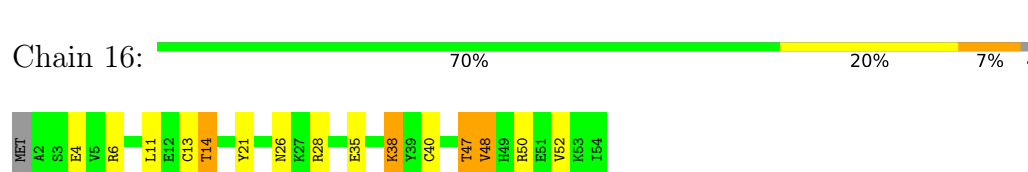
- Molecule 27: 50S ribosomal protein L32



- Molecule 27: 50S ribosomal protein L32



- Molecule 28: 50S ribosomal protein L33



- Molecule 28: 50S ribosomal protein L33

Chain 26:  80% 11% 7% .



- Molecule 29: 50S ribosomal protein L34

Chain 17:  10% 69% 22% 6% .



- Molecule 29: 50S ribosomal protein L34

Chain 27:  10% 73% 22% . .



- Molecule 30: 50S ribosomal protein L35

Chain 18:  2% 66% 31% . .



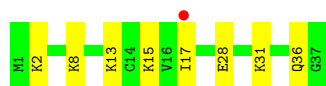
- Molecule 30: 50S ribosomal protein L35

Chain 28:  74% 22% . .



- Molecule 31: 50S ribosomal protein L36

Chain 19:  3% 78% 22%



- Molecule 31: 50S ribosomal protein L36

Chain 29:  76% 24%

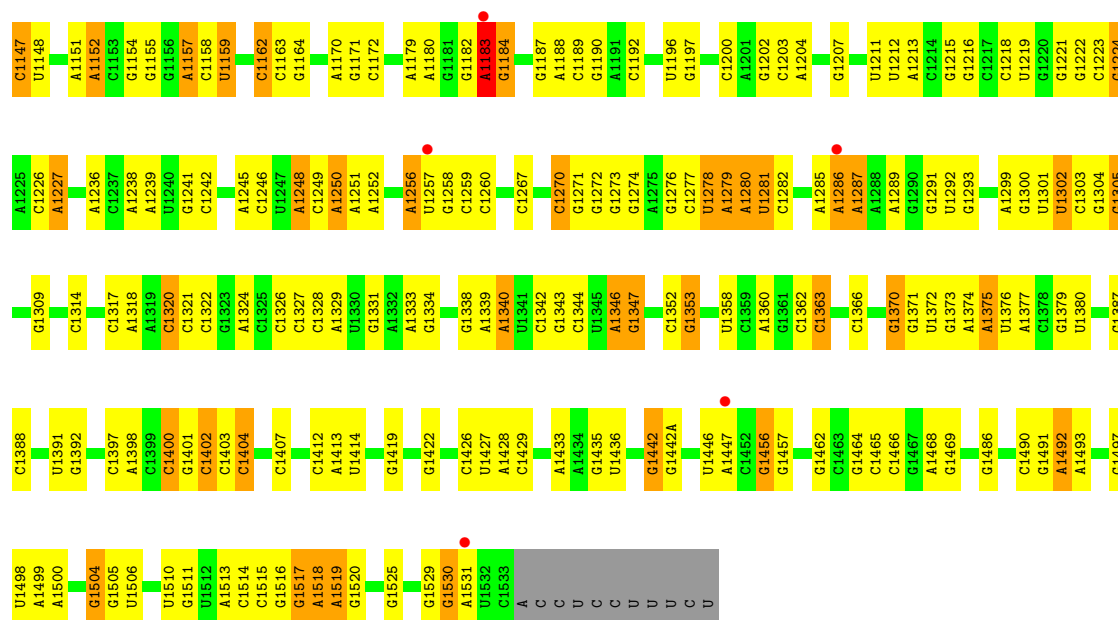


- Molecule 32: 16S Ribosomal RNA

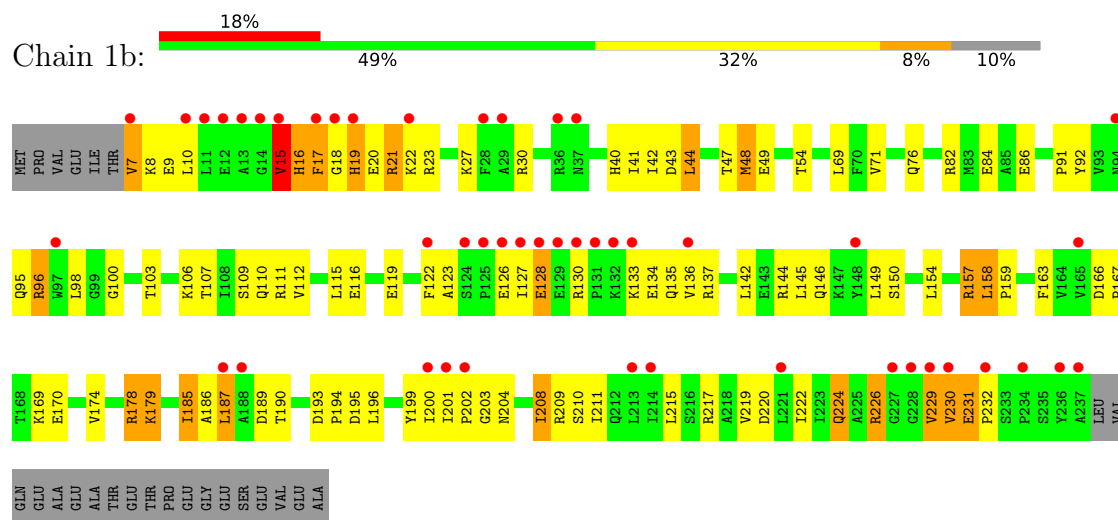


Chain 2a:

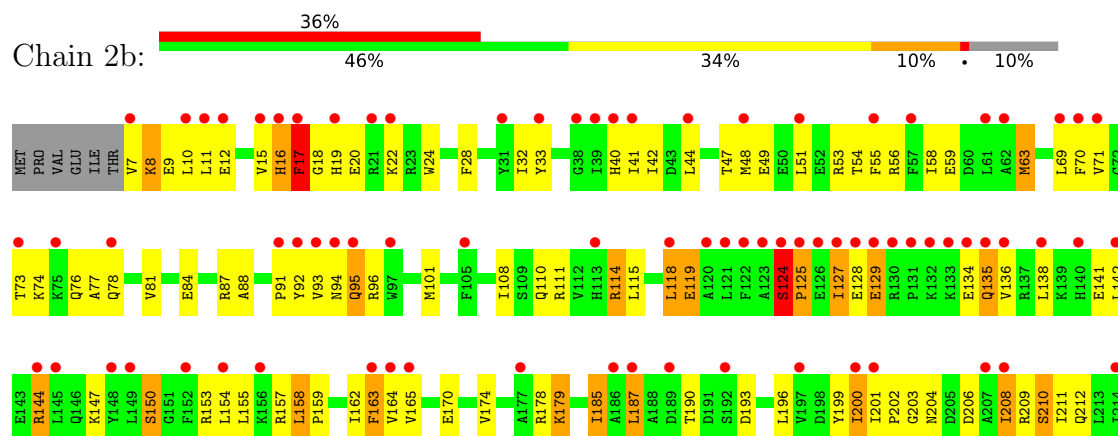


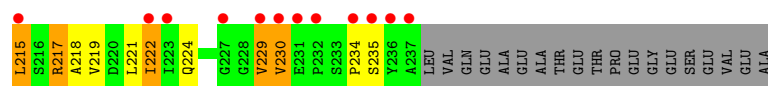


• Molecule 33: 30S ribosomal protein S2

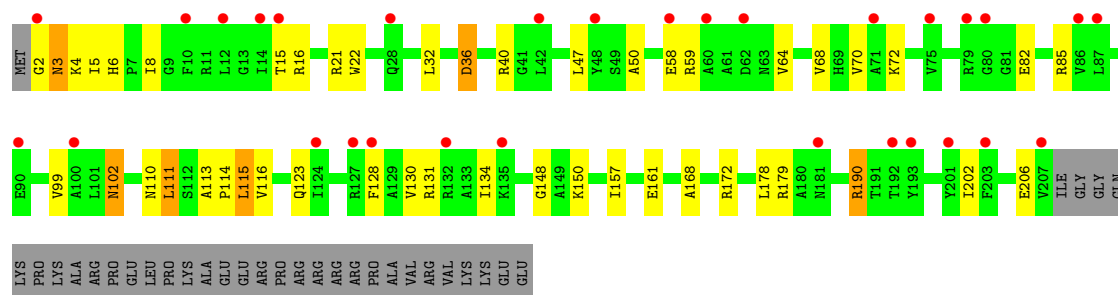


• Molecule 33: 30S ribosomal protein S2

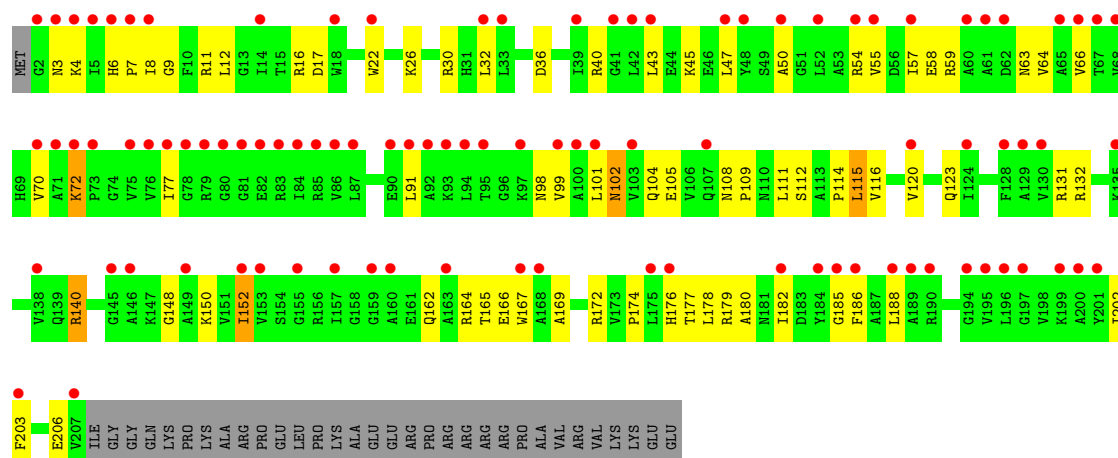
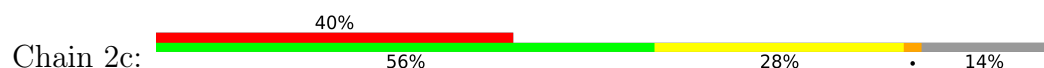




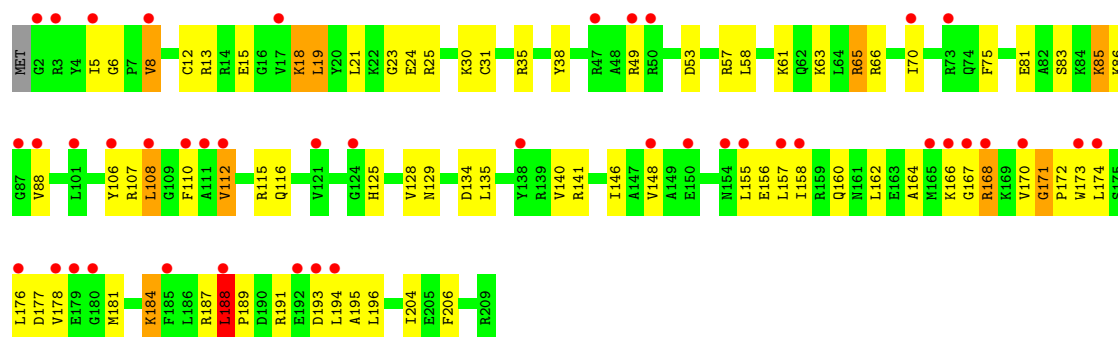
• Molecule 34: 30S ribosomal protein S3



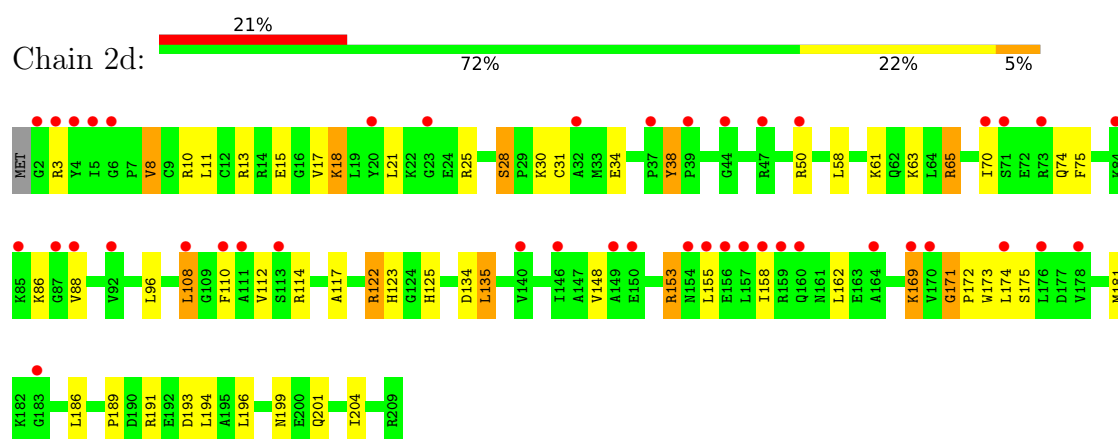
• Molecule 34: 30S ribosomal protein S3



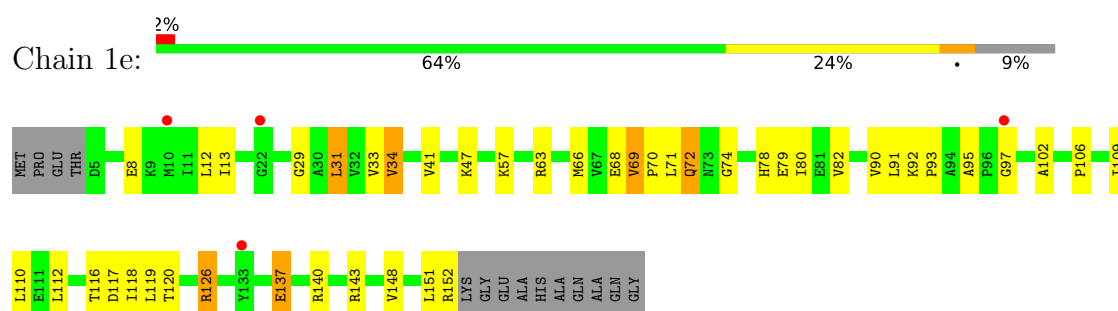
• Molecule 35: 30S ribosomal protein S4



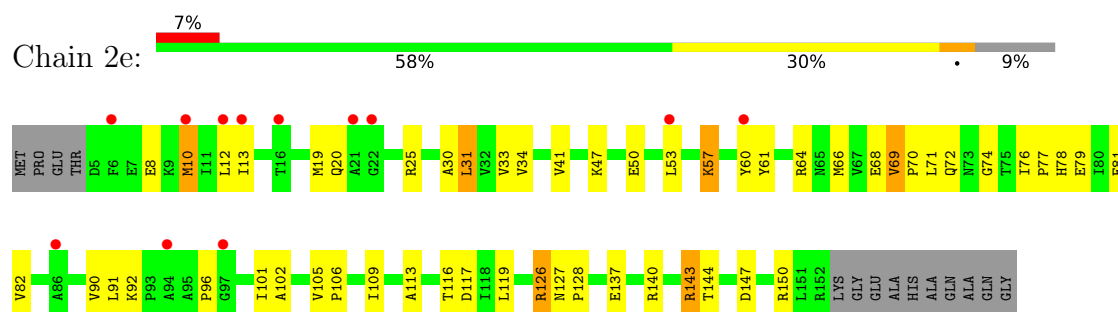
• Molecule 35: 30S ribosomal protein S4



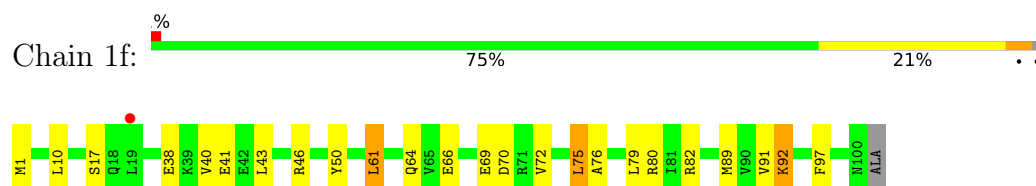
- Molecule 36: 30S ribosomal protein S5



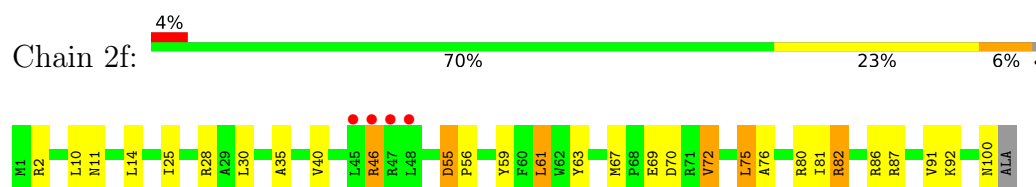
- Molecule 36: 30S ribosomal protein S5



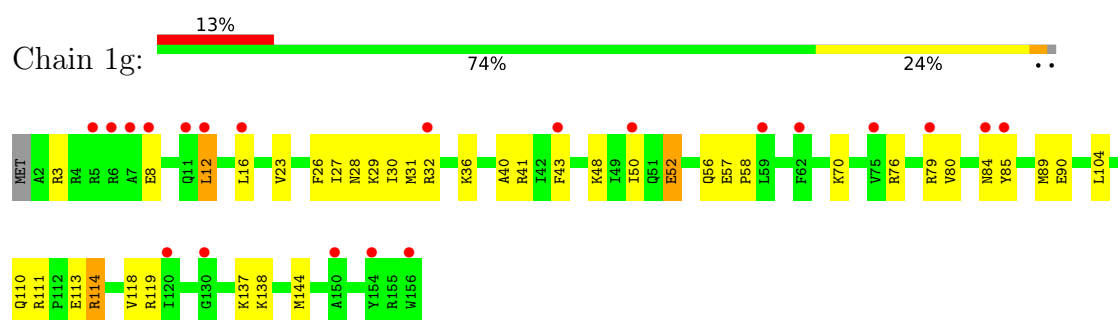
- Molecule 37: 30S ribosomal protein S6



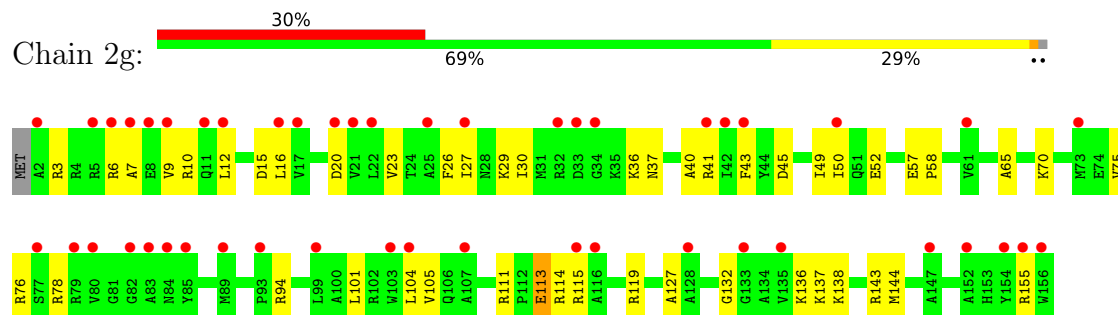
- Molecule 37: 30S ribosomal protein S6



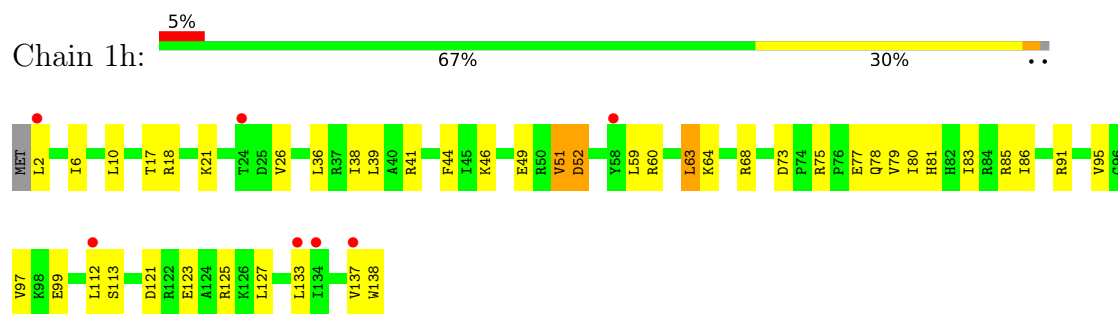
- Molecule 38: 30S ribosomal protein S7



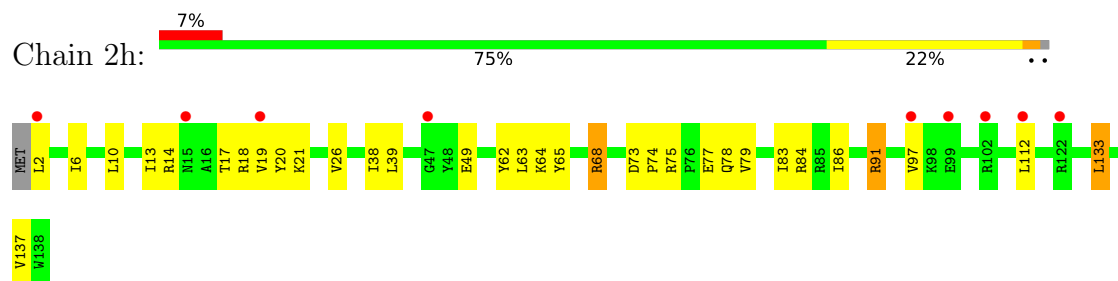
• Molecule 38: 30S ribosomal protein S7



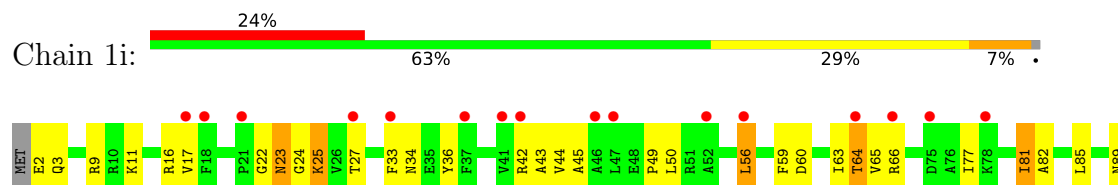
• Molecule 39: 30S ribosomal protein S8

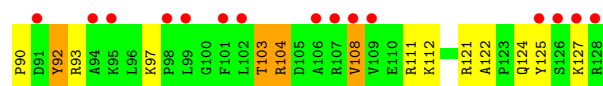


• Molecule 39: 30S ribosomal protein S8

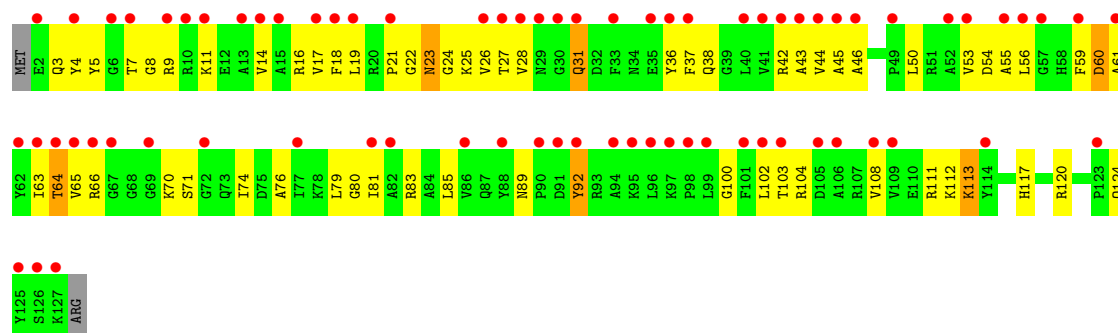


• Molecule 40: 30S ribosomal protein S9

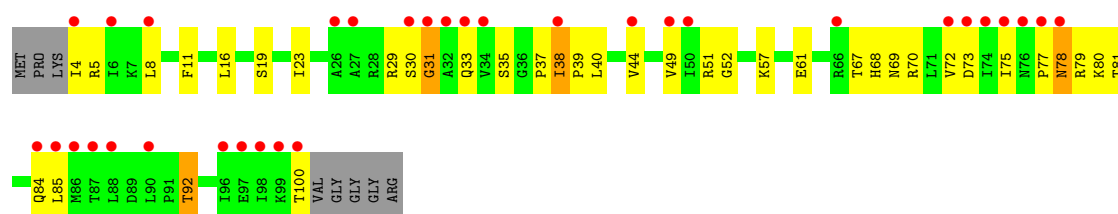




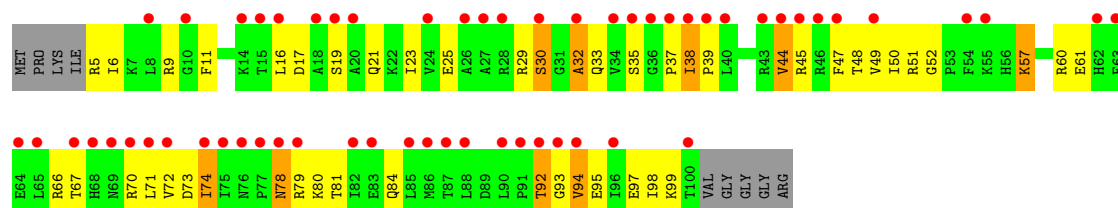
• Molecule 40: 30S ribosomal protein S9



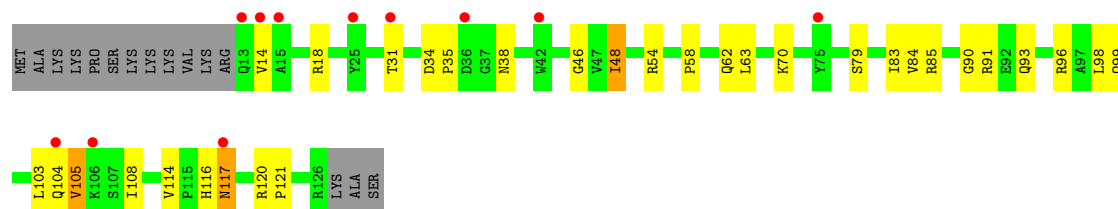
• Molecule 41: 30S ribosomal protein S10



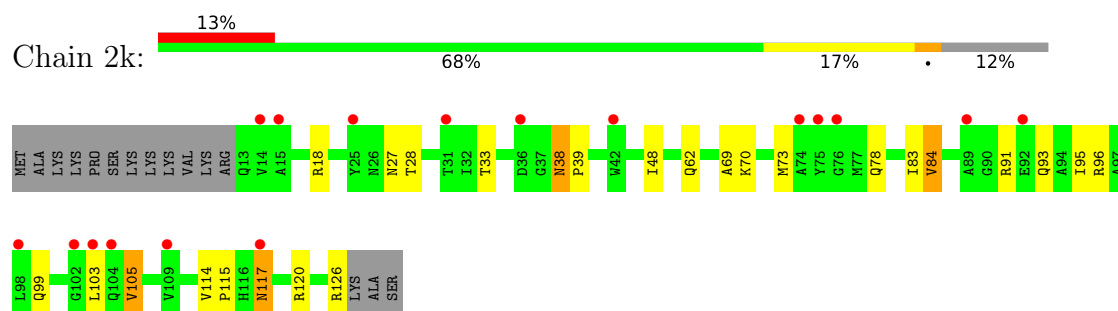
• Molecule 41: 30S ribosomal protein S10



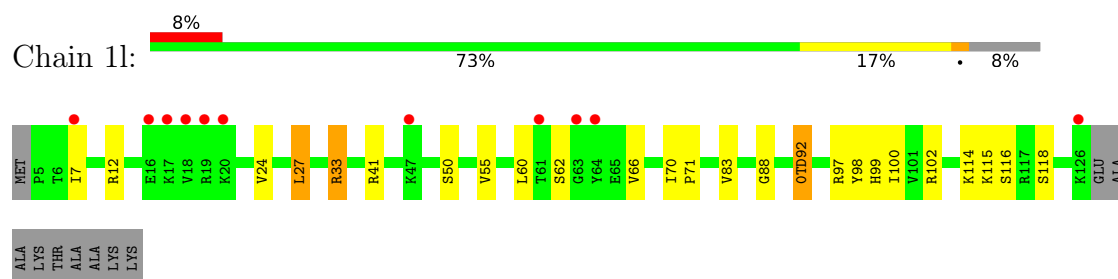
• Molecule 42: 30S ribosomal protein S11



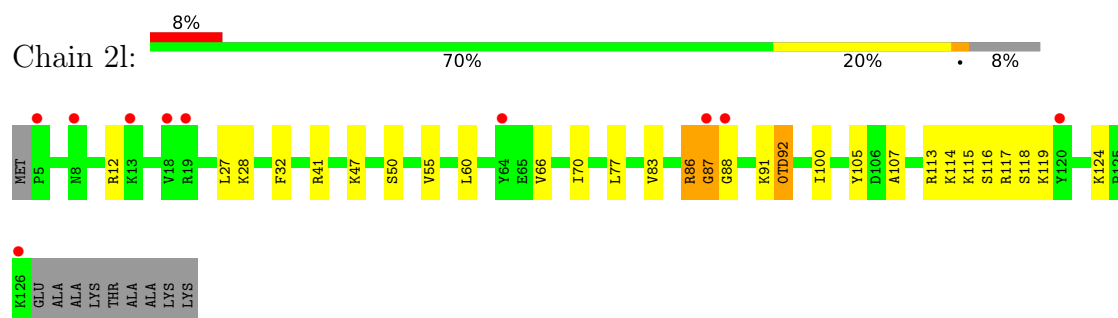
- Molecule 42: 30S ribosomal protein S11



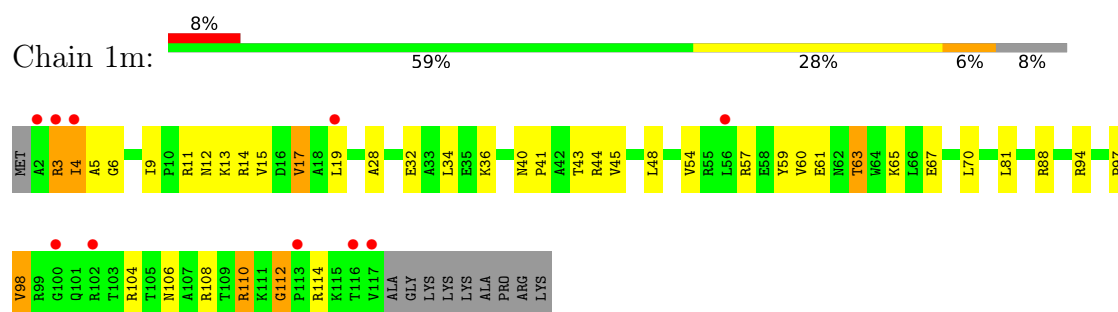
- Molecule 43: 30S ribosomal protein S12



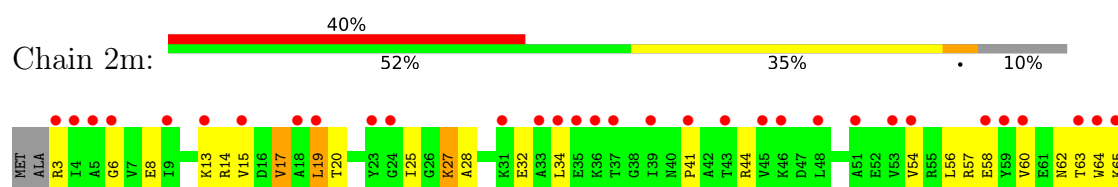
- Molecule 43: 30S ribosomal protein S12



- Molecule 44: 30S ribosomal protein S13



- Molecule 44: 30S ribosomal protein S13





- Molecule 45: 30S ribosomal protein S14 type Z



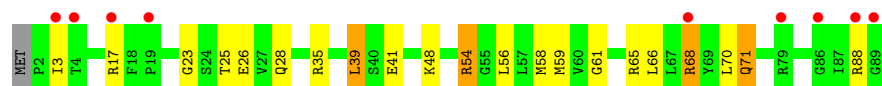
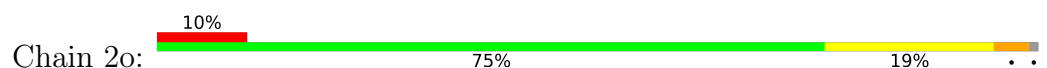
- Molecule 45: 30S ribosomal protein S14 type Z



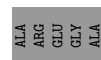
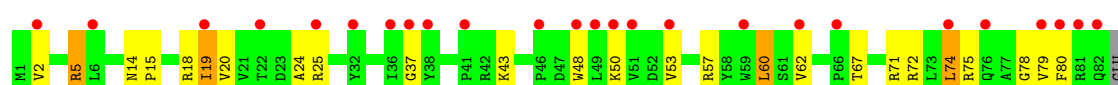
- Molecule 46: 30S ribosomal protein S15



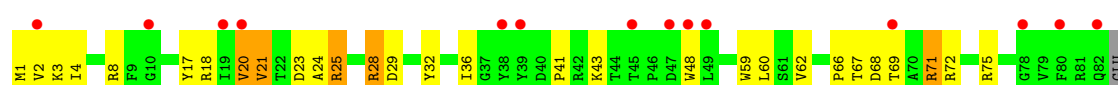
- Molecule 46: 30S ribosomal protein S15



- Molecule 47: 30S ribosomal protein S16

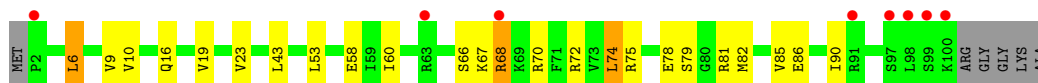
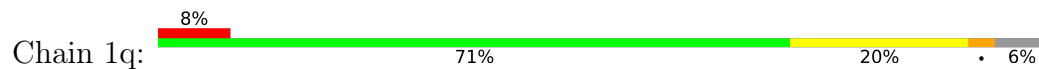


- Molecule 47: 30S ribosomal protein S16

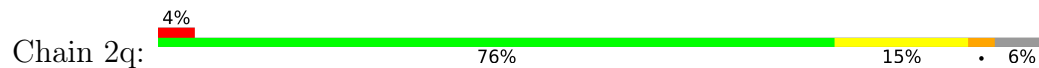


ALA
ARG
GLU
GLY
ALA

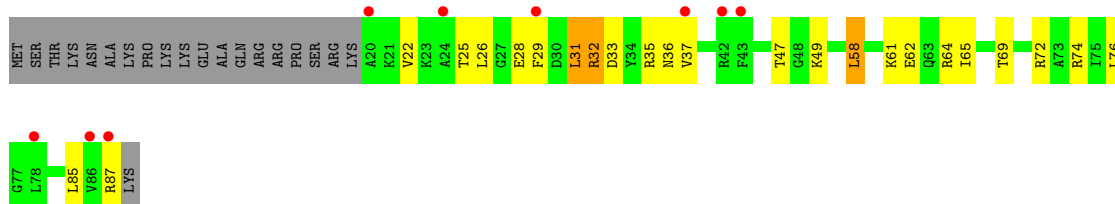
• Molecule 48: 30S ribosomal protein S17



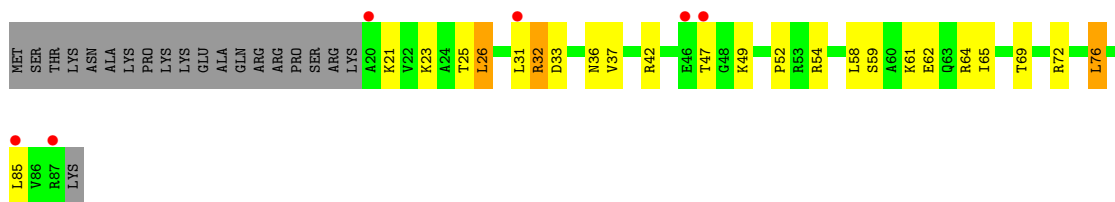
• Molecule 48: 30S ribosomal protein S17



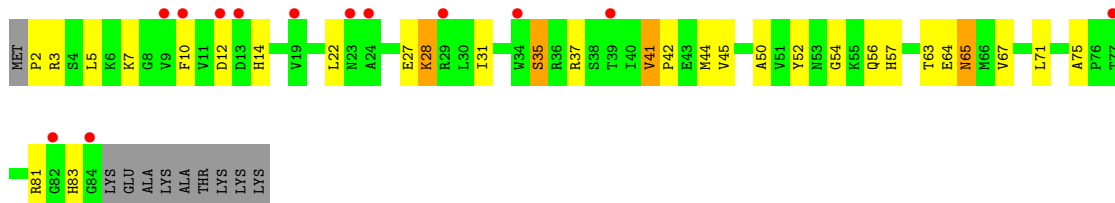
• Molecule 49: 30S ribosomal protein S18



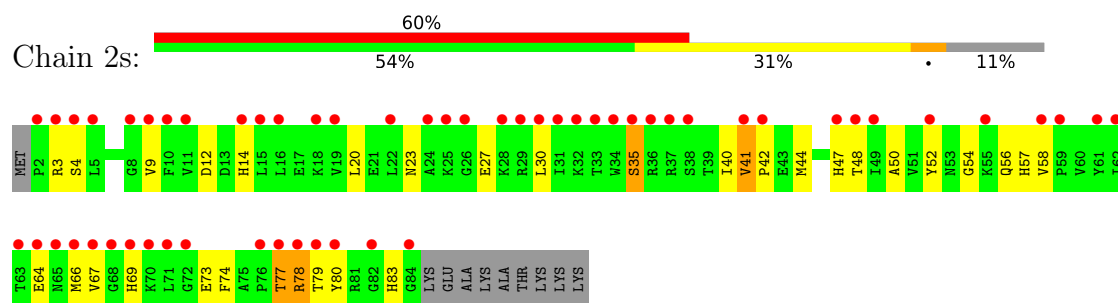
• Molecule 49: 30S ribosomal protein S18



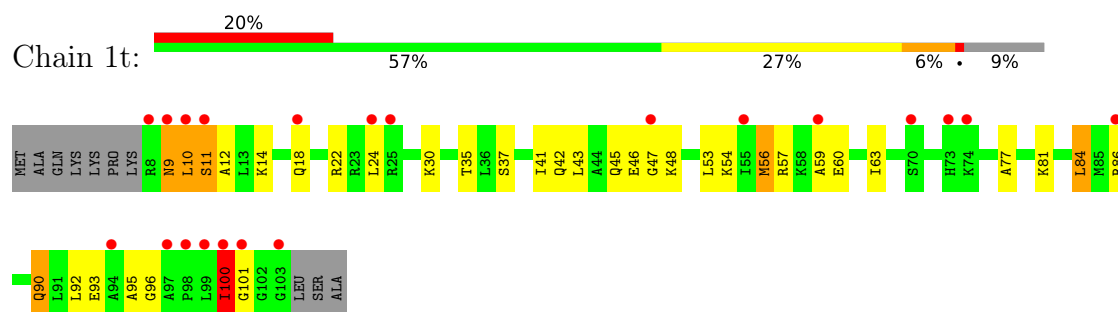
• Molecule 50: 30S ribosomal protein S19



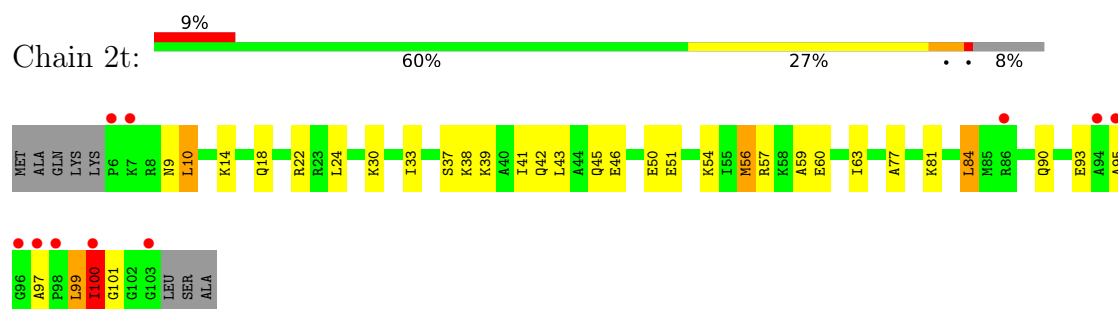
- Molecule 50: 30S ribosomal protein S19



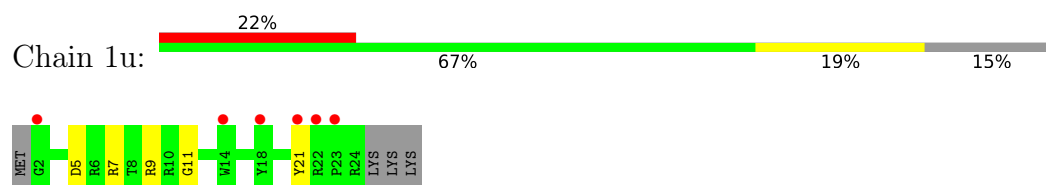
- Molecule 51: 30S ribosomal protein S20



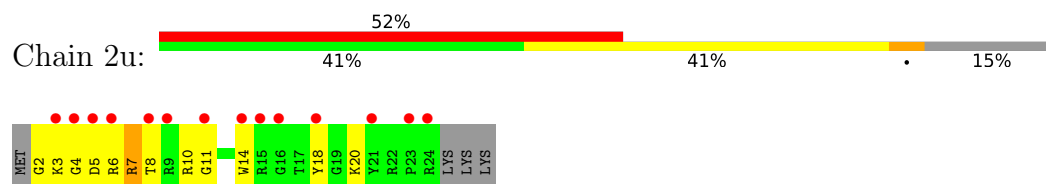
- Molecule 51: 30S ribosomal protein S20



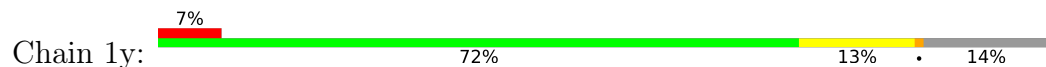
- Molecule 52: 30S ribosomal protein Thx

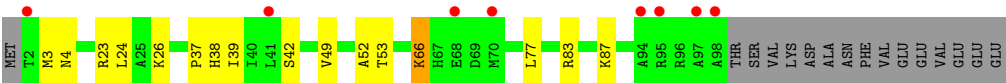


- Molecule 52: 30S ribosomal protein Thx



- Molecule 53: Ribosome-associated inhibitor A





● Molecule 53: Ribosome-associated inhibitor A



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	209.16Å 448.37Å 618.12Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	173.22 – 2.30 173.22 – 2.30	Depositor EDS
% Data completeness (in resolution range)	97.5 (173.22-2.30) 97.5 (173.22-2.30)	Depositor EDS
R_{merge}	0.15	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.18 (at 2.29Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.2_1309)	Depositor
R, R_{free}	0.207 , 0.247 0.207 , 0.246	Depositor DCC
R_{free} test set	123763 reflections (4.89%)	wwPDB-VP
Wilson B-factor (Å ²)	48.4	Xtriage
Anisotropy	0.173	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 54.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.44$, $\langle L^2 \rangle = 0.26$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	298502	wwPDB-VP
Average B, all atoms (Å ²)	55.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.49% 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: 0TD, 5MC, UR3, 4OC, M2G, 2MA, ZN, MG, PSU, MPD, 2MU, 7MG, 2MG, MA6, SF4, 5MU, OMG

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	0.39	0/69029	0.56	9/107746 (0.0%)
1	2A	0.32	0/68901	0.54	6/107544 (0.0%)
2	1B	0.31	0/2876	0.50	0/4486
2	2B	0.30	0/2878	0.49	0/4490
3	1D	0.62	0/2181	0.91	5/2940 (0.2%)
3	2D	0.51	0/2186	0.89	4/2944 (0.1%)
4	1E	0.62	0/1592	0.95	2/2149 (0.1%)
4	2E	0.52	0/1592	1.01	10/2149 (0.5%)
5	1F	0.61	1/1619 (0.1%)	0.86	1/2193 (0.0%)
5	2F	0.50	0/1615	0.93	3/2188 (0.1%)
6	1G	0.45	0/1451	0.94	7/1961 (0.4%)
6	2G	0.47	0/1449	0.94	3/1957 (0.2%)
7	1H	0.51	0/1356	0.88	1/1834 (0.1%)
7	2H	0.45	0/1350	0.97	5/1826 (0.3%)
8	1I	0.46	0/1109	0.94	3/1512 (0.2%)
8	2I	0.43	0/1091	0.89	1/1490 (0.1%)
9	1N	0.56	0/1148	0.88	0/1547
9	2N	0.42	0/1144	0.87	2/1543 (0.1%)
10	1O	0.59	0/943	0.93	2/1269 (0.2%)
10	2O	0.48	0/943	0.84	0/1269
11	1P	0.59	0/1152	0.92	0/1533
11	2P	0.44	0/1152	0.86	3/1533 (0.2%)
12	1Q	0.61	0/1143	0.86	0/1527
12	2Q	0.50	0/1143	0.87	0/1527
13	1R	0.62	0/982	0.91	0/1312
13	2R	0.52	0/982	0.87	0/1312
14	1S	0.51	0/887	0.87	0/1180
14	2S	0.47	0/880	0.90	0/1172
15	1T	0.57	0/1105	0.88	0/1477
15	2T	0.48	0/1097	0.86	2/1468 (0.1%)
16	1U	0.64	0/977	0.83	0/1301

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
16	2U	0.50	0/977	0.88	1/1301 (0.1%)
17	1V	0.54	0/786	0.88	0/1053
17	2V	0.49	0/782	0.88	0/1049
18	1W	0.62	0/897	0.84	0/1205
18	2W	0.56	0/897	0.82	0/1205
19	1X	0.59	0/764	0.90	0/1025
19	2X	0.51	0/764	0.86	0/1025
20	1Y	0.51	0/823	0.98	1/1099 (0.1%)
20	2Y	0.44	0/823	0.86	0/1100
21	1Z	0.46	0/1620	0.86	0/2200
21	2Z	0.45	0/1590	0.92	1/2162 (0.0%)
22	10	0.58	0/616	0.88	0/821
22	20	0.43	0/616	0.86	2/821 (0.2%)
23	11	0.56	0/761	0.83	0/1013
23	21	0.50	0/766	0.84	0/1018
24	12	0.51	0/590	0.78	0/781
24	22	0.42	0/594	0.77	0/785
25	13	0.59	0/474	0.92	0/635
25	23	0.48	0/469	0.88	0/630
26	14	0.49	0/559	1.16	7/754 (0.9%)
26	24	0.54	0/549	1.11	5/741 (0.7%)
27	15	0.61	0/473	0.89	0/639
27	25	0.53	0/469	0.80	0/635
28	16	0.58	0/460	0.81	2/613 (0.3%)
28	26	0.50	0/456	0.80	0/608
29	17	0.68	0/426	0.84	1/561 (0.2%)
29	27	0.54	0/426	0.83	0/561
30	18	0.61	0/525	0.81	0/691
30	28	0.49	0/525	0.86	0/691
31	19	0.60	0/310	0.87	0/407
31	29	0.44	0/310	0.86	0/407
32	1a	0.26	0/35795	0.46	1/55864 (0.0%)
32	2a	0.24	0/35890	0.44	3/56012 (0.0%)
33	1b	0.44	0/1876	0.98	5/2533 (0.2%)
33	2b	0.47	0/1860	0.96	5/2518 (0.2%)
34	1c	0.42	0/1582	0.86	2/2137 (0.1%)
34	2c	0.46	0/1566	0.93	5/2119 (0.2%)
35	1d	0.45	0/1695	0.93	5/2274 (0.2%)
35	2d	0.42	0/1698	0.90	4/2277 (0.2%)
36	1e	0.46	0/1149	0.88	2/1548 (0.1%)
36	2e	0.44	0/1149	0.91	6/1548 (0.4%)
37	1f	0.47	0/827	0.87	0/1120
37	2f	0.44	0/829	0.85	2/1123 (0.2%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
38	1g	0.40	0/1254	0.81	0/1683
38	2g	0.39	0/1248	0.83	0/1676
39	1h	0.41	0/1118	0.81	0/1506
39	2h	0.37	0/1108	0.85	0/1494
40	1i	0.41	0/1005	0.90	0/1351
40	2i	0.44	0/985	0.90	1/1329 (0.1%)
41	1j	0.43	0/732	0.94	0/993
41	2j	0.44	0/723	0.94	1/984 (0.1%)
42	1k	0.47	0/849	0.94	5/1150 (0.4%)
42	2k	0.45	0/848	0.91	2/1149 (0.2%)
43	1l	0.43	0/937	0.83	0/1260
43	2l	0.44	0/937	0.95	5/1260 (0.4%)
44	1m	0.42	0/924	0.92	5/1242 (0.4%)
44	2m	0.41	0/905	0.95	1/1217 (0.1%)
45	1n	0.43	0/501	0.74	0/664
45	2n	0.43	0/501	0.84	0/664
46	1o	0.43	0/739	0.88	1/985 (0.1%)
46	2o	0.41	0/739	0.85	0/985
47	1p	0.42	0/697	0.90	1/939 (0.1%)
47	2p	0.46	0/693	0.81	0/935
48	1q	0.41	0/836	0.81	0/1117
48	2q	0.39	0/836	0.81	0/1117
49	1r	0.42	0/560	0.91	1/746 (0.1%)
49	2r	0.40	0/560	0.80	0/746
50	1s	0.40	0/663	0.99	2/895 (0.2%)
50	2s	0.45	0/660	0.90	1/893 (0.1%)
51	1t	0.44	0/734	0.90	1/969 (0.1%)
51	2t	0.40	0/736	0.83	1/976 (0.1%)
52	1u	0.36	0/203	0.73	0/266
52	2u	0.42	0/203	0.80	0/266
53	1y	0.46	0/776	0.78	0/1048
53	2y	0.39	0/761	0.75	0/1030
All	All	0.38	1/309937 (0.0%)	0.64	157/463223 (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
14	1S	0	1
19	1X	0	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
19	2X	0	1
33	1b	0	1
43	2l	0	1
All	All	0	5

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	1F	132	VAL	CA-CB	5.65	1.60	1.53

The worst 5 of 157 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
35	1d	188	LEU	CA-C-N	10.70	131.39	119.83
35	1d	188	LEU	C-N-CA	10.70	131.39	119.83
43	2l	88	GLY	N-CA-C	8.59	123.75	112.25
1	2A	1992	G	C2'-C3'-O3'	8.21	121.81	109.50
33	1b	128	GLU	N-CA-C	-8.11	102.95	113.17

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
14	1S	58	LEU	Peptide
19	1X	93	GLU	Peptide
33	1b	231	GLU	Peptide
19	2X	93	GLU	Peptide
43	2l	86	ARG	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	31203	523	0
1	2A	61758	0	31151	759	0
2	1B	2572	0	1305	26	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	2B	2573	0	1306	37	0
3	1D	2131	0	2207	42	0
3	2D	2136	0	2218	52	0
4	1E	1559	0	1618	41	0
4	2E	1559	0	1618	43	0
5	1F	1584	0	1625	42	0
5	2F	1580	0	1619	40	0
6	1G	1426	0	1445	44	0
6	2G	1424	0	1441	60	0
7	1H	1330	0	1407	20	0
7	2H	1324	0	1402	39	0
8	1I	1094	0	1127	27	0
8	2I	1076	0	1094	22	0
9	1N	1121	0	1195	14	0
9	2N	1117	0	1184	17	0
10	1O	933	0	996	19	0
10	2O	933	0	996	14	0
11	1P	1135	0	1212	29	0
11	2P	1135	0	1212	29	0
12	1Q	1122	0	1179	24	0
12	2Q	1122	0	1179	23	0
13	1R	968	0	1033	21	0
13	2R	968	0	1033	21	0
14	1S	877	0	938	18	0
14	2S	870	0	923	27	0
15	1T	1091	0	1151	36	0
15	2T	1083	0	1136	24	0
16	1U	959	0	1019	22	0
16	2U	959	0	1019	20	0
17	1V	775	0	841	14	0
17	2V	771	0	830	24	0
18	1W	886	0	940	14	0
18	2W	886	0	940	16	0
19	1X	750	0	814	17	0
19	2X	750	0	814	17	0
20	1Y	810	0	892	15	0
20	2Y	810	0	887	22	0
21	1Z	1587	0	1598	23	0
21	2Z	1557	0	1564	32	0
22	10	608	0	622	10	0
22	20	608	0	622	11	0
23	11	754	0	823	13	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
23	21	759	0	837	21	0
24	12	588	0	643	5	0
24	22	592	0	654	12	0
25	13	469	0	518	8	0
25	23	464	0	514	6	0
26	14	546	0	522	27	0
26	24	536	0	514	44	0
27	15	459	0	476	7	0
27	25	455	0	465	6	0
28	16	453	0	473	8	0
28	26	449	0	469	4	0
29	17	418	0	467	14	0
29	27	418	0	467	9	0
30	18	517	0	582	24	0
30	28	517	0	582	20	0
31	19	307	0	335	6	0
31	29	307	0	335	5	0
32	1a	32246	0	16296	380	0
32	2a	32331	0	16339	490	0
33	1b	1842	0	1862	56	0
33	2b	1825	0	1828	73	0
34	1c	1558	0	1557	31	0
34	2c	1542	0	1517	53	0
35	1d	1665	0	1687	60	0
35	2d	1668	0	1703	42	0
36	1e	1133	0	1191	25	0
36	2e	1133	0	1191	29	0
37	1f	814	0	808	14	0
37	2f	816	0	808	18	0
38	1g	1235	0	1249	24	0
38	2g	1229	0	1238	21	0
39	1h	1098	0	1143	22	0
39	2h	1088	0	1126	15	0
40	1i	986	0	990	33	0
40	2i	966	0	953	50	0
41	1j	719	0	672	27	0
41	2j	710	0	661	40	0
42	1k	834	0	838	16	0
42	2k	833	0	836	15	0
43	1l	932	0	981	18	0
43	2l	932	0	981	19	0
44	1m	914	0	954	29	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
44	2m	895	0	920	34	0
45	1n	492	0	529	14	0
45	2n	492	0	529	23	0
46	1o	728	0	760	19	0
46	2o	728	0	760	15	0
47	1p	681	0	697	18	0
47	2p	677	0	686	19	0
48	1q	823	0	891	16	0
48	2q	823	0	891	12	0
49	1r	555	0	618	13	0
49	2r	555	0	618	14	0
50	1s	648	0	658	25	0
50	2s	645	0	635	33	0
51	1t	732	0	809	22	0
51	2t	733	0	795	26	0
52	1u	199	0	208	2	0
52	2u	199	0	208	8	0
53	1y	764	0	786	10	0
53	2y	749	0	757	32	0
54	10	5	0	0	0	0
54	11	4	0	0	0	0
54	13	2	0	0	0	0
54	14	1	0	0	0	0
54	15	2	0	0	0	0
54	17	2	0	0	0	0
54	18	1	0	0	0	0
54	19	2	0	0	0	0
54	1A	1075	0	0	0	0
54	1B	30	0	0	0	0
54	1D	14	0	0	0	0
54	1E	6	0	0	0	0
54	1F	10	0	0	0	0
54	1G	4	0	0	0	0
54	1H	2	0	0	0	0
54	1N	3	0	0	0	0
54	1O	1	0	0	0	0
54	1P	2	0	0	0	0
54	1Q	4	0	0	0	0
54	1R	3	0	0	0	0
54	1T	3	0	0	0	0
54	1U	2	0	0	0	0
54	1V	3	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
54	1W	2	0	0	0	0
54	1X	1	0	0	0	0
54	1Z	1	0	0	0	0
54	1a	280	0	0	0	0
54	1b	1	0	0	0	0
54	1d	5	0	0	0	0
54	1e	4	0	0	0	0
54	1f	1	0	0	0	0
54	1g	3	0	0	0	0
54	1h	2	0	0	0	0
54	1i	1	0	0	0	0
54	1l	2	0	0	0	0
54	1n	2	0	0	0	0
54	1o	1	0	0	0	0
54	1q	2	0	0	0	0
54	1r	1	0	0	0	0
54	1t	1	0	0	0	0
54	1y	4	0	0	0	0
54	20	2	0	0	0	0
54	21	1	0	0	0	0
54	26	1	0	0	0	0
54	27	1	0	0	0	0
54	28	2	0	0	0	0
54	2A	761	0	0	0	0
54	2B	19	0	0	0	0
54	2D	9	0	0	0	0
54	2E	5	0	0	0	0
54	2F	3	0	0	0	0
54	2G	3	0	0	0	0
54	2I	1	0	0	0	0
54	2N	1	0	0	0	0
54	2O	2	0	0	0	0
54	2P	2	0	0	0	0
54	2Q	2	0	0	0	0
54	2R	1	0	0	0	0
54	2T	3	0	0	0	0
54	2V	1	0	0	0	0
54	2W	2	0	0	0	0
54	2X	1	0	0	0	0
54	2a	193	0	0	0	0
54	2e	1	0	0	0	0
54	2f	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
54	2j	1	0	0	0	0
54	2l	1	0	0	0	0
54	2r	1	0	0	0	0
54	2t	1	0	0	0	0
55	18	8	0	14	5	0
55	1A	8	0	14	1	0
55	1T	8	0	14	0	0
55	1a	8	0	14	8	0
55	2A	16	0	28	2	0
55	2B	8	0	14	0	0
56	1B	12	0	12	1	0
56	1F	12	0	12	3	0
57	14	1	0	0	0	0
57	15	1	0	0	0	0
57	16	1	0	0	0	0
57	19	1	0	0	0	0
57	1Y	1	0	0	0	0
57	1n	1	0	0	0	0
57	24	1	0	0	0	0
57	25	1	0	0	0	0
57	26	1	0	0	0	0
57	29	1	0	0	0	0
57	2Y	1	0	0	0	0
57	2n	1	0	0	0	0
58	1d	8	0	0	0	0
58	2d	8	0	0	0	0
59	10	25	0	0	0	0
59	11	25	0	0	0	0
59	12	15	0	0	0	0
59	13	25	0	0	0	0
59	14	4	0	0	0	0
59	15	25	0	0	0	0
59	16	22	0	0	0	0
59	17	19	0	0	2	0
59	18	31	0	0	2	0
59	19	9	0	0	1	0
59	1A	4154	0	0	66	0
59	1B	109	0	0	1	0
59	1D	119	0	0	2	0
59	1E	81	0	0	4	0
59	1F	66	0	0	3	0
59	1G	20	0	0	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
59	1H	16	0	0	0	0
59	1I	9	0	0	0	0
59	1N	55	0	0	0	0
59	1O	29	0	0	1	0
59	1P	56	0	0	2	0
59	1Q	46	0	0	2	0
59	1R	37	0	0	2	0
59	1S	11	0	0	0	0
59	1T	39	0	0	3	0
59	1U	49	0	0	6	0
59	1V	34	0	0	3	0
59	1W	27	0	0	0	0
59	1X	27	0	0	0	0
59	1Y	20	0	0	1	0
59	1Z	13	0	0	1	0
59	1a	599	0	0	20	0
59	1b	1	0	0	0	0
59	1c	1	0	0	0	0
59	1d	8	0	0	1	0
59	1e	5	0	0	1	0
59	1f	3	0	0	0	0
59	1h	1	0	0	0	0
59	1i	1	0	0	0	0
59	1j	1	0	0	0	0
59	1k	1	0	0	0	0
59	1l	5	0	0	0	0
59	1m	2	0	0	0	0
59	1o	7	0	0	2	0
59	1p	3	0	0	0	0
59	1t	1	0	0	0	0
59	1y	7	0	0	1	0
59	20	13	0	0	0	0
59	21	22	0	0	1	0
59	22	4	0	0	1	0
59	23	3	0	0	0	0
59	24	2	0	0	2	0
59	25	10	0	0	0	0
59	26	5	0	0	0	0
59	27	9	0	0	1	0
59	28	16	0	0	0	0
59	29	3	0	0	0	0
59	2A	2665	0	0	77	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
59	2B	69	0	0	8	0
59	2D	59	0	0	0	0
59	2E	33	0	0	2	0
59	2F	26	0	0	0	0
59	2G	9	0	0	0	0
59	2H	4	0	0	0	0
59	2I	4	0	0	1	0
59	2N	6	0	0	0	0
59	2O	23	0	0	3	0
59	2P	30	0	0	1	0
59	2Q	28	0	0	1	0
59	2R	21	0	0	1	0
59	2S	7	0	0	1	0
59	2T	11	0	0	0	0
59	2U	20	0	0	1	0
59	2V	6	0	0	0	0
59	2W	20	0	0	1	0
59	2X	10	0	0	0	0
59	2Y	4	0	0	0	0
59	2Z	16	0	0	2	0
59	2a	459	0	0	36	0
59	2d	6	0	0	0	0
59	2e	2	0	0	0	0
59	2f	1	0	0	0	0
59	2j	2	0	0	1	0
59	2l	5	0	0	0	0
59	2m	2	0	0	0	0
59	2o	2	0	0	0	0
59	2p	3	0	0	0	0
59	2q	1	0	0	0	0
59	2r	5	0	0	0	0
59	2t	2	0	0	0	0
59	2y	5	0	0	0	0
All	All	298502	0	194517	3979	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 8.

The worst 5 of 3979 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1A:1128:U:H3	1:1A:1132:A:N6	1.32	1.27
1:2A:2128:C:N4	1:2A:2160:G:H1	1.46	1.11
32:2a:1003:G:H2'	32:2a:1004:A:H4'	1.32	1.10
32:1a:78:G:H1	32:1a:91:C:N4	1.49	1.09
1:2A:2602:A:H1'	1:2A:2603:G:H5''	1.36	1.08

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%)	260 (95%)	13 (5%)	0	100	100
4	1E	202/206 (98%)	195 (96%)	6 (3%)	1 (0%)	24	31
4	2E	202/206 (98%)	196 (97%)	6 (3%)	0	100	100
5	1F	201/210 (96%)	197 (98%)	4 (2%)	0	100	100
5	2F	201/210 (96%)	196 (98%)	3 (2%)	2 (1%)	12	15
6	1G	179/182 (98%)	167 (93%)	11 (6%)	1 (1%)	21	27
6	2G	179/182 (98%)	170 (95%)	8 (4%)	1 (1%)	21	27
7	1H	172/180 (96%)	167 (97%)	5 (3%)	0	100	100
7	2H	171/180 (95%)	165 (96%)	6 (4%)	0	100	100
8	1I	145/148 (98%)	133 (92%)	11 (8%)	1 (1%)	18	23
8	2I	144/148 (97%)	135 (94%)	9 (6%)	0	100	100
9	1N	138/140 (99%)	136 (99%)	2 (1%)	0	100	100
9	2N	138/140 (99%)	136 (99%)	2 (1%)	0	100	100
10	1O	120/122 (98%)	114 (95%)	6 (5%)	0	100	100
10	2O	120/122 (98%)	115 (96%)	5 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
11	1P	147/150 (98%)	141 (96%)	6 (4%)	0	100	100
11	2P	147/150 (98%)	141 (96%)	5 (3%)	1 (1%)	18	23
12	1Q	139/141 (99%)	134 (96%)	5 (4%)	0	100	100
12	2Q	139/141 (99%)	134 (96%)	5 (4%)	0	100	100
13	1R	116/118 (98%)	113 (97%)	3 (3%)	0	100	100
13	2R	116/118 (98%)	114 (98%)	2 (2%)	0	100	100
14	1S	108/112 (96%)	104 (96%)	3 (3%)	1 (1%)	14	17
14	2S	108/112 (96%)	105 (97%)	3 (3%)	0	100	100
15	1T	129/146 (88%)	124 (96%)	5 (4%)	0	100	100
15	2T	129/146 (88%)	125 (97%)	4 (3%)	0	100	100
16	1U	114/118 (97%)	114 (100%)	0	0	100	100
16	2U	114/118 (97%)	114 (100%)	0	0	100	100
17	1V	99/101 (98%)	97 (98%)	2 (2%)	0	100	100
17	2V	99/101 (98%)	96 (97%)	3 (3%)	0	100	100
18	1W	110/113 (97%)	109 (99%)	1 (1%)	0	100	100
18	2W	110/113 (97%)	110 (100%)	0	0	100	100
19	1X	93/96 (97%)	92 (99%)	1 (1%)	0	100	100
19	2X	93/96 (97%)	91 (98%)	2 (2%)	0	100	100
20	1Y	105/110 (96%)	99 (94%)	6 (6%)	0	100	100
20	2Y	105/110 (96%)	101 (96%)	4 (4%)	0	100	100
21	1Z	201/206 (98%)	196 (98%)	5 (2%)	0	100	100
21	2Z	199/206 (97%)	194 (98%)	5 (2%)	0	100	100
22	10	75/85 (88%)	73 (97%)	2 (3%)	0	100	100
22	20	75/85 (88%)	73 (97%)	2 (3%)	0	100	100
23	11	95/98 (97%)	94 (99%)	0	1 (1%)	11	13
23	21	95/98 (97%)	93 (98%)	1 (1%)	1 (1%)	11	13
24	12	68/72 (94%)	67 (98%)	1 (2%)	0	100	100
24	22	68/72 (94%)	67 (98%)	1 (2%)	0	100	100
25	13	57/60 (95%)	55 (96%)	2 (4%)	0	100	100
25	23	57/60 (95%)	55 (96%)	2 (4%)	0	100	100
26	14	67/71 (94%)	56 (84%)	5 (8%)	6 (9%)	0	0

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
26	24	67/71 (94%)	53 (79%)	11 (16%)	3 (4%)	2	1
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%)	49 (96%)	2 (4%)	0	100	100
29	17	46/49 (94%)	46 (100%)	0	0	100	100
29	27	46/49 (94%)	46 (100%)	0	0	100	100
30	18	62/65 (95%)	61 (98%)	1 (2%)	0	100	100
30	28	62/65 (95%)	61 (98%)	1 (2%)	0	100	100
31	19	35/37 (95%)	35 (100%)	0	0	100	100
31	29	35/37 (95%)	35 (100%)	0	0	100	100
33	1b	229/256 (90%)	202 (88%)	20 (9%)	7 (3%)	3	2
33	2b	229/256 (90%)	205 (90%)	19 (8%)	5 (2%)	5	4
34	1c	204/239 (85%)	190 (93%)	14 (7%)	0	100	100
34	2c	204/239 (85%)	187 (92%)	17 (8%)	0	100	100
35	1d	206/209 (99%)	197 (96%)	9 (4%)	0	100	100
35	2d	206/209 (99%)	199 (97%)	7 (3%)	0	100	100
36	1e	146/162 (90%)	144 (99%)	2 (1%)	0	100	100
36	2e	146/162 (90%)	145 (99%)	1 (1%)	0	100	100
37	1f	98/101 (97%)	96 (98%)	2 (2%)	0	100	100
37	2f	98/101 (97%)	96 (98%)	2 (2%)	0	100	100
38	1g	153/156 (98%)	148 (97%)	5 (3%)	0	100	100
38	2g	153/156 (98%)	148 (97%)	4 (3%)	1 (1%)	18	23
39	1h	135/138 (98%)	133 (98%)	2 (2%)	0	100	100
39	2h	135/138 (98%)	130 (96%)	5 (4%)	0	100	100
40	1i	125/128 (98%)	115 (92%)	9 (7%)	1 (1%)	16	20
40	2i	124/128 (97%)	113 (91%)	8 (6%)	3 (2%)	4	4
41	1j	95/105 (90%)	83 (87%)	8 (8%)	4 (4%)	2	1
41	2j	94/105 (90%)	85 (90%)	7 (7%)	2 (2%)	5	4
42	1k	112/129 (87%)	103 (92%)	7 (6%)	2 (2%)	6	6
42	2k	112/129 (87%)	106 (95%)	5 (4%)	1 (1%)	14	17

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
43	1l	119/132 (90%)	117 (98%)	2 (2%)	0	100	100
43	2l	119/132 (90%)	116 (98%)	3 (2%)	0	100	100
44	1m	114/126 (90%)	105 (92%)	7 (6%)	2 (2%)	6	6
44	2m	112/126 (89%)	105 (94%)	6 (5%)	1 (1%)	14	17
45	1n	58/61 (95%)	56 (97%)	2 (3%)	0	100	100
45	2n	58/61 (95%)	56 (97%)	2 (3%)	0	100	100
46	1o	86/89 (97%)	82 (95%)	4 (5%)	0	100	100
46	2o	86/89 (97%)	82 (95%)	4 (5%)	0	100	100
47	1p	80/88 (91%)	77 (96%)	3 (4%)	0	100	100
47	2p	80/88 (91%)	76 (95%)	4 (5%)	0	100	100
48	1q	97/105 (92%)	94 (97%)	2 (2%)	1 (1%)	12	15
48	2q	97/105 (92%)	95 (98%)	2 (2%)	0	100	100
49	1r	66/88 (75%)	65 (98%)	1 (2%)	0	100	100
49	2r	66/88 (75%)	65 (98%)	1 (2%)	0	100	100
50	1s	81/93 (87%)	78 (96%)	3 (4%)	0	100	100
50	2s	81/93 (87%)	79 (98%)	2 (2%)	0	100	100
51	1t	94/106 (89%)	86 (92%)	6 (6%)	2 (2%)	5	4
51	2t	96/106 (91%)	88 (92%)	6 (6%)	2 (2%)	5	4
52	1u	21/27 (78%)	19 (90%)	2 (10%)	0	100	100
52	2u	21/27 (78%)	19 (90%)	1 (5%)	1 (5%)	2	1
53	1y	95/113 (84%)	94 (99%)	1 (1%)	0	100	100
53	2y	94/113 (83%)	89 (95%)	4 (4%)	1 (1%)	11	13
All	All	11629/12354 (94%)	11139 (96%)	435 (4%)	55 (0%)	24	31

5 of 55 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
26	14	49	PHE
33	1b	16	HIS
33	1b	17	PHE
33	1b	22	LYS
51	1t	95	ALA

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%)	192 (90%)	22 (10%)	7	8
3	2D	215/218 (99%)	193 (90%)	22 (10%)	7	8
4	1E	164/166 (99%)	139 (85%)	25 (15%)	3	3
4	2E	164/166 (99%)	138 (84%)	26 (16%)	2	2
5	1F	160/166 (96%)	140 (88%)	20 (12%)	4	5
5	2F	159/166 (96%)	142 (89%)	17 (11%)	6	8
6	1G	144/156 (92%)	125 (87%)	19 (13%)	4	4
6	2G	142/156 (91%)	119 (84%)	23 (16%)	2	2
7	1H	144/148 (97%)	133 (92%)	11 (8%)	12	16
7	2H	143/148 (97%)	125 (87%)	18 (13%)	4	5
8	1I	111/124 (90%)	87 (78%)	24 (22%)	1	1
8	2I	108/124 (87%)	93 (86%)	15 (14%)	3	4
9	1N	119/119 (100%)	103 (87%)	16 (13%)	4	4
9	2N	118/119 (99%)	104 (88%)	14 (12%)	5	6
10	1O	100/100 (100%)	94 (94%)	6 (6%)	17	25
10	2O	100/100 (100%)	92 (92%)	8 (8%)	11	15
11	1P	115/116 (99%)	101 (88%)	14 (12%)	5	5
11	2P	115/116 (99%)	103 (90%)	12 (10%)	7	8
12	1Q	111/111 (100%)	100 (90%)	11 (10%)	7	9
12	2Q	111/111 (100%)	100 (90%)	11 (10%)	7	9
13	1R	101/101 (100%)	85 (84%)	16 (16%)	2	2
13	2R	101/101 (100%)	86 (85%)	15 (15%)	3	3
14	1S	87/88 (99%)	75 (86%)	12 (14%)	3	4
14	2S	85/88 (97%)	71 (84%)	14 (16%)	2	2
15	1T	115/127 (91%)	102 (89%)	13 (11%)	5	7
15	2T	113/127 (89%)	102 (90%)	11 (10%)	8	10

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
16	1U	93/94 (99%)	80 (86%)	13 (14%)	3	3
16	2U	93/94 (99%)	82 (88%)	11 (12%)	5	6
17	1V	81/82 (99%)	68 (84%)	13 (16%)	2	2
17	2V	80/82 (98%)	67 (84%)	13 (16%)	2	2
18	1W	90/92 (98%)	78 (87%)	12 (13%)	4	4
18	2W	90/92 (98%)	80 (89%)	10 (11%)	6	7
19	1X	77/78 (99%)	71 (92%)	6 (8%)	11	16
19	2X	77/78 (99%)	71 (92%)	6 (8%)	11	16
20	1Y	86/91 (94%)	80 (93%)	6 (7%)	14	19
20	2Y	86/91 (94%)	77 (90%)	9 (10%)	6	8
21	1Z	169/179 (94%)	143 (85%)	26 (15%)	2	3
21	2Z	165/179 (92%)	144 (87%)	21 (13%)	4	5
22	10	61/67 (91%)	57 (93%)	4 (7%)	15	21
22	20	61/67 (91%)	58 (95%)	3 (5%)	22	34
23	11	79/83 (95%)	69 (87%)	10 (13%)	4	5
23	21	81/83 (98%)	71 (88%)	10 (12%)	4	5
24	12	65/67 (97%)	62 (95%)	3 (5%)	24	36
24	22	66/67 (98%)	61 (92%)	5 (8%)	12	16
25	13	51/52 (98%)	47 (92%)	4 (8%)	11	16
25	23	50/52 (96%)	44 (88%)	6 (12%)	5	5
26	14	58/63 (92%)	47 (81%)	11 (19%)	1	1
26	24	54/63 (86%)	43 (80%)	11 (20%)	1	1
27	15	51/52 (98%)	44 (86%)	7 (14%)	3	4
27	25	50/52 (96%)	43 (86%)	7 (14%)	3	3
28	16	51/52 (98%)	44 (86%)	7 (14%)	3	4
28	26	50/52 (96%)	44 (88%)	6 (12%)	5	5
29	17	41/42 (98%)	37 (90%)	4 (10%)	7	10
29	27	41/42 (98%)	38 (93%)	3 (7%)	13	18
30	18	54/55 (98%)	51 (94%)	3 (6%)	19	28
30	28	54/55 (98%)	49 (91%)	5 (9%)	8	11
31	19	34/34 (100%)	33 (97%)	1 (3%)	37	55

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
31	29	34/34 (100%)	33 (97%)	1 (3%)	37	55
33	1b	191/220 (87%)	158 (83%)	33 (17%)	2	2
33	2b	187/220 (85%)	150 (80%)	37 (20%)	1	1
34	1c	144/188 (77%)	132 (92%)	12 (8%)	10	14
34	2c	140/188 (74%)	126 (90%)	14 (10%)	7	9
35	1d	171/181 (94%)	151 (88%)	20 (12%)	5	6
35	2d	172/181 (95%)	156 (91%)	16 (9%)	8	11
36	1e	114/123 (93%)	102 (90%)	12 (10%)	6	8
36	2e	114/123 (93%)	99 (87%)	15 (13%)	4	4
37	1f	85/90 (94%)	77 (91%)	8 (9%)	8	11
37	2f	85/90 (94%)	76 (89%)	9 (11%)	6	8
38	1g	120/127 (94%)	108 (90%)	12 (10%)	7	9
38	2g	119/127 (94%)	104 (87%)	15 (13%)	4	5
39	1h	116/119 (98%)	101 (87%)	15 (13%)	4	4
39	2h	114/119 (96%)	101 (89%)	13 (11%)	5	6
40	1i	91/99 (92%)	75 (82%)	16 (18%)	2	2
40	2i	88/99 (89%)	77 (88%)	11 (12%)	4	5
41	1j	68/92 (74%)	64 (94%)	4 (6%)	18	26
41	2j	68/92 (74%)	61 (90%)	7 (10%)	7	8
42	1k	83/99 (84%)	74 (89%)	9 (11%)	6	7
42	2k	83/99 (84%)	75 (90%)	8 (10%)	8	10
43	1l	96/108 (89%)	91 (95%)	5 (5%)	21	31
43	2l	96/108 (89%)	92 (96%)	4 (4%)	26	40
44	1m	90/101 (89%)	78 (87%)	12 (13%)	4	4
44	2m	87/101 (86%)	76 (87%)	11 (13%)	4	5
45	1n	49/50 (98%)	43 (88%)	6 (12%)	5	5
45	2n	49/50 (98%)	42 (86%)	7 (14%)	3	3
46	1o	78/80 (98%)	69 (88%)	9 (12%)	5	6
46	2o	78/80 (98%)	68 (87%)	10 (13%)	4	4
47	1p	69/74 (93%)	60 (87%)	9 (13%)	4	4
47	2p	68/74 (92%)	57 (84%)	11 (16%)	2	2

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
48	1q	94/97 (97%)	88 (94%)	6 (6%)	16	23
48	2q	94/97 (97%)	87 (93%)	7 (7%)	13	17
49	1r	59/77 (77%)	48 (81%)	11 (19%)	1	1
49	2r	59/77 (77%)	49 (83%)	10 (17%)	2	2
50	1s	68/80 (85%)	60 (88%)	8 (12%)	5	6
50	2s	67/80 (84%)	60 (90%)	7 (10%)	7	8
51	1t	71/82 (87%)	61 (86%)	10 (14%)	3	3
51	2t	70/82 (85%)	61 (87%)	9 (13%)	4	4
52	1u	18/22 (82%)	16 (89%)	2 (11%)	6	7
52	2u	18/22 (82%)	16 (89%)	2 (11%)	6	7
53	1y	82/98 (84%)	79 (96%)	3 (4%)	30	45
53	2y	79/98 (81%)	68 (86%)	11 (14%)	3	4
All	All	9524/10260 (93%)	8396 (88%)	1128 (12%)	5	6

5 of 1128 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
33	2b	221	LEU
35	2d	108	LEU
33	2b	217	ARG
43	2l	41	ARG
35	1d	49	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 172 such sidechains are listed below:

Mol	Chain	Res	Type
24	22	56	GLN
39	2h	78	GLN
31	29	36	GLN
34	2c	181	ASN
41	2j	84	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	1A	2865/2915 (98%)	410 (14%)	41 (1%)

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Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	2A	2858/2915 (98%)	485 (16%)	41 (1%)
2	1B	119/121 (98%)	10 (8%)	0
2	2B	119/121 (98%)	14 (11%)	0
32	1a	1497/1521 (98%)	231 (15%)	0
32	2a	1501/1521 (98%)	252 (16%)	0
All	All	8959/9114 (98%)	1402 (15%)	82 (0%)

5 of 1402 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	1A	12	U
1	1A	13	A
1	1A	34	C
1	1A	35	G
1	1A	45	C

5 of 82 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	2A	1057	A
1	2A	2126	A
1	2A	1067	A
1	2A	1420	U
1	2A	2406	U

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
1	5MU	1A	1961	1	19,22,23	1.33	4 (21%)	27,32,35	2.30	7 (25%)
1	2MA	1A	2515	1,54	22,25,26	1.48	5 (22%)	32,37,40	2.48	9 (28%)
1	2MA	2A	2503	1,54	22,25,26	1.49	5 (22%)	32,37,40	2.37	9 (28%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
43	0TD	1l	92	43	8,9,10	8.01	6 (75%)	6,11,13	4.26	2 (33%)
1	PSU	1A	1933	1	18,21,22	1.35	2 (11%)	21,30,33	1.97	4 (19%)
1	2MU	2A	2552	1,54	19,22,24	1.32	3 (15%)	25,31,36	1.95	5 (20%)
32	UR3	2a	1498	32,54	19,22,23	0.96	1 (5%)	26,32,35	1.72	3 (11%)
32	7MG	1a	527	32,54	23,26,27	1.31	3 (13%)	27,39,42	2.52	6 (22%)
32	PSU	1a	516	32,54	18,21,22	1.40	2 (11%)	21,30,33	2.01	5 (23%)
1	5MC	2A	1942	1	19,22,23	1.75	3 (15%)	26,32,35	1.27	2 (7%)
32	M2G	1a	966	32	24,27,28	1.32	4 (16%)	33,40,43	1.85	5 (15%)
1	PSU	1A	2617	1	18,21,22	1.44	3 (16%)	21,30,33	1.96	4 (19%)
32	5MC	1a	1404	32	19,22,23	1.66	3 (15%)	26,32,35	1.20	3 (11%)
32	MA6	1a	1518	32	23,26,27	1.59	5 (21%)	33,38,41	2.25	13 (39%)
1	PSU	2A	1911	1	18,21,22	1.44	2 (11%)	21,30,33	2.00	4 (19%)
1	5MC	1A	1984	1,54	19,22,23	1.57	2 (10%)	26,32,35	1.46	4 (15%)
1	PSU	1A	1939	1	18,21,22	1.36	3 (16%)	21,30,33	1.88	4 (19%)
32	PSU	2a	516	32,54	18,21,22	1.30	2 (11%)	21,30,33	2.19	5 (23%)
32	M2G	2a	966	32,54	24,27,28	1.24	3 (12%)	33,40,43	1.88	6 (18%)
1	5MU	1A	1937	1,54	19,22,23	1.46	5 (26%)	27,32,35	2.28	8 (29%)
1	4OC	1A	1942	1,54	19,22,24	0.82	0	25,31,35	0.94	1 (4%)
32	5MC	2a	1404	32	19,22,23	1.86	3 (15%)	26,32,35	1.31	4 (15%)
1	4OC	2A	1920	1	19,22,24	0.82	0	25,31,35	0.99	1 (4%)
32	5MC	2a	1400	32	19,22,23	1.79	3 (15%)	26,32,35	1.15	3 (11%)
1	5MC	2A	1962	1,54	19,22,23	1.56	3 (15%)	26,32,35	1.28	3 (11%)
32	MA6	1a	1519	32	23,26,27	1.56	4 (17%)	33,38,41	2.30	10 (30%)
32	5MC	1a	967	32	19,22,23	1.67	3 (15%)	26,32,35	1.16	3 (11%)
32	2MG	2a	1207	32	23,26,27	1.22	3 (13%)	33,38,41	2.17	8 (24%)
32	MA6	2a	1519	32	23,26,27	1.61	5 (21%)	33,38,41	2.38	13 (39%)
32	4OC	1a	1402	32	20,23,24	0.74	1 (5%)	25,32,35	0.96	1 (4%)
32	UR3	1a	1498	32	19,22,23	0.97	0	26,32,35	1.82	3 (11%)
1	2MU	1A	2564	1,54	19,22,24	1.32	3 (15%)	25,31,36	1.87	6 (24%)
32	5MC	1a	1407	32	19,22,23	1.86	3 (15%)	26,32,35	1.27	3 (11%)
1	5MU	2A	1939	1,54	19,22,23	1.35	5 (26%)	27,32,35	2.51	7 (25%)
1	OMG	2A	2251	1,54	23,26,27	1.14	2 (8%)	32,38,41	2.00	6 (18%)
32	5MC	2a	967	32	19,22,23	1.88	3 (15%)	26,32,35	1.15	3 (11%)
1	5MC	1A	1964	1,54	19,22,23	1.55	3 (15%)	26,32,35	1.10	2 (7%)
32	5MC	1a	1400	32	19,22,23	1.80	3 (15%)	26,32,35	1.29	2 (7%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	OMG	1A	2263	1,54	23,26,27	1.27	3 (13%)	32,38,41	2.03	6 (18%)
1	PSU	2A	1917	1	18,21,22	1.35	2 (11%)	21,30,33	2.12	3 (14%)
32	MA6	2a	1518	32	23,26,27	1.57	4 (17%)	33,38,41	2.27	12 (36%)
32	4OC	2a	1402	32	20,23,24	0.74	0	25,32,35	0.95	1 (4%)
43	0TD	2l	92	43	8,9,10	4.87	2 (25%)	6,11,13	2.22	2 (33%)
32	2MG	1a	1207	32,54	23,26,27	1.24	2 (8%)	33,38,41	2.52	12 (36%)
32	7MG	2a	527	32	23,26,27	1.43	4 (17%)	27,39,42	2.56	5 (18%)
32	5MC	2a	1407	32	19,22,23	1.58	3 (15%)	26,32,35	1.20	3 (11%)
1	PSU	2A	2605	1	18,21,22	1.35	3 (16%)	21,30,33	1.97	5 (23%)
1	5MU	2A	1915	1	19,22,23	1.51	4 (21%)	27,32,35	2.16	8 (29%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	5MU	1A	1961	1	-	0/7/25/26	0/2/2/2
1	2MA	1A	2515	1,54	-	1/7/25/26	0/3/3/3
1	2MA	2A	2503	1,54	-	0/7/25/26	0/3/3/3
43	0TD	1l	92	43	-	2/7/12/14	-
1	PSU	1A	1933	1	-	0/7/25/26	0/2/2/2
1	2MU	2A	2552	1,54	-	0/9/27/28	0/2/2/2
32	UR3	2a	1498	32,54	-	0/7/25/26	0/2/2/2
32	7MG	1a	527	32,54	-	2/7/37/38	0/3/3/3
32	PSU	1a	516	32,54	-	0/7/25/26	0/2/2/2
1	5MC	2A	1942	1	-	0/7/25/26	0/2/2/2
32	M2G	1a	966	32	-	0/11/29/30	0/3/3/3
1	PSU	1A	2617	1	-	0/7/25/26	0/2/2/2
32	5MC	1a	1404	32	-	0/7/25/26	0/2/2/2
32	MA6	1a	1518	32	-	3/11/29/30	0/3/3/3
1	PSU	2A	1911	1	-	0/7/25/26	0/2/2/2
1	5MC	1A	1984	1,54	-	0/7/25/26	0/2/2/2
1	PSU	1A	1939	1	-	0/7/25/26	0/2/2/2
32	PSU	2a	516	32,54	-	0/7/25/26	0/2/2/2
32	M2G	2a	966	32,54	-	0/11/29/30	0/3/3/3
1	5MU	1A	1937	1,54	-	2/7/25/26	0/2/2/2
1	4OC	1A	1942	1,54	-	1/9/27/30	0/2/2/2
32	5MC	2a	1404	32	-	0/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	4OC	2A	1920	1	-	0/9/27/30	0/2/2/2
32	5MC	2a	1400	32	-	0/7/25/26	0/2/2/2
1	5MC	2A	1962	1,54	-	0/7/25/26	0/2/2/2
32	MA6	1a	1519	32	-	2/11/29/30	0/3/3/3
32	5MC	1a	967	32	-	0/7/25/26	0/2/2/2
32	2MG	2a	1207	32	-	0/9/27/28	0/3/3/3
32	MA6	2a	1519	32	-	5/11/29/30	0/3/3/3
32	4OC	1a	1402	32	-	2/9/29/30	0/2/2/2
32	UR3	1a	1498	32	-	0/7/25/26	0/2/2/2
1	2MU	1A	2564	1,54	-	0/9/27/28	0/2/2/2
32	5MC	1a	1407	32	-	0/7/25/26	0/2/2/2
1	5MU	2A	1939	1,54	-	0/7/25/26	0/2/2/2
1	OMG	2A	2251	1,54	-	1/9/27/28	0/3/3/3
32	5MC	2a	967	32	-	0/7/25/26	0/2/2/2
1	5MC	1A	1964	1,54	-	0/7/25/26	0/2/2/2
32	5MC	1a	1400	32	-	0/7/25/26	0/2/2/2
1	OMG	1A	2263	1,54	-	1/9/27/28	0/3/3/3
1	PSU	2A	1917	1	-	0/7/25/26	0/2/2/2
32	MA6	2a	1518	32	-	1/11/29/30	0/3/3/3
32	4OC	2a	1402	32	-	1/9/29/30	0/2/2/2
43	0TD	2l	92	43	-	3/7/12/14	-
32	2MG	1a	1207	32,54	-	0/9/27/28	0/3/3/3
32	7MG	2a	527	32	-	0/7/37/38	0/3/3/3
32	5MC	2a	1407	32	-	0/7/25/26	0/2/2/2
1	PSU	2A	2605	1	-	0/7/25/26	0/2/2/2
1	5MU	2A	1915	1	-	2/7/25/26	0/2/2/2

The worst 5 of 140 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
43	1l	92	0TD	CB-SB	-17.14	1.65	1.82
43	1l	92	0TD	CB-CA	-13.64	1.50	1.54
43	2l	92	0TD	CB-SB	-12.72	1.69	1.82
32	2a	967	5MC	C5-C4	7.09	1.49	1.44
32	2a	1404	5MC	C5-C4	6.91	1.49	1.44

The worst 5 of 244 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	2a	527	7MG	N9-C4-N3	8.67	138.17	125.46
32	1a	527	7MG	N9-C4-N3	8.43	137.81	125.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1A	2515	2MA	C5-C4-N3	-8.39	118.34	127.18
43	1l	92	0TD	CB-CA-N	-7.92	93.06	109.10
32	1a	1498	UR3	C4-N3-C2	-7.34	118.67	124.58

There are no chirality outliers.

5 of 29 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	1A	1937	5MU	O4'-C1'-N1-C2
1	1A	1937	5MU	O4'-C1'-N1-C6
1	1A	2263	OMG	C1'-C2'-O2'-CM2
32	1a	1518	MA6	C5-C6-N6-C9
43	1l	92	0TD	SB-CB-CG-OD2

There are no ring outliers.

19 monomers are involved in 27 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	1A	1961	5MU	1	0
1	2A	2503	2MA	1	0
43	1l	92	0TD	1	0
1	2A	2552	2MU	1	0
32	1a	966	M2G	1	0
32	1a	1404	5MC	1	0
32	1a	1518	MA6	3	0
32	2a	1404	5MC	1	0
32	2a	1400	5MC	4	0
32	1a	1519	MA6	4	0
32	2a	1519	MA6	1	0
32	1a	1402	4OC	2	0
32	1a	1498	UR3	1	0
1	2A	1939	5MU	3	0
1	2A	2251	OMG	1	0
32	2a	1518	MA6	1	0
32	2a	1402	4OC	1	0
43	2l	92	0TD	2	0
1	2A	1915	5MU	1	0

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry

Of 2540 ligands modelled in this entry, 2529 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
56	ARG	1B	230	54	10,11,11	0.82	1 (10%)	9,13,13	1.27	1 (11%)
55	MPD	1T	8004	-	7,7,7	0.33	0	9,10,10	0.32	0
55	MPD	18	102	-	7,7,7	0.23	0	9,10,10	0.58	0
55	MPD	2A	3748	-	7,7,7	0.33	0	9,10,10	0.26	0
55	MPD	1a	1880	-	7,7,7	0.62	0	9,10,10	0.69	0
55	MPD	2B	3020	-	7,7,7	0.33	0	9,10,10	0.37	0
58	SF4	2d	501	35	0,12,12	-	-	-	-	-
56	ARG	1F	311	-	10,11,11	0.73	1 (10%)	9,13,13	1.08	1 (11%)
55	MPD	2A	3747	-	7,7,7	0.39	0	9,10,10	0.51	0
55	MPD	1A	4028	-	7,7,7	0.32	0	9,10,10	0.16	0
58	SF4	1d	501	35	0,12,12	-	-	-	-	-

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
56	ARG	1B	230	54	-	2/11/11/11	-
55	MPD	1T	8004	-	-	2/5/5/5	-
55	MPD	18	102	-	-	2/5/5/5	-
55	MPD	2A	3748	-	-	5/5/5/5	-
55	MPD	1a	1880	-	-	1/5/5/5	-
55	MPD	2B	3020	-	-	1/5/5/5	-
58	SF4	2d	501	35	-	-	0/6/5/5
56	ARG	1F	311	-	-	3/11/11/11	-
55	MPD	2A	3747	-	-	0/5/5/5	-
55	MPD	1A	4028	-	-	1/5/5/5	-
58	SF4	1d	501	35	-	-	0/6/5/5

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
56	1B	230	ARG	OXT-C	-2.47	1.22	1.30
56	1F	311	ARG	OXT-C	-2.04	1.24	1.30

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
56	1F	311	ARG	OXT-C-O	-3.05	117.16	124.08
56	1B	230	ARG	OXT-C-O	-2.82	117.69	124.08

There are no chirality outliers.

5 of 17 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
55	18	102	MPD	C2-C3-C4-C5
55	2A	3748	MPD	C2-C3-C4-O4
55	2A	3748	MPD	C2-C3-C4-C5
56	1F	311	ARG	C-CA-CB-CG
56	1B	230	ARG	NE-CD-CG-CB

There are no ring outliers.

6 monomers are involved in 20 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
56	1B	230	ARG	1	0
55	18	102	MPD	5	0
55	1a	1880	MPD	8	0
56	1F	311	ARG	3	0
55	2A	3747	MPD	2	0
55	1A	4028	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%)	-0.46	111 (3%) 43 45	23, 40, 90, 100	0
1	2A	2856/2915 (97%)	-0.35	98 (3%) 48 50	26, 44, 91, 104	0
2	1B	120/121 (99%)	-0.15	1 (0%) 82 83	34, 56, 71, 86	0
2	2B	120/121 (99%)	0.21	1 (0%) 82 83	41, 61, 74, 87	0
3	1D	275/276 (99%)	0.03	7 (2%) 58 60	23, 37, 53, 78	0
3	2D	275/276 (99%)	0.02	5 (1%) 67 69	25, 41, 55, 77	0
4	1E	204/206 (99%)	0.20	3 (1%) 72 73	22, 43, 63, 72	0
4	2E	204/206 (99%)	0.20	2 (0%) 79 80	26, 47, 65, 74	0
5	1F	203/210 (96%)	0.33	5 (2%) 58 60	20, 46, 72, 84	0
5	2F	203/210 (96%)	0.50	7 (3%) 48 50	25, 52, 73, 85	0
6	1G	181/182 (99%)	0.81	11 (6%) 27 29	54, 70, 81, 90	0
6	2G	181/182 (99%)	1.64	56 (30%) 1 1	58, 73, 83, 91	0
7	1H	174/180 (96%)	1.06	16 (9%) 14 16	45, 62, 73, 78	0
7	2H	173/180 (96%)	1.47	38 (21%) 2 2	54, 67, 76, 80	0
8	1I	147/148 (99%)	1.22	18 (12%) 8 9	43, 71, 80, 84	0
8	2I	146/148 (98%)	1.39	27 (18%) 3 4	47, 71, 81, 84	0
9	1N	140/140 (100%)	-0.03	2 (1%) 73 75	25, 36, 60, 81	0
9	2N	140/140 (100%)	0.78	4 (2%) 53 56	39, 58, 74, 81	0
10	1O	122/122 (100%)	-0.10	2 (1%) 70 72	25, 37, 57, 64	0
10	2O	122/122 (100%)	0.39	1 (0%) 82 83	38, 52, 66, 74	0
11	1P	149/150 (99%)	0.18	3 (2%) 65 66	19, 43, 67, 78	0
11	2P	149/150 (99%)	0.66	9 (6%) 27 29	32, 62, 79, 85	0
12	1Q	141/141 (100%)	0.25	3 (2%) 63 65	28, 44, 58, 72	0
12	2Q	141/141 (100%)	0.37	3 (2%) 63 65	33, 49, 61, 74	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
13	1R	118/118 (100%)	-0.13	0 100 100	27, 38, 54, 63	0
13	2R	118/118 (100%)	-0.01	0 100 100	32, 42, 56, 64	0
14	1S	110/112 (98%)	0.67	5 (4%) 38 40	42, 56, 67, 71	0
14	2S	110/112 (98%)	1.29	16 (14%) 6 7	48, 60, 70, 74	0
15	1T	131/146 (89%)	0.55	9 (6%) 23 25	34, 47, 72, 82	0
15	2T	131/146 (89%)	0.36	5 (3%) 44 46	39, 49, 74, 83	0
16	1U	116/118 (98%)	0.11	2 (1%) 69 70	25, 36, 53, 68	0
16	2U	116/118 (98%)	0.33	1 (0%) 81 82	30, 43, 57, 70	0
17	1V	101/101 (100%)	0.48	2 (1%) 65 66	26, 48, 63, 73	0
17	2V	101/101 (100%)	0.64	1 (0%) 79 80	30, 54, 67, 74	0
18	1W	112/113 (99%)	-0.05	2 (1%) 67 69	28, 34, 55, 87	0
18	2W	112/113 (99%)	0.07	3 (2%) 56 58	32, 38, 58, 87	0
19	1X	95/96 (98%)	0.40	7 (7%) 20 22	32, 42, 63, 74	0
19	2X	95/96 (98%)	0.67	5 (5%) 32 34	37, 47, 67, 76	0
20	1Y	107/110 (97%)	0.83	6 (5%) 30 32	39, 54, 69, 78	0
20	2Y	107/110 (97%)	1.18	14 (13%) 7 8	43, 58, 72, 80	0
21	1Z	203/206 (98%)	1.03	15 (7%) 20 22	45, 63, 78, 83	0
21	2Z	201/206 (97%)	1.16	18 (8%) 15 16	50, 66, 78, 82	0
22	10	77/85 (90%)	-0.15	2 (2%) 57 59	26, 35, 52, 63	0
22	20	77/85 (90%)	0.93	3 (3%) 43 45	41, 57, 68, 81	0
23	11	97/98 (98%)	0.16	1 (1%) 79 80	26, 41, 68, 76	0
23	21	97/98 (98%)	0.43	3 (3%) 51 53	35, 51, 72, 75	0
24	12	70/72 (97%)	0.69	5 (7%) 22 24	40, 53, 65, 82	0
24	22	70/72 (97%)	0.73	2 (2%) 53 56	45, 59, 68, 81	0
25	13	59/60 (98%)	0.23	3 (5%) 33 35	28, 40, 67, 80	0
25	23	59/60 (98%)	0.72	5 (8%) 16 18	34, 45, 70, 80	0
26	14	69/71 (97%)	1.32	13 (18%) 3 4	67, 81, 90, 94	0
26	24	69/71 (97%)	2.36	37 (53%) 0 0	70, 82, 90, 94	0
27	15	59/60 (98%)	-0.11	1 (1%) 69 70	22, 37, 59, 69	0
27	25	59/60 (98%)	-0.09	1 (1%) 69 70	25, 40, 61, 70	0
28	16	53/54 (98%)	0.24	0 100 100	34, 45, 61, 64	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
28	26	53/54 (98%)	0.29	0 100 100	39, 49, 61, 66	0
29	17	48/49 (97%)	0.08	5 (10%) 11 13	22, 30, 58, 68	0
29	27	48/49 (97%)	0.04	5 (10%) 11 13	26, 33, 60, 68	0
30	18	64/65 (98%)	0.09	1 (1%) 70 72	30, 38, 45, 61	0
30	28	64/65 (98%)	0.15	0 100 100	33, 42, 49, 64	0
31	19	37/37 (100%)	-0.08	1 (2%) 56 58	29, 39, 55, 56	0
31	29	37/37 (100%)	0.67	0 100 100	45, 60, 72, 75	0
32	1a	1488/1521 (97%)	0.05	31 (2%) 63 65	34, 63, 89, 102	0
32	2a	1492/1521 (98%)	0.27	34 (2%) 61 63	44, 73, 92, 103	0
33	1b	231/256 (90%)	1.38	47 (20%) 3 3	65, 78, 86, 91	0
33	2b	231/256 (90%)	1.91	91 (39%) 1 0	67, 79, 87, 93	0
34	1c	206/239 (86%)	1.30	30 (14%) 6 6	63, 74, 83, 89	0
34	2c	206/239 (86%)	2.05	96 (46%) 0 0	65, 76, 84, 90	0
35	1d	208/209 (99%)	1.45	43 (20%) 2 3	55, 69, 79, 84	0
35	2d	208/209 (99%)	1.42	43 (20%) 2 3	57, 69, 78, 84	0
36	1e	148/162 (91%)	0.71	4 (2%) 56 58	46, 61, 72, 87	0
36	2e	148/162 (91%)	1.16	12 (8%) 18 19	56, 70, 79, 87	0
37	1f	100/101 (99%)	0.84	1 (1%) 79 80	53, 64, 74, 79	0
37	2f	100/101 (99%)	0.97	4 (4%) 42 44	53, 64, 74, 79	0
38	1g	155/156 (99%)	1.18	21 (13%) 7 8	62, 72, 81, 84	0
38	2g	155/156 (99%)	1.69	47 (30%) 1 1	66, 74, 81, 84	0
39	1h	137/138 (99%)	0.90	7 (5%) 33 35	54, 67, 74, 77	0
39	2h	137/138 (99%)	1.03	9 (6%) 24 26	56, 68, 75, 78	0
40	1i	127/128 (99%)	1.51	31 (24%) 2 2	60, 78, 85, 88	0
40	2i	126/128 (98%)	2.26	73 (57%) 0 0	64, 79, 86, 89	0
41	1j	97/105 (92%)	1.71	33 (34%) 1 1	59, 79, 88, 91	0
41	2j	96/105 (91%)	2.34	58 (60%) 0 0	65, 80, 88, 91	0
42	1k	114/129 (88%)	1.02	11 (9%) 13 15	46, 63, 77, 79	0
42	2k	114/129 (88%)	1.21	17 (14%) 5 6	48, 65, 77, 80	0
43	1l	121/132 (91%)	0.90	11 (9%) 15 16	48, 58, 70, 75	0
43	2l	121/132 (91%)	0.88	10 (8%) 17 19	51, 60, 70, 77	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
44	1m	116/126 (92%)	0.90	10 (8%) 16 17	54, 71, 79, 84	0
44	2m	114/126 (90%)	2.01	50 (43%) 0 0	73, 82, 87, 91	0
45	1n	60/61 (98%)	1.28	9 (15%) 5 6	64, 71, 78, 79	0
45	2n	60/61 (98%)	2.12	33 (55%) 0 0	67, 74, 80, 87	0
46	1o	88/89 (98%)	0.83	6 (6%) 23 25	46, 64, 77, 79	0
46	2o	88/89 (98%)	1.02	9 (10%) 12 13	50, 65, 78, 80	0
47	1p	82/88 (93%)	1.69	25 (30%) 1 1	58, 68, 78, 81	0
47	2p	82/88 (93%)	1.59	14 (17%) 4 5	59, 68, 77, 83	0
48	1q	99/105 (94%)	1.09	8 (8%) 18 19	53, 66, 75, 79	0
48	2q	99/105 (94%)	0.93	4 (4%) 42 44	53, 66, 76, 80	0
49	1r	68/88 (77%)	0.92	9 (13%) 7 8	55, 65, 77, 79	0
49	2r	68/88 (77%)	0.95	6 (8%) 15 17	55, 66, 77, 79	0
50	1s	83/93 (89%)	1.45	13 (15%) 5 6	67, 77, 83, 85	0
50	2s	83/93 (89%)	2.34	56 (67%) 0 0	70, 79, 84, 86	0
51	1t	96/106 (90%)	1.40	21 (21%) 2 2	57, 68, 79, 83	0
51	2t	98/106 (92%)	1.05	10 (10%) 12 13	57, 69, 81, 83	0
52	1u	23/27 (85%)	1.53	6 (26%) 1 2	69, 72, 76, 78	0
52	2u	23/27 (85%)	2.18	14 (60%) 0 0	71, 74, 77, 80	0
53	1y	97/113 (85%)	0.69	8 (8%) 17 19	44, 56, 70, 74	0
53	2y	96/113 (84%)	1.19	15 (15%) 5 6	57, 71, 79, 83	0
All	All	20766/21468 (96%)	0.41	1722 (8%) 17 19	19, 58, 85, 104	0

The worst 5 of 1722 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
45	2n	2	ALA	8.7
26	24	56	VAL	7.9
1	1A	1122	C	7.8
40	2i	102	LEU	6.8
15	1T	131	ALA	6.6

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($\text{\AA}^2$)	Q<0.9
1	5MU	2A	1915	21/22	0.80	0.15	70,82,87,103	0
1	PSU	2A	1917	20/21	0.85	0.13	62,74,84,89	0
1	5MU	1A	1937	21/22	0.87	0.13	65,79,86,95	0
32	M2G	2a	966	25/26	0.87	0.14	52,68,81,90	0
1	PSU	2A	1911	20/21	0.88	0.11	62,68,73,82	0
32	2MG	2a	1207	24/25	0.88	0.12	75,83,90,94	0
1	PSU	1A	1939	20/21	0.89	0.11	63,73,82,86	0
43	0TD	2l	92	10/11	0.91	0.12	57,63,66,74	0
32	PSU	2a	516	20/21	0.92	0.10	69,76,81,82	0
1	4OC	2A	1920	21/23	0.92	0.11	57,62,67,67	0
43	0TD	1l	92	10/11	0.93	0.14	54,59,68,68	0
32	5MC	2a	967	21/22	0.93	0.10	61,68,77,86	0
32	2MG	1a	1207	24/25	0.93	0.10	60,68,71,74	0
32	7MG	2a	527	24/25	0.93	0.12	57,66,70,73	0
32	4OC	2a	1402	22/23	0.94	0.10	53,64,74,82	0
32	5MC	1a	967	21/22	0.94	0.11	51,61,73,83	0
1	PSU	1A	1933	20/21	0.95	0.08	59,66,68,81	0
32	5MC	2a	1404	21/22	0.95	0.09	54,61,64,67	0
32	5MC	2a	1407	21/22	0.95	0.10	46,62,69,70	0
32	UR3	2a	1498	21/22	0.95	0.09	53,60,65,73	0
32	PSU	1a	516	20/21	0.95	0.08	49,58,65,67	0
32	5MC	1a	1400	21/22	0.96	0.09	37,50,57,58	0
32	5MC	1a	1407	21/22	0.96	0.09	41,48,54,56	0
32	5MC	2a	1400	21/22	0.96	0.10	62,68,74,77	0
32	UR3	1a	1498	21/22	0.96	0.08	35,46,53,56	0
1	5MC	2A	1942	21/22	0.96	0.08	36,45,52,53	0
32	MA6	1a	1519	24/25	0.96	0.10	40,45,52,52	0
1	4OC	1A	1942	21/23	0.96	0.11	52,60,63,65	0
32	MA6	2a	1518	24/25	0.96	0.08	47,58,65,68	0
32	7MG	1a	527	24/25	0.96	0.08	40,48,55,55	0
32	MA6	1a	1518	24/25	0.97	0.09	37,44,51,56	0
32	4OC	1a	1402	22/23	0.97	0.07	41,47,51,56	0
32	5MC	1a	1404	21/22	0.97	0.07	33,43,49,51	0
32	M2G	1a	966	25/26	0.97	0.08	48,53,59,65	0
32	MA6	2a	1519	24/25	0.97	0.09	51,61,64,69	0
1	5MC	1A	1964	21/22	0.97	0.07	34,41,47,52	0
1	5MU	1A	1961	21/22	0.98	0.06	24,30,34,37	0
1	5MC	1A	1984	21/22	0.98	0.06	29,36,41,47	0
1	5MU	2A	1939	21/22	0.98	0.06	28,33,37,42	0
1	2MA	1A	2515	23/24	0.98	0.07	17,23,28,31	0
1	5MC	2A	1962	21/22	0.98	0.08	32,38,44,54	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
1	OMG	2A	2251	24/25	0.98	0.07	27,31,35,37	0
1	2MA	2A	2503	23/24	0.98	0.06	21,28,32,37	0
1	2MU	2A	2552	21/23	0.98	0.06	27,33,38,38	0
1	PSU	2A	2605	20/21	0.98	0.06	27,31,39,41	0
1	2MU	1A	2564	21/23	0.98	0.06	24,29,33,36	0
1	PSU	1A	2617	20/21	0.98	0.07	23,29,35,38	0
1	OMG	1A	2263	24/25	0.99	0.06	22,28,29,33	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
54	MG	1A	3990	1/1	0.44	0.29	83,83,83,83	0
54	MG	1a	1788	1/1	0.46	0.22	85,85,85,85	0
54	MG	1A	3747	1/1	0.52	0.16	62,62,62,62	0
54	MG	1a	1773	1/1	0.56	0.26	85,85,85,85	0
54	MG	1A	3513	1/1	0.57	0.21	58,58,58,58	0
54	MG	1a	1850	1/1	0.57	0.21	94,94,94,94	0
54	MG	2O	202	1/1	0.59	0.37	94,94,94,94	0
54	MG	1A	3295	1/1	0.60	0.28	84,84,84,84	0
54	MG	1A	3496	1/1	0.62	0.18	56,56,56,56	0
54	MG	1a	1719	1/1	0.62	0.19	94,94,94,94	0
54	MG	14	502	1/1	0.64	0.14	83,83,83,83	0
54	MG	1A	3528	1/1	0.64	0.23	61,61,61,61	0
54	MG	1A	3612	1/1	0.64	0.43	66,66,66,66	0
54	MG	2a	1787	1/1	0.64	0.27	82,82,82,82	0
54	MG	1a	1744	1/1	0.65	0.38	88,88,88,88	0
54	MG	1A	3579	1/1	0.65	0.22	74,74,74,74	0
54	MG	1T	8003	1/1	0.65	0.21	72,72,72,72	0
54	MG	1a	1836	1/1	0.66	0.24	83,83,83,83	0
54	MG	2A	3478	1/1	0.67	0.28	64,64,64,64	0
54	MG	2B	3015	1/1	0.68	0.18	87,87,87,87	0
54	MG	2A	3360	1/1	0.68	0.20	72,72,72,72	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	2a	1667	1/1	0.68	0.23	83,83,83,83	0
54	MG	1A	3964	1/1	0.68	0.19	68,68,68,68	0
54	MG	1A	3810	1/1	0.69	0.26	80,80,80,80	0
54	MG	2A	3408	1/1	0.70	0.33	74,74,74,74	0
54	MG	1B	221	1/1	0.70	0.15	48,48,48,48	0
54	MG	1A	3377	1/1	0.70	0.28	67,67,67,67	0
54	MG	2A	3509	1/1	0.71	0.19	75,75,75,75	0
54	MG	1A	3949	1/1	0.71	0.23	69,69,69,69	0
54	MG	1a	1732	1/1	0.71	0.24	92,92,92,92	0
54	MG	1a	1791	1/1	0.71	0.14	72,72,72,72	0
54	MG	1A	3593	1/1	0.71	0.15	62,62,62,62	0
54	MG	2A	3502	1/1	0.72	0.17	61,61,61,61	0
54	MG	1a	1872	1/1	0.72	0.26	83,83,83,83	0
54	MG	2A	3720	1/1	0.72	0.17	55,55,55,55	0
54	MG	2A	3231	1/1	0.72	0.14	61,61,61,61	0
54	MG	1a	1803	1/1	0.72	0.21	87,87,87,87	0
54	MG	1A	3664	1/1	0.72	0.13	60,60,60,60	0
54	MG	1A	3889	1/1	0.72	0.22	47,47,47,47	0
54	MG	1A	3788	1/1	0.73	0.27	66,66,66,66	0
54	MG	2A	3495	1/1	0.73	0.12	54,54,54,54	0
54	MG	1A	3577	1/1	0.73	0.23	41,41,41,41	0
54	MG	1A	3833	1/1	0.73	0.18	60,60,60,60	0
54	MG	2A	3582	1/1	0.73	0.16	70,70,70,70	0
54	MG	1A	3882	1/1	0.73	0.23	74,74,74,74	0
54	MG	1A	3643	1/1	0.73	0.21	72,72,72,72	0
54	MG	1A	3415	1/1	0.73	0.15	63,63,63,63	0
54	MG	1A	3694	1/1	0.73	0.25	69,69,69,69	0
54	MG	1A	3511	1/1	0.73	0.15	64,64,64,64	0
54	MG	2a	1788	1/1	0.73	0.15	102,102,102,102	0
54	MG	2A	3729	1/1	0.74	0.12	59,59,59,59	0
54	MG	2A	3438	1/1	0.74	0.16	56,56,56,56	0
54	MG	2A	3465	1/1	0.74	0.23	67,67,67,67	0
54	MG	1A	3331	1/1	0.74	0.23	75,75,75,75	0
54	MG	2a	1689	1/1	0.74	0.23	70,70,70,70	0
54	MG	2A	3593	1/1	0.74	0.14	48,48,48,48	0
54	MG	1a	1834	1/1	0.74	0.20	59,59,59,59	0
54	MG	1a	1751	1/1	0.75	0.22	67,67,67,67	0
54	MG	1A	3583	1/1	0.75	0.16	43,43,43,43	0
54	MG	1A	3631	1/1	0.75	0.38	74,74,74,74	0
54	MG	2A	3426	1/1	0.75	0.18	58,58,58,58	0
54	MG	2A	3157	1/1	0.75	0.24	68,68,68,68	0
54	MG	2A	3584	1/1	0.76	0.24	49,49,49,49	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	1a	1815	1/1	0.76	0.16	75,75,75,75	0
54	MG	1A	3553	1/1	0.76	0.24	68,68,68,68	0
54	MG	1a	1752	1/1	0.76	0.20	73,73,73,73	0
54	MG	1B	207	1/1	0.76	0.23	68,68,68,68	0
54	MG	2E	303	1/1	0.76	0.27	72,72,72,72	0
54	MG	1A	3866	1/1	0.76	0.13	64,64,64,64	0
54	MG	1A	3573	1/1	0.76	0.21	59,59,59,59	0
54	MG	1a	1793	1/1	0.76	0.15	67,67,67,67	0
54	MG	2a	1693	1/1	0.76	0.35	88,88,88,88	0
54	MG	2a	1724	1/1	0.76	0.30	82,82,82,82	0
54	MG	2A	3306	1/1	0.76	0.14	56,56,56,56	0
54	MG	1a	1749	1/1	0.76	0.19	70,70,70,70	0
54	MG	1A	3328	1/1	0.77	0.16	19,19,19,19	0
54	MG	1A	3890	1/1	0.77	0.22	62,62,62,62	0
54	MG	1A	3432	1/1	0.77	0.19	67,67,67,67	0
54	MG	1a	1762	1/1	0.77	0.23	80,80,80,80	0
54	MG	2A	3534	1/1	0.77	0.29	78,78,78,78	0
54	MG	1A	3858	1/1	0.77	0.14	68,68,68,68	0
54	MG	1A	3639	1/1	0.77	0.11	65,65,65,65	0
54	MG	1A	3407	1/1	0.77	0.19	66,66,66,66	0
54	MG	2A	3598	1/1	0.77	0.15	72,72,72,72	0
54	MG	2A	3129	1/1	0.77	0.11	63,63,63,63	0
54	MG	1g	203	1/1	0.78	0.28	78,78,78,78	0
54	MG	2A	3609	1/1	0.78	0.13	58,58,58,58	0
54	MG	2A	3717	1/1	0.78	0.14	60,60,60,60	0
54	MG	2A	3464	1/1	0.78	0.23	63,63,63,63	0
54	MG	1q	202	1/1	0.78	0.25	73,73,73,73	0
54	MG	1A	3825	1/1	0.78	0.20	70,70,70,70	0
54	MG	1A	3224	1/1	0.78	0.15	69,69,69,69	0
54	MG	1a	1841	1/1	0.78	0.20	61,61,61,61	0
54	MG	2a	1649	1/1	0.78	0.17	75,75,75,75	0
54	MG	2a	1650	1/1	0.78	0.30	74,74,74,74	0
54	MG	2a	1656	1/1	0.78	0.22	69,69,69,69	0
54	MG	2A	3277	1/1	0.78	0.17	58,58,58,58	0
54	MG	2a	1668	1/1	0.78	0.31	77,77,77,77	0
54	MG	1a	1685	1/1	0.78	0.18	75,75,75,75	0
54	MG	2A	3569	1/1	0.78	0.20	55,55,55,55	0
54	MG	1a	1859	1/1	0.78	0.19	72,72,72,72	0
54	MG	1B	225	1/1	0.78	0.27	68,68,68,68	0
54	MG	1a	1878	1/1	0.78	0.20	66,66,66,66	0
54	MG	2A	3384	1/1	0.79	0.13	46,46,46,46	0
54	MG	1A	3973	1/1	0.79	0.15	44,44,44,44	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	2G	3002	1/1	0.79	0.20	79,79,79,79	0
54	MG	2A	3418	1/1	0.79	0.17	71,71,71,71	0
54	MG	2a	1637	1/1	0.79	0.19	92,92,92,92	0
54	MG	2a	1641	1/1	0.79	0.29	70,70,70,70	0
54	MG	1A	3975	1/1	0.79	0.18	52,52,52,52	0
54	MG	2A	3576	1/1	0.79	0.14	49,49,49,49	0
54	MG	2A	3431	1/1	0.79	0.19	57,57,57,57	0
54	MG	2a	1666	1/1	0.79	0.30	78,78,78,78	0
54	MG	1A	3870	1/1	0.79	0.23	71,71,71,71	0
54	MG	1A	3171	1/1	0.79	0.14	56,56,56,56	0
54	MG	2a	1687	1/1	0.79	0.26	82,82,82,82	0
54	MG	1a	1874	1/1	0.79	0.14	66,66,66,66	0
54	MG	2A	3468	1/1	0.79	0.20	72,72,72,72	0
54	MG	2a	1719	1/1	0.79	0.22	76,76,76,76	0
54	MG	1A	3960	1/1	0.79	0.15	71,71,71,71	0
54	MG	2A	3481	1/1	0.79	0.15	69,69,69,69	0
54	MG	1A	3566	1/1	0.79	0.15	60,60,60,60	0
54	MG	2j	8001	1/1	0.79	0.12	82,82,82,82	0
54	MG	1A	4003	1/1	0.80	0.23	66,66,66,66	0
54	MG	1A	3365	1/1	0.80	0.19	69,69,69,69	0
54	MG	2A	3336	1/1	0.80	0.15	55,55,55,55	0
54	MG	1A	3752	1/1	0.80	0.21	57,57,57,57	0
54	MG	2A	3365	1/1	0.80	0.23	68,68,68,68	0
54	MG	1A	3763	1/1	0.80	0.18	53,53,53,53	0
54	MG	1B	227	1/1	0.80	0.14	76,76,76,76	0
54	MG	1a	1800	1/1	0.80	0.18	70,70,70,70	0
54	MG	1F	307	1/1	0.80	0.17	49,49,49,49	0
54	MG	1F	309	1/1	0.80	0.16	69,69,69,69	0
54	MG	2a	1633	1/1	0.80	0.32	69,69,69,69	0
54	MG	1A	3576	1/1	0.80	0.21	57,57,57,57	0
54	MG	1A	3916	1/1	0.80	0.30	68,68,68,68	0
54	MG	1a	1602	1/1	0.80	0.14	73,73,73,73	0
54	MG	1a	1659	1/1	0.80	0.28	76,76,76,76	0
54	MG	1a	1676	1/1	0.80	0.35	75,75,75,75	0
54	MG	2a	1664	1/1	0.80	0.29	79,79,79,79	0
54	MG	1A	3530	1/1	0.80	0.18	69,69,69,69	0
54	MG	2A	3486	1/1	0.80	0.13	63,63,63,63	0
54	MG	1a	1702	1/1	0.80	0.21	67,67,67,67	0
54	MG	1A	3426	1/1	0.80	0.14	34,34,34,34	0
54	MG	1A	3963	1/1	0.80	0.20	67,67,67,67	0
54	MG	2A	3526	1/1	0.80	0.18	66,66,66,66	0
54	MG	2a	1706	1/1	0.80	0.19	74,74,74,74	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	2a	1710	1/1	0.80	0.30	71,71,71,71	0
54	MG	1A	3830	1/1	0.80	0.14	65,65,65,65	0
54	MG	2a	1721	1/1	0.80	0.24	71,71,71,71	0
54	MG	1A	3557	1/1	0.80	0.16	61,61,61,61	0
54	MG	2a	1778	1/1	0.80	0.14	79,79,79,79	0
54	MG	1A	3371	1/1	0.80	0.14	65,65,65,65	0
54	MG	2A	3174	1/1	0.80	0.22	61,61,61,61	0
54	MG	2a	1789	1/1	0.80	0.37	80,80,80,80	0
54	MG	1A	3706	1/1	0.80	0.17	64,64,64,64	0
55	MPD	1a	1880	8/8	0.80	0.22	48,59,72,72	0
54	MG	1A	3431	1/1	0.81	0.13	61,61,61,61	0
54	MG	1A	3688	1/1	0.81	0.26	80,80,80,80	0
54	MG	2B	3006	1/1	0.81	0.27	72,72,72,72	0
54	MG	2A	3414	1/1	0.81	0.26	65,65,65,65	0
54	MG	1a	1822	1/1	0.81	0.26	68,68,68,68	0
54	MG	2A	3527	1/1	0.81	0.13	66,66,66,66	0
54	MG	1A	3786	1/1	0.81	0.21	64,64,64,64	0
54	MG	2a	1630	1/1	0.81	0.24	71,71,71,71	0
54	MG	1a	1684	1/1	0.81	0.37	73,73,73,73	0
54	MG	1a	1768	1/1	0.81	0.17	71,71,71,71	0
54	MG	1A	3434	1/1	0.81	0.29	72,72,72,72	0
54	MG	1A	3450	1/1	0.81	0.15	57,57,57,57	0
54	MG	2A	3329	1/1	0.81	0.19	60,60,60,60	0
54	MG	1A	4051	1/1	0.81	0.22	52,52,52,52	0
54	MG	1W	3001	1/1	0.81	0.24	59,59,59,59	0
54	MG	1A	3646	1/1	0.81	0.31	81,81,81,81	0
54	MG	2A	3633	1/1	0.82	0.30	68,68,68,68	0
54	MG	2A	3513	1/1	0.82	0.22	58,58,58,58	0
54	MG	2A	3524	1/1	0.82	0.15	64,64,64,64	0
54	MG	1B	217	1/1	0.82	0.20	70,70,70,70	0
54	MG	2B	3001	1/1	0.82	0.13	68,68,68,68	0
54	MG	2B	3002	1/1	0.82	0.17	72,72,72,72	0
54	MG	2a	1686	1/1	0.82	0.26	66,66,66,66	0
54	MG	1a	1696	1/1	0.82	0.25	68,68,68,68	0
54	MG	2A	3528	1/1	0.82	0.29	67,67,67,67	0
54	MG	2D	301	1/1	0.82	0.24	55,55,55,55	0
54	MG	2A	3387	1/1	0.82	0.21	55,55,55,55	0
54	MG	1A	3625	1/1	0.82	0.16	63,63,63,63	0
54	MG	2A	3292	1/1	0.82	0.16	55,55,55,55	0
54	MG	2a	1609	1/1	0.82	0.33	74,74,74,74	0
54	MG	2a	1618	1/1	0.82	0.11	75,75,75,75	0
54	MG	1a	1811	1/1	0.82	0.26	78,78,78,78	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	2A	3055	1/1	0.82	0.12	54,54,54,54	0
54	MG	2A	3498	1/1	0.82	0.16	58,58,58,58	0
54	MG	2a	1638	1/1	0.82	0.19	62,62,62,62	0
54	MG	1a	1705	1/1	0.82	0.16	56,56,56,56	0
54	MG	1a	1613	1/1	0.82	0.43	71,71,71,71	0
55	MPD	2B	3020	8/8	0.82	0.23	47,70,77,79	0
54	MG	1A	3680	1/1	0.83	0.12	66,66,66,66	0
54	MG	1A	3922	1/1	0.83	0.10	30,30,30,30	0
54	MG	1A	3571	1/1	0.83	0.13	65,65,65,65	0
54	MG	1a	1776	1/1	0.83	0.27	80,80,80,80	0
54	MG	2A	3388	1/1	0.83	0.17	55,55,55,55	0
54	MG	1a	1689	1/1	0.83	0.39	73,73,73,73	0
54	MG	1b	3001	1/1	0.83	0.18	87,87,87,87	0
54	MG	1d	506	1/1	0.83	0.10	93,93,93,93	0
54	MG	2A	3420	1/1	0.83	0.16	54,54,54,54	0
54	MG	2a	1661	1/1	0.83	0.34	74,74,74,74	0
54	MG	1A	3038	1/1	0.83	0.18	60,60,60,60	0
54	MG	1A	3697	1/1	0.83	0.20	53,53,53,53	0
54	MG	2A	3035	1/1	0.83	0.21	67,67,67,67	0
54	MG	1A	3400	1/1	0.83	0.18	61,61,61,61	0
54	MG	1A	3721	1/1	0.83	0.21	64,64,64,64	0
54	MG	2A	3467	1/1	0.83	0.19	67,67,67,67	0
54	MG	1a	1805	1/1	0.83	0.17	68,68,68,68	0
54	MG	1A	3294	1/1	0.83	0.15	74,74,74,74	0
54	MG	2a	1705	1/1	0.83	0.17	75,75,75,75	0
54	MG	2A	3226	1/1	0.83	0.31	69,69,69,69	0
54	MG	2A	3484	1/1	0.83	0.18	66,66,66,66	0
54	MG	2B	3010	1/1	0.83	0.23	80,80,80,80	0
54	MG	1a	1736	1/1	0.83	0.23	66,66,66,66	0
54	MG	1A	3219	1/1	0.83	0.21	65,65,65,65	0
54	MG	2a	1771	1/1	0.83	0.15	86,86,86,86	0
54	MG	2a	1774	1/1	0.83	0.18	66,66,66,66	0
54	MG	1a	1832	1/1	0.83	0.19	72,72,72,72	0
54	MG	1A	3418	1/1	0.83	0.15	55,55,55,55	0
54	MG	1A	3765	1/1	0.83	0.16	71,71,71,71	0
54	MG	2R	8001	1/1	0.83	0.15	52,52,52,52	0
54	MG	2I	101	1/1	0.83	0.09	69,69,69,69	0
54	MG	2a	1603	1/1	0.83	0.17	69,69,69,69	0
55	MPD	2A	3747	8/8	0.83	0.27	37,47,59,61	0
54	MG	1A	3312	1/1	0.83	0.23	72,72,72,72	0
54	MG	1A	3590	1/1	0.84	0.19	72,72,72,72	0
54	MG	2A	3247	1/1	0.84	0.21	55,55,55,55	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	2a	1640	1/1	0.84	0.30	66,66,66,66	0
54	MG	2A	3627	1/1	0.84	0.15	60,60,60,60	0
54	MG	1A	3084	1/1	0.84	0.20	58,58,58,58	0
54	MG	1A	3768	1/1	0.84	0.19	67,67,67,67	0
54	MG	1A	3770	1/1	0.84	0.12	34,34,34,34	0
54	MG	2a	1659	1/1	0.84	0.32	75,75,75,75	0
54	MG	2A	3725	1/1	0.84	0.13	61,61,61,61	0
54	MG	2A	3310	1/1	0.84	0.17	62,62,62,62	0
54	MG	1A	3192	1/1	0.84	0.26	68,68,68,68	0
54	MG	1A	3621	1/1	0.84	0.15	65,65,65,65	0
54	MG	2B	3004	1/1	0.84	0.11	77,77,77,77	0
54	MG	2a	1672	1/1	0.84	0.35	73,73,73,73	0
54	MG	2a	1679	1/1	0.84	0.28	67,67,67,67	0
54	MG	1A	3405	1/1	0.84	0.25	65,65,65,65	0
54	MG	1A	3196	1/1	0.84	0.24	72,72,72,72	0
54	MG	2B	3014	1/1	0.84	0.14	65,65,65,65	0
54	MG	1a	1801	1/1	0.84	0.16	80,80,80,80	0
54	MG	1A	3561	1/1	0.84	0.18	62,62,62,62	0
54	MG	1A	3726	1/1	0.84	0.12	50,50,50,50	0
54	MG	1A	3581	1/1	0.84	0.17	67,67,67,67	0
54	MG	2a	1715	1/1	0.84	0.24	71,71,71,71	0
54	MG	1A	3409	1/1	0.84	0.16	58,58,58,58	0
54	MG	1a	1820	1/1	0.84	0.21	76,76,76,76	0
54	MG	1A	3754	1/1	0.84	0.23	59,59,59,59	0
54	MG	2a	1765	1/1	0.84	0.22	68,68,68,68	0
54	MG	2A	3171	1/1	0.84	0.16	56,56,56,56	0
54	MG	2a	1605	1/1	0.84	0.16	63,63,63,63	0
54	MG	2a	1608	1/1	0.84	0.37	69,69,69,69	0
54	MG	1a	1614	1/1	0.84	0.27	74,74,74,74	0
54	MG	2A	3191	1/1	0.84	0.11	53,53,53,53	0
54	MG	2a	1620	1/1	0.84	0.30	77,77,77,77	0
54	MG	2A	3455	1/1	0.84	0.17	62,62,62,62	0
55	MPD	1T	8004	8/8	0.84	0.24	56,61,69,80	0
54	MG	2a	1631	1/1	0.84	0.24	77,77,77,77	0
54	MG	1a	1648	1/1	0.84	0.30	56,56,56,56	0
54	MG	2a	1635	1/1	0.84	0.17	67,67,67,67	0
57	ZN	24	501	1/1	0.84	0.10	257,257,257,257	0
54	MG	1a	1673	1/1	0.85	0.25	71,71,71,71	0
54	MG	2a	1604	1/1	0.85	0.21	66,66,66,66	0
54	MG	1a	1675	1/1	0.85	0.47	70,70,70,70	0
54	MG	1A	3745	1/1	0.85	0.11	71,71,71,71	0
54	MG	2A	3499	1/1	0.85	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
54	MG	1A	3666	1/1	0.85	0.10	64,64,64,64	0
54	MG	1A	3956	1/1	0.85	0.22	60,60,60,60	0
54	MG	2a	1622	1/1	0.85	0.34	74,74,74,74	0
54	MG	2a	1626	1/1	0.85	0.22	70,70,70,70	0
54	MG	2A	3237	1/1	0.85	0.28	65,65,65,65	0
54	MG	2A	3516	1/1	0.85	0.13	58,58,58,58	0
54	MG	2A	3244	1/1	0.85	0.17	56,56,56,56	0
54	MG	1A	3267	1/1	0.85	0.10	82,82,82,82	0
54	MG	2A	3251	1/1	0.85	0.17	53,53,53,53	0
54	MG	1E	304	1/1	0.85	0.15	59,59,59,59	0
54	MG	1a	1699	1/1	0.85	0.29	73,73,73,73	0
54	MG	2A	3549	1/1	0.85	0.11	51,51,51,51	0
54	MG	1A	3454	1/1	0.85	0.15	31,31,31,31	0
54	MG	2A	3572	1/1	0.85	0.16	52,52,52,52	0
54	MG	1a	1829	1/1	0.85	0.30	70,70,70,70	0
54	MG	1A	3758	1/1	0.85	0.17	66,66,66,66	0
54	MG	1R	203	1/1	0.85	0.14	48,48,48,48	0
54	MG	2a	1663	1/1	0.85	0.27	67,67,67,67	0
54	MG	1a	1730	1/1	0.85	0.12	62,62,62,62	0
54	MG	1T	8002	1/1	0.85	0.19	61,61,61,61	0
54	MG	2A	3367	1/1	0.85	0.16	66,66,66,66	0
54	MG	2A	3620	1/1	0.85	0.12	42,42,42,42	0
54	MG	2A	3625	1/1	0.85	0.16	43,43,43,43	0
54	MG	1a	1845	1/1	0.85	0.30	68,68,68,68	0
54	MG	1A	3638	1/1	0.85	0.19	35,35,35,35	0
54	MG	2A	3668	1/1	0.85	0.15	73,73,73,73	0
54	MG	2A	3684	1/1	0.85	0.13	62,62,62,62	0
54	MG	1A	3274	1/1	0.85	0.25	74,74,74,74	0
54	MG	2A	3391	1/1	0.85	0.22	71,71,71,71	0
54	MG	1a	1863	1/1	0.85	0.14	64,64,64,64	0
54	MG	2a	1707	1/1	0.85	0.14	65,65,65,65	0
54	MG	1a	1869	1/1	0.85	0.23	74,74,74,74	0
54	MG	2A	3737	1/1	0.85	0.12	37,37,37,37	0
54	MG	2a	1718	1/1	0.85	0.32	82,82,82,82	0
54	MG	10	104	1/1	0.85	0.15	64,64,64,64	0
54	MG	1A	3506	1/1	0.85	0.19	36,36,36,36	0
54	MG	1A	3708	1/1	0.85	0.12	64,64,64,64	0
54	MG	2a	1733	1/1	0.85	0.12	83,83,83,83	0
54	MG	2a	1739	1/1	0.85	0.13	79,79,79,79	0
54	MG	1a	1753	1/1	0.85	0.16	62,62,62,62	0
54	MG	2B	3007	1/1	0.85	0.13	76,76,76,76	0
54	MG	1A	4004	1/1	0.85	0.10	56,56,56,56	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	1A	3616	1/1	0.85	0.10	55,55,55,55	0
54	MG	1a	1631	1/1	0.85	0.33	70,70,70,70	0
54	MG	1a	1774	1/1	0.85	0.21	68,68,68,68	0
54	MG	2A	3048	1/1	0.85	0.18	66,66,66,66	0
54	MG	1B	202	1/1	0.85	0.18	63,63,63,63	0
54	MG	2N	8001	1/1	0.85	0.12	78,78,78,78	0
54	MG	1a	1658	1/1	0.85	0.29	61,61,61,61	0
54	MG	2A	3144	1/1	0.85	0.12	53,53,53,53	0
54	MG	1A	3531	1/1	0.85	0.20	66,66,66,66	0
54	MG	2a	1601	1/1	0.85	0.18	69,69,69,69	0
54	MG	1a	1677	1/1	0.86	0.30	63,63,63,63	0
54	MG	1a	1680	1/1	0.86	0.22	69,69,69,69	0
54	MG	1a	1837	1/1	0.86	0.18	74,74,74,74	0
54	MG	1a	1838	1/1	0.86	0.17	66,66,66,66	0
54	MG	1A	3998	1/1	0.86	0.28	51,51,51,51	0
54	MG	1A	3480	1/1	0.86	0.12	28,28,28,28	0
54	MG	2A	3437	1/1	0.86	0.16	52,52,52,52	0
54	MG	1A	3568	1/1	0.86	0.16	55,55,55,55	0
54	MG	1A	4030	1/1	0.86	0.33	53,53,53,53	0
54	MG	1A	4035	1/1	0.86	0.12	27,27,27,27	0
54	MG	1a	1866	1/1	0.86	0.19	69,69,69,69	0
54	MG	1A	3640	1/1	0.86	0.27	71,71,71,71	0
54	MG	1A	3485	1/1	0.86	0.13	72,72,72,72	0
54	MG	2A	3475	1/1	0.86	0.10	62,62,62,62	0
54	MG	1a	1707	1/1	0.86	0.21	74,74,74,74	0
54	MG	1a	1718	1/1	0.86	0.14	58,58,58,58	0
54	MG	1A	3399	1/1	0.86	0.18	54,54,54,54	0
54	MG	1B	216	1/1	0.86	0.26	58,58,58,58	0
54	MG	2a	1623	1/1	0.86	0.37	73,73,73,73	0
54	MG	2a	1625	1/1	0.86	0.31	73,73,73,73	0
54	MG	2A	3487	1/1	0.86	0.12	73,73,73,73	0
54	MG	2A	3490	1/1	0.86	0.14	66,66,66,66	0
54	MG	1A	3649	1/1	0.86	0.19	59,59,59,59	0
54	MG	1A	3655	1/1	0.86	0.10	40,40,40,40	0
54	MG	2A	3023	1/1	0.86	0.13	54,54,54,54	0
54	MG	1A	3501	1/1	0.86	0.12	69,69,69,69	0
54	MG	1A	3425	1/1	0.86	0.18	57,57,57,57	0
54	MG	2A	3511	1/1	0.86	0.14	62,62,62,62	0
54	MG	2A	3512	1/1	0.86	0.12	54,54,54,54	0
54	MG	2a	1644	1/1	0.86	0.21	75,75,75,75	0
54	MG	2a	1645	1/1	0.86	0.28	67,67,67,67	0
54	MG	2a	1646	1/1	0.86	0.22	77,77,77,77	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	2a	1648	1/1	0.86	0.35	76,76,76,76	0
54	MG	1a	1750	1/1	0.86	0.14	69,69,69,69	0
54	MG	2A	3124	1/1	0.86	0.10	66,66,66,66	0
54	MG	1A	3670	1/1	0.86	0.18	64,64,64,64	0
54	MG	1A	3679	1/1	0.86	0.13	69,69,69,69	0
54	MG	2a	1660	1/1	0.86	0.34	72,72,72,72	0
54	MG	1A	3507	1/1	0.86	0.14	32,32,32,32	0
54	MG	2a	1662	1/1	0.86	0.32	79,79,79,79	0
54	MG	2A	3162	1/1	0.86	0.19	57,57,57,57	0
54	MG	2A	3530	1/1	0.86	0.10	50,50,50,50	0
54	MG	1O	8001	1/1	0.86	0.14	62,62,62,62	0
54	MG	1A	3125	1/1	0.86	0.15	49,49,49,49	0
54	MG	2A	3182	1/1	0.86	0.12	49,49,49,49	0
54	MG	1A	3297	1/1	0.86	0.28	71,71,71,71	0
54	MG	2A	3206	1/1	0.86	0.20	56,56,56,56	0
54	MG	2A	3223	1/1	0.86	0.13	58,58,58,58	0
54	MG	1A	3525	1/1	0.86	0.11	57,57,57,57	0
54	MG	1A	3592	1/1	0.86	0.12	54,54,54,54	0
54	MG	1a	1783	1/1	0.86	0.11	87,87,87,87	0
54	MG	1A	3066	1/1	0.86	0.22	64,64,64,64	0
54	MG	2A	3614	1/1	0.86	0.12	42,42,42,42	0
54	MG	1A	3719	1/1	0.86	0.12	47,47,47,47	0
54	MG	1A	3597	1/1	0.86	0.12	62,62,62,62	0
54	MG	1a	1606	1/1	0.86	0.22	63,63,63,63	0
54	MG	2A	3289	1/1	0.86	0.17	69,69,69,69	0
54	MG	2A	3635	1/1	0.86	0.21	65,65,65,65	0
54	MG	2A	3642	1/1	0.86	0.13	77,77,77,77	0
54	MG	2A	3659	1/1	0.86	0.11	76,76,76,76	0
54	MG	2a	1727	1/1	0.86	0.17	69,69,69,69	0
54	MG	1A	3372	1/1	0.86	0.10	39,39,39,39	0
54	MG	2A	3303	1/1	0.86	0.21	61,61,61,61	0
54	MG	1A	3615	1/1	0.86	0.14	60,60,60,60	0
54	MG	1A	3443	1/1	0.86	0.10	48,48,48,48	0
54	MG	2A	3722	1/1	0.86	0.15	57,57,57,57	0
54	MG	1A	3413	1/1	0.86	0.17	68,68,68,68	0
54	MG	1A	3969	1/1	0.86	0.18	61,61,61,61	0
54	MG	1A	3753	1/1	0.86	0.13	57,57,57,57	0
54	MG	1A	3027	1/1	0.86	0.10	60,60,60,60	0
54	MG	1a	1823	1/1	0.86	0.16	75,75,75,75	0
54	MG	1a	1824	1/1	0.86	0.23	73,73,73,73	0
54	MG	1a	1827	1/1	0.86	0.28	73,73,73,73	0
54	MG	1A	3988	1/1	0.86	0.10	81,81,81,81	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	1A	3462	1/1	0.86	0.12	60,60,60,60	0
54	MG	2B	3012	1/1	0.86	0.20	77,77,77,77	0
54	MG	1a	1701	1/1	0.87	0.26	64,64,64,64	0
54	MG	1A	3644	1/1	0.87	0.14	48,48,48,48	0
54	MG	1A	3375	1/1	0.87	0.13	49,49,49,49	0
54	MG	1A	3580	1/1	0.87	0.09	59,59,59,59	0
54	MG	1A	3522	1/1	0.87	0.19	61,61,61,61	0
54	MG	1G	3002	1/1	0.87	0.11	62,62,62,62	0
54	MG	2A	3288	1/1	0.87	0.13	51,51,51,51	0
54	MG	1A	3319	1/1	0.87	0.10	65,65,65,65	0
54	MG	1A	3965	1/1	0.87	0.12	63,63,63,63	0
54	MG	1a	1735	1/1	0.87	0.13	68,68,68,68	0
54	MG	1A	3321	1/1	0.87	0.14	50,50,50,50	0
54	MG	2A	3535	1/1	0.87	0.24	71,71,71,71	0
54	MG	2A	3537	1/1	0.87	0.10	55,55,55,55	0
54	MG	1A	3324	1/1	0.87	0.25	61,61,61,61	0
54	MG	2A	3551	1/1	0.87	0.12	61,61,61,61	0
54	MG	2A	3312	1/1	0.87	0.14	65,65,65,65	0
54	MG	1A	3292	1/1	0.87	0.18	58,58,58,58	0
54	MG	2A	3335	1/1	0.87	0.20	63,63,63,63	0
54	MG	10	102	1/1	0.87	0.10	51,51,51,51	0
54	MG	1A	3596	1/1	0.87	0.16	47,47,47,47	0
54	MG	1a	1873	1/1	0.87	0.13	65,65,65,65	0
54	MG	1A	3011	1/1	0.87	0.16	62,62,62,62	0
54	MG	1A	3995	1/1	0.87	0.16	44,44,44,44	0
54	MG	1A	3555	1/1	0.87	0.12	53,53,53,53	0
54	MG	1A	3344	1/1	0.87	0.17	59,59,59,59	0
54	MG	1A	3348	1/1	0.87	0.12	44,44,44,44	0
54	MG	2A	3626	1/1	0.87	0.18	47,47,47,47	0
54	MG	1A	4019	1/1	0.87	0.30	58,58,58,58	0
54	MG	2A	3628	1/1	0.87	0.12	56,56,56,56	0
54	MG	1a	1641	1/1	0.87	0.45	75,75,75,75	0
54	MG	1A	3261	1/1	0.87	0.11	64,64,64,64	0
54	MG	2A	3419	1/1	0.87	0.14	54,54,54,54	0
54	MG	1A	3367	1/1	0.87	0.14	54,54,54,54	0
54	MG	2A	3422	1/1	0.87	0.15	56,56,56,56	0
54	MG	1A	3570	1/1	0.87	0.19	71,71,71,71	0
54	MG	2A	3703	1/1	0.87	0.09	59,59,59,59	0
54	MG	2a	1685	1/1	0.87	0.29	64,64,64,64	0
54	MG	2A	3709	1/1	0.87	0.11	50,50,50,50	0
54	MG	2A	3057	1/1	0.87	0.19	63,63,63,63	0
54	MG	1a	1669	1/1	0.87	0.13	70,70,70,70	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	1A	3725	1/1	0.87	0.13	51,51,51,51	0
54	MG	2A	3445	1/1	0.87	0.23	66,66,66,66	0
54	MG	2A	3132	1/1	0.87	0.10	60,60,60,60	0
54	MG	2A	3462	1/1	0.87	0.18	53,53,53,53	0
54	MG	2A	3752	1/1	0.87	0.15	46,46,46,46	0
54	MG	2A	3136	1/1	0.87	0.24	64,64,64,64	0
54	MG	1B	203	1/1	0.87	0.16	70,70,70,70	0
54	MG	2A	3466	1/1	0.87	0.10	51,51,51,51	0
54	MG	2B	3005	1/1	0.87	0.24	60,60,60,60	0
54	MG	2A	3152	1/1	0.87	0.15	61,61,61,61	0
54	MG	1B	206	1/1	0.87	0.10	51,51,51,51	0
54	MG	2a	1731	1/1	0.87	0.16	73,73,73,73	0
54	MG	2B	3009	1/1	0.87	0.22	64,64,64,64	0
54	MG	1A	3419	1/1	0.87	0.15	49,49,49,49	0
54	MG	2a	1752	1/1	0.87	0.12	67,67,67,67	0
54	MG	2A	3476	1/1	0.87	0.12	55,55,55,55	0
54	MG	1B	208	1/1	0.87	0.35	72,72,72,72	0
54	MG	1B	211	1/1	0.87	0.22	69,69,69,69	0
54	MG	1A	3199	1/1	0.87	0.32	70,70,70,70	0
54	MG	2A	3187	1/1	0.87	0.24	61,61,61,61	0
54	MG	1A	3891	1/1	0.87	0.20	73,73,73,73	0
54	MG	2A	3488	1/1	0.87	0.11	58,58,58,58	0
54	MG	2A	3196	1/1	0.87	0.11	49,49,49,49	0
54	MG	2A	3200	1/1	0.87	0.31	57,57,57,57	0
54	MG	20	101	1/1	0.87	0.10	64,64,64,64	0
54	MG	1A	3128	1/1	0.87	0.38	65,65,65,65	0
54	MG	1A	3428	1/1	0.87	0.10	48,48,48,48	0
54	MG	1a	1700	1/1	0.87	0.13	66,66,66,66	0
54	MG	2A	3374	1/1	0.88	0.09	57,57,57,57	0
54	MG	2A	3380	1/1	0.88	0.11	35,35,35,35	0
54	MG	1A	3674	1/1	0.88	0.12	58,58,58,58	0
54	MG	1A	3439	1/1	0.88	0.13	49,49,49,49	0
54	MG	2A	3755	1/1	0.88	0.28	52,52,52,52	0
54	MG	1A	3402	1/1	0.88	0.20	73,73,73,73	0
54	MG	2A	3389	1/1	0.88	0.12	56,56,56,56	0
54	MG	1A	3836	1/1	0.88	0.11	57,57,57,57	0
54	MG	1A	3847	1/1	0.88	0.12	59,59,59,59	0
54	MG	2A	3410	1/1	0.88	0.12	57,57,57,57	0
54	MG	1A	3849	1/1	0.88	0.10	53,53,53,53	0
54	MG	1A	3447	1/1	0.88	0.13	53,53,53,53	0
54	MG	1a	1720	1/1	0.88	0.10	65,65,65,65	0
54	MG	1a	1728	1/1	0.88	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
54	MG	2B	3013	1/1	0.88	0.09	76,76,76,76	0
54	MG	1e	201	1/1	0.88	0.24	65,65,65,65	0
54	MG	1A	3861	1/1	0.88	0.10	54,54,54,54	0
54	MG	2B	3018	1/1	0.88	0.18	76,76,76,76	0
54	MG	1A	3540	1/1	0.88	0.12	52,52,52,52	0
54	MG	1A	3695	1/1	0.88	0.13	51,51,51,51	0
54	MG	2E	305	1/1	0.88	0.20	65,65,65,65	0
54	MG	1A	3601	1/1	0.88	0.18	38,38,38,38	0
54	MG	2A	3040	1/1	0.88	0.18	58,58,58,58	0
54	MG	2A	3453	1/1	0.88	0.26	52,52,52,52	0
54	MG	1a	1740	1/1	0.88	0.30	69,69,69,69	0
54	MG	2T	3001	1/1	0.88	0.22	65,65,65,65	0
54	MG	1A	3884	1/1	0.88	0.08	27,27,27,27	0
54	MG	1A	3705	1/1	0.88	0.15	67,67,67,67	0
54	MG	28	8001	1/1	0.88	0.10	66,66,66,66	0
54	MG	2A	3080	1/1	0.88	0.11	50,50,50,50	0
54	MG	2A	3081	1/1	0.88	0.25	55,55,55,55	0
54	MG	2A	3082	1/1	0.88	0.21	59,59,59,59	0
54	MG	2A	3093	1/1	0.88	0.15	61,61,61,61	0
54	MG	2A	3474	1/1	0.88	0.22	65,65,65,65	0
54	MG	2A	3096	1/1	0.88	0.21	63,63,63,63	0
54	MG	2a	1617	1/1	0.88	0.23	65,65,65,65	0
54	MG	2A	3100	1/1	0.88	0.11	54,54,54,54	0
54	MG	1A	3150	1/1	0.88	0.18	58,58,58,58	0
54	MG	1P	202	1/1	0.88	0.14	73,73,73,73	0
54	MG	1A	3152	1/1	0.88	0.17	66,66,66,66	0
54	MG	2a	1624	1/1	0.88	0.35	73,73,73,73	0
54	MG	1A	3712	1/1	0.88	0.11	36,36,36,36	0
54	MG	2A	3140	1/1	0.88	0.12	54,54,54,54	0
54	MG	1A	3353	1/1	0.88	0.12	53,53,53,53	0
54	MG	1A	3938	1/1	0.88	0.14	56,56,56,56	0
54	MG	1a	1772	1/1	0.88	0.14	77,77,77,77	0
54	MG	1A	3939	1/1	0.88	0.12	61,61,61,61	0
54	MG	2a	1636	1/1	0.88	0.10	64,64,64,64	0
54	MG	2A	3163	1/1	0.88	0.20	62,62,62,62	0
54	MG	2A	3500	1/1	0.88	0.16	62,62,62,62	0
54	MG	1A	3474	1/1	0.88	0.13	35,35,35,35	0
54	MG	2A	3504	1/1	0.88	0.15	63,63,63,63	0
54	MG	2a	1642	1/1	0.88	0.24	80,80,80,80	0
54	MG	2A	3508	1/1	0.88	0.10	59,59,59,59	0
54	MG	1A	3360	1/1	0.88	0.17	55,55,55,55	0
54	MG	1A	3629	1/1	0.88	0.20	68,68,68,68	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	1a	1605	1/1	0.88	0.15	61,61,61,61	0
54	MG	2A	3189	1/1	0.88	0.17	57,57,57,57	0
54	MG	2A	3190	1/1	0.88	0.25	61,61,61,61	0
54	MG	2a	1654	1/1	0.88	0.23	60,60,60,60	0
54	MG	2a	1655	1/1	0.88	0.24	69,69,69,69	0
54	MG	1A	3567	1/1	0.88	0.13	49,49,49,49	0
54	MG	1A	3634	1/1	0.88	0.29	43,43,43,43	0
54	MG	1A	3166	1/1	0.88	0.24	61,61,61,61	0
54	MG	2A	3204	1/1	0.88	0.35	66,66,66,66	0
54	MG	1A	3492	1/1	0.88	0.08	60,60,60,60	0
54	MG	2A	3219	1/1	0.88	0.21	62,62,62,62	0
54	MG	1A	3100	1/1	0.88	0.12	50,50,50,50	0
54	MG	2A	3224	1/1	0.88	0.21	49,49,49,49	0
54	MG	1a	1644	1/1	0.88	0.12	57,57,57,57	0
54	MG	2A	3230	1/1	0.88	0.20	62,62,62,62	0
54	MG	2A	3553	1/1	0.88	0.13	76,76,76,76	0
54	MG	2A	3568	1/1	0.88	0.12	42,42,42,42	0
54	MG	1a	1809	1/1	0.88	0.18	62,62,62,62	0
54	MG	1A	3497	1/1	0.88	0.10	45,45,45,45	0
54	MG	1A	3762	1/1	0.88	0.16	52,52,52,52	0
54	MG	2A	3578	1/1	0.88	0.15	71,71,71,71	0
54	MG	1A	3369	1/1	0.88	0.09	39,39,39,39	0
54	MG	2a	1698	1/1	0.88	0.18	69,69,69,69	0
54	MG	1a	1664	1/1	0.88	0.18	58,58,58,58	0
54	MG	2A	3265	1/1	0.88	0.17	55,55,55,55	0
54	MG	1A	3262	1/1	0.88	0.22	60,60,60,60	0
54	MG	1A	3190	1/1	0.88	0.11	61,61,61,61	0
54	MG	1A	3067	1/1	0.88	0.17	60,60,60,60	0
54	MG	1A	3283	1/1	0.88	0.11	60,60,60,60	0
54	MG	2A	3624	1/1	0.88	0.12	66,66,66,66	0
54	MG	2A	3294	1/1	0.88	0.14	56,56,56,56	0
54	MG	2A	3302	1/1	0.88	0.10	57,57,57,57	0
54	MG	2a	1725	1/1	0.88	0.16	64,64,64,64	0
54	MG	1A	4008	1/1	0.88	0.14	33,33,33,33	0
54	MG	2a	1729	1/1	0.88	0.12	71,71,71,71	0
54	MG	1A	3062	1/1	0.88	0.18	46,46,46,46	0
54	MG	1A	3791	1/1	0.88	0.15	60,60,60,60	0
54	MG	1A	3794	1/1	0.88	0.18	65,65,65,65	0
54	MG	1A	3803	1/1	0.88	0.13	50,50,50,50	0
54	MG	1a	1690	1/1	0.88	0.37	71,71,71,71	0
54	MG	2A	3663	1/1	0.88	0.10	74,74,74,74	0
54	MG	1a	1694	1/1	0.88	0.26	67,67,67,67	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	2A	3680	1/1	0.88	0.17	53,53,53,53	0
54	MG	2a	1780	1/1	0.88	0.19	66,66,66,66	0
54	MG	2A	3346	1/1	0.88	0.10	55,55,55,55	0
54	MG	2A	3692	1/1	0.88	0.08	52,52,52,52	0
54	MG	2A	3696	1/1	0.88	0.08	56,56,56,56	0
54	MG	2e	201	1/1	0.88	0.18	71,71,71,71	0
54	MG	2A	3350	1/1	0.88	0.10	43,43,43,43	0
54	MG	2l	3001	1/1	0.88	0.42	64,64,64,64	0
54	MG	2A	3353	1/1	0.88	0.12	44,44,44,44	0
54	MG	2A	3713	1/1	0.88	0.13	57,57,57,57	0
54	MG	1a	1846	1/1	0.88	0.14	74,74,74,74	0
54	MG	1A	3808	1/1	0.88	0.10	55,55,55,55	0
56	ARG	1F	311	12/12	0.88	0.12	44,63,72,77	0
54	MG	1A	3341	1/1	0.88	0.12	46,46,46,46	0
54	MG	1a	1654	1/1	0.89	0.26	64,64,64,64	0
54	MG	2A	3279	1/1	0.89	0.17	37,37,37,37	0
54	MG	1a	1761	1/1	0.89	0.25	64,64,64,64	0
54	MG	2A	3519	1/1	0.89	0.15	60,60,60,60	0
54	MG	1A	3894	1/1	0.89	0.16	62,62,62,62	0
54	MG	1A	3516	1/1	0.89	0.15	60,60,60,60	0
54	MG	2a	1614	1/1	0.89	0.15	55,55,55,55	0
54	MG	1l	3002	1/1	0.89	0.20	72,72,72,72	0
54	MG	1A	3715	1/1	0.89	0.18	48,48,48,48	0
54	MG	1r	3001	1/1	0.89	0.19	65,65,65,65	0
54	MG	1y	204	1/1	0.89	0.15	93,93,93,93	0
54	MG	1A	3928	1/1	0.89	0.21	58,58,58,58	0
54	MG	1a	1671	1/1	0.89	0.31	63,63,63,63	0
54	MG	2A	3544	1/1	0.89	0.09	55,55,55,55	0
54	MG	1A	3799	1/1	0.89	0.10	51,51,51,51	0
54	MG	1a	1777	1/1	0.89	0.09	55,55,55,55	0
54	MG	2A	3049	1/1	0.89	0.15	50,50,50,50	0
54	MG	2A	3554	1/1	0.89	0.16	43,43,43,43	0
54	MG	2A	3342	1/1	0.89	0.12	45,45,45,45	0
54	MG	1A	3716	1/1	0.89	0.17	48,48,48,48	0
54	MG	2A	3348	1/1	0.89	0.09	62,62,62,62	0
54	MG	2A	3056	1/1	0.89	0.19	62,62,62,62	0
54	MG	1a	1785	1/1	0.89	0.21	76,76,76,76	0
54	MG	2A	3062	1/1	0.89	0.16	53,53,53,53	0
54	MG	2A	3063	1/1	0.89	0.17	61,61,61,61	0
54	MG	1a	1786	1/1	0.89	0.25	70,70,70,70	0
54	MG	2A	3368	1/1	0.89	0.14	64,64,64,64	0
54	MG	1B	218	1/1	0.89	0.13	48,48,48,48	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	1A	3943	1/1	0.89	0.10	38,38,38,38	0
54	MG	2A	3383	1/1	0.89	0.17	52,52,52,52	0
54	MG	1A	3595	1/1	0.89	0.12	48,48,48,48	0
54	MG	1a	1794	1/1	0.89	0.21	58,58,58,58	0
54	MG	1A	3668	1/1	0.89	0.17	52,52,52,52	0
54	MG	1A	3813	1/1	0.89	0.13	31,31,31,31	0
54	MG	1A	3819	1/1	0.89	0.21	76,76,76,76	0
54	MG	2A	3395	1/1	0.89	0.14	51,51,51,51	0
54	MG	1a	1804	1/1	0.89	0.11	65,65,65,65	0
54	MG	2A	3135	1/1	0.89	0.29	61,61,61,61	0
54	MG	1A	3382	1/1	0.89	0.07	32,32,32,32	0
54	MG	2A	3416	1/1	0.89	0.16	61,61,61,61	0
54	MG	2A	3138	1/1	0.89	0.24	61,61,61,61	0
54	MG	1A	3635	1/1	0.89	0.17	59,59,59,59	0
54	MG	1A	3967	1/1	0.89	0.12	81,81,81,81	0
54	MG	1a	1697	1/1	0.89	0.13	60,60,60,60	0
54	MG	2A	3693	1/1	0.89	0.09	57,57,57,57	0
54	MG	1A	3677	1/1	0.89	0.14	54,54,54,54	0
54	MG	1A	3835	1/1	0.89	0.10	47,47,47,47	0
54	MG	1A	3559	1/1	0.89	0.09	46,46,46,46	0
54	MG	1A	3838	1/1	0.89	0.09	55,55,55,55	0
54	MG	2A	3172	1/1	0.89	0.15	61,61,61,61	0
54	MG	1a	1825	1/1	0.89	0.20	77,77,77,77	0
54	MG	2a	1702	1/1	0.89	0.15	65,65,65,65	0
54	MG	2A	3454	1/1	0.89	0.11	58,58,58,58	0
54	MG	2A	3179	1/1	0.89	0.27	56,56,56,56	0
54	MG	2A	3461	1/1	0.89	0.17	52,52,52,52	0
54	MG	1A	3466	1/1	0.89	0.14	53,53,53,53	0
54	MG	2A	3186	1/1	0.89	0.14	53,53,53,53	0
54	MG	1A	3610	1/1	0.89	0.12	35,35,35,35	0
54	MG	1a	1715	1/1	0.89	0.25	65,65,65,65	0
54	MG	1a	1716	1/1	0.89	0.12	74,74,74,74	0
54	MG	2B	3003	1/1	0.89	0.26	71,71,71,71	0
54	MG	1A	3471	1/1	0.89	0.11	29,29,29,29	0
54	MG	1A	3451	1/1	0.89	0.11	48,48,48,48	0
54	MG	1A	3374	1/1	0.89	0.12	57,57,57,57	0
54	MG	1a	1723	1/1	0.89	0.14	64,64,64,64	0
54	MG	2A	3477	1/1	0.89	0.10	49,49,49,49	0
54	MG	1a	1603	1/1	0.89	0.23	77,77,77,77	0
54	MG	2A	3209	1/1	0.89	0.13	63,63,63,63	0
54	MG	2a	1755	1/1	0.89	0.11	82,82,82,82	0
54	MG	2A	3212	1/1	0.89	0.20	70,70,70,70	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	2A	3214	1/1	0.89	0.29	49,49,49,49	0
54	MG	1A	3699	1/1	0.89	0.13	41,41,41,41	0
54	MG	1A	4017	1/1	0.89	0.17	62,62,62,62	0
54	MG	1a	1857	1/1	0.89	0.21	68,68,68,68	0
54	MG	2D	306	1/1	0.89	0.13	60,60,60,60	0
54	MG	1A	3878	1/1	0.89	0.12	65,65,65,65	0
54	MG	1A	3701	1/1	0.89	0.25	68,68,68,68	0
54	MG	2G	3001	1/1	0.89	0.18	76,76,76,76	0
54	MG	1A	3704	1/1	0.89	0.11	58,58,58,58	0
54	MG	1a	1637	1/1	0.89	0.24	68,68,68,68	0
54	MG	2A	3501	1/1	0.89	0.17	72,72,72,72	0
54	MG	1A	3455	1/1	0.89	0.10	50,50,50,50	0
54	MG	2A	3246	1/1	0.89	0.10	51,51,51,51	0
54	MG	1A	3459	1/1	0.89	0.15	55,55,55,55	0
54	MG	1A	3663	1/1	0.89	0.18	37,37,37,37	0
54	MG	1a	1653	1/1	0.89	0.21	64,64,64,64	0
54	MG	1A	3611	1/1	0.90	0.16	54,54,54,54	0
54	MG	1A	3982	1/1	0.90	0.20	62,62,62,62	0
54	MG	2A	3460	1/1	0.90	0.12	54,54,54,54	0
54	MG	1A	3987	1/1	0.90	0.10	44,44,44,44	0
54	MG	1A	3313	1/1	0.90	0.14	70,70,70,70	0
54	MG	1A	3318	1/1	0.90	0.13	44,44,44,44	0
54	MG	2B	3011	1/1	0.90	0.11	61,61,61,61	0
54	MG	1a	1706	1/1	0.90	0.10	47,47,47,47	0
54	MG	1A	3529	1/1	0.90	0.10	55,55,55,55	0
54	MG	1a	1714	1/1	0.90	0.18	62,62,62,62	0
54	MG	1l	101	1/1	0.90	0.17	66,66,66,66	0
54	MG	2A	3469	1/1	0.90	0.10	62,62,62,62	0
54	MG	2A	3472	1/1	0.90	0.22	65,65,65,65	0
54	MG	2A	3194	1/1	0.90	0.11	53,53,53,53	0
54	MG	2D	309	1/1	0.90	0.24	65,65,65,65	0
54	MG	1l	103	1/1	0.90	0.15	60,60,60,60	0
54	MG	1A	3488	1/1	0.90	0.12	45,45,45,45	0
54	MG	1a	1839	1/1	0.90	0.09	67,67,67,67	0
54	MG	17	102	1/1	0.90	0.15	63,63,63,63	0
54	MG	2G	3003	1/1	0.90	0.09	65,65,65,65	0
54	MG	2A	3480	1/1	0.90	0.18	53,53,53,53	0
54	MG	18	101	1/1	0.90	0.09	60,60,60,60	0
54	MG	1a	1721	1/1	0.90	0.17	71,71,71,71	0
54	MG	1a	1849	1/1	0.90	0.12	66,66,66,66	0
54	MG	1A	4000	1/1	0.90	0.17	78,78,78,78	0
54	MG	1a	1725	1/1	0.90	0.18	67,67,67,67	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	1A	3690	1/1	0.90	0.14	51,51,51,51	0
54	MG	1A	3134	1/1	0.90	0.10	45,45,45,45	0
54	MG	2A	3228	1/1	0.90	0.23	64,64,64,64	0
54	MG	1a	1864	1/1	0.90	0.15	70,70,70,70	0
54	MG	1A	3766	1/1	0.90	0.17	56,56,56,56	0
54	MG	1A	3578	1/1	0.90	0.28	58,58,58,58	0
54	MG	1A	3363	1/1	0.90	0.10	33,33,33,33	0
54	MG	1A	3545	1/1	0.90	0.32	64,64,64,64	0
54	MG	2A	3507	1/1	0.90	0.08	52,52,52,52	0
54	MG	1a	1742	1/1	0.90	0.21	55,55,55,55	0
54	MG	1a	1634	1/1	0.90	0.25	61,61,61,61	0
54	MG	2A	3253	1/1	0.90	0.12	50,50,50,50	0
54	MG	2A	3260	1/1	0.90	0.10	53,53,53,53	0
54	MG	2A	3264	1/1	0.90	0.23	59,59,59,59	0
54	MG	2A	3515	1/1	0.90	0.16	34,34,34,34	0
54	MG	1a	1745	1/1	0.90	0.21	73,73,73,73	0
54	MG	2A	3275	1/1	0.90	0.18	58,58,58,58	0
54	MG	2A	3520	1/1	0.90	0.24	38,38,38,38	0
54	MG	2A	3521	1/1	0.90	0.22	57,57,57,57	0
54	MG	2A	3522	1/1	0.90	0.12	55,55,55,55	0
54	MG	2A	3523	1/1	0.90	0.11	51,51,51,51	0
54	MG	1d	502	1/1	0.90	0.38	77,77,77,77	0
54	MG	1A	3549	1/1	0.90	0.15	63,63,63,63	0
54	MG	1A	3789	1/1	0.90	0.13	58,58,58,58	0
54	MG	1e	202	1/1	0.90	0.28	58,58,58,58	0
54	MG	2A	3529	1/1	0.90	0.12	54,54,54,54	0
54	MG	1A	4076	1/1	0.90	0.21	57,57,57,57	0
54	MG	1a	1647	1/1	0.90	0.29	57,57,57,57	0
54	MG	2A	3301	1/1	0.90	0.11	48,48,48,48	0
54	MG	2A	3536	1/1	0.90	0.08	63,63,63,63	0
54	MG	1q	201	1/1	0.90	0.17	55,55,55,55	0
54	MG	2A	3539	1/1	0.90	0.09	38,38,38,38	0
54	MG	2a	1652	1/1	0.90	0.21	57,57,57,57	0
54	MG	1A	3908	1/1	0.90	0.10	27,27,27,27	0
54	MG	2A	3546	1/1	0.90	0.09	58,58,58,58	0
54	MG	1a	1756	1/1	0.90	0.14	57,57,57,57	0
54	MG	2a	1658	1/1	0.90	0.16	60,60,60,60	0
54	MG	1a	1758	1/1	0.90	0.15	73,73,73,73	0
54	MG	2A	3010	1/1	0.90	0.22	60,60,60,60	0
54	MG	2A	3315	1/1	0.90	0.17	57,57,57,57	0
54	MG	2A	3556	1/1	0.90	0.10	62,62,62,62	0
54	MG	2A	3566	1/1	0.90	0.09	63,63,63,63	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	1a	1759	1/1	0.90	0.15	65,65,65,65	0
54	MG	1A	3112	1/1	0.90	0.11	67,67,67,67	0
54	MG	1B	204	1/1	0.90	0.25	65,65,65,65	0
54	MG	1a	1764	1/1	0.90	0.18	65,65,65,65	0
54	MG	2a	1670	1/1	0.90	0.09	65,65,65,65	0
54	MG	1A	3585	1/1	0.90	0.11	54,54,54,54	0
54	MG	2a	1675	1/1	0.90	0.37	69,69,69,69	0
54	MG	2a	1678	1/1	0.90	0.12	66,66,66,66	0
54	MG	2A	3347	1/1	0.90	0.08	34,34,34,34	0
54	MG	2a	1680	1/1	0.90	0.13	75,75,75,75	0
54	MG	1A	3589	1/1	0.90	0.14	57,57,57,57	0
54	MG	1a	1660	1/1	0.90	0.17	69,69,69,69	0
54	MG	1A	3933	1/1	0.90	0.13	68,68,68,68	0
54	MG	1a	1665	1/1	0.90	0.11	67,67,67,67	0
54	MG	2A	3612	1/1	0.90	0.14	33,33,33,33	0
54	MG	1A	3554	1/1	0.90	0.16	58,58,58,58	0
54	MG	1A	3591	1/1	0.90	0.08	55,55,55,55	0
54	MG	1a	1784	1/1	0.90	0.09	66,66,66,66	0
54	MG	2A	3372	1/1	0.90	0.07	51,51,51,51	0
54	MG	1A	3174	1/1	0.90	0.19	57,57,57,57	0
54	MG	2A	3090	1/1	0.90	0.09	63,63,63,63	0
54	MG	2a	1711	1/1	0.90	0.19	79,79,79,79	0
54	MG	1A	3945	1/1	0.90	0.09	37,37,37,37	0
54	MG	2A	3629	1/1	0.90	0.10	62,62,62,62	0
54	MG	1a	1787	1/1	0.90	0.14	64,64,64,64	0
54	MG	2A	3097	1/1	0.90	0.13	57,57,57,57	0
54	MG	2A	3098	1/1	0.90	0.15	53,53,53,53	0
54	MG	1A	3429	1/1	0.90	0.20	57,57,57,57	0
54	MG	2A	3113	1/1	0.90	0.15	57,57,57,57	0
54	MG	2a	1728	1/1	0.90	0.12	77,77,77,77	0
54	MG	2A	3392	1/1	0.90	0.20	65,65,65,65	0
54	MG	2A	3671	1/1	0.90	0.09	36,36,36,36	0
54	MG	2A	3679	1/1	0.90	0.10	56,56,56,56	0
54	MG	2a	1736	1/1	0.90	0.15	67,67,67,67	0
54	MG	1A	3718	1/1	0.90	0.20	47,47,47,47	0
54	MG	2a	1740	1/1	0.90	0.10	80,80,80,80	0
54	MG	2a	1751	1/1	0.90	0.10	65,65,65,65	0
54	MG	1A	3821	1/1	0.90	0.15	36,36,36,36	0
54	MG	1a	1681	1/1	0.90	0.18	61,61,61,61	0
54	MG	2A	3411	1/1	0.90	0.16	62,62,62,62	0
54	MG	1a	1795	1/1	0.90	0.12	71,71,71,71	0
54	MG	1D	314	1/1	0.90	0.16	72,72,72,72	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	2A	3137	1/1	0.90	0.17	57,57,57,57	0
54	MG	1A	3206	1/1	0.90	0.33	65,65,65,65	0
54	MG	1a	1688	1/1	0.90	0.37	70,70,70,70	0
54	MG	2A	3719	1/1	0.90	0.14	56,56,56,56	0
54	MG	1A	3130	1/1	0.90	0.17	55,55,55,55	0
54	MG	1A	3467	1/1	0.90	0.10	43,43,43,43	0
54	MG	2A	3427	1/1	0.90	0.12	51,51,51,51	0
54	MG	1a	1691	1/1	0.90	0.16	56,56,56,56	0
54	MG	2r	101	1/1	0.90	0.12	68,68,68,68	0
54	MG	1A	3304	1/1	0.90	0.26	62,62,62,62	0
54	MG	1A	3604	1/1	0.90	0.12	59,59,59,59	0
54	MG	2A	3444	1/1	0.90	0.15	61,61,61,61	0
55	MPD	2A	3748	8/8	0.90	0.18	54,65,67,73	0
54	MG	2A	3166	1/1	0.90	0.10	61,61,61,61	0
54	MG	2A	3448	1/1	0.90	0.16	66,66,66,66	0
57	ZN	2Y	501	1/1	0.90	0.16	169,169,169,169	0
54	MG	1A	3282	1/1	0.90	0.28	60,60,60,60	0
54	MG	1A	3632	1/1	0.91	0.13	56,56,56,56	0
54	MG	2A	3400	1/1	0.91	0.14	40,40,40,40	0
54	MG	2A	3405	1/1	0.91	0.13	53,53,53,53	0
54	MG	1A	4001	1/1	0.91	0.19	68,68,68,68	0
54	MG	2A	3409	1/1	0.91	0.09	44,44,44,44	0
54	MG	2A	3099	1/1	0.91	0.20	53,53,53,53	0
54	MG	1A	3453	1/1	0.91	0.12	40,40,40,40	0
54	MG	2A	3727	1/1	0.91	0.10	70,70,70,70	0
54	MG	2A	3413	1/1	0.91	0.19	59,59,59,59	0
54	MG	2A	3107	1/1	0.91	0.12	53,53,53,53	0
54	MG	2A	3751	1/1	0.91	0.25	48,48,48,48	0
54	MG	1a	1782	1/1	0.91	0.09	75,75,75,75	0
54	MG	2A	3119	1/1	0.91	0.12	49,49,49,49	0
54	MG	2A	3120	1/1	0.91	0.24	55,55,55,55	0
54	MG	1A	3713	1/1	0.91	0.13	33,33,33,33	0
54	MG	2A	3421	1/1	0.91	0.10	69,69,69,69	0
54	MG	1a	1649	1/1	0.91	0.22	58,58,58,58	0
54	MG	1A	3138	1/1	0.91	0.19	60,60,60,60	0
54	MG	2A	3133	1/1	0.91	0.34	57,57,57,57	0
54	MG	2A	3428	1/1	0.91	0.15	57,57,57,57	0
54	MG	2B	3008	1/1	0.91	0.09	66,66,66,66	0
54	MG	1A	3203	1/1	0.91	0.16	61,61,61,61	0
54	MG	1A	3527	1/1	0.91	0.11	32,32,32,32	0
54	MG	1A	4022	1/1	0.91	0.18	55,55,55,55	0
54	MG	2A	3442	1/1	0.91	0.14	51,51,51,51	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	2A	3443	1/1	0.91	0.09	41,41,41,41	0
54	MG	1A	4026	1/1	0.91	0.12	46,46,46,46	0
54	MG	1A	3456	1/1	0.91	0.15	62,62,62,62	0
54	MG	1A	3205	1/1	0.91	0.14	57,57,57,57	0
54	MG	2A	3148	1/1	0.91	0.12	51,51,51,51	0
54	MG	1A	3057	1/1	0.91	0.14	53,53,53,53	0
54	MG	1A	4064	1/1	0.91	0.23	40,40,40,40	0
54	MG	2A	3457	1/1	0.91	0.11	62,62,62,62	0
54	MG	2A	3458	1/1	0.91	0.08	57,57,57,57	0
54	MG	2A	3159	1/1	0.91	0.19	46,46,46,46	0
54	MG	1A	3864	1/1	0.91	0.13	48,48,48,48	0
54	MG	1A	3284	1/1	0.91	0.10	59,59,59,59	0
54	MG	2A	3164	1/1	0.91	0.20	58,58,58,58	0
54	MG	1A	3868	1/1	0.91	0.10	39,39,39,39	0
54	MG	1A	3737	1/1	0.91	0.13	57,57,57,57	0
54	MG	1A	3738	1/1	0.91	0.09	34,34,34,34	0
54	MG	2W	8001	1/1	0.91	0.15	50,50,50,50	0
54	MG	1A	3647	1/1	0.91	0.10	49,49,49,49	0
54	MG	1A	3207	1/1	0.91	0.12	60,60,60,60	0
54	MG	1a	1817	1/1	0.91	0.08	98,98,98,98	0
54	MG	2A	3473	1/1	0.91	0.08	51,51,51,51	0
54	MG	2a	1602	1/1	0.91	0.10	58,58,58,58	0
54	MG	2A	3183	1/1	0.91	0.10	66,66,66,66	0
54	MG	1A	3887	1/1	0.91	0.12	56,56,56,56	0
54	MG	1A	3468	1/1	0.91	0.16	64,64,64,64	0
54	MG	2a	1607	1/1	0.91	0.09	72,72,72,72	0
54	MG	1A	3657	1/1	0.91	0.12	55,55,55,55	0
54	MG	1A	3548	1/1	0.91	0.09	57,57,57,57	0
54	MG	2a	1610	1/1	0.91	0.18	61,61,61,61	0
54	MG	1B	219	1/1	0.91	0.09	44,44,44,44	0
54	MG	1a	1826	1/1	0.91	0.15	70,70,70,70	0
54	MG	2A	3483	1/1	0.91	0.09	37,37,37,37	0
54	MG	2A	3195	1/1	0.91	0.23	66,66,66,66	0
54	MG	2a	1621	1/1	0.91	0.10	56,56,56,56	0
54	MG	1A	3893	1/1	0.91	0.21	40,40,40,40	0
54	MG	1B	222	1/1	0.91	0.13	65,65,65,65	0
54	MG	2A	3202	1/1	0.91	0.14	49,49,49,49	0
54	MG	1A	3065	1/1	0.91	0.12	39,39,39,39	0
54	MG	2A	3491	1/1	0.91	0.09	51,51,51,51	0
54	MG	1A	3898	1/1	0.91	0.08	50,50,50,50	0
54	MG	1B	229	1/1	0.91	0.08	60,60,60,60	0
54	MG	1D	311	1/1	0.91	0.13	69,69,69,69	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	2A	3213	1/1	0.91	0.10	60,60,60,60	0
54	MG	1A	3552	1/1	0.91	0.12	45,45,45,45	0
54	MG	2A	3218	1/1	0.91	0.21	60,60,60,60	0
54	MG	1a	1703	1/1	0.91	0.33	66,66,66,66	0
54	MG	2A	3505	1/1	0.91	0.10	73,73,73,73	0
54	MG	2A	3506	1/1	0.91	0.11	59,59,59,59	0
54	MG	1a	1704	1/1	0.91	0.16	68,68,68,68	0
54	MG	2a	1643	1/1	0.91	0.17	76,76,76,76	0
54	MG	1A	3339	1/1	0.91	0.14	54,54,54,54	0
54	MG	1F	306	1/1	0.91	0.24	48,48,48,48	0
54	MG	1A	3191	1/1	0.91	0.18	55,55,55,55	0
54	MG	1a	1708	1/1	0.91	0.12	55,55,55,55	0
54	MG	1A	3600	1/1	0.91	0.12	57,57,57,57	0
54	MG	2A	3234	1/1	0.91	0.17	65,65,65,65	0
54	MG	2a	1651	1/1	0.91	0.34	67,67,67,67	0
54	MG	1A	3676	1/1	0.91	0.23	71,71,71,71	0
54	MG	1H	8001	1/1	0.91	0.17	62,62,62,62	0
54	MG	1H	8002	1/1	0.91	0.12	58,58,58,58	0
54	MG	1a	1865	1/1	0.91	0.12	46,46,46,46	0
54	MG	1N	202	1/1	0.91	0.12	61,61,61,61	0
54	MG	2A	3252	1/1	0.91	0.10	54,54,54,54	0
54	MG	1A	3380	1/1	0.91	0.09	26,26,26,26	0
54	MG	1A	3785	1/1	0.91	0.17	58,58,58,58	0
54	MG	1Q	203	1/1	0.91	0.13	50,50,50,50	0
54	MG	1A	3252	1/1	0.91	0.26	59,59,59,59	0
54	MG	2A	3272	1/1	0.91	0.13	46,46,46,46	0
54	MG	2a	1665	1/1	0.91	0.27	66,66,66,66	0
54	MG	1a	1726	1/1	0.91	0.13	65,65,65,65	0
54	MG	1A	3608	1/1	0.91	0.13	37,37,37,37	0
54	MG	1a	1729	1/1	0.91	0.07	56,56,56,56	0
54	MG	2A	3287	1/1	0.91	0.10	48,48,48,48	0
54	MG	1d	504	1/1	0.91	0.28	67,67,67,67	0
54	MG	2a	1674	1/1	0.91	0.16	74,74,74,74	0
54	MG	1A	3687	1/1	0.91	0.08	61,61,61,61	0
54	MG	1A	3950	1/1	0.91	0.09	77,77,77,77	0
54	MG	1A	3383	1/1	0.91	0.07	34,34,34,34	0
54	MG	1A	3435	1/1	0.91	0.17	52,52,52,52	0
54	MG	2a	1681	1/1	0.91	0.15	74,74,74,74	0
54	MG	1a	1738	1/1	0.91	0.10	64,64,64,64	0
54	MG	1n	502	1/1	0.91	0.07	46,46,46,46	0
54	MG	1A	3797	1/1	0.91	0.21	65,65,65,65	0
54	MG	1a	1741	1/1	0.91	0.21	65,65,65,65	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	2A	3561	1/1	0.91	0.12	50,50,50,50	0
54	MG	2a	1695	1/1	0.91	0.14	67,67,67,67	0
54	MG	1A	3345	1/1	0.91	0.17	61,61,61,61	0
54	MG	1A	3500	1/1	0.91	0.07	19,19,19,19	0
54	MG	2A	3319	1/1	0.91	0.09	42,42,42,42	0
54	MG	2A	3001	1/1	0.91	0.12	57,57,57,57	0
54	MG	17	101	1/1	0.91	0.14	64,64,64,64	0
54	MG	2a	1709	1/1	0.91	0.13	66,66,66,66	0
54	MG	1A	3806	1/1	0.91	0.19	62,62,62,62	0
54	MG	2A	3340	1/1	0.91	0.08	54,54,54,54	0
54	MG	2A	3024	1/1	0.91	0.21	49,49,49,49	0
54	MG	2A	3025	1/1	0.91	0.09	44,44,44,44	0
54	MG	1A	3441	1/1	0.91	0.16	64,64,64,64	0
54	MG	2A	3603	1/1	0.91	0.12	78,78,78,78	0
54	MG	2A	3605	1/1	0.91	0.09	36,36,36,36	0
54	MG	19	101	1/1	0.91	0.29	62,62,62,62	0
54	MG	2a	1726	1/1	0.91	0.18	57,57,57,57	0
54	MG	2A	3349	1/1	0.91	0.11	46,46,46,46	0
54	MG	1A	3158	1/1	0.91	0.10	49,49,49,49	0
54	MG	1A	3811	1/1	0.91	0.19	32,32,32,32	0
54	MG	2A	3355	1/1	0.91	0.13	49,49,49,49	0
54	MG	1a	1754	1/1	0.91	0.18	66,66,66,66	0
54	MG	1A	3623	1/1	0.91	0.14	29,29,29,29	0
54	MG	1A	3814	1/1	0.91	0.14	60,60,60,60	0
54	MG	2A	3060	1/1	0.91	0.24	42,42,42,42	0
54	MG	2a	1749	1/1	0.91	0.09	85,85,85,85	0
54	MG	2A	3061	1/1	0.91	0.16	50,50,50,50	0
54	MG	1A	3311	1/1	0.91	0.09	46,46,46,46	0
54	MG	2A	3634	1/1	0.91	0.13	50,50,50,50	0
54	MG	2A	3376	1/1	0.91	0.11	58,58,58,58	0
54	MG	2A	3636	1/1	0.91	0.12	66,66,66,66	0
54	MG	2A	3637	1/1	0.91	0.11	49,49,49,49	0
54	MG	2A	3638	1/1	0.91	0.09	55,55,55,55	0
54	MG	1A	3358	1/1	0.91	0.11	27,27,27,27	0
54	MG	2a	1786	1/1	0.91	0.19	67,67,67,67	0
54	MG	2A	3381	1/1	0.91	0.09	39,39,39,39	0
54	MG	2A	3382	1/1	0.91	0.10	58,58,58,58	0
54	MG	2A	3667	1/1	0.91	0.10	49,49,49,49	0
54	MG	2a	1791	1/1	0.91	0.09	61,61,61,61	0
54	MG	2a	1792	1/1	0.91	0.11	67,67,67,67	0
54	MG	1a	1618	1/1	0.91	0.11	65,65,65,65	0
54	MG	1A	3127	1/1	0.91	0.26	57,57,57,57	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	2A	3385	1/1	0.91	0.16	43,43,43,43	0
54	MG	2A	3386	1/1	0.91	0.11	45,45,45,45	0
55	MPD	1A	4028	8/8	0.91	0.16	39,59,65,70	0
54	MG	1a	1633	1/1	0.91	0.29	67,67,67,67	0
54	MG	2A	3086	1/1	0.91	0.18	57,57,57,57	0
54	MG	1a	1770	1/1	0.91	0.15	58,58,58,58	0
54	MG	2A	3694	1/1	0.91	0.10	41,41,41,41	0
54	MG	1A	3997	1/1	0.91	0.21	58,58,58,58	0
54	MG	2A	3697	1/1	0.91	0.10	67,67,67,67	0
54	MG	1A	3826	1/1	0.91	0.06	8,8,8,8	0
54	MG	2A	3708	1/1	0.91	0.15	51,51,51,51	0
54	MG	1A	4033	1/1	0.92	0.23	47,47,47,47	0
54	MG	1d	505	1/1	0.92	0.20	60,60,60,60	0
54	MG	1a	1625	1/1	0.92	0.11	53,53,53,53	0
54	MG	1A	3477	1/1	0.92	0.13	39,39,39,39	0
54	MG	2D	302	1/1	0.92	0.24	52,52,52,52	0
54	MG	1A	4044	1/1	0.92	0.32	52,52,52,52	0
54	MG	2D	308	1/1	0.92	0.07	31,31,31,31	0
54	MG	2A	3241	1/1	0.92	0.07	48,48,48,48	0
54	MG	2A	3243	1/1	0.92	0.27	46,46,46,46	0
54	MG	1A	3478	1/1	0.92	0.14	36,36,36,36	0
54	MG	1i	3001	1/1	0.92	0.15	62,62,62,62	0
54	MG	1A	3534	1/1	0.92	0.16	67,67,67,67	0
54	MG	2A	3250	1/1	0.92	0.09	62,62,62,62	0
54	MG	1a	1638	1/1	0.92	0.25	61,61,61,61	0
54	MG	1o	3001	1/1	0.92	0.29	65,65,65,65	0
54	MG	2Q	3002	1/1	0.92	0.10	63,63,63,63	0
54	MG	1a	1640	1/1	0.92	0.15	61,61,61,61	0
54	MG	2A	3256	1/1	0.92	0.42	61,61,61,61	0
54	MG	2T	3002	1/1	0.92	0.16	69,69,69,69	0
54	MG	2A	3259	1/1	0.92	0.08	51,51,51,51	0
54	MG	1A	3636	1/1	0.92	0.15	37,37,37,37	0
54	MG	20	102	1/1	0.92	0.10	60,60,60,60	0
54	MG	1a	1757	1/1	0.92	0.10	71,71,71,71	0
54	MG	26	502	1/1	0.92	0.15	68,68,68,68	0
54	MG	1y	201	1/1	0.92	0.26	72,72,72,72	0
54	MG	1A	3176	1/1	0.92	0.14	46,46,46,46	0
54	MG	1A	3905	1/1	0.92	0.14	55,55,55,55	0
54	MG	1A	3544	1/1	0.92	0.12	58,58,58,58	0
54	MG	1A	3914	1/1	0.92	0.12	49,49,49,49	0
54	MG	1a	1650	1/1	0.92	0.33	65,65,65,65	0
54	MG	1A	3411	1/1	0.92	0.15	35,35,35,35	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	1a	1769	1/1	0.92	0.11	58,58,58,58	0
54	MG	2A	3036	1/1	0.92	0.13	64,64,64,64	0
54	MG	2A	3038	1/1	0.92	0.16	53,53,53,53	0
54	MG	2A	3300	1/1	0.92	0.09	55,55,55,55	0
54	MG	2A	3517	1/1	0.92	0.11	57,57,57,57	0
54	MG	1A	3641	1/1	0.92	0.11	62,62,62,62	0
54	MG	2A	3041	1/1	0.92	0.10	50,50,50,50	0
54	MG	1a	1771	1/1	0.92	0.17	79,79,79,79	0
54	MG	1a	1655	1/1	0.92	0.38	69,69,69,69	0
54	MG	1B	210	1/1	0.92	0.10	56,56,56,56	0
54	MG	1A	3926	1/1	0.92	0.11	65,65,65,65	0
54	MG	2A	3313	1/1	0.92	0.12	52,52,52,52	0
54	MG	1a	1775	1/1	0.92	0.12	59,59,59,59	0
54	MG	2a	1629	1/1	0.92	0.16	61,61,61,61	0
54	MG	1A	3709	1/1	0.92	0.07	53,53,53,53	0
54	MG	2A	3323	1/1	0.92	0.11	59,59,59,59	0
54	MG	1A	3642	1/1	0.92	0.17	39,39,39,39	0
54	MG	2A	3333	1/1	0.92	0.10	38,38,38,38	0
54	MG	1a	1780	1/1	0.92	0.11	53,53,53,53	0
54	MG	1A	3934	1/1	0.92	0.08	35,35,35,35	0
54	MG	2A	3065	1/1	0.92	0.28	47,47,47,47	0
54	MG	2A	3068	1/1	0.92	0.14	61,61,61,61	0
54	MG	2A	3540	1/1	0.92	0.12	47,47,47,47	0
54	MG	1a	1667	1/1	0.92	0.14	63,63,63,63	0
54	MG	1A	3936	1/1	0.92	0.10	55,55,55,55	0
54	MG	1A	3177	1/1	0.92	0.14	52,52,52,52	0
54	MG	2A	3550	1/1	0.92	0.08	53,53,53,53	0
54	MG	1A	3352	1/1	0.92	0.10	53,53,53,53	0
54	MG	2a	1647	1/1	0.92	0.34	67,67,67,67	0
54	MG	1A	3550	1/1	0.92	0.12	57,57,57,57	0
54	MG	2A	3352	1/1	0.92	0.07	25,25,25,25	0
54	MG	2A	3092	1/1	0.92	0.19	59,59,59,59	0
54	MG	1A	3494	1/1	0.92	0.11	41,41,41,41	0
54	MG	1B	228	1/1	0.92	0.10	65,65,65,65	0
54	MG	2A	3363	1/1	0.92	0.08	64,64,64,64	0
54	MG	1A	3948	1/1	0.92	0.10	49,49,49,49	0
54	MG	2A	3571	1/1	0.92	0.10	44,44,44,44	0
54	MG	1A	3416	1/1	0.92	0.13	33,33,33,33	0
54	MG	1a	1683	1/1	0.92	0.11	58,58,58,58	0
54	MG	1a	1799	1/1	0.92	0.10	65,65,65,65	0
54	MG	2A	3580	1/1	0.92	0.10	39,39,39,39	0
54	MG	1A	3815	1/1	0.92	0.09	47,47,47,47	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	1E	301	1/1	0.92	0.25	40,40,40,40	0
54	MG	2A	3587	1/1	0.92	0.12	52,52,52,52	0
54	MG	2A	3118	1/1	0.92	0.19	45,45,45,45	0
54	MG	1a	1686	1/1	0.92	0.10	64,64,64,64	0
54	MG	1A	3272	1/1	0.92	0.16	30,30,30,30	0
54	MG	1A	3355	1/1	0.92	0.10	43,43,43,43	0
54	MG	2a	1669	1/1	0.92	0.13	77,77,77,77	0
54	MG	2A	3125	1/1	0.92	0.09	44,44,44,44	0
54	MG	2a	1671	1/1	0.92	0.34	70,70,70,70	0
54	MG	1A	3169	1/1	0.92	0.13	53,53,53,53	0
54	MG	2a	1673	1/1	0.92	0.09	68,68,68,68	0
54	MG	1A	3502	1/1	0.92	0.11	56,56,56,56	0
54	MG	2A	3618	1/1	0.92	0.12	37,37,37,37	0
54	MG	2a	1676	1/1	0.92	0.33	62,62,62,62	0
54	MG	2a	1677	1/1	0.92	0.24	66,66,66,66	0
54	MG	1a	1812	1/1	0.92	0.09	51,51,51,51	0
54	MG	1G	3001	1/1	0.92	0.07	72,72,72,72	0
54	MG	1A	3279	1/1	0.92	0.34	69,69,69,69	0
54	MG	1a	1818	1/1	0.92	0.08	69,69,69,69	0
54	MG	2a	1683	1/1	0.92	0.23	69,69,69,69	0
54	MG	1A	3744	1/1	0.92	0.17	51,51,51,51	0
54	MG	1A	3458	1/1	0.92	0.14	48,48,48,48	0
54	MG	2A	3396	1/1	0.92	0.12	50,50,50,50	0
54	MG	2a	1688	1/1	0.92	0.17	58,58,58,58	0
54	MG	2A	3398	1/1	0.92	0.18	56,56,56,56	0
54	MG	2A	3141	1/1	0.92	0.17	59,59,59,59	0
54	MG	2A	3404	1/1	0.92	0.20	70,70,70,70	0
54	MG	1A	3509	1/1	0.92	0.10	62,62,62,62	0
54	MG	2A	3407	1/1	0.92	0.12	41,41,41,41	0
54	MG	1A	3974	1/1	0.92	0.11	75,75,75,75	0
54	MG	1A	3361	1/1	0.92	0.09	47,47,47,47	0
54	MG	2A	3658	1/1	0.92	0.07	52,52,52,52	0
54	MG	1Q	202	1/1	0.92	0.12	55,55,55,55	0
54	MG	1A	3979	1/1	0.92	0.13	62,62,62,62	0
54	MG	1A	3846	1/1	0.92	0.09	47,47,47,47	0
54	MG	2a	1712	1/1	0.92	0.14	62,62,62,62	0
54	MG	1a	1830	1/1	0.92	0.13	84,84,84,84	0
54	MG	1a	1831	1/1	0.92	0.16	67,67,67,67	0
54	MG	2A	3165	1/1	0.92	0.19	64,64,64,64	0
54	MG	1T	8001	1/1	0.92	0.10	60,60,60,60	0
54	MG	2a	1723	1/1	0.92	0.15	68,68,68,68	0
54	MG	2A	3683	1/1	0.92	0.08	51,51,51,51	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	1A	3460	1/1	0.92	0.12	55,55,55,55	0
54	MG	2A	3688	1/1	0.92	0.10	67,67,67,67	0
54	MG	1a	1835	1/1	0.92	0.21	60,60,60,60	0
54	MG	1A	3391	1/1	0.92	0.11	49,49,49,49	0
54	MG	1A	3854	1/1	0.92	0.09	42,42,42,42	0
54	MG	2A	3180	1/1	0.92	0.10	49,49,49,49	0
54	MG	1Z	8001	1/1	0.92	0.15	64,64,64,64	0
54	MG	2A	3700	1/1	0.92	0.09	49,49,49,49	0
54	MG	1A	3994	1/1	0.92	0.13	38,38,38,38	0
54	MG	1A	3855	1/1	0.92	0.09	62,62,62,62	0
54	MG	1A	3617	1/1	0.92	0.09	24,24,24,24	0
54	MG	2A	3712	1/1	0.92	0.07	67,67,67,67	0
54	MG	1A	3761	1/1	0.92	0.12	58,58,58,58	0
54	MG	2A	3716	1/1	0.92	0.10	54,54,54,54	0
54	MG	2a	1757	1/1	0.92	0.08	49,49,49,49	0
54	MG	1a	1848	1/1	0.92	0.13	64,64,64,64	0
54	MG	2a	1769	1/1	0.92	0.17	50,50,50,50	0
54	MG	1A	3305	1/1	0.92	0.19	54,54,54,54	0
54	MG	15	102	1/1	0.92	0.09	55,55,55,55	0
54	MG	2A	3447	1/1	0.92	0.20	48,48,48,48	0
54	MG	15	103	1/1	0.92	0.15	71,71,71,71	0
54	MG	2a	1782	1/1	0.92	0.11	65,65,65,65	0
54	MG	1A	3047	1/1	0.92	0.34	63,63,63,63	0
54	MG	1A	3254	1/1	0.92	0.13	53,53,53,53	0
54	MG	1A	3368	1/1	0.92	0.07	24,24,24,24	0
54	MG	2A	3203	1/1	0.92	0.26	58,58,58,58	0
54	MG	1A	3692	1/1	0.92	0.08	55,55,55,55	0
54	MG	1A	3769	1/1	0.92	0.12	57,57,57,57	0
54	MG	2A	3208	1/1	0.92	0.18	48,48,48,48	0
54	MG	2f	3001	1/1	0.92	0.15	53,53,53,53	0
54	MG	1A	3154	1/1	0.92	0.16	67,67,67,67	0
54	MG	2A	3463	1/1	0.92	0.12	55,55,55,55	0
54	MG	1a	1871	1/1	0.92	0.08	75,75,75,75	0
54	MG	1A	4020	1/1	0.92	0.09	63,63,63,63	0
54	MG	1A	3772	1/1	0.92	0.08	50,50,50,50	0
54	MG	2A	3216	1/1	0.92	0.23	64,64,64,64	0
54	MG	1a	1739	1/1	0.92	0.24	60,60,60,60	0
54	MG	1a	1607	1/1	0.92	0.21	54,54,54,54	0
54	MG	2A	3222	1/1	0.92	0.17	53,53,53,53	0
54	MG	1a	1879	1/1	0.92	0.08	72,72,72,72	0
57	ZN	14	501	1/1	0.92	0.11	225,225,225,225	0
54	MG	1A	3888	1/1	0.92	0.07	58,58,58,58	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	1A	3779	1/1	0.92	0.10	29,29,29,29	0
54	MG	1a	1657	1/1	0.93	0.18	53,53,53,53	0
54	MG	1A	3957	1/1	0.93	0.13	40,40,40,40	0
54	MG	2A	3482	1/1	0.93	0.14	36,36,36,36	0
54	MG	1A	3958	1/1	0.93	0.08	63,63,63,63	0
54	MG	1A	3959	1/1	0.93	0.08	70,70,70,70	0
54	MG	2A	3016	1/1	0.93	0.17	59,59,59,59	0
54	MG	1a	1661	1/1	0.93	0.24	44,44,44,44	0
54	MG	1A	3102	1/1	0.93	0.11	48,48,48,48	0
54	MG	1D	303	1/1	0.93	0.19	36,36,36,36	0
54	MG	2A	3029	1/1	0.93	0.15	47,47,47,47	0
54	MG	2A	3032	1/1	0.93	0.08	46,46,46,46	0
54	MG	2A	3034	1/1	0.93	0.12	49,49,49,49	0
54	MG	2A	3257	1/1	0.93	0.23	58,58,58,58	0
54	MG	1A	3449	1/1	0.93	0.11	54,54,54,54	0
54	MG	1a	1778	1/1	0.93	0.09	67,67,67,67	0
54	MG	2A	3037	1/1	0.93	0.26	52,52,52,52	0
54	MG	1a	1668	1/1	0.93	0.10	59,59,59,59	0
54	MG	2A	3267	1/1	0.93	0.12	60,60,60,60	0
54	MG	1a	1781	1/1	0.93	0.13	62,62,62,62	0
54	MG	1D	313	1/1	0.93	0.13	52,52,52,52	0
54	MG	1A	3837	1/1	0.93	0.07	29,29,29,29	0
54	MG	1A	3499	1/1	0.93	0.07	55,55,55,55	0
54	MG	2A	3280	1/1	0.93	0.09	48,48,48,48	0
54	MG	1a	1674	1/1	0.93	0.15	63,63,63,63	0
54	MG	1E	303	1/1	0.93	0.12	31,31,31,31	0
54	MG	2A	3514	1/1	0.93	0.15	60,60,60,60	0
54	MG	1A	3843	1/1	0.93	0.22	53,53,53,53	0
54	MG	2A	3058	1/1	0.93	0.15	58,58,58,58	0
54	MG	2a	1606	1/1	0.93	0.16	57,57,57,57	0
54	MG	2A	3293	1/1	0.93	0.10	42,42,42,42	0
54	MG	1E	305	1/1	0.93	0.08	38,38,38,38	0
54	MG	2A	3296	1/1	0.93	0.09	42,42,42,42	0
54	MG	1a	1679	1/1	0.93	0.22	55,55,55,55	0
54	MG	2a	1612	1/1	0.93	0.23	63,63,63,63	0
54	MG	2a	1613	1/1	0.93	0.23	68,68,68,68	0
54	MG	1A	3844	1/1	0.93	0.12	58,58,58,58	0
54	MG	1A	3751	1/1	0.93	0.10	27,27,27,27	0
54	MG	1A	3049	1/1	0.93	0.26	55,55,55,55	0
54	MG	1a	1797	1/1	0.93	0.09	74,74,74,74	0
54	MG	2A	3070	1/1	0.93	0.09	46,46,46,46	0
54	MG	2A	3071	1/1	0.93	0.21	52,52,52,52	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	2A	3075	1/1	0.93	0.18	46,46,46,46	0
54	MG	1A	3410	1/1	0.93	0.09	36,36,36,36	0
54	MG	2A	3533	1/1	0.93	0.13	58,58,58,58	0
54	MG	1A	3976	1/1	0.93	0.14	50,50,50,50	0
54	MG	1G	3003	1/1	0.93	0.09	63,63,63,63	0
54	MG	1a	1687	1/1	0.93	0.07	52,52,52,52	0
54	MG	1A	3672	1/1	0.93	0.09	68,68,68,68	0
54	MG	1A	3980	1/1	0.93	0.15	58,58,58,58	0
54	MG	1A	3981	1/1	0.93	0.11	58,58,58,58	0
54	MG	1a	1810	1/1	0.93	0.16	60,60,60,60	0
54	MG	1A	3609	1/1	0.93	0.13	54,54,54,54	0
54	MG	2A	3547	1/1	0.93	0.14	63,63,63,63	0
54	MG	2a	1639	1/1	0.93	0.20	73,73,73,73	0
54	MG	1A	3985	1/1	0.93	0.08	75,75,75,75	0
54	MG	1A	3035	1/1	0.93	0.17	57,57,57,57	0
54	MG	1A	3213	1/1	0.93	0.30	63,63,63,63	0
54	MG	2A	3105	1/1	0.93	0.16	55,55,55,55	0
54	MG	1R	201	1/1	0.93	0.14	53,53,53,53	0
54	MG	1A	3989	1/1	0.93	0.10	48,48,48,48	0
54	MG	2A	3558	1/1	0.93	0.08	32,32,32,32	0
54	MG	2A	3116	1/1	0.93	0.09	65,65,65,65	0
54	MG	2A	3117	1/1	0.93	0.12	52,52,52,52	0
54	MG	1A	3862	1/1	0.93	0.07	54,54,54,54	0
54	MG	1A	3991	1/1	0.93	0.07	50,50,50,50	0
54	MG	1A	3014	1/1	0.93	0.20	58,58,58,58	0
54	MG	2A	3366	1/1	0.93	0.08	53,53,53,53	0
54	MG	2a	1653	1/1	0.93	0.26	62,62,62,62	0
54	MG	2A	3121	1/1	0.93	0.15	58,58,58,58	0
54	MG	2A	3122	1/1	0.93	0.14	44,44,44,44	0
54	MG	2A	3369	1/1	0.93	0.10	51,51,51,51	0
54	MG	2A	3370	1/1	0.93	0.06	33,33,33,33	0
54	MG	1A	3563	1/1	0.93	0.15	53,53,53,53	0
54	MG	2A	3585	1/1	0.93	0.12	38,38,38,38	0
54	MG	1A	3684	1/1	0.93	0.10	39,39,39,39	0
54	MG	2A	3588	1/1	0.93	0.10	88,88,88,88	0
54	MG	2A	3591	1/1	0.93	0.08	43,43,43,43	0
54	MG	2A	3375	1/1	0.93	0.07	51,51,51,51	0
54	MG	1A	3221	1/1	0.93	0.18	54,54,54,54	0
54	MG	1A	3876	1/1	0.93	0.14	37,37,37,37	0
54	MG	10	105	1/1	0.93	0.09	65,65,65,65	0
54	MG	1A	3335	1/1	0.93	0.10	37,37,37,37	0
54	MG	1A	3689	1/1	0.93	0.11	71,71,71,71	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	1A	3620	1/1	0.93	0.15	40,40,40,40	0
54	MG	2A	3616	1/1	0.93	0.10	47,47,47,47	0
54	MG	1a	1717	1/1	0.93	0.12	64,64,64,64	0
54	MG	1A	3089	1/1	0.93	0.12	47,47,47,47	0
54	MG	2A	3622	1/1	0.93	0.08	69,69,69,69	0
54	MG	1A	3783	1/1	0.93	0.12	37,37,37,37	0
54	MG	2A	3142	1/1	0.93	0.09	47,47,47,47	0
54	MG	1A	3515	1/1	0.93	0.12	34,34,34,34	0
54	MG	2A	3146	1/1	0.93	0.08	61,61,61,61	0
54	MG	1A	3247	1/1	0.93	0.28	61,61,61,61	0
54	MG	1A	3518	1/1	0.93	0.11	65,65,65,65	0
54	MG	1a	1842	1/1	0.93	0.17	64,64,64,64	0
54	MG	1a	1844	1/1	0.93	0.08	54,54,54,54	0
54	MG	1A	4025	1/1	0.93	0.08	70,70,70,70	0
54	MG	19	103	1/1	0.93	0.09	66,66,66,66	0
54	MG	1A	3129	1/1	0.93	0.13	49,49,49,49	0
54	MG	1A	3099	1/1	0.93	0.18	59,59,59,59	0
54	MG	1A	3257	1/1	0.93	0.19	51,51,51,51	0
54	MG	2A	3644	1/1	0.93	0.07	58,58,58,58	0
54	MG	2a	1694	1/1	0.93	0.11	50,50,50,50	0
54	MG	1a	1731	1/1	0.93	0.07	54,54,54,54	0
54	MG	2a	1696	1/1	0.93	0.13	73,73,73,73	0
54	MG	2a	1697	1/1	0.93	0.16	66,66,66,66	0
54	MG	1A	3170	1/1	0.93	0.08	38,38,38,38	0
54	MG	2A	3661	1/1	0.93	0.07	46,46,46,46	0
54	MG	2a	1703	1/1	0.93	0.15	69,69,69,69	0
54	MG	1a	1861	1/1	0.93	0.08	52,52,52,52	0
54	MG	2A	3178	1/1	0.93	0.12	59,59,59,59	0
54	MG	1a	1862	1/1	0.93	0.17	64,64,64,64	0
54	MG	2A	3415	1/1	0.93	0.20	49,49,49,49	0
54	MG	2A	3674	1/1	0.93	0.08	25,25,25,25	0
54	MG	1A	4043	1/1	0.93	0.10	32,32,32,32	0
54	MG	2A	3417	1/1	0.93	0.22	52,52,52,52	0
54	MG	2a	1714	1/1	0.93	0.09	69,69,69,69	0
54	MG	2A	3681	1/1	0.93	0.07	70,70,70,70	0
54	MG	1A	3200	1/1	0.93	0.30	63,63,63,63	0
54	MG	1A	3397	1/1	0.93	0.09	33,33,33,33	0
54	MG	1A	3002	1/1	0.93	0.09	54,54,54,54	0
54	MG	1a	1868	1/1	0.93	0.07	71,71,71,71	0
54	MG	1A	3584	1/1	0.93	0.11	47,47,47,47	0
54	MG	2A	3425	1/1	0.93	0.13	55,55,55,55	0
54	MG	1a	1870	1/1	0.93	0.07	93,93,93,93	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	1a	1627	1/1	0.93	0.13	54,54,54,54	0
54	MG	2A	3698	1/1	0.93	0.10	39,39,39,39	0
54	MG	1A	3437	1/1	0.93	0.13	41,41,41,41	0
54	MG	1A	3586	1/1	0.93	0.13	55,55,55,55	0
54	MG	1A	3932	1/1	0.93	0.06	55,55,55,55	0
54	MG	2A	3197	1/1	0.93	0.10	47,47,47,47	0
54	MG	2a	1737	1/1	0.93	0.08	67,67,67,67	0
54	MG	2A	3198	1/1	0.93	0.11	56,56,56,56	0
54	MG	2A	3199	1/1	0.93	0.09	56,56,56,56	0
54	MG	2a	1741	1/1	0.93	0.08	82,82,82,82	0
54	MG	1A	3812	1/1	0.93	0.10	46,46,46,46	0
54	MG	1A	3269	1/1	0.93	0.10	53,53,53,53	0
54	MG	1a	1639	1/1	0.93	0.14	47,47,47,47	0
54	MG	1A	3542	1/1	0.93	0.12	49,49,49,49	0
54	MG	2A	3449	1/1	0.93	0.11	60,60,60,60	0
54	MG	2A	3723	1/1	0.93	0.35	44,44,44,44	0
54	MG	2A	3205	1/1	0.93	0.32	66,66,66,66	0
54	MG	1A	3314	1/1	0.93	0.14	73,73,73,73	0
54	MG	2A	3207	1/1	0.93	0.09	46,46,46,46	0
54	MG	2A	3730	1/1	0.93	0.17	56,56,56,56	0
54	MG	1a	1642	1/1	0.93	0.24	70,70,70,70	0
54	MG	2A	3740	1/1	0.93	0.09	54,54,54,54	0
54	MG	2A	3746	1/1	0.93	0.10	55,55,55,55	0
54	MG	1a	1643	1/1	0.93	0.10	62,62,62,62	0
54	MG	1A	3442	1/1	0.93	0.14	61,61,61,61	0
54	MG	1B	215	1/1	0.93	0.09	59,59,59,59	0
54	MG	2A	3757	1/1	0.93	0.16	64,64,64,64	0
54	MG	1e	204	1/1	0.93	0.12	62,62,62,62	0
54	MG	1f	8001	1/1	0.93	0.14	52,52,52,52	0
54	MG	1A	3648	1/1	0.93	0.06	29,29,29,29	0
54	MG	1h	3001	1/1	0.93	0.29	65,65,65,65	0
54	MG	1h	3002	1/1	0.93	0.19	58,58,58,58	0
54	MG	1A	3547	1/1	0.93	0.08	41,41,41,41	0
54	MG	1A	3731	1/1	0.93	0.06	38,38,38,38	0
54	MG	2A	3225	1/1	0.93	0.16	54,54,54,54	0
54	MG	1A	3827	1/1	0.93	0.12	27,27,27,27	0
54	MG	1a	1765	1/1	0.93	0.14	48,48,48,48	0
54	MG	2A	3229	1/1	0.93	0.09	51,51,51,51	0
54	MG	1a	1767	1/1	0.93	0.07	79,79,79,79	0
54	MG	1A	3317	1/1	0.93	0.19	45,45,45,45	0
54	MG	2A	3232	1/1	0.93	0.12	52,52,52,52	0
54	MG	1A	3444	1/1	0.93	0.19	61,61,61,61	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	2B	3017	1/1	0.93	0.08	68,68,68,68	0
54	MG	1A	4057	1/1	0.94	0.16	38,38,38,38	0
54	MG	1A	3491	1/1	0.94	0.12	24,24,24,24	0
54	MG	2D	307	1/1	0.94	0.13	37,37,37,37	0
54	MG	2A	3258	1/1	0.94	0.23	44,44,44,44	0
54	MG	1A	3420	1/1	0.94	0.13	24,24,24,24	0
54	MG	2A	3046	1/1	0.94	0.11	48,48,48,48	0
54	MG	1A	3422	1/1	0.94	0.13	32,32,32,32	0
54	MG	2F	302	1/1	0.94	0.09	41,41,41,41	0
54	MG	1A	3572	1/1	0.94	0.09	30,30,30,30	0
54	MG	2A	3051	1/1	0.94	0.30	57,57,57,57	0
54	MG	2A	3052	1/1	0.94	0.16	43,43,43,43	0
54	MG	2I	3001	1/1	0.94	0.07	52,52,52,52	0
54	MG	2A	3274	1/1	0.94	0.11	53,53,53,53	0
54	MG	1A	3036	1/1	0.94	0.10	41,41,41,41	0
54	MG	2P	201	1/1	0.94	0.12	55,55,55,55	0
54	MG	2P	202	1/1	0.94	0.07	55,55,55,55	0
54	MG	1A	3022	1/1	0.94	0.08	46,46,46,46	0
54	MG	1A	3903	1/1	0.94	0.08	67,67,67,67	0
54	MG	1A	3182	1/1	0.94	0.16	61,61,61,61	0
54	MG	2A	3285	1/1	0.94	0.08	32,32,32,32	0
54	MG	2T	3003	1/1	0.94	0.14	68,68,68,68	0
54	MG	1A	3652	1/1	0.94	0.07	56,56,56,56	0
54	MG	1A	3653	1/1	0.94	0.14	40,40,40,40	0
54	MG	1A	3187	1/1	0.94	0.26	56,56,56,56	0
54	MG	1a	1789	1/1	0.94	0.06	67,67,67,67	0
54	MG	1a	1790	1/1	0.94	0.09	52,52,52,52	0
54	MG	1A	3656	1/1	0.94	0.07	26,26,26,26	0
54	MG	1A	3430	1/1	0.94	0.11	56,56,56,56	0
54	MG	2A	3297	1/1	0.94	0.07	43,43,43,43	0
54	MG	1A	3662	1/1	0.94	0.07	48,48,48,48	0
54	MG	1A	3076	1/1	0.94	0.07	44,44,44,44	0
54	MG	1A	3782	1/1	0.94	0.07	35,35,35,35	0
54	MG	1a	1798	1/1	0.94	0.08	48,48,48,48	0
54	MG	1A	3503	1/1	0.94	0.11	52,52,52,52	0
54	MG	2A	3308	1/1	0.94	0.17	56,56,56,56	0
54	MG	2A	3083	1/1	0.94	0.12	69,69,69,69	0
54	MG	2A	3532	1/1	0.94	0.14	47,47,47,47	0
54	MG	1A	3004	1/1	0.94	0.09	44,44,44,44	0
54	MG	1A	3030	1/1	0.94	0.06	33,33,33,33	0
54	MG	2A	3314	1/1	0.94	0.13	38,38,38,38	0
54	MG	1A	3669	1/1	0.94	0.06	46,46,46,46	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	1A	3941	1/1	0.94	0.16	66,66,66,66	0
54	MG	2A	3538	1/1	0.94	0.08	49,49,49,49	0
54	MG	2A	3321	1/1	0.94	0.05	33,33,33,33	0
54	MG	1B	231	1/1	0.94	0.06	59,59,59,59	0
54	MG	2A	3541	1/1	0.94	0.12	43,43,43,43	0
54	MG	2A	3326	1/1	0.94	0.09	30,30,30,30	0
54	MG	1a	1808	1/1	0.94	0.11	67,67,67,67	0
54	MG	1D	302	1/1	0.94	0.20	60,60,60,60	0
54	MG	2a	1628	1/1	0.94	0.20	66,66,66,66	0
54	MG	1A	3373	1/1	0.94	0.12	52,52,52,52	0
54	MG	1A	3944	1/1	0.94	0.05	24,24,24,24	0
54	MG	2A	3104	1/1	0.94	0.10	46,46,46,46	0
54	MG	2a	1632	1/1	0.94	0.30	59,59,59,59	0
54	MG	1A	3142	1/1	0.94	0.08	51,51,51,51	0
54	MG	2A	3106	1/1	0.94	0.17	56,56,56,56	0
54	MG	1a	1814	1/1	0.94	0.08	67,67,67,67	0
54	MG	2A	3109	1/1	0.94	0.10	47,47,47,47	0
54	MG	2A	3112	1/1	0.94	0.14	50,50,50,50	0
54	MG	2A	3562	1/1	0.94	0.07	50,50,50,50	0
54	MG	1A	3322	1/1	0.94	0.11	30,30,30,30	0
54	MG	1A	3052	1/1	0.94	0.18	44,44,44,44	0
54	MG	1A	3378	1/1	0.94	0.11	36,36,36,36	0
54	MG	2A	3354	1/1	0.94	0.07	56,56,56,56	0
54	MG	1a	1819	1/1	0.94	0.30	64,64,64,64	0
54	MG	2A	3358	1/1	0.94	0.19	69,69,69,69	0
54	MG	2A	3577	1/1	0.94	0.08	57,57,57,57	0
54	MG	1A	3955	1/1	0.94	0.10	60,60,60,60	0
54	MG	1A	3151	1/1	0.94	0.10	41,41,41,41	0
54	MG	1F	305	1/1	0.94	0.34	66,66,66,66	0
54	MG	1A	3804	1/1	0.94	0.18	37,37,37,37	0
54	MG	1A	3381	1/1	0.94	0.07	24,24,24,24	0
54	MG	1F	308	1/1	0.94	0.12	41,41,41,41	0
54	MG	1A	3682	1/1	0.94	0.10	59,59,59,59	0
54	MG	1a	1693	1/1	0.94	0.08	40,40,40,40	0
54	MG	1A	3594	1/1	0.94	0.10	58,58,58,58	0
54	MG	2A	3596	1/1	0.94	0.08	58,58,58,58	0
54	MG	1a	1695	1/1	0.94	0.38	67,67,67,67	0
54	MG	2A	3599	1/1	0.94	0.10	57,57,57,57	0
54	MG	1A	3278	1/1	0.94	0.10	56,56,56,56	0
54	MG	1A	3448	1/1	0.94	0.11	67,67,67,67	0
54	MG	1A	3032	1/1	0.94	0.19	56,56,56,56	0
54	MG	2A	3611	1/1	0.94	0.06	34,34,34,34	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	1A	3598	1/1	0.94	0.10	35,35,35,35	0
54	MG	1N	201	1/1	0.94	0.12	44,44,44,44	0
54	MG	1A	3390	1/1	0.94	0.09	42,42,42,42	0
54	MG	1A	3337	1/1	0.94	0.07	35,35,35,35	0
54	MG	2A	3619	1/1	0.94	0.07	53,53,53,53	0
54	MG	1A	3603	1/1	0.94	0.08	53,53,53,53	0
54	MG	1A	3696	1/1	0.94	0.27	38,38,38,38	0
54	MG	1a	1843	1/1	0.94	0.08	67,67,67,67	0
54	MG	2A	3153	1/1	0.94	0.14	48,48,48,48	0
54	MG	2A	3155	1/1	0.94	0.19	52,52,52,52	0
54	MG	1A	3394	1/1	0.94	0.08	26,26,26,26	0
54	MG	1A	3698	1/1	0.94	0.16	51,51,51,51	0
54	MG	1A	3395	1/1	0.94	0.16	32,32,32,32	0
54	MG	2A	3632	1/1	0.94	0.07	72,72,72,72	0
54	MG	1a	1711	1/1	0.94	0.13	69,69,69,69	0
54	MG	1A	3536	1/1	0.94	0.09	33,33,33,33	0
54	MG	1A	3338	1/1	0.94	0.09	46,46,46,46	0
54	MG	1A	3984	1/1	0.94	0.19	59,59,59,59	0
54	MG	2A	3170	1/1	0.94	0.16	59,59,59,59	0
54	MG	1U	201	1/1	0.94	0.35	61,61,61,61	0
54	MG	1V	202	1/1	0.94	0.14	64,64,64,64	0
54	MG	2A	3173	1/1	0.94	0.09	55,55,55,55	0
54	MG	2A	3655	1/1	0.94	0.06	54,54,54,54	0
54	MG	1V	203	1/1	0.94	0.18	63,63,63,63	0
54	MG	1A	3061	1/1	0.94	0.12	49,49,49,49	0
54	MG	1W	3002	1/1	0.94	0.09	52,52,52,52	0
54	MG	1A	3109	1/1	0.94	0.12	45,45,45,45	0
54	MG	1A	3110	1/1	0.94	0.08	43,43,43,43	0
54	MG	1A	3841	1/1	0.94	0.12	49,49,49,49	0
54	MG	2A	3185	1/1	0.94	0.23	50,50,50,50	0
54	MG	2a	1701	1/1	0.94	0.08	70,70,70,70	0
54	MG	1a	1727	1/1	0.94	0.12	54,54,54,54	0
54	MG	2A	3677	1/1	0.94	0.11	52,52,52,52	0
54	MG	2a	1704	1/1	0.94	0.18	67,67,67,67	0
54	MG	1A	3546	1/1	0.94	0.15	42,42,42,42	0
54	MG	1A	3285	1/1	0.94	0.13	53,53,53,53	0
54	MG	1A	3210	1/1	0.94	0.30	58,58,58,58	0
54	MG	1l	104	1/1	0.94	0.07	41,41,41,41	0
54	MG	1A	3349	1/1	0.94	0.11	30,30,30,30	0
54	MG	2A	3687	1/1	0.94	0.07	39,39,39,39	0
54	MG	1a	1875	1/1	0.94	0.10	77,77,77,77	0
54	MG	1A	3996	1/1	0.94	0.13	59,59,59,59	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	1A	3034	1/1	0.94	0.07	53,53,53,53	0
54	MG	1a	1737	1/1	0.94	0.14	54,54,54,54	0
54	MG	2A	3433	1/1	0.94	0.09	32,32,32,32	0
54	MG	1A	3624	1/1	0.94	0.11	60,60,60,60	0
54	MG	1A	3999	1/1	0.94	0.16	39,39,39,39	0
54	MG	1A	3115	1/1	0.94	0.09	46,46,46,46	0
54	MG	1A	3857	1/1	0.94	0.10	23,23,23,23	0
54	MG	1A	4002	1/1	0.94	0.14	68,68,68,68	0
54	MG	1A	3469	1/1	0.94	0.11	25,25,25,25	0
54	MG	2A	3711	1/1	0.94	0.09	50,50,50,50	0
54	MG	1A	3860	1/1	0.94	0.07	48,48,48,48	0
54	MG	1a	1746	1/1	0.94	0.07	56,56,56,56	0
54	MG	1g	202	1/1	0.94	0.42	66,66,66,66	0
54	MG	1a	1604	1/1	0.94	0.15	54,54,54,54	0
54	MG	1A	3412	1/1	0.94	0.13	27,27,27,27	0
54	MG	1A	4010	1/1	0.94	0.07	34,34,34,34	0
54	MG	1A	3064	1/1	0.94	0.07	44,44,44,44	0
54	MG	1l	3001	1/1	0.94	0.23	62,62,62,62	0
54	MG	2a	1745	1/1	0.94	0.07	46,46,46,46	0
54	MG	1a	1608	1/1	0.94	0.20	54,54,54,54	0
54	MG	1a	1609	1/1	0.94	0.10	57,57,57,57	0
54	MG	2A	3728	1/1	0.94	0.12	58,58,58,58	0
54	MG	2A	3220	1/1	0.94	0.14	58,58,58,58	0
54	MG	1A	3728	1/1	0.94	0.12	68,68,68,68	0
54	MG	2a	1759	1/1	0.94	0.09	75,75,75,75	0
54	MG	2a	1761	1/1	0.94	0.09	65,65,65,65	0
54	MG	1A	3414	1/1	0.94	0.08	33,33,33,33	0
54	MG	2a	1768	1/1	0.94	0.07	52,52,52,52	0
54	MG	2A	3738	1/1	0.94	0.07	46,46,46,46	0
54	MG	1A	3357	1/1	0.94	0.09	51,51,51,51	0
54	MG	1a	1619	1/1	0.94	0.10	65,65,65,65	0
54	MG	2A	3750	1/1	0.94	0.18	48,48,48,48	0
54	MG	2a	1779	1/1	0.94	0.13	78,78,78,78	0
54	MG	1a	1620	1/1	0.94	0.07	48,48,48,48	0
54	MG	2A	3227	1/1	0.94	0.09	51,51,51,51	0
54	MG	2a	1784	1/1	0.94	0.11	64,64,64,64	0
54	MG	1a	1624	1/1	0.94	0.17	52,52,52,52	0
54	MG	2A	3471	1/1	0.94	0.10	30,30,30,30	0
54	MG	2A	3758	1/1	0.94	0.09	52,52,52,52	0
54	MG	1A	3298	1/1	0.94	0.09	62,62,62,62	0
54	MG	2A	3002	1/1	0.94	0.08	38,38,38,38	0
54	MG	1A	3873	1/1	0.94	0.08	48,48,48,48	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	1a	1766	1/1	0.94	0.21	71,71,71,71	0
54	MG	2A	3017	1/1	0.94	0.15	54,54,54,54	0
54	MG	1A	4027	1/1	0.94	0.11	55,55,55,55	0
54	MG	2A	3239	1/1	0.94	0.18	49,49,49,49	0
54	MG	1A	3739	1/1	0.94	0.08	45,45,45,45	0
54	MG	1A	3562	1/1	0.94	0.08	54,54,54,54	0
54	MG	1A	3482	1/1	0.94	0.13	30,30,30,30	0
54	MG	1A	3746	1/1	0.94	0.10	59,59,59,59	0
54	MG	2A	3033	1/1	0.94	0.21	54,54,54,54	0
54	MG	2A	3248	1/1	0.94	0.10	43,43,43,43	0
54	MG	1A	3010	1/1	0.94	0.08	49,49,49,49	0
54	MG	1A	4047	1/1	0.94	0.09	59,59,59,59	0
54	MG	1A	3230	1/1	0.94	0.13	44,44,44,44	0
54	MG	1A	4055	1/1	0.94	0.15	42,42,42,42	0
54	MG	2A	3493	1/1	0.94	0.08	53,53,53,53	0
54	MG	1A	3162	1/1	0.95	0.19	40,40,40,40	0
54	MG	1A	3204	1/1	0.95	0.11	60,60,60,60	0
54	MG	2A	3255	1/1	0.95	0.15	45,45,45,45	0
54	MG	1D	304	1/1	0.95	0.13	61,61,61,61	0
54	MG	1a	1670	1/1	0.95	0.27	68,68,68,68	0
54	MG	2A	3497	1/1	0.95	0.08	47,47,47,47	0
54	MG	2D	304	1/1	0.95	0.11	36,36,36,36	0
54	MG	2A	3059	1/1	0.95	0.09	45,45,45,45	0
54	MG	1A	3954	1/1	0.95	0.07	24,24,24,24	0
54	MG	1A	3807	1/1	0.95	0.08	52,52,52,52	0
54	MG	1A	3618	1/1	0.95	0.10	32,32,32,32	0
54	MG	1A	3164	1/1	0.95	0.12	45,45,45,45	0
54	MG	1A	3558	1/1	0.95	0.06	62,62,62,62	0
54	MG	2A	3268	1/1	0.95	0.10	57,57,57,57	0
54	MG	2A	3067	1/1	0.95	0.07	49,49,49,49	0
54	MG	1a	1806	1/1	0.95	0.09	52,52,52,52	0
54	MG	1A	3622	1/1	0.95	0.12	53,53,53,53	0
54	MG	1A	3700	1/1	0.95	0.14	41,41,41,41	0
54	MG	2A	3278	1/1	0.95	0.06	50,50,50,50	0
54	MG	1E	306	1/1	0.95	0.19	68,68,68,68	0
54	MG	1F	302	1/1	0.95	0.20	40,40,40,40	0
54	MG	2A	3282	1/1	0.95	0.06	52,52,52,52	0
54	MG	2A	3283	1/1	0.95	0.10	19,19,19,19	0
54	MG	1A	3962	1/1	0.95	0.08	59,59,59,59	0
54	MG	1A	3058	1/1	0.95	0.15	49,49,49,49	0
54	MG	1A	3702	1/1	0.95	0.13	43,43,43,43	0
54	MG	2A	3084	1/1	0.95	0.09	49,49,49,49	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	2A	3291	1/1	0.95	0.14	54,54,54,54	0
54	MG	2A	3085	1/1	0.95	0.07	46,46,46,46	0
54	MG	1A	3560	1/1	0.95	0.08	57,57,57,57	0
54	MG	2A	3088	1/1	0.95	0.32	47,47,47,47	0
54	MG	1A	3493	1/1	0.95	0.11	53,53,53,53	0
54	MG	1F	310	1/1	0.95	0.09	53,53,53,53	0
54	MG	28	8002	1/1	0.95	0.12	51,51,51,51	0
54	MG	2A	3298	1/1	0.95	0.06	33,33,33,33	0
54	MG	1A	3388	1/1	0.95	0.14	31,31,31,31	0
54	MG	1A	3495	1/1	0.95	0.07	45,45,45,45	0
54	MG	2A	3531	1/1	0.95	0.09	62,62,62,62	0
54	MG	1A	3436	1/1	0.95	0.07	43,43,43,43	0
54	MG	1A	3711	1/1	0.95	0.06	40,40,40,40	0
54	MG	1A	3831	1/1	0.95	0.17	53,53,53,53	0
54	MG	1A	3059	1/1	0.95	0.14	26,26,26,26	0
54	MG	2A	3309	1/1	0.95	0.09	39,39,39,39	0
54	MG	1A	3090	1/1	0.95	0.12	55,55,55,55	0
54	MG	1A	3714	1/1	0.95	0.08	45,45,45,45	0
54	MG	1A	3392	1/1	0.95	0.12	27,27,27,27	0
54	MG	1A	3637	1/1	0.95	0.08	49,49,49,49	0
54	MG	2A	3108	1/1	0.95	0.10	60,60,60,60	0
54	MG	1A	3092	1/1	0.95	0.12	35,35,35,35	0
54	MG	1a	1833	1/1	0.95	0.09	48,48,48,48	0
54	MG	1A	3346	1/1	0.95	0.07	35,35,35,35	0
54	MG	1R	202	1/1	0.95	0.12	50,50,50,50	0
54	MG	1A	3293	1/1	0.95	0.07	50,50,50,50	0
54	MG	2A	3331	1/1	0.95	0.08	47,47,47,47	0
54	MG	1A	3218	1/1	0.95	0.26	48,48,48,48	0
54	MG	1A	3173	1/1	0.95	0.21	52,52,52,52	0
54	MG	2A	3555	1/1	0.95	0.07	52,52,52,52	0
54	MG	1A	3039	1/1	0.95	0.09	48,48,48,48	0
54	MG	2A	3338	1/1	0.95	0.07	33,33,33,33	0
54	MG	1a	1840	1/1	0.95	0.11	58,58,58,58	0
54	MG	1A	3133	1/1	0.95	0.08	42,42,42,42	0
54	MG	2A	3565	1/1	0.95	0.09	57,57,57,57	0
54	MG	2A	3343	1/1	0.95	0.07	56,56,56,56	0
54	MG	2A	3344	1/1	0.95	0.11	42,42,42,42	0
54	MG	1U	202	1/1	0.95	0.16	47,47,47,47	0
54	MG	1A	3041	1/1	0.95	0.11	54,54,54,54	0
54	MG	2A	3127	1/1	0.95	0.09	44,44,44,44	0
54	MG	2A	3128	1/1	0.95	0.13	45,45,45,45	0
54	MG	1A	3408	1/1	0.95	0.09	38,38,38,38	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	1A	3001	1/1	0.95	0.08	33,33,33,33	0
54	MG	1A	3741	1/1	0.95	0.10	56,56,56,56	0
54	MG	1A	3517	1/1	0.95	0.11	22,22,22,22	0
54	MG	10	101	1/1	0.95	0.07	52,52,52,52	0
54	MG	1A	3248	1/1	0.95	0.35	58,58,58,58	0
54	MG	10	103	1/1	0.95	0.08	53,53,53,53	0
54	MG	1a	1858	1/1	0.95	0.07	54,54,54,54	0
54	MG	1A	3186	1/1	0.95	0.34	43,43,43,43	0
54	MG	1a	1860	1/1	0.95	0.11	66,66,66,66	0
54	MG	1A	3654	1/1	0.95	0.07	34,34,34,34	0
54	MG	2A	3145	1/1	0.95	0.09	49,49,49,49	0
54	MG	1A	3587	1/1	0.95	0.12	50,50,50,50	0
54	MG	2A	3147	1/1	0.95	0.08	47,47,47,47	0
54	MG	2A	3371	1/1	0.95	0.10	70,70,70,70	0
54	MG	1A	3139	1/1	0.95	0.06	45,45,45,45	0
54	MG	2A	3373	1/1	0.95	0.06	50,50,50,50	0
54	MG	1A	4006	1/1	0.95	0.10	55,55,55,55	0
54	MG	13	101	1/1	0.95	0.10	62,62,62,62	0
54	MG	2A	3154	1/1	0.95	0.14	45,45,45,45	0
54	MG	2A	3378	1/1	0.95	0.08	47,47,47,47	0
54	MG	1A	3021	1/1	0.95	0.15	34,34,34,34	0
54	MG	1A	4009	1/1	0.95	0.11	41,41,41,41	0
54	MG	1A	3659	1/1	0.95	0.08	54,54,54,54	0
54	MG	1A	3757	1/1	0.95	0.07	50,50,50,50	0
54	MG	1A	3008	1/1	0.95	0.07	40,40,40,40	0
54	MG	1A	3759	1/1	0.95	0.12	45,45,45,45	0
54	MG	1A	4021	1/1	0.95	0.22	34,34,34,34	0
54	MG	1A	3056	1/1	0.95	0.08	47,47,47,47	0
54	MG	2A	3168	1/1	0.95	0.31	46,46,46,46	0
54	MG	2A	3631	1/1	0.95	0.06	64,64,64,64	0
54	MG	1A	3263	1/1	0.95	0.19	49,49,49,49	0
54	MG	1A	3417	1/1	0.95	0.13	40,40,40,40	0
54	MG	1A	3033	1/1	0.95	0.12	44,44,44,44	0
54	MG	1A	3119	1/1	0.95	0.31	47,47,47,47	0
54	MG	1A	3767	1/1	0.95	0.06	43,43,43,43	0
54	MG	2A	3176	1/1	0.95	0.12	45,45,45,45	0
54	MG	2A	3399	1/1	0.95	0.07	61,61,61,61	0
54	MG	1d	503	1/1	0.95	0.33	69,69,69,69	0
54	MG	2A	3402	1/1	0.95	0.09	52,52,52,52	0
54	MG	1A	3124	1/1	0.95	0.12	45,45,45,45	0
54	MG	2a	1684	1/1	0.95	0.39	59,59,59,59	0
54	MG	1a	1747	1/1	0.95	0.15	54,54,54,54	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	2A	3406	1/1	0.95	0.08	42,42,42,42	0
54	MG	1a	1748	1/1	0.95	0.07	58,58,58,58	0
54	MG	1A	3326	1/1	0.95	0.10	33,33,33,33	0
54	MG	2A	3665	1/1	0.95	0.07	53,53,53,53	0
54	MG	1A	3543	1/1	0.95	0.20	46,46,46,46	0
54	MG	1a	1612	1/1	0.95	0.35	62,62,62,62	0
54	MG	1A	3904	1/1	0.95	0.06	51,51,51,51	0
54	MG	2A	3188	1/1	0.95	0.06	57,57,57,57	0
54	MG	1A	4048	1/1	0.95	0.15	35,35,35,35	0
54	MG	2A	3678	1/1	0.95	0.07	54,54,54,54	0
54	MG	2a	1699	1/1	0.95	0.07	53,53,53,53	0
54	MG	1A	4050	1/1	0.95	0.17	29,29,29,29	0
54	MG	1A	3675	1/1	0.95	0.14	60,60,60,60	0
54	MG	1A	3776	1/1	0.95	0.07	21,21,21,21	0
54	MG	1a	1621	1/1	0.95	0.06	48,48,48,48	0
54	MG	1A	4056	1/1	0.95	0.25	41,41,41,41	0
54	MG	1A	3912	1/1	0.95	0.06	39,39,39,39	0
54	MG	1A	3777	1/1	0.95	0.07	40,40,40,40	0
54	MG	2A	3689	1/1	0.95	0.07	45,45,45,45	0
54	MG	2A	3690	1/1	0.95	0.06	63,63,63,63	0
54	MG	1n	503	1/1	0.95	0.13	59,59,59,59	0
54	MG	1a	1629	1/1	0.95	0.26	65,65,65,65	0
54	MG	2a	1713	1/1	0.95	0.11	61,61,61,61	0
54	MG	2A	3201	1/1	0.95	0.14	53,53,53,53	0
54	MG	2A	3695	1/1	0.95	0.10	57,57,57,57	0
54	MG	2a	1716	1/1	0.95	0.15	64,64,64,64	0
54	MG	1A	4070	1/1	0.95	0.13	32,32,32,32	0
54	MG	1A	4075	1/1	0.95	0.14	39,39,39,39	0
54	MG	2a	1720	1/1	0.95	0.07	63,63,63,63	0
54	MG	1A	3915	1/1	0.95	0.10	34,34,34,34	0
54	MG	2a	1722	1/1	0.95	0.15	64,64,64,64	0
54	MG	1A	3475	1/1	0.95	0.14	40,40,40,40	0
54	MG	2A	3701	1/1	0.95	0.09	63,63,63,63	0
54	MG	1y	203	1/1	0.95	0.07	61,61,61,61	0
54	MG	2A	3705	1/1	0.95	0.13	57,57,57,57	0
54	MG	1A	3919	1/1	0.95	0.11	35,35,35,35	0
54	MG	2A	3441	1/1	0.95	0.11	70,70,70,70	0
54	MG	2A	3710	1/1	0.95	0.07	45,45,45,45	0
54	MG	1A	3921	1/1	0.95	0.09	61,61,61,61	0
54	MG	1A	3780	1/1	0.95	0.13	48,48,48,48	0
54	MG	2A	3211	1/1	0.95	0.10	56,56,56,56	0
54	MG	2A	3715	1/1	0.95	0.10	50,50,50,50	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	2A	3009	1/1	0.95	0.08	44,44,44,44	0
54	MG	1A	3476	1/1	0.95	0.08	39,39,39,39	0
54	MG	2A	3014	1/1	0.95	0.08	53,53,53,53	0
54	MG	2A	3215	1/1	0.95	0.09	54,54,54,54	0
54	MG	2A	3721	1/1	0.95	0.11	59,59,59,59	0
54	MG	1A	3273	1/1	0.95	0.11	55,55,55,55	0
54	MG	2A	3217	1/1	0.95	0.27	61,61,61,61	0
54	MG	2a	1754	1/1	0.95	0.14	84,84,84,84	0
54	MG	1A	3930	1/1	0.95	0.09	60,60,60,60	0
54	MG	2A	3022	1/1	0.95	0.21	44,44,44,44	0
54	MG	1A	3605	1/1	0.95	0.23	40,40,40,40	0
54	MG	1a	1645	1/1	0.95	0.09	61,61,61,61	0
54	MG	2a	1763	1/1	0.95	0.07	51,51,51,51	0
54	MG	1A	3681	1/1	0.95	0.07	29,29,29,29	0
54	MG	2A	3735	1/1	0.95	0.09	38,38,38,38	0
54	MG	1A	3607	1/1	0.95	0.20	52,52,52,52	0
54	MG	1A	3935	1/1	0.95	0.08	53,53,53,53	0
54	MG	1A	3376	1/1	0.95	0.09	45,45,45,45	0
54	MG	2A	3741	1/1	0.95	0.16	50,50,50,50	0
54	MG	2A	3743	1/1	0.95	0.11	63,63,63,63	0
54	MG	2A	3745	1/1	0.95	0.35	67,67,67,67	0
54	MG	1A	3479	1/1	0.95	0.15	42,42,42,42	0
54	MG	2a	1783	1/1	0.95	0.06	62,62,62,62	0
54	MG	1B	220	1/1	0.95	0.06	34,34,34,34	0
54	MG	1A	3330	1/1	0.95	0.09	33,33,33,33	0
54	MG	1A	3940	1/1	0.95	0.05	43,43,43,43	0
54	MG	1B	223	1/1	0.95	0.07	69,69,69,69	0
54	MG	2A	3756	1/1	0.95	0.15	52,52,52,52	0
54	MG	2A	3039	1/1	0.95	0.13	55,55,55,55	0
54	MG	2A	3233	1/1	0.95	0.09	58,58,58,58	0
54	MG	2a	1793	1/1	0.95	0.13	51,51,51,51	0
54	MG	2A	3761	1/1	0.95	0.17	37,37,37,37	0
54	MG	2A	3763	1/1	0.95	0.08	40,40,40,40	0
54	MG	1A	3796	1/1	0.95	0.10	60,60,60,60	0
54	MG	2A	3236	1/1	0.95	0.09	49,49,49,49	0
54	MG	1A	3481	1/1	0.95	0.08	57,57,57,57	0
54	MG	2A	3238	1/1	0.95	0.21	47,47,47,47	0
54	MG	2A	3044	1/1	0.95	0.09	44,44,44,44	0
54	MG	2A	3045	1/1	0.95	0.11	41,41,41,41	0
54	MG	1A	3201	1/1	0.95	0.15	47,47,47,47	0
54	MG	2A	3047	1/1	0.95	0.10	46,46,46,46	0
54	MG	1a	1662	1/1	0.95	0.37	64,64,64,64	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	ARG	1B	230	12/12	0.95	0.08	29,41,51,51	0
54	MG	1a	1663	1/1	0.95	0.18	58,58,58,58	0
54	MG	2A	3050	1/1	0.95	0.18	54,54,54,54	0
54	MG	1A	3800	1/1	0.95	0.08	38,38,38,38	0
54	MG	1A	3483	1/1	0.95	0.10	31,31,31,31	0
54	MG	1A	3651	1/1	0.96	0.10	58,58,58,58	0
54	MG	1A	3095	1/1	0.96	0.31	45,45,45,45	0
54	MG	2A	3742	1/1	0.96	0.11	56,56,56,56	0
54	MG	2A	3210	1/1	0.96	0.07	53,53,53,53	0
54	MG	1A	3564	1/1	0.96	0.10	26,26,26,26	0
54	MG	1A	3074	1/1	0.96	0.09	36,36,36,36	0
54	MG	2A	3450	1/1	0.96	0.15	58,58,58,58	0
54	MG	2A	3451	1/1	0.96	0.11	39,39,39,39	0
54	MG	1A	3051	1/1	0.96	0.22	48,48,48,48	0
54	MG	1A	3202	1/1	0.96	0.20	49,49,49,49	0
54	MG	1A	3484	1/1	0.96	0.08	41,41,41,41	0
54	MG	1A	3778	1/1	0.96	0.05	34,34,34,34	0
54	MG	1Q	201	1/1	0.96	0.08	33,33,33,33	0
54	MG	1A	3658	1/1	0.96	0.05	19,19,19,19	0
54	MG	2A	3762	1/1	0.96	0.08	53,53,53,53	0
54	MG	1y	202	1/1	0.96	0.09	59,59,59,59	0
54	MG	1A	3167	1/1	0.96	0.12	53,53,53,53	0
54	MG	1A	3781	1/1	0.96	0.08	48,48,48,48	0
54	MG	1A	3660	1/1	0.96	0.07	23,23,23,23	0
54	MG	1A	3168	1/1	0.96	0.06	32,32,32,32	0
54	MG	1A	3784	1/1	0.96	0.04	36,36,36,36	0
54	MG	1A	3489	1/1	0.96	0.08	61,61,61,61	0
54	MG	2A	3012	1/1	0.96	0.04	39,39,39,39	0
54	MG	1A	3574	1/1	0.96	0.10	31,31,31,31	0
54	MG	1A	3961	1/1	0.96	0.10	45,45,45,45	0
54	MG	1A	3787	1/1	0.96	0.06	25,25,25,25	0
54	MG	1V	201	1/1	0.96	0.07	55,55,55,55	0
54	MG	1A	3490	1/1	0.96	0.17	66,66,66,66	0
54	MG	1A	3101	1/1	0.96	0.08	47,47,47,47	0
54	MG	1A	3354	1/1	0.96	0.08	63,63,63,63	0
54	MG	2A	3026	1/1	0.96	0.09	45,45,45,45	0
54	MG	2B	3016	1/1	0.96	0.06	67,67,67,67	0
54	MG	2A	3027	1/1	0.96	0.10	45,45,45,45	0
54	MG	1A	3079	1/1	0.96	0.12	40,40,40,40	0
54	MG	1X	8001	1/1	0.96	0.11	43,43,43,43	0
54	MG	1A	3671	1/1	0.96	0.12	36,36,36,36	0
54	MG	2D	303	1/1	0.96	0.26	44,44,44,44	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	1A	3012	1/1	0.96	0.08	38,38,38,38	0
54	MG	1A	3673	1/1	0.96	0.06	55,55,55,55	0
54	MG	2A	3245	1/1	0.96	0.08	56,56,56,56	0
54	MG	1A	3209	1/1	0.96	0.07	44,44,44,44	0
54	MG	1a	1755	1/1	0.96	0.17	58,58,58,58	0
54	MG	1A	3802	1/1	0.96	0.06	47,47,47,47	0
54	MG	2A	3249	1/1	0.96	0.08	49,49,49,49	0
54	MG	2F	301	1/1	0.96	0.08	44,44,44,44	0
54	MG	1A	3977	1/1	0.96	0.07	24,24,24,24	0
54	MG	1A	3359	1/1	0.96	0.10	11,11,11,11	0
54	MG	11	102	1/1	0.96	0.07	49,49,49,49	0
54	MG	2A	3042	1/1	0.96	0.13	47,47,47,47	0
54	MG	1A	3288	1/1	0.96	0.14	57,57,57,57	0
54	MG	1A	3289	1/1	0.96	0.07	31,31,31,31	0
54	MG	2O	201	1/1	0.96	0.13	58,58,58,58	0
54	MG	1A	3362	1/1	0.96	0.09	39,39,39,39	0
54	MG	13	102	1/1	0.96	0.07	49,49,49,49	0
54	MG	1A	3172	1/1	0.96	0.22	48,48,48,48	0
54	MG	1A	3809	1/1	0.96	0.25	46,46,46,46	0
54	MG	2A	3261	1/1	0.96	0.17	47,47,47,47	0
54	MG	1A	3986	1/1	0.96	0.06	19,19,19,19	0
54	MG	1A	3364	1/1	0.96	0.06	33,33,33,33	0
54	MG	2A	3266	1/1	0.96	0.11	55,55,55,55	0
54	MG	2V	201	1/1	0.96	0.18	60,60,60,60	0
54	MG	2A	3510	1/1	0.96	0.09	47,47,47,47	0
54	MG	1A	3212	1/1	0.96	0.09	48,48,48,48	0
54	MG	1A	3504	1/1	0.96	0.11	26,26,26,26	0
54	MG	2A	3269	1/1	0.96	0.17	38,38,38,38	0
54	MG	2A	3271	1/1	0.96	0.24	47,47,47,47	0
54	MG	27	3001	1/1	0.96	0.12	43,43,43,43	0
54	MG	1A	3685	1/1	0.96	0.06	70,70,70,70	0
54	MG	1A	3366	1/1	0.96	0.09	46,46,46,46	0
54	MG	1A	3992	1/1	0.96	0.06	19,19,19,19	0
54	MG	1A	3993	1/1	0.96	0.29	54,54,54,54	0
54	MG	1A	3086	1/1	0.96	0.23	45,45,45,45	0
54	MG	1A	3818	1/1	0.96	0.06	47,47,47,47	0
54	MG	1A	3508	1/1	0.96	0.07	46,46,46,46	0
54	MG	1A	3820	1/1	0.96	0.11	31,31,31,31	0
54	MG	1A	3217	1/1	0.96	0.20	49,49,49,49	0
54	MG	2A	3525	1/1	0.96	0.09	51,51,51,51	0
54	MG	2A	3066	1/1	0.96	0.06	45,45,45,45	0
54	MG	2A	3286	1/1	0.96	0.05	31,31,31,31	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	1A	3822	1/1	0.96	0.08	34,34,34,34	0
54	MG	1a	1610	1/1	0.96	0.12	45,45,45,45	0
54	MG	1A	3691	1/1	0.96	0.08	54,54,54,54	0
54	MG	2a	1616	1/1	0.96	0.06	48,48,48,48	0
54	MG	1A	3510	1/1	0.96	0.13	31,31,31,31	0
54	MG	1A	3088	1/1	0.96	0.31	47,47,47,47	0
54	MG	2A	3078	1/1	0.96	0.09	56,56,56,56	0
54	MG	1A	3060	1/1	0.96	0.09	49,49,49,49	0
54	MG	1A	3514	1/1	0.96	0.08	23,23,23,23	0
54	MG	1A	3832	1/1	0.96	0.09	50,50,50,50	0
54	MG	1A	4007	1/1	0.96	0.12	17,17,17,17	0
54	MG	2A	3299	1/1	0.96	0.06	35,35,35,35	0
54	MG	1A	3301	1/1	0.96	0.23	48,48,48,48	0
54	MG	1A	3602	1/1	0.96	0.24	32,32,32,32	0
54	MG	1A	3147	1/1	0.96	0.17	46,46,46,46	0
54	MG	2A	3542	1/1	0.96	0.14	34,34,34,34	0
54	MG	2A	3543	1/1	0.96	0.05	42,42,42,42	0
54	MG	1A	4011	1/1	0.96	0.10	58,58,58,58	0
54	MG	1a	1630	1/1	0.96	0.18	64,64,64,64	0
54	MG	2A	3307	1/1	0.96	0.11	53,53,53,53	0
54	MG	2A	3548	1/1	0.96	0.06	55,55,55,55	0
54	MG	1A	4015	1/1	0.96	0.24	41,41,41,41	0
54	MG	1A	3116	1/1	0.96	0.11	49,49,49,49	0
54	MG	2A	3094	1/1	0.96	0.10	40,40,40,40	0
54	MG	2A	3552	1/1	0.96	0.09	57,57,57,57	0
54	MG	2A	3311	1/1	0.96	0.07	49,49,49,49	0
54	MG	1A	3225	1/1	0.96	0.10	49,49,49,49	0
54	MG	1a	1635	1/1	0.96	0.07	37,37,37,37	0
54	MG	1a	1636	1/1	0.96	0.10	47,47,47,47	0
54	MG	2A	3557	1/1	0.96	0.09	52,52,52,52	0
54	MG	1A	3839	1/1	0.96	0.22	60,60,60,60	0
54	MG	2A	3318	1/1	0.96	0.10	37,37,37,37	0
54	MG	1A	3069	1/1	0.96	0.10	37,37,37,37	0
54	MG	1A	3231	1/1	0.96	0.08	44,44,44,44	0
54	MG	1a	1807	1/1	0.96	0.08	73,73,73,73	0
54	MG	2A	3324	1/1	0.96	0.07	44,44,44,44	0
54	MG	2A	3325	1/1	0.96	0.07	50,50,50,50	0
54	MG	2A	3570	1/1	0.96	0.08	57,57,57,57	0
54	MG	1A	4024	1/1	0.96	0.22	36,36,36,36	0
54	MG	1A	3526	1/1	0.96	0.07	48,48,48,48	0
54	MG	2A	3575	1/1	0.96	0.06	43,43,43,43	0
54	MG	2A	3330	1/1	0.96	0.08	31,31,31,31	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	1A	3234	1/1	0.96	0.12	37,37,37,37	0
54	MG	2A	3332	1/1	0.96	0.07	50,50,50,50	0
54	MG	1A	3235	1/1	0.96	0.12	41,41,41,41	0
54	MG	2A	3111	1/1	0.96	0.07	54,54,54,54	0
54	MG	1A	3236	1/1	0.96	0.18	59,59,59,59	0
54	MG	1A	4031	1/1	0.96	0.24	38,38,38,38	0
54	MG	2A	3586	1/1	0.96	0.07	62,62,62,62	0
54	MG	1A	3850	1/1	0.96	0.10	33,33,33,33	0
54	MG	1a	1816	1/1	0.96	0.09	73,73,73,73	0
54	MG	1A	3852	1/1	0.96	0.08	46,46,46,46	0
54	MG	1A	3614	1/1	0.96	0.07	38,38,38,38	0
54	MG	2A	3345	1/1	0.96	0.05	35,35,35,35	0
54	MG	1A	3243	1/1	0.96	0.13	33,33,33,33	0
54	MG	1A	3320	1/1	0.96	0.14	33,33,33,33	0
54	MG	2A	3600	1/1	0.96	0.09	67,67,67,67	0
54	MG	1a	1821	1/1	0.96	0.09	72,72,72,72	0
54	MG	2A	3123	1/1	0.96	0.30	48,48,48,48	0
54	MG	2A	3607	1/1	0.96	0.09	67,67,67,67	0
54	MG	1A	3532	1/1	0.96	0.16	61,61,61,61	0
54	MG	2A	3351	1/1	0.96	0.04	35,35,35,35	0
54	MG	1A	3385	1/1	0.96	0.13	40,40,40,40	0
54	MG	1A	3386	1/1	0.96	0.10	41,41,41,41	0
54	MG	1A	4053	1/1	0.96	0.20	45,45,45,45	0
54	MG	1A	3717	1/1	0.96	0.18	39,39,39,39	0
54	MG	2A	3356	1/1	0.96	0.08	48,48,48,48	0
54	MG	2A	3130	1/1	0.96	0.32	42,42,42,42	0
54	MG	1A	3537	1/1	0.96	0.07	31,31,31,31	0
54	MG	1A	3538	1/1	0.96	0.06	36,36,36,36	0
54	MG	2A	3364	1/1	0.96	0.14	49,49,49,49	0
54	MG	2A	3134	1/1	0.96	0.14	49,49,49,49	0
54	MG	2a	1691	1/1	0.96	0.10	71,71,71,71	0
54	MG	2a	1692	1/1	0.96	0.06	77,77,77,77	0
54	MG	1A	4060	1/1	0.96	0.23	32,32,32,32	0
54	MG	1A	3246	1/1	0.96	0.13	54,54,54,54	0
54	MG	1A	4067	1/1	0.96	0.11	42,42,42,42	0
54	MG	2A	3630	1/1	0.96	0.06	52,52,52,52	0
54	MG	1A	3869	1/1	0.96	0.07	50,50,50,50	0
54	MG	1a	1666	1/1	0.96	0.08	53,53,53,53	0
54	MG	1A	4074	1/1	0.96	0.06	43,43,43,43	0
54	MG	1A	3457	1/1	0.96	0.10	51,51,51,51	0
54	MG	1A	3871	1/1	0.96	0.05	45,45,45,45	0
54	MG	1A	3073	1/1	0.96	0.07	38,38,38,38	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	1A	3727	1/1	0.96	0.09	42,42,42,42	0
54	MG	1a	1672	1/1	0.96	0.14	58,58,58,58	0
54	MG	2A	3639	1/1	0.96	0.08	59,59,59,59	0
54	MG	2A	3640	1/1	0.96	0.07	63,63,63,63	0
54	MG	2a	1708	1/1	0.96	0.09	55,55,55,55	0
54	MG	2A	3641	1/1	0.96	0.11	49,49,49,49	0
54	MG	2A	3377	1/1	0.96	0.08	57,57,57,57	0
54	MG	1A	3628	1/1	0.96	0.09	20,20,20,20	0
54	MG	2A	3646	1/1	0.96	0.09	71,71,71,71	0
54	MG	2A	3651	1/1	0.96	0.06	66,66,66,66	0
54	MG	2A	3379	1/1	0.96	0.06	30,30,30,30	0
54	MG	1A	3730	1/1	0.96	0.07	53,53,53,53	0
54	MG	1A	3323	1/1	0.96	0.13	28,28,28,28	0
54	MG	2a	1717	1/1	0.96	0.09	77,77,77,77	0
54	MG	1A	3886	1/1	0.96	0.04	29,29,29,29	0
54	MG	1A	3735	1/1	0.96	0.11	39,39,39,39	0
54	MG	2A	3156	1/1	0.96	0.05	36,36,36,36	0
54	MG	1a	1678	1/1	0.96	0.27	64,64,64,64	0
54	MG	1A	3736	1/1	0.96	0.06	54,54,54,54	0
54	MG	2A	3670	1/1	0.96	0.13	38,38,38,38	0
54	MG	1A	3630	1/1	0.96	0.04	41,41,41,41	0
54	MG	2A	3672	1/1	0.96	0.06	39,39,39,39	0
54	MG	2A	3673	1/1	0.96	0.06	38,38,38,38	0
54	MG	1A	3189	1/1	0.96	0.23	44,44,44,44	0
54	MG	1a	1855	1/1	0.96	0.06	59,59,59,59	0
54	MG	1a	1682	1/1	0.96	0.11	47,47,47,47	0
54	MG	2a	1730	1/1	0.96	0.07	55,55,55,55	0
54	MG	1A	3093	1/1	0.96	0.11	54,54,54,54	0
54	MG	1A	3892	1/1	0.96	0.12	38,38,38,38	0
54	MG	1A	3633	1/1	0.96	0.17	46,46,46,46	0
54	MG	2A	3397	1/1	0.96	0.05	36,36,36,36	0
54	MG	1A	3743	1/1	0.96	0.09	45,45,45,45	0
54	MG	2A	3685	1/1	0.96	0.06	60,60,60,60	0
54	MG	1A	3465	1/1	0.96	0.05	59,59,59,59	0
54	MG	1A	3253	1/1	0.96	0.24	34,34,34,34	0
54	MG	2a	1748	1/1	0.96	0.10	75,75,75,75	0
54	MG	2A	3401	1/1	0.96	0.07	43,43,43,43	0
54	MG	2a	1750	1/1	0.96	0.08	79,79,79,79	0
54	MG	1A	3126	1/1	0.96	0.09	44,44,44,44	0
54	MG	2A	3691	1/1	0.96	0.06	54,54,54,54	0
54	MG	2a	1753	1/1	0.96	0.08	74,74,74,74	0
54	MG	2A	3403	1/1	0.96	0.09	36,36,36,36	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	2A	3175	1/1	0.96	0.07	52,52,52,52	0
54	MG	1A	3256	1/1	0.96	0.07	35,35,35,35	0
54	MG	2A	3177	1/1	0.96	0.13	39,39,39,39	0
54	MG	2a	1760	1/1	0.96	0.08	63,63,63,63	0
54	MG	1A	3906	1/1	0.96	0.25	38,38,38,38	0
54	MG	1A	3907	1/1	0.96	0.05	13,13,13,13	0
54	MG	1A	3748	1/1	0.96	0.20	54,54,54,54	0
54	MG	1A	3911	1/1	0.96	0.10	28,28,28,28	0
54	MG	1A	3749	1/1	0.96	0.06	27,27,27,27	0
54	MG	1A	3913	1/1	0.96	0.06	22,22,22,22	0
54	MG	2A	3704	1/1	0.96	0.07	48,48,48,48	0
54	MG	2a	1775	1/1	0.96	0.17	57,57,57,57	0
54	MG	1a	1698	1/1	0.96	0.12	60,60,60,60	0
54	MG	2A	3706	1/1	0.96	0.06	51,51,51,51	0
54	MG	2A	3707	1/1	0.96	0.13	39,39,39,39	0
54	MG	1A	3750	1/1	0.96	0.11	33,33,33,33	0
54	MG	1D	310	1/1	0.96	0.08	52,52,52,52	0
54	MG	1a	1876	1/1	0.96	0.17	41,41,41,41	0
54	MG	1A	3551	1/1	0.96	0.12	50,50,50,50	0
54	MG	1A	3159	1/1	0.96	0.10	53,53,53,53	0
54	MG	1A	3401	1/1	0.96	0.08	32,32,32,32	0
54	MG	1A	3472	1/1	0.96	0.11	36,36,36,36	0
54	MG	1A	3756	1/1	0.96	0.07	47,47,47,47	0
54	MG	2A	3424	1/1	0.96	0.23	61,61,61,61	0
54	MG	2A	3718	1/1	0.96	0.08	67,67,67,67	0
54	MG	1A	3923	1/1	0.96	0.04	43,43,43,43	0
54	MG	1A	3473	1/1	0.96	0.06	33,33,33,33	0
54	MG	1A	3193	1/1	0.96	0.12	46,46,46,46	0
54	MG	1A	3403	1/1	0.96	0.07	25,25,25,25	0
54	MG	2A	3429	1/1	0.96	0.06	36,36,36,36	0
54	MG	2t	3001	1/1	0.96	0.15	52,52,52,52	0
54	MG	2A	3430	1/1	0.96	0.09	52,52,52,52	0
54	MG	2A	3726	1/1	0.96	0.08	58,58,58,58	0
55	MPD	18	102	8/8	0.96	0.09	30,34,40,47	0
54	MG	1A	3931	1/1	0.96	0.07	35,35,35,35	0
54	MG	1A	3194	1/1	0.96	0.26	42,42,42,42	0
54	MG	1A	3161	1/1	0.96	0.08	49,49,49,49	0
54	MG	1A	3198	1/1	0.96	0.28	56,56,56,56	0
54	MG	2A	3732	1/1	0.96	0.17	47,47,47,47	0
54	MG	1A	3764	1/1	0.96	0.06	29,29,29,29	0
54	MG	2A	3736	1/1	0.96	0.21	50,50,50,50	0
54	MG	1A	3343	1/1	0.96	0.06	31,31,31,31	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	1A	3650	1/1	0.96	0.14	61,61,61,61	0
54	MG	2A	3496	1/1	0.97	0.06	41,41,41,41	0
54	MG	2A	3064	1/1	0.97	0.04	38,38,38,38	0
54	MG	1A	4063	1/1	0.97	0.13	41,41,41,41	0
54	MG	1A	3521	1/1	0.97	0.20	31,31,31,31	0
54	MG	1A	4066	1/1	0.97	0.10	38,38,38,38	0
54	MG	1A	3083	1/1	0.97	0.08	38,38,38,38	0
54	MG	2A	3069	1/1	0.97	0.11	44,44,44,44	0
54	MG	1A	4069	1/1	0.97	0.21	40,40,40,40	0
54	MG	1A	3523	1/1	0.97	0.10	49,49,49,49	0
54	MG	2A	3276	1/1	0.97	0.06	40,40,40,40	0
54	MG	2A	3073	1/1	0.97	0.08	49,49,49,49	0
54	MG	1A	4071	1/1	0.97	0.06	39,39,39,39	0
54	MG	2A	3076	1/1	0.97	0.22	51,51,51,51	0
54	MG	2A	3077	1/1	0.97	0.18	48,48,48,48	0
54	MG	2A	3281	1/1	0.97	0.05	33,33,33,33	0
54	MG	1a	1802	1/1	0.97	0.06	63,63,63,63	0
54	MG	2A	3079	1/1	0.97	0.09	44,44,44,44	0
54	MG	2B	3019	1/1	0.97	0.07	51,51,51,51	0
54	MG	1A	4072	1/1	0.97	0.12	36,36,36,36	0
54	MG	1a	1646	1/1	0.97	0.10	39,39,39,39	0
54	MG	1A	3175	1/1	0.97	0.05	43,43,43,43	0
54	MG	1A	3918	1/1	0.97	0.07	52,52,52,52	0
54	MG	2D	305	1/1	0.97	0.17	49,49,49,49	0
54	MG	2A	3518	1/1	0.97	0.08	35,35,35,35	0
54	MG	1A	3255	1/1	0.97	0.25	45,45,45,45	0
54	MG	1B	201	1/1	0.97	0.22	44,44,44,44	0
54	MG	1a	1652	1/1	0.97	0.11	44,44,44,44	0
54	MG	2E	302	1/1	0.97	0.06	41,41,41,41	0
54	MG	1A	3920	1/1	0.97	0.04	47,47,47,47	0
54	MG	2A	3089	1/1	0.97	0.04	33,33,33,33	0
54	MG	1A	3070	1/1	0.97	0.21	43,43,43,43	0
54	MG	2A	3091	1/1	0.97	0.05	34,34,34,34	0
54	MG	2F	303	1/1	0.97	0.20	43,43,43,43	0
54	MG	1A	3153	1/1	0.97	0.12	46,46,46,46	0
54	MG	1a	1813	1/1	0.97	0.05	81,81,81,81	0
54	MG	1A	3384	1/1	0.97	0.08	43,43,43,43	0
54	MG	1A	3924	1/1	0.97	0.07	61,61,61,61	0
54	MG	1A	3259	1/1	0.97	0.09	40,40,40,40	0
54	MG	1B	209	1/1	0.97	0.04	39,39,39,39	0
54	MG	2A	3304	1/1	0.97	0.12	37,37,37,37	0
54	MG	1A	3927	1/1	0.97	0.07	63,63,63,63	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	1A	3693	1/1	0.97	0.25	54,54,54,54	0
54	MG	2Q	3001	1/1	0.97	0.04	44,44,44,44	0
54	MG	1B	212	1/1	0.97	0.06	59,59,59,59	0
54	MG	1B	213	1/1	0.97	0.07	55,55,55,55	0
54	MG	1A	3792	1/1	0.97	0.06	26,26,26,26	0
54	MG	1A	3260	1/1	0.97	0.05	44,44,44,44	0
54	MG	1A	3327	1/1	0.97	0.04	32,32,32,32	0
54	MG	1A	3533	1/1	0.97	0.17	27,27,27,27	0
54	MG	1A	3613	1/1	0.97	0.19	42,42,42,42	0
54	MG	1A	3180	1/1	0.97	0.19	48,48,48,48	0
54	MG	1A	3801	1/1	0.97	0.05	45,45,45,45	0
54	MG	2A	3114	1/1	0.97	0.06	47,47,47,47	0
54	MG	2A	3545	1/1	0.97	0.05	75,75,75,75	0
54	MG	2A	3115	1/1	0.97	0.05	50,50,50,50	0
54	MG	2A	3322	1/1	0.97	0.05	40,40,40,40	0
54	MG	1A	3937	1/1	0.97	0.05	71,71,71,71	0
54	MG	1A	3535	1/1	0.97	0.04	26,26,26,26	0
54	MG	1B	224	1/1	0.97	0.04	44,44,44,44	0
54	MG	1A	3211	1/1	0.97	0.16	40,40,40,40	0
54	MG	1B	226	1/1	0.97	0.05	37,37,37,37	0
54	MG	1A	3072	1/1	0.97	0.10	37,37,37,37	0
54	MG	1A	3805	1/1	0.97	0.05	63,63,63,63	0
54	MG	1A	3464	1/1	0.97	0.09	47,47,47,47	0
54	MG	1A	3539	1/1	0.97	0.09	36,36,36,36	0
54	MG	2A	3334	1/1	0.97	0.06	31,31,31,31	0
54	MG	1D	301	1/1	0.97	0.16	37,37,37,37	0
54	MG	1A	3333	1/1	0.97	0.10	47,47,47,47	0
54	MG	1A	3946	1/1	0.97	0.12	56,56,56,56	0
54	MG	2A	3564	1/1	0.97	0.05	57,57,57,57	0
54	MG	2a	1615	1/1	0.97	0.21	63,63,63,63	0
54	MG	2A	3339	1/1	0.97	0.05	36,36,36,36	0
54	MG	1A	3947	1/1	0.97	0.06	50,50,50,50	0
54	MG	2A	3567	1/1	0.97	0.04	46,46,46,46	0
54	MG	2a	1619	1/1	0.97	0.08	48,48,48,48	0
54	MG	1D	309	1/1	0.97	0.13	40,40,40,40	0
54	MG	1A	3541	1/1	0.97	0.04	27,27,27,27	0
54	MG	1A	3707	1/1	0.97	0.10	43,43,43,43	0
54	MG	1D	312	1/1	0.97	0.08	54,54,54,54	0
54	MG	1A	3334	1/1	0.97	0.09	37,37,37,37	0
54	MG	1A	3396	1/1	0.97	0.08	26,26,26,26	0
54	MG	1A	3265	1/1	0.97	0.07	40,40,40,40	0
54	MG	2a	1627	1/1	0.97	0.09	49,49,49,49	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	1a	1853	1/1	0.97	0.06	54,54,54,54	0
54	MG	1A	3627	1/1	0.97	0.11	42,42,42,42	0
54	MG	2A	3579	1/1	0.97	0.09	56,56,56,56	0
54	MG	1A	3336	1/1	0.97	0.09	45,45,45,45	0
54	MG	2A	3581	1/1	0.97	0.08	48,48,48,48	0
54	MG	1A	3155	1/1	0.97	0.09	54,54,54,54	0
54	MG	2a	1634	1/1	0.97	0.07	37,37,37,37	0
54	MG	2A	3143	1/1	0.97	0.07	40,40,40,40	0
54	MG	1A	3268	1/1	0.97	0.12	45,45,45,45	0
54	MG	1A	3215	1/1	0.97	0.10	50,50,50,50	0
54	MG	1F	303	1/1	0.97	0.12	34,34,34,34	0
54	MG	1A	3340	1/1	0.97	0.06	25,25,25,25	0
54	MG	2A	3359	1/1	0.97	0.04	40,40,40,40	0
54	MG	2A	3592	1/1	0.97	0.10	47,47,47,47	0
54	MG	1A	3404	1/1	0.97	0.05	33,33,33,33	0
54	MG	2A	3594	1/1	0.97	0.07	46,46,46,46	0
54	MG	2A	3150	1/1	0.97	0.20	46,46,46,46	0
54	MG	2A	3151	1/1	0.97	0.04	48,48,48,48	0
54	MG	1A	3216	1/1	0.97	0.13	44,44,44,44	0
54	MG	1A	3107	1/1	0.97	0.21	38,38,38,38	0
54	MG	2A	3602	1/1	0.97	0.05	32,32,32,32	0
54	MG	1A	3722	1/1	0.97	0.05	32,32,32,32	0
54	MG	2A	3604	1/1	0.97	0.09	35,35,35,35	0
54	MG	1a	1867	1/1	0.97	0.05	47,47,47,47	0
54	MG	1A	3966	1/1	0.97	0.06	48,48,48,48	0
54	MG	1A	3724	1/1	0.97	0.07	66,66,66,66	0
54	MG	2A	3158	1/1	0.97	0.09	44,44,44,44	0
54	MG	1A	3968	1/1	0.97	0.14	44,44,44,44	0
54	MG	2A	3160	1/1	0.97	0.14	44,44,44,44	0
54	MG	2A	3161	1/1	0.97	0.10	51,51,51,51	0
54	MG	1A	3108	1/1	0.97	0.06	41,41,41,41	0
54	MG	1A	3970	1/1	0.97	0.08	62,62,62,62	0
54	MG	1a	1709	1/1	0.97	0.07	39,39,39,39	0
54	MG	2A	3621	1/1	0.97	0.10	56,56,56,56	0
54	MG	1A	3972	1/1	0.97	0.07	26,26,26,26	0
54	MG	2A	3623	1/1	0.97	0.15	61,61,61,61	0
54	MG	1a	1712	1/1	0.97	0.04	50,50,50,50	0
54	MG	2A	3167	1/1	0.97	0.21	41,41,41,41	0
54	MG	1A	3275	1/1	0.97	0.12	41,41,41,41	0
54	MG	2A	3169	1/1	0.97	0.16	41,41,41,41	0
54	MG	1A	3160	1/1	0.97	0.22	44,44,44,44	0
54	MG	1N	203	1/1	0.97	0.06	53,53,53,53	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	1a	1881	1/1	0.97	0.06	68,68,68,68	0
54	MG	1A	3220	1/1	0.97	0.31	39,39,39,39	0
54	MG	1A	3729	1/1	0.97	0.09	27,27,27,27	0
54	MG	1A	3026	1/1	0.97	0.22	34,34,34,34	0
54	MG	1A	3350	1/1	0.97	0.13	37,37,37,37	0
54	MG	1A	3733	1/1	0.97	0.05	55,55,55,55	0
54	MG	1A	3351	1/1	0.97	0.05	24,24,24,24	0
54	MG	2A	3393	1/1	0.97	0.08	43,43,43,43	0
54	MG	1A	3842	1/1	0.97	0.07	41,41,41,41	0
54	MG	1A	3983	1/1	0.97	0.09	74,74,74,74	0
54	MG	1e	203	1/1	0.97	0.09	58,58,58,58	0
54	MG	2a	1682	1/1	0.97	0.09	51,51,51,51	0
54	MG	1A	3222	1/1	0.97	0.09	36,36,36,36	0
54	MG	2A	3184	1/1	0.97	0.08	45,45,45,45	0
54	MG	1A	3132	1/1	0.97	0.05	39,39,39,39	0
54	MG	2A	3645	1/1	0.97	0.05	77,77,77,77	0
54	MG	1g	201	1/1	0.97	0.10	62,62,62,62	0
54	MG	2A	3650	1/1	0.97	0.05	61,61,61,61	0
54	MG	1A	3017	1/1	0.97	0.17	37,37,37,37	0
54	MG	2a	1690	1/1	0.97	0.05	71,71,71,71	0
54	MG	1A	3227	1/1	0.97	0.23	37,37,37,37	0
54	MG	2A	3656	1/1	0.97	0.15	61,61,61,61	0
54	MG	2A	3657	1/1	0.97	0.06	40,40,40,40	0
54	MG	1A	3229	1/1	0.97	0.08	47,47,47,47	0
54	MG	1A	3742	1/1	0.97	0.06	47,47,47,47	0
54	MG	1a	1734	1/1	0.97	0.09	47,47,47,47	0
54	MG	2A	3192	1/1	0.97	0.07	44,44,44,44	0
54	MG	1A	3851	1/1	0.97	0.10	44,44,44,44	0
54	MG	2A	3666	1/1	0.97	0.08	54,54,54,54	0
54	MG	2a	1700	1/1	0.97	0.24	47,47,47,47	0
54	MG	1A	3165	1/1	0.97	0.12	37,37,37,37	0
54	MG	1A	3853	1/1	0.97	0.08	40,40,40,40	0
54	MG	2A	3669	1/1	0.97	0.04	38,38,38,38	0
54	MG	1A	3068	1/1	0.97	0.23	49,49,49,49	0
54	MG	1A	3423	1/1	0.97	0.06	16,16,16,16	0
54	MG	1A	3856	1/1	0.97	0.10	33,33,33,33	0
54	MG	1A	3232	1/1	0.97	0.11	42,42,42,42	0
54	MG	1A	3197	1/1	0.97	0.06	52,52,52,52	0
54	MG	1A	3427	1/1	0.97	0.07	39,39,39,39	0
54	MG	1A	3498	1/1	0.97	0.07	50,50,50,50	0
54	MG	1A	3135	1/1	0.97	0.20	41,41,41,41	0
54	MG	1A	3863	1/1	0.97	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
54	MG	1A	3136	1/1	0.97	0.19	39,39,39,39	0
54	MG	1A	3237	1/1	0.97	0.12	36,36,36,36	0
54	MG	2A	3423	1/1	0.97	0.05	33,33,33,33	0
54	MG	2A	3003	1/1	0.97	0.05	51,51,51,51	0
54	MG	2A	3686	1/1	0.97	0.06	43,43,43,43	0
54	MG	2A	3006	1/1	0.97	0.10	46,46,46,46	0
54	MG	2A	3007	1/1	0.97	0.08	36,36,36,36	0
54	MG	2A	3008	1/1	0.97	0.05	30,30,30,30	0
54	MG	1A	3302	1/1	0.97	0.13	34,34,34,34	0
54	MG	1A	4005	1/1	0.97	0.08	97,97,97,97	0
54	MG	1A	3077	1/1	0.97	0.15	53,53,53,53	0
54	MG	1A	3755	1/1	0.97	0.12	47,47,47,47	0
54	MG	2A	3015	1/1	0.97	0.22	36,36,36,36	0
54	MG	2A	3434	1/1	0.97	0.09	56,56,56,56	0
54	MG	2A	3436	1/1	0.97	0.14	49,49,49,49	0
54	MG	1A	3661	1/1	0.97	0.05	46,46,46,46	0
54	MG	1A	3433	1/1	0.97	0.06	10,10,10,10	0
54	MG	2A	3699	1/1	0.97	0.05	44,44,44,44	0
54	MG	2A	3439	1/1	0.97	0.05	46,46,46,46	0
54	MG	2A	3021	1/1	0.97	0.06	31,31,31,31	0
54	MG	2A	3702	1/1	0.97	0.07	55,55,55,55	0
54	MG	1A	3874	1/1	0.97	0.04	24,24,24,24	0
54	MG	2A	3221	1/1	0.97	0.25	45,45,45,45	0
54	MG	1A	3505	1/1	0.97	0.09	28,28,28,28	0
54	MG	1A	4013	1/1	0.97	0.06	43,43,43,43	0
54	MG	2a	1744	1/1	0.97	0.08	75,75,75,75	0
54	MG	2A	3446	1/1	0.97	0.07	58,58,58,58	0
54	MG	1A	3244	1/1	0.97	0.15	36,36,36,36	0
54	MG	1a	1760	1/1	0.97	0.13	63,63,63,63	0
54	MG	1A	3880	1/1	0.97	0.12	39,39,39,39	0
54	MG	2A	3028	1/1	0.97	0.06	33,33,33,33	0
54	MG	1A	3881	1/1	0.97	0.07	28,28,28,28	0
54	MG	2A	3031	1/1	0.97	0.11	27,27,27,27	0
54	MG	2A	3714	1/1	0.97	0.04	56,56,56,56	0
54	MG	1a	1763	1/1	0.97	0.13	59,59,59,59	0
54	MG	1A	3665	1/1	0.97	0.12	60,60,60,60	0
54	MG	1A	3307	1/1	0.97	0.06	46,46,46,46	0
54	MG	1A	3309	1/1	0.97	0.06	47,47,47,47	0
54	MG	2A	3459	1/1	0.97	0.13	49,49,49,49	0
54	MG	2a	1762	1/1	0.97	0.05	54,54,54,54	0
54	MG	1A	3370	1/1	0.97	0.09	54,54,54,54	0
54	MG	2A	3235	1/1	0.97	0.08	48,48,48,48	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	2a	1767	1/1	0.97	0.09	70,70,70,70	0
54	MG	1A	3310	1/1	0.97	0.15	45,45,45,45	0
54	MG	1A	3440	1/1	0.97	0.06	42,42,42,42	0
54	MG	2a	1770	1/1	0.97	0.06	82,82,82,82	0
54	MG	1A	3512	1/1	0.97	0.06	61,61,61,61	0
54	MG	2a	1772	1/1	0.97	0.05	58,58,58,58	0
54	MG	1A	3245	1/1	0.97	0.18	35,35,35,35	0
54	MG	1a	1611	1/1	0.97	0.05	38,38,38,38	0
54	MG	2A	3242	1/1	0.97	0.17	48,48,48,48	0
54	MG	1A	3048	1/1	0.97	0.04	28,28,28,28	0
54	MG	1A	3080	1/1	0.97	0.09	52,52,52,52	0
54	MG	1A	3771	1/1	0.97	0.06	44,44,44,44	0
54	MG	2A	3733	1/1	0.97	0.09	33,33,33,33	0
54	MG	2A	3734	1/1	0.97	0.24	41,41,41,41	0
54	MG	2a	1785	1/1	0.97	0.07	76,76,76,76	0
54	MG	1A	4036	1/1	0.97	0.15	35,35,35,35	0
54	MG	1A	3120	1/1	0.97	0.05	37,37,37,37	0
54	MG	1A	3902	1/1	0.97	0.05	69,69,69,69	0
54	MG	1A	4045	1/1	0.97	0.14	36,36,36,36	0
54	MG	1a	1622	1/1	0.97	0.05	47,47,47,47	0
54	MG	1A	3773	1/1	0.97	0.04	31,31,31,31	0
54	MG	1A	3774	1/1	0.97	0.10	43,43,43,43	0
54	MG	2A	3054	1/1	0.97	0.09	44,44,44,44	0
54	MG	2A	3744	1/1	0.97	0.10	40,40,40,40	0
54	MG	1A	3775	1/1	0.97	0.04	36,36,36,36	0
54	MG	1A	3251	1/1	0.97	0.12	52,52,52,52	0
54	MG	2A	3749	1/1	0.97	0.17	39,39,39,39	0
54	MG	1A	4052	1/1	0.97	0.15	45,45,45,45	0
54	MG	1A	3678	1/1	0.97	0.06	62,62,62,62	0
54	MG	2A	3485	1/1	0.97	0.05	54,54,54,54	0
54	MG	2A	3754	1/1	0.97	0.28	46,46,46,46	0
54	MG	1A	4054	1/1	0.97	0.13	44,44,44,44	0
54	MG	1A	3082	1/1	0.97	0.13	53,53,53,53	0
54	MG	1A	3909	1/1	0.97	0.04	28,28,28,28	0
54	MG	2A	3489	1/1	0.97	0.06	33,33,33,33	0
54	MG	2A	3759	1/1	0.97	0.21	46,46,46,46	0
54	MG	2A	3262	1/1	0.97	0.09	58,58,58,58	0
54	MG	2A	3263	1/1	0.97	0.06	41,41,41,41	0
54	MG	1A	3519	1/1	0.97	0.06	59,59,59,59	0
54	MG	1A	3599	1/1	0.97	0.09	50,50,50,50	0
57	ZN	29	501	1/1	0.97	0.14	131,131,131,131	0
58	SF4	1d	501	8/8	0.97	0.07	64,70,74,95	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	1A	3520	1/1	0.98	0.07	32,32,32,32	0
54	MG	1A	3823	1/1	0.98	0.19	36,36,36,36	0
54	MG	1D	305	1/1	0.98	0.04	38,38,38,38	0
54	MG	2E	304	1/1	0.98	0.06	35,35,35,35	0
54	MG	1D	306	1/1	0.98	0.18	46,46,46,46	0
54	MG	1D	308	1/1	0.98	0.06	45,45,45,45	0
54	MG	1A	3824	1/1	0.98	0.19	33,33,33,33	0
54	MG	1A	3271	1/1	0.98	0.09	37,37,37,37	0
54	MG	1A	3113	1/1	0.98	0.12	34,34,34,34	0
54	MG	2A	3560	1/1	0.98	0.05	23,23,23,23	0
54	MG	1a	1692	1/1	0.98	0.11	44,44,44,44	0
54	MG	1A	3114	1/1	0.98	0.18	33,33,33,33	0
54	MG	2A	3563	1/1	0.98	0.04	50,50,50,50	0
54	MG	1A	3829	1/1	0.98	0.04	25,25,25,25	0
54	MG	1A	3524	1/1	0.98	0.08	29,29,29,29	0
54	MG	1A	3720	1/1	0.98	0.08	33,33,33,33	0
54	MG	1E	302	1/1	0.98	0.03	42,42,42,42	0
54	MG	1A	3045	1/1	0.98	0.08	33,33,33,33	0
54	MG	1A	3063	1/1	0.98	0.03	31,31,31,31	0
54	MG	1A	3276	1/1	0.98	0.16	29,29,29,29	0
54	MG	1A	3438	1/1	0.98	0.04	27,27,27,27	0
54	MG	1F	301	1/1	0.98	0.17	36,36,36,36	0
54	MG	2A	3574	1/1	0.98	0.05	30,30,30,30	0
54	MG	1a	1877	1/1	0.98	0.05	55,55,55,55	0
54	MG	1A	3214	1/1	0.98	0.17	42,42,42,42	0
54	MG	2W	8002	1/1	0.98	0.13	60,60,60,60	0
54	MG	2X	8001	1/1	0.98	0.04	47,47,47,47	0
54	MG	1A	3118	1/1	0.98	0.14	43,43,43,43	0
54	MG	1F	304	1/1	0.98	0.07	33,33,33,33	0
54	MG	1A	3280	1/1	0.98	0.10	48,48,48,48	0
54	MG	1A	3840	1/1	0.98	0.04	39,39,39,39	0
54	MG	1A	3003	1/1	0.98	0.12	24,24,24,24	0
54	MG	1A	3085	1/1	0.98	0.33	38,38,38,38	0
54	MG	2A	3583	1/1	0.98	0.04	34,34,34,34	0
54	MG	1a	1710	1/1	0.98	0.09	38,38,38,38	0
54	MG	1A	3121	1/1	0.98	0.09	35,35,35,35	0
54	MG	1A	3978	1/1	0.98	0.07	29,29,29,29	0
54	MG	1a	1713	1/1	0.98	0.07	44,44,44,44	0
54	MG	1A	3732	1/1	0.98	0.04	32,32,32,32	0
54	MG	1A	3123	1/1	0.98	0.09	23,23,23,23	0
54	MG	1A	3286	1/1	0.98	0.17	41,41,41,41	0
54	MG	1A	3848	1/1	0.98	0.06	41,41,41,41	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	1A	3287	1/1	0.98	0.05	39,39,39,39	0
54	MG	1A	3006	1/1	0.98	0.03	30,30,30,30	0
54	MG	2a	1611	1/1	0.98	0.05	41,41,41,41	0
54	MG	2A	3597	1/1	0.98	0.06	72,72,72,72	0
54	MG	1A	3087	1/1	0.98	0.25	34,34,34,34	0
54	MG	1A	3452	1/1	0.98	0.07	56,56,56,56	0
54	MG	1A	3740	1/1	0.98	0.04	22,22,22,22	0
54	MG	2A	3601	1/1	0.98	0.03	50,50,50,50	0
54	MG	1A	3290	1/1	0.98	0.15	36,36,36,36	0
54	MG	1A	3291	1/1	0.98	0.21	43,43,43,43	0
54	MG	1A	3023	1/1	0.98	0.12	34,34,34,34	0
54	MG	1A	3223	1/1	0.98	0.11	32,32,32,32	0
54	MG	2A	3606	1/1	0.98	0.04	48,48,48,48	0
54	MG	1Q	204	1/1	0.98	0.14	55,55,55,55	0
54	MG	2A	3608	1/1	0.98	0.05	64,64,64,64	0
54	MG	1A	3050	1/1	0.98	0.08	44,44,44,44	0
54	MG	2A	3610	1/1	0.98	0.10	44,44,44,44	0
54	MG	1A	3859	1/1	0.98	0.04	33,33,33,33	0
54	MG	1A	3015	1/1	0.98	0.10	38,38,38,38	0
54	MG	2A	3613	1/1	0.98	0.12	49,49,49,49	0
54	MG	1t	3001	1/1	0.98	0.05	49,49,49,49	0
54	MG	2A	3615	1/1	0.98	0.03	34,34,34,34	0
54	MG	1A	3296	1/1	0.98	0.06	31,31,31,31	0
54	MG	2A	3617	1/1	0.98	0.04	23,23,23,23	0
54	MG	1A	3226	1/1	0.98	0.19	42,42,42,42	0
54	MG	2A	3394	1/1	0.98	0.07	33,33,33,33	0
54	MG	1A	3461	1/1	0.98	0.05	44,44,44,44	0
54	MG	1A	3016	1/1	0.98	0.15	42,42,42,42	0
54	MG	1A	3865	1/1	0.98	0.11	35,35,35,35	0
54	MG	2A	3193	1/1	0.98	0.06	41,41,41,41	0
54	MG	1A	3463	1/1	0.98	0.04	53,53,53,53	0
54	MG	1A	3867	1/1	0.98	0.08	32,32,32,32	0
54	MG	2A	3004	1/1	0.98	0.07	26,26,26,26	0
54	MG	2A	3005	1/1	0.98	0.13	45,45,45,45	0
54	MG	1A	3299	1/1	0.98	0.10	22,22,22,22	0
54	MG	1A	3228	1/1	0.98	0.21	41,41,41,41	0
54	MG	1a	1743	1/1	0.98	0.05	53,53,53,53	0
54	MG	1A	3053	1/1	0.98	0.17	36,36,36,36	0
54	MG	1A	3379	1/1	0.98	0.05	27,27,27,27	0
54	MG	1A	3872	1/1	0.98	0.04	42,42,42,42	0
54	MG	2A	3013	1/1	0.98	0.11	24,24,24,24	0
54	MG	1A	3303	1/1	0.98	0.22	31,31,31,31	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	1A	3131	1/1	0.98	0.05	46,46,46,46	0
54	MG	2A	3412	1/1	0.98	0.04	60,60,60,60	0
54	MG	1A	3875	1/1	0.98	0.04	50,50,50,50	0
54	MG	1A	3470	1/1	0.98	0.12	49,49,49,49	0
54	MG	2A	3018	1/1	0.98	0.15	35,35,35,35	0
54	MG	2A	3019	1/1	0.98	0.23	46,46,46,46	0
54	MG	2a	1657	1/1	0.98	0.09	52,52,52,52	0
54	MG	1A	3178	1/1	0.98	0.09	38,38,38,38	0
54	MG	2A	3643	1/1	0.98	0.05	63,63,63,63	0
54	MG	1A	3760	1/1	0.98	0.07	34,34,34,34	0
54	MG	1A	4014	1/1	0.98	0.03	33,33,33,33	0
54	MG	1A	3306	1/1	0.98	0.05	29,29,29,29	0
54	MG	2A	3647	1/1	0.98	0.14	58,58,58,58	0
54	MG	2A	3649	1/1	0.98	0.04	56,56,56,56	0
54	MG	1A	4016	1/1	0.98	0.06	62,62,62,62	0
54	MG	1A	3094	1/1	0.98	0.13	37,37,37,37	0
54	MG	1A	4018	1/1	0.98	0.05	44,44,44,44	0
54	MG	1A	3883	1/1	0.98	0.05	38,38,38,38	0
54	MG	1A	3308	1/1	0.98	0.08	46,46,46,46	0
54	MG	2A	3030	1/1	0.98	0.14	39,39,39,39	0
54	MG	1A	3885	1/1	0.98	0.04	67,67,67,67	0
54	MG	1A	3181	1/1	0.98	0.10	36,36,36,36	0
54	MG	2A	3662	1/1	0.98	0.05	59,59,59,59	0
54	MG	1A	4023	1/1	0.98	0.04	60,60,60,60	0
54	MG	2A	3664	1/1	0.98	0.05	61,61,61,61	0
54	MG	1A	3565	1/1	0.98	0.06	50,50,50,50	0
54	MG	1A	3387	1/1	0.98	0.09	25,25,25,25	0
54	MG	2A	3432	1/1	0.98	0.06	35,35,35,35	0
54	MG	1A	3055	1/1	0.98	0.26	42,42,42,42	0
54	MG	1a	1601	1/1	0.98	0.07	57,57,57,57	0
54	MG	1A	3389	1/1	0.98	0.13	35,35,35,35	0
54	MG	1A	4029	1/1	0.98	0.07	49,49,49,49	0
54	MG	1A	3569	1/1	0.98	0.06	37,37,37,37	0
54	MG	1A	3183	1/1	0.98	0.14	41,41,41,41	0
54	MG	2A	3440	1/1	0.98	0.04	45,45,45,45	0
54	MG	2A	3675	1/1	0.98	0.08	61,61,61,61	0
54	MG	2A	3676	1/1	0.98	0.04	48,48,48,48	0
54	MG	1A	4032	1/1	0.98	0.19	35,35,35,35	0
54	MG	2A	3043	1/1	0.98	0.03	23,23,23,23	0
54	MG	1A	3096	1/1	0.98	0.05	40,40,40,40	0
54	MG	1A	4034	1/1	0.98	0.10	31,31,31,31	0
54	MG	1A	3238	1/1	0.98	0.19	38,38,38,38	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	1A	3895	1/1	0.98	0.03	35,35,35,35	0
54	MG	1A	4037	1/1	0.98	0.12	32,32,32,32	0
54	MG	1A	4038	1/1	0.98	0.04	37,37,37,37	0
54	MG	2A	3240	1/1	0.98	0.12	34,34,34,34	0
54	MG	1A	4039	1/1	0.98	0.08	41,41,41,41	0
54	MG	1a	1779	1/1	0.98	0.06	56,56,56,56	0
54	MG	2A	3452	1/1	0.98	0.07	48,48,48,48	0
54	MG	1A	4042	1/1	0.98	0.11	36,36,36,36	0
54	MG	2A	3053	1/1	0.98	0.04	39,39,39,39	0
54	MG	1a	1615	1/1	0.98	0.10	28,28,28,28	0
54	MG	1a	1616	1/1	0.98	0.08	48,48,48,48	0
54	MG	1a	1617	1/1	0.98	0.04	50,50,50,50	0
54	MG	1A	3239	1/1	0.98	0.13	43,43,43,43	0
54	MG	1A	3900	1/1	0.98	0.03	29,29,29,29	0
54	MG	1A	3901	1/1	0.98	0.08	46,46,46,46	0
54	MG	1A	3315	1/1	0.98	0.09	34,34,34,34	0
54	MG	1A	3575	1/1	0.98	0.06	33,33,33,33	0
54	MG	1a	1623	1/1	0.98	0.05	43,43,43,43	0
54	MG	2A	3254	1/1	0.98	0.27	39,39,39,39	0
54	MG	1A	3316	1/1	0.98	0.07	39,39,39,39	0
54	MG	1A	3241	1/1	0.98	0.14	37,37,37,37	0
54	MG	1a	1626	1/1	0.98	0.06	43,43,43,43	0
54	MG	1A	3486	1/1	0.98	0.09	31,31,31,31	0
54	MG	1a	1628	1/1	0.98	0.04	37,37,37,37	0
54	MG	1A	3487	1/1	0.98	0.06	25,25,25,25	0
54	MG	1A	3398	1/1	0.98	0.07	22,22,22,22	0
54	MG	1A	3242	1/1	0.98	0.13	40,40,40,40	0
54	MG	1a	1632	1/1	0.98	0.07	36,36,36,36	0
54	MG	2A	3072	1/1	0.98	0.18	36,36,36,36	0
54	MG	1A	3582	1/1	0.98	0.09	50,50,50,50	0
54	MG	1A	3097	1/1	0.98	0.12	42,42,42,42	0
54	MG	2A	3479	1/1	0.98	0.06	38,38,38,38	0
54	MG	1A	4058	1/1	0.98	0.07	37,37,37,37	0
54	MG	1A	3188	1/1	0.98	0.10	40,40,40,40	0
54	MG	1A	3683	1/1	0.98	0.08	57,57,57,57	0
54	MG	2A	3270	1/1	0.98	0.07	41,41,41,41	0
54	MG	1A	3037	1/1	0.98	0.13	39,39,39,39	0
54	MG	1A	4065	1/1	0.98	0.09	49,49,49,49	0
54	MG	1A	3137	1/1	0.98	0.18	42,42,42,42	0
54	MG	1A	3028	1/1	0.98	0.15	28,28,28,28	0
54	MG	2a	1734	1/1	0.98	0.06	64,64,64,64	0
54	MG	2a	1735	1/1	0.98	0.08	64,64,64,64	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	1A	4068	1/1	0.98	0.27	43,43,43,43	0
54	MG	1A	3075	1/1	0.98	0.09	41,41,41,41	0
54	MG	1A	3790	1/1	0.98	0.05	21,21,21,21	0
54	MG	1A	3406	1/1	0.98	0.03	30,30,30,30	0
54	MG	2A	3492	1/1	0.98	0.14	57,57,57,57	0
54	MG	2a	1743	1/1	0.98	0.06	61,61,61,61	0
54	MG	2A	3087	1/1	0.98	0.08	47,47,47,47	0
54	MG	1A	3325	1/1	0.98	0.05	21,21,21,21	0
54	MG	2a	1747	1/1	0.98	0.09	78,78,78,78	0
54	MG	2A	3731	1/1	0.98	0.14	23,23,23,23	0
54	MG	1A	4073	1/1	0.98	0.17	40,40,40,40	0
54	MG	1A	3793	1/1	0.98	0.09	55,55,55,55	0
54	MG	1A	3141	1/1	0.98	0.19	36,36,36,36	0
54	MG	1A	3795	1/1	0.98	0.05	68,68,68,68	0
54	MG	1a	1651	1/1	0.98	0.10	38,38,38,38	0
54	MG	1A	3007	1/1	0.98	0.11	35,35,35,35	0
54	MG	2A	3095	1/1	0.98	0.04	38,38,38,38	0
54	MG	2a	1756	1/1	0.98	0.05	57,57,57,57	0
54	MG	2A	3290	1/1	0.98	0.07	33,33,33,33	0
54	MG	2a	1758	1/1	0.98	0.10	50,50,50,50	0
54	MG	1A	3195	1/1	0.98	0.10	47,47,47,47	0
54	MG	1A	3929	1/1	0.98	0.04	52,52,52,52	0
54	MG	1A	3143	1/1	0.98	0.05	44,44,44,44	0
54	MG	1a	1656	1/1	0.98	0.04	37,37,37,37	0
54	MG	2A	3295	1/1	0.98	0.04	33,33,33,33	0
54	MG	1A	3144	1/1	0.98	0.14	41,41,41,41	0
54	MG	2a	1766	1/1	0.98	0.04	63,63,63,63	0
54	MG	2A	3101	1/1	0.98	0.05	34,34,34,34	0
54	MG	2A	3102	1/1	0.98	0.09	49,49,49,49	0
54	MG	2A	3103	1/1	0.98	0.13	37,37,37,37	0
54	MG	1A	3332	1/1	0.98	0.08	28,28,28,28	0
54	MG	2A	3753	1/1	0.98	0.20	39,39,39,39	0
54	MG	1A	3145	1/1	0.98	0.09	43,43,43,43	0
54	MG	2a	1773	1/1	0.98	0.12	59,59,59,59	0
54	MG	1a	1828	1/1	0.98	0.04	55,55,55,55	0
54	MG	1A	3103	1/1	0.98	0.14	44,44,44,44	0
54	MG	2a	1776	1/1	0.98	0.04	76,76,76,76	0
54	MG	2a	1777	1/1	0.98	0.04	72,72,72,72	0
54	MG	1A	3258	1/1	0.98	0.11	40,40,40,40	0
54	MG	1A	3104	1/1	0.98	0.19	41,41,41,41	0
54	MG	1A	3105	1/1	0.98	0.05	57,57,57,57	0
54	MG	2A	3760	1/1	0.98	0.43	40,40,40,40	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	1A	3106	1/1	0.98	0.15	30,30,30,30	0
54	MG	1B	214	1/1	0.98	0.03	42,42,42,42	0
54	MG	1A	3703	1/1	0.98	0.04	41,41,41,41	0
54	MG	1A	3040	1/1	0.98	0.10	39,39,39,39	0
54	MG	1A	3078	1/1	0.98	0.26	38,38,38,38	0
54	MG	1A	3942	1/1	0.98	0.05	59,59,59,59	0
54	MG	1A	3031	1/1	0.98	0.12	24,24,24,24	0
54	MG	2a	1790	1/1	0.98	0.06	61,61,61,61	0
54	MG	1A	3342	1/1	0.98	0.06	57,57,57,57	0
54	MG	2A	3316	1/1	0.98	0.04	40,40,40,40	0
54	MG	2A	3317	1/1	0.98	0.04	37,37,37,37	0
54	MG	1A	3266	1/1	0.98	0.15	28,28,28,28	0
54	MG	1A	3157	1/1	0.98	0.10	39,39,39,39	0
54	MG	2A	3320	1/1	0.98	0.06	47,47,47,47	0
54	MG	1A	3710	1/1	0.98	0.07	55,55,55,55	0
54	MG	1A	3816	1/1	0.98	0.05	32,32,32,32	0
54	MG	1A	3817	1/1	0.98	0.04	45,45,45,45	0
54	MG	1A	3043	1/1	0.98	0.08	17,17,17,17	0
54	MG	2A	3126	1/1	0.98	0.05	28,28,28,28	0
54	MG	1A	3951	1/1	0.98	0.06	31,31,31,31	0
54	MG	2A	3327	1/1	0.98	0.11	34,34,34,34	0
54	MG	2A	3328	1/1	0.98	0.12	36,36,36,36	0
54	MG	1A	3952	1/1	0.98	0.04	33,33,33,33	0
54	MG	1A	3953	1/1	0.98	0.06	19,19,19,19	0
54	MG	1A	3081	1/1	0.98	0.16	46,46,46,46	0
54	MG	2A	3131	1/1	0.98	0.12	39,39,39,39	0
54	MG	1a	1854	1/1	0.98	0.04	52,52,52,52	0
57	ZN	1n	501	1/1	0.98	0.04	65,65,65,65	0
54	MG	1A	3347	1/1	0.98	0.07	24,24,24,24	0
54	MG	1a	1856	1/1	0.98	0.04	58,58,58,58	0
57	ZN	25	101	1/1	0.98	0.04	64,64,64,64	0
54	MG	1A	3270	1/1	0.98	0.18	32,32,32,32	0
57	ZN	2n	501	1/1	0.98	0.06	84,84,84,84	0
54	MG	2A	3337	1/1	0.98	0.06	32,32,32,32	0
58	SF4	2d	501	8/8	0.98	0.05	61,78,84,104	0
54	MG	1A	3140	1/1	0.99	0.23	31,31,31,31	0
54	MG	1A	3645	1/1	0.99	0.09	30,30,30,30	0
54	MG	1A	4046	1/1	0.99	0.07	29,29,29,29	0
54	MG	1A	3798	1/1	0.99	0.04	71,71,71,71	0
54	MG	2A	3284	1/1	0.99	0.03	41,41,41,41	0
54	MG	2A	3020	1/1	0.99	0.16	44,44,44,44	0
54	MG	1a	1847	1/1	0.99	0.03	42,42,42,42	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	1A	3122	1/1	0.99	0.17	37,37,37,37	0
54	MG	1A	4049	1/1	0.99	0.14	41,41,41,41	0
54	MG	1A	3281	1/1	0.99	0.08	39,39,39,39	0
54	MG	2A	3110	1/1	0.99	0.07	28,28,28,28	0
54	MG	2A	3589	1/1	0.99	0.03	54,54,54,54	0
54	MG	2A	3590	1/1	0.99	0.03	49,49,49,49	0
54	MG	1a	1851	1/1	0.99	0.03	68,68,68,68	0
54	MG	1a	1852	1/1	0.99	0.03	52,52,52,52	0
54	MG	1A	3917	1/1	0.99	0.03	15,15,15,15	0
54	MG	2A	3390	1/1	0.99	0.04	31,31,31,31	0
54	MG	2A	3595	1/1	0.99	0.04	33,33,33,33	0
54	MG	1A	3556	1/1	0.99	0.09	39,39,39,39	0
54	MG	1A	3019	1/1	0.99	0.12	30,30,30,30	0
54	MG	1A	3249	1/1	0.99	0.18	35,35,35,35	0
54	MG	1A	3250	1/1	0.99	0.12	39,39,39,39	0
54	MG	2A	3494	1/1	0.99	0.07	27,27,27,27	0
54	MG	1A	3393	1/1	0.99	0.12	26,26,26,26	0
54	MG	1A	3356	1/1	0.99	0.03	11,11,11,11	0
54	MG	1A	3606	1/1	0.99	0.19	32,32,32,32	0
54	MG	1A	4059	1/1	0.99	0.16	28,28,28,28	0
54	MG	1A	3925	1/1	0.99	0.05	54,54,54,54	0
54	MG	1A	4061	1/1	0.99	0.09	37,37,37,37	0
54	MG	1A	4062	1/1	0.99	0.07	37,37,37,37	0
54	MG	2A	3305	1/1	0.99	0.06	19,19,19,19	0
54	MG	2A	3503	1/1	0.99	0.13	35,35,35,35	0
54	MG	1A	3020	1/1	0.99	0.19	39,39,39,39	0
54	MG	1A	3091	1/1	0.99	0.05	42,42,42,42	0
54	MG	2A	3724	1/1	0.99	0.03	66,66,66,66	0
54	MG	2a	1732	1/1	0.99	0.03	62,62,62,62	0
54	MG	1A	3029	1/1	0.99	0.04	40,40,40,40	0
54	MG	1G	3004	1/1	0.99	0.04	45,45,45,45	0
54	MG	1A	3146	1/1	0.99	0.13	28,28,28,28	0
54	MG	1A	3005	1/1	0.99	0.12	24,24,24,24	0
54	MG	1A	3149	1/1	0.99	0.05	28,28,28,28	0
54	MG	2a	1738	1/1	0.99	0.04	71,71,71,71	0
54	MG	1A	3013	1/1	0.99	0.04	17,17,17,17	0
54	MG	1A	3111	1/1	0.99	0.11	38,38,38,38	0
54	MG	1A	3009	1/1	0.99	0.04	26,26,26,26	0
54	MG	2a	1742	1/1	0.99	0.03	69,69,69,69	0
54	MG	1a	1792	1/1	0.99	0.05	62,62,62,62	0
54	MG	1P	201	1/1	0.99	0.15	26,26,26,26	0
54	MG	1A	3329	1/1	0.99	0.08	39,39,39,39	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	2a	1746	1/1	0.99	0.06	56,56,56,56	0
54	MG	1A	3445	1/1	0.99	0.07	31,31,31,31	0
54	MG	2A	3139	1/1	0.99	0.10	28,28,28,28	0
54	MG	1A	3446	1/1	0.99	0.09	30,30,30,30	0
54	MG	2A	3739	1/1	0.99	0.04	52,52,52,52	0
54	MG	1A	3667	1/1	0.99	0.06	47,47,47,47	0
54	MG	1A	3619	1/1	0.99	0.10	37,37,37,37	0
54	MG	1A	3877	1/1	0.99	0.07	40,40,40,40	0
54	MG	1A	3054	1/1	0.99	0.15	34,34,34,34	0
54	MG	1A	3879	1/1	0.99	0.05	38,38,38,38	0
54	MG	1a	1722	1/1	0.99	0.06	40,40,40,40	0
54	MG	1A	3042	1/1	0.99	0.04	24,24,24,24	0
54	MG	1B	205	1/1	0.99	0.09	39,39,39,39	0
54	MG	2A	3149	1/1	0.99	0.05	28,28,28,28	0
54	MG	1A	3024	1/1	0.99	0.11	18,18,18,18	0
54	MG	1A	3179	1/1	0.99	0.11	34,34,34,34	0
54	MG	1A	3723	1/1	0.99	0.04	44,44,44,44	0
54	MG	1A	3264	1/1	0.99	0.16	29,29,29,29	0
54	MG	2a	1764	1/1	0.99	0.04	64,64,64,64	0
54	MG	1A	4012	1/1	0.99	0.11	23,23,23,23	0
54	MG	1A	3828	1/1	0.99	0.06	27,27,27,27	0
54	MG	1A	3233	1/1	0.99	0.08	37,37,37,37	0
54	MG	2A	3435	1/1	0.99	0.08	43,43,43,43	0
54	MG	1a	1733	1/1	0.99	0.07	34,34,34,34	0
54	MG	1A	3626	1/1	0.99	0.10	30,30,30,30	0
54	MG	1A	3300	1/1	0.99	0.07	12,12,12,12	0
54	MG	2A	3341	1/1	0.99	0.06	36,36,36,36	0
54	MG	1A	3156	1/1	0.99	0.17	30,30,30,30	0
54	MG	2A	3648	1/1	0.99	0.04	48,48,48,48	0
54	MG	1A	3044	1/1	0.99	0.08	32,32,32,32	0
54	MG	2A	3074	1/1	0.99	0.05	23,23,23,23	0
54	MG	1A	3834	1/1	0.99	0.04	45,45,45,45	0
54	MG	2A	3652	1/1	0.99	0.06	38,38,38,38	0
54	MG	2A	3653	1/1	0.99	0.05	38,38,38,38	0
54	MG	2A	3654	1/1	0.99	0.03	56,56,56,56	0
54	MG	2a	1781	1/1	0.99	0.04	60,60,60,60	0
54	MG	1A	3208	1/1	0.99	0.14	42,42,42,42	0
54	MG	1A	3117	1/1	0.99	0.12	39,39,39,39	0
54	MG	1A	3071	1/1	0.99	0.16	32,32,32,32	0
54	MG	1A	3184	1/1	0.99	0.09	35,35,35,35	0
54	MG	1A	3896	1/1	0.99	0.05	49,49,49,49	0
54	MG	2A	3660	1/1	0.99	0.08	47,47,47,47	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	1A	3897	1/1	0.99	0.12	44,44,44,44	0
54	MG	1A	3734	1/1	0.99	0.03	41,41,41,41	0
54	MG	1A	3899	1/1	0.99	0.04	47,47,47,47	0
54	MG	1A	3240	1/1	0.99	0.20	38,38,38,38	0
54	MG	1A	3588	1/1	0.99	0.06	21,21,21,21	0
54	MG	1A	3185	1/1	0.99	0.13	37,37,37,37	0
54	MG	2A	3357	1/1	0.99	0.06	41,41,41,41	0
54	MG	2A	3456	1/1	0.99	0.02	24,24,24,24	0
54	MG	1A	3025	1/1	0.99	0.16	40,40,40,40	0
54	MG	2A	3559	1/1	0.99	0.03	55,55,55,55	0
54	MG	1A	3421	1/1	0.99	0.08	24,24,24,24	0
54	MG	1A	3845	1/1	0.99	0.07	22,22,22,22	0
54	MG	2A	3362	1/1	0.99	0.04	34,34,34,34	0
54	MG	1A	3046	1/1	0.99	0.13	13,13,13,13	0
54	MG	1A	3018	1/1	0.99	0.11	33,33,33,33	0
54	MG	2E	301	1/1	0.99	0.04	50,50,50,50	0
54	MG	1A	3971	1/1	0.99	0.04	31,31,31,31	0
54	MG	2A	3181	1/1	0.99	0.03	46,46,46,46	0
54	MG	1A	3424	1/1	0.99	0.04	46,46,46,46	0
54	MG	1A	3277	1/1	0.99	0.18	29,29,29,29	0
54	MG	2A	3273	1/1	0.99	0.09	44,44,44,44	0
57	ZN	1Y	501	1/1	0.99	0.05	56,56,56,56	0
54	MG	1D	307	1/1	0.99	0.11	17,17,17,17	0
57	ZN	15	101	1/1	0.99	0.02	50,50,50,50	0
57	ZN	16	501	1/1	0.99	0.05	39,39,39,39	0
57	ZN	19	102	1/1	0.99	0.03	37,37,37,37	0
54	MG	2A	3682	1/1	0.99	0.03	40,40,40,40	0
54	MG	2A	3011	1/1	0.99	0.06	28,28,28,28	0
54	MG	2A	3470	1/1	0.99	0.11	50,50,50,50	0
54	MG	2A	3573	1/1	0.99	0.03	50,50,50,50	0
57	ZN	26	501	1/1	0.99	0.03	60,60,60,60	0
54	MG	1A	4040	1/1	0.99	0.14	37,37,37,37	0
54	MG	1A	4041	1/1	0.99	0.09	37,37,37,37	0
54	MG	1A	3910	1/1	0.99	0.03	42,42,42,42	0
54	MG	1A	3163	1/1	0.99	0.18	34,34,34,34	0
54	MG	1a	1796	1/1	1.00	0.02	68,68,68,68	0
54	MG	1a	1724	1/1	1.00	0.06	36,36,36,36	0
54	MG	1A	3098	1/1	1.00	0.07	12,12,12,12	0
54	MG	1A	3686	1/1	1.00	0.03	50,50,50,50	0
54	MG	1A	3148	1/1	1.00	0.02	33,33,33,33	0
54	MG	2A	3361	1/1	1.00	0.01	34,34,34,34	0

6.5 Other polymers [i](#)

There are no such residues in this entry.