



wwPDB X-ray Structure Validation Summary Report ⓘ

Aug 6, 2026 – 04:10 AM EDT

PDB ID : 8FC1 / pdb_00008fc1
Title : Crystal structure of the Thermus thermophilus 70S ribosome in complex with protein Y, hygromycin A, and erythromycin at 2.50Å resolution
Authors : Chen, C.-W.; Syroegin, E.A.; Svetlov, M.S.; Polikanov, Y.S.
Deposited on : 2022-12-01
Resolution : 2.50 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
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.015 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.50

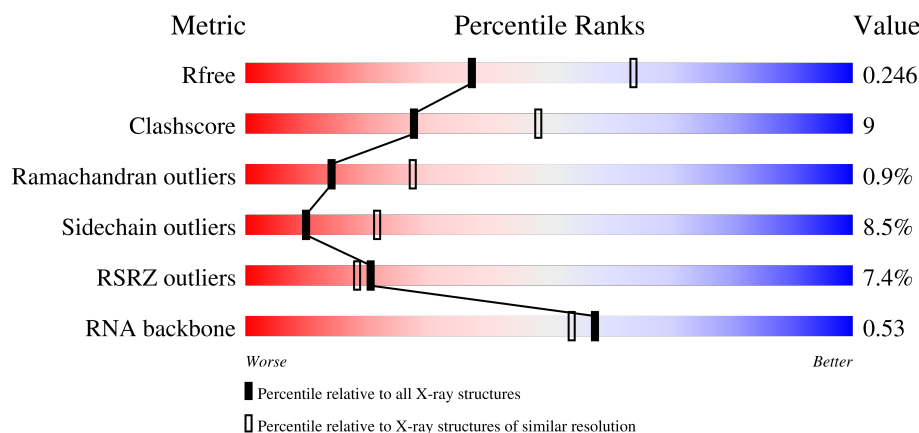
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 Å.

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



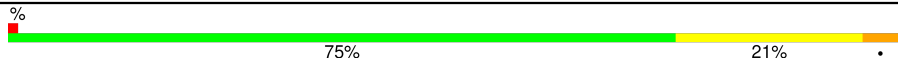
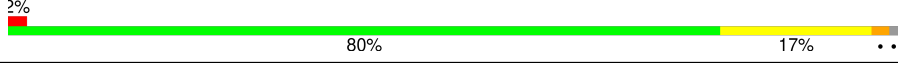
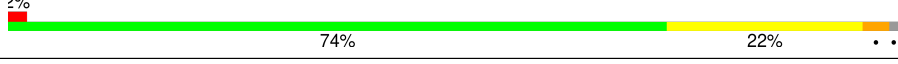
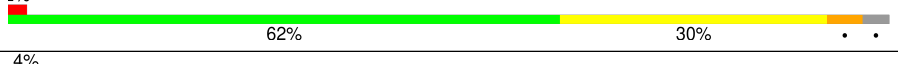
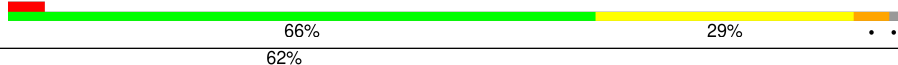
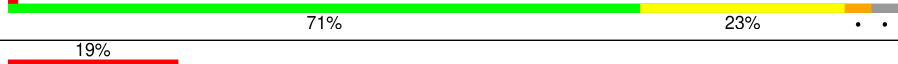
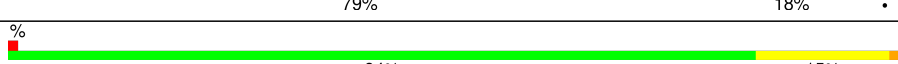
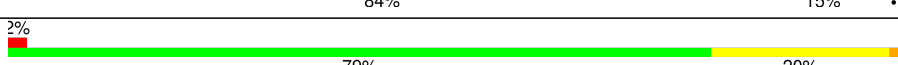
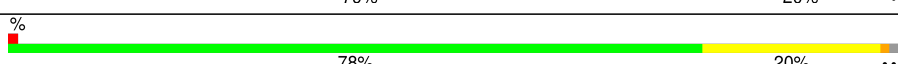
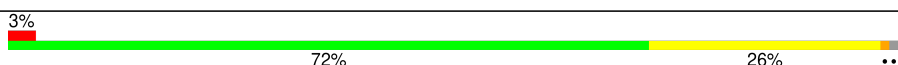
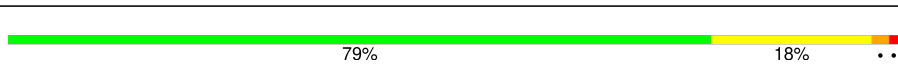
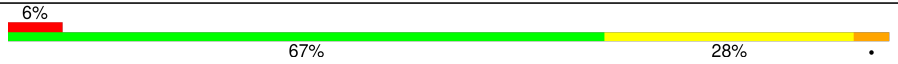
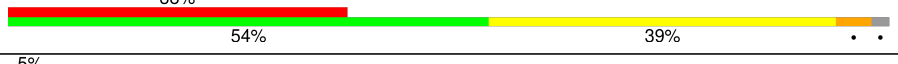
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	5829 (2.50-2.50)
Clashscore	190562	6492 (2.50-2.50)
Ramachandran outliers	187476	6378 (2.50-2.50)
Sidechain outliers	187428	6380 (2.50-2.50)
RSRZ outliers	180081	5833 (2.50-2.50)
RNA backbone	3983	1003 (2.78-2.22)

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

Mol	Chain	Length	Quality of chain
1	1A	2915	3% 66% 27% 6%
1	2A	2915	4% 58% 33% 7%
2	1B	121	% 71% 24%
2	2B	121	5% 45% 45% 9%

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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	1877	-	-	-	X
54	MG	2a	3006	-	-	-	X
54	MG	2a	3010	-	-	-	X
57	MPD	1a	1880	-	-	X	-

2 Entry composition

There are 61 unique types of molecules in this entry. The entry contains 296967 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	1040	Total	Mg	0	0
			1040	1040		
54	1B	29	Total	Mg	0	0
			29	29		
54	1D	18	Total	Mg	0	0
			18	18		
54	1E	8	Total	Mg	0	0
			8	8		
54	1F	18	Total	Mg	0	0
			18	18		
54	1G	4	Total	Mg	0	0
			4	4		
54	1H	2	Total	Mg	0	0
			2	2		
54	1N	4	Total	Mg	0	0
			4	4		
54	1O	1	Total	Mg	0	0
			1	1		
54	1P	5	Total	Mg	0	0
			5	5		
54	1Q	5	Total	Mg	0	0
			5	5		
54	1R	5	Total	Mg	0	0
			5	5		
54	1T	5	Total	Mg	0	0
			5	5		
54	1U	7	Total	Mg	0	0
			7	7		
54	1V	6	Total	Mg	0	0
			6	6		
54	1W	3	Total	Mg	0	0
			3	3		
54	1Y	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	8	Total 8	Mg 8	0	0
54	11	5	Total 5	Mg 5	0	0
54	13	3	Total 3	Mg 3	0	0
54	14	1	Total 1	Mg 1	0	0
54	15	8	Total 8	Mg 8	0	0
54	17	6	Total 6	Mg 6	0	0
54	18	2	Total 2	Mg 2	0	0
54	19	2	Total 2	Mg 2	0	0
54	1a	279	Total 279	Mg 279	0	0
54	1b	1	Total 1	Mg 1	0	0
54	1d	5	Total 5	Mg 5	0	0
54	1e	3	Total 3	Mg 3	0	0
54	1f	2	Total 2	Mg 2	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	1k	1	Total 1	Mg 1	0	0
54	1l	2	Total 2	Mg 2	0	0
54	1m	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

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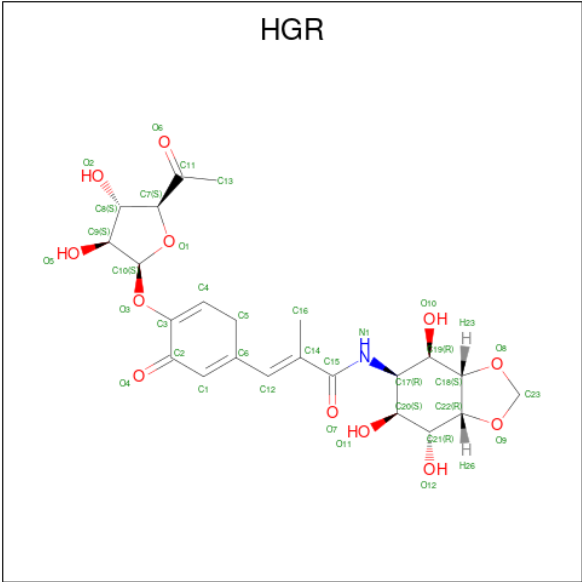
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
54	1t	1	Total 1 Mg 1	0	0
54	1y	3	Total 3 Mg 3	0	0
54	2A	730	Total 730 Mg 730	0	0
54	2B	18	Total 18 Mg 18	0	0
54	2D	13	Total 13 Mg 13	0	0
54	2E	6	Total 6 Mg 6	0	0
54	2F	4	Total 4 Mg 4	0	0
54	2G	2	Total 2 Mg 2	0	0
54	2I	1	Total 1 Mg 1	0	0
54	2O	2	Total 2 Mg 2	0	0
54	2P	1	Total 1 Mg 1	0	0
54	2Q	1	Total 1 Mg 1	0	0
54	2R	3	Total 3 Mg 3	0	0
54	2T	3	Total 3 Mg 3	0	0
54	2U	1	Total 1 Mg 1	0	0
54	2V	2	Total 2 Mg 2	0	0
54	2W	2	Total 2 Mg 2	0	0
54	2X	1	Total 1 Mg 1	0	0
54	2Y	1	Total 1 Mg 1	0	0
54	20	1	Total 1 Mg 1	0	0
54	21	2	Total 2 Mg 2	0	0

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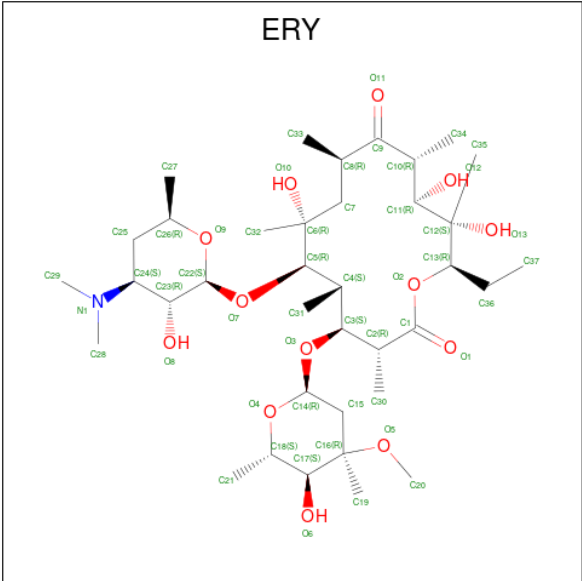
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
54	23	1	Total 1	Mg 1	0	0
54	25	3	Total 3	Mg 3	0	0
54	27	2	Total 2	Mg 2	0	0
54	28	2	Total 2	Mg 2	0	0
54	2a	190	Total 190	Mg 190	0	0
54	2e	2	Total 2	Mg 2	0	0
54	2f	1	Total 1	Mg 1	0	0
54	2j	1	Total 1	Mg 1	0	0
54	2k	1	Total 1	Mg 1	0	0
54	2n	1	Total 1	Mg 1	0	0
54	2r	2	Total 2	Mg 2	0	0
54	2t	1	Total 1	Mg 1	0	0
54	2y	1	Total 1	Mg 1	0	0

- Molecule 55 is Hygromycin A (CCD ID: HGR) (formula: $C_{23}H_{29}NO_{12}$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
55	1A	1	Total	C	N	O	0	0
			36	23	1	12		
55	2A	1	Total	C	N	O	0	0
			36	23	1	12		

- Molecule 56 is ERYTHROMYCIN A (CCD ID: ERY) (formula: $C_{37}H_{67}NO_{13}$) (labeled as "Ligand of Interest" by depositor).



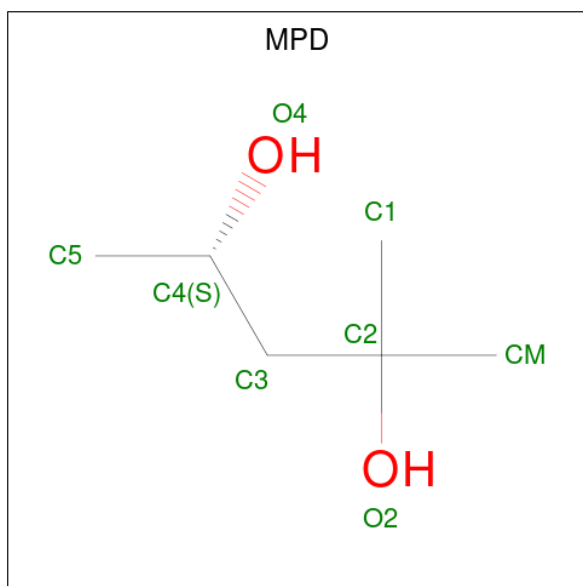
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
56	1A	1	Total	C	N	O	0	0
			51	37	1	13		

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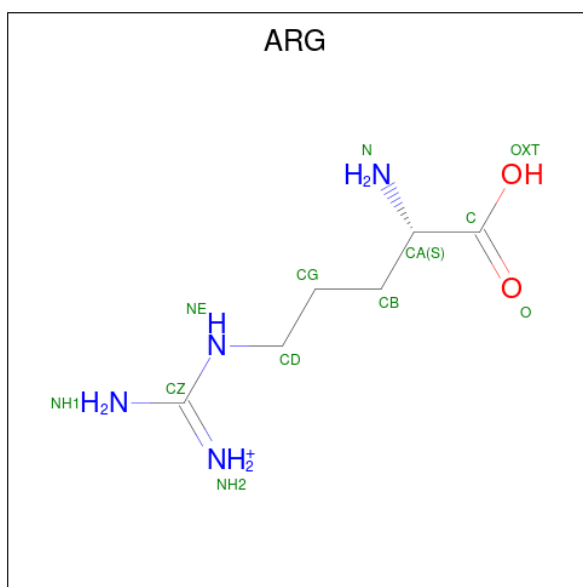
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
56	2A	1	Total	C	N	O	0	0
			51	37	1	13		

- Molecule 57 is (4S)-2-METHYL-2,4-PENTANEDIOL (CCD ID: MPD) (formula: $C_6H_{14}O_2$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
57	1A	1	Total	C	O	0	0
			8	6	2		
57	1T	1	Total	C	O	0	0
			8	6	2		
57	18	1	Total	C	O	0	0
			8	6	2		
57	1a	1	Total	C	O	0	0
			8	6	2		
57	2A	1	Total	C	O	0	0
			8	6	2		
57	2A	1	Total	C	O	0	0
			8	6	2		
57	2B	1	Total	C	O	0	0
			8	6	2		

- Molecule 58 is ARGinine (CCD ID: ARG) (formula: $C_6H_{15}N_4O_2$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
58	1B	1	Total	C	N	O	0	0
			12	6	4	2		
58	1F	1	Total	C	N	O	0	0
			12	6	4	2		

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

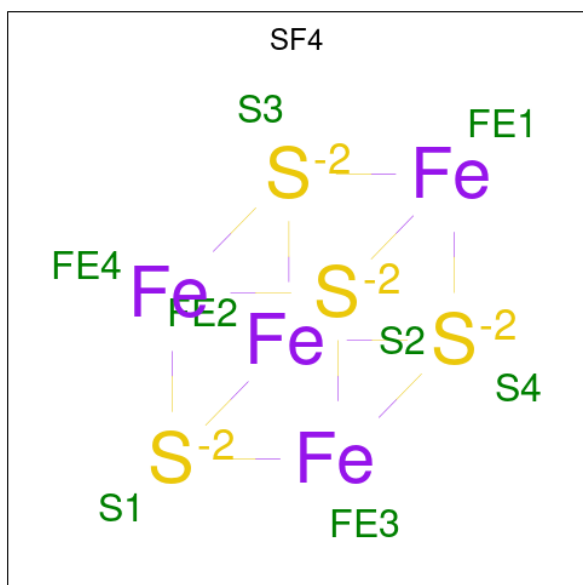
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
59	1Y	1	Total	Zn	0	0
			1	1		
59	14	1	Total	Zn	0	0
			1	1		
59	15	1	Total	Zn	0	0
			1	1		
59	16	1	Total	Zn	0	0
			1	1		
59	19	1	Total	Zn	0	0
			1	1		
59	1n	1	Total	Zn	0	0
			1	1		
59	2Y	1	Total	Zn	0	0
			1	1		
59	24	1	Total	Zn	0	0
			1	1		
59	25	1	Total	Zn	0	0
			1	1		
59	26	1	Total	Zn	0	0
			1	1		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
59	29	1	Total	Zn	0	0
			1	1		
59	2n	1	Total	Zn	0	0
			1	1		

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



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

- Molecule 61 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
61	1A	3898	Total	O	0	0
			3898	3898		
61	1B	94	Total	O	0	0
			94	94		
61	1D	103	Total	O	0	0
			103	103		
61	1E	68	Total	O	0	0
			68	68		
61	1F	64	Total	O	0	0
			64	64		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
61	1G	16	Total 16	O 16	0	0
61	1H	15	Total 15	O 15	0	0
61	1I	5	Total 5	O 5	0	0
61	1N	45	Total 45	O 45	0	0
61	1O	22	Total 22	O 22	0	0
61	1P	56	Total 56	O 56	0	0
61	1Q	37	Total 37	O 37	0	0
61	1R	29	Total 29	O 29	0	0
61	1S	12	Total 12	O 12	0	0
61	1T	37	Total 37	O 37	0	0
61	1U	41	Total 41	O 41	0	0
61	1V	34	Total 34	O 34	0	0
61	1W	27	Total 27	O 27	0	0
61	1X	27	Total 27	O 27	0	0
61	1Y	16	Total 16	O 16	0	0
61	1Z	5	Total 5	O 5	0	0
61	10	21	Total 21	O 21	0	0
61	11	28	Total 28	O 28	0	0
61	12	14	Total 14	O 14	0	0
61	13	22	Total 22	O 22	0	0
61	14	4	Total 4	O 4	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
61	15	25	Total 25	O 25	0	0
61	16	21	Total 21	O 21	0	0
61	17	13	Total 13	O 13	0	0
61	18	23	Total 23	O 23	0	0
61	19	2	Total 2	O 2	0	0
61	1a	447	Total 447	O 447	0	0
61	1b	1	Total 1	O 1	0	0
61	1c	2	Total 2	O 2	0	0
61	1d	9	Total 9	O 9	0	0
61	1e	5	Total 5	O 5	0	0
61	1f	1	Total 1	O 1	0	0
61	1h	1	Total 1	O 1	0	0
61	1j	1	Total 1	O 1	0	0
61	1l	3	Total 3	O 3	0	0
61	1o	2	Total 2	O 2	0	0
61	1p	2	Total 2	O 2	0	0
61	1y	1	Total 1	O 1	0	0
61	2A	1941	Total 1941	O 1941	0	0
61	2B	45	Total 45	O 45	0	0
61	2D	45	Total 45	O 45	0	0
61	2E	25	Total 25	O 25	0	0

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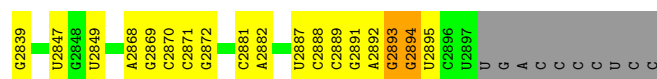
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
61	2F	15	Total 15	O 15	0	0
61	2G	2	Total 2	O 2	0	0
61	2H	1	Total 1	O 1	0	0
61	2I	1	Total 1	O 1	0	0
61	2N	3	Total 3	O 3	0	0
61	2O	10	Total 10	O 10	0	0
61	2P	19	Total 19	O 19	0	0
61	2Q	13	Total 13	O 13	0	0
61	2R	17	Total 17	O 17	0	0
61	2T	6	Total 6	O 6	0	0
61	2U	7	Total 7	O 7	0	0
61	2V	4	Total 4	O 4	0	0
61	2W	20	Total 20	O 20	0	0
61	2X	7	Total 7	O 7	0	0
61	2Y	2	Total 2	O 2	0	0
61	2Z	7	Total 7	O 7	0	0
61	20	5	Total 5	O 5	0	0
61	21	15	Total 15	O 15	0	0
61	22	1	Total 1	O 1	0	0
61	23	2	Total 2	O 2	0	0
61	25	7	Total 7	O 7	0	0

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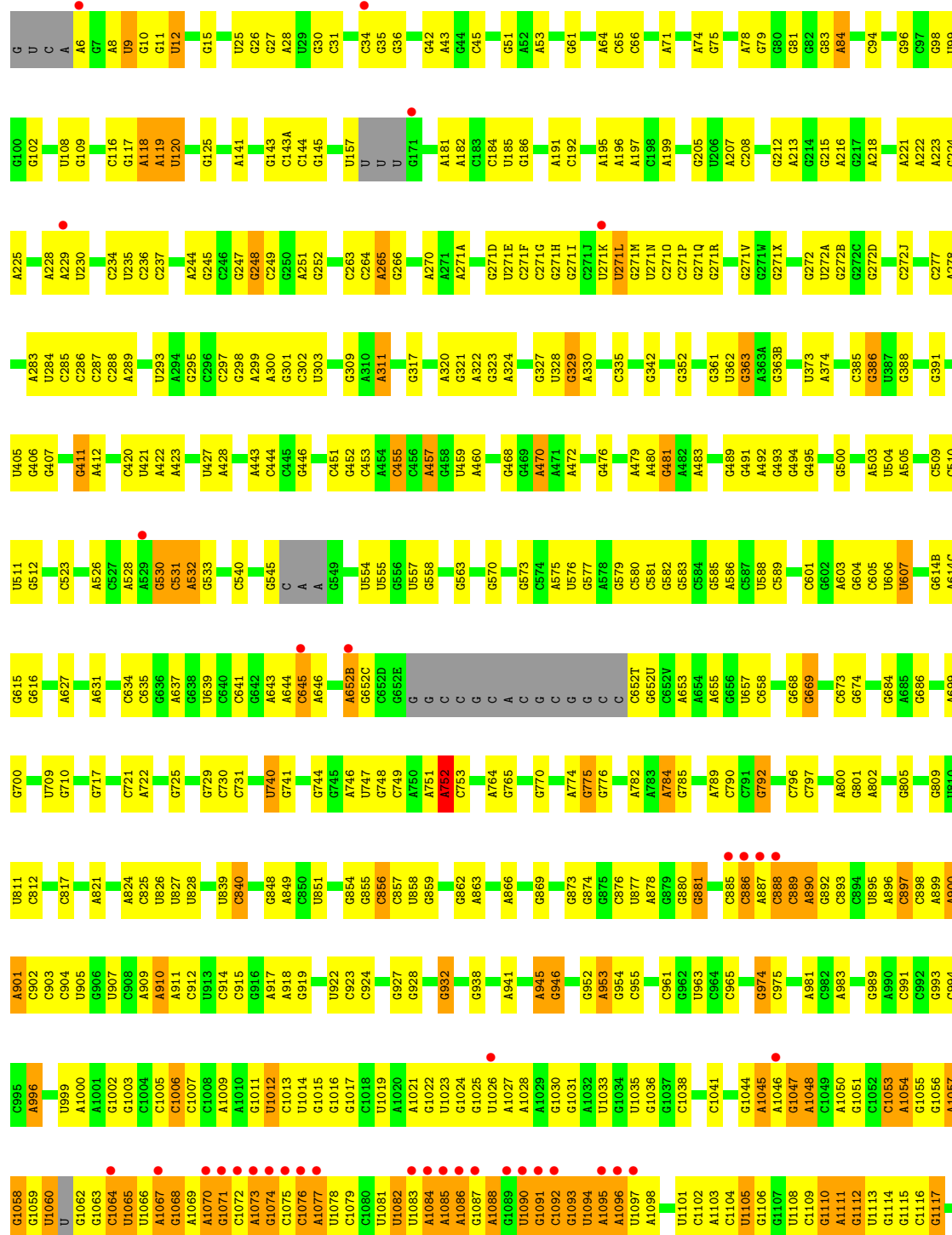
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
61	26	2	Total 2	O 2	0	0
61	27	8	Total 8	O 8	0	0
61	28	9	Total 9	O 9	0	0
61	2a	266	Total 266	O 266	0	0
61	2d	4	Total 4	O 4	0	0
61	2e	1	Total 1	O 1	0	0
61	2l	1	Total 1	O 1	0	0
61	2o	2	Total 2	O 2	0	0
61	2q	1	Total 1	O 1	0	0
61	2r	3	Total 3	O 3	0	0
61	2u	1	Total 1	O 1	0	0

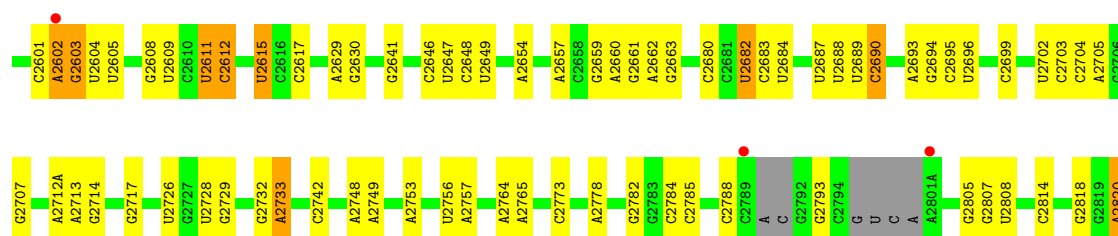
U2726	U2605	G2458	A2336	G2238	C2143	G2061	G1929	C1797	G1575	G1525	U1405	G1264	G1114
G2732	G2608	G2458	U2344	U2243	U2144	G2069	G1930	U1798	A1676	G1530	U1406	A1265	G1115
A2733	U2609	C2461	G2345	U2244	C2146	G2069	U1931	G1799	A1677	C1530	U1407	A1266	C1116
G2734	C2610	C2462	A2346	U2245	G2147	U2074	G1933	G1800	C1532	C1531	U1267	U1267	A1128
G2735	U2611	C2463	C2347	C2248	G2148	U2075	A1937	A1802	C1686	G	A1268	A1269	A1129
A2748	C2612	C2464	U2348	G2251	G2149	G2080	A1938	A1803	G1687	U	U1130	G1270	U1130
G2751	C2617	A2469	G2349	G2251	U2150	G2081	U1939	C1804	U1688	A	G1271	G1271	G1131
G2752	C2618	G2472	G2350	A2268	G2152	U2086	U1939	C1805	U1693	C	A1272	A1272	C1136
A2753	C2619	G2472	G2351	G2270	G2153	G2087	C1942	A1810	G1537	G1537	G1421	U1273	C1136
G2758	C2627	C2475	G2352	G2271	G2154	G2093	U1955	G1811	G1542	A1542	G1422	C1289	U1141
G2759	C2628	A2476	G2353	A2273	G2156	U2096	C1962	G1812	C1543	C1543	G1427	C1290	U1141
G2760	C2629	A2477	G2354	A2274	A2157	C2097	U1962	G1813	A1700	A1557	A1428	C1291	A1155
G2761	C2630	A2478	G2355	A2275	G2158	U2098	U1962	A1814	A1701	A1558	C1429	U1292	A1156
G2762	U2491	G2479	G2356	G2277	G2159	U2099	C1967	A1815	G1703	A1559	C1430	C1293	U1165
G2763	U2492	G2480	G2357	G2278	G2160	G2100	C1968	G1816	A1566	U1431	C1431	C1294	C1166
A2764	U2493	U2493	G2372	G2279	C2161	G2101	A1969	U1818	G1707	G1442	G1442	U1300	U1167
A2765	G2502	C2377	A2378	G2280	G2162	U2102	A1970	G1822	C1712	A1445	A1445	A1301	G1171
G2766	C2503	G2379	G2380	C2283	C2163	C2103	A1971	G1823	U1713	A1456	A1456	A1302	G1173
G2777	A2504	G2381	G2382	A2286	G2164	G2104	A1972	G1824	G1740	A1579	A1579	G1303	A1174
G2778	U2505	G2383	G2384	A2287	G2165	G2105	C1972	G1825	G1741	A1580	A1580	G1315	U1175
U2779	U2506	G2385	G2386	G2290	G2166	G2106	U1993	G1826	U1739	A1581	A1452	G1315	G1176
A2780	A2518	G2387	G2388	U2291	G2167	C2107	U1993	A1829	G1740	A1582	A1452	A1301	A1177
A2781	C2521	G2389	U2390	C2292	U2172	G2110	G1997	G1830	A1584	A1586	A1452	A1301	G1178
G2789	U2522	G2391	G2392	G2299	G2173	G2111	G2000	G1832	G1593	C1584	G1459	A1321	C1179
A2790	G2529	G2393	G2394	G2303	G2174	U2113	A2014	A1847	G1594	A1595	C1467	C1330	C1180
G2791	G2535	U2406	G2407	G2304	C2178	G2115	A2014	U1864	C1607	A1614	A1471	C1331	G1187
G2792	G2536	G2408	G2409	G2305	U2180	A2117	A2020	G1865	U1758	A1608	A1476	C1332	U1188
G2793	U2537	G2410	G2411	G2306	G2181	U2118	C2021	G1866	A1759	A1609	A1477	U1352	U1189
U2794	C2538	G2412	G2413	G2307	G2182	A2119	U2022	A1876	A1762	A1610	A1478	A1353	G1191
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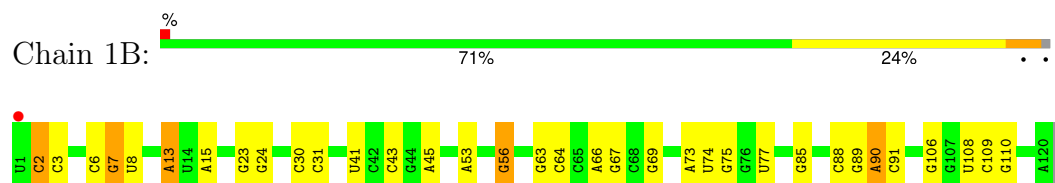
• Molecule 1: 23S Ribosomal RNA



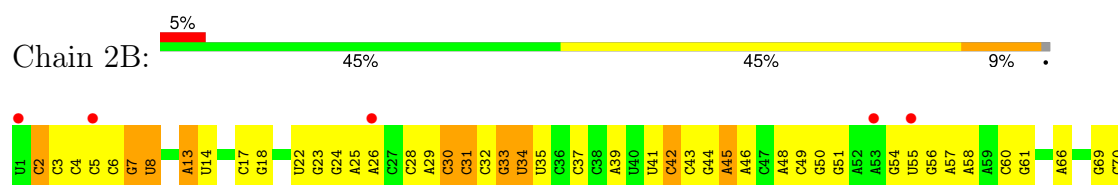
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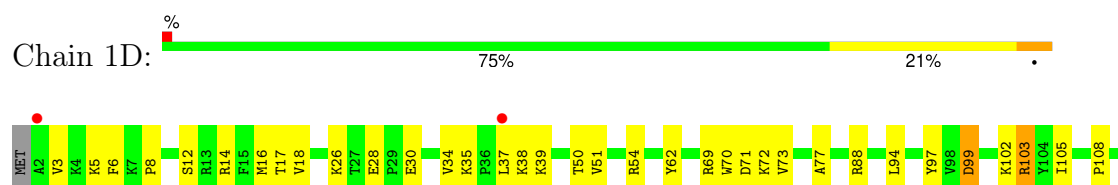
• Molecule 2: 5S Ribosomal RNA



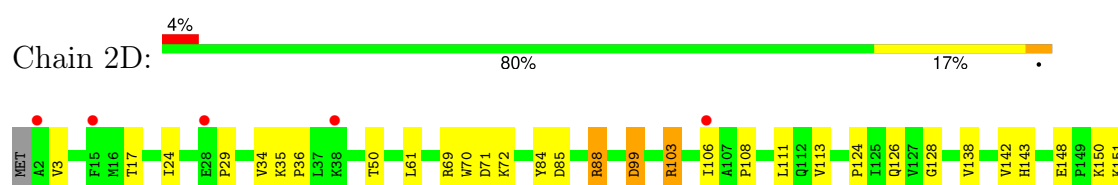
• Molecule 2: 5S Ribosomal RNA



• Molecule 3: 50S ribosomal protein L2

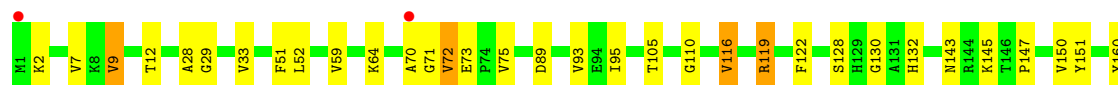
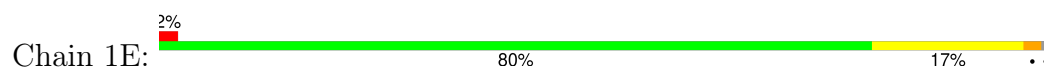


• Molecule 3: 50S ribosomal protein L2

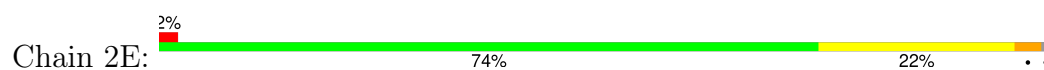




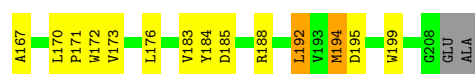
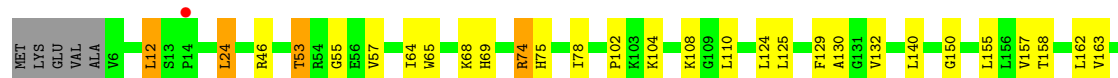
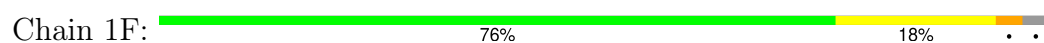
• Molecule 4: 50S ribosomal protein L3



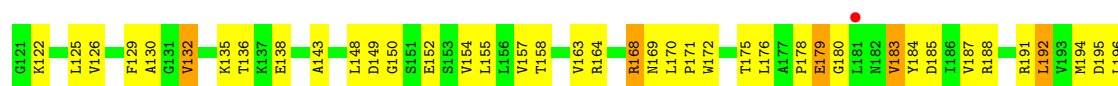
• Molecule 4: 50S ribosomal protein L3



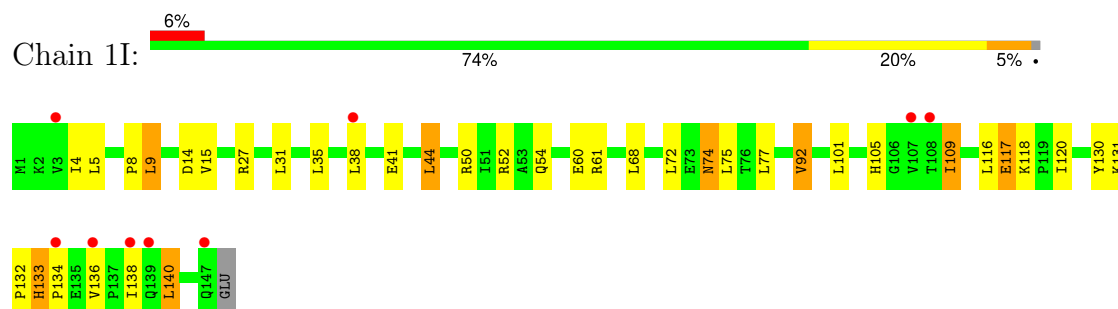
• Molecule 5: 50S ribosomal protein L4



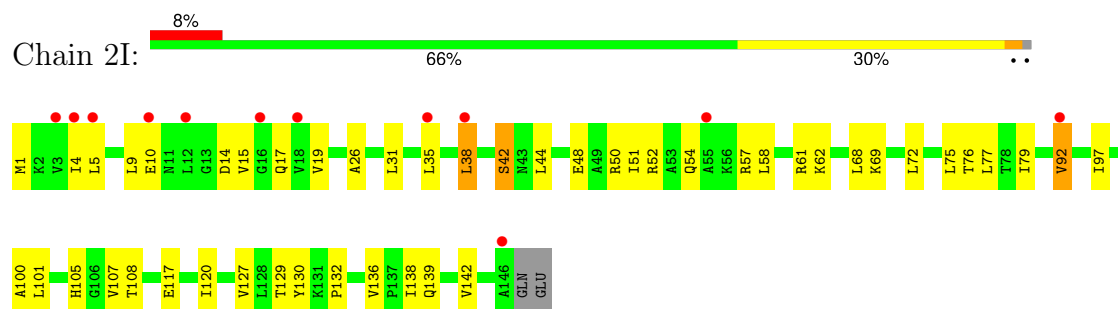
• Molecule 5: 50S ribosomal protein L4



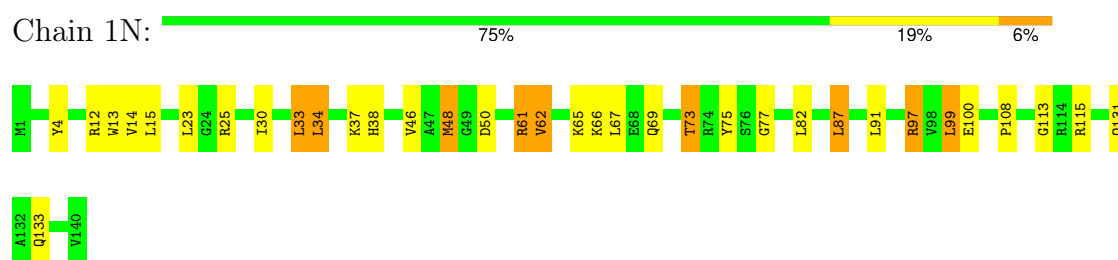
- Molecule 8: 50S ribosomal protein L9



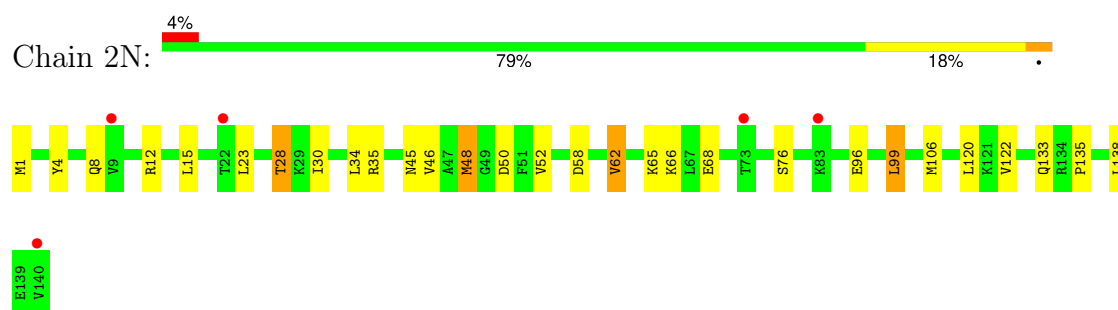
- Molecule 8: 50S ribosomal protein L9



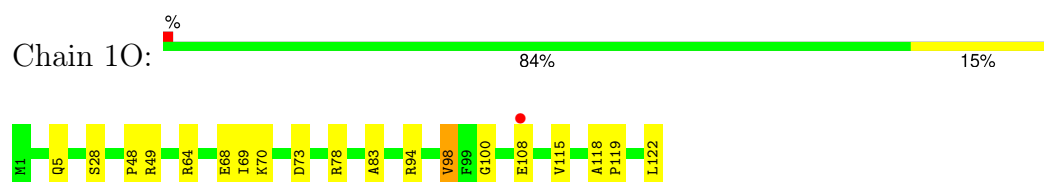
- Molecule 9: 50S ribosomal protein L13



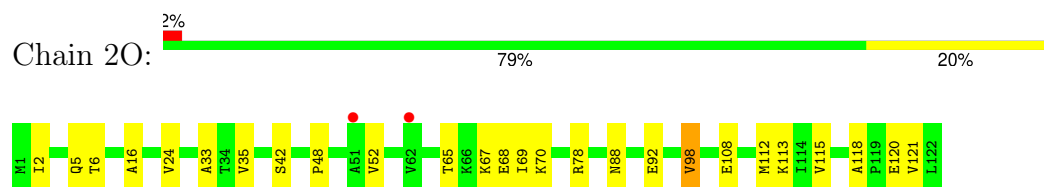
- Molecule 9: 50S ribosomal protein L13



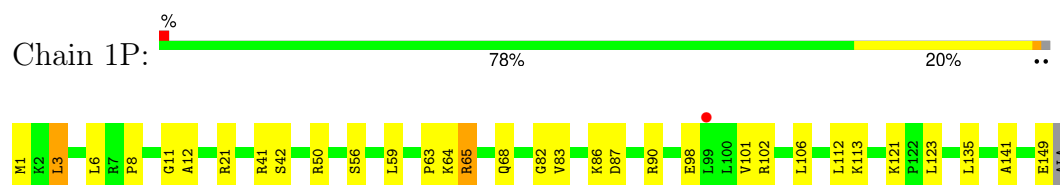
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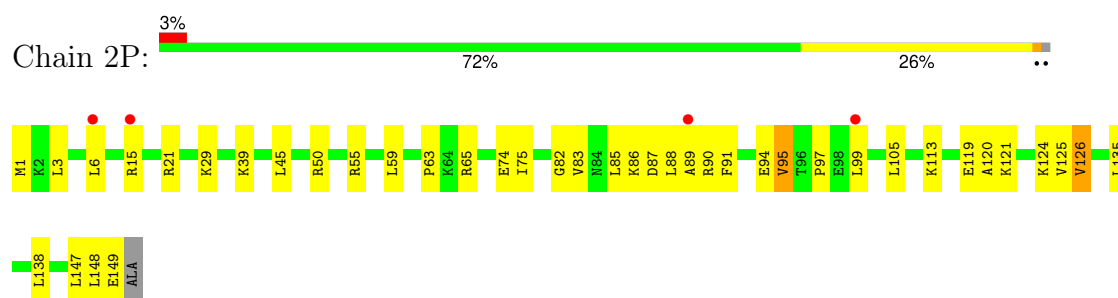
- Molecule 10: 50S ribosomal protein L14



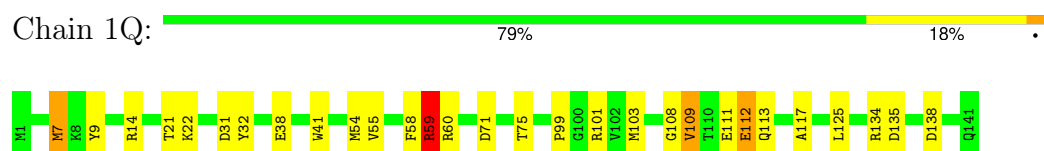
- Molecule 11: 50S ribosomal protein L15



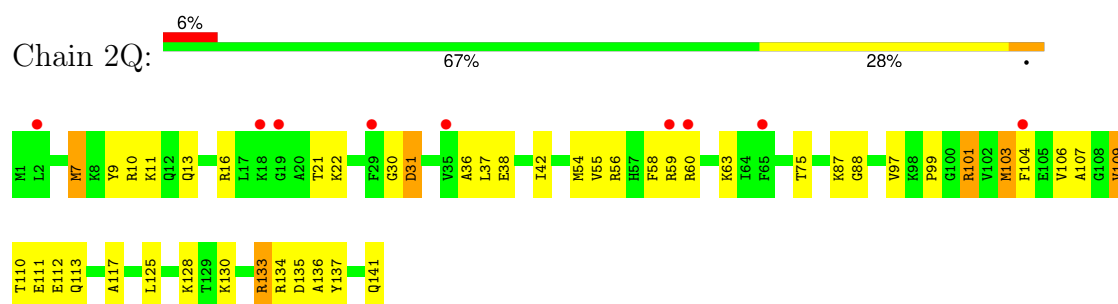
- Molecule 11: 50S ribosomal protein L15



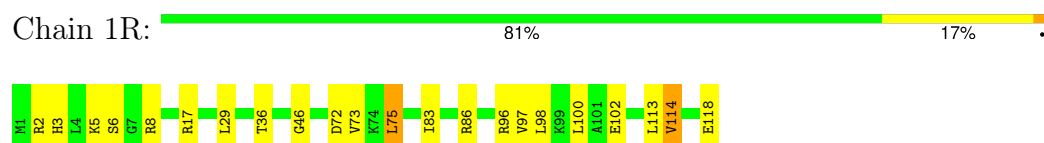
- Molecule 12: 50S ribosomal protein L16



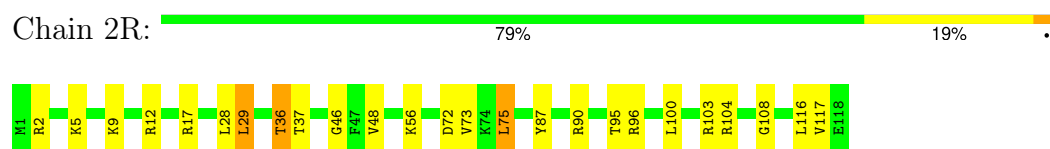
- Molecule 12: 50S ribosomal protein L16



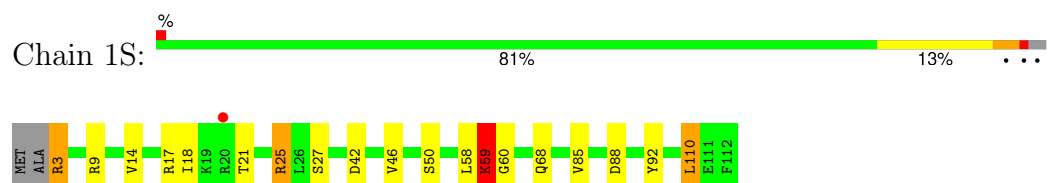
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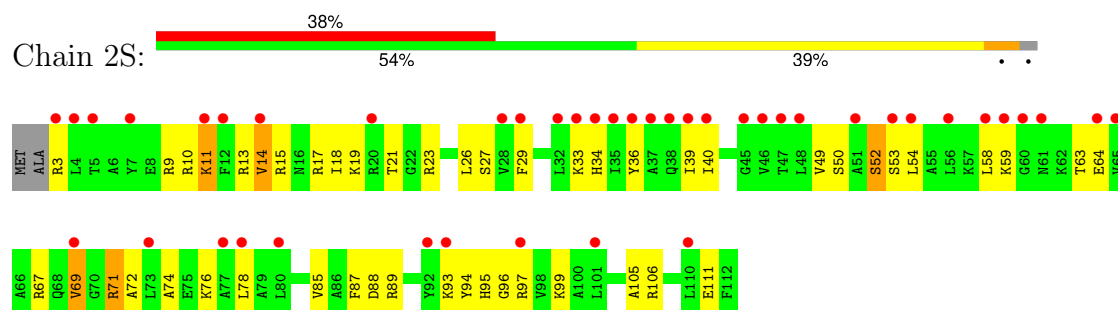
- Molecule 13: 50S ribosomal protein L17



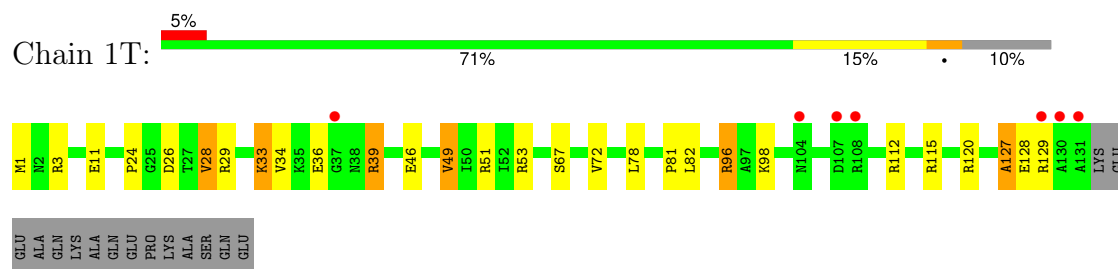
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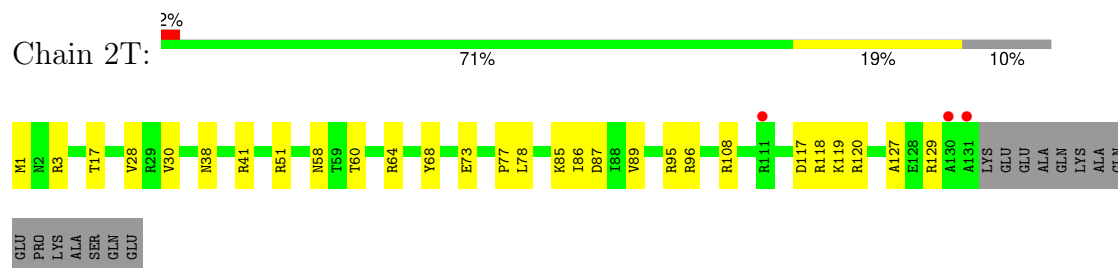
- Molecule 14: 50S ribosomal protein L18



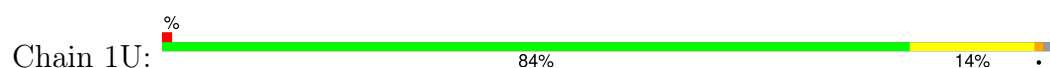
- Molecule 15: 50S ribosomal protein L19



- Molecule 15: 50S ribosomal protein L19



- Molecule 16: 50S ribosomal protein L20

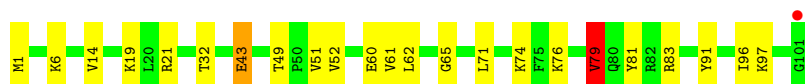
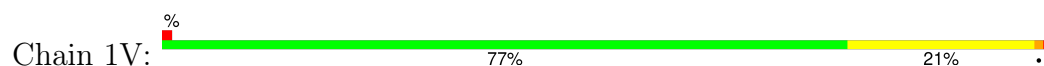




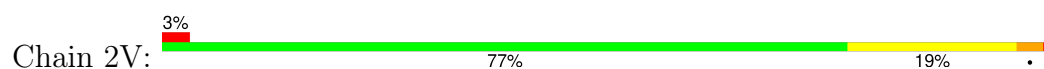
- Molecule 16: 50S ribosomal protein L20



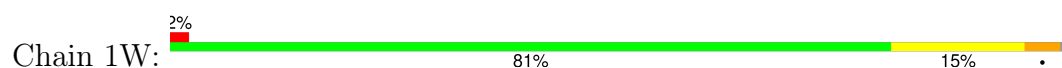
- Molecule 17: 50S ribosomal protein L21



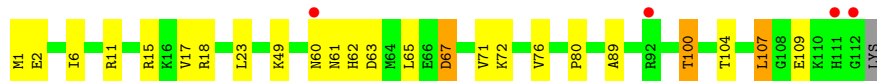
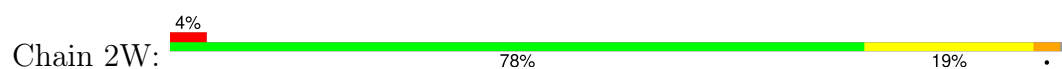
- Molecule 17: 50S ribosomal protein L21



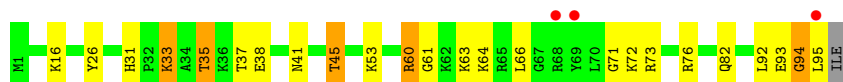
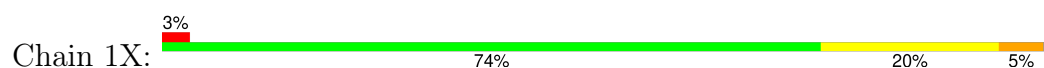
- Molecule 18: 50S ribosomal protein L22



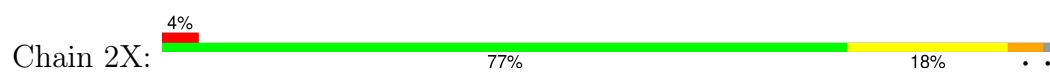
- Molecule 18: 50S ribosomal protein L22



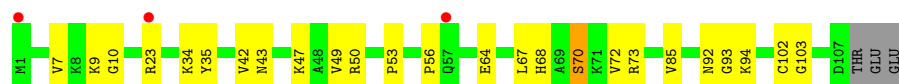
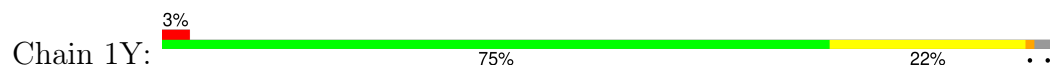
- Molecule 19: 50S ribosomal protein L23



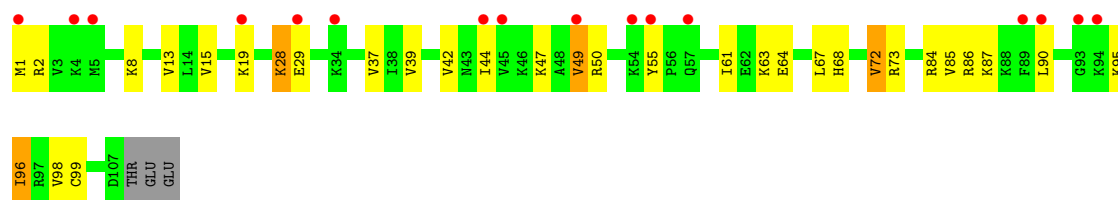
- Molecule 19: 50S ribosomal protein L23



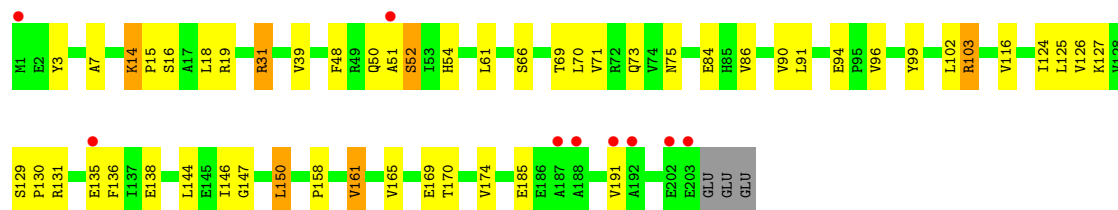
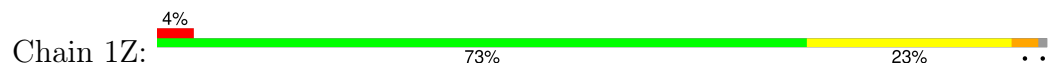
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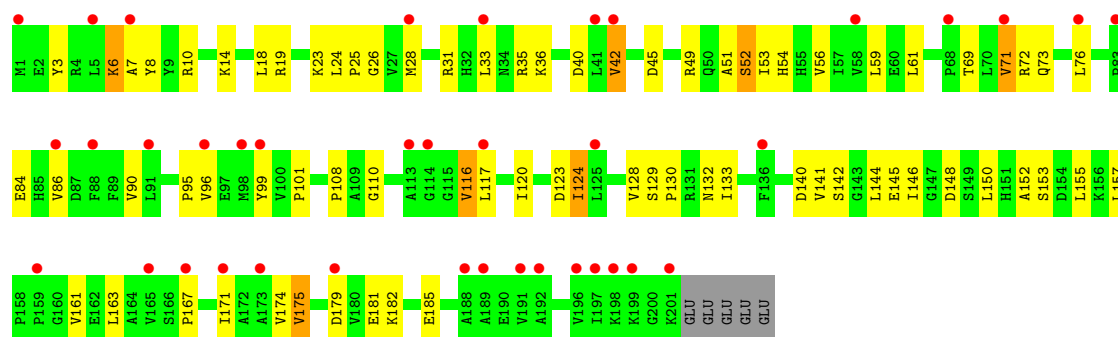
- Molecule 20: 50S ribosomal protein L24



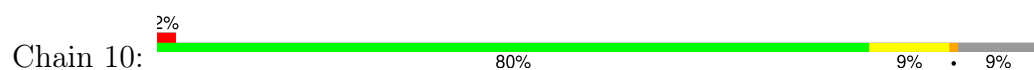
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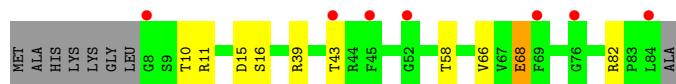
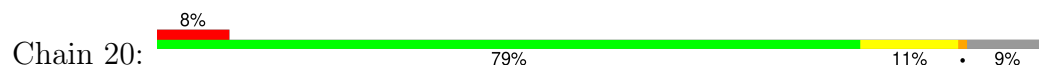
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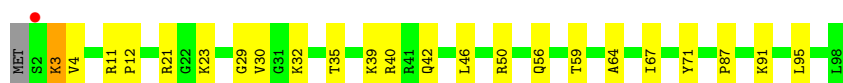
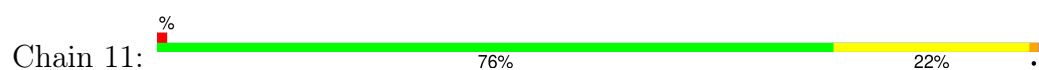
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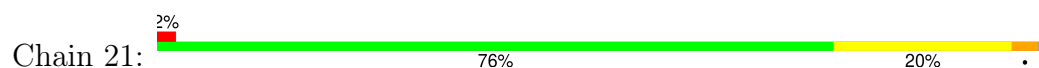
- Molecule 22: 50S ribosomal protein L27



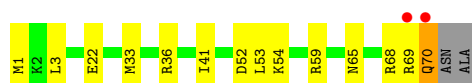
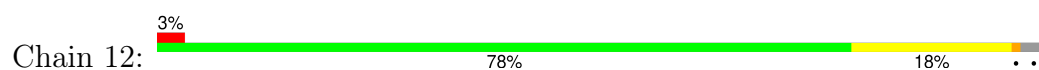
- Molecule 23: 50S ribosomal protein L28



- Molecule 23: 50S ribosomal protein L28



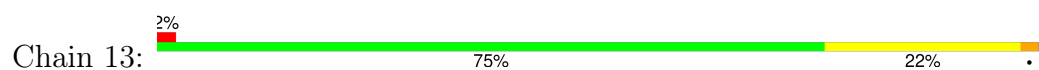
- Molecule 24: 50S ribosomal protein L29



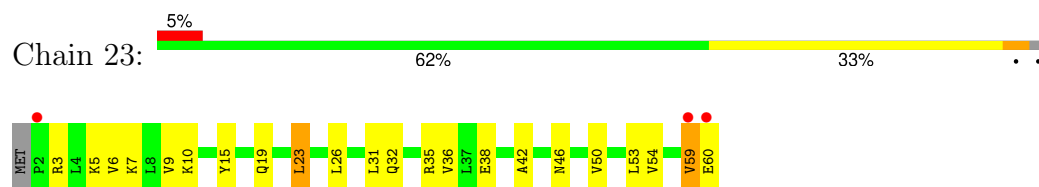
- Molecule 24: 50S ribosomal protein L29



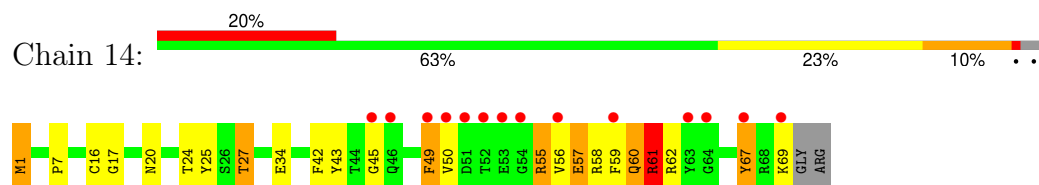
- Molecule 25: 50S ribosomal protein L30



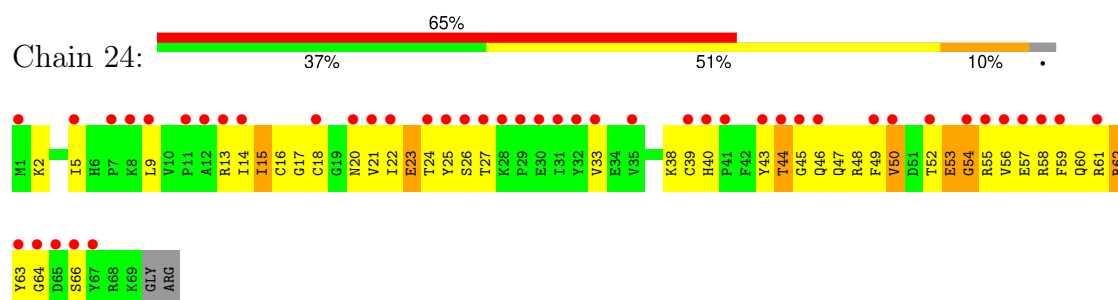
- Molecule 25: 50S ribosomal protein L30



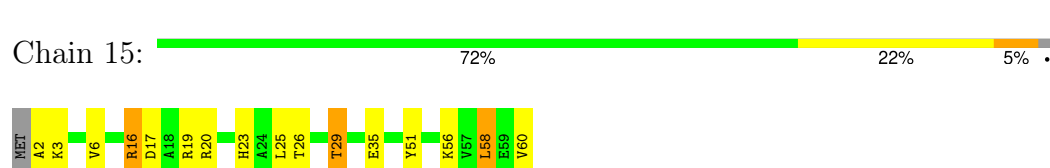
- Molecule 26: 50S ribosomal protein L31



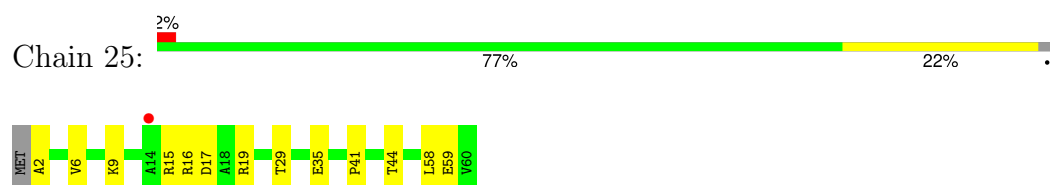
- Molecule 26: 50S ribosomal protein L31



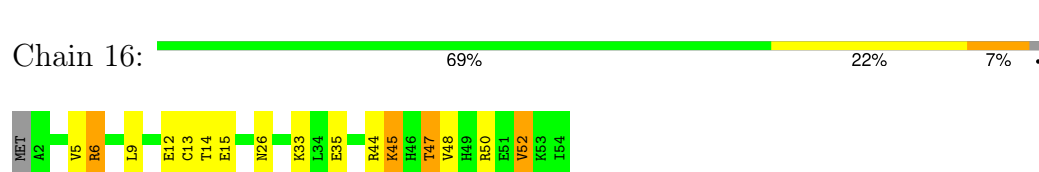
- Molecule 27: 50S ribosomal protein L32



- Molecule 27: 50S ribosomal protein L32

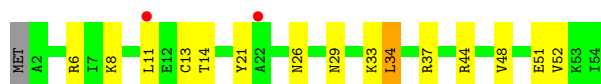


- Molecule 28: 50S ribosomal protein L33

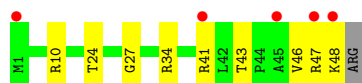
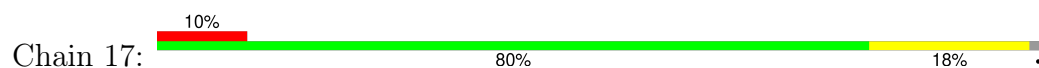


- Molecule 28: 50S ribosomal protein L33

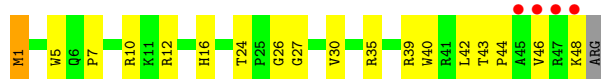




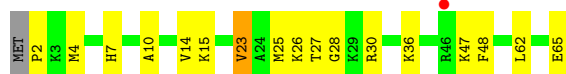
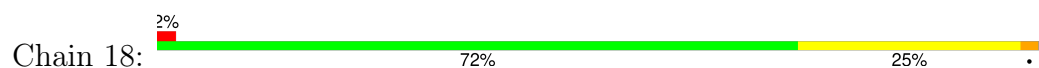
- Molecule 29: 50S ribosomal protein L34



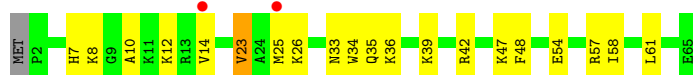
- Molecule 29: 50S ribosomal protein L34



- Molecule 30: 50S ribosomal protein L35



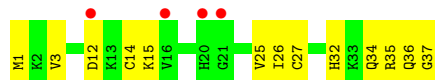
- Molecule 30: 50S ribosomal protein L35



- Molecule 31: 50S ribosomal protein L36

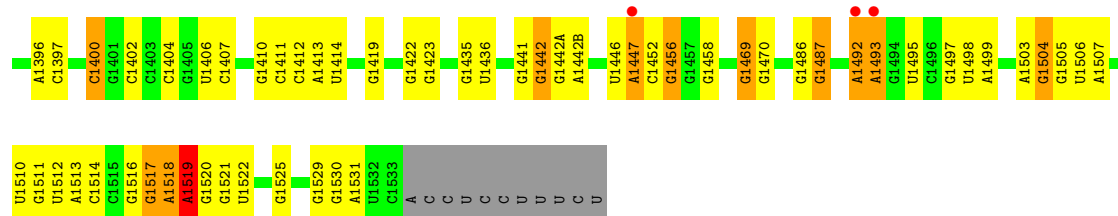


- Molecule 31: 50S ribosomal protein L36

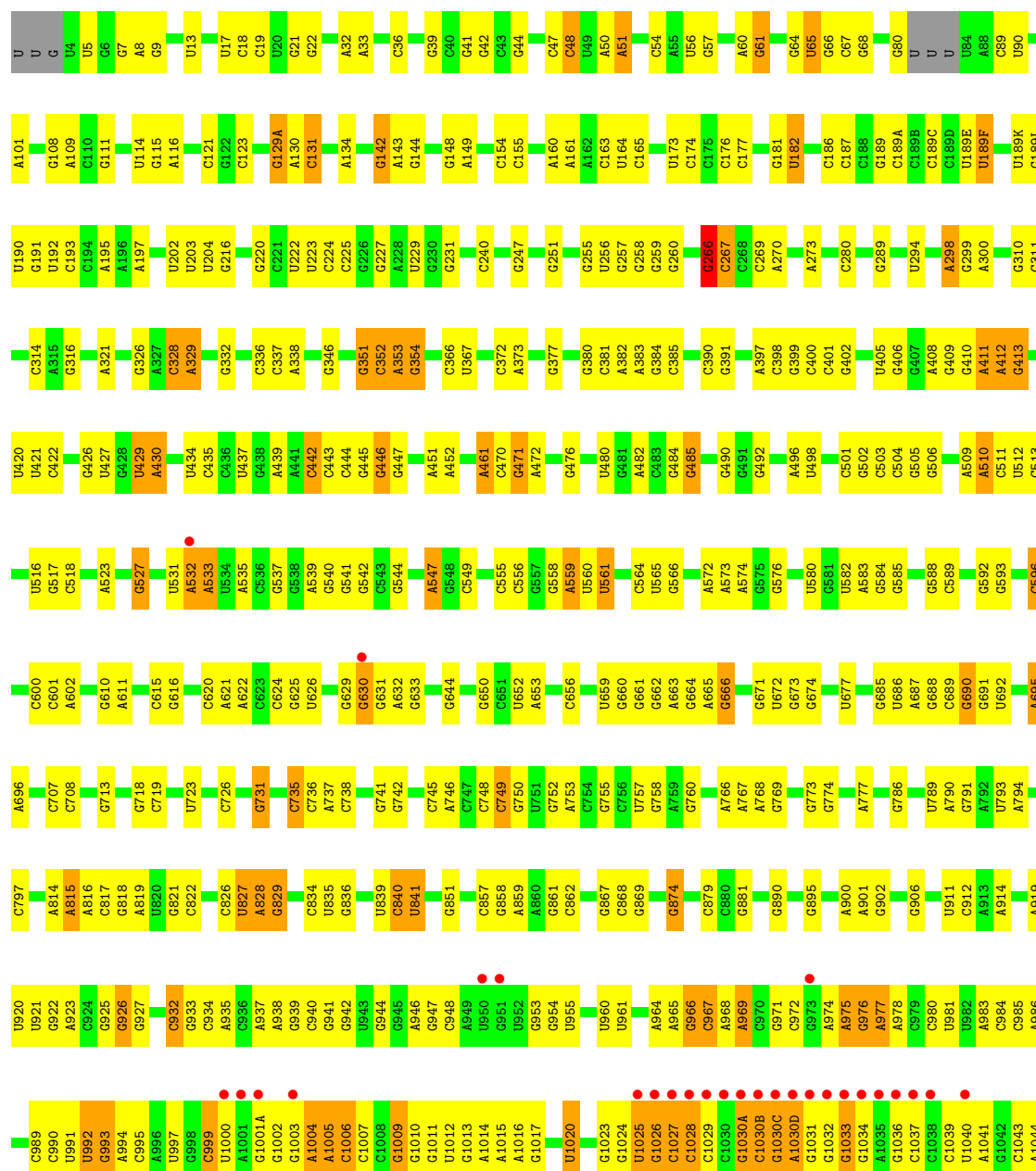


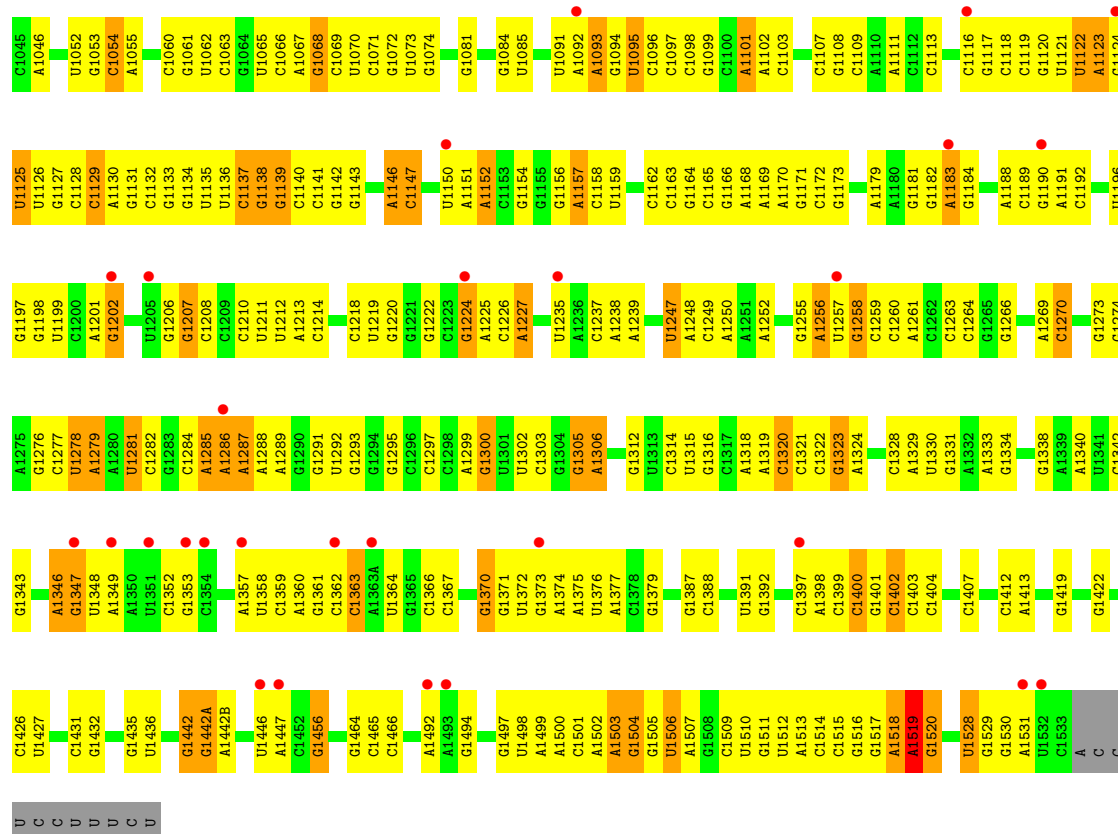
- Molecule 32: 16S Ribosomal RNA



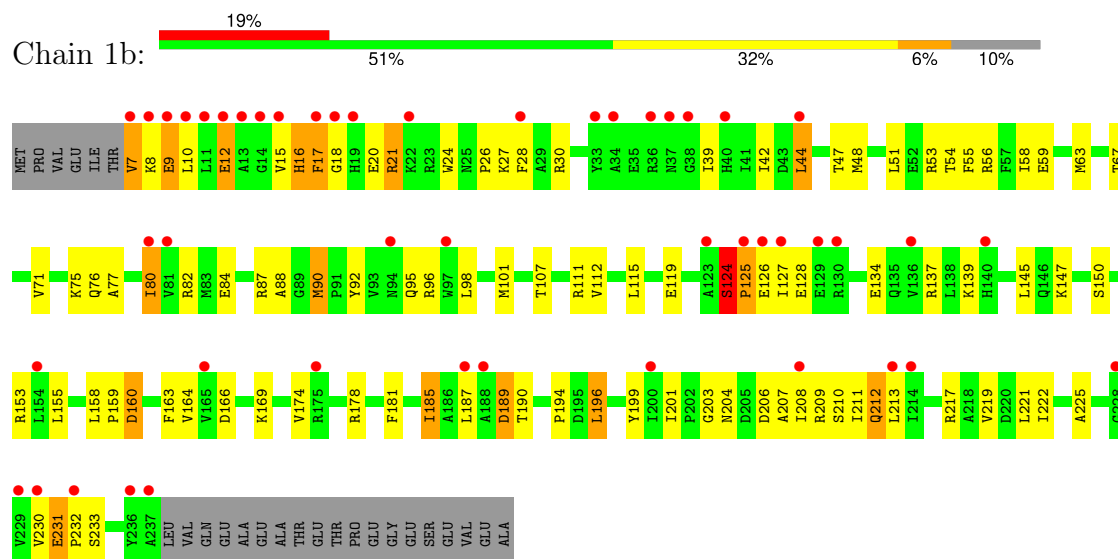


• Molecule 32: 16S Ribosomal RNA

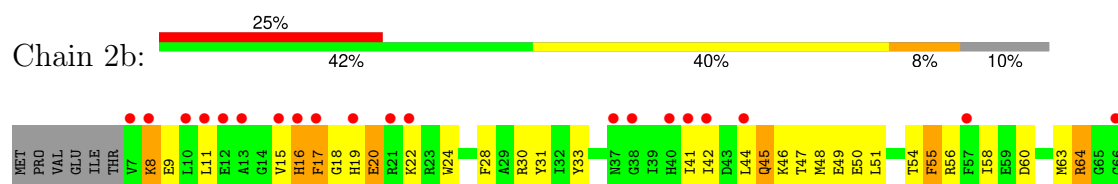


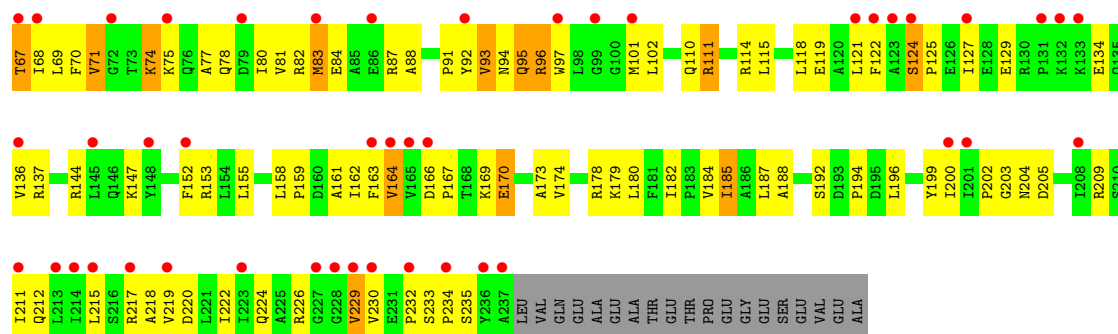


• Molecule 33: 30S ribosomal protein S2

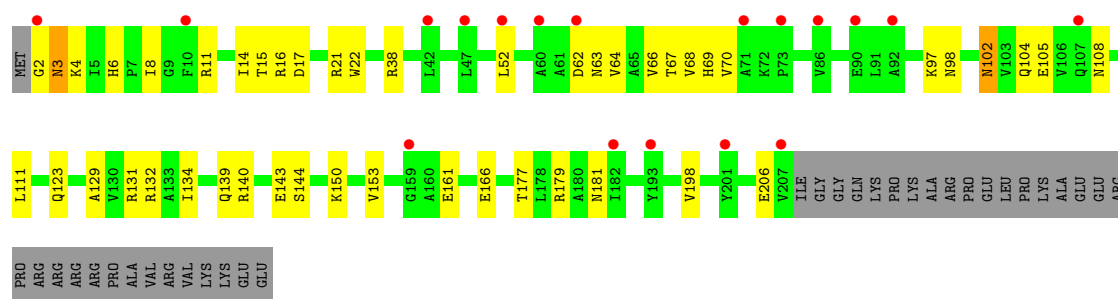


• Molecule 33: 30S ribosomal protein S2

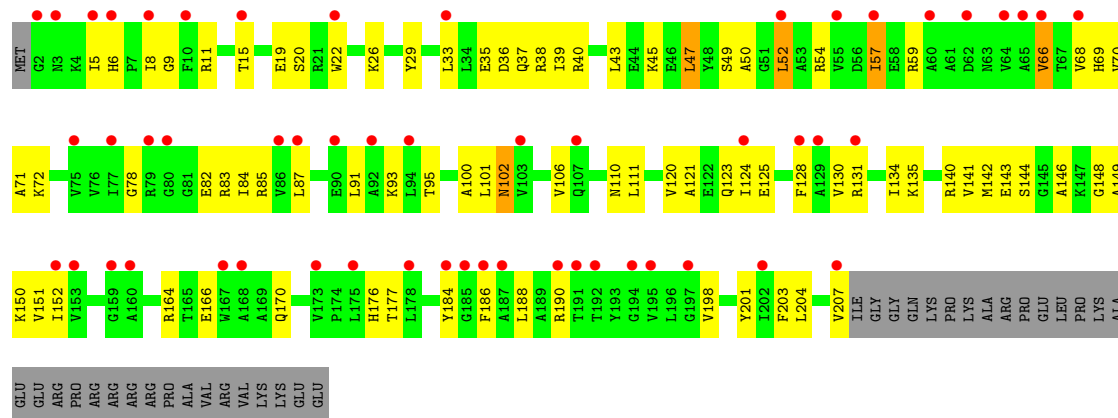




• Molecule 34: 30S ribosomal protein S3

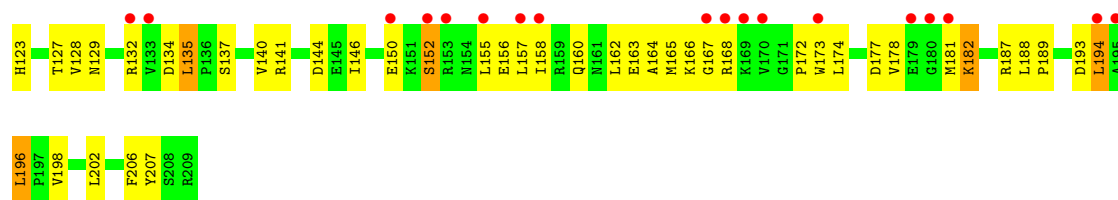


• Molecule 34: 30S ribosomal protein S3

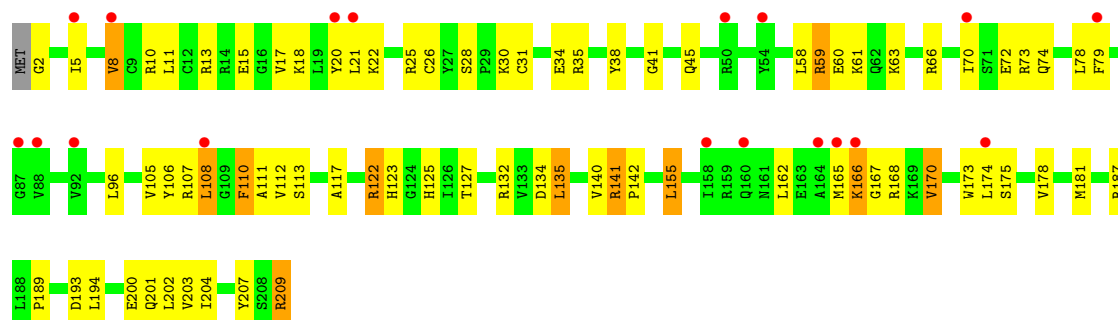


• Molecule 35: 30S ribosomal protein S4

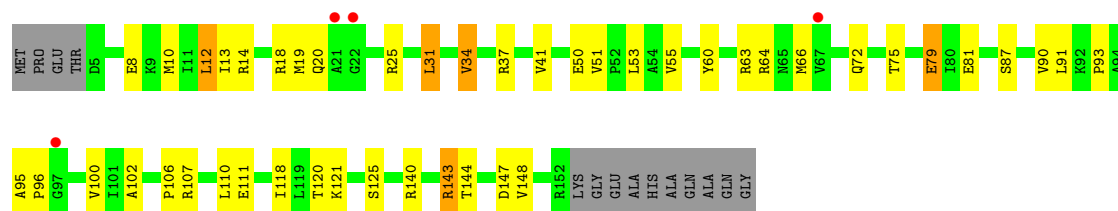




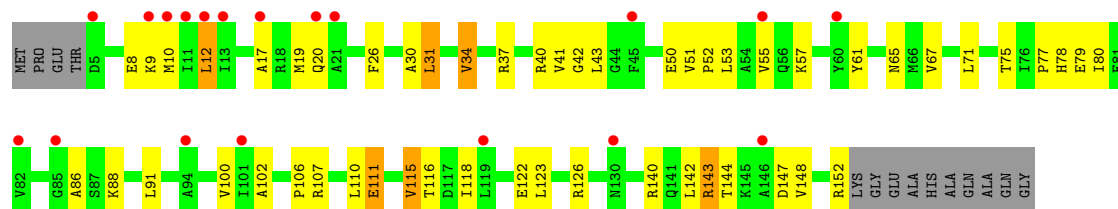
• Molecule 35: 30S ribosomal protein S4



• Molecule 36: 30S ribosomal protein S5



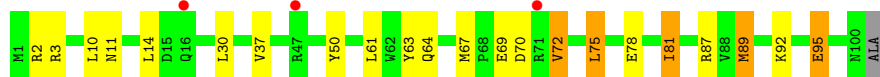
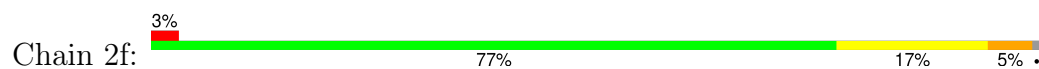
• Molecule 36: 30S ribosomal protein S5



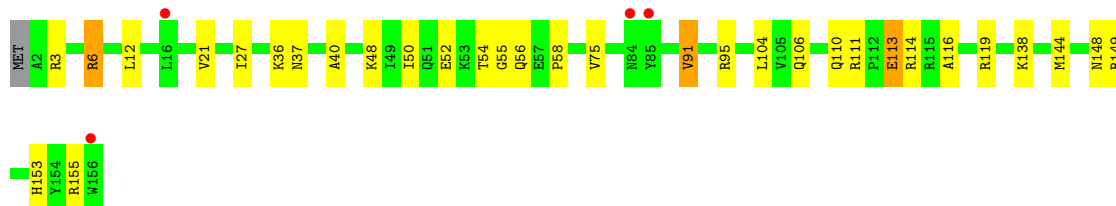
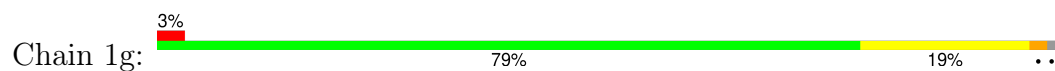
• Molecule 37: 30S ribosomal protein S6



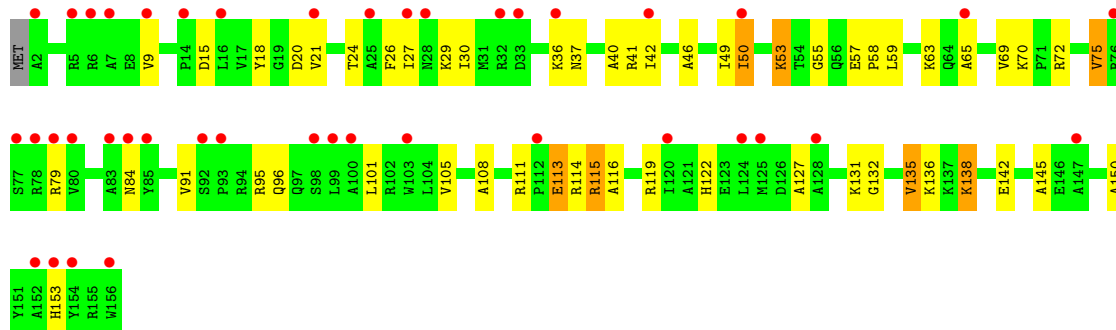
- Molecule 37: 30S ribosomal protein S6



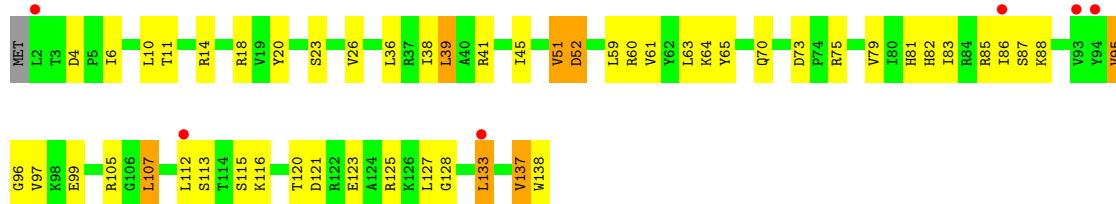
- Molecule 38: 30S ribosomal protein S7



- Molecule 38: 30S ribosomal protein S7

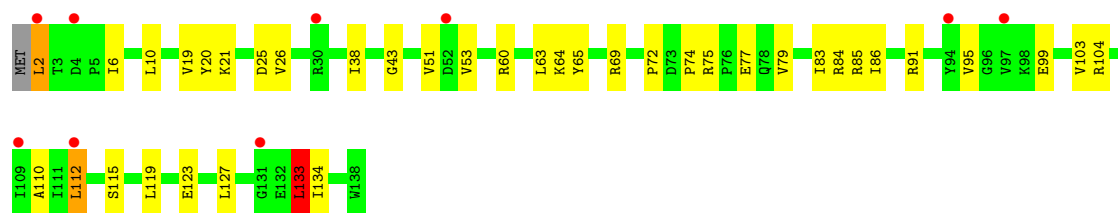


- Molecule 39: 30S ribosomal protein S8

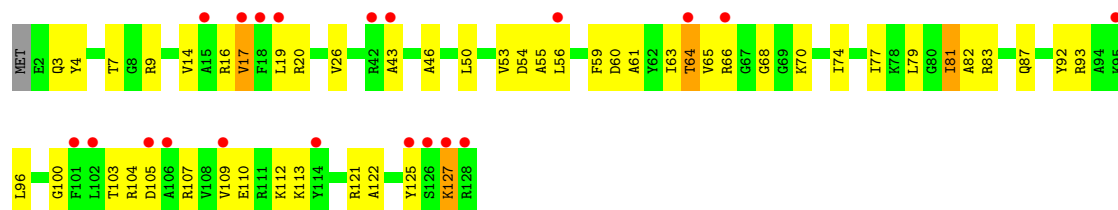


- Molecule 39: 30S ribosomal protein S8

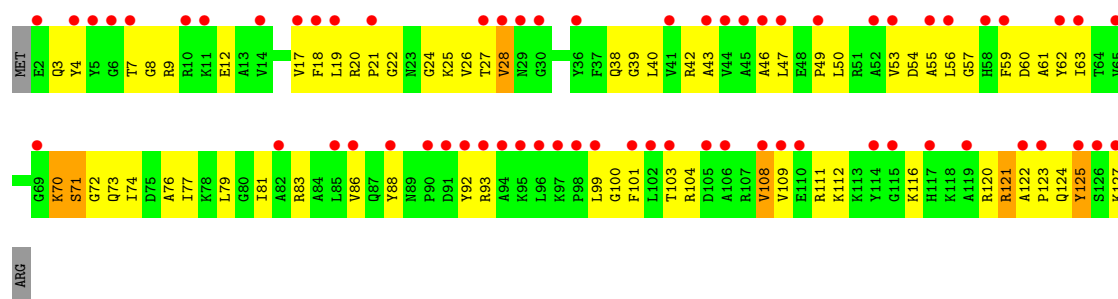




• Molecule 40: 30S ribosomal protein S9



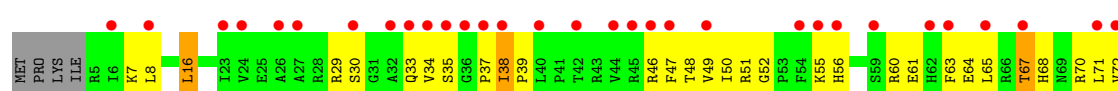
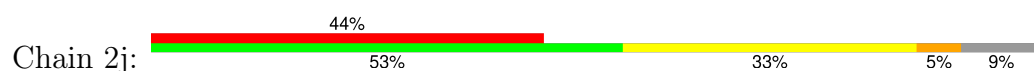
• Molecule 40: 30S ribosomal protein S9

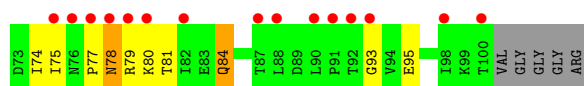


• Molecule 41: 30S ribosomal protein S10



• Molecule 41: 30S ribosomal protein S10

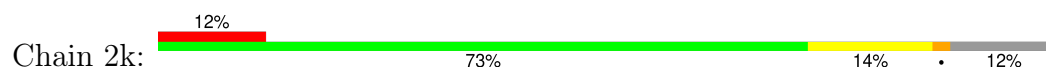




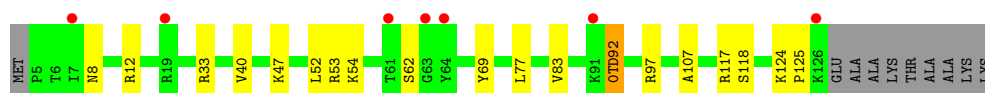
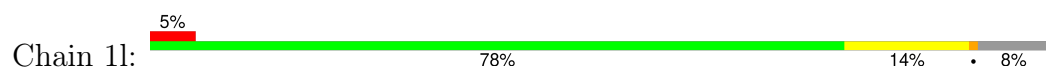
- Molecule 42: 30S ribosomal protein S11



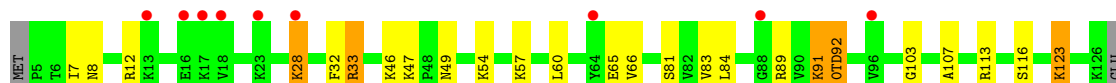
- Molecule 42: 30S ribosomal protein S11



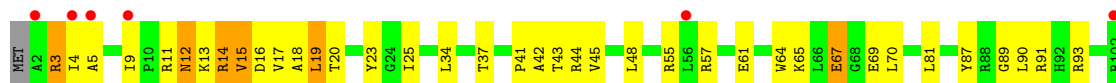
- Molecule 43: 30S ribosomal protein S12

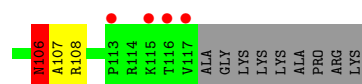


- Molecule 43: 30S ribosomal protein S12

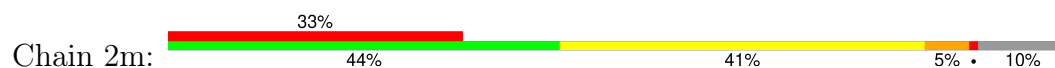


- Molecule 44: 30S ribosomal protein S13





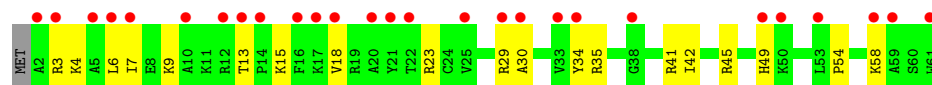
- Molecule 44: 30S ribosomal protein S13



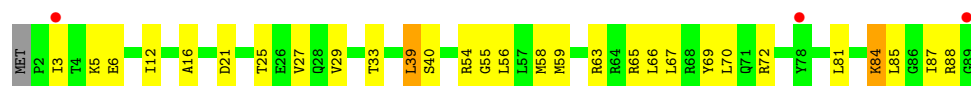
- Molecule 45: 30S ribosomal protein S14 type Z



- Molecule 45: 30S ribosomal protein S14 type Z



- Molecule 46: 30S ribosomal protein S15

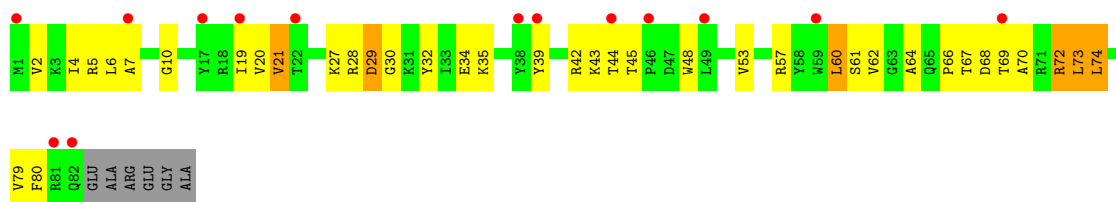


- Molecule 46: 30S ribosomal protein S15

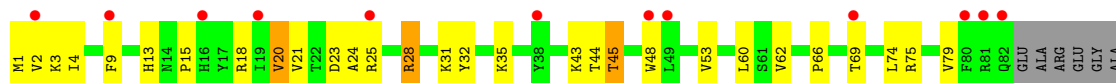


- Molecule 47: 30S ribosomal protein S16

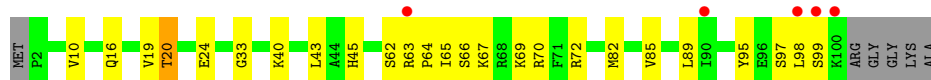




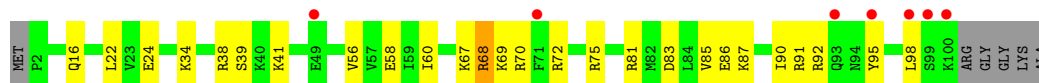
- Molecule 47: 30S ribosomal protein S16



- Molecule 48: 30S ribosomal protein S17



- Molecule 48: 30S ribosomal protein S17



- Molecule 49: 30S ribosomal protein S18

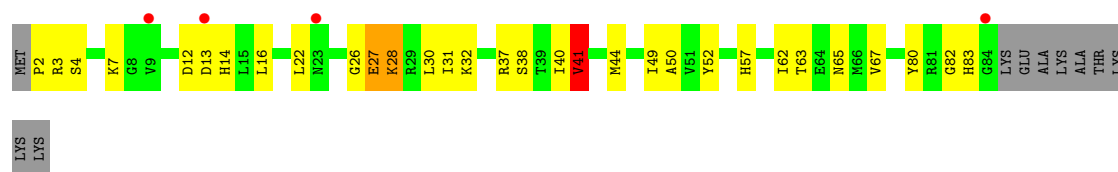


- Molecule 49: 30S ribosomal protein S18

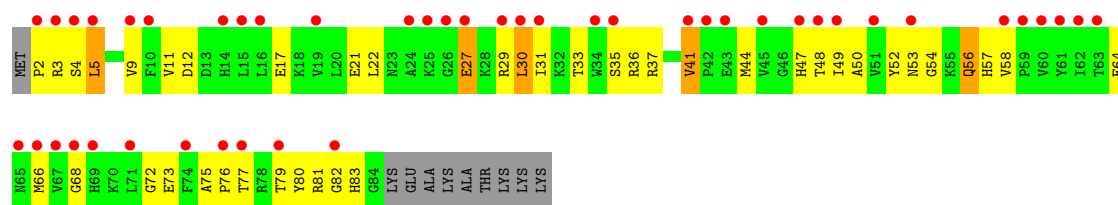
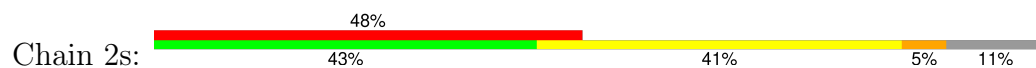


- Molecule 50: 30S ribosomal protein S19

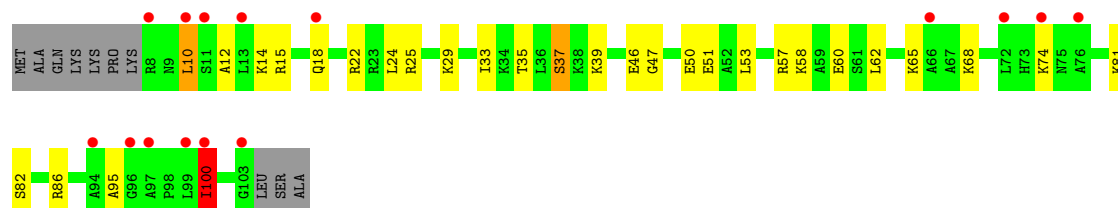




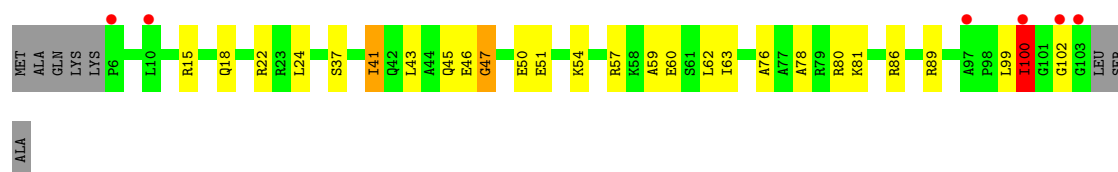
- Molecule 50: 30S ribosomal protein S19



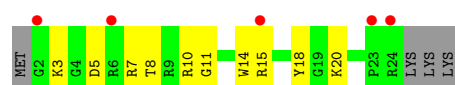
- Molecule 51: 30S ribosomal protein S20



- Molecule 51: 30S ribosomal protein S20

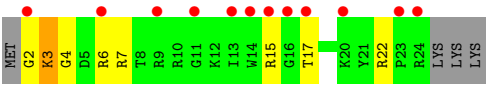


- Molecule 52: 30S ribosomal protein Thx

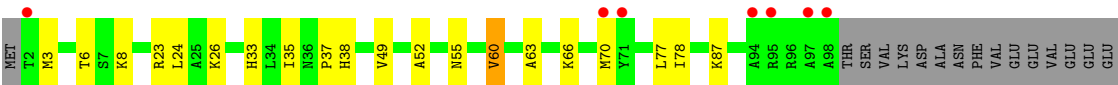


- Molecule 52: 30S ribosomal protein Thx

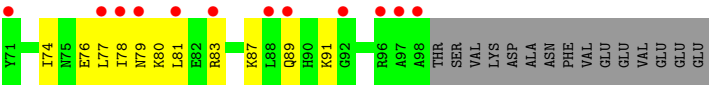
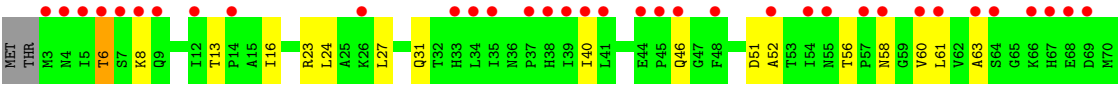




● Molecule 53: Ribosome-associated inhibitor A



● 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	208.57Å 448.58Å 617.47Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	151.65 – 2.50 151.65 – 2.50	Depositor EDS
% Data completeness (in resolution range)	99.9 (151.65-2.50) 99.9 (151.65-2.50)	Depositor EDS
R_{merge}	0.17	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.22 (at 2.52Å)	Xtriage
Refinement program	PHENIX 1.8.2	Depositor
R, R_{free}	0.206 , 0.246 0.206 , 0.246	Depositor DCC
R_{free} test set	98630 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å ²)	57.6	Xtriage
Anisotropy	0.189	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 64.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	296967	wwPDB-VP
Average B, all atoms (Å ²)	65.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.54% 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: MA6, PSU, HGR, G7M, 2MG, 5MC, OMC, ERY, OMG, UR3, 2MA, 4OC, 5MU, MPD, 0TD, ZN, 2MU, M2G, MG, SF4

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	0.31	0/69030	0.49	5/107750 (0.0%)
1	2A	0.24	0/68902	0.43	2/107548 (0.0%)
2	1B	0.25	0/2876	0.44	0/4486
2	2B	0.21	0/2878	0.40	0/4490
3	1D	0.30	0/2181	0.55	0/2940
3	2D	0.24	0/2186	0.48	0/2944
4	1E	0.27	0/1592	0.51	0/2149
4	2E	0.21	0/1592	0.45	0/2149
5	1F	0.26	0/1619	0.50	0/2193
5	2F	0.22	0/1615	0.48	0/2188
6	1G	0.21	0/1451	0.41	0/1961
6	2G	0.23	0/1449	0.44	0/1957
7	1H	0.23	0/1356	0.44	0/1834
7	2H	0.19	0/1350	0.40	0/1826
8	1I	0.20	0/1109	0.42	0/1512
8	2I	0.17	0/1091	0.40	0/1490
9	1N	0.27	0/1148	0.48	0/1547
9	2N	0.19	0/1144	0.38	0/1543
10	1O	0.28	0/943	0.47	0/1269
10	2O	0.23	0/943	0.47	0/1269
11	1P	0.28	0/1152	0.52	0/1533
11	2P	0.22	0/1152	0.45	0/1533
12	1Q	0.28	0/1143	0.49	0/1527
12	2Q	0.19	0/1143	0.43	0/1527
13	1R	0.29	0/982	0.53	0/1312
13	2R	0.25	0/982	0.46	0/1312
14	1S	0.23	0/887	0.46	0/1180
14	2S	0.20	0/880	0.45	0/1172
15	1T	0.26	0/1105	0.50	0/1477
15	2T	0.21	0/1097	0.45	0/1468
16	1U	0.30	0/977	0.53	0/1301

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
16	2U	0.19	0/977	0.40	0/1301
17	1V	0.27	0/786	0.47	0/1053
17	2V	0.20	0/782	0.40	0/1049
18	1W	0.29	0/897	0.46	0/1205
18	2W	0.23	0/897	0.43	0/1205
19	1X	0.28	0/764	0.52	0/1025
19	2X	0.21	0/764	0.44	0/1025
20	1Y	0.26	0/823	0.52	0/1099
20	2Y	0.20	0/823	0.46	0/1100
21	1Z	0.23	0/1620	0.46	0/2200
21	2Z	0.20	0/1590	0.45	0/2162
22	10	0.29	0/616	0.54	0/821
22	20	0.20	0/616	0.45	0/821
23	11	0.27	0/761	0.46	0/1013
23	21	0.23	0/766	0.41	0/1018
24	12	0.23	0/590	0.45	0/781
24	22	0.21	0/594	0.43	0/785
25	13	0.28	0/474	0.52	0/635
25	23	0.19	0/469	0.40	0/630
26	14	0.26	0/559	0.59	0/754
26	24	0.30	0/549	0.70	0/741
27	15	0.32	0/473	0.60	0/639
27	25	0.26	0/469	0.45	0/635
28	16	0.26	0/460	0.50	0/613
28	26	0.21	0/456	0.45	0/608
29	17	0.33	0/426	0.50	0/561
29	27	0.25	0/426	0.50	0/561
30	18	0.27	0/525	0.51	0/691
30	28	0.21	0/525	0.41	0/691
31	19	0.31	0/310	0.50	0/407
31	29	0.20	0/310	0.42	0/407
32	1a	0.21	0/35795	0.40	0/55864
32	2a	0.20	1/35890 (0.0%)	0.39	2/56012 (0.0%)
33	1b	0.22	0/1876	0.48	0/2533
33	2b	0.25	0/1860	0.51	2/2518 (0.1%)
34	1c	0.19	0/1582	0.42	0/2137
34	2c	0.22	0/1566	0.41	0/2119
35	1d	0.20	0/1695	0.44	0/2274
35	2d	0.19	0/1698	0.42	0/2277
36	1e	0.21	0/1149	0.44	0/1548
36	2e	0.20	0/1149	0.41	0/1548
37	1f	0.21	0/827	0.40	0/1120
37	2f	0.20	0/829	0.41	0/1123

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
38	1g	0.19	0/1254	0.40	0/1683
38	2g	0.20	0/1248	0.40	0/1676
39	1h	0.19	0/1118	0.42	0/1506
39	2h	0.17	0/1108	0.40	0/1494
40	1i	0.20	0/1005	0.46	0/1351
40	2i	0.23	0/985	0.47	0/1329
41	1j	0.24	0/732	0.40	0/993
41	2j	0.23	0/723	0.41	0/984
42	1k	0.20	0/849	0.45	0/1150
42	2k	0.20	0/848	0.44	0/1149
43	1l	0.20	0/937	0.43	0/1260
43	2l	0.18	0/937	0.40	0/1260
44	1m	0.19	0/924	0.46	0/1242
44	2m	0.23	0/905	0.46	0/1217
45	1n	0.20	0/501	0.48	0/664
45	2n	0.21	0/501	0.43	0/664
46	1o	0.20	0/739	0.40	0/985
46	2o	0.21	0/739	0.40	0/985
47	1p	0.20	0/697	0.49	0/939
47	2p	0.20	0/693	0.45	0/935
48	1q	0.21	0/836	0.42	0/1117
48	2q	0.21	0/836	0.41	0/1117
49	1r	0.21	0/560	0.52	0/746
49	2r	0.20	0/560	0.38	0/746
50	1s	0.19	0/663	0.51	1/895 (0.1%)
50	2s	0.22	0/660	0.44	0/893
51	1t	0.21	0/734	0.50	0/969
51	2t	0.19	0/736	0.42	0/976
52	1u	0.21	0/203	0.48	0/266
52	2u	0.23	0/203	0.48	0/266
53	1y	0.20	0/776	0.40	0/1048
53	2y	0.20	0/761	0.37	0/1030
All	All	0.25	1/309939 (0.0%)	0.44	12/463231 (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
26	14	0	1
26	24	0	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
33	1b	0	1
All	All	0	3

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	2a	1498	UR3	O3'-P	5.25	1.61	1.56

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1A	1042	G	OP1-P-O3'	-8.93	81.21	108.00
1	1A	1042	G	OP2-P-O3'	-6.96	87.13	108.00
50	1s	41	VAL	CB-CA-C	6.42	115.62	109.33
33	2b	232	PRO	CA-C-N	6.00	138.01	120.97
33	2b	232	PRO	C-N-CA	6.00	138.01	120.97

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
26	14	67	TYR	Peptide
33	1b	231	GLU	Peptide
26	24	18	CYS	Peptide

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	1A	61869	0	31205	610	0
1	2A	61758	0	31152	750	0
2	1B	2572	0	1305	24	0
2	2B	2573	0	1306	60	0
3	1D	2131	0	2207	54	0
3	2D	2136	0	2218	36	0
4	1E	1559	0	1618	27	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	2E	1559	0	1618	36	0
5	1F	1584	0	1625	26	0
5	2F	1580	0	1619	52	0
6	1G	1426	0	1445	42	0
6	2G	1424	0	1441	89	0
7	1H	1330	0	1407	26	0
7	2H	1324	0	1402	41	0
8	1I	1094	0	1127	25	0
8	2I	1076	0	1094	29	0
9	1N	1121	0	1195	25	0
9	2N	1117	0	1184	20	0
10	1O	933	0	996	13	0
10	2O	933	0	996	18	0
11	1P	1135	0	1212	25	0
11	2P	1135	0	1212	28	0
12	1Q	1122	0	1179	19	0
12	2Q	1122	0	1179	28	0
13	1R	968	0	1033	16	0
13	2R	968	0	1033	16	0
14	1S	877	0	938	17	0
14	2S	870	0	923	30	0
15	1T	1091	0	1151	21	0
15	2T	1083	0	1136	25	0
16	1U	959	0	1019	15	0
16	2U	959	0	1019	26	0
17	1V	775	0	841	16	0
17	2V	771	0	830	16	0
18	1W	886	0	940	14	0
18	2W	886	0	940	11	0
19	1X	750	0	814	18	0
19	2X	750	0	814	15	0
20	1Y	810	0	892	16	0
20	2Y	810	0	887	21	0
21	1Z	1587	0	1598	31	0
21	2Z	1557	0	1564	49	0
22	10	608	0	622	9	0
22	20	608	0	622	4	0
23	11	754	0	823	13	0
23	21	759	0	837	18	0
24	12	588	0	643	11	0
24	22	592	0	654	10	0
25	13	469	0	518	8	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
25	23	464	0	514	14	0
26	14	546	0	522	21	0
26	24	536	0	514	36	0
27	15	459	0	476	11	0
27	25	455	0	465	7	0
28	16	453	0	473	7	0
28	26	449	0	469	8	0
29	17	418	0	467	5	0
29	27	418	0	467	10	0
30	18	517	0	582	15	0
30	28	517	0	582	16	0
31	19	307	0	335	1	0
31	29	307	0	335	10	0
32	1a	32246	0	16295	415	0
32	2a	32331	0	16338	532	0
33	1b	1842	0	1862	65	0
33	2b	1825	0	1828	86	0
34	1c	1558	0	1557	33	0
34	2c	1542	0	1517	62	0
35	1d	1665	0	1687	56	0
35	2d	1668	0	1703	58	0
36	1e	1133	0	1191	29	0
36	2e	1133	0	1191	36	0
37	1f	814	0	808	17	0
37	2f	816	0	808	16	0
38	1g	1235	0	1249	20	0
38	2g	1229	0	1238	30	0
39	1h	1098	0	1143	39	0
39	2h	1088	0	1126	22	0
40	1i	986	0	990	34	0
40	2i	966	0	953	51	0
41	1j	719	0	672	26	0
41	2j	710	0	661	30	0
42	1k	834	0	838	20	0
42	2k	833	0	836	11	0
43	1l	932	0	981	14	0
43	2l	932	0	981	18	0
44	1m	914	0	954	33	0
44	2m	895	0	920	45	0
45	1n	492	0	529	19	0
45	2n	492	0	529	17	0
46	1o	728	0	760	18	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
46	2o	728	0	760	20	0
47	1p	681	0	697	28	0
47	2p	677	0	686	21	0
48	1q	823	0	891	18	0
48	2q	823	0	891	18	0
49	1r	555	0	618	9	0
49	2r	555	0	618	12	0
50	1s	648	0	658	20	0
50	2s	645	0	635	39	0
51	1t	732	0	809	24	0
51	2t	733	0	795	17	0
52	1u	199	0	208	7	0
52	2u	199	0	208	7	0
53	1y	764	0	786	17	0
53	2y	749	0	757	18	0
54	10	8	0	0	0	0
54	11	5	0	0	0	0
54	13	3	0	0	0	0
54	14	1	0	0	0	0
54	15	8	0	0	0	0
54	17	6	0	0	0	0
54	18	2	0	0	0	0
54	19	2	0	0	0	0
54	1A	1040	0	0	0	0
54	1B	29	0	0	0	0
54	1D	18	0	0	0	0
54	1E	8	0	0	0	0
54	1F	18	0	0	0	0
54	1G	4	0	0	0	0
54	1H	2	0	0	0	0
54	1N	4	0	0	0	0
54	1O	1	0	0	0	0
54	1P	5	0	0	0	0
54	1Q	5	0	0	0	0
54	1R	5	0	0	0	0
54	1T	5	0	0	0	0
54	1U	7	0	0	0	0
54	1V	6	0	0	0	0
54	1W	3	0	0	0	0
54	1Y	1	0	0	0	0
54	1Z	1	0	0	0	0
54	1a	279	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
54	1b	1	0	0	0	0
54	1d	5	0	0	0	0
54	1e	3	0	0	0	0
54	1f	2	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	1k	1	0	0	0	0
54	1l	2	0	0	0	0
54	1m	2	0	0	0	0
54	1n	2	0	0	0	0
54	1o	1	0	0	0	0
54	1t	1	0	0	0	0
54	1y	3	0	0	0	0
54	20	1	0	0	0	0
54	21	2	0	0	0	0
54	23	1	0	0	0	0
54	25	3	0	0	0	0
54	27	2	0	0	0	0
54	28	2	0	0	0	0
54	2A	730	0	0	0	0
54	2B	18	0	0	0	0
54	2D	13	0	0	0	0
54	2E	6	0	0	0	0
54	2F	4	0	0	0	0
54	2G	2	0	0	0	0
54	2I	1	0	0	0	0
54	2O	2	0	0	0	0
54	2P	1	0	0	0	0
54	2Q	1	0	0	0	0
54	2R	3	0	0	0	0
54	2T	3	0	0	0	0
54	2U	1	0	0	0	0
54	2V	2	0	0	0	0
54	2W	2	0	0	0	0
54	2X	1	0	0	0	0
54	2Y	1	0	0	0	0
54	2a	190	0	0	0	0
54	2e	2	0	0	0	0
54	2f	1	0	0	0	0
54	2j	1	0	0	0	0
54	2k	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
54	2n	1	0	0	0	0
54	2r	2	0	0	0	0
54	2t	1	0	0	0	0
54	2y	1	0	0	0	0
55	1A	36	0	29	1	0
55	2A	36	0	29	1	0
56	1A	51	0	67	0	0
56	2A	51	0	67	1	0
57	18	8	0	14	3	0
57	1A	8	0	14	1	0
57	1T	8	0	14	0	0
57	1a	8	0	13	6	0
57	2A	16	0	28	0	0
57	2B	8	0	14	0	0
58	1B	12	0	12	0	0
58	1F	12	0	12	1	0
59	14	1	0	0	0	0
59	15	1	0	0	0	0
59	16	1	0	0	0	0
59	19	1	0	0	0	0
59	1Y	1	0	0	0	0
59	1n	1	0	0	0	0
59	24	1	0	0	0	0
59	25	1	0	0	0	0
59	26	1	0	0	0	0
59	29	1	0	0	0	0
59	2Y	1	0	0	0	0
59	2n	1	0	0	0	0
60	1d	8	0	0	0	0
60	2d	8	0	0	1	0
61	10	21	0	0	1	0
61	11	28	0	0	1	0
61	12	14	0	0	2	0
61	13	22	0	0	1	0
61	14	4	0	0	0	0
61	15	25	0	0	0	0
61	16	21	0	0	0	0
61	17	13	0	0	0	0
61	18	23	0	0	1	0
61	19	2	0	0	0	0
61	1A	3898	0	0	87	0
61	1B	94	0	0	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
61	1D	103	0	0	2	0
61	1E	68	0	0	1	0
61	1F	64	0	0	0	0
61	1G	16	0	0	0	0
61	1H	15	0	0	0	0
61	1I	5	0	0	0	0
61	1N	45	0	0	1	0
61	1O	22	0	0	1	0
61	1P	56	0	0	3	0
61	1Q	37	0	0	1	0
61	1R	29	0	0	0	0
61	1S	12	0	0	2	0
61	1T	37	0	0	3	0
61	1U	41	0	0	4	0
61	1V	34	0	0	1	0
61	1W	27	0	0	1	0
61	1X	27	0	0	1	0
61	1Y	16	0	0	1	0
61	1Z	5	0	0	0	0
61	1a	447	0	0	18	0
61	1b	1	0	0	0	0
61	1c	2	0	0	0	0
61	1d	9	0	0	2	0
61	1e	5	0	0	1	0
61	1f	1	0	0	0	0
61	1h	1	0	0	0	0
61	1j	1	0	0	0	0
61	1l	3	0	0	1	0
61	1o	2	0	0	0	0
61	1p	2	0	0	0	0
61	1y	1	0	0	0	0
61	20	5	0	0	0	0
61	21	15	0	0	0	0
61	22	1	0	0	1	0
61	23	2	0	0	0	0
61	25	7	0	0	1	0
61	26	2	0	0	0	0
61	27	8	0	0	0	0
61	28	9	0	0	1	0
61	2A	1941	0	0	97	0
61	2B	45	0	0	13	0
61	2D	45	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
61	2E	25	0	0	1	0
61	2F	15	0	0	0	0
61	2G	2	0	0	0	0
61	2H	1	0	0	0	0
61	2I	1	0	0	0	0
61	2N	3	0	0	1	0
61	2O	10	0	0	0	0
61	2P	19	0	0	1	0
61	2Q	13	0	0	0	0
61	2R	17	0	0	2	0
61	2T	6	0	0	0	0
61	2U	7	0	0	0	0
61	2V	4	0	0	1	0
61	2W	20	0	0	0	0
61	2X	7	0	0	0	0
61	2Y	2	0	0	0	0
61	2Z	7	0	0	0	0
61	2a	266	0	0	18	0
61	2d	4	0	0	0	0
61	2e	1	0	0	0	0
61	2l	1	0	0	0	0
61	2o	2	0	0	0	0
61	2q	1	0	0	0	0
61	2r	3	0	0	0	0
61	2u	1	0	0	0	0
All	All	296967	0	194709	4218	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 9.

The worst 5 of 4218 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1A:1082:U:H3	1:1A:1086:A:N6	1.38	1.21
1:1A:1082:U:O4	1:1A:1086:A:N1	1.98	0.95
1:1A:1798:U:H5'	3:1D:259:THR:HG22	1.48	0.95
10:2O:48:PRO:HB3	32:2a:1422:G:H5''	1.49	0.94
1:2A:2100:G:H1	1:2A:2189:U:H3	1.11	0.94

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%)	258 (94%)	14 (5%)	1 (0%)	30	49
3	2D	273/276 (99%)	257 (94%)	15 (6%)	1 (0%)	30	49
4	1E	202/206 (98%)	191 (95%)	9 (4%)	2 (1%)	12	24
4	2E	202/206 (98%)	192 (95%)	8 (4%)	2 (1%)	12	24
5	1F	201/210 (96%)	197 (98%)	3 (2%)	1 (0%)	24	43
5	2F	201/210 (96%)	190 (94%)	10 (5%)	1 (0%)	24	43
6	1G	179/182 (98%)	163 (91%)	12 (7%)	4 (2%)	5	9
6	2G	179/182 (98%)	149 (83%)	26 (14%)	4 (2%)	5	9
7	1H	172/180 (96%)	161 (94%)	10 (6%)	1 (1%)	21	38
7	2H	171/180 (95%)	148 (86%)	23 (14%)	0	100	100
8	1I	145/148 (98%)	128 (88%)	16 (11%)	1 (1%)	18	34
8	2I	144/148 (97%)	130 (90%)	13 (9%)	1 (1%)	18	34
9	1N	138/140 (99%)	133 (96%)	5 (4%)	0	100	100
9	2N	138/140 (99%)	134 (97%)	4 (3%)	0	100	100
10	1O	120/122 (98%)	113 (94%)	6 (5%)	1 (1%)	16	31
10	2O	120/122 (98%)	112 (93%)	7 (6%)	1 (1%)	16	31
11	1P	147/150 (98%)	141 (96%)	6 (4%)	0	100	100
11	2P	147/150 (98%)	140 (95%)	6 (4%)	1 (1%)	18	34
12	1Q	139/141 (99%)	134 (96%)	4 (3%)	1 (1%)	18	34
12	2Q	139/141 (99%)	130 (94%)	9 (6%)	0	100	100
13	1R	116/118 (98%)	114 (98%)	2 (2%)	0	100	100
13	2R	116/118 (98%)	113 (97%)	3 (3%)	0	100	100
14	1S	108/112 (96%)	102 (94%)	5 (5%)	1 (1%)	14	27
14	2S	108/112 (96%)	96 (89%)	11 (10%)	1 (1%)	14	27
15	1T	129/146 (88%)	120 (93%)	8 (6%)	1 (1%)	16	31

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
15	2T	129/146 (88%)	122 (95%)	7 (5%)	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%)	95 (96%)	2 (2%)	2 (2%)	6	10
17	2V	99/101 (98%)	95 (96%)	3 (3%)	1 (1%)	12	24
18	1W	110/113 (97%)	110 (100%)	0	0	100	100
18	2W	110/113 (97%)	108 (98%)	2 (2%)	0	100	100
19	1X	93/96 (97%)	90 (97%)	2 (2%)	1 (1%)	11	22
19	2X	93/96 (97%)	87 (94%)	5 (5%)	1 (1%)	11	22
20	1Y	105/110 (96%)	95 (90%)	10 (10%)	0	100	100
20	2Y	105/110 (96%)	99 (94%)	6 (6%)	0	100	100
21	1Z	201/206 (98%)	186 (92%)	14 (7%)	1 (0%)	24	43
21	2Z	199/206 (97%)	177 (89%)	20 (10%)	2 (1%)	12	24
22	10	75/85 (88%)	71 (95%)	4 (5%)	0	100	100
22	20	75/85 (88%)	71 (95%)	4 (5%)	0	100	100
23	11	95/98 (97%)	93 (98%)	1 (1%)	1 (1%)	11	22
23	21	95/98 (97%)	93 (98%)	1 (1%)	1 (1%)	11	22
24	12	68/72 (94%)	67 (98%)	1 (2%)	0	100	100
24	22	68/72 (94%)	64 (94%)	4 (6%)	0	100	100
25	13	57/60 (95%)	56 (98%)	1 (2%)	0	100	100
25	23	57/60 (95%)	54 (95%)	3 (5%)	0	100	100
26	14	67/71 (94%)	53 (79%)	10 (15%)	4 (6%)	1	1
26	24	67/71 (94%)	45 (67%)	15 (22%)	7 (10%)	0	0
27	15	57/60 (95%)	57 (100%)	0	0	100	100
27	25	57/60 (95%)	54 (95%)	2 (4%)	1 (2%)	6	12
28	16	51/54 (94%)	49 (96%)	2 (4%)	0	100	100
28	26	51/54 (94%)	46 (90%)	5 (10%)	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%)	62 (100%)	0	0	100	100
30	28	62/65 (95%)	61 (98%)	1 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
31	19	35/37 (95%)	35 (100%)	0	0	100	100
31	29	35/37 (95%)	33 (94%)	2 (6%)	0	100	100
33	1b	229/256 (90%)	193 (84%)	28 (12%)	8 (4%)	3	4
33	2b	229/256 (90%)	191 (83%)	32 (14%)	6 (3%)	4	7
34	1c	204/239 (85%)	188 (92%)	15 (7%)	1 (0%)	24	43
34	2c	204/239 (85%)	176 (86%)	26 (13%)	2 (1%)	12	24
35	1d	206/209 (99%)	188 (91%)	17 (8%)	1 (0%)	24	43
35	2d	206/209 (99%)	197 (96%)	9 (4%)	0	100	100
36	1e	146/162 (90%)	137 (94%)	9 (6%)	0	100	100
36	2e	146/162 (90%)	138 (94%)	8 (6%)	0	100	100
37	1f	98/101 (97%)	93 (95%)	4 (4%)	1 (1%)	12	24
37	2f	98/101 (97%)	93 (95%)	5 (5%)	0	100	100
38	1g	153/156 (98%)	148 (97%)	4 (3%)	1 (1%)	18	34
38	2g	153/156 (98%)	142 (93%)	9 (6%)	2 (1%)	9	18
39	1h	135/138 (98%)	129 (96%)	6 (4%)	0	100	100
39	2h	135/138 (98%)	124 (92%)	10 (7%)	1 (1%)	18	34
40	1i	125/128 (98%)	113 (90%)	11 (9%)	1 (1%)	16	31
40	2i	124/128 (97%)	107 (86%)	14 (11%)	3 (2%)	4	8
41	1j	95/105 (90%)	78 (82%)	13 (14%)	4 (4%)	2	2
41	2j	94/105 (90%)	80 (85%)	10 (11%)	4 (4%)	2	2
42	1k	112/129 (87%)	104 (93%)	8 (7%)	0	100	100
42	2k	112/129 (87%)	100 (89%)	11 (10%)	1 (1%)	14	27
43	1l	119/132 (90%)	115 (97%)	4 (3%)	0	100	100
43	2l	119/132 (90%)	112 (94%)	7 (6%)	0	100	100
44	1m	114/126 (90%)	103 (90%)	7 (6%)	4 (4%)	3	4
44	2m	112/126 (89%)	100 (89%)	8 (7%)	4 (4%)	2	3
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%)	83 (96%)	3 (4%)	0	100	100
46	2o	86/89 (97%)	79 (92%)	6 (7%)	1 (1%)	10	20
47	1p	80/88 (91%)	70 (88%)	9 (11%)	1 (1%)	9	18

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
47	2p	80/88 (91%)	69 (86%)	10 (12%)	1 (1%)	9	18
48	1q	97/105 (92%)	87 (90%)	9 (9%)	1 (1%)	12	24
48	2q	97/105 (92%)	89 (92%)	7 (7%)	1 (1%)	12	24
49	1r	66/88 (75%)	63 (96%)	3 (4%)	0	100	100
49	2r	66/88 (75%)	64 (97%)	2 (3%)	0	100	100
50	1s	81/93 (87%)	69 (85%)	10 (12%)	2 (2%)	4	7
50	2s	81/93 (87%)	68 (84%)	11 (14%)	2 (2%)	4	7
51	1t	94/106 (89%)	87 (93%)	4 (4%)	3 (3%)	3	4
51	2t	96/106 (91%)	88 (92%)	5 (5%)	3 (3%)	3	5
52	1u	21/27 (78%)	21 (100%)	0	0	100	100
52	2u	21/27 (78%)	16 (76%)	4 (19%)	1 (5%)	2	2
53	1y	95/113 (84%)	95 (100%)	0	0	100	100
53	2y	94/113 (83%)	90 (96%)	4 (4%)	0	100	100
All	All	11629/12354 (94%)	10793 (93%)	728 (6%)	108 (1%)	14	27

5 of 108 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	1E	71	GLY
5	1F	130	ALA
6	1G	47	LYS
6	1G	50	ALA
26	14	49	PHE

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%)	195 (91%)	19 (9%)	9	20
3	2D	215/218 (99%)	199 (93%)	16 (7%)	13	27
4	1E	164/166 (99%)	154 (94%)	10 (6%)	17	35

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	2E	164/166 (99%)	153 (93%)	11 (7%)	15	31
5	1F	160/166 (96%)	144 (90%)	16 (10%)	7	15
5	2F	159/166 (96%)	140 (88%)	19 (12%)	5	11
6	1G	144/156 (92%)	132 (92%)	12 (8%)	10	22
6	2G	142/156 (91%)	126 (89%)	16 (11%)	5	12
7	1H	144/148 (97%)	131 (91%)	13 (9%)	9	19
7	2H	143/148 (97%)	129 (90%)	14 (10%)	7	16
8	1I	111/124 (90%)	98 (88%)	13 (12%)	5	11
8	2I	108/124 (87%)	98 (91%)	10 (9%)	8	18
9	1N	119/119 (100%)	107 (90%)	12 (10%)	7	15
9	2N	118/119 (99%)	107 (91%)	11 (9%)	8	18
10	1O	100/100 (100%)	96 (96%)	4 (4%)	28	54
10	2O	100/100 (100%)	97 (97%)	3 (3%)	36	64
11	1P	115/116 (99%)	108 (94%)	7 (6%)	17	35
11	2P	115/116 (99%)	106 (92%)	9 (8%)	11	24
12	1Q	111/111 (100%)	105 (95%)	6 (5%)	20	41
12	2Q	111/111 (100%)	98 (88%)	13 (12%)	5	11
13	1R	101/101 (100%)	92 (91%)	9 (9%)	9	20
13	2R	101/101 (100%)	95 (94%)	6 (6%)	18	37
14	1S	87/88 (99%)	79 (91%)	8 (9%)	8	19
14	2S	85/88 (97%)	75 (88%)	10 (12%)	5	11
15	1T	115/127 (91%)	106 (92%)	9 (8%)	11	24
15	2T	113/127 (89%)	106 (94%)	7 (6%)	16	34
16	1U	93/94 (99%)	89 (96%)	4 (4%)	26	51
16	2U	93/94 (99%)	87 (94%)	6 (6%)	15	32
17	1V	81/82 (99%)	75 (93%)	6 (7%)	13	27
17	2V	80/82 (98%)	73 (91%)	7 (9%)	9	20
18	1W	90/92 (98%)	83 (92%)	7 (8%)	11	24
18	2W	90/92 (98%)	80 (89%)	10 (11%)	6	12
19	1X	77/78 (99%)	72 (94%)	5 (6%)	15	32
19	2X	77/78 (99%)	74 (96%)	3 (4%)	28	55

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
20	1Y	86/91 (94%)	80 (93%)	6 (7%)	14	29
20	2Y	86/91 (94%)	75 (87%)	11 (13%)	4	9
21	1Z	169/179 (94%)	151 (89%)	18 (11%)	6	13
21	2Z	165/179 (92%)	152 (92%)	13 (8%)	11	24
22	10	61/67 (91%)	59 (97%)	2 (3%)	33	61
22	20	61/67 (91%)	57 (93%)	4 (7%)	15	32
23	11	79/83 (95%)	73 (92%)	6 (8%)	12	26
23	21	81/83 (98%)	75 (93%)	6 (7%)	13	27
24	12	65/67 (97%)	63 (97%)	2 (3%)	35	62
24	22	66/67 (98%)	56 (85%)	10 (15%)	3	5
25	13	51/52 (98%)	46 (90%)	5 (10%)	7	16
25	23	50/52 (96%)	45 (90%)	5 (10%)	7	15
26	14	58/63 (92%)	52 (90%)	6 (10%)	7	14
26	24	54/63 (86%)	45 (83%)	9 (17%)	2	4
27	15	51/52 (98%)	45 (88%)	6 (12%)	5	11
27	25	50/52 (96%)	47 (94%)	3 (6%)	17	36
28	16	51/52 (98%)	43 (84%)	8 (16%)	2	5
28	26	50/52 (96%)	44 (88%)	6 (12%)	5	10
29	17	41/42 (98%)	38 (93%)	3 (7%)	13	27
29	27	41/42 (98%)	37 (90%)	4 (10%)	7	16
30	18	54/55 (98%)	52 (96%)	2 (4%)	30	57
30	28	54/55 (98%)	52 (96%)	2 (4%)	30	57
31	19	34/34 (100%)	33 (97%)	1 (3%)	37	65
31	29	34/34 (100%)	32 (94%)	2 (6%)	18	37
33	1b	191/220 (87%)	169 (88%)	22 (12%)	5	11
33	2b	187/220 (85%)	162 (87%)	25 (13%)	4	8
34	1c	144/188 (77%)	137 (95%)	7 (5%)	22	45
34	2c	140/188 (74%)	126 (90%)	14 (10%)	7	15
35	1d	171/181 (94%)	157 (92%)	14 (8%)	10	23
35	2d	172/181 (95%)	151 (88%)	21 (12%)	5	10
36	1e	114/123 (93%)	108 (95%)	6 (5%)	20	42

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
36	2e	114/123 (93%)	103 (90%)	11 (10%)	8	17
37	1f	85/90 (94%)	77 (91%)	8 (9%)	8	18
37	2f	85/90 (94%)	77 (91%)	8 (9%)	8	18
38	1g	120/127 (94%)	115 (96%)	5 (4%)	26	52
38	2g	119/127 (94%)	107 (90%)	12 (10%)	7	15
39	1h	116/119 (98%)	106 (91%)	10 (9%)	10	21
39	2h	114/119 (96%)	102 (90%)	12 (10%)	6	14
40	1i	91/99 (92%)	85 (93%)	6 (7%)	15	32
40	2i	88/99 (89%)	78 (89%)	10 (11%)	5	12
41	1j	68/92 (74%)	59 (87%)	9 (13%)	4	8
41	2j	68/92 (74%)	56 (82%)	12 (18%)	2	3
42	1k	83/99 (84%)	77 (93%)	6 (7%)	13	28
42	2k	83/99 (84%)	77 (93%)	6 (7%)	13	28
43	1l	96/108 (89%)	95 (99%)	1 (1%)	68	86
43	2l	96/108 (89%)	89 (93%)	7 (7%)	13	27
44	1m	90/101 (89%)	84 (93%)	6 (7%)	15	31
44	2m	87/101 (86%)	77 (88%)	10 (12%)	5	11
45	1n	49/50 (98%)	44 (90%)	5 (10%)	7	15
45	2n	49/50 (98%)	43 (88%)	6 (12%)	5	10
46	1o	78/80 (98%)	73 (94%)	5 (6%)	16	33
46	2o	78/80 (98%)	74 (95%)	4 (5%)	21	43
47	1p	69/74 (93%)	57 (83%)	12 (17%)	2	3
47	2p	68/74 (92%)	60 (88%)	8 (12%)	5	11
48	1q	94/97 (97%)	90 (96%)	4 (4%)	26	51
48	2q	94/97 (97%)	87 (93%)	7 (7%)	13	27
49	1r	59/77 (77%)	57 (97%)	2 (3%)	32	60
49	2r	59/77 (77%)	55 (93%)	4 (7%)	14	31
50	1s	68/80 (85%)	63 (93%)	5 (7%)	13	27
50	2s	67/80 (84%)	58 (87%)	9 (13%)	4	8
51	1t	71/82 (87%)	65 (92%)	6 (8%)	10	22
51	2t	70/82 (85%)	62 (89%)	8 (11%)	5	12

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
52	1u	18/22 (82%)	17 (94%)	1 (6%)	19	39
52	2u	18/22 (82%)	18 (100%)	0	100	100
53	1y	82/98 (84%)	81 (99%)	1 (1%)	63	83
53	2y	79/98 (81%)	73 (92%)	6 (8%)	12	26
All	All	9524/10260 (93%)	8712 (92%)	812 (8%)	10	22

5 of 812 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
10	2O	69	ILE
24	22	25	VAL
51	2t	41	ILE
12	2Q	16	ARG
9	2N	138	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 139 such sidechains are listed below:

Mol	Chain	Res	Type
37	2f	94	GLN
38	2g	86	GLN
47	2p	13	HIS
38	1g	148	ASN
38	1g	64	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	1A	2865/2915 (98%)	403 (14%)	35 (1%)
1	2A	2858/2915 (98%)	463 (16%)	37 (1%)
2	1B	119/121 (98%)	13 (10%)	0
2	2B	119/121 (98%)	17 (14%)	0
32	1a	1497/1521 (98%)	246 (16%)	0
32	2a	1501/1521 (98%)	259 (17%)	0
All	All	8959/9114 (98%)	1401 (15%)	72 (0%)

5 of 1401 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	1A	12	U
1	1A	13	A
1	1A	15	G
1	1A	33	U
1	1A	34	C

5 of 72 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	2A	1491	G
1	2A	2756	U
1	2A	1992	G
1	2A	2406	U
1	1A	1762	A

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

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	PSU	1A	1911	1	18,21,22	1.36	2 (11%)	21,30,33	2.03	4 (19%)
1	2MA	1A	2503	1,54	22,25,26	1.48	6 (27%)	32,37,40	2.42	9 (28%)
1	OMG	1A	2251	1,54	23,26,27	1.23	3 (13%)	32,38,41	2.05	7 (21%)
1	5MU	2A	1939	1	19,22,23	1.50	6 (31%)	27,32,35	2.28	8 (29%)
32	4OC	2a	1402	32	20,23,24	0.76	0	25,32,35	0.93	1 (4%)
1	5MC	1A	1962	1,54	19,22,23	1.74	3 (15%)	26,32,35	1.19	4 (15%)
32	PSU	1a	516	32,54	18,21,22	1.37	2 (11%)	21,30,33	2.00	4 (19%)
32	M2G	2a	966	32	24,27,28	1.33	4 (16%)	33,40,43	1.84	5 (15%)
1	5MU	1A	1939	1,54	19,22,23	1.36	4 (21%)	27,32,35	2.27	6 (22%)
32	UR3	2a	1498	32	19,22,23	1.04	2 (10%)	26,32,35	1.70	3 (11%)
1	5MC	1A	1942	1,54	19,22,23	1.41	3 (15%)	26,32,35	1.10	2 (7%)
32	2MG	2a	1207	32	23,26,27	1.28	4 (17%)	33,38,41	2.06	5 (15%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
32	MA6	2a	1519	32	23,26,27	0.43	0	33,38,41	2.15	9 (27%)
1	OMG	2A	2251	1,54	23,26,27	1.20	3 (13%)	32,38,41	2.03	6 (18%)
32	MA6	1a	1518	32	23,26,27	0.39	0	33,38,41	1.89	8 (24%)
1	5MC	2A	1962	1	19,22,23	1.61	3 (15%)	26,32,35	1.12	2 (7%)
1	PSU	1A	1917	1,54	18,21,22	1.40	2 (11%)	21,30,33	2.02	3 (14%)
32	5MC	2a	1404	32	19,22,23	1.72	3 (15%)	26,32,35	1.17	3 (11%)
43	0TD	2l	92	43	8,9,10	4.34	1 (12%)	6,11,13	1.92	3 (50%)
1	5MU	1A	1915	1,54	19,22,23	1.49	5 (26%)	27,32,35	2.25	9 (33%)
32	G7M	1a	527	32,54	23,26,27	2.32	5 (21%)	34,39,42	2.95	10 (29%)
1	2MU	1A	2552	1,54	19,22,24	1.26	3 (15%)	25,31,36	1.75	6 (24%)
32	5MC	2a	1400	32	19,22,23	1.64	3 (15%)	26,32,35	1.20	2 (7%)
1	PSU	2A	1911	1	18,21,22	1.38	2 (11%)	21,30,33	2.07	4 (19%)
1	2MU	2A	2552	1,54	19,22,24	1.26	3 (15%)	25,31,36	1.88	6 (24%)
32	5MC	2a	967	32	19,22,23	1.87	2 (10%)	26,32,35	1.10	2 (7%)
1	PSU	2A	1917	1	18,21,22	1.37	2 (11%)	21,30,33	2.07	3 (14%)
32	PSU	2a	516	32,54	18,21,22	1.36	3 (16%)	21,30,33	2.01	5 (23%)
1	PSU	1A	2605	1	18,21,22	1.46	3 (16%)	21,30,33	2.16	5 (23%)
1	2MA	2A	2503	1,54	22,25,26	1.45	4 (18%)	32,37,40	2.35	8 (25%)
32	MA6	1a	1519	32	23,26,27	0.42	0	33,38,41	1.98	9 (27%)
32	MA6	2a	1518	32	23,26,27	0.40	0	33,38,41	2.02	9 (27%)
32	4OC	1a	1402	32	20,23,24	0.72	0	25,32,35	0.96	1 (4%)
43	0TD	1l	92	43	8,9,10	4.65	1 (12%)	6,11,13	2.13	3 (50%)
1	OMC	1A	1920	1,54	19,22,23	0.80	0	25,31,34	0.87	1 (4%)
32	UR3	1a	1498	32	19,22,23	0.92	0	26,32,35	1.82	3 (11%)
32	5MC	2a	1407	32	19,22,23	1.64	3 (15%)	26,32,35	1.19	3 (11%)
32	G7M	2a	527	32,54	23,26,27	2.36	5 (21%)	34,39,42	3.04	10 (29%)
32	5MC	1a	967	32	19,22,23	1.52	3 (15%)	26,32,35	1.03	2 (7%)
1	OMC	2A	1920	1	19,22,23	0.78	0	25,31,34	0.95	1 (4%)
32	5MC	1a	1400	32	19,22,23	1.73	3 (15%)	26,32,35	1.22	2 (7%)
1	5MC	2A	1942	1	19,22,23	1.80	3 (15%)	26,32,35	1.25	3 (11%)
32	2MG	1a	1207	32	23,26,27	1.22	2 (8%)	33,38,41	2.23	8 (24%)
1	PSU	2A	2605	1	18,21,22	1.42	3 (16%)	21,30,33	2.14	5 (23%)
32	M2G	1a	966	32	24,27,28	1.29	5 (20%)	33,40,43	1.81	6 (18%)
32	5MC	1a	1407	32	19,22,23	1.52	3 (15%)	26,32,35	1.20	3 (11%)
32	5MC	1a	1404	32	19,22,23	1.54	2 (10%)	26,32,35	1.04	2 (7%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	5MU	2A	1915	1	19,22,23	1.49	4 (21%)	27,32,35	2.24	9 (33%)

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	PSU	1A	1911	1	-	0/7/25/26	0/2/2/2
1	2MA	1A	2503	1,54	-	1/7/25/26	0/3/3/3
1	OMG	1A	2251	1,54	-	0/9/27/28	0/3/3/3
1	5MU	2A	1939	1	-	0/7/25/26	0/2/2/2
32	4OC	2a	1402	32	-	2/9/29/30	0/2/2/2
1	5MC	1A	1962	1,54	-	2/7/25/26	0/2/2/2
32	PSU	1a	516	32,54	-	0/7/25/26	0/2/2/2
32	M2G	2a	966	32	-	0/11/29/30	0/3/3/3
1	5MU	1A	1939	1,54	-	0/7/25/26	0/2/2/2
32	UR3	2a	1498	32	-	0/7/25/26	0/2/2/2
1	5MC	1A	1942	1,54	-	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	-	2/11/29/30	0/3/3/3
1	OMG	2A	2251	1,54	-	0/9/27/28	0/3/3/3
32	MA6	1a	1518	32	-	0/11/29/30	0/3/3/3
1	5MC	2A	1962	1	-	2/7/25/26	0/2/2/2
1	PSU	1A	1917	1,54	-	0/7/25/26	0/2/2/2
32	5MC	2a	1404	32	-	0/7/25/26	0/2/2/2
43	0TD	2l	92	43	-	1/7/12/14	-
1	5MU	1A	1915	1,54	-	2/7/25/26	0/2/2/2
32	G7M	1a	527	32,54	-	1/7/25/26	0/3/3/3
1	2MU	1A	2552	1,54	-	0/9/27/28	0/2/2/2
32	5MC	2a	1400	32	-	0/7/25/26	0/2/2/2
1	PSU	2A	1911	1	-	0/7/25/26	0/2/2/2
1	2MU	2A	2552	1,54	-	2/9/27/28	0/2/2/2
32	5MC	2a	967	32	-	0/7/25/26	0/2/2/2
1	PSU	2A	1917	1	-	0/7/25/26	0/2/2/2
32	PSU	2a	516	32,54	-	1/7/25/26	0/2/2/2
1	PSU	1A	2605	1	-	0/7/25/26	0/2/2/2
1	2MA	2A	2503	1,54	-	0/7/25/26	0/3/3/3
32	MA6	1a	1519	32	-	2/11/29/30	0/3/3/3
32	MA6	2a	1518	32	-	0/11/29/30	0/3/3/3
32	4OC	1a	1402	32	-	0/9/29/30	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
43	0TD	1l	92	43	-	3/7/12/14	-
1	OMC	1A	1920	1,54	-	1/9/27/28	0/2/2/2
32	UR3	1a	1498	32	-	0/7/25/26	0/2/2/2
32	5MC	2a	1407	32	-	0/7/25/26	0/2/2/2
32	G7M	2a	527	32,54	-	2/7/25/26	0/3/3/3
32	5MC	1a	967	32	-	0/7/25/26	0/2/2/2
1	OMC	2A	1920	1	-	2/9/27/28	0/2/2/2
32	5MC	1a	1400	32	-	0/7/25/26	0/2/2/2
1	5MC	2A	1942	1	-	0/7/25/26	0/2/2/2
32	2MG	1a	1207	32	-	0/9/27/28	0/3/3/3
1	PSU	2A	2605	1	-	0/7/25/26	0/2/2/2
32	M2G	1a	966	32	-	0/11/29/30	0/3/3/3
32	5MC	1a	1407	32	-	0/7/25/26	0/2/2/2
32	5MC	1a	1404	32	-	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 123 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
43	1l	92	0TD	CB-SB	-12.75	1.69	1.82
43	2l	92	0TD	CB-SB	-11.92	1.70	1.82
32	2a	527	G7M	C8-N7	7.55	1.45	1.33
32	1a	527	G7M	C8-N7	7.38	1.45	1.33
32	2a	967	5MC	C5-C4	7.00	1.49	1.44

The worst 5 of 232 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	2a	527	G7M	CN7-N7-C8	-8.36	112.13	124.79
1	1A	2503	2MA	C5-C4-N3	-8.28	118.46	127.18
1	2A	2503	2MA	C5-C4-N3	-8.12	118.63	127.18
32	1a	527	G7M	CN7-N7-C8	-8.08	112.55	124.79
32	1a	1498	UR3	C4-N3-C2	-7.34	118.67	124.58

There are no chirality outliers.

5 of 28 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	1A	1915	5MU	O4'-C1'-N1-C2
1	1A	1915	5MU	O4'-C1'-N1-C6
43	1l	92	0TD	O-C-CA-CB

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Mol	Chain	Res	Type	Atoms
43	1l	92	0TD	CG-CB-SB-CSB
1	2A	1915	5MU	O4'-C1'-N1-C2

There are no ring outliers.

19 monomers are involved in 25 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	2A	1939	5MU	1	0
32	2a	1402	4OC	1	0
32	2a	966	M2G	1	0
1	1A	1939	5MU	2	0
32	2a	1207	2MG	2	0
32	2a	1519	MA6	3	0
1	2A	2251	OMG	1	0
32	1a	1518	MA6	2	0
43	2l	92	0TD	3	0
1	1A	2552	2MU	1	0
32	2a	1400	5MC	1	0
32	2a	967	5MC	1	0
1	2A	1917	PSU	1	0
32	1a	1519	MA6	2	0
32	2a	1518	MA6	1	0
43	1l	92	0TD	1	0
1	1A	1920	OMC	1	0
1	2A	1920	OMC	1	0
32	1a	1400	5MC	2	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 2534 ligands modelled in this entry, 2519 are monoatomic - leaving 15 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the

expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
58	ARG	1F	319	-	10,11,11	0.73	1 (10%)	9,13,13	0.88	1 (11%)
57	MPD	1T	206	-	7,7,7	0.37	0	9,10,10	0.23	0
57	MPD	18	103	-	7,7,7	0.32	0	9,10,10	0.40	0
56	ERY	1A	4042	-	53,53,53	0.94	2 (3%)	82,82,82	1.31	10 (12%)
57	MPD	2A	3733	-	7,7,7	0.39	0	9,10,10	0.49	0
57	MPD	2A	3734	-	7,7,7	0.32	0	9,10,10	0.19	0
55	HGR	1A	4041	-	39,39,39	2.39	8 (20%)	48,58,58	1.82	13 (27%)
57	MPD	1A	4043	-	7,7,7	0.34	0	9,10,10	0.22	0
57	MPD	2B	219	-	7,7,7	0.33	0	9,10,10	0.19	0
58	ARG	1B	230	54	10,11,11	0.79	1 (10%)	9,13,13	0.96	1 (11%)
60	SF4	1d	306	35	0,12,12	-	-	-	-	-
56	ERY	2A	3732	-	53,53,53	0.96	2 (3%)	82,82,82	1.39	11 (13%)
57	MPD	1a	1880	32	7,7,7	0.45	0	9,10,10	0.58	0
60	SF4	2d	501	35	0,12,12	-	-	-	-	-
55	HGR	2A	3731	-	39,39,39	2.42	9 (23%)	48,58,58	1.68	13 (27%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
58	ARG	1F	319	-	-	3/11/11/11	-
57	MPD	1T	206	-	-	0/5/5/5	-
57	MPD	18	103	-	-	2/5/5/5	-
56	ERY	1A	4042	-	-	0/72/107/107	0/3/3/3
57	MPD	2A	3733	-	-	0/5/5/5	-
57	MPD	2A	3734	-	-	1/5/5/5	-
55	HGR	1A	4041	-	-	5/20/79/79	0/4/4/4
57	MPD	1A	4043	-	-	2/5/5/5	-
57	MPD	2B	219	-	-	1/5/5/5	-
58	ARG	1B	230	54	-	0/11/11/11	-
60	SF4	1d	306	35	-	-	0/6/5/5
56	ERY	2A	3732	-	-	4/72/107/107	0/3/3/3
57	MPD	1a	1880	32	-	5/5/5/5	-
60	SF4	2d	501	35	-	-	0/6/5/5
55	HGR	2A	3731	-	-	5/20/79/79	0/4/4/4

The worst 5 of 23 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
55	2A	3731	HGR	C12-C14	9.37	1.55	1.33
55	1A	4041	HGR	C12-C14	8.86	1.54	1.33
55	1A	4041	HGR	C5-C4	-5.62	1.39	1.49
55	2A	3731	HGR	C5-C4	-5.47	1.39	1.49
55	1A	4041	HGR	C5-C6	-5.24	1.39	1.50

The worst 5 of 49 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
55	2A	3731	HGR	C4-C5-C6	4.72	122.42	112.35
55	1A	4041	HGR	C4-C5-C6	4.56	122.08	112.35
56	2A	3732	ERY	O5-C16-C17	3.90	109.51	103.86
56	2A	3732	ERY	C13-O2-C1	-3.73	111.68	118.20
55	1A	4041	HGR	O9-C22-C18	-3.70	98.20	106.03

There are no chirality outliers.

5 of 28 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
56	2A	3732	ERY	C15-C16-O5-C20
56	2A	3732	ERY	C19-C16-O5-C20
57	18	103	MPD	C2-C3-C4-O4
57	18	103	MPD	C2-C3-C4-C5
57	2B	219	MPD	C2-C3-C4-O4

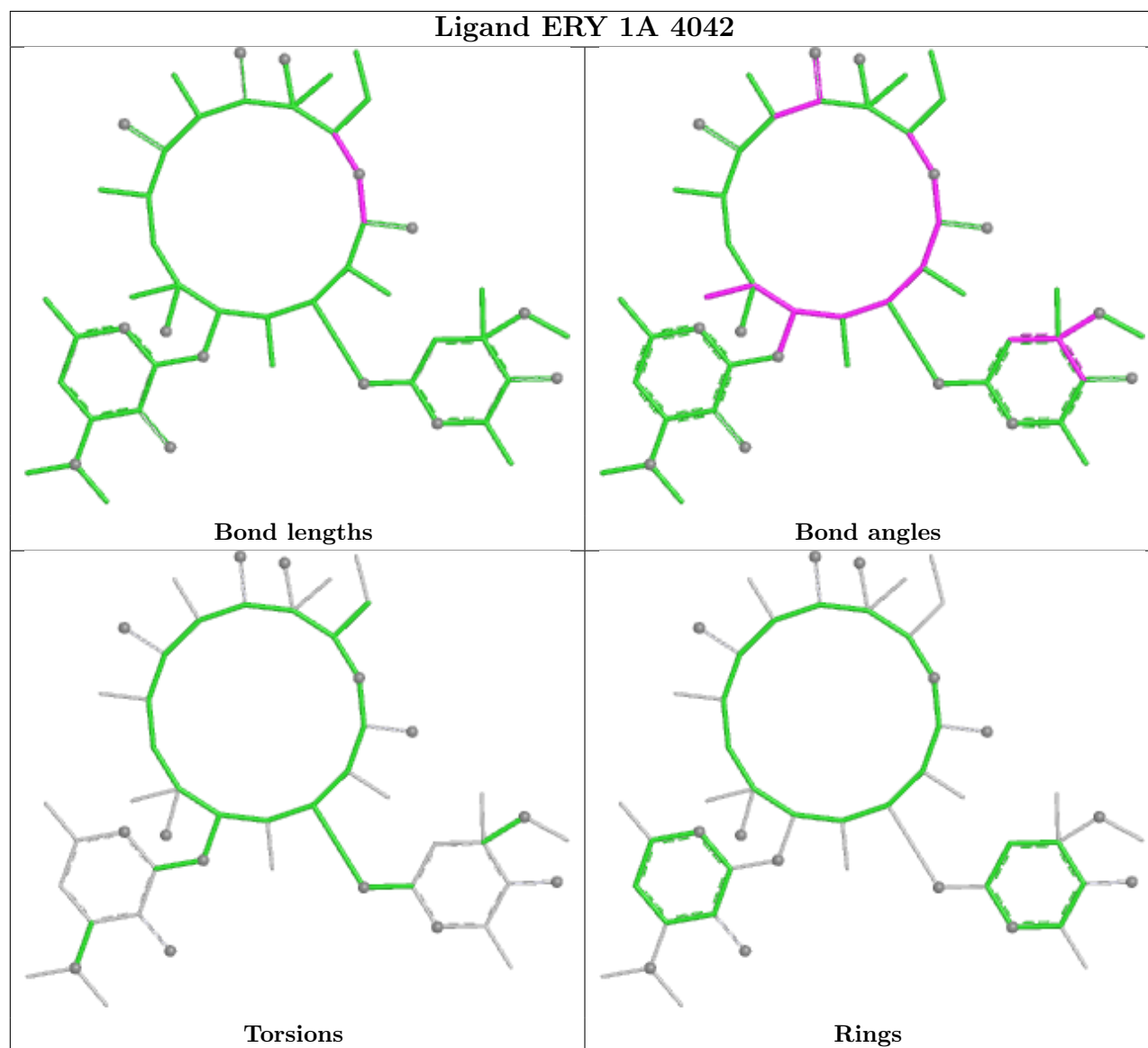
There are no ring outliers.

8 monomers are involved in 15 short contacts:

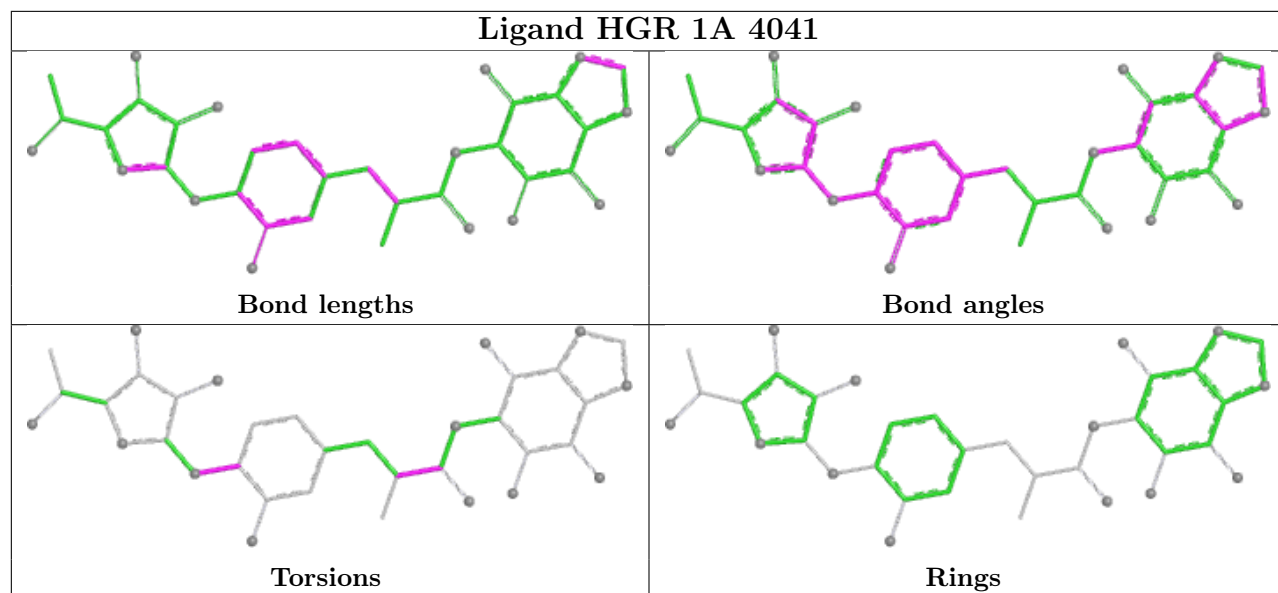
Mol	Chain	Res	Type	Clashes	Symm-Clashes
58	1F	319	ARG	1	0
57	18	103	MPD	3	0
55	1A	4041	HGR	1	0
57	1A	4043	MPD	1	0
56	2A	3732	ERY	1	0
57	1a	1880	MPD	6	0
60	2d	501	SF4	1	0
55	2A	3731	HGR	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will

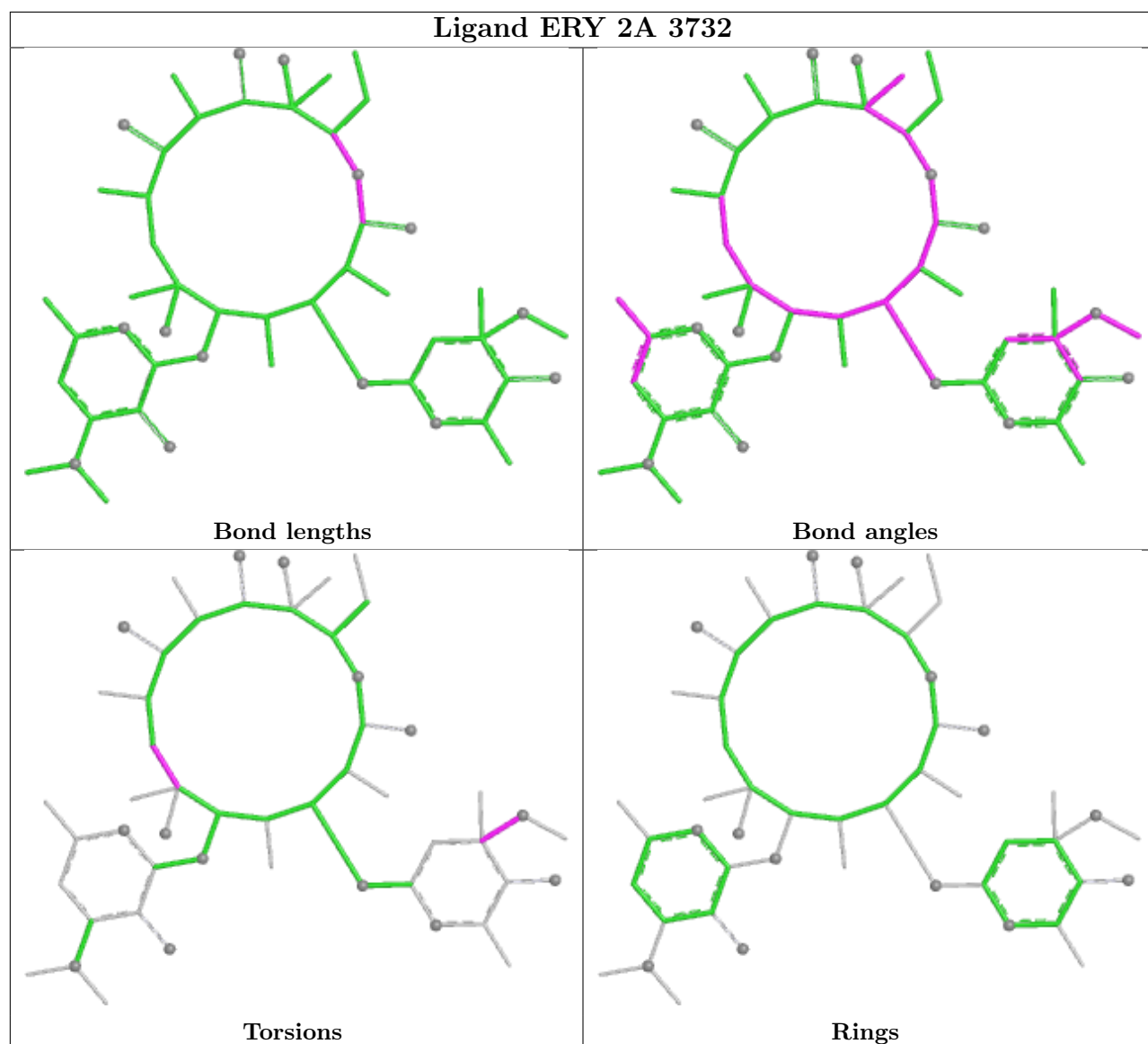
also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

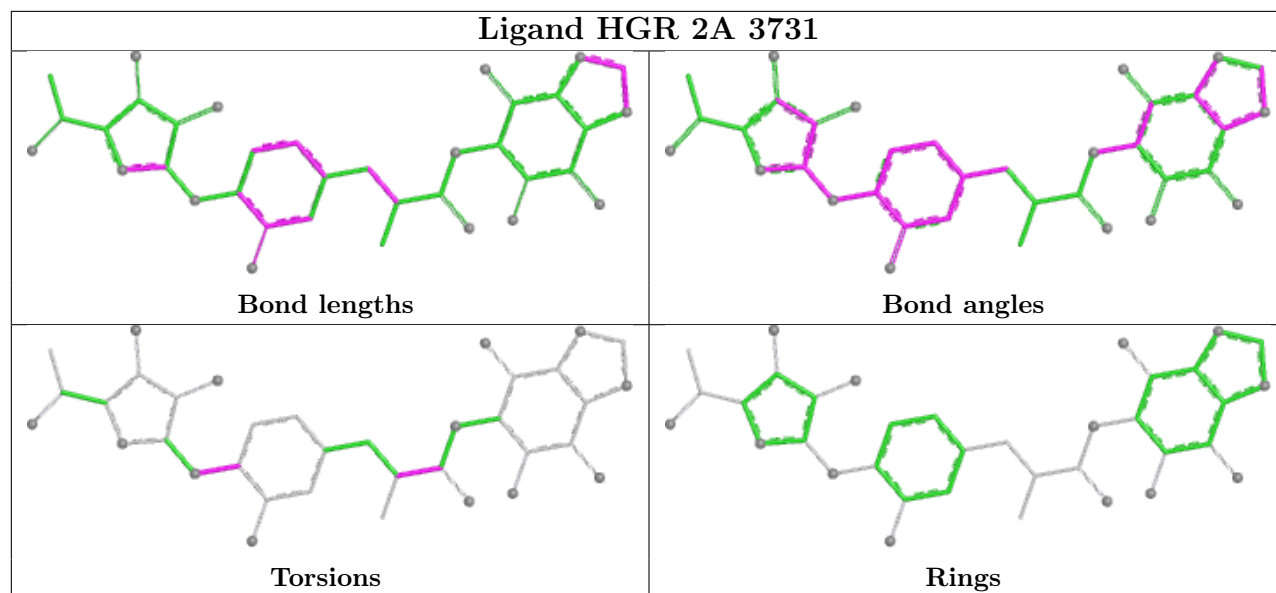


Ligand HGR 1A 4041



Ligand ERY 2A 3732





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%)	-0.51	90 (3%)	51	47	26, 43, 97, 110	0
1	2A	2856/2915 (97%)	-0.04	117 (4%)	41	37	39, 63, 100, 111	0
2	1B	120/121 (99%)	-0.36	1 (0%)	82	80	37, 55, 69, 84	0
2	2B	120/121 (99%)	0.98	6 (5%)	34	30	68, 88, 96, 98	0
3	1D	275/276 (99%)	-0.03	4 (1%)	72	68	27, 43, 56, 79	0
3	2D	275/276 (99%)	0.40	10 (3%)	46	41	36, 56, 68, 82	0
4	1E	204/206 (99%)	0.11	4 (1%)	65	61	26, 46, 64, 79	0
4	2E	204/206 (99%)	0.42	5 (2%)	58	54	38, 62, 75, 85	0
5	1F	203/210 (96%)	0.02	1 (0%)	87	85	24, 48, 72, 87	0
5	2F	203/210 (96%)	0.65	4 (1%)	65	61	41, 73, 83, 92	0
6	1G	181/182 (99%)	0.69	8 (4%)	39	34	52, 68, 81, 90	0
6	2G	181/182 (99%)	2.34	112 (61%)	0	0	81, 89, 94, 97	0
7	1H	174/180 (96%)	0.37	2 (1%)	78	75	43, 58, 70, 79	0
7	2H	173/180 (96%)	1.43	34 (19%)	3	2	74, 84, 90, 94	0
8	1I	147/148 (99%)	0.91	9 (6%)	27	23	48, 76, 85, 87	0
8	2I	146/148 (98%)	1.04	12 (8%)	17	15	58, 78, 87, 91	0
9	1N	140/140 (100%)	0.01	0	100	100	33, 44, 65, 80	0
9	2N	140/140 (100%)	0.80	5 (3%)	46	41	50, 69, 81, 84	0
10	1O	122/122 (100%)	0.14	1 (0%)	82	80	37, 45, 65, 68	0
10	2O	122/122 (100%)	0.44	2 (1%)	70	67	50, 60, 72, 78	0
11	1P	149/150 (99%)	0.05	1 (0%)	84	81	26, 50, 71, 83	0
11	2P	149/150 (99%)	0.53	4 (2%)	56	51	43, 71, 86, 90	0
12	1Q	141/141 (100%)	-0.06	0	100	100	33, 45, 59, 72	0
12	2Q	141/141 (100%)	0.95	9 (6%)	25	22	52, 71, 79, 87	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
13	1R	118/118 (100%)	-0.10	0 100 100	33, 42, 58, 65	0
13	2R	118/118 (100%)	0.23	0 100 100	45, 57, 67, 74	0
14	1S	110/112 (98%)	0.26	1 (0%) 81 78	45, 55, 66, 70	0
14	2S	110/112 (98%)	1.74	43 (39%) 1 0	72, 82, 86, 90	0
15	1T	131/146 (89%)	0.38	7 (5%) 32 28	40, 50, 72, 83	0
15	2T	131/146 (89%)	0.49	3 (2%) 61 57	52, 63, 79, 86	0
16	1U	116/118 (98%)	-0.17	1 (0%) 81 78	28, 38, 50, 69	0
16	2U	116/118 (98%)	0.53	0 100 100	47, 66, 78, 86	0
17	1V	101/101 (100%)	-0.06	1 (0%) 79 76	29, 46, 62, 72	0
17	2V	101/101 (100%)	0.82	3 (2%) 52 48	49, 76, 82, 89	0
18	1W	112/113 (99%)	-0.10	2 (1%) 67 64	31, 38, 58, 86	0
18	2W	112/113 (99%)	0.41	4 (3%) 46 41	46, 56, 74, 87	0
19	1X	95/96 (98%)	0.15	3 (3%) 50 46	32, 43, 64, 79	0
19	2X	95/96 (98%)	0.81	4 (4%) 40 36	55, 66, 79, 86	0
20	1Y	107/110 (97%)	0.42	3 (2%) 55 50	40, 54, 72, 82	0
20	2Y	107/110 (97%)	1.28	16 (14%) 5 4	65, 75, 83, 89	0
21	1Z	203/206 (98%)	0.50	9 (4%) 39 34	45, 62, 77, 87	0
21	2Z	201/206 (97%)	1.50	38 (18%) 3 2	73, 82, 88, 90	0
22	10	77/85 (90%)	0.05	2 (2%) 57 52	35, 43, 60, 68	0
22	20	77/85 (90%)	1.07	7 (9%) 15 13	59, 69, 78, 83	0
23	11	97/98 (98%)	0.27	1 (1%) 79 76	34, 49, 71, 84	0
23	21	97/98 (98%)	0.68	2 (2%) 63 59	47, 61, 79, 86	0
24	12	70/72 (97%)	0.31	2 (2%) 53 49	42, 55, 65, 84	0
24	22	70/72 (97%)	0.67	1 (1%) 73 70	67, 75, 82, 83	0
25	13	59/60 (98%)	-0.12	1 (1%) 69 65	30, 42, 63, 76	0
25	23	59/60 (98%)	0.60	3 (5%) 33 29	57, 67, 82, 93	0
26	14	69/71 (97%)	1.14	14 (20%) 3 2	61, 77, 92, 96	0
26	24	69/71 (97%)	2.35	46 (66%) 0 0	83, 93, 99, 100	0
27	15	59/60 (98%)	-0.21	0 100 100	28, 40, 58, 64	0
27	25	59/60 (98%)	0.25	1 (1%) 69 65	41, 56, 70, 75	0
28	16	53/54 (98%)	-0.09	0 100 100	39, 47, 61, 67	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
28	26	53/54 (98%)	0.67	2 (3%) 44 39	60, 67, 74, 79	0
29	17	48/49 (97%)	0.07	5 (10%) 11 10	28, 35, 59, 71	0
29	27	48/49 (97%)	0.38	4 (8%) 17 15	39, 48, 70, 78	0
30	18	64/65 (98%)	-0.16	1 (1%) 70 67	35, 40, 47, 59	0
30	28	64/65 (98%)	0.55	2 (3%) 51 47	54, 62, 68, 71	0
31	19	37/37 (100%)	0.05	0 100 100	37, 46, 61, 67	0
31	29	37/37 (100%)	1.08	4 (10%) 11 9	61, 72, 80, 82	0
32	1a	1488/1521 (97%)	0.13	29 (1%) 66 62	41, 73, 96, 110	0
32	2a	1492/1521 (98%)	0.49	56 (3%) 44 39	53, 81, 100, 110	0
33	1b	231/256 (90%)	1.34	48 (20%) 2 2	68, 82, 90, 94	0
33	2b	231/256 (90%)	1.65	65 (28%) 1 1	80, 88, 94, 97	0
34	1c	206/239 (86%)	0.98	18 (8%) 16 14	64, 76, 87, 91	0
34	2c	206/239 (86%)	1.59	54 (26%) 1 1	79, 88, 93, 95	0
35	1d	208/209 (99%)	1.07	23 (11%) 10 8	62, 76, 85, 88	0
35	2d	208/209 (99%)	1.19	18 (8%) 16 14	66, 76, 84, 87	0
36	1e	148/162 (91%)	0.58	4 (2%) 56 51	52, 70, 78, 91	0
36	2e	148/162 (91%)	1.17	19 (12%) 7 6	66, 78, 86, 93	0
37	1f	100/101 (99%)	0.70	2 (2%) 65 61	59, 70, 78, 82	0
37	2f	100/101 (99%)	0.79	3 (3%) 52 48	63, 74, 83, 86	0
38	1g	155/156 (99%)	0.61	4 (2%) 57 52	68, 76, 83, 89	0
38	2g	155/156 (99%)	1.56	41 (26%) 1 1	81, 86, 91, 95	0
39	1h	137/138 (99%)	0.80	6 (4%) 39 34	63, 71, 78, 83	0
39	2h	137/138 (99%)	1.07	9 (6%) 24 21	69, 79, 84, 88	0
40	1i	127/128 (99%)	1.32	20 (15%) 5 4	65, 82, 89, 91	0
40	2i	126/128 (98%)	2.12	65 (51%) 0 0	81, 90, 95, 96	0
41	1j	97/105 (92%)	1.60	28 (28%) 1 1	64, 83, 91, 93	0
41	2j	96/105 (91%)	1.96	46 (47%) 0 0	83, 90, 94, 98	0
42	1k	114/129 (88%)	0.68	6 (5%) 32 28	48, 68, 78, 83	0
42	2k	114/129 (88%)	1.24	16 (14%) 6 5	66, 78, 85, 87	0
43	1l	121/132 (91%)	0.74	7 (5%) 29 25	53, 64, 75, 81	0
43	2l	121/132 (91%)	0.85	9 (7%) 20 18	64, 73, 78, 85	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
44	1m	116/126 (92%)	0.93	10 (8%) 16 14	64, 78, 83, 88	0
44	2m	114/126 (90%)	1.83	41 (35%) 1 1	84, 89, 93, 95	0
45	1n	60/61 (98%)	0.85	2 (3%) 49 45	68, 75, 81, 83	0
45	2n	60/61 (98%)	2.05	27 (45%) 0 0	83, 88, 93, 95	0
46	1o	88/89 (98%)	0.72	3 (3%) 48 43	51, 69, 79, 84	0
46	2o	88/89 (98%)	0.92	6 (6%) 23 20	64, 77, 83, 89	0
47	1p	82/88 (93%)	1.33	14 (17%) 4 3	69, 77, 85, 89	0
47	2p	82/88 (93%)	1.25	12 (14%) 6 4	66, 75, 83, 91	0
48	1q	99/105 (94%)	0.95	5 (5%) 33 29	59, 72, 82, 84	0
48	2q	99/105 (94%)	0.96	7 (7%) 22 19	63, 75, 82, 85	0
49	1r	68/88 (77%)	0.60	0 100 100	59, 68, 80, 85	0
49	2r	68/88 (77%)	0.97	3 (4%) 39 34	70, 77, 84, 89	0
50	1s	83/93 (89%)	0.97	4 (4%) 35 31	70, 80, 86, 93	0
50	2s	83/93 (89%)	2.05	45 (54%) 0 0	82, 91, 95, 98	0
51	1t	96/106 (90%)	1.19	15 (15%) 5 4	68, 76, 85, 86	0
51	2t	98/106 (92%)	0.88	6 (6%) 27 23	65, 75, 85, 88	0
52	1u	23/27 (85%)	1.22	5 (21%) 2 2	70, 74, 79, 79	0
52	2u	23/27 (85%)	2.29	12 (52%) 0 0	84, 89, 91, 93	0
53	1y	97/113 (85%)	0.93	7 (7%) 21 19	57, 67, 79, 82	0
53	2y	96/113 (84%)	2.01	47 (48%) 0 0	76, 84, 90, 93	0
All	All	20766/21468 (96%)	0.43	1544 (7%) 20 18	24, 69, 93, 111	0

The worst 5 of 1544 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
7	1H	2	SER	6.7
45	2n	2	ALA	6.4
53	2y	98	ALA	6.1
1	1A	1087	G	6.0
1	2A	2602	A	5.7

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

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum,

median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
1	5MU	2A	1915	21/22	0.83	0.12	85,90,94,108	0
32	2MG	2a	1207	24/25	0.84	0.13	87,93,99,103	0
32	5MC	2a	967	21/22	0.86	0.14	75,80,86,92	0
1	5MU	1A	1915	21/22	0.86	0.13	75,82,90,93	0
32	M2G	2a	966	25/26	0.88	0.14	70,75,90,97	0
32	G7M	2a	527	24/25	0.89	0.13	75,77,79,84	0
1	PSU	2A	1917	20/21	0.89	0.09	80,85,95,100	0
43	0TD	1l	92	10/11	0.91	0.12	59,62,66,79	0
43	0TD	2l	92	10/11	0.91	0.11	68,72,75,85	0
1	PSU	1A	1917	20/21	0.92	0.09	66,75,86,86	0
1	PSU	1A	1911	20/21	0.92	0.10	64,73,76,86	0
32	PSU	2a	516	20/21	0.92	0.09	77,81,88,88	0
1	PSU	2A	1911	20/21	0.92	0.10	72,75,83,91	0
32	2MG	1a	1207	24/25	0.93	0.09	73,78,81,83	0
32	4OC	2a	1402	22/23	0.93	0.11	68,72,77,81	0
1	OMC	2A	1920	21/22	0.93	0.11	70,74,81,84	0
32	5MC	1a	967	21/22	0.94	0.12	63,69,77,82	0
32	5MC	2a	1404	21/22	0.94	0.09	65,72,77,79	0
32	UR3	2a	1498	21/22	0.94	0.10	64,70,75,78	0
32	MA6	2a	1519	24/25	0.94	0.13	64,74,78,79	0
32	5MC	2a	1400	21/22	0.94	0.13	73,80,82,85	0
32	5MC	2a	1407	21/22	0.95	0.09	63,72,76,82	0
32	G7M	1a	527	24/25	0.95	0.09	51,57,62,65	0
32	MA6	2a	1518	24/25	0.95	0.11	66,73,78,78	0
32	5MC	1a	1407	21/22	0.95	0.11	56,61,66,72	0
32	PSU	1a	516	20/21	0.95	0.08	65,69,73,75	0
32	4OC	1a	1402	22/23	0.96	0.10	51,60,65,67	0
32	M2G	1a	966	25/26	0.96	0.09	49,62,70,80	0
32	UR3	1a	1498	21/22	0.96	0.10	52,57,60,70	0
32	MA6	1a	1518	24/25	0.96	0.10	47,53,57,58	0
1	5MC	2A	1942	21/22	0.96	0.09	53,59,62,75	0
32	5MC	1a	1400	21/22	0.96	0.09	49,57,63,63	0
1	5MC	2A	1962	21/22	0.97	0.07	45,52,59,65	0
1	OMG	2A	2251	24/25	0.97	0.09	43,47,50,51	0
1	2MA	2A	2503	23/24	0.97	0.08	35,43,47,49	0
32	5MC	1a	1404	21/22	0.97	0.08	50,54,57,61	0
32	MA6	1a	1519	24/25	0.97	0.09	49,54,59,61	0
1	PSU	1A	2605	20/21	0.97	0.08	29,34,37,38	0
1	5MU	2A	1939	21/22	0.97	0.07	38,45,49,51	0
1	OMC	1A	1920	21/22	0.97	0.08	56,64,67,69	0
1	2MA	1A	2503	23/24	0.98	0.05	24,28,32,33	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
1	2MU	2A	2552	21/23	0.98	0.07	41,45,50,54	0
1	PSU	2A	2605	20/21	0.98	0.06	37,45,51,51	0
1	2MU	1A	2552	21/23	0.98	0.08	29,36,38,45	0
1	5MU	1A	1939	21/22	0.98	0.06	30,35,38,41	0
1	5MC	1A	1942	21/22	0.98	0.07	39,43,47,49	0
1	5MC	1A	1962	21/22	0.98	0.06	34,42,47,51	0
1	OMG	1A	2251	24/25	0.98	0.07	26,32,35,37	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	3769	1/1	0.42	0.24	73,73,73,73	0
54	MG	2a	3049	1/1	0.43	0.25	86,86,86,86	0
54	MG	2O	202	1/1	0.46	0.23	87,87,87,87	0
54	MG	1a	1772	1/1	0.46	0.18	92,92,92,92	0
54	MG	2a	3010	1/1	0.49	0.40	92,92,92,92	0
54	MG	1A	3719	1/1	0.51	0.24	82,82,82,82	0
54	MG	1a	1680	1/1	0.53	0.32	87,87,87,87	0
54	MG	1A	3458	1/1	0.54	0.22	56,56,56,56	0
54	MG	2A	3270	1/1	0.58	0.34	88,88,88,88	0
54	MG	2A	3724	1/1	0.59	0.16	88,88,88,88	0
54	MG	1a	1797	1/1	0.59	0.22	95,95,95,95	0
54	MG	2B	211	1/1	0.60	0.21	86,86,86,86	0
54	MG	1A	3384	1/1	0.60	0.26	63,63,63,63	0
54	MG	2A	3478	1/1	0.60	0.23	77,77,77,77	0
54	MG	1a	1867	1/1	0.60	0.26	89,89,89,89	0
54	MG	2A	3521	1/1	0.61	0.23	77,77,77,77	0
54	MG	1A	3723	1/1	0.61	0.32	71,71,71,71	0
54	MG	1A	4001	1/1	0.61	0.17	85,85,85,85	0
54	MG	1a	1869	1/1	0.62	0.14	85,85,85,85	0
54	MG	1a	1774	1/1	0.62	0.18	87,87,87,87	0
54	MG	2B	213	1/1	0.62	0.14	84,84,84,84	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	1a	1704	1/1	0.63	0.24	81,81,81,81	0
54	MG	2a	3175	1/1	0.63	0.27	91,91,91,91	0
54	MG	1a	1665	1/1	0.64	0.21	86,86,86,86	0
54	MG	1A	3661	1/1	0.65	0.33	43,43,43,43	0
54	MG	2A	3635	1/1	0.67	0.37	69,69,69,69	0
54	MG	1A	3805	1/1	0.67	0.25	47,47,47,47	0
54	MG	1A	3697	1/1	0.68	0.20	68,68,68,68	0
54	MG	1B	206	1/1	0.68	0.39	81,81,81,81	0
54	MG	1a	1635	1/1	0.68	0.24	82,82,82,82	0
54	MG	1A	3844	1/1	0.68	0.31	47,47,47,47	0
54	MG	2A	3477	1/1	0.68	0.26	83,83,83,83	0
54	MG	1a	1874	1/1	0.69	0.20	86,86,86,86	0
54	MG	1a	1611	1/1	0.69	0.27	88,88,88,88	0
54	MG	1a	1821	1/1	0.69	0.27	86,86,86,86	0
54	MG	2a	3106	1/1	0.69	0.40	86,86,86,86	0
54	MG	2a	3118	1/1	0.69	0.23	82,82,82,82	0
54	MG	2B	214	1/1	0.69	0.12	95,95,95,95	0
54	MG	2A	3321	1/1	0.70	0.29	73,73,73,73	0
54	MG	2A	3441	1/1	0.70	0.14	77,77,77,77	0
54	MG	1A	3294	1/1	0.70	0.22	83,83,83,83	0
54	MG	2G	201	1/1	0.70	0.22	86,86,86,86	0
54	MG	1A	3668	1/1	0.70	0.17	70,70,70,70	0
54	MG	2A	3500	1/1	0.70	0.21	85,85,85,85	0
54	MG	2A	3090	1/1	0.70	0.16	75,75,75,75	0
54	MG	2A	3094	1/1	0.70	0.39	89,89,89,89	0
54	MG	1a	1696	1/1	0.70	0.24	86,86,86,86	0
54	MG	2a	3139	1/1	0.70	0.24	84,84,84,84	0
54	MG	2B	204	1/1	0.70	0.16	84,84,84,84	0
54	MG	2r	102	1/1	0.70	0.21	78,78,78,78	0
54	MG	1a	1604	1/1	0.71	0.24	77,77,77,77	0
54	MG	2A	3542	1/1	0.71	0.20	83,83,83,83	0
54	MG	1A	3541	1/1	0.71	0.14	65,65,65,65	0
54	MG	1a	1878	1/1	0.71	0.12	93,93,93,93	0
54	MG	2A	3468	1/1	0.71	0.20	82,82,82,82	0
54	MG	1g	202	1/1	0.71	0.21	83,83,83,83	0
54	MG	1a	1841	1/1	0.71	0.15	77,77,77,77	0
54	MG	1A	3670	1/1	0.71	0.17	67,67,67,67	0
54	MG	2D	309	1/1	0.71	0.29	88,88,88,88	0
54	MG	1H	201	1/1	0.72	0.27	77,77,77,77	0
54	MG	2A	3634	1/1	0.72	0.15	70,70,70,70	0
54	MG	1a	1803	1/1	0.72	0.25	77,77,77,77	0
54	MG	1b	301	1/1	0.72	0.27	87,87,87,87	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	2A	3095	1/1	0.72	0.31	81,81,81,81	0
54	MG	2j	201	1/1	0.72	0.19	84,84,84,84	0
54	MG	2A	3522	1/1	0.72	0.24	85,85,85,85	0
54	MG	10	106	1/1	0.73	0.22	69,69,69,69	0
54	MG	1A	3976	1/1	0.73	0.20	76,76,76,76	0
54	MG	2a	3038	1/1	0.73	0.20	94,94,94,94	0
54	MG	1a	1824	1/1	0.73	0.17	84,84,84,84	0
54	MG	1B	220	1/1	0.73	0.20	53,53,53,53	0
54	MG	1a	1850	1/1	0.73	0.22	72,72,72,72	0
54	MG	1B	226	1/1	0.73	0.15	73,73,73,73	0
54	MG	1A	3907	1/1	0.73	0.18	72,72,72,72	0
54	MG	1a	1666	1/1	0.73	0.35	80,80,80,80	0
54	MG	2A	3543	1/1	0.73	0.14	74,74,74,74	0
54	MG	1T	204	1/1	0.74	0.22	78,78,78,78	0
54	MG	2G	202	1/1	0.74	0.20	91,91,91,91	0
54	MG	1a	1629	1/1	0.74	0.35	76,76,76,76	0
54	MG	2A	3461	1/1	0.74	0.16	75,75,75,75	0
54	MG	1A	3853	1/1	0.74	0.20	64,64,64,64	0
54	MG	1A	3601	1/1	0.74	0.21	58,58,58,58	0
54	MG	2a	3059	1/1	0.74	0.32	91,91,91,91	0
54	MG	2a	3061	1/1	0.74	0.34	84,84,84,84	0
54	MG	2a	3099	1/1	0.74	0.30	77,77,77,77	0
54	MG	2A	3261	1/1	0.74	0.25	81,81,81,81	0
54	MG	2B	209	1/1	0.74	0.32	80,80,80,80	0
54	MG	1a	1852	1/1	0.74	0.23	76,76,76,76	0
54	MG	2A	3506	1/1	0.74	0.24	82,82,82,82	0
54	MG	2A	3298	1/1	0.74	0.21	90,90,90,90	0
54	MG	2A	3320	1/1	0.74	0.17	71,71,71,71	0
54	MG	2A	3630	1/1	0.75	0.11	100,100,100,100	0
54	MG	1a	1610	1/1	0.75	0.29	73,73,73,73	0
54	MG	1A	3674	1/1	0.75	0.20	82,82,82,82	0
54	MG	2A	3366	1/1	0.75	0.22	83,83,83,83	0
54	MG	2I	201	1/1	0.75	0.15	78,78,78,78	0
54	MG	2a	3137	1/1	0.75	0.16	80,80,80,80	0
54	MG	1A	3776	1/1	0.75	0.25	72,72,72,72	0
54	MG	1A	4032	1/1	0.75	0.18	65,65,65,65	0
54	MG	1A	3864	1/1	0.75	0.19	64,64,64,64	0
54	MG	1A	3455	1/1	0.75	0.22	66,66,66,66	0
54	MG	2A	3585	1/1	0.76	0.17	67,67,67,67	0
54	MG	1A	3604	1/1	0.76	0.25	64,64,64,64	0
54	MG	1A	3713	1/1	0.76	0.26	78,78,78,78	0
54	MG	2A	3275	1/1	0.76	0.39	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	3721	1/1	0.76	0.19	78,78,78,78	0
54	MG	2A	3295	1/1	0.76	0.24	71,71,71,71	0
54	MG	1a	1693	1/1	0.76	0.19	88,88,88,88	0
54	MG	1A	3887	1/1	0.76	0.16	71,71,71,71	0
54	MG	1A	3895	1/1	0.76	0.15	60,60,60,60	0
54	MG	1a	1771	1/1	0.76	0.13	94,94,94,94	0
54	MG	2A	3430	1/1	0.76	0.34	83,83,83,83	0
54	MG	2A	3131	1/1	0.76	0.34	81,81,81,81	0
54	MG	2E	306	1/1	0.76	0.25	79,79,79,79	0
54	MG	2A	3567	1/1	0.76	0.28	87,87,87,87	0
54	MG	2A	3568	1/1	0.76	0.19	82,82,82,82	0
57	MPD	2B	219	8/8	0.76	0.25	72,74,84,90	0
54	MG	1A	3666	1/1	0.77	0.14	70,70,70,70	0
54	MG	1A	3492	1/1	0.77	0.16	64,64,64,64	0
54	MG	1P	204	1/1	0.77	0.26	48,48,48,48	0
54	MG	1A	4015	1/1	0.77	0.27	36,36,36,36	0
54	MG	2a	3037	1/1	0.77	0.13	85,85,85,85	0
54	MG	1e	203	1/1	0.77	0.12	77,77,77,77	0
54	MG	2A	3452	1/1	0.77	0.17	69,69,69,69	0
54	MG	1A	4030	1/1	0.77	0.17	66,66,66,66	0
54	MG	1a	1681	1/1	0.77	0.14	90,90,90,90	0
54	MG	2a	3085	1/1	0.77	0.27	89,89,89,89	0
54	MG	2A	3725	1/1	0.77	0.21	87,87,87,87	0
54	MG	1a	1692	1/1	0.77	0.25	79,79,79,79	0
54	MG	1a	1829	1/1	0.77	0.19	83,83,83,83	0
54	MG	1A	3477	1/1	0.77	0.17	66,66,66,66	0
54	MG	1A	3828	1/1	0.77	0.17	79,79,79,79	0
54	MG	2a	3148	1/1	0.77	0.15	82,82,82,82	0
54	MG	1A	3561	1/1	0.77	0.23	64,64,64,64	0
54	MG	1a	1863	1/1	0.77	0.21	78,78,78,78	0
54	MG	1a	1769	1/1	0.77	0.25	85,85,85,85	0
54	MG	1a	1868	1/1	0.77	0.16	80,80,80,80	0
54	MG	1A	3445	1/1	0.78	0.19	80,80,80,80	0
54	MG	1a	1877	1/1	0.78	0.41	73,73,73,73	0
54	MG	18	102	1/1	0.78	0.31	52,52,52,52	0
54	MG	1A	3014	1/1	0.78	0.35	70,70,70,70	0
54	MG	1d	303	1/1	0.78	0.21	76,76,76,76	0
54	MG	2a	3024	1/1	0.78	0.33	82,82,82,82	0
54	MG	2A	3323	1/1	0.78	0.18	67,67,67,67	0
54	MG	1A	3829	1/1	0.78	0.24	39,39,39,39	0
54	MG	2A	3378	1/1	0.78	0.28	84,84,84,84	0
54	MG	1a	1703	1/1	0.78	0.30	80,80,80,80	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	2A	3689	1/1	0.78	0.14	73,73,73,73	0
54	MG	2A	3437	1/1	0.78	0.12	87,87,87,87	0
54	MG	2a	3087	1/1	0.78	0.25	73,73,73,73	0
54	MG	2A	3022	1/1	0.78	0.40	63,63,63,63	0
54	MG	2A	3052	1/1	0.78	0.21	64,64,64,64	0
54	MG	2A	3728	1/1	0.78	0.24	64,64,64,64	0
54	MG	2A	3058	1/1	0.78	0.20	59,59,59,59	0
54	MG	1A	3906	1/1	0.78	0.15	49,49,49,49	0
54	MG	1A	3197	1/1	0.78	0.30	75,75,75,75	0
54	MG	1A	3969	1/1	0.78	0.22	67,67,67,67	0
54	MG	1A	3848	1/1	0.78	0.23	70,70,70,70	0
54	MG	2n	101	1/1	0.78	0.34	81,81,81,81	0
54	MG	1A	3987	1/1	0.78	0.24	58,58,58,58	0
54	MG	1A	3391	1/1	0.78	0.15	58,58,58,58	0
54	MG	2A	3162	1/1	0.79	0.25	76,76,76,76	0
54	MG	2A	3180	1/1	0.79	0.16	76,76,76,76	0
54	MG	2A	3181	1/1	0.79	0.25	76,76,76,76	0
54	MG	2A	3216	1/1	0.79	0.22	69,69,69,69	0
54	MG	1a	1777	1/1	0.79	0.16	82,82,82,82	0
54	MG	2a	3006	1/1	0.79	0.42	87,87,87,87	0
54	MG	15	107	1/1	0.79	0.21	59,59,59,59	0
54	MG	1A	3480	1/1	0.79	0.17	61,61,61,61	0
54	MG	1A	3730	1/1	0.79	0.20	73,73,73,73	0
54	MG	1A	3488	1/1	0.79	0.16	55,55,55,55	0
54	MG	2a	3044	1/1	0.79	0.17	91,91,91,91	0
54	MG	1B	222	1/1	0.79	0.14	61,61,61,61	0
54	MG	1A	3200	1/1	0.79	0.18	86,86,86,86	0
54	MG	1y	202	1/1	0.79	0.22	73,73,73,73	0
54	MG	1a	1712	1/1	0.79	0.20	76,76,76,76	0
54	MG	2A	3697	1/1	0.79	0.17	62,62,62,62	0
54	MG	2A	3024	1/1	0.79	0.17	67,67,67,67	0
54	MG	2A	3386	1/1	0.79	0.14	68,68,68,68	0
54	MG	2a	3110	1/1	0.79	0.19	74,74,74,74	0
54	MG	2A	3047	1/1	0.79	0.20	74,74,74,74	0
54	MG	1a	1738	1/1	0.79	0.22	72,72,72,72	0
54	MG	1a	1861	1/1	0.79	0.16	84,84,84,84	0
54	MG	2A	3074	1/1	0.79	0.19	67,67,67,67	0
54	MG	1A	3703	1/1	0.79	0.15	71,71,71,71	0
54	MG	2e	201	1/1	0.79	0.29	77,77,77,77	0
54	MG	1A	3312	1/1	0.79	0.21	60,60,60,60	0
54	MG	1A	4017	1/1	0.79	0.17	66,66,66,66	0
54	MG	2B	216	1/1	0.79	0.15	86,86,86,86	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	1A	3335	1/1	0.79	0.21	78,78,78,78	0
58	ARG	1F	319	12/12	0.79	0.18	61,72,79,80	0
54	MG	1A	4011	1/1	0.80	0.16	84,84,84,84	0
54	MG	2A	3362	1/1	0.80	0.14	51,51,51,51	0
54	MG	1a	1745	1/1	0.80	0.25	70,70,70,70	0
54	MG	2A	3578	1/1	0.80	0.18	71,71,71,71	0
54	MG	2A	3374	1/1	0.80	0.21	82,82,82,82	0
54	MG	2a	3021	1/1	0.80	0.32	79,79,79,79	0
54	MG	2A	3618	1/1	0.80	0.13	48,48,48,48	0
54	MG	2a	3027	1/1	0.80	0.21	83,83,83,83	0
54	MG	2A	3623	1/1	0.80	0.19	44,44,44,44	0
54	MG	1A	3296	1/1	0.80	0.16	77,77,77,77	0
54	MG	2A	3631	1/1	0.80	0.28	64,64,64,64	0
54	MG	2A	3164	1/1	0.80	0.27	88,88,88,88	0
54	MG	1A	3810	1/1	0.80	0.20	67,67,67,67	0
54	MG	2a	3060	1/1	0.80	0.25	73,73,73,73	0
54	MG	1A	3943	1/1	0.80	0.16	75,75,75,75	0
54	MG	2a	3064	1/1	0.80	0.28	89,89,89,89	0
54	MG	2a	3066	1/1	0.80	0.21	82,82,82,82	0
54	MG	2a	3067	1/1	0.80	0.08	95,95,95,95	0
54	MG	2a	3073	1/1	0.80	0.38	82,82,82,82	0
54	MG	2A	3192	1/1	0.80	0.39	82,82,82,82	0
54	MG	2A	3706	1/1	0.80	0.11	88,88,88,88	0
54	MG	2a	3098	1/1	0.80	0.30	83,83,83,83	0
54	MG	2A	3211	1/1	0.80	0.28	76,76,76,76	0
54	MG	1A	3811	1/1	0.80	0.19	61,61,61,61	0
54	MG	1A	3974	1/1	0.80	0.14	59,59,59,59	0
54	MG	1A	3814	1/1	0.80	0.24	69,69,69,69	0
54	MG	2B	202	1/1	0.80	0.29	82,82,82,82	0
54	MG	2A	3273	1/1	0.80	0.31	80,80,80,80	0
54	MG	1A	3986	1/1	0.80	0.23	59,59,59,59	0
54	MG	1A	3556	1/1	0.80	0.17	67,67,67,67	0
54	MG	2a	3185	1/1	0.80	0.16	83,83,83,83	0
54	MG	2A	3089	1/1	0.80	0.24	78,78,78,78	0
54	MG	1A	3149	1/1	0.80	0.29	66,66,66,66	0
54	MG	2A	3526	1/1	0.80	0.18	47,47,47,47	0
54	MG	2A	3535	1/1	0.80	0.18	73,73,73,73	0
54	MG	2A	3539	1/1	0.80	0.19	90,90,90,90	0
54	MG	1a	1717	1/1	0.80	0.26	71,71,71,71	0
54	MG	2A	3620	1/1	0.81	0.26	79,79,79,79	0
54	MG	1a	1864	1/1	0.81	0.12	95,95,95,95	0
54	MG	1A	3581	1/1	0.81	0.16	62,62,62,62	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	1a	1749	1/1	0.81	0.25	77,77,77,77	0
54	MG	2A	3140	1/1	0.81	0.24	80,80,80,80	0
54	MG	1A	3473	1/1	0.81	0.18	63,63,63,63	0
54	MG	1a	1669	1/1	0.81	0.22	76,76,76,76	0
54	MG	2A	3691	1/1	0.81	0.17	66,66,66,66	0
54	MG	2A	3165	1/1	0.81	0.18	61,61,61,61	0
54	MG	2A	3705	1/1	0.81	0.17	65,65,65,65	0
54	MG	2A	3459	1/1	0.81	0.21	73,73,73,73	0
54	MG	2A	3460	1/1	0.81	0.14	79,79,79,79	0
54	MG	2A	3174	1/1	0.81	0.10	79,79,79,79	0
54	MG	1A	3522	1/1	0.81	0.10	67,67,67,67	0
54	MG	2a	3079	1/1	0.81	0.22	83,83,83,83	0
54	MG	1A	3607	1/1	0.81	0.14	62,62,62,62	0
54	MG	2A	3729	1/1	0.81	0.34	74,74,74,74	0
54	MG	2a	3088	1/1	0.81	0.26	81,81,81,81	0
54	MG	1A	3923	1/1	0.81	0.11	30,30,30,30	0
54	MG	1a	1794	1/1	0.81	0.17	78,78,78,78	0
54	MG	1A	3089	1/1	0.81	0.21	67,67,67,67	0
54	MG	1A	3953	1/1	0.81	0.12	55,55,55,55	0
54	MG	1A	3543	1/1	0.81	0.16	64,64,64,64	0
54	MG	1A	3555	1/1	0.81	0.12	59,59,59,59	0
54	MG	2a	3138	1/1	0.81	0.22	75,75,75,75	0
54	MG	1A	3154	1/1	0.81	0.21	77,77,77,77	0
54	MG	2A	3284	1/1	0.81	0.32	64,64,64,64	0
54	MG	2a	3171	1/1	0.81	0.20	84,84,84,84	0
54	MG	2A	3043	1/1	0.81	0.29	76,76,76,76	0
54	MG	1a	1713	1/1	0.81	0.29	77,77,77,77	0
54	MG	1a	1842	1/1	0.81	0.21	87,87,87,87	0
54	MG	1A	3395	1/1	0.81	0.16	70,70,70,70	0
54	MG	1a	1722	1/1	0.81	0.26	76,76,76,76	0
54	MG	2a	3005	1/1	0.81	0.19	66,66,66,66	0
54	MG	1a	1737	1/1	0.81	0.16	82,82,82,82	0
54	MG	1a	1641	1/1	0.81	0.13	79,79,79,79	0
54	MG	1A	3539	1/1	0.82	0.15	79,79,79,79	0
54	MG	2A	3182	1/1	0.82	0.14	72,72,72,72	0
54	MG	2A	3514	1/1	0.82	0.15	76,76,76,76	0
54	MG	2A	3184	1/1	0.82	0.27	80,80,80,80	0
54	MG	2A	3188	1/1	0.82	0.27	66,66,66,66	0
54	MG	1A	3605	1/1	0.82	0.32	46,46,46,46	0
54	MG	2A	3208	1/1	0.82	0.13	68,68,68,68	0
54	MG	1A	3168	1/1	0.82	0.27	70,70,70,70	0
54	MG	1A	3724	1/1	0.82	0.17	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	3032	1/1	0.82	0.14	91,91,91,91	0
54	MG	2A	3248	1/1	0.82	0.21	63,63,63,63	0
54	MG	1A	3656	1/1	0.82	0.22	77,77,77,77	0
54	MG	2A	3266	1/1	0.82	0.31	82,82,82,82	0
54	MG	1a	1786	1/1	0.82	0.14	77,77,77,77	0
54	MG	1A	3742	1/1	0.82	0.13	50,50,50,50	0
54	MG	1A	4036	1/1	0.82	0.20	73,73,73,73	0
54	MG	1a	1799	1/1	0.82	0.20	80,80,80,80	0
54	MG	2A	3286	1/1	0.82	0.21	70,70,70,70	0
54	MG	2A	3626	1/1	0.82	0.15	82,82,82,82	0
54	MG	2A	3034	1/1	0.82	0.33	81,81,81,81	0
54	MG	1A	3328	1/1	0.82	0.12	70,70,70,70	0
54	MG	1a	1820	1/1	0.82	0.18	84,84,84,84	0
54	MG	1A	3330	1/1	0.82	0.16	64,64,64,64	0
54	MG	2A	3053	1/1	0.82	0.27	74,74,74,74	0
54	MG	2A	3356	1/1	0.82	0.14	74,74,74,74	0
54	MG	1A	3801	1/1	0.82	0.15	39,39,39,39	0
54	MG	1A	3667	1/1	0.82	0.24	73,73,73,73	0
54	MG	1A	3262	1/1	0.82	0.26	71,71,71,71	0
54	MG	1A	3362	1/1	0.82	0.16	76,76,76,76	0
54	MG	2A	3385	1/1	0.82	0.13	70,70,70,70	0
54	MG	2a	3129	1/1	0.82	0.21	70,70,70,70	0
54	MG	2a	3131	1/1	0.82	0.12	83,83,83,83	0
54	MG	1A	3504	1/1	0.82	0.12	33,33,33,33	0
54	MG	1Z	301	1/1	0.82	0.17	73,73,73,73	0
54	MG	2A	3104	1/1	0.82	0.23	65,65,65,65	0
54	MG	2A	3118	1/1	0.82	0.29	74,74,74,74	0
54	MG	2A	3442	1/1	0.82	0.18	73,73,73,73	0
54	MG	2A	3446	1/1	0.82	0.17	65,65,65,65	0
54	MG	1A	3826	1/1	0.82	0.16	65,65,65,65	0
54	MG	1A	3981	1/1	0.82	0.17	58,58,58,58	0
54	MG	1A	3589	1/1	0.82	0.16	68,68,68,68	0
54	MG	1A	3376	1/1	0.82	0.13	65,65,65,65	0
54	MG	1A	3990	1/1	0.82	0.16	61,61,61,61	0
54	MG	1A	3999	1/1	0.82	0.11	75,75,75,75	0
54	MG	1a	1760	1/1	0.82	0.10	64,64,64,64	0
54	MG	1a	1679	1/1	0.83	0.17	66,66,66,66	0
54	MG	1a	1781	1/1	0.83	0.18	89,89,89,89	0
54	MG	1a	1785	1/1	0.83	0.15	73,73,73,73	0
54	MG	1m	202	1/1	0.83	0.23	79,79,79,79	0
54	MG	2A	3501	1/1	0.83	0.12	75,75,75,75	0
54	MG	1O	201	1/1	0.83	0.17	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	3511	1/1	0.83	0.20	77,77,77,77	0
54	MG	2A	3213	1/1	0.83	0.18	72,72,72,72	0
54	MG	1A	3546	1/1	0.83	0.20	66,66,66,66	0
54	MG	2a	3016	1/1	0.83	0.16	79,79,79,79	0
54	MG	2a	3019	1/1	0.83	0.23	80,80,80,80	0
54	MG	2A	3219	1/1	0.83	0.11	62,62,62,62	0
54	MG	2A	3230	1/1	0.83	0.26	72,72,72,72	0
54	MG	1R	205	1/1	0.83	0.23	61,61,61,61	0
54	MG	1A	3893	1/1	0.83	0.20	39,39,39,39	0
54	MG	2a	3036	1/1	0.83	0.22	78,78,78,78	0
54	MG	2A	3262	1/1	0.83	0.14	65,65,65,65	0
54	MG	2A	3037	1/1	0.83	0.30	74,74,74,74	0
54	MG	2a	3041	1/1	0.83	0.27	80,80,80,80	0
54	MG	1W	201	1/1	0.83	0.25	57,57,57,57	0
54	MG	1A	3456	1/1	0.83	0.14	41,41,41,41	0
54	MG	2a	3050	1/1	0.83	0.36	87,87,87,87	0
54	MG	2A	3048	1/1	0.83	0.17	73,73,73,73	0
54	MG	1A	3639	1/1	0.83	0.21	64,64,64,64	0
54	MG	1A	3167	1/1	0.83	0.27	77,77,77,77	0
54	MG	1A	3464	1/1	0.83	0.23	66,66,66,66	0
54	MG	1a	1835	1/1	0.83	0.23	78,78,78,78	0
54	MG	2A	3087	1/1	0.83	0.23	90,90,90,90	0
54	MG	2a	3071	1/1	0.83	0.26	69,69,69,69	0
54	MG	1a	1716	1/1	0.83	0.27	71,71,71,71	0
54	MG	1A	3472	1/1	0.83	0.22	69,69,69,69	0
54	MG	2A	3335	1/1	0.83	0.23	71,71,71,71	0
54	MG	1a	1718	1/1	0.83	0.17	67,67,67,67	0
54	MG	2A	3673	1/1	0.83	0.10	76,76,76,76	0
54	MG	2A	3685	1/1	0.83	0.19	74,74,74,74	0
54	MG	1A	3583	1/1	0.83	0.11	53,53,53,53	0
54	MG	2A	3102	1/1	0.83	0.35	70,70,70,70	0
54	MG	2A	3368	1/1	0.83	0.15	78,78,78,78	0
54	MG	1a	1860	1/1	0.83	0.12	90,90,90,90	0
54	MG	1A	3437	1/1	0.83	0.18	66,66,66,66	0
54	MG	2A	3707	1/1	0.83	0.18	75,75,75,75	0
54	MG	2a	3136	1/1	0.83	0.23	76,76,76,76	0
54	MG	1A	3669	1/1	0.83	0.30	44,44,44,44	0
54	MG	2A	3722	1/1	0.83	0.25	76,76,76,76	0
54	MG	1B	216	1/1	0.83	0.17	51,51,51,51	0
54	MG	2a	3143	1/1	0.83	0.21	73,73,73,73	0
54	MG	2A	3142	1/1	0.83	0.16	76,76,76,76	0
54	MG	2a	3170	1/1	0.83	0.24	68,68,68,68	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	1a	1638	1/1	0.83	0.20	71,71,71,71	0
54	MG	2A	3163	1/1	0.83	0.11	67,67,67,67	0
54	MG	2a	3179	1/1	0.83	0.19	67,67,67,67	0
54	MG	1a	1758	1/1	0.83	0.19	76,76,76,76	0
54	MG	1A	3278	1/1	0.83	0.34	75,75,75,75	0
54	MG	1a	1642	1/1	0.83	0.15	65,65,65,65	0
54	MG	1A	3861	1/1	0.83	0.22	68,68,68,68	0
54	MG	1A	3225	1/1	0.83	0.12	77,77,77,77	0
54	MG	2y	3200	1/1	0.83	0.13	74,74,74,74	0
54	MG	1A	3871	1/1	0.83	0.11	66,66,66,66	0
54	MG	2A	3466	1/1	0.83	0.34	68,68,68,68	0
54	MG	1a	1646	1/1	0.84	0.22	76,76,76,76	0
54	MG	1e	201	1/1	0.84	0.29	71,71,71,71	0
54	MG	2a	3026	1/1	0.84	0.23	75,75,75,75	0
54	MG	2A	3607	1/1	0.84	0.12	74,74,74,74	0
54	MG	1a	1656	1/1	0.84	0.16	73,73,73,73	0
54	MG	1a	1805	1/1	0.84	0.31	83,83,83,83	0
54	MG	2A	3622	1/1	0.84	0.23	85,85,85,85	0
54	MG	1a	1813	1/1	0.84	0.31	78,78,78,78	0
54	MG	1a	1817	1/1	0.84	0.12	75,75,75,75	0
54	MG	1A	3937	1/1	0.84	0.14	35,35,35,35	0
54	MG	1A	3736	1/1	0.84	0.17	37,37,37,37	0
54	MG	2A	3031	1/1	0.84	0.27	84,84,84,84	0
54	MG	1A	3662	1/1	0.84	0.19	66,66,66,66	0
54	MG	1B	221	1/1	0.84	0.19	72,72,72,72	0
54	MG	1a	1751	1/1	0.84	0.18	76,76,76,76	0
54	MG	1a	1756	1/1	0.84	0.25	68,68,68,68	0
54	MG	2A	3210	1/1	0.84	0.17	70,70,70,70	0
54	MG	1A	3325	1/1	0.84	0.19	64,64,64,64	0
54	MG	1A	3606	1/1	0.84	0.35	66,66,66,66	0
54	MG	1a	1761	1/1	0.84	0.20	79,79,79,79	0
54	MG	2A	3054	1/1	0.84	0.19	72,72,72,72	0
54	MG	1a	1690	1/1	0.84	0.33	76,76,76,76	0
54	MG	2a	3086	1/1	0.84	0.15	80,80,80,80	0
54	MG	2A	3231	1/1	0.84	0.43	75,75,75,75	0
54	MG	2A	3474	1/1	0.84	0.11	84,84,84,84	0
54	MG	2A	3069	1/1	0.84	0.28	72,72,72,72	0
54	MG	1F	314	1/1	0.84	0.15	52,52,52,52	0
54	MG	2a	3100	1/1	0.84	0.24	80,80,80,80	0
54	MG	2A	3491	1/1	0.84	0.14	52,52,52,52	0
54	MG	1a	1862	1/1	0.84	0.14	82,82,82,82	0
54	MG	2a	3116	1/1	0.84	0.35	87,87,87,87	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	1A	3261	1/1	0.84	0.22	69,69,69,69	0
54	MG	2A	3503	1/1	0.84	0.16	76,76,76,76	0
54	MG	1N	202	1/1	0.84	0.21	66,66,66,66	0
54	MG	1a	1617	1/1	0.84	0.11	70,70,70,70	0
54	MG	1A	3193	1/1	0.84	0.24	77,77,77,77	0
54	MG	2A	3276	1/1	0.84	0.33	70,70,70,70	0
54	MG	2A	3277	1/1	0.84	0.36	70,70,70,70	0
54	MG	2A	3096	1/1	0.84	0.18	64,64,64,64	0
54	MG	1a	1782	1/1	0.84	0.19	79,79,79,79	0
54	MG	2a	3149	1/1	0.84	0.12	71,71,71,71	0
54	MG	2A	3536	1/1	0.84	0.15	68,68,68,68	0
54	MG	2A	3538	1/1	0.84	0.13	75,75,75,75	0
54	MG	1P	203	1/1	0.84	0.25	74,74,74,74	0
54	MG	2U	201	1/1	0.84	0.22	79,79,79,79	0
54	MG	2a	3002	1/1	0.84	0.17	75,75,75,75	0
54	MG	2A	3109	1/1	0.84	0.23	55,55,55,55	0
54	MG	1A	3310	1/1	0.84	0.17	59,59,59,59	0
54	MG	2a	3008	1/1	0.84	0.20	62,62,62,62	0
54	MG	2A	3555	1/1	0.84	0.10	63,63,63,63	0
54	MG	2a	3013	1/1	0.84	0.34	79,79,79,79	0
57	MPD	1a	1880	8/8	0.84	0.16	60,72,78,78	0
57	MPD	2A	3733	8/8	0.84	0.27	54,60,66,66	0
54	MG	1A	3172	1/1	0.84	0.15	50,50,50,50	0
54	MG	1T	201	1/1	0.84	0.26	62,62,62,62	0
54	MG	1a	1798	1/1	0.85	0.10	83,83,83,83	0
54	MG	2A	3530	1/1	0.85	0.19	63,63,63,63	0
54	MG	1a	1697	1/1	0.85	0.29	63,63,63,63	0
54	MG	2A	3036	1/1	0.85	0.17	66,66,66,66	0
54	MG	1A	3748	1/1	0.85	0.11	39,39,39,39	0
54	MG	1A	4025	1/1	0.85	0.29	44,44,44,44	0
54	MG	1a	1811	1/1	0.85	0.18	85,85,85,85	0
54	MG	2A	3271	1/1	0.85	0.20	63,63,63,63	0
54	MG	1a	1709	1/1	0.85	0.20	73,73,73,73	0
54	MG	1A	4028	1/1	0.85	0.19	66,66,66,66	0
54	MG	18	101	1/1	0.85	0.21	74,74,74,74	0
54	MG	2A	3573	1/1	0.85	0.10	49,49,49,49	0
54	MG	2A	3574	1/1	0.85	0.18	60,60,60,60	0
54	MG	2a	3040	1/1	0.85	0.15	73,73,73,73	0
54	MG	1a	1715	1/1	0.85	0.25	76,76,76,76	0
54	MG	1A	3767	1/1	0.85	0.13	64,64,64,64	0
54	MG	2A	3596	1/1	0.85	0.11	73,73,73,73	0
54	MG	1A	3947	1/1	0.85	0.12	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	2A	3612	1/1	0.85	0.15	51,51,51,51	0
54	MG	1a	1831	1/1	0.85	0.19	86,86,86,86	0
54	MG	1A	4034	1/1	0.85	0.17	79,79,79,79	0
54	MG	2A	3299	1/1	0.85	0.14	43,43,43,43	0
54	MG	1a	1840	1/1	0.85	0.13	73,73,73,73	0
54	MG	1A	3702	1/1	0.85	0.24	85,85,85,85	0
54	MG	1A	4037	1/1	0.85	0.18	71,71,71,71	0
54	MG	1a	1623	1/1	0.85	0.40	75,75,75,75	0
54	MG	1a	1744	1/1	0.85	0.27	78,78,78,78	0
54	MG	1a	1853	1/1	0.85	0.19	67,67,67,67	0
54	MG	1B	205	1/1	0.85	0.12	61,61,61,61	0
54	MG	1A	3954	1/1	0.85	0.10	55,55,55,55	0
54	MG	2A	3112	1/1	0.85	0.16	78,78,78,78	0
54	MG	2a	3096	1/1	0.85	0.17	73,73,73,73	0
54	MG	2a	3097	1/1	0.85	0.30	84,84,84,84	0
54	MG	2A	3113	1/1	0.85	0.14	76,76,76,76	0
54	MG	1A	3321	1/1	0.85	0.34	56,56,56,56	0
54	MG	2A	3703	1/1	0.85	0.13	68,68,68,68	0
54	MG	2A	3125	1/1	0.85	0.17	66,66,66,66	0
54	MG	2A	3389	1/1	0.85	0.18	49,49,49,49	0
54	MG	1A	3784	1/1	0.85	0.17	58,58,58,58	0
54	MG	1A	3609	1/1	0.85	0.19	72,72,72,72	0
54	MG	1A	3804	1/1	0.85	0.15	50,50,50,50	0
54	MG	1A	3875	1/1	0.85	0.13	73,73,73,73	0
54	MG	1A	3557	1/1	0.85	0.13	40,40,40,40	0
54	MG	1a	1870	1/1	0.85	0.26	75,75,75,75	0
54	MG	1A	3640	1/1	0.85	0.24	56,56,56,56	0
54	MG	1A	3993	1/1	0.85	0.22	61,61,61,61	0
54	MG	1A	3462	1/1	0.85	0.23	74,74,74,74	0
54	MG	1A	3526	1/1	0.85	0.14	60,60,60,60	0
54	MG	1A	4006	1/1	0.85	0.23	54,54,54,54	0
54	MG	2a	3167	1/1	0.85	0.13	75,75,75,75	0
54	MG	2a	3169	1/1	0.85	0.23	76,76,76,76	0
54	MG	1a	1686	1/1	0.85	0.27	82,82,82,82	0
54	MG	1A	3689	1/1	0.85	0.21	65,65,65,65	0
54	MG	1A	4012	1/1	0.85	0.25	88,88,88,88	0
54	MG	2B	217	1/1	0.85	0.10	79,79,79,79	0
54	MG	2a	3181	1/1	0.85	0.17	82,82,82,82	0
54	MG	2A	3485	1/1	0.85	0.20	82,82,82,82	0
54	MG	2a	3188	1/1	0.85	0.18	88,88,88,88	0
54	MG	2A	3205	1/1	0.85	0.36	76,76,76,76	0
54	MG	2A	3207	1/1	0.85	0.15	73,73,73,73	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	1h	202	1/1	0.85	0.19	67,67,67,67	0
54	MG	1a	1788	1/1	0.85	0.15	72,72,72,72	0
54	MG	1a	1793	1/1	0.85	0.19	74,74,74,74	0
54	MG	2A	3002	1/1	0.85	0.23	70,70,70,70	0
54	MG	2A	3010	1/1	0.85	0.33	73,73,73,73	0
54	MG	1A	4013	1/1	0.85	0.19	66,66,66,66	0
54	MG	1A	3283	1/1	0.85	0.12	56,56,56,56	0
54	MG	1A	3813	1/1	0.86	0.11	75,75,75,75	0
54	MG	1a	1667	1/1	0.86	0.43	74,74,74,74	0
54	MG	2A	3403	1/1	0.86	0.18	57,57,57,57	0
54	MG	2A	3406	1/1	0.86	0.17	60,60,60,60	0
54	MG	2A	3421	1/1	0.86	0.20	80,80,80,80	0
54	MG	2A	3185	1/1	0.86	0.14	71,71,71,71	0
54	MG	1A	3552	1/1	0.86	0.14	64,64,64,64	0
54	MG	1A	3034	1/1	0.86	0.10	59,59,59,59	0
54	MG	2a	3051	1/1	0.86	0.35	67,67,67,67	0
54	MG	2a	3053	1/1	0.86	0.32	72,72,72,72	0
54	MG	2A	3636	1/1	0.86	0.14	79,79,79,79	0
54	MG	2A	3653	1/1	0.86	0.10	94,94,94,94	0
54	MG	1A	3379	1/1	0.86	0.08	41,41,41,41	0
54	MG	1A	3273	1/1	0.86	0.27	71,71,71,71	0
54	MG	2A	3450	1/1	0.86	0.17	66,66,66,66	0
54	MG	1a	1682	1/1	0.86	0.15	60,60,60,60	0
54	MG	1A	3833	1/1	0.86	0.14	45,45,45,45	0
54	MG	1A	3635	1/1	0.86	0.24	42,42,42,42	0
54	MG	1a	1775	1/1	0.86	0.20	76,76,76,76	0
54	MG	2a	3082	1/1	0.86	0.41	68,68,68,68	0
54	MG	1A	3959	1/1	0.86	0.13	49,49,49,49	0
54	MG	1a	1780	1/1	0.86	0.12	80,80,80,80	0
54	MG	2A	3714	1/1	0.86	0.11	59,59,59,59	0
54	MG	2A	3083	1/1	0.86	0.21	72,72,72,72	0
54	MG	2a	3092	1/1	0.86	0.40	86,86,86,86	0
54	MG	10	107	1/1	0.86	0.15	70,70,70,70	0
54	MG	2A	3233	1/1	0.86	0.12	60,60,60,60	0
54	MG	1A	3847	1/1	0.86	0.10	60,60,60,60	0
54	MG	2A	3490	1/1	0.86	0.17	71,71,71,71	0
54	MG	1A	3035	1/1	0.86	0.13	55,55,55,55	0
54	MG	2a	3105	1/1	0.86	0.54	83,83,83,83	0
54	MG	2A	3093	1/1	0.86	0.20	82,82,82,82	0
54	MG	2a	3108	1/1	0.86	0.37	71,71,71,71	0
54	MG	1A	3691	1/1	0.86	0.12	66,66,66,66	0
54	MG	2A	3269	1/1	0.86	0.23	60,60,60,60	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	1A	3471	1/1	0.86	0.21	71,71,71,71	0
54	MG	2a	3121	1/1	0.86	0.11	81,81,81,81	0
54	MG	2a	3122	1/1	0.86	0.19	67,67,67,67	0
54	MG	1a	1789	1/1	0.86	0.20	64,64,64,64	0
54	MG	1B	210	1/1	0.86	0.23	70,70,70,70	0
54	MG	1A	3652	1/1	0.86	0.14	60,60,60,60	0
54	MG	1A	3038	1/1	0.86	0.27	69,69,69,69	0
54	MG	1d	301	1/1	0.86	0.28	74,74,74,74	0
54	MG	2D	311	1/1	0.86	0.11	36,36,36,36	0
54	MG	2a	3140	1/1	0.86	0.22	72,72,72,72	0
54	MG	2E	303	1/1	0.86	0.14	39,39,39,39	0
54	MG	1A	3704	1/1	0.86	0.10	62,62,62,62	0
54	MG	1A	3877	1/1	0.86	0.11	56,56,56,56	0
54	MG	2a	3153	1/1	0.86	0.13	82,82,82,82	0
54	MG	1A	3033	1/1	0.86	0.15	55,55,55,55	0
54	MG	1B	229	1/1	0.86	0.08	68,68,68,68	0
54	MG	1A	3809	1/1	0.86	0.10	39,39,39,39	0
54	MG	2A	3312	1/1	0.86	0.17	70,70,70,70	0
54	MG	28	102	1/1	0.86	0.20	66,66,66,66	0
54	MG	1F	316	1/1	0.86	0.20	56,56,56,56	0
54	MG	2A	3546	1/1	0.86	0.12	50,50,50,50	0
54	MG	2A	3143	1/1	0.86	0.14	54,54,54,54	0
54	MG	1a	1814	1/1	0.86	0.18	81,81,81,81	0
54	MG	1A	3238	1/1	0.86	0.23	65,65,65,65	0
54	MG	2A	3355	1/1	0.86	0.20	75,75,75,75	0
54	MG	1a	1743	1/1	0.86	0.23	72,72,72,72	0
54	MG	2A	3019	1/1	0.86	0.52	58,58,58,58	0
54	MG	2A	3170	1/1	0.86	0.23	61,61,61,61	0
54	MG	1a	1651	1/1	0.86	0.13	67,67,67,67	0
54	MG	2A	3179	1/1	0.86	0.25	76,76,76,76	0
54	MG	1A	3901	1/1	0.86	0.09	33,33,33,33	0
54	MG	1A	3134	1/1	0.86	0.15	51,51,51,51	0
54	MG	1A	3775	1/1	0.87	0.13	51,51,51,51	0
54	MG	1A	3890	1/1	0.87	0.17	71,71,71,71	0
54	MG	2A	3410	1/1	0.87	0.31	78,78,78,78	0
54	MG	2B	210	1/1	0.87	0.24	77,77,77,77	0
54	MG	11	104	1/1	0.87	0.16	63,63,63,63	0
54	MG	2A	3422	1/1	0.87	0.13	66,66,66,66	0
54	MG	2A	3427	1/1	0.87	0.12	71,71,71,71	0
54	MG	1A	3228	1/1	0.87	0.24	66,66,66,66	0
54	MG	2A	3436	1/1	0.87	0.15	76,76,76,76	0
54	MG	1A	3112	1/1	0.87	0.10	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	3439	1/1	0.87	0.11	41,41,41,41	0
54	MG	2D	313	1/1	0.87	0.35	70,70,70,70	0
54	MG	1A	3899	1/1	0.87	0.19	75,75,75,75	0
54	MG	1a	1601	1/1	0.87	0.38	78,78,78,78	0
54	MG	1a	1730	1/1	0.87	0.21	75,75,75,75	0
54	MG	2A	3156	1/1	0.87	0.18	72,72,72,72	0
54	MG	1a	1733	1/1	0.87	0.12	72,72,72,72	0
54	MG	1A	3259	1/1	0.87	0.16	45,45,45,45	0
54	MG	1A	3127	1/1	0.87	0.22	58,58,58,58	0
54	MG	2I	102	1/1	0.87	0.15	84,84,84,84	0
54	MG	1A	3679	1/1	0.87	0.12	63,63,63,63	0
54	MG	2A	3462	1/1	0.87	0.16	72,72,72,72	0
54	MG	2a	3004	1/1	0.87	0.11	56,56,56,56	0
54	MG	2A	3465	1/1	0.87	0.16	67,67,67,67	0
54	MG	1a	1614	1/1	0.87	0.11	67,67,67,67	0
54	MG	2a	3007	1/1	0.87	0.10	73,73,73,73	0
54	MG	1A	4035	1/1	0.87	0.21	66,66,66,66	0
54	MG	1A	3204	1/1	0.87	0.15	70,70,70,70	0
54	MG	1a	1750	1/1	0.87	0.17	76,76,76,76	0
54	MG	2a	3015	1/1	0.87	0.18	74,74,74,74	0
54	MG	1A	3690	1/1	0.87	0.21	41,41,41,41	0
54	MG	2a	3018	1/1	0.87	0.25	69,69,69,69	0
54	MG	2A	3479	1/1	0.87	0.17	69,69,69,69	0
54	MG	2A	3481	1/1	0.87	0.16	73,73,73,73	0
54	MG	2A	3483	1/1	0.87	0.10	75,75,75,75	0
54	MG	1A	3401	1/1	0.87	0.13	64,64,64,64	0
54	MG	2A	3486	1/1	0.87	0.10	76,76,76,76	0
54	MG	1a	1757	1/1	0.87	0.16	67,67,67,67	0
54	MG	1A	3693	1/1	0.87	0.10	61,61,61,61	0
54	MG	1A	3610	1/1	0.87	0.14	36,36,36,36	0
54	MG	1A	3612	1/1	0.87	0.12	55,55,55,55	0
54	MG	2a	3039	1/1	0.87	0.14	68,68,68,68	0
54	MG	2A	3197	1/1	0.87	0.26	70,70,70,70	0
54	MG	1a	1765	1/1	0.87	0.20	57,57,57,57	0
54	MG	2A	3206	1/1	0.87	0.16	66,66,66,66	0
54	MG	2a	3046	1/1	0.87	0.17	76,76,76,76	0
54	MG	2a	3048	1/1	0.87	0.21	84,84,84,84	0
54	MG	1a	1645	1/1	0.87	0.24	62,62,62,62	0
54	MG	1A	3958	1/1	0.87	0.09	34,34,34,34	0
54	MG	1I	202	1/1	0.87	0.18	75,75,75,75	0
54	MG	2A	3524	1/1	0.87	0.21	69,69,69,69	0
54	MG	2a	3056	1/1	0.87	0.16	73,73,73,73	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	1A	3613	1/1	0.87	0.21	67,67,67,67	0
54	MG	2A	3527	1/1	0.87	0.12	69,69,69,69	0
54	MG	1a	1773	1/1	0.87	0.18	83,83,83,83	0
54	MG	1a	1655	1/1	0.87	0.26	59,59,59,59	0
54	MG	1A	3621	1/1	0.87	0.13	69,69,69,69	0
54	MG	2A	3537	1/1	0.87	0.13	79,79,79,79	0
54	MG	1a	1662	1/1	0.87	0.15	81,81,81,81	0
54	MG	1A	3623	1/1	0.87	0.11	47,47,47,47	0
54	MG	1A	3429	1/1	0.87	0.20	60,60,60,60	0
54	MG	2A	3238	1/1	0.87	0.38	51,51,51,51	0
54	MG	1D	317	1/1	0.87	0.15	76,76,76,76	0
54	MG	1a	1668	1/1	0.87	0.20	73,73,73,73	0
54	MG	1A	3977	1/1	0.87	0.10	59,59,59,59	0
54	MG	2A	3264	1/1	0.87	0.10	73,73,73,73	0
54	MG	2A	3570	1/1	0.87	0.18	57,57,57,57	0
54	MG	2A	3571	1/1	0.87	0.16	46,46,46,46	0
54	MG	1a	1673	1/1	0.87	0.33	71,71,71,71	0
54	MG	1a	1676	1/1	0.87	0.19	75,75,75,75	0
54	MG	1a	1790	1/1	0.87	0.14	73,73,73,73	0
54	MG	1a	1678	1/1	0.87	0.20	55,55,55,55	0
54	MG	1F	315	1/1	0.87	0.23	72,72,72,72	0
54	MG	2A	3602	1/1	0.87	0.15	71,71,71,71	0
54	MG	1A	3435	1/1	0.87	0.27	60,60,60,60	0
54	MG	1A	3355	1/1	0.87	0.14	54,54,54,54	0
54	MG	2a	3112	1/1	0.87	0.10	84,84,84,84	0
54	MG	2A	3055	1/1	0.87	0.35	80,80,80,80	0
54	MG	2A	3280	1/1	0.87	0.23	65,65,65,65	0
54	MG	2A	3283	1/1	0.87	0.31	73,73,73,73	0
54	MG	1H	202	1/1	0.87	0.15	58,58,58,58	0
54	MG	2a	3124	1/1	0.87	0.14	74,74,74,74	0
54	MG	2A	3060	1/1	0.87	0.18	67,67,67,67	0
54	MG	2A	3294	1/1	0.87	0.17	65,65,65,65	0
54	MG	2a	3134	1/1	0.87	0.12	92,92,92,92	0
54	MG	2A	3068	1/1	0.87	0.21	70,70,70,70	0
54	MG	1A	3852	1/1	0.87	0.10	49,49,49,49	0
54	MG	1a	1804	1/1	0.87	0.28	77,77,77,77	0
54	MG	2A	3077	1/1	0.87	0.20	74,74,74,74	0
54	MG	2A	3081	1/1	0.87	0.23	68,68,68,68	0
54	MG	2A	3661	1/1	0.87	0.12	48,48,48,48	0
54	MG	1A	3047	1/1	0.87	0.24	61,61,61,61	0
54	MG	2A	3680	1/1	0.87	0.13	81,81,81,81	0
54	MG	1A	3449	1/1	0.87	0.17	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	3373	1/1	0.87	0.14	63,63,63,63	0
54	MG	1a	1694	1/1	0.87	0.24	62,62,62,62	0
54	MG	1A	3866	1/1	0.87	0.12	64,64,64,64	0
54	MG	2A	3699	1/1	0.87	0.15	71,71,71,71	0
54	MG	2A	3702	1/1	0.87	0.14	68,68,68,68	0
54	MG	1A	4004	1/1	0.87	0.23	52,52,52,52	0
54	MG	1a	1700	1/1	0.87	0.28	62,62,62,62	0
54	MG	1A	3510	1/1	0.87	0.10	31,31,31,31	0
54	MG	2A	3097	1/1	0.87	0.18	77,77,77,77	0
54	MG	1A	3520	1/1	0.87	0.20	60,60,60,60	0
54	MG	2e	202	1/1	0.87	0.17	77,77,77,77	0
54	MG	2A	3718	1/1	0.87	0.22	75,75,75,75	0
54	MG	1A	3590	1/1	0.87	0.14	61,61,61,61	0
54	MG	1a	1710	1/1	0.87	0.12	72,72,72,72	0
54	MG	2A	3723	1/1	0.87	0.16	85,85,85,85	0
57	MPD	1T	206	8/8	0.87	0.24	71,73,77,78	0
54	MG	2A	3387	1/1	0.87	0.16	74,74,74,74	0
54	MG	2A	3111	1/1	0.87	0.20	65,65,65,65	0
54	MG	2A	3391	1/1	0.87	0.17	75,75,75,75	0
54	MG	2A	3395	1/1	0.87	0.18	74,74,74,74	0
54	MG	1a	1729	1/1	0.88	0.16	72,72,72,72	0
54	MG	1A	3952	1/1	0.88	0.12	47,47,47,47	0
54	MG	2A	3161	1/1	0.88	0.15	71,71,71,71	0
54	MG	1a	1732	1/1	0.88	0.12	78,78,78,78	0
54	MG	1A	3201	1/1	0.88	0.25	68,68,68,68	0
54	MG	1a	1632	1/1	0.88	0.16	68,68,68,68	0
54	MG	1A	3722	1/1	0.88	0.23	43,43,43,43	0
54	MG	1A	3133	1/1	0.88	0.19	47,47,47,47	0
54	MG	2A	3173	1/1	0.88	0.30	71,71,71,71	0
54	MG	1A	3588	1/1	0.88	0.16	64,64,64,64	0
54	MG	2A	3470	1/1	0.88	0.13	74,74,74,74	0
54	MG	2A	3177	1/1	0.88	0.13	59,59,59,59	0
54	MG	1a	1872	1/1	0.88	0.11	58,58,58,58	0
54	MG	1A	3349	1/1	0.88	0.17	66,66,66,66	0
54	MG	1a	1876	1/1	0.88	0.15	62,62,62,62	0
54	MG	1a	1746	1/1	0.88	0.21	62,62,62,62	0
54	MG	1a	1643	1/1	0.88	0.16	61,61,61,61	0
54	MG	1A	3518	1/1	0.88	0.13	40,40,40,40	0
54	MG	1A	3737	1/1	0.88	0.19	35,35,35,35	0
54	MG	1a	1753	1/1	0.88	0.15	66,66,66,66	0
54	MG	2A	3194	1/1	0.88	0.48	80,80,80,80	0
54	MG	2A	3494	1/1	0.88	0.13	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	1650	1/1	0.88	0.28	65,65,65,65	0
54	MG	1D	301	1/1	0.88	0.18	50,50,50,50	0
54	MG	1f	201	1/1	0.88	0.21	78,78,78,78	0
54	MG	1a	1652	1/1	0.88	0.29	74,74,74,74	0
54	MG	1D	311	1/1	0.88	0.38	57,57,57,57	0
54	MG	1D	313	1/1	0.88	0.18	53,53,53,53	0
54	MG	1a	1764	1/1	0.88	0.14	72,72,72,72	0
54	MG	1n	101	1/1	0.88	0.38	76,76,76,76	0
54	MG	1A	3850	1/1	0.88	0.11	60,60,60,60	0
54	MG	1a	1663	1/1	0.88	0.20	75,75,75,75	0
54	MG	1a	1664	1/1	0.88	0.10	76,76,76,76	0
54	MG	2A	3528	1/1	0.88	0.14	66,66,66,66	0
54	MG	2a	3042	1/1	0.88	0.22	65,65,65,65	0
54	MG	2a	3043	1/1	0.88	0.12	85,85,85,85	0
54	MG	2A	3017	1/1	0.88	0.14	65,65,65,65	0
54	MG	2a	3045	1/1	0.88	0.24	73,73,73,73	0
54	MG	1F	311	1/1	0.88	0.23	61,61,61,61	0
54	MG	1F	312	1/1	0.88	0.17	45,45,45,45	0
54	MG	2A	3247	1/1	0.88	0.45	81,81,81,81	0
54	MG	1A	3739	1/1	0.88	0.20	59,59,59,59	0
54	MG	2A	3250	1/1	0.88	0.14	67,67,67,67	0
54	MG	2A	3251	1/1	0.88	0.18	51,51,51,51	0
54	MG	1A	3982	1/1	0.88	0.15	70,70,70,70	0
54	MG	1A	3207	1/1	0.88	0.24	67,67,67,67	0
54	MG	1a	1779	1/1	0.88	0.15	79,79,79,79	0
54	MG	1A	3293	1/1	0.88	0.10	74,74,74,74	0
54	MG	2A	3267	1/1	0.88	0.30	64,64,64,64	0
54	MG	2A	3039	1/1	0.88	0.27	77,77,77,77	0
54	MG	2A	3040	1/1	0.88	0.16	59,59,59,59	0
54	MG	2a	3068	1/1	0.88	0.20	78,78,78,78	0
54	MG	1A	3760	1/1	0.88	0.11	53,53,53,53	0
54	MG	1A	3524	1/1	0.88	0.10	46,46,46,46	0
54	MG	2A	3575	1/1	0.88	0.16	64,64,64,64	0
54	MG	2A	3274	1/1	0.88	0.20	60,60,60,60	0
54	MG	1a	1784	1/1	0.88	0.09	83,83,83,83	0
54	MG	2A	3049	1/1	0.88	0.38	82,82,82,82	0
54	MG	2A	3051	1/1	0.88	0.15	55,55,55,55	0
54	MG	2A	3604	1/1	0.88	0.13	51,51,51,51	0
54	MG	1A	3869	1/1	0.88	0.15	55,55,55,55	0
54	MG	2A	3282	1/1	0.88	0.39	73,73,73,73	0
54	MG	2A	3616	1/1	0.88	0.13	40,40,40,40	0
54	MG	1A	3022	1/1	0.88	0.12	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	3872	1/1	0.88	0.12	69,69,69,69	0
54	MG	2A	3285	1/1	0.88	0.20	61,61,61,61	0
54	MG	2a	3103	1/1	0.88	0.22	65,65,65,65	0
54	MG	1P	205	1/1	0.88	0.28	61,61,61,61	0
54	MG	1a	1684	1/1	0.88	0.26	70,70,70,70	0
54	MG	1a	1685	1/1	0.88	0.37	78,78,78,78	0
54	MG	2a	3109	1/1	0.88	0.33	57,57,57,57	0
54	MG	1A	3536	1/1	0.88	0.09	32,32,32,32	0
54	MG	2A	3633	1/1	0.88	0.18	70,70,70,70	0
54	MG	2a	3113	1/1	0.88	0.28	58,58,58,58	0
54	MG	2a	3114	1/1	0.88	0.37	72,72,72,72	0
54	MG	1a	1688	1/1	0.88	0.10	53,53,53,53	0
54	MG	1A	3188	1/1	0.88	0.16	63,63,63,63	0
54	MG	1A	3780	1/1	0.88	0.18	72,72,72,72	0
54	MG	1A	3115	1/1	0.88	0.11	55,55,55,55	0
54	MG	2A	3322	1/1	0.88	0.14	78,78,78,78	0
54	MG	2a	3127	1/1	0.88	0.23	79,79,79,79	0
54	MG	1A	3792	1/1	0.88	0.09	36,36,36,36	0
54	MG	1A	3797	1/1	0.88	0.10	46,46,46,46	0
54	MG	2A	3350	1/1	0.88	0.11	45,45,45,45	0
54	MG	1A	4018	1/1	0.88	0.15	48,48,48,48	0
54	MG	1a	1699	1/1	0.88	0.24	57,57,57,57	0
54	MG	1A	3027	1/1	0.88	0.26	72,72,72,72	0
54	MG	1A	3388	1/1	0.88	0.11	27,27,27,27	0
54	MG	1A	3905	1/1	0.88	0.12	55,55,55,55	0
54	MG	2a	3141	1/1	0.88	0.21	70,70,70,70	0
54	MG	1a	1706	1/1	0.88	0.35	71,71,71,71	0
54	MG	2a	3144	1/1	0.88	0.12	67,67,67,67	0
54	MG	1A	4031	1/1	0.88	0.10	60,60,60,60	0
54	MG	2A	3098	1/1	0.88	0.12	73,73,73,73	0
54	MG	1a	1826	1/1	0.88	0.11	76,76,76,76	0
54	MG	2a	3166	1/1	0.88	0.14	77,77,77,77	0
54	MG	1A	3617	1/1	0.88	0.13	61,61,61,61	0
54	MG	2A	3716	1/1	0.88	0.17	81,81,81,81	0
54	MG	1a	1602	1/1	0.88	0.21	77,77,77,77	0
54	MG	1A	3315	1/1	0.88	0.19	38,38,38,38	0
54	MG	1a	1609	1/1	0.88	0.32	62,62,62,62	0
54	MG	2a	3177	1/1	0.88	0.18	67,67,67,67	0
54	MG	1A	3199	1/1	0.88	0.11	55,55,55,55	0
54	MG	2A	3116	1/1	0.88	0.22	56,56,56,56	0
54	MG	2A	3408	1/1	0.88	0.14	57,57,57,57	0
54	MG	2a	3186	1/1	0.88	0.16	75,75,75,75	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	1A	3128	1/1	0.88	0.31	60,60,60,60	0
54	MG	2A	3121	1/1	0.88	0.15	74,74,74,74	0
54	MG	2A	3124	1/1	0.88	0.12	46,46,46,46	0
54	MG	2A	3426	1/1	0.88	0.14	58,58,58,58	0
54	MG	1A	3407	1/1	0.88	0.17	67,67,67,67	0
54	MG	2A	3126	1/1	0.88	0.14	72,72,72,72	0
54	MG	2A	3432	1/1	0.88	0.23	54,54,54,54	0
54	MG	2A	3129	1/1	0.88	0.13	67,67,67,67	0
54	MG	1A	3266	1/1	0.88	0.10	74,74,74,74	0
54	MG	2A	3138	1/1	0.88	0.17	66,66,66,66	0
54	MG	1a	1723	1/1	0.88	0.14	58,58,58,58	0
54	MG	1a	1727	1/1	0.88	0.11	64,64,64,64	0
54	MG	1B	225	1/1	0.89	0.11	52,52,52,52	0
54	MG	2A	3512	1/1	0.89	0.10	60,60,60,60	0
54	MG	2A	3513	1/1	0.89	0.15	65,65,65,65	0
54	MG	1a	1639	1/1	0.89	0.24	74,74,74,74	0
54	MG	1A	3576	1/1	0.89	0.10	44,44,44,44	0
54	MG	1B	228	1/1	0.89	0.11	76,76,76,76	0
54	MG	2A	3523	1/1	0.89	0.19	71,71,71,71	0
54	MG	1A	3301	1/1	0.89	0.13	66,66,66,66	0
54	MG	1A	3651	1/1	0.89	0.17	69,69,69,69	0
54	MG	1A	3390	1/1	0.89	0.22	78,78,78,78	0
54	MG	1A	3344	1/1	0.89	0.15	59,59,59,59	0
54	MG	1D	316	1/1	0.89	0.16	70,70,70,70	0
54	MG	2A	3533	1/1	0.89	0.10	73,73,73,73	0
54	MG	1a	1747	1/1	0.89	0.31	75,75,75,75	0
54	MG	1a	1748	1/1	0.89	0.19	66,66,66,66	0
54	MG	1A	3657	1/1	0.89	0.11	48,48,48,48	0
54	MG	1A	3248	1/1	0.89	0.11	73,73,73,73	0
54	MG	2a	3031	1/1	0.89	0.17	75,75,75,75	0
54	MG	2A	3115	1/1	0.89	0.24	65,65,65,65	0
54	MG	1A	3352	1/1	0.89	0.14	58,58,58,58	0
54	MG	1a	1657	1/1	0.89	0.13	77,77,77,77	0
54	MG	1A	3663	1/1	0.89	0.21	34,34,34,34	0
54	MG	2A	3551	1/1	0.89	0.09	59,59,59,59	0
54	MG	1A	3854	1/1	0.89	0.11	35,35,35,35	0
54	MG	1A	3744	1/1	0.89	0.13	58,58,58,58	0
54	MG	2A	3309	1/1	0.89	0.13	70,70,70,70	0
54	MG	1F	317	1/1	0.89	0.15	75,75,75,75	0
54	MG	1A	3596	1/1	0.89	0.23	64,64,64,64	0
54	MG	1a	1762	1/1	0.89	0.22	72,72,72,72	0
54	MG	1a	1763	1/1	0.89	0.30	76,76,76,76	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	2a	3047	1/1	0.89	0.34	72,72,72,72	0
54	MG	1A	3527	1/1	0.89	0.11	54,54,54,54	0
54	MG	2A	3141	1/1	0.89	0.14	54,54,54,54	0
54	MG	2A	3580	1/1	0.89	0.13	68,68,68,68	0
54	MG	2A	3583	1/1	0.89	0.13	75,75,75,75	0
54	MG	2A	3339	1/1	0.89	0.10	52,52,52,52	0
54	MG	2a	3055	1/1	0.89	0.13	76,76,76,76	0
54	MG	1A	3867	1/1	0.89	0.11	41,41,41,41	0
54	MG	2a	3058	1/1	0.89	0.23	79,79,79,79	0
54	MG	2A	3351	1/1	0.89	0.10	54,54,54,54	0
54	MG	1e	202	1/1	0.89	0.12	62,62,62,62	0
54	MG	2A	3144	1/1	0.89	0.16	60,60,60,60	0
54	MG	2A	3154	1/1	0.89	0.28	64,64,64,64	0
54	MG	2A	3155	1/1	0.89	0.17	70,70,70,70	0
54	MG	1A	3762	1/1	0.89	0.10	62,62,62,62	0
54	MG	2A	3373	1/1	0.89	0.14	59,59,59,59	0
54	MG	1A	4005	1/1	0.89	0.15	47,47,47,47	0
54	MG	1A	3250	1/1	0.89	0.33	66,66,66,66	0
54	MG	1A	3280	1/1	0.89	0.24	48,48,48,48	0
54	MG	1A	3430	1/1	0.89	0.15	61,61,61,61	0
54	MG	2a	3083	1/1	0.89	0.33	77,77,77,77	0
54	MG	1A	3673	1/1	0.89	0.14	62,62,62,62	0
54	MG	1T	203	1/1	0.89	0.20	65,65,65,65	0
54	MG	2A	3171	1/1	0.89	0.15	56,56,56,56	0
54	MG	1A	4014	1/1	0.89	0.10	93,93,93,93	0
54	MG	2a	3090	1/1	0.89	0.17	70,70,70,70	0
54	MG	1V	205	1/1	0.89	0.17	72,72,72,72	0
54	MG	2A	3638	1/1	0.89	0.12	70,70,70,70	0
54	MG	1A	3882	1/1	0.89	0.27	43,43,43,43	0
54	MG	2A	3407	1/1	0.89	0.12	68,68,68,68	0
54	MG	2A	3016	1/1	0.89	0.30	77,77,77,77	0
54	MG	2A	3678	1/1	0.89	0.13	73,73,73,73	0
54	MG	1A	3192	1/1	0.89	0.11	53,53,53,53	0
54	MG	2a	3104	1/1	0.89	0.32	71,71,71,71	0
54	MG	2A	3683	1/1	0.89	0.11	50,50,50,50	0
54	MG	1A	3544	1/1	0.89	0.07	28,28,28,28	0
54	MG	1A	3790	1/1	0.89	0.27	73,73,73,73	0
54	MG	2A	3690	1/1	0.89	0.09	57,57,57,57	0
54	MG	11	102	1/1	0.89	0.13	62,62,62,62	0
54	MG	1A	3486	1/1	0.89	0.21	73,73,73,73	0
54	MG	14	101	1/1	0.89	0.08	82,82,82,82	0
54	MG	2A	3190	1/1	0.89	0.20	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	3191	1/1	0.89	0.31	76,76,76,76	0
54	MG	1A	3375	1/1	0.89	0.15	63,63,63,63	0
54	MG	1A	3198	1/1	0.89	0.12	55,55,55,55	0
54	MG	1A	3904	1/1	0.89	0.10	52,52,52,52	0
54	MG	2A	3709	1/1	0.89	0.14	65,65,65,65	0
54	MG	2A	3198	1/1	0.89	0.41	75,75,75,75	0
54	MG	2A	3200	1/1	0.89	0.26	76,76,76,76	0
54	MG	2a	3130	1/1	0.89	0.12	64,64,64,64	0
54	MG	2A	3448	1/1	0.89	0.20	72,72,72,72	0
54	MG	2A	3720	1/1	0.89	0.14	73,73,73,73	0
54	MG	1A	3616	1/1	0.89	0.11	57,57,57,57	0
54	MG	1A	3696	1/1	0.89	0.10	51,51,51,51	0
54	MG	2A	3458	1/1	0.89	0.11	69,69,69,69	0
54	MG	1a	1603	1/1	0.89	0.15	75,75,75,75	0
54	MG	1A	3499	1/1	0.89	0.09	27,27,27,27	0
54	MG	1A	3699	1/1	0.89	0.10	71,71,71,71	0
54	MG	1A	3067	1/1	0.89	0.13	57,57,57,57	0
54	MG	2B	201	1/1	0.89	0.10	86,86,86,86	0
54	MG	1A	3206	1/1	0.89	0.08	50,50,50,50	0
54	MG	2B	203	1/1	0.89	0.21	79,79,79,79	0
54	MG	1a	1812	1/1	0.89	0.08	78,78,78,78	0
54	MG	2a	3165	1/1	0.89	0.27	79,79,79,79	0
54	MG	1B	207	1/1	0.89	0.43	73,73,73,73	0
54	MG	2A	3226	1/1	0.89	0.26	58,58,58,58	0
54	MG	2A	3229	1/1	0.89	0.11	77,77,77,77	0
54	MG	2A	3476	1/1	0.89	0.12	69,69,69,69	0
54	MG	1a	1714	1/1	0.89	0.16	68,68,68,68	0
54	MG	2a	3172	1/1	0.89	0.10	76,76,76,76	0
54	MG	1A	3624	1/1	0.89	0.09	45,45,45,45	0
54	MG	1A	3821	1/1	0.89	0.12	65,65,65,65	0
54	MG	2A	3066	1/1	0.89	0.07	66,66,66,66	0
54	MG	1a	1625	1/1	0.89	0.12	64,64,64,64	0
54	MG	2D	312	1/1	0.89	0.14	73,73,73,73	0
54	MG	1a	1628	1/1	0.89	0.33	70,70,70,70	0
54	MG	1A	3822	1/1	0.89	0.13	56,56,56,56	0
54	MG	2a	3190	1/1	0.89	0.16	68,68,68,68	0
54	MG	1a	1828	1/1	0.89	0.18	56,56,56,56	0
54	MG	1A	3563	1/1	0.89	0.36	41,41,41,41	0
54	MG	1A	3955	1/1	0.89	0.10	62,62,62,62	0
54	MG	2A	3263	1/1	0.89	0.40	69,69,69,69	0
54	MG	1a	1636	1/1	0.89	0.31	66,66,66,66	0
54	MG	2P	201	1/1	0.89	0.12	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	2A	3265	1/1	0.89	0.14	74,74,74,74	0
54	MG	2V	202	1/1	0.89	0.24	65,65,65,65	0
54	MG	1a	1837	1/1	0.89	0.23	72,72,72,72	0
54	MG	25	101	1/1	0.89	0.50	57,57,57,57	0
54	MG	25	103	1/1	0.89	0.14	74,74,74,74	0
54	MG	1h	201	1/1	0.90	0.18	59,59,59,59	0
54	MG	2A	3449	1/1	0.90	0.28	47,47,47,47	0
54	MG	1A	3525	1/1	0.90	0.12	61,61,61,61	0
54	MG	1l	201	1/1	0.90	0.30	71,71,71,71	0
54	MG	2A	3187	1/1	0.90	0.22	78,78,78,78	0
54	MG	1B	224	1/1	0.90	0.19	74,74,74,74	0
54	MG	1A	3302	1/1	0.90	0.17	50,50,50,50	0
54	MG	1a	1644	1/1	0.90	0.25	59,59,59,59	0
54	MG	1A	3685	1/1	0.90	0.08	24,24,24,24	0
54	MG	2A	3193	1/1	0.90	0.20	67,67,67,67	0
54	MG	1y	203	1/1	0.90	0.13	90,90,90,90	0
54	MG	1B	227	1/1	0.90	0.19	76,76,76,76	0
54	MG	1A	3808	1/1	0.90	0.10	64,64,64,64	0
54	MG	2T	203	1/1	0.90	0.18	63,63,63,63	0
54	MG	1A	3105	1/1	0.90	0.11	63,63,63,63	0
54	MG	1A	3533	1/1	0.90	0.12	63,63,63,63	0
54	MG	20	101	1/1	0.90	0.12	59,59,59,59	0
54	MG	1A	3110	1/1	0.90	0.15	52,52,52,52	0
54	MG	1A	3211	1/1	0.90	0.27	70,70,70,70	0
54	MG	1D	315	1/1	0.90	0.10	68,68,68,68	0
54	MG	1a	1659	1/1	0.90	0.33	79,79,79,79	0
54	MG	2A	3032	1/1	0.90	0.31	68,68,68,68	0
54	MG	2A	3212	1/1	0.90	0.13	62,62,62,62	0
54	MG	1A	3316	1/1	0.90	0.15	54,54,54,54	0
54	MG	1A	3968	1/1	0.90	0.09	61,61,61,61	0
54	MG	1E	301	1/1	0.90	0.34	52,52,52,52	0
54	MG	2A	3224	1/1	0.90	0.21	66,66,66,66	0
54	MG	2A	3225	1/1	0.90	0.47	57,57,57,57	0
54	MG	1E	303	1/1	0.90	0.30	57,57,57,57	0
54	MG	1A	3277	1/1	0.90	0.14	73,73,73,73	0
54	MG	2A	3505	1/1	0.90	0.10	78,78,78,78	0
54	MG	2A	3041	1/1	0.90	0.14	54,54,54,54	0
54	MG	1A	3620	1/1	0.90	0.10	58,58,58,58	0
54	MG	1A	3823	1/1	0.90	0.26	46,46,46,46	0
54	MG	2A	3234	1/1	0.90	0.14	70,70,70,70	0
54	MG	2A	3235	1/1	0.90	0.15	75,75,75,75	0
54	MG	2A	3518	1/1	0.90	0.14	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	2a	3029	1/1	0.90	0.20	76,76,76,76	0
54	MG	2a	3030	1/1	0.90	0.19	69,69,69,69	0
54	MG	2A	3519	1/1	0.90	0.11	85,85,85,85	0
54	MG	1A	3322	1/1	0.90	0.31	48,48,48,48	0
54	MG	2a	3033	1/1	0.90	0.28	70,70,70,70	0
54	MG	2A	3239	1/1	0.90	0.35	65,65,65,65	0
54	MG	1A	3980	1/1	0.90	0.17	52,52,52,52	0
54	MG	1A	3031	1/1	0.90	0.08	25,25,25,25	0
54	MG	1a	1677	1/1	0.90	0.16	67,67,67,67	0
54	MG	1A	3327	1/1	0.90	0.14	70,70,70,70	0
54	MG	1A	3984	1/1	0.90	0.12	46,46,46,46	0
54	MG	1A	3630	1/1	0.90	0.09	70,70,70,70	0
54	MG	2A	3056	1/1	0.90	0.22	63,63,63,63	0
54	MG	2A	3534	1/1	0.90	0.12	63,63,63,63	0
54	MG	1A	3843	1/1	0.90	0.09	20,20,20,20	0
54	MG	1A	3152	1/1	0.90	0.15	62,62,62,62	0
54	MG	2A	3061	1/1	0.90	0.17	76,76,76,76	0
54	MG	2A	3063	1/1	0.90	0.23	61,61,61,61	0
54	MG	2A	3065	1/1	0.90	0.09	51,51,51,51	0
54	MG	1A	3720	1/1	0.90	0.13	56,56,56,56	0
54	MG	1A	3998	1/1	0.90	0.13	55,55,55,55	0
54	MG	1A	3721	1/1	0.90	0.35	49,49,49,49	0
54	MG	1A	3637	1/1	0.90	0.21	42,42,42,42	0
54	MG	1A	3483	1/1	0.90	0.14	48,48,48,48	0
54	MG	1A	3061	1/1	0.90	0.14	56,56,56,56	0
54	MG	1V	204	1/1	0.90	0.13	65,65,65,65	0
54	MG	2A	3085	1/1	0.90	0.46	58,58,58,58	0
54	MG	1A	3644	1/1	0.90	0.11	29,29,29,29	0
54	MG	2a	3062	1/1	0.90	0.15	81,81,81,81	0
54	MG	2a	3063	1/1	0.90	0.24	75,75,75,75	0
54	MG	1A	3732	1/1	0.90	0.13	69,69,69,69	0
54	MG	1A	3647	1/1	0.90	0.12	39,39,39,39	0
54	MG	10	102	1/1	0.90	0.22	46,46,46,46	0
54	MG	2A	3577	1/1	0.90	0.13	64,64,64,64	0
54	MG	1A	3648	1/1	0.90	0.14	69,69,69,69	0
54	MG	1A	3405	1/1	0.90	0.17	58,58,58,58	0
54	MG	2a	3077	1/1	0.90	0.17	66,66,66,66	0
54	MG	1a	1825	1/1	0.90	0.12	79,79,79,79	0
54	MG	1A	3489	1/1	0.90	0.14	64,64,64,64	0
54	MG	2A	3590	1/1	0.90	0.15	58,58,58,58	0
54	MG	2A	3592	1/1	0.90	0.10	56,56,56,56	0
54	MG	1a	1705	1/1	0.90	0.26	62,62,62,62	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	2A	3599	1/1	0.90	0.12	75,75,75,75	0
54	MG	2A	3300	1/1	0.90	0.18	67,67,67,67	0
54	MG	1A	3290	1/1	0.90	0.33	51,51,51,51	0
54	MG	2A	3103	1/1	0.90	0.23	64,64,64,64	0
54	MG	2a	3095	1/1	0.90	0.27	79,79,79,79	0
54	MG	2A	3610	1/1	0.90	0.16	49,49,49,49	0
54	MG	2A	3319	1/1	0.90	0.09	44,44,44,44	0
54	MG	1l	105	1/1	0.90	0.10	47,47,47,47	0
54	MG	1A	3340	1/1	0.90	0.10	46,46,46,46	0
54	MG	1a	1711	1/1	0.90	0.20	69,69,69,69	0
54	MG	15	103	1/1	0.90	0.26	46,46,46,46	0
54	MG	2A	3326	1/1	0.90	0.26	76,76,76,76	0
54	MG	2A	3624	1/1	0.90	0.15	61,61,61,61	0
54	MG	2A	3328	1/1	0.90	0.25	72,72,72,72	0
54	MG	2A	3332	1/1	0.90	0.15	76,76,76,76	0
54	MG	1A	3658	1/1	0.90	0.18	56,56,56,56	0
54	MG	2A	3114	1/1	0.90	0.31	70,70,70,70	0
54	MG	2A	3341	1/1	0.90	0.09	45,45,45,45	0
54	MG	2A	3349	1/1	0.90	0.15	67,67,67,67	0
54	MG	17	106	1/1	0.90	0.16	62,62,62,62	0
54	MG	1a	1843	1/1	0.90	0.08	77,77,77,77	0
54	MG	1a	1849	1/1	0.90	0.12	63,63,63,63	0
54	MG	2A	3656	1/1	0.90	0.10	62,62,62,62	0
54	MG	1A	3502	1/1	0.90	0.11	42,42,42,42	0
54	MG	2A	3666	1/1	0.90	0.16	57,57,57,57	0
54	MG	2a	3126	1/1	0.90	0.27	78,78,78,78	0
54	MG	2A	3671	1/1	0.90	0.14	60,60,60,60	0
54	MG	2a	3128	1/1	0.90	0.21	73,73,73,73	0
54	MG	1A	4029	1/1	0.90	0.23	59,59,59,59	0
54	MG	19	102	1/1	0.90	0.14	61,61,61,61	0
54	MG	2A	3679	1/1	0.90	0.16	63,63,63,63	0
54	MG	1A	3160	1/1	0.90	0.69	51,51,51,51	0
54	MG	1A	3886	1/1	0.90	0.14	52,52,52,52	0
54	MG	1A	3768	1/1	0.90	0.23	69,69,69,69	0
54	MG	2A	3375	1/1	0.90	0.30	73,73,73,73	0
54	MG	2A	3376	1/1	0.90	0.12	70,70,70,70	0
54	MG	1A	3889	1/1	0.90	0.10	47,47,47,47	0
54	MG	2A	3694	1/1	0.90	0.15	56,56,56,56	0
54	MG	2A	3696	1/1	0.90	0.08	55,55,55,55	0
54	MG	1a	1607	1/1	0.90	0.18	69,69,69,69	0
54	MG	2a	3145	1/1	0.90	0.20	72,72,72,72	0
54	MG	1A	3506	1/1	0.90	0.12	52,52,52,52	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	1A	3664	1/1	0.90	0.15	55,55,55,55	0
54	MG	1A	3036	1/1	0.90	0.10	41,41,41,41	0
54	MG	2a	3156	1/1	0.90	0.23	72,72,72,72	0
54	MG	2a	3160	1/1	0.90	0.19	79,79,79,79	0
54	MG	1a	1735	1/1	0.90	0.13	70,70,70,70	0
54	MG	1B	201	1/1	0.90	0.20	64,64,64,64	0
54	MG	2A	3399	1/1	0.90	0.12	45,45,45,45	0
54	MG	2a	3168	1/1	0.90	0.20	75,75,75,75	0
54	MG	1B	203	1/1	0.90	0.38	77,77,77,77	0
54	MG	2A	3404	1/1	0.90	0.14	54,54,54,54	0
54	MG	2A	3405	1/1	0.90	0.12	57,57,57,57	0
54	MG	1a	1620	1/1	0.90	0.19	71,71,71,71	0
54	MG	1A	3595	1/1	0.90	0.12	48,48,48,48	0
54	MG	2a	3176	1/1	0.90	0.14	72,72,72,72	0
54	MG	1A	3783	1/1	0.90	0.13	66,66,66,66	0
54	MG	1a	1879	1/1	0.90	0.20	75,75,75,75	0
54	MG	2A	3414	1/1	0.90	0.23	66,66,66,66	0
54	MG	1A	3350	1/1	0.90	0.12	63,63,63,63	0
54	MG	1B	209	1/1	0.90	0.11	58,58,58,58	0
54	MG	2A	3727	1/1	0.90	0.13	74,74,74,74	0
54	MG	2A	3167	1/1	0.90	0.24	61,61,61,61	0
54	MG	2A	3169	1/1	0.90	0.15	67,67,67,67	0
54	MG	2A	3428	1/1	0.90	0.23	67,67,67,67	0
54	MG	1d	302	1/1	0.90	0.36	82,82,82,82	0
54	MG	1A	3785	1/1	0.90	0.17	52,52,52,52	0
54	MG	2r	101	1/1	0.90	0.22	80,80,80,80	0
54	MG	1B	211	1/1	0.90	0.29	71,71,71,71	0
54	MG	1A	3032	1/1	0.90	0.15	65,65,65,65	0
54	MG	1A	3130	1/1	0.90	0.16	64,64,64,64	0
54	MG	1A	3450	1/1	0.90	0.09	27,27,27,27	0
54	MG	2B	212	1/1	0.90	0.09	95,95,95,95	0
54	MG	1f	202	1/1	0.90	0.13	55,55,55,55	0
54	MG	1a	1754	1/1	0.90	0.16	77,77,77,77	0
59	ZN	24	501	1/1	0.90	0.09	140,140,140,140	0
54	MG	2A	3520	1/1	0.91	0.16	76,76,76,76	0
54	MG	2A	3110	1/1	0.91	0.12	69,69,69,69	0
54	MG	1A	3222	1/1	0.91	0.20	55,55,55,55	0
54	MG	1A	3945	1/1	0.91	0.10	62,62,62,62	0
54	MG	1A	3571	1/1	0.91	0.12	52,52,52,52	0
54	MG	1a	1739	1/1	0.91	0.16	72,72,72,72	0
54	MG	1a	1740	1/1	0.91	0.21	60,60,60,60	0
54	MG	1a	1871	1/1	0.91	0.27	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	3289	1/1	0.91	0.20	68,68,68,68	0
54	MG	2A	3531	1/1	0.91	0.34	57,57,57,57	0
54	MG	2A	3532	1/1	0.91	0.12	62,62,62,62	0
54	MG	1A	3385	1/1	0.91	0.12	50,50,50,50	0
54	MG	2A	3120	1/1	0.91	0.20	52,52,52,52	0
54	MG	1A	3706	1/1	0.91	0.10	80,80,80,80	0
54	MG	1a	1875	1/1	0.91	0.32	70,70,70,70	0
54	MG	1A	3709	1/1	0.91	0.09	35,35,35,35	0
54	MG	2A	3308	1/1	0.91	0.19	68,68,68,68	0
54	MG	1A	3819	1/1	0.91	0.10	49,49,49,49	0
54	MG	2A	3540	1/1	0.91	0.26	65,65,65,65	0
54	MG	1a	1640	1/1	0.91	0.21	78,78,78,78	0
54	MG	1A	3712	1/1	0.91	0.11	67,67,67,67	0
54	MG	2a	3025	1/1	0.91	0.27	70,70,70,70	0
54	MG	2A	3544	1/1	0.91	0.11	60,60,60,60	0
54	MG	2A	3132	1/1	0.91	0.14	62,62,62,62	0
54	MG	2A	3550	1/1	0.91	0.14	65,65,65,65	0
54	MG	2A	3133	1/1	0.91	0.37	72,72,72,72	0
54	MG	1A	3515	1/1	0.91	0.08	74,74,74,74	0
54	MG	2A	3557	1/1	0.91	0.26	59,59,59,59	0
54	MG	2A	3559	1/1	0.91	0.09	64,64,64,64	0
54	MG	1A	3966	1/1	0.91	0.23	33,33,33,33	0
54	MG	1A	3141	1/1	0.91	0.10	57,57,57,57	0
54	MG	1A	3587	1/1	0.91	0.12	61,61,61,61	0
54	MG	1d	304	1/1	0.91	0.28	71,71,71,71	0
54	MG	1A	3827	1/1	0.91	0.27	52,52,52,52	0
54	MG	1A	3049	1/1	0.91	0.28	57,57,57,57	0
54	MG	1E	305	1/1	0.91	0.12	31,31,31,31	0
54	MG	1A	3650	1/1	0.91	0.11	31,31,31,31	0
54	MG	1A	3461	1/1	0.91	0.08	66,66,66,66	0
54	MG	1A	3836	1/1	0.91	0.09	65,65,65,65	0
54	MG	2A	3581	1/1	0.91	0.12	70,70,70,70	0
54	MG	1A	3837	1/1	0.91	0.11	72,72,72,72	0
54	MG	2A	3584	1/1	0.91	0.09	54,54,54,54	0
54	MG	1a	1658	1/1	0.91	0.21	52,52,52,52	0
54	MG	2A	3587	1/1	0.91	0.16	61,61,61,61	0
54	MG	1A	3838	1/1	0.91	0.07	33,33,33,33	0
54	MG	2A	3363	1/1	0.91	0.15	84,84,84,84	0
54	MG	1A	3343	1/1	0.91	0.23	65,65,65,65	0
54	MG	1G	203	1/1	0.91	0.10	57,57,57,57	0
54	MG	2A	3369	1/1	0.91	0.13	51,51,51,51	0
54	MG	1A	3591	1/1	0.91	0.15	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	1t	201	1/1	0.91	0.10	66,66,66,66	0
54	MG	2A	3172	1/1	0.91	0.15	66,66,66,66	0
54	MG	1A	3593	1/1	0.91	0.16	57,57,57,57	0
54	MG	1A	3311	1/1	0.91	0.27	74,74,74,74	0
54	MG	1A	3995	1/1	0.91	0.11	65,65,65,65	0
54	MG	2a	3065	1/1	0.91	0.30	80,80,80,80	0
54	MG	2A	3178	1/1	0.91	0.11	71,71,71,71	0
54	MG	2A	3005	1/1	0.91	0.10	63,63,63,63	0
54	MG	1A	3470	1/1	0.91	0.21	77,77,77,77	0
54	MG	2a	3070	1/1	0.91	0.08	72,72,72,72	0
54	MG	1a	1776	1/1	0.91	0.16	79,79,79,79	0
54	MG	2A	3625	1/1	0.91	0.10	69,69,69,69	0
54	MG	1A	3738	1/1	0.91	0.11	47,47,47,47	0
54	MG	2A	3627	1/1	0.91	0.14	72,72,72,72	0
54	MG	2A	3628	1/1	0.91	0.09	63,63,63,63	0
54	MG	2A	3396	1/1	0.91	0.11	67,67,67,67	0
54	MG	1a	1670	1/1	0.91	0.13	66,66,66,66	0
54	MG	2A	3632	1/1	0.91	0.14	64,64,64,64	0
54	MG	2A	3400	1/1	0.91	0.14	60,60,60,60	0
54	MG	1A	3598	1/1	0.91	0.17	71,71,71,71	0
54	MG	2A	3186	1/1	0.91	0.20	70,70,70,70	0
54	MG	2a	3091	1/1	0.91	0.15	70,70,70,70	0
54	MG	2A	3023	1/1	0.91	0.20	74,74,74,74	0
54	MG	1R	202	1/1	0.91	0.15	48,48,48,48	0
54	MG	2A	3639	1/1	0.91	0.12	62,62,62,62	0
54	MG	1A	3231	1/1	0.91	0.22	47,47,47,47	0
54	MG	1A	3529	1/1	0.91	0.09	52,52,52,52	0
54	MG	2A	3657	1/1	0.91	0.12	61,61,61,61	0
54	MG	1A	3531	1/1	0.91	0.17	73,73,73,73	0
54	MG	1A	3759	1/1	0.91	0.09	51,51,51,51	0
54	MG	1A	3314	1/1	0.91	0.17	65,65,65,65	0
54	MG	1A	3004	1/1	0.91	0.11	52,52,52,52	0
54	MG	1A	3766	1/1	0.91	0.15	57,57,57,57	0
54	MG	2a	3107	1/1	0.91	0.41	66,66,66,66	0
54	MG	1A	3537	1/1	0.91	0.07	23,23,23,23	0
54	MG	1A	3208	1/1	0.91	0.08	55,55,55,55	0
54	MG	2A	3044	1/1	0.91	0.11	62,62,62,62	0
54	MG	2a	3111	1/1	0.91	0.43	74,74,74,74	0
54	MG	1A	3611	1/1	0.91	0.11	60,60,60,60	0
54	MG	2A	3433	1/1	0.91	0.12	63,63,63,63	0
54	MG	1A	4019	1/1	0.91	0.10	57,57,57,57	0
54	MG	2A	3209	1/1	0.91	0.33	60,60,60,60	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	2a	3117	1/1	0.91	0.14	76,76,76,76	0
54	MG	10	108	1/1	0.91	0.14	69,69,69,69	0
54	MG	2A	3695	1/1	0.91	0.16	74,74,74,74	0
54	MG	1A	3879	1/1	0.91	0.10	50,50,50,50	0
54	MG	1A	3249	1/1	0.91	0.23	70,70,70,70	0
54	MG	1A	3885	1/1	0.91	0.09	41,41,41,41	0
54	MG	1A	3676	1/1	0.91	0.14	56,56,56,56	0
54	MG	2A	3218	1/1	0.91	0.22	73,73,73,73	0
54	MG	1A	3432	1/1	0.91	0.13	71,71,71,71	0
54	MG	2A	3221	1/1	0.91	0.20	67,67,67,67	0
54	MG	2A	3454	1/1	0.91	0.10	58,58,58,58	0
54	MG	2A	3457	1/1	0.91	0.16	62,62,62,62	0
54	MG	2A	3710	1/1	0.91	0.08	70,70,70,70	0
54	MG	15	105	1/1	0.91	0.22	72,72,72,72	0
54	MG	15	106	1/1	0.91	0.23	38,38,38,38	0
54	MG	2A	3717	1/1	0.91	0.09	56,56,56,56	0
54	MG	2A	3059	1/1	0.91	0.12	54,54,54,54	0
54	MG	2A	3719	1/1	0.91	0.10	79,79,79,79	0
54	MG	2a	3142	1/1	0.91	0.11	82,82,82,82	0
54	MG	1A	3888	1/1	0.91	0.07	50,50,50,50	0
54	MG	1A	3093	1/1	0.91	0.12	52,52,52,52	0
54	MG	1A	3687	1/1	0.91	0.12	33,33,33,33	0
54	MG	1A	3254	1/1	0.91	0.13	55,55,55,55	0
54	MG	1A	3786	1/1	0.91	0.09	36,36,36,36	0
54	MG	1A	4039	1/1	0.91	0.15	66,66,66,66	0
54	MG	2A	3726	1/1	0.91	0.23	69,69,69,69	0
54	MG	2A	3473	1/1	0.91	0.09	79,79,79,79	0
54	MG	2a	3161	1/1	0.91	0.16	78,78,78,78	0
54	MG	1A	3619	1/1	0.91	0.11	42,42,42,42	0
54	MG	1A	3443	1/1	0.91	0.11	71,71,71,71	0
54	MG	2A	3240	1/1	0.91	0.21	68,68,68,68	0
54	MG	2A	3243	1/1	0.91	0.19	62,62,62,62	0
54	MG	2A	3245	1/1	0.91	0.08	66,66,66,66	0
54	MG	1A	3214	1/1	0.91	0.21	56,56,56,56	0
54	MG	2B	205	1/1	0.91	0.34	71,71,71,71	0
54	MG	2B	207	1/1	0.91	0.24	76,76,76,76	0
54	MG	2A	3078	1/1	0.91	0.09	60,60,60,60	0
54	MG	1A	3799	1/1	0.91	0.14	55,55,55,55	0
54	MG	1A	3447	1/1	0.91	0.11	36,36,36,36	0
54	MG	2A	3487	1/1	0.91	0.17	87,87,87,87	0
54	MG	2A	3489	1/1	0.91	0.22	72,72,72,72	0
54	MG	2a	3183	1/1	0.91	0.11	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	1A	3448	1/1	0.91	0.14	53,53,53,53	0
54	MG	1A	3909	1/1	0.91	0.17	43,43,43,43	0
54	MG	1a	1613	1/1	0.91	0.23	75,75,75,75	0
54	MG	2B	218	1/1	0.91	0.13	79,79,79,79	0
54	MG	2D	302	1/1	0.91	0.16	57,57,57,57	0
54	MG	1A	3915	1/1	0.91	0.08	57,57,57,57	0
54	MG	1a	1725	1/1	0.91	0.20	53,53,53,53	0
54	MG	1a	1726	1/1	0.91	0.14	86,86,86,86	0
54	MG	1A	3698	1/1	0.91	0.18	39,39,39,39	0
54	MG	1A	3924	1/1	0.91	0.15	35,35,35,35	0
54	MG	2A	3508	1/1	0.91	0.16	72,72,72,72	0
57	MPD	1A	4043	8/8	0.91	0.18	56,63,69,69	0
54	MG	1a	1854	1/1	0.91	0.17	74,74,74,74	0
54	MG	1a	1858	1/1	0.91	0.14	86,86,86,86	0
54	MG	1A	3931	1/1	0.91	0.12	31,31,31,31	0
57	MPD	2A	3734	8/8	0.91	0.23	72,77,82,83	0
54	MG	1a	1731	1/1	0.91	0.14	61,61,61,61	0
54	MG	1A	3220	1/1	0.91	0.38	74,74,74,74	0
54	MG	1a	1627	1/1	0.91	0.40	77,77,77,77	0
54	MG	1A	3174	1/1	0.92	0.16	59,59,59,59	0
54	MG	1A	3076	1/1	0.92	0.08	44,44,44,44	0
54	MG	27	101	1/1	0.92	0.34	62,62,62,62	0
54	MG	2A	3134	1/1	0.92	0.32	66,66,66,66	0
54	MG	2A	3314	1/1	0.92	0.10	68,68,68,68	0
54	MG	2a	3003	1/1	0.92	0.10	71,71,71,71	0
54	MG	1A	3281	1/1	0.92	0.14	64,64,64,64	0
54	MG	1A	3324	1/1	0.92	0.23	65,65,65,65	0
54	MG	1a	1661	1/1	0.92	0.16	65,65,65,65	0
54	MG	1A	3868	1/1	0.92	0.11	43,43,43,43	0
54	MG	1N	204	1/1	0.92	0.13	60,60,60,60	0
54	MG	1g	201	1/1	0.92	0.28	74,74,74,74	0
54	MG	2A	3151	1/1	0.92	0.17	65,65,65,65	0
54	MG	1A	3282	1/1	0.92	0.09	60,60,60,60	0
54	MG	1a	1766	1/1	0.92	0.27	70,70,70,70	0
54	MG	2A	3556	1/1	0.92	0.10	76,76,76,76	0
54	MG	2A	3338	1/1	0.92	0.10	41,41,41,41	0
54	MG	1A	3465	1/1	0.92	0.11	56,56,56,56	0
54	MG	2A	3563	1/1	0.92	0.28	67,67,67,67	0
54	MG	2A	3566	1/1	0.92	0.10	74,74,74,74	0
54	MG	2A	3160	1/1	0.92	0.29	50,50,50,50	0
54	MG	2A	3344	1/1	0.92	0.10	46,46,46,46	0
54	MG	1i	201	1/1	0.92	0.21	76,76,76,76	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	1A	3469	1/1	0.92	0.14	48,48,48,48	0
54	MG	1A	3011	1/1	0.92	0.22	70,70,70,70	0
54	MG	1A	3683	1/1	0.92	0.07	33,33,33,33	0
54	MG	1A	3119	1/1	0.92	0.32	47,47,47,47	0
54	MG	1n	102	1/1	0.92	0.10	61,61,61,61	0
54	MG	1A	4007	1/1	0.92	0.13	62,62,62,62	0
54	MG	1a	1671	1/1	0.92	0.30	64,64,64,64	0
54	MG	1a	1672	1/1	0.92	0.30	74,74,74,74	0
54	MG	1a	1778	1/1	0.92	0.09	73,73,73,73	0
54	MG	2A	3370	1/1	0.92	0.12	49,49,49,49	0
54	MG	1A	3686	1/1	0.92	0.13	58,58,58,58	0
54	MG	2A	3006	1/1	0.92	0.10	57,57,57,57	0
54	MG	2A	3176	1/1	0.92	0.19	62,62,62,62	0
54	MG	1A	3399	1/1	0.92	0.10	49,49,49,49	0
54	MG	2A	3012	1/1	0.92	0.12	68,68,68,68	0
54	MG	2A	3384	1/1	0.92	0.12	73,73,73,73	0
54	MG	1A	3012	1/1	0.92	0.13	55,55,55,55	0
54	MG	2A	3603	1/1	0.92	0.09	45,45,45,45	0
54	MG	1A	3404	1/1	0.92	0.09	52,52,52,52	0
54	MG	2A	3018	1/1	0.92	0.41	55,55,55,55	0
54	MG	1A	3255	1/1	0.92	0.24	53,53,53,53	0
54	MG	2a	3054	1/1	0.92	0.34	72,72,72,72	0
54	MG	1W	202	1/1	0.92	0.20	61,61,61,61	0
54	MG	1A	3339	1/1	0.92	0.16	62,62,62,62	0
54	MG	1A	3622	1/1	0.92	0.10	57,57,57,57	0
54	MG	2A	3398	1/1	0.92	0.08	40,40,40,40	0
54	MG	2A	3026	1/1	0.92	0.12	62,62,62,62	0
54	MG	1a	1683	1/1	0.92	0.11	66,66,66,66	0
54	MG	2A	3402	1/1	0.92	0.11	51,51,51,51	0
54	MG	2A	3189	1/1	0.92	0.13	70,70,70,70	0
54	MG	1A	3484	1/1	0.92	0.08	30,30,30,30	0
54	MG	2A	3033	1/1	0.92	0.27	57,57,57,57	0
54	MG	1a	1792	1/1	0.92	0.10	76,76,76,76	0
54	MG	1A	3802	1/1	0.92	0.17	48,48,48,48	0
54	MG	1A	3411	1/1	0.92	0.11	29,29,29,29	0
54	MG	1a	1796	1/1	0.92	0.12	65,65,65,65	0
54	MG	1A	3627	1/1	0.92	0.10	66,66,66,66	0
54	MG	2A	3418	1/1	0.92	0.10	57,57,57,57	0
54	MG	2a	3075	1/1	0.92	0.26	72,72,72,72	0
54	MG	2A	3419	1/1	0.92	0.19	75,75,75,75	0
54	MG	1A	3903	1/1	0.92	0.09	45,45,45,45	0
54	MG	2A	3201	1/1	0.92	0.11	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	2A	3203	1/1	0.92	0.31	76,76,76,76	0
54	MG	2a	3084	1/1	0.92	0.34	72,72,72,72	0
54	MG	1A	3807	1/1	0.92	0.14	60,60,60,60	0
54	MG	1a	1802	1/1	0.92	0.12	75,75,75,75	0
54	MG	1A	3701	1/1	0.92	0.15	62,62,62,62	0
54	MG	2A	3658	1/1	0.92	0.07	86,86,86,86	0
54	MG	2a	3089	1/1	0.92	0.28	62,62,62,62	0
54	MG	2A	3660	1/1	0.92	0.15	44,44,44,44	0
54	MG	1A	4033	1/1	0.92	0.12	62,62,62,62	0
54	MG	1A	3629	1/1	0.92	0.35	40,40,40,40	0
54	MG	2A	3667	1/1	0.92	0.10	77,77,77,77	0
54	MG	1A	3418	1/1	0.92	0.11	31,31,31,31	0
54	MG	1A	3632	1/1	0.92	0.23	41,41,41,41	0
54	MG	2A	3438	1/1	0.92	0.11	64,64,64,64	0
54	MG	17	105	1/1	0.92	0.18	65,65,65,65	0
54	MG	1A	3910	1/1	0.92	0.23	39,39,39,39	0
54	MG	1A	3634	1/1	0.92	0.28	40,40,40,40	0
54	MG	2A	3443	1/1	0.92	0.27	75,75,75,75	0
54	MG	2A	3445	1/1	0.92	0.14	76,76,76,76	0
54	MG	2A	3217	1/1	0.92	0.13	64,64,64,64	0
54	MG	1A	3918	1/1	0.92	0.10	51,51,51,51	0
54	MG	2A	3692	1/1	0.92	0.10	56,56,56,56	0
54	MG	1A	3922	1/1	0.92	0.10	55,55,55,55	0
54	MG	1a	1823	1/1	0.92	0.13	76,76,76,76	0
54	MG	1A	3295	1/1	0.92	0.11	49,49,49,49	0
54	MG	1A	3257	1/1	0.92	0.31	51,51,51,51	0
54	MG	2A	3455	1/1	0.92	0.14	69,69,69,69	0
54	MG	2A	3701	1/1	0.92	0.11	64,64,64,64	0
54	MG	1A	3930	1/1	0.92	0.09	51,51,51,51	0
54	MG	1A	3575	1/1	0.92	0.27	40,40,40,40	0
54	MG	1A	3297	1/1	0.92	0.12	71,71,71,71	0
54	MG	1A	3300	1/1	0.92	0.20	52,52,52,52	0
54	MG	1a	1832	1/1	0.92	0.13	76,76,76,76	0
54	MG	1a	1834	1/1	0.92	0.16	69,69,69,69	0
54	MG	2a	3125	1/1	0.92	0.16	65,65,65,65	0
54	MG	1B	215	1/1	0.92	0.08	65,65,65,65	0
54	MG	2A	3712	1/1	0.92	0.09	49,49,49,49	0
54	MG	1A	3582	1/1	0.92	0.15	65,65,65,65	0
54	MG	1a	1838	1/1	0.92	0.13	73,73,73,73	0
54	MG	1a	1612	1/1	0.92	0.11	36,36,36,36	0
54	MG	2A	3241	1/1	0.92	0.26	51,51,51,51	0
54	MG	1B	218	1/1	0.92	0.08	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	3215	1/1	0.92	0.20	46,46,46,46	0
54	MG	1A	3949	1/1	0.92	0.09	59,59,59,59	0
54	MG	1A	3950	1/1	0.92	0.09	65,65,65,65	0
54	MG	2A	3092	1/1	0.92	0.18	61,61,61,61	0
54	MG	2A	3480	1/1	0.92	0.09	68,68,68,68	0
54	MG	1A	3951	1/1	0.92	0.08	70,70,70,70	0
54	MG	2A	3482	1/1	0.92	0.10	61,61,61,61	0
54	MG	2A	3253	1/1	0.92	0.20	65,65,65,65	0
54	MG	2A	3256	1/1	0.92	0.16	56,56,56,56	0
54	MG	2A	3258	1/1	0.92	0.27	50,50,50,50	0
54	MG	2a	3147	1/1	0.92	0.19	81,81,81,81	0
54	MG	1A	3441	1/1	0.92	0.11	33,33,33,33	0
54	MG	2A	3488	1/1	0.92	0.14	68,68,68,68	0
54	MG	1A	3507	1/1	0.92	0.09	33,33,33,33	0
54	MG	1A	3351	1/1	0.92	0.14	38,38,38,38	0
54	MG	2a	3158	1/1	0.92	0.10	54,54,54,54	0
54	MG	1A	3511	1/1	0.92	0.14	71,71,71,71	0
54	MG	2B	206	1/1	0.92	0.25	73,73,73,73	0
54	MG	1a	1631	1/1	0.92	0.27	71,71,71,71	0
54	MG	1A	3155	1/1	0.92	0.16	57,57,57,57	0
54	MG	1a	1634	1/1	0.92	0.11	56,56,56,56	0
54	MG	1A	3099	1/1	0.92	0.12	59,59,59,59	0
54	MG	1A	3839	1/1	0.92	0.18	37,37,37,37	0
54	MG	1A	3967	1/1	0.92	0.08	34,34,34,34	0
54	MG	1D	314	1/1	0.92	0.26	49,49,49,49	0
54	MG	2B	215	1/1	0.92	0.17	77,77,77,77	0
54	MG	2a	3173	1/1	0.92	0.18	63,63,63,63	0
54	MG	1A	3659	1/1	0.92	0.15	53,53,53,53	0
54	MG	1A	3263	1/1	0.92	0.14	53,53,53,53	0
54	MG	1A	3970	1/1	0.92	0.18	60,60,60,60	0
54	MG	2D	301	1/1	0.92	0.23	53,53,53,53	0
54	MG	1A	3971	1/1	0.92	0.12	73,73,73,73	0
54	MG	2D	307	1/1	0.92	0.28	60,60,60,60	0
54	MG	2D	308	1/1	0.92	0.24	50,50,50,50	0
54	MG	2A	3278	1/1	0.92	0.19	53,53,53,53	0
54	MG	2A	3279	1/1	0.92	0.30	66,66,66,66	0
54	MG	2a	3189	1/1	0.92	0.30	65,65,65,65	0
54	MG	1A	3002	1/1	0.92	0.09	49,49,49,49	0
54	MG	2A	3117	1/1	0.92	0.18	63,63,63,63	0
54	MG	1A	3597	1/1	0.92	0.09	46,46,46,46	0
54	MG	1A	3849	1/1	0.92	0.10	64,64,64,64	0
54	MG	2F	302	1/1	0.92	0.10	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	1a	1647	1/1	0.92	0.23	63,63,63,63	0
54	MG	1A	3106	1/1	0.92	0.21	37,37,37,37	0
54	MG	1A	3751	1/1	0.92	0.16	65,65,65,65	0
54	MG	2A	3291	1/1	0.92	0.30	78,78,78,78	0
54	MG	2A	3529	1/1	0.92	0.08	46,46,46,46	0
54	MG	1A	3756	1/1	0.92	0.11	66,66,66,66	0
54	MG	2A	3128	1/1	0.92	0.24	46,46,46,46	0
54	MG	1a	1755	1/1	0.92	0.18	65,65,65,65	0
54	MG	2A	3130	1/1	0.92	0.25	61,61,61,61	0
54	MG	2I	101	1/1	0.92	0.14	59,59,59,59	0
54	MG	1A	3039	1/1	0.92	0.12	56,56,56,56	0
54	MG	1A	3270	1/1	0.93	0.22	49,49,49,49	0
54	MG	2F	301	1/1	0.93	0.34	48,48,48,48	0
54	MG	1I	101	1/1	0.93	0.24	50,50,50,50	0
54	MG	1A	3272	1/1	0.93	0.12	68,68,68,68	0
54	MG	2A	3272	1/1	0.93	0.34	72,72,72,72	0
54	MG	1I	103	1/1	0.93	0.11	58,58,58,58	0
54	MG	2O	201	1/1	0.93	0.14	79,79,79,79	0
54	MG	2A	3517	1/1	0.93	0.07	81,81,81,81	0
54	MG	1a	1708	1/1	0.93	0.14	64,64,64,64	0
54	MG	2R	203	1/1	0.93	0.15	56,56,56,56	0
54	MG	1A	3066	1/1	0.93	0.15	72,72,72,72	0
54	MG	1A	4009	1/1	0.93	0.12	84,84,84,84	0
54	MG	2V	201	1/1	0.93	0.22	59,59,59,59	0
54	MG	1A	3860	1/1	0.93	0.24	60,60,60,60	0
54	MG	2W	201	1/1	0.93	0.23	70,70,70,70	0
54	MG	2A	3105	1/1	0.93	0.08	73,73,73,73	0
54	MG	2A	3106	1/1	0.93	0.20	53,53,53,53	0
54	MG	1A	3010	1/1	0.93	0.15	61,61,61,61	0
54	MG	1A	3158	1/1	0.93	0.07	53,53,53,53	0
54	MG	25	102	1/1	0.93	0.20	50,50,50,50	0
54	MG	1A	3628	1/1	0.93	0.13	45,45,45,45	0
54	MG	1A	3213	1/1	0.93	0.21	45,45,45,45	0
54	MG	1A	3345	1/1	0.93	0.28	46,46,46,46	0
54	MG	1a	1856	1/1	0.93	0.10	70,70,70,70	0
54	MG	1A	3348	1/1	0.93	0.17	46,46,46,46	0
54	MG	2A	3290	1/1	0.93	0.27	52,52,52,52	0
54	MG	1A	3068	1/1	0.93	0.25	51,51,51,51	0
54	MG	1a	1720	1/1	0.93	0.21	63,63,63,63	0
54	MG	1A	3020	1/1	0.93	0.33	43,43,43,43	0
54	MG	2A	3297	1/1	0.93	0.14	65,65,65,65	0
54	MG	2a	3009	1/1	0.93	0.13	76,76,76,76	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	19	101	1/1	0.93	0.21	65,65,65,65	0
54	MG	2a	3011	1/1	0.93	0.12	74,74,74,74	0
54	MG	1A	3740	1/1	0.93	0.32	43,43,43,43	0
54	MG	1A	3125	1/1	0.93	0.09	44,44,44,44	0
54	MG	2A	3305	1/1	0.93	0.14	45,45,45,45	0
54	MG	1A	3084	1/1	0.93	0.17	54,54,54,54	0
54	MG	1A	3553	1/1	0.93	0.17	61,61,61,61	0
54	MG	2A	3311	1/1	0.93	0.22	72,72,72,72	0
54	MG	1A	3086	1/1	0.93	0.30	50,50,50,50	0
54	MG	1a	1605	1/1	0.93	0.24	63,63,63,63	0
54	MG	2A	3318	1/1	0.93	0.09	43,43,43,43	0
54	MG	2A	3554	1/1	0.93	0.08	74,74,74,74	0
54	MG	1A	3754	1/1	0.93	0.08	39,39,39,39	0
54	MG	1a	1873	1/1	0.93	0.22	64,64,64,64	0
54	MG	1A	3645	1/1	0.93	0.08	31,31,31,31	0
54	MG	1A	3757	1/1	0.93	0.09	61,61,61,61	0
54	MG	2A	3561	1/1	0.93	0.09	71,71,71,71	0
54	MG	1A	3358	1/1	0.93	0.05	34,34,34,34	0
54	MG	2A	3565	1/1	0.93	0.08	83,83,83,83	0
54	MG	1A	3227	1/1	0.93	0.13	41,41,41,41	0
54	MG	2A	3139	1/1	0.93	0.10	56,56,56,56	0
54	MG	2A	3331	1/1	0.93	0.10	58,58,58,58	0
54	MG	1A	3761	1/1	0.93	0.09	41,41,41,41	0
54	MG	1A	3649	1/1	0.93	0.14	57,57,57,57	0
54	MG	1a	1741	1/1	0.93	0.13	71,71,71,71	0
54	MG	1a	1615	1/1	0.93	0.17	76,76,76,76	0
54	MG	1a	1616	1/1	0.93	0.11	76,76,76,76	0
54	MG	2A	3342	1/1	0.93	0.09	65,65,65,65	0
54	MG	2A	3148	1/1	0.93	0.14	54,54,54,54	0
54	MG	2A	3346	1/1	0.93	0.11	45,45,45,45	0
54	MG	1A	3897	1/1	0.93	0.09	40,40,40,40	0
54	MG	1A	3764	1/1	0.93	0.07	50,50,50,50	0
54	MG	1A	3558	1/1	0.93	0.08	49,49,49,49	0
54	MG	2A	3353	1/1	0.93	0.09	42,42,42,42	0
54	MG	1A	3560	1/1	0.93	0.08	69,69,69,69	0
54	MG	2A	3157	1/1	0.93	0.15	63,63,63,63	0
54	MG	1A	3364	1/1	0.93	0.09	48,48,48,48	0
54	MG	2A	3595	1/1	0.93	0.09	72,72,72,72	0
54	MG	1A	3466	1/1	0.93	0.09	51,51,51,51	0
54	MG	2A	3364	1/1	0.93	0.14	56,56,56,56	0
54	MG	1A	3774	1/1	0.93	0.20	49,49,49,49	0
54	MG	1B	212	1/1	0.93	0.07	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	1A	3565	1/1	0.93	0.07	36,36,36,36	0
54	MG	1A	3569	1/1	0.93	0.09	54,54,54,54	0
54	MG	2A	3609	1/1	0.93	0.07	50,50,50,50	0
54	MG	2A	3166	1/1	0.93	0.17	68,68,68,68	0
54	MG	1A	3777	1/1	0.93	0.12	50,50,50,50	0
54	MG	2A	3168	1/1	0.93	0.14	53,53,53,53	0
54	MG	2A	3617	1/1	0.93	0.07	69,69,69,69	0
54	MG	1A	3467	1/1	0.93	0.10	63,63,63,63	0
54	MG	2A	3619	1/1	0.93	0.11	66,66,66,66	0
54	MG	1A	3574	1/1	0.93	0.23	73,73,73,73	0
54	MG	2a	3076	1/1	0.93	0.13	74,74,74,74	0
54	MG	2A	3621	1/1	0.93	0.12	68,68,68,68	0
54	MG	1a	1759	1/1	0.93	0.16	70,70,70,70	0
54	MG	2a	3080	1/1	0.93	0.18	61,61,61,61	0
54	MG	2a	3081	1/1	0.93	0.26	76,76,76,76	0
54	MG	1A	3919	1/1	0.93	0.09	72,72,72,72	0
54	MG	1A	3369	1/1	0.93	0.13	60,60,60,60	0
54	MG	1A	3372	1/1	0.93	0.08	55,55,55,55	0
54	MG	1A	3580	1/1	0.93	0.09	44,44,44,44	0
54	MG	1A	3927	1/1	0.93	0.09	32,32,32,32	0
54	MG	1A	3665	1/1	0.93	0.30	45,45,45,45	0
54	MG	2A	3629	1/1	0.93	0.14	73,73,73,73	0
54	MG	2A	3001	1/1	0.93	0.37	66,66,66,66	0
54	MG	1A	3177	1/1	0.93	0.23	47,47,47,47	0
54	MG	2A	3003	1/1	0.93	0.11	66,66,66,66	0
54	MG	2A	3004	1/1	0.93	0.09	47,47,47,47	0
54	MG	2A	3401	1/1	0.93	0.11	82,82,82,82	0
54	MG	1a	1768	1/1	0.93	0.09	77,77,77,77	0
54	MG	1A	3087	1/1	0.93	0.26	47,47,47,47	0
54	MG	1a	1770	1/1	0.93	0.10	75,75,75,75	0
54	MG	1D	305	1/1	0.93	0.22	50,50,50,50	0
54	MG	2A	3652	1/1	0.93	0.07	71,71,71,71	0
54	MG	2a	3102	1/1	0.93	0.33	62,62,62,62	0
54	MG	1D	309	1/1	0.93	0.13	64,64,64,64	0
54	MG	1A	3232	1/1	0.93	0.11	44,44,44,44	0
54	MG	1A	3586	1/1	0.93	0.07	66,66,66,66	0
54	MG	1A	3377	1/1	0.93	0.07	41,41,41,41	0
54	MG	1A	3233	1/1	0.93	0.28	41,41,41,41	0
54	MG	2A	3416	1/1	0.93	0.17	66,66,66,66	0
54	MG	2A	3662	1/1	0.93	0.08	56,56,56,56	0
54	MG	2A	3417	1/1	0.93	0.11	46,46,46,46	0
54	MG	1A	3190	1/1	0.93	0.25	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	3239	1/1	0.93	0.21	41,41,41,41	0
54	MG	2A	3195	1/1	0.93	0.07	65,65,65,65	0
54	MG	2A	3025	1/1	0.93	0.10	54,54,54,54	0
54	MG	2a	3115	1/1	0.93	0.33	68,68,68,68	0
54	MG	2A	3423	1/1	0.93	0.07	47,47,47,47	0
54	MG	2A	3424	1/1	0.93	0.07	47,47,47,47	0
54	MG	1A	3677	1/1	0.93	0.24	65,65,65,65	0
54	MG	2a	3120	1/1	0.93	0.15	70,70,70,70	0
54	MG	2A	3684	1/1	0.93	0.09	71,71,71,71	0
54	MG	1A	3305	1/1	0.93	0.11	45,45,45,45	0
54	MG	1A	3132	1/1	0.93	0.07	40,40,40,40	0
54	MG	2A	3202	1/1	0.93	0.23	53,53,53,53	0
54	MG	1E	307	1/1	0.93	0.14	32,32,32,32	0
54	MG	2A	3204	1/1	0.93	0.34	73,73,73,73	0
54	MG	2A	3435	1/1	0.93	0.09	58,58,58,58	0
54	MG	1a	1783	1/1	0.93	0.13	58,58,58,58	0
54	MG	1A	3684	1/1	0.93	0.09	64,64,64,64	0
54	MG	1A	3058	1/1	0.93	0.17	58,58,58,58	0
54	MG	1A	3392	1/1	0.93	0.09	39,39,39,39	0
54	MG	1A	3962	1/1	0.93	0.10	51,51,51,51	0
54	MG	1A	3816	1/1	0.93	0.17	69,69,69,69	0
54	MG	1A	3498	1/1	0.93	0.13	60,60,60,60	0
54	MG	1A	3194	1/1	0.93	0.27	44,44,44,44	0
54	MG	2A	3045	1/1	0.93	0.18	76,76,76,76	0
54	MG	1A	3599	1/1	0.93	0.09	66,66,66,66	0
54	MG	1A	3501	1/1	0.93	0.07	27,27,27,27	0
54	MG	1A	3196	1/1	0.93	0.28	53,53,53,53	0
54	MG	2A	3711	1/1	0.93	0.12	62,62,62,62	0
54	MG	2A	3451	1/1	0.93	0.10	59,59,59,59	0
54	MG	1a	1675	1/1	0.93	0.32	69,69,69,69	0
54	MG	1A	3972	1/1	0.93	0.08	64,64,64,64	0
54	MG	2A	3222	1/1	0.93	0.16	70,70,70,70	0
54	MG	2A	3456	1/1	0.93	0.09	68,68,68,68	0
54	MG	2a	3154	1/1	0.93	0.09	80,80,80,80	0
54	MG	1A	3695	1/1	0.93	0.14	53,53,53,53	0
54	MG	1A	3060	1/1	0.93	0.08	58,58,58,58	0
54	MG	1A	3135	1/1	0.93	0.23	49,49,49,49	0
54	MG	1A	3831	1/1	0.93	0.10	39,39,39,39	0
54	MG	2a	3162	1/1	0.93	0.10	74,74,74,74	0
54	MG	1A	3320	1/1	0.93	0.18	47,47,47,47	0
54	MG	1a	1809	1/1	0.93	0.10	76,76,76,76	0
54	MG	2A	3463	1/1	0.93	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	1810	1/1	0.93	0.07	76,76,76,76	0
54	MG	1R	203	1/1	0.93	0.12	52,52,52,52	0
54	MG	2A	3467	1/1	0.93	0.08	73,73,73,73	0
54	MG	2A	3062	1/1	0.93	0.10	50,50,50,50	0
54	MG	1A	3138	1/1	0.93	0.07	59,59,59,59	0
54	MG	2A	3064	1/1	0.93	0.10	63,63,63,63	0
54	MG	1A	3260	1/1	0.93	0.11	59,59,59,59	0
54	MG	2A	3475	1/1	0.93	0.14	63,63,63,63	0
54	MG	1A	3041	1/1	0.93	0.14	61,61,61,61	0
54	MG	2A	3242	1/1	0.93	0.11	69,69,69,69	0
54	MG	1a	1816	1/1	0.93	0.15	75,75,75,75	0
54	MG	1A	3424	1/1	0.93	0.05	30,30,30,30	0
54	MG	2a	3184	1/1	0.93	0.12	73,73,73,73	0
54	MG	1A	3425	1/1	0.93	0.10	32,32,32,32	0
54	MG	1a	1689	1/1	0.93	0.13	68,68,68,68	0
54	MG	2a	3187	1/1	0.93	0.11	74,74,74,74	0
54	MG	1A	3614	1/1	0.93	0.11	57,57,57,57	0
54	MG	2A	3080	1/1	0.93	0.13	63,63,63,63	0
54	MG	2A	3252	1/1	0.93	0.12	47,47,47,47	0
54	MG	1A	3845	1/1	0.93	0.08	40,40,40,40	0
54	MG	2A	3255	1/1	0.93	0.41	48,48,48,48	0
54	MG	2f	201	1/1	0.93	0.11	57,57,57,57	0
54	MG	2A	3082	1/1	0.93	0.16	65,65,65,65	0
54	MG	2A	3257	1/1	0.93	0.13	40,40,40,40	0
54	MG	1A	3143	1/1	0.93	0.34	50,50,50,50	0
54	MG	1A	3062	1/1	0.93	0.22	50,50,50,50	0
54	MG	2t	201	1/1	0.93	0.16	53,53,53,53	0
54	MG	2D	303	1/1	0.93	0.33	50,50,50,50	0
54	MG	2D	304	1/1	0.93	0.28	60,60,60,60	0
54	MG	1A	3065	1/1	0.93	0.08	41,41,41,41	0
54	MG	2A	3499	1/1	0.93	0.11	69,69,69,69	0
54	MG	10	103	1/1	0.93	0.09	52,52,52,52	0
54	MG	1a	1830	1/1	0.93	0.11	79,79,79,79	0
54	MG	2A	3091	1/1	0.93	0.15	57,57,57,57	0
54	MG	1A	4002	1/1	0.93	0.07	52,52,52,52	0
54	MG	1A	3434	1/1	0.93	0.09	46,46,46,46	0
54	MG	1A	3008	1/1	0.94	0.06	46,46,46,46	0
54	MG	1A	3478	1/1	0.94	0.08	66,66,66,66	0
54	MG	2A	3560	1/1	0.94	0.10	45,45,45,45	0
54	MG	1B	202	1/1	0.94	0.25	70,70,70,70	0
54	MG	1A	3169	1/1	0.94	0.06	36,36,36,36	0
54	MG	1a	1752	1/1	0.94	0.07	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	1k	201	1/1	0.94	0.12	54,54,54,54	0
54	MG	1A	3579	1/1	0.94	0.14	61,61,61,61	0
54	MG	1A	3170	1/1	0.94	0.16	54,54,54,54	0
54	MG	1m	201	1/1	0.94	0.07	76,76,76,76	0
54	MG	2A	3365	1/1	0.94	0.10	46,46,46,46	0
54	MG	1A	3210	1/1	0.94	0.18	50,50,50,50	0
54	MG	1A	3778	1/1	0.94	0.06	55,55,55,55	0
54	MG	1A	3397	1/1	0.94	0.15	51,51,51,51	0
54	MG	2a	3017	1/1	0.94	0.10	57,57,57,57	0
54	MG	1A	3025	1/1	0.94	0.45	43,43,43,43	0
54	MG	1A	3265	1/1	0.94	0.09	53,53,53,53	0
54	MG	2a	3020	1/1	0.94	0.08	66,66,66,66	0
54	MG	1A	3107	1/1	0.94	0.45	42,42,42,42	0
54	MG	2a	3023	1/1	0.94	0.41	76,76,76,76	0
54	MG	2A	3175	1/1	0.94	0.06	58,58,58,58	0
54	MG	1A	3497	1/1	0.94	0.10	55,55,55,55	0
54	MG	1A	3787	1/1	0.94	0.09	61,61,61,61	0
54	MG	1A	3920	1/1	0.94	0.07	64,64,64,64	0
54	MG	2a	3028	1/1	0.94	0.10	66,66,66,66	0
54	MG	1A	3921	1/1	0.94	0.07	60,60,60,60	0
54	MG	1A	3326	1/1	0.94	0.12	59,59,59,59	0
54	MG	1A	3671	1/1	0.94	0.15	48,48,48,48	0
54	MG	2A	3388	1/1	0.94	0.10	63,63,63,63	0
54	MG	1A	3796	1/1	0.94	0.10	57,57,57,57	0
54	MG	2a	3034	1/1	0.94	0.21	66,66,66,66	0
54	MG	2A	3390	1/1	0.94	0.14	70,70,70,70	0
54	MG	1A	3268	1/1	0.94	0.11	52,52,52,52	0
54	MG	2A	3015	1/1	0.94	0.21	48,48,48,48	0
54	MG	1A	3409	1/1	0.94	0.07	37,37,37,37	0
54	MG	2A	3605	1/1	0.94	0.09	51,51,51,51	0
54	MG	1A	3592	1/1	0.94	0.09	27,27,27,27	0
54	MG	1A	3410	1/1	0.94	0.09	32,32,32,32	0
54	MG	1A	3175	1/1	0.94	0.23	60,60,60,60	0
54	MG	1D	303	1/1	0.94	0.13	46,46,46,46	0
54	MG	1A	3271	1/1	0.94	0.16	36,36,36,36	0
54	MG	1D	307	1/1	0.94	0.09	47,47,47,47	0
54	MG	1A	3419	1/1	0.94	0.09	37,37,37,37	0
54	MG	1A	3333	1/1	0.94	0.13	57,57,57,57	0
54	MG	2A	3030	1/1	0.94	0.20	42,42,42,42	0
54	MG	1A	3334	1/1	0.94	0.08	51,51,51,51	0
54	MG	1A	3600	1/1	0.94	0.11	33,33,33,33	0
54	MG	1A	3109	1/1	0.94	0.14	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	2A	3411	1/1	0.94	0.18	67,67,67,67	0
54	MG	1A	3217	1/1	0.94	0.13	52,52,52,52	0
54	MG	2A	3035	1/1	0.94	0.21	68,68,68,68	0
54	MG	1A	3218	1/1	0.94	0.10	51,51,51,51	0
54	MG	1A	3521	1/1	0.94	0.10	30,30,30,30	0
54	MG	2A	3038	1/1	0.94	0.13	58,58,58,58	0
54	MG	1A	3341	1/1	0.94	0.12	61,61,61,61	0
54	MG	1A	3219	1/1	0.94	0.33	46,46,46,46	0
54	MG	1a	1787	1/1	0.94	0.09	68,68,68,68	0
54	MG	1A	3279	1/1	0.94	0.23	55,55,55,55	0
54	MG	1E	308	1/1	0.94	0.19	75,75,75,75	0
54	MG	1A	3964	1/1	0.94	0.09	24,24,24,24	0
54	MG	2A	3046	1/1	0.94	0.21	76,76,76,76	0
54	MG	1A	3178	1/1	0.94	0.12	57,57,57,57	0
54	MG	2A	3431	1/1	0.94	0.12	67,67,67,67	0
54	MG	2A	3646	1/1	0.94	0.09	67,67,67,67	0
54	MG	1F	313	1/1	0.94	0.27	48,48,48,48	0
54	MG	2a	3074	1/1	0.94	0.28	56,56,56,56	0
54	MG	1A	3442	1/1	0.94	0.13	35,35,35,35	0
54	MG	2A	3434	1/1	0.94	0.21	63,63,63,63	0
54	MG	1a	1795	1/1	0.94	0.10	78,78,78,78	0
54	MG	1A	3528	1/1	0.94	0.09	52,52,52,52	0
54	MG	2A	3220	1/1	0.94	0.10	57,57,57,57	0
54	MG	1A	3221	1/1	0.94	0.44	44,44,44,44	0
54	MG	1A	3615	1/1	0.94	0.09	33,33,33,33	0
54	MG	2A	3665	1/1	0.94	0.07	81,81,81,81	0
54	MG	1G	202	1/1	0.94	0.25	63,63,63,63	0
54	MG	1a	1800	1/1	0.94	0.10	58,58,58,58	0
54	MG	2A	3668	1/1	0.94	0.08	76,76,76,76	0
54	MG	2A	3057	1/1	0.94	0.09	51,51,51,51	0
54	MG	2A	3672	1/1	0.94	0.08	47,47,47,47	0
54	MG	2A	3444	1/1	0.94	0.10	48,48,48,48	0
54	MG	2A	3677	1/1	0.94	0.17	74,74,74,74	0
54	MG	1A	3530	1/1	0.94	0.08	31,31,31,31	0
54	MG	1A	3705	1/1	0.94	0.06	74,74,74,74	0
54	MG	1A	3973	1/1	0.94	0.09	68,68,68,68	0
54	MG	2A	3682	1/1	0.94	0.08	60,60,60,60	0
54	MG	1A	3184	1/1	0.94	0.41	46,46,46,46	0
54	MG	1N	203	1/1	0.94	0.14	47,47,47,47	0
54	MG	1A	3045	1/1	0.94	0.17	39,39,39,39	0
54	MG	2A	3236	1/1	0.94	0.07	63,63,63,63	0
54	MG	2A	3453	1/1	0.94	0.07	59,59,59,59	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	1A	3286	1/1	0.94	0.19	60,60,60,60	0
54	MG	1A	3226	1/1	0.94	0.10	62,62,62,62	0
54	MG	1A	3716	1/1	0.94	0.13	66,66,66,66	0
54	MG	2A	3067	1/1	0.94	0.16	57,57,57,57	0
54	MG	1A	3353	1/1	0.94	0.10	33,33,33,33	0
54	MG	1a	1815	1/1	0.94	0.11	66,66,66,66	0
54	MG	1Q	203	1/1	0.94	0.10	51,51,51,51	0
54	MG	2A	3075	1/1	0.94	0.39	60,60,60,60	0
54	MG	1Q	204	1/1	0.94	0.13	47,47,47,47	0
54	MG	1a	1819	1/1	0.94	0.07	72,72,72,72	0
54	MG	2A	3079	1/1	0.94	0.12	59,59,59,59	0
54	MG	1A	3453	1/1	0.94	0.07	21,21,21,21	0
54	MG	1a	1687	1/1	0.94	0.15	56,56,56,56	0
54	MG	1A	3291	1/1	0.94	0.10	58,58,58,58	0
54	MG	1R	204	1/1	0.94	0.12	48,48,48,48	0
54	MG	2A	3472	1/1	0.94	0.12	56,56,56,56	0
54	MG	1A	3625	1/1	0.94	0.12	48,48,48,48	0
54	MG	1a	1691	1/1	0.94	0.14	65,65,65,65	0
54	MG	2A	3715	1/1	0.94	0.13	71,71,71,71	0
54	MG	1a	1827	1/1	0.94	0.09	56,56,56,56	0
54	MG	1A	3003	1/1	0.94	0.07	36,36,36,36	0
54	MG	1A	3991	1/1	0.94	0.10	62,62,62,62	0
54	MG	1A	3545	1/1	0.94	0.19	48,48,48,48	0
54	MG	1a	1695	1/1	0.94	0.16	52,52,52,52	0
54	MG	1U	206	1/1	0.94	0.28	44,44,44,44	0
54	MG	1V	203	1/1	0.94	0.10	46,46,46,46	0
54	MG	1A	3994	1/1	0.94	0.09	71,71,71,71	0
54	MG	2a	3132	1/1	0.94	0.11	71,71,71,71	0
54	MG	1A	3191	1/1	0.94	0.07	58,58,58,58	0
54	MG	1A	3997	1/1	0.94	0.08	32,32,32,32	0
54	MG	1a	1839	1/1	0.94	0.08	51,51,51,51	0
54	MG	1A	3019	1/1	0.94	0.37	34,34,34,34	0
54	MG	1Y	201	1/1	0.94	0.12	55,55,55,55	0
54	MG	1A	3631	1/1	0.94	0.11	64,64,64,64	0
54	MG	2A	3730	1/1	0.94	0.08	68,68,68,68	0
54	MG	10	101	1/1	0.94	0.17	43,43,43,43	0
54	MG	1A	4000	1/1	0.94	0.11	50,50,50,50	0
54	MG	1A	3855	1/1	0.94	0.06	46,46,46,46	0
54	MG	2A	3495	1/1	0.94	0.19	57,57,57,57	0
54	MG	2A	3497	1/1	0.94	0.19	73,73,73,73	0
54	MG	1A	3116	1/1	0.94	0.18	44,44,44,44	0
54	MG	1A	3633	1/1	0.94	0.30	37,37,37,37	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	2a	3151	1/1	0.94	0.16	80,80,80,80	0
54	MG	2B	208	1/1	0.94	0.24	71,71,71,71	0
54	MG	2A	3281	1/1	0.94	0.34	74,74,74,74	0
54	MG	1A	3091	1/1	0.94	0.08	42,42,42,42	0
54	MG	1A	3865	1/1	0.94	0.07	48,48,48,48	0
54	MG	1A	3153	1/1	0.94	0.11	52,52,52,52	0
54	MG	1A	4008	1/1	0.94	0.20	41,41,41,41	0
54	MG	2A	3510	1/1	0.94	0.11	66,66,66,66	0
54	MG	2a	3164	1/1	0.94	0.14	76,76,76,76	0
54	MG	1A	3741	1/1	0.94	0.17	43,43,43,43	0
54	MG	2A	3287	1/1	0.94	0.11	64,64,64,64	0
54	MG	1A	3092	1/1	0.94	0.16	44,44,44,44	0
54	MG	2A	3119	1/1	0.94	0.09	57,57,57,57	0
54	MG	1a	1719	1/1	0.94	0.20	63,63,63,63	0
54	MG	13	102	1/1	0.94	0.15	72,72,72,72	0
54	MG	2A	3122	1/1	0.94	0.10	56,56,56,56	0
54	MG	2A	3123	1/1	0.94	0.14	49,49,49,49	0
54	MG	2D	305	1/1	0.94	0.44	49,49,49,49	0
54	MG	1a	1721	1/1	0.94	0.11	56,56,56,56	0
54	MG	1A	3126	1/1	0.94	0.09	40,40,40,40	0
54	MG	15	102	1/1	0.94	0.26	39,39,39,39	0
54	MG	1A	3054	1/1	0.94	0.20	34,34,34,34	0
54	MG	2a	3180	1/1	0.94	0.09	59,59,59,59	0
54	MG	2A	3307	1/1	0.94	0.15	62,62,62,62	0
54	MG	1A	3749	1/1	0.94	0.10	59,59,59,59	0
54	MG	1A	3874	1/1	0.94	0.15	32,32,32,32	0
54	MG	1A	3643	1/1	0.94	0.07	50,50,50,50	0
54	MG	1A	3001	1/1	0.94	0.06	39,39,39,39	0
54	MG	1A	3878	1/1	0.94	0.06	58,58,58,58	0
54	MG	2A	3317	1/1	0.94	0.07	54,54,54,54	0
54	MG	1A	4022	1/1	0.94	0.14	64,64,64,64	0
54	MG	1A	3562	1/1	0.94	0.14	58,58,58,58	0
54	MG	1A	4026	1/1	0.94	0.08	66,66,66,66	0
54	MG	1A	3164	1/1	0.94	0.30	41,41,41,41	0
54	MG	1A	3883	1/1	0.94	0.08	68,68,68,68	0
54	MG	1A	3758	1/1	0.94	0.18	37,37,37,37	0
54	MG	1A	3101	1/1	0.94	0.11	46,46,46,46	0
54	MG	1A	3566	1/1	0.94	0.08	44,44,44,44	0
54	MG	2A	3541	1/1	0.94	0.16	60,60,60,60	0
54	MG	2A	3146	1/1	0.94	0.27	60,60,60,60	0
54	MG	1a	1742	1/1	0.94	0.12	44,44,44,44	0
54	MG	1A	3567	1/1	0.94	0.08	43,43,43,43	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	2A	3152	1/1	0.94	0.10	48,48,48,48	0
54	MG	1A	3205	1/1	0.94	0.10	60,60,60,60	0
54	MG	1A	3474	1/1	0.94	0.12	53,53,53,53	0
54	MG	1A	3572	1/1	0.94	0.19	48,48,48,48	0
54	MG	1A	3573	1/1	0.94	0.10	57,57,57,57	0
58	ARG	1B	230	12/12	0.94	0.09	32,44,59,61	0
54	MG	2A	3158	1/1	0.94	0.15	76,76,76,76	0
54	MG	28	101	1/1	0.94	0.10	68,68,68,68	0
54	MG	1A	3415	1/1	0.95	0.09	37,37,37,37	0
54	MG	1A	3798	1/1	0.95	0.11	30,30,30,30	0
54	MG	2A	3586	1/1	0.95	0.09	67,67,67,67	0
54	MG	2A	3397	1/1	0.95	0.08	61,61,61,61	0
54	MG	2A	3589	1/1	0.95	0.08	60,60,60,60	0
54	MG	1A	3416	1/1	0.95	0.07	35,35,35,35	0
54	MG	2a	3014	1/1	0.95	0.19	63,63,63,63	0
54	MG	2A	3591	1/1	0.95	0.07	52,52,52,52	0
54	MG	1a	1818	1/1	0.95	0.11	72,72,72,72	0
54	MG	2A	3593	1/1	0.95	0.06	58,58,58,58	0
54	MG	1A	3108	1/1	0.95	0.19	40,40,40,40	0
54	MG	10	105	1/1	0.95	0.07	55,55,55,55	0
54	MG	1A	3908	1/1	0.95	0.10	61,61,61,61	0
54	MG	1A	3485	1/1	0.95	0.16	52,52,52,52	0
54	MG	1a	1698	1/1	0.95	0.30	74,74,74,74	0
54	MG	1A	3803	1/1	0.95	0.08	42,42,42,42	0
54	MG	2A	3214	1/1	0.95	0.24	60,60,60,60	0
54	MG	2A	3215	1/1	0.95	0.13	65,65,65,65	0
54	MG	1A	3304	1/1	0.95	0.06	45,45,45,45	0
54	MG	2A	3409	1/1	0.95	0.12	51,51,51,51	0
54	MG	1a	1702	1/1	0.95	0.20	61,61,61,61	0
54	MG	2A	3613	1/1	0.95	0.09	56,56,56,56	0
54	MG	2A	3615	1/1	0.95	0.05	29,29,29,29	0
54	MG	1A	3223	1/1	0.95	0.15	36,36,36,36	0
54	MG	1A	3564	1/1	0.95	0.07	29,29,29,29	0
54	MG	1A	3057	1/1	0.95	0.15	54,54,54,54	0
54	MG	1A	3490	1/1	0.95	0.10	57,57,57,57	0
54	MG	1a	1707	1/1	0.95	0.29	60,60,60,60	0
54	MG	2A	3223	1/1	0.95	0.11	55,55,55,55	0
54	MG	1A	4040	1/1	0.95	0.08	61,61,61,61	0
54	MG	1A	3017	1/1	0.95	0.19	36,36,36,36	0
54	MG	1A	3495	1/1	0.95	0.05	34,34,34,34	0
54	MG	2A	3228	1/1	0.95	0.21	60,60,60,60	0
54	MG	1A	3812	1/1	0.95	0.06	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	15	104	1/1	0.95	0.10	43,43,43,43	0
54	MG	1A	3496	1/1	0.95	0.09	61,61,61,61	0
54	MG	2A	3232	1/1	0.95	0.10	63,63,63,63	0
54	MG	1A	3202	1/1	0.95	0.15	42,42,42,42	0
54	MG	1A	3636	1/1	0.95	0.14	44,44,44,44	0
54	MG	2A	3086	1/1	0.95	0.07	45,45,45,45	0
54	MG	15	108	1/1	0.95	0.07	56,56,56,56	0
54	MG	1a	1847	1/1	0.95	0.11	73,73,73,73	0
54	MG	2a	3052	1/1	0.95	0.14	55,55,55,55	0
54	MG	17	101	1/1	0.95	0.08	38,38,38,38	0
54	MG	17	102	1/1	0.95	0.10	48,48,48,48	0
54	MG	17	104	1/1	0.95	0.17	43,43,43,43	0
54	MG	1B	208	1/1	0.95	0.06	56,56,56,56	0
54	MG	2A	3640	1/1	0.95	0.08	69,69,69,69	0
54	MG	1A	3714	1/1	0.95	0.11	67,67,67,67	0
54	MG	2A	3649	1/1	0.95	0.06	69,69,69,69	0
54	MG	1A	3820	1/1	0.95	0.13	36,36,36,36	0
54	MG	1A	3015	1/1	0.95	0.18	32,32,32,32	0
54	MG	1A	3040	1/1	0.95	0.14	42,42,42,42	0
54	MG	2A	3249	1/1	0.95	0.13	69,69,69,69	0
54	MG	1A	3948	1/1	0.95	0.11	50,50,50,50	0
54	MG	1A	3366	1/1	0.95	0.12	37,37,37,37	0
54	MG	1B	217	1/1	0.95	0.09	58,58,58,58	0
54	MG	1A	3825	1/1	0.95	0.09	57,57,57,57	0
54	MG	2a	3069	1/1	0.95	0.19	74,74,74,74	0
54	MG	1a	1866	1/1	0.95	0.15	67,67,67,67	0
54	MG	1B	219	1/1	0.95	0.07	38,38,38,38	0
54	MG	2A	3108	1/1	0.95	0.09	74,74,74,74	0
54	MG	1A	3642	1/1	0.95	0.13	63,63,63,63	0
54	MG	2A	3259	1/1	0.95	0.05	70,70,70,70	0
54	MG	2A	3260	1/1	0.95	0.29	73,73,73,73	0
54	MG	1A	3080	1/1	0.95	0.23	53,53,53,53	0
54	MG	2A	3675	1/1	0.95	0.07	49,49,49,49	0
54	MG	2A	3676	1/1	0.95	0.06	47,47,47,47	0
54	MG	1A	3439	1/1	0.95	0.07	48,48,48,48	0
54	MG	1A	3505	1/1	0.95	0.09	32,32,32,32	0
54	MG	1A	3727	1/1	0.95	0.15	51,51,51,51	0
54	MG	1A	3957	1/1	0.95	0.06	36,36,36,36	0
54	MG	2A	3681	1/1	0.95	0.05	76,76,76,76	0
54	MG	1A	3440	1/1	0.95	0.08	34,34,34,34	0
54	MG	1A	3319	1/1	0.95	0.21	40,40,40,40	0
54	MG	2A	3464	1/1	0.95	0.09	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	3733	1/1	0.95	0.08	53,53,53,53	0
54	MG	2A	3686	1/1	0.95	0.09	41,41,41,41	0
54	MG	1A	3734	1/1	0.95	0.14	51,51,51,51	0
54	MG	1A	3965	1/1	0.95	0.05	32,32,32,32	0
54	MG	2a	3094	1/1	0.95	0.27	59,59,59,59	0
54	MG	1a	1619	1/1	0.95	0.11	70,70,70,70	0
54	MG	1A	3144	1/1	0.95	0.14	47,47,47,47	0
54	MG	1A	3585	1/1	0.95	0.09	51,51,51,51	0
54	MG	1A	3236	1/1	0.95	0.15	44,44,44,44	0
54	MG	1A	3444	1/1	0.95	0.08	35,35,35,35	0
54	MG	1D	312	1/1	0.95	0.17	37,37,37,37	0
54	MG	1A	3655	1/1	0.95	0.07	30,30,30,30	0
54	MG	1A	3148	1/1	0.95	0.14	38,38,38,38	0
54	MG	1A	3323	1/1	0.95	0.16	46,46,46,46	0
54	MG	1a	1633	1/1	0.95	0.08	42,42,42,42	0
54	MG	1A	3209	1/1	0.95	0.29	48,48,48,48	0
54	MG	1A	3241	1/1	0.95	0.30	45,45,45,45	0
54	MG	1A	3975	1/1	0.95	0.09	68,68,68,68	0
54	MG	1A	3660	1/1	0.95	0.16	50,50,50,50	0
54	MG	2A	3484	1/1	0.95	0.08	38,38,38,38	0
54	MG	2A	3136	1/1	0.95	0.12	72,72,72,72	0
54	MG	2A	3137	1/1	0.95	0.22	72,72,72,72	0
54	MG	2A	3713	1/1	0.95	0.25	71,71,71,71	0
54	MG	2A	3288	1/1	0.95	0.14	65,65,65,65	0
54	MG	1A	3243	1/1	0.95	0.29	51,51,51,51	0
54	MG	1A	3752	1/1	0.95	0.07	35,35,35,35	0
54	MG	1A	3452	1/1	0.95	0.06	32,32,32,32	0
54	MG	1F	306	1/1	0.95	0.17	42,42,42,42	0
54	MG	1A	3387	1/1	0.95	0.06	39,39,39,39	0
54	MG	1A	3863	1/1	0.95	0.10	55,55,55,55	0
54	MG	2A	3496	1/1	0.95	0.12	48,48,48,48	0
54	MG	1A	3100	1/1	0.95	0.06	55,55,55,55	0
54	MG	1A	3284	1/1	0.95	0.39	49,49,49,49	0
54	MG	2A	3147	1/1	0.95	0.13	67,67,67,67	0
54	MG	1A	3120	1/1	0.95	0.14	51,51,51,51	0
54	MG	2A	3150	1/1	0.95	0.08	52,52,52,52	0
54	MG	1A	3289	1/1	0.95	0.16	40,40,40,40	0
54	MG	1A	3992	1/1	0.95	0.07	63,63,63,63	0
54	MG	2A	3153	1/1	0.95	0.13	63,63,63,63	0
54	MG	1F	318	1/1	0.95	0.06	55,55,55,55	0
54	MG	1a	1653	1/1	0.95	0.07	48,48,48,48	0
54	MG	2a	3135	1/1	0.95	0.17	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	2A	3316	1/1	0.95	0.06	41,41,41,41	0
54	MG	1a	1654	1/1	0.95	0.21	66,66,66,66	0
54	MG	1G	201	1/1	0.95	0.16	66,66,66,66	0
54	MG	2A	3515	1/1	0.95	0.07	45,45,45,45	0
54	MG	1A	3052	1/1	0.95	0.23	42,42,42,42	0
54	MG	1A	3396	1/1	0.95	0.06	58,58,58,58	0
54	MG	1G	204	1/1	0.95	0.11	51,51,51,51	0
54	MG	2A	3008	1/1	0.95	0.09	51,51,51,51	0
54	MG	1A	3870	1/1	0.95	0.08	47,47,47,47	0
54	MG	2A	3324	1/1	0.95	0.07	47,47,47,47	0
54	MG	2a	3146	1/1	0.95	0.13	68,68,68,68	0
54	MG	2A	3011	1/1	0.95	0.07	47,47,47,47	0
54	MG	1a	1660	1/1	0.95	0.10	74,74,74,74	0
54	MG	2A	3329	1/1	0.95	0.15	45,45,45,45	0
54	MG	1A	3996	1/1	0.95	0.06	65,65,65,65	0
54	MG	1N	201	1/1	0.95	0.13	46,46,46,46	0
54	MG	2A	3333	1/1	0.95	0.19	65,65,65,65	0
54	MG	1A	3102	1/1	0.95	0.12	45,45,45,45	0
54	MG	1A	3292	1/1	0.95	0.13	52,52,52,52	0
54	MG	1A	3538	1/1	0.95	0.06	42,42,42,42	0
54	MG	1A	3103	1/1	0.95	0.26	50,50,50,50	0
54	MG	1P	202	1/1	0.95	0.22	36,36,36,36	0
54	MG	1A	3675	1/1	0.95	0.10	35,35,35,35	0
54	MG	1A	3064	1/1	0.95	0.07	44,44,44,44	0
54	MG	1A	3542	1/1	0.95	0.05	61,61,61,61	0
54	MG	2A	3028	1/1	0.95	0.09	56,56,56,56	0
54	MG	2A	3029	1/1	0.95	0.08	52,52,52,52	0
54	MG	1Q	201	1/1	0.95	0.12	40,40,40,40	0
54	MG	1A	3258	1/1	0.95	0.17	47,47,47,47	0
54	MG	1A	3681	1/1	0.95	0.10	38,38,38,38	0
54	MG	2A	3357	1/1	0.95	0.12	43,43,43,43	0
54	MG	2A	3360	1/1	0.95	0.23	72,72,72,72	0
54	MG	1a	1674	1/1	0.95	0.18	75,75,75,75	0
54	MG	2F	303	1/1	0.95	0.14	66,66,66,66	0
54	MG	2A	3547	1/1	0.95	0.07	56,56,56,56	0
54	MG	2a	3178	1/1	0.95	0.10	82,82,82,82	0
54	MG	1A	3682	1/1	0.95	0.06	46,46,46,46	0
54	MG	1A	3779	1/1	0.95	0.06	49,49,49,49	0
54	MG	2A	3553	1/1	0.95	0.07	66,66,66,66	0
54	MG	1A	3129	1/1	0.95	0.11	54,54,54,54	0
54	MG	1A	3162	1/1	0.95	0.22	45,45,45,45	0
54	MG	2R	202	1/1	0.95	0.09	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	3367	1/1	0.95	0.07	44,44,44,44	0
54	MG	2T	201	1/1	0.95	0.22	71,71,71,71	0
54	MG	2T	202	1/1	0.95	0.19	72,72,72,72	0
54	MG	1A	3030	1/1	0.95	0.06	33,33,33,33	0
54	MG	1A	3548	1/1	0.95	0.07	53,53,53,53	0
54	MG	1a	1801	1/1	0.95	0.05	76,76,76,76	0
54	MG	2A	3371	1/1	0.95	0.06	48,48,48,48	0
54	MG	1A	3891	1/1	0.95	0.05	30,30,30,30	0
54	MG	1U	201	1/1	0.95	0.17	42,42,42,42	0
54	MG	1A	3551	1/1	0.95	0.39	37,37,37,37	0
54	MG	1U	207	1/1	0.95	0.17	40,40,40,40	0
54	MG	1a	1806	1/1	0.95	0.11	65,65,65,65	0
54	MG	2A	3383	1/1	0.95	0.26	60,60,60,60	0
54	MG	1a	1808	1/1	0.95	0.07	61,61,61,61	0
55	HGR	2A	3731	36/36	0.95	0.11	36,44,52,57	0
54	MG	1A	4016	1/1	0.95	0.09	19,19,19,19	0
54	MG	27	102	1/1	0.95	0.23	47,47,47,47	0
57	MPD	18	103	8/8	0.95	0.12	36,41,45,49	0
54	MG	1A	3088	1/1	0.95	0.41	46,46,46,46	0
54	MG	2A	3199	1/1	0.95	0.10	58,58,58,58	0
54	MG	1A	3412	1/1	0.95	0.06	38,38,38,38	0
54	MG	1A	3791	1/1	0.95	0.12	62,62,62,62	0
54	MG	1A	3413	1/1	0.95	0.08	42,42,42,42	0
54	MG	1A	3479	1/1	0.95	0.09	58,58,58,58	0
54	MG	2A	3393	1/1	0.95	0.13	71,71,71,71	0
54	MG	1D	308	1/1	0.96	0.19	39,39,39,39	0
54	MG	1A	3694	1/1	0.96	0.12	52,52,52,52	0
54	MG	1D	310	1/1	0.96	0.10	55,55,55,55	0
54	MG	2A	3572	1/1	0.96	0.08	73,73,73,73	0
54	MG	1A	3298	1/1	0.96	0.10	31,31,31,31	0
54	MG	1a	1637	1/1	0.96	0.06	45,45,45,45	0
54	MG	2a	3001	1/1	0.96	0.07	54,54,54,54	0
54	MG	1A	3361	1/1	0.96	0.16	43,43,43,43	0
54	MG	1A	3171	1/1	0.96	0.04	32,32,32,32	0
54	MG	2A	3382	1/1	0.96	0.07	64,64,64,64	0
54	MG	1A	3094	1/1	0.96	0.28	42,42,42,42	0
54	MG	1A	3532	1/1	0.96	0.07	53,53,53,53	0
54	MG	1A	3700	1/1	0.96	0.08	66,66,66,66	0
54	MG	1A	3173	1/1	0.96	0.30	46,46,46,46	0
54	MG	1A	3303	1/1	0.96	0.14	39,39,39,39	0
54	MG	1A	3142	1/1	0.96	0.07	50,50,50,50	0
54	MG	1A	3095	1/1	0.96	0.18	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	2a	3012	1/1	0.96	0.07	60,60,60,60	0
54	MG	2A	3588	1/1	0.96	0.07	57,57,57,57	0
54	MG	1A	3817	1/1	0.96	0.11	62,62,62,62	0
54	MG	1a	1648	1/1	0.96	0.12	49,49,49,49	0
54	MG	1A	3818	1/1	0.96	0.06	81,81,81,81	0
54	MG	2A	3394	1/1	0.96	0.06	72,72,72,72	0
54	MG	1F	304	1/1	0.96	0.21	39,39,39,39	0
54	MG	1A	3176	1/1	0.96	0.06	41,41,41,41	0
54	MG	1F	307	1/1	0.96	0.27	33,33,33,33	0
54	MG	2A	3597	1/1	0.96	0.10	72,72,72,72	0
54	MG	2A	3598	1/1	0.96	0.09	71,71,71,71	0
54	MG	1F	309	1/1	0.96	0.24	59,59,59,59	0
54	MG	1A	3960	1/1	0.96	0.15	60,60,60,60	0
54	MG	1A	3059	1/1	0.96	0.13	29,29,29,29	0
54	MG	1A	3708	1/1	0.96	0.14	59,59,59,59	0
54	MG	1A	3457	1/1	0.96	0.06	43,43,43,43	0
54	MG	2A	3606	1/1	0.96	0.09	66,66,66,66	0
54	MG	1A	3146	1/1	0.96	0.15	48,48,48,48	0
54	MG	1A	3824	1/1	0.96	0.10	74,74,74,74	0
54	MG	1A	3459	1/1	0.96	0.09	62,62,62,62	0
54	MG	1A	3460	1/1	0.96	0.17	62,62,62,62	0
54	MG	1A	3313	1/1	0.96	0.34	41,41,41,41	0
54	MG	2A	3614	1/1	0.96	0.07	61,61,61,61	0
54	MG	1A	3717	1/1	0.96	0.06	51,51,51,51	0
54	MG	1A	3718	1/1	0.96	0.17	48,48,48,48	0
54	MG	1A	3830	1/1	0.96	0.09	52,52,52,52	0
54	MG	1A	3383	1/1	0.96	0.07	58,58,58,58	0
54	MG	2A	3413	1/1	0.96	0.07	42,42,42,42	0
54	MG	1A	3179	1/1	0.96	0.15	37,37,37,37	0
54	MG	1A	3834	1/1	0.96	0.09	43,43,43,43	0
54	MG	1A	3267	1/1	0.96	0.10	54,54,54,54	0
54	MG	1A	3181	1/1	0.96	0.15	61,61,61,61	0
54	MG	1A	3317	1/1	0.96	0.05	21,21,21,21	0
54	MG	2A	3420	1/1	0.96	0.07	39,39,39,39	0
54	MG	1A	3389	1/1	0.96	0.06	22,22,22,22	0
54	MG	1A	3841	1/1	0.96	0.22	42,42,42,42	0
54	MG	1A	3842	1/1	0.96	0.10	70,70,70,70	0
54	MG	1A	3725	1/1	0.96	0.17	46,46,46,46	0
54	MG	2A	3425	1/1	0.96	0.10	65,65,65,65	0
54	MG	1A	3269	1/1	0.96	0.29	36,36,36,36	0
54	MG	1A	3729	1/1	0.96	0.09	64,64,64,64	0
54	MG	2A	3071	1/1	0.96	0.12	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	2A	3072	1/1	0.96	0.06	34,34,34,34	0
54	MG	1Q	202	1/1	0.96	0.06	35,35,35,35	0
54	MG	1A	3846	1/1	0.96	0.05	25,25,25,25	0
54	MG	1A	3183	1/1	0.96	0.11	53,53,53,53	0
54	MG	1Q	205	1/1	0.96	0.12	62,62,62,62	0
54	MG	1A	3028	1/1	0.96	0.24	41,41,41,41	0
54	MG	2A	3641	1/1	0.96	0.05	65,65,65,65	0
54	MG	2A	3645	1/1	0.96	0.06	70,70,70,70	0
54	MG	1A	3393	1/1	0.96	0.05	30,30,30,30	0
54	MG	1A	3081	1/1	0.96	0.31	44,44,44,44	0
54	MG	2A	3651	1/1	0.96	0.10	60,60,60,60	0
54	MG	1A	3150	1/1	0.96	0.08	42,42,42,42	0
54	MG	1A	3274	1/1	0.96	0.13	50,50,50,50	0
54	MG	2A	3655	1/1	0.96	0.08	69,69,69,69	0
54	MG	2A	3440	1/1	0.96	0.08	59,59,59,59	0
54	MG	2a	3072	1/1	0.96	0.06	63,63,63,63	0
54	MG	2A	3084	1/1	0.96	0.13	51,51,51,51	0
54	MG	1T	202	1/1	0.96	0.09	68,68,68,68	0
54	MG	2A	3246	1/1	0.96	0.10	56,56,56,56	0
54	MG	1A	3276	1/1	0.96	0.18	33,33,33,33	0
54	MG	1A	3151	1/1	0.96	0.29	41,41,41,41	0
54	MG	2A	3664	1/1	0.96	0.06	35,35,35,35	0
54	MG	1A	3856	1/1	0.96	0.15	50,50,50,50	0
54	MG	1a	1833	1/1	0.96	0.09	68,68,68,68	0
54	MG	1U	202	1/1	0.96	0.16	40,40,40,40	0
54	MG	1U	204	1/1	0.96	0.27	65,65,65,65	0
54	MG	2A	3669	1/1	0.96	0.13	78,78,78,78	0
54	MG	1U	205	1/1	0.96	0.30	35,35,35,35	0
54	MG	1A	3402	1/1	0.96	0.08	40,40,40,40	0
54	MG	1A	4003	1/1	0.96	0.06	28,28,28,28	0
54	MG	1A	3051	1/1	0.96	0.31	52,52,52,52	0
54	MG	1A	3570	1/1	0.96	0.06	30,30,30,30	0
54	MG	1A	3085	1/1	0.96	0.37	40,40,40,40	0
54	MG	2A	3099	1/1	0.96	0.16	65,65,65,65	0
54	MG	2A	3101	1/1	0.96	0.14	58,58,58,58	0
54	MG	2a	3093	1/1	0.96	0.30	63,63,63,63	0
54	MG	1V	206	1/1	0.96	0.07	61,61,61,61	0
54	MG	1A	3745	1/1	0.96	0.06	40,40,40,40	0
54	MG	1A	3406	1/1	0.96	0.15	62,62,62,62	0
54	MG	1A	3487	1/1	0.96	0.10	59,59,59,59	0
54	MG	1A	3750	1/1	0.96	0.13	48,48,48,48	0
54	MG	2A	3107	1/1	0.96	0.05	35,35,35,35	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	2A	3268	1/1	0.96	0.10	60,60,60,60	0
54	MG	2A	3688	1/1	0.96	0.09	72,72,72,72	0
54	MG	1A	3654	1/1	0.96	0.06	44,44,44,44	0
54	MG	1A	3329	1/1	0.96	0.05	43,43,43,43	0
54	MG	1A	3753	1/1	0.96	0.07	58,58,58,58	0
54	MG	10	104	1/1	0.96	0.08	64,64,64,64	0
54	MG	1A	3026	1/1	0.96	0.25	40,40,40,40	0
54	MG	1A	3873	1/1	0.96	0.14	43,43,43,43	0
54	MG	1A	3755	1/1	0.96	0.08	37,37,37,37	0
54	MG	1A	3332	1/1	0.96	0.10	29,29,29,29	0
54	MG	2A	3698	1/1	0.96	0.05	75,75,75,75	0
54	MG	1A	3577	1/1	0.96	0.07	57,57,57,57	0
54	MG	1A	3063	1/1	0.96	0.06	38,38,38,38	0
54	MG	1A	3157	1/1	0.96	0.15	46,46,46,46	0
54	MG	1A	3069	1/1	0.96	0.10	42,42,42,42	0
54	MG	1A	3414	1/1	0.96	0.07	48,48,48,48	0
54	MG	1A	3337	1/1	0.96	0.05	34,34,34,34	0
54	MG	1A	3584	1/1	0.96	0.10	45,45,45,45	0
54	MG	2A	3708	1/1	0.96	0.07	80,80,80,80	0
54	MG	1A	3159	1/1	0.96	0.28	49,49,49,49	0
54	MG	1A	3285	1/1	0.96	0.07	49,49,49,49	0
54	MG	1A	3131	1/1	0.96	0.09	64,64,64,64	0
54	MG	1a	1724	1/1	0.96	0.06	43,43,43,43	0
54	MG	1A	3420	1/1	0.96	0.06	45,45,45,45	0
54	MG	1A	3770	1/1	0.96	0.14	52,52,52,52	0
54	MG	1A	3892	1/1	0.96	0.04	56,56,56,56	0
54	MG	1a	1728	1/1	0.96	0.12	46,46,46,46	0
54	MG	2A	3292	1/1	0.96	0.18	74,74,74,74	0
54	MG	1A	3287	1/1	0.96	0.07	39,39,39,39	0
54	MG	1A	4038	1/1	0.96	0.14	57,57,57,57	0
54	MG	2a	3133	1/1	0.96	0.10	64,64,64,64	0
54	MG	1A	3070	1/1	0.96	0.23	45,45,45,45	0
54	MG	17	103	1/1	0.96	0.24	41,41,41,41	0
54	MG	1A	3072	1/1	0.96	0.27	39,39,39,39	0
54	MG	1A	3508	1/1	0.96	0.13	40,40,40,40	0
54	MG	2A	3301	1/1	0.96	0.06	38,38,38,38	0
54	MG	2A	3502	1/1	0.96	0.07	47,47,47,47	0
54	MG	2A	3302	1/1	0.96	0.07	57,57,57,57	0
54	MG	2A	3303	1/1	0.96	0.10	29,29,29,29	0
54	MG	1A	3346	1/1	0.96	0.07	31,31,31,31	0
54	MG	1A	3347	1/1	0.96	0.08	42,42,42,42	0
54	MG	1B	204	1/1	0.96	0.07	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	3513	1/1	0.96	0.08	29,29,29,29	0
54	MG	1A	3781	1/1	0.96	0.08	51,51,51,51	0
54	MG	1A	3433	1/1	0.96	0.06	26,26,26,26	0
54	MG	2A	3145	1/1	0.96	0.08	44,44,44,44	0
54	MG	1A	3165	1/1	0.96	0.17	42,42,42,42	0
54	MG	2a	3150	1/1	0.96	0.11	73,73,73,73	0
54	MG	2A	3516	1/1	0.96	0.09	68,68,68,68	0
54	MG	1A	3680	1/1	0.96	0.20	55,55,55,55	0
54	MG	1A	3519	1/1	0.96	0.07	58,58,58,58	0
54	MG	2a	3155	1/1	0.96	0.09	81,81,81,81	0
54	MG	2A	3149	1/1	0.96	0.12	60,60,60,60	0
54	MG	1A	3073	1/1	0.96	0.06	47,47,47,47	0
54	MG	1a	1606	1/1	0.96	0.10	72,72,72,72	0
54	MG	1A	3911	1/1	0.96	0.09	63,63,63,63	0
54	MG	1a	1608	1/1	0.96	0.07	63,63,63,63	0
54	MG	1A	3913	1/1	0.96	0.10	50,50,50,50	0
54	MG	2A	3325	1/1	0.96	0.06	36,36,36,36	0
54	MG	1A	3788	1/1	0.96	0.06	49,49,49,49	0
54	MG	2A	3327	1/1	0.96	0.16	70,70,70,70	0
54	MG	1A	3111	1/1	0.96	0.14	49,49,49,49	0
54	MG	1o	101	1/1	0.96	0.14	53,53,53,53	0
54	MG	1A	3603	1/1	0.96	0.11	36,36,36,36	0
54	MG	2A	3159	1/1	0.96	0.33	55,55,55,55	0
54	MG	1y	201	1/1	0.96	0.07	72,72,72,72	0
54	MG	1A	3253	1/1	0.96	0.28	40,40,40,40	0
54	MG	2D	306	1/1	0.96	0.08	48,48,48,48	0
54	MG	2A	3336	1/1	0.96	0.06	51,51,51,51	0
54	MG	1A	3795	1/1	0.96	0.06	36,36,36,36	0
54	MG	1A	3523	1/1	0.96	0.08	46,46,46,46	0
54	MG	2D	310	1/1	0.96	0.09	61,61,61,61	0
54	MG	2A	3340	1/1	0.96	0.10	59,59,59,59	0
54	MG	1A	3136	1/1	0.96	0.20	39,39,39,39	0
54	MG	1A	3074	1/1	0.96	0.12	32,32,32,32	0
54	MG	2A	3343	1/1	0.96	0.08	68,68,68,68	0
54	MG	1A	3925	1/1	0.96	0.07	34,34,34,34	0
54	MG	1A	3608	1/1	0.96	0.10	44,44,44,44	0
54	MG	1a	1622	1/1	0.96	0.09	55,55,55,55	0
54	MG	2A	3007	1/1	0.96	0.08	49,49,49,49	0
54	MG	1A	3929	1/1	0.96	0.08	27,27,27,27	0
54	MG	2A	3548	1/1	0.96	0.08	44,44,44,44	0
54	MG	2A	3549	1/1	0.96	0.14	39,39,39,39	0
54	MG	2A	3352	1/1	0.96	0.09	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	3009	1/1	0.96	0.07	49,49,49,49	0
54	MG	2A	3552	1/1	0.96	0.06	88,88,88,88	0
54	MG	2k	201	1/1	0.96	0.12	69,69,69,69	0
54	MG	2R	201	1/1	0.96	0.24	55,55,55,55	0
54	MG	1a	1624	1/1	0.96	0.10	54,54,54,54	0
54	MG	1A	3354	1/1	0.96	0.10	26,26,26,26	0
54	MG	1A	3692	1/1	0.96	0.07	58,58,58,58	0
54	MG	2A	3013	1/1	0.96	0.07	28,28,28,28	0
55	HGR	1A	4041	36/36	0.96	0.08	21,29,35,39	0
54	MG	2A	3014	1/1	0.96	0.09	55,55,55,55	0
54	MG	2A	3558	1/1	0.96	0.07	65,65,65,65	0
54	MG	1A	3256	1/1	0.96	0.19	43,43,43,43	0
54	MG	1A	3938	1/1	0.96	0.08	46,46,46,46	0
54	MG	1a	1630	1/1	0.96	0.11	50,50,50,50	0
54	MG	2Y	201	1/1	0.96	0.14	59,59,59,59	0
54	MG	1A	3939	1/1	0.96	0.07	69,69,69,69	0
54	MG	1A	3942	1/1	0.96	0.05	60,60,60,60	0
54	MG	2A	3021	1/1	0.96	0.06	52,52,52,52	0
54	MG	23	101	1/1	0.96	0.12	62,62,62,62	0
54	MG	2A	3183	1/1	0.96	0.08	55,55,55,55	0
59	ZN	2n	102	1/1	0.96	0.07	108,108,108,108	0
54	MG	1A	3638	1/1	0.97	0.09	45,45,45,45	0
54	MG	1A	3840	1/1	0.97	0.29	39,39,39,39	0
54	MG	1A	3212	1/1	0.97	0.30	46,46,46,46	0
54	MG	1A	3113	1/1	0.97	0.26	36,36,36,36	0
54	MG	2A	3659	1/1	0.97	0.07	48,48,48,48	0
54	MG	2a	3035	1/1	0.97	0.06	46,46,46,46	0
54	MG	1A	3114	1/1	0.97	0.28	42,42,42,42	0
54	MG	2A	3313	1/1	0.97	0.06	51,51,51,51	0
54	MG	1a	1649	1/1	0.97	0.11	53,53,53,53	0
54	MG	2A	3663	1/1	0.97	0.06	43,43,43,43	0
54	MG	2A	3020	1/1	0.97	0.10	50,50,50,50	0
54	MG	1A	3023	1/1	0.97	0.16	40,40,40,40	0
54	MG	1A	3559	1/1	0.97	0.06	57,57,57,57	0
54	MG	1A	3216	1/1	0.97	0.11	53,53,53,53	0
54	MG	1A	3077	1/1	0.97	0.25	45,45,45,45	0
54	MG	1A	3979	1/1	0.97	0.08	81,81,81,81	0
54	MG	2A	3670	1/1	0.97	0.06	72,72,72,72	0
54	MG	1A	3147	1/1	0.97	0.05	37,37,37,37	0
54	MG	2A	3027	1/1	0.97	0.06	41,41,41,41	0
54	MG	1A	3117	1/1	0.97	0.18	36,36,36,36	0
54	MG	1A	3096	1/1	0.97	0.07	43,43,43,43	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	2A	3493	1/1	0.97	0.06	57,57,57,57	0
54	MG	1A	3983	1/1	0.97	0.10	51,51,51,51	0
54	MG	1A	3182	1/1	0.97	0.16	35,35,35,35	0
54	MG	1A	3985	1/1	0.97	0.12	59,59,59,59	0
54	MG	1A	3394	1/1	0.97	0.09	35,35,35,35	0
54	MG	1A	3653	1/1	0.97	0.08	36,36,36,36	0
54	MG	1P	201	1/1	0.97	0.34	36,36,36,36	0
54	MG	1A	3988	1/1	0.97	0.04	28,28,28,28	0
54	MG	2A	3334	1/1	0.97	0.08	58,58,58,58	0
54	MG	1A	3098	1/1	0.97	0.03	22,22,22,22	0
54	MG	2A	3504	1/1	0.97	0.09	59,59,59,59	0
54	MG	1A	3122	1/1	0.97	0.33	44,44,44,44	0
54	MG	2A	3337	1/1	0.97	0.06	53,53,53,53	0
54	MG	1A	3858	1/1	0.97	0.06	43,43,43,43	0
54	MG	1A	3859	1/1	0.97	0.06	48,48,48,48	0
54	MG	1A	3185	1/1	0.97	0.17	33,33,33,33	0
54	MG	1A	3187	1/1	0.97	0.27	43,43,43,43	0
54	MG	1A	3481	1/1	0.97	0.06	60,60,60,60	0
54	MG	1A	3400	1/1	0.97	0.06	64,64,64,64	0
54	MG	1A	3124	1/1	0.97	0.09	36,36,36,36	0
54	MG	1A	3331	1/1	0.97	0.07	56,56,56,56	0
54	MG	1A	3403	1/1	0.97	0.06	55,55,55,55	0
54	MG	2A	3700	1/1	0.97	0.06	64,64,64,64	0
54	MG	1A	3189	1/1	0.97	0.28	42,42,42,42	0
54	MG	2A	3050	1/1	0.97	0.15	49,49,49,49	0
54	MG	1A	3578	1/1	0.97	0.11	55,55,55,55	0
54	MG	2a	3078	1/1	0.97	0.08	69,69,69,69	0
54	MG	2A	3704	1/1	0.97	0.05	65,65,65,65	0
54	MG	1A	3229	1/1	0.97	0.16	44,44,44,44	0
54	MG	2A	3354	1/1	0.97	0.06	40,40,40,40	0
54	MG	2A	3196	1/1	0.97	0.07	61,61,61,61	0
54	MG	1A	3763	1/1	0.97	0.05	27,27,27,27	0
54	MG	1A	3079	1/1	0.97	0.17	45,45,45,45	0
54	MG	2A	3359	1/1	0.97	0.09	62,62,62,62	0
54	MG	1A	3765	1/1	0.97	0.08	50,50,50,50	0
54	MG	2A	3361	1/1	0.97	0.08	49,49,49,49	0
54	MG	1A	3053	1/1	0.97	0.11	37,37,37,37	0
54	MG	1U	203	1/1	0.97	0.31	41,41,41,41	0
54	MG	1A	3491	1/1	0.97	0.07	58,58,58,58	0
54	MG	1A	3408	1/1	0.97	0.08	39,39,39,39	0
54	MG	1A	3024	1/1	0.97	0.06	28,28,28,28	0
54	MG	1A	3338	1/1	0.97	0.12	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	3880	1/1	0.97	0.05	63,63,63,63	0
54	MG	1A	3881	1/1	0.97	0.07	48,48,48,48	0
54	MG	1A	3771	1/1	0.97	0.05	32,32,32,32	0
54	MG	1A	3773	1/1	0.97	0.10	32,32,32,32	0
54	MG	1A	3884	1/1	0.97	0.06	36,36,36,36	0
54	MG	1A	3235	1/1	0.97	0.23	42,42,42,42	0
54	MG	1W	203	1/1	0.97	0.06	56,56,56,56	0
54	MG	2a	3101	1/1	0.97	0.31	61,61,61,61	0
54	MG	1A	3156	1/1	0.97	0.21	38,38,38,38	0
54	MG	2A	3070	1/1	0.97	0.24	49,49,49,49	0
54	MG	2A	3545	1/1	0.97	0.09	59,59,59,59	0
54	MG	1A	3237	1/1	0.97	0.32	36,36,36,36	0
54	MG	1A	3342	1/1	0.97	0.05	29,29,29,29	0
54	MG	2A	3073	1/1	0.97	0.11	53,53,53,53	0
54	MG	1A	3288	1/1	0.97	0.09	37,37,37,37	0
54	MG	1A	4027	1/1	0.97	0.06	46,46,46,46	0
54	MG	2A	3076	1/1	0.97	0.09	60,60,60,60	0
54	MG	1A	3678	1/1	0.97	0.07	56,56,56,56	0
54	MG	1a	1701	1/1	0.97	0.10	65,65,65,65	0
54	MG	1A	3083	1/1	0.97	0.14	40,40,40,40	0
54	MG	1A	3417	1/1	0.97	0.06	31,31,31,31	0
54	MG	2A	3392	1/1	0.97	0.12	54,54,54,54	0
54	MG	1A	3782	1/1	0.97	0.14	36,36,36,36	0
54	MG	1A	3055	1/1	0.97	0.23	34,34,34,34	0
54	MG	2A	3227	1/1	0.97	0.12	56,56,56,56	0
54	MG	2a	3119	1/1	0.97	0.05	74,74,74,74	0
54	MG	1A	3594	1/1	0.97	0.06	55,55,55,55	0
54	MG	1A	3898	1/1	0.97	0.06	29,29,29,29	0
54	MG	1A	3104	1/1	0.97	0.20	44,44,44,44	0
54	MG	1A	3242	1/1	0.97	0.27	44,44,44,44	0
54	MG	1A	3422	1/1	0.97	0.07	23,23,23,23	0
54	MG	2A	3088	1/1	0.97	0.07	47,47,47,47	0
54	MG	13	101	1/1	0.97	0.11	43,43,43,43	0
54	MG	2A	3569	1/1	0.97	0.11	73,73,73,73	0
54	MG	1A	3056	1/1	0.97	0.10	39,39,39,39	0
54	MG	1A	3244	1/1	0.97	0.21	45,45,45,45	0
54	MG	2A	3237	1/1	0.97	0.29	44,44,44,44	0
54	MG	15	101	1/1	0.97	0.11	45,45,45,45	0
54	MG	1a	1859	1/1	0.97	0.13	60,60,60,60	0
54	MG	1A	3514	1/1	0.97	0.05	43,43,43,43	0
54	MG	2A	3576	1/1	0.97	0.08	41,41,41,41	0
54	MG	1A	3426	1/1	0.97	0.05	29,29,29,29	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	1A	3516	1/1	0.97	0.06	36,36,36,36	0
54	MG	1A	3427	1/1	0.97	0.08	36,36,36,36	0
54	MG	2A	3412	1/1	0.97	0.07	45,45,45,45	0
54	MG	2E	301	1/1	0.97	0.22	54,54,54,54	0
54	MG	1A	3246	1/1	0.97	0.28	38,38,38,38	0
54	MG	2E	305	1/1	0.97	0.07	43,43,43,43	0
54	MG	1a	1865	1/1	0.97	0.05	71,71,71,71	0
54	MG	1A	3161	1/1	0.97	0.15	45,45,45,45	0
54	MG	1A	3018	1/1	0.97	0.19	31,31,31,31	0
54	MG	1A	3800	1/1	0.97	0.06	42,42,42,42	0
54	MG	2F	304	1/1	0.97	0.22	52,52,52,52	0
54	MG	1A	3006	1/1	0.97	0.05	36,36,36,36	0
54	MG	1A	3251	1/1	0.97	0.29	41,41,41,41	0
54	MG	1A	3016	1/1	0.97	0.30	41,41,41,41	0
54	MG	1A	3356	1/1	0.97	0.11	28,28,28,28	0
54	MG	2a	3152	1/1	0.97	0.06	66,66,66,66	0
54	MG	1A	3357	1/1	0.97	0.06	30,30,30,30	0
54	MG	1B	213	1/1	0.97	0.07	52,52,52,52	0
54	MG	2Q	201	1/1	0.97	0.04	58,58,58,58	0
54	MG	1A	3203	1/1	0.97	0.16	51,51,51,51	0
54	MG	2a	3157	1/1	0.97	0.09	75,75,75,75	0
54	MG	1A	3359	1/1	0.97	0.06	15,15,15,15	0
54	MG	1A	3166	1/1	0.97	0.18	41,41,41,41	0
54	MG	1A	3071	1/1	0.97	0.34	34,34,34,34	0
54	MG	1A	3928	1/1	0.97	0.04	35,35,35,35	0
54	MG	2a	3163	1/1	0.97	0.16	65,65,65,65	0
54	MG	2A	3600	1/1	0.97	0.04	50,50,50,50	0
54	MG	1A	3363	1/1	0.97	0.10	30,30,30,30	0
54	MG	1A	3618	1/1	0.97	0.06	44,44,44,44	0
54	MG	1A	3707	1/1	0.97	0.07	55,55,55,55	0
54	MG	1A	3934	1/1	0.97	0.18	48,48,48,48	0
54	MG	2W	202	1/1	0.97	0.07	68,68,68,68	0
54	MG	2X	101	1/1	0.97	0.09	67,67,67,67	0
54	MG	1A	3048	1/1	0.97	0.05	30,30,30,30	0
54	MG	1A	3815	1/1	0.97	0.07	79,79,79,79	0
54	MG	1A	3446	1/1	0.97	0.11	34,34,34,34	0
54	MG	1A	3940	1/1	0.97	0.08	69,69,69,69	0
54	MG	1A	3941	1/1	0.97	0.07	63,63,63,63	0
54	MG	1A	3307	1/1	0.97	0.11	57,57,57,57	0
54	MG	1A	3367	1/1	0.97	0.09	55,55,55,55	0
54	MG	1A	3368	1/1	0.97	0.08	48,48,48,48	0
54	MG	1g	203	1/1	0.97	0.07	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	1A	3946	1/1	0.97	0.07	58,58,58,58	0
54	MG	1A	3715	1/1	0.97	0.10	46,46,46,46	0
54	MG	1A	3308	1/1	0.97	0.27	48,48,48,48	0
54	MG	1a	1618	1/1	0.97	0.05	53,53,53,53	0
54	MG	1A	3451	1/1	0.97	0.10	34,34,34,34	0
54	MG	1A	3626	1/1	0.97	0.06	56,56,56,56	0
54	MG	1A	3370	1/1	0.97	0.07	58,58,58,58	0
54	MG	1A	3309	1/1	0.97	0.14	41,41,41,41	0
54	MG	1A	3137	1/1	0.97	0.19	39,39,39,39	0
54	MG	1A	3021	1/1	0.97	0.23	45,45,45,45	0
54	MG	1a	1626	1/1	0.97	0.05	59,59,59,59	0
54	MG	1A	3139	1/1	0.97	0.19	33,33,33,33	0
54	MG	1A	3547	1/1	0.97	0.06	24,24,24,24	0
54	MG	1D	318	1/1	0.97	0.11	52,52,52,52	0
54	MG	1A	3140	1/1	0.97	0.25	36,36,36,36	0
54	MG	1A	3726	1/1	0.97	0.09	58,58,58,58	0
54	MG	1A	3832	1/1	0.97	0.12	53,53,53,53	0
54	MG	1A	3005	1/1	0.97	0.09	30,30,30,30	0
54	MG	1A	3963	1/1	0.97	0.06	70,70,70,70	0
54	MG	1F	301	1/1	0.97	0.11	40,40,40,40	0
54	MG	1A	3380	1/1	0.97	0.08	30,30,30,30	0
56	ERY	1A	4042	51/51	0.97	0.08	20,37,45,53	0
56	ERY	2A	3732	51/51	0.97	0.09	38,48,57,63	0
54	MG	1F	305	1/1	0.97	0.12	46,46,46,46	0
54	MG	1A	3835	1/1	0.97	0.09	55,55,55,55	0
54	MG	1A	3381	1/1	0.97	0.12	41,41,41,41	0
54	MG	2a	3022	1/1	0.97	0.04	54,54,54,54	0
54	MG	2A	3469	1/1	0.97	0.09	42,42,42,42	0
54	MG	1F	308	1/1	0.97	0.13	36,36,36,36	0
54	MG	2A	3471	1/1	0.97	0.05	65,65,65,65	0
54	MG	1A	3731	1/1	0.97	0.07	50,50,50,50	0
54	MG	1F	310	1/1	0.97	0.10	45,45,45,45	0
54	MG	1A	3554	1/1	0.97	0.07	34,34,34,34	0
59	ZN	29	501	1/1	0.97	0.04	77,77,77,77	0
54	MG	2A	3654	1/1	0.97	0.06	52,52,52,52	0
60	SF4	1d	306	8/8	0.97	0.07	68,77,83,90	0
60	SF4	2d	501	8/8	0.97	0.06	74,89,98,98	0
54	MG	1V	202	1/1	0.98	0.20	38,38,38,38	0
54	MG	2E	302	1/1	0.98	0.08	53,53,53,53	0
54	MG	1A	3118	1/1	0.98	0.09	46,46,46,46	0
54	MG	1D	302	1/1	0.98	0.07	57,57,57,57	0
54	MG	2A	3637	1/1	0.98	0.04	83,83,83,83	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	1A	3378	1/1	0.98	0.04	28,28,28,28	0
54	MG	1D	304	1/1	0.98	0.04	45,45,45,45	0
54	MG	1A	3746	1/1	0.98	0.04	57,57,57,57	0
54	MG	1A	3747	1/1	0.98	0.05	80,80,80,80	0
54	MG	2A	3643	1/1	0.98	0.07	45,45,45,45	0
54	MG	1A	3641	1/1	0.98	0.14	41,41,41,41	0
54	MG	1A	3932	1/1	0.98	0.05	21,21,21,21	0
54	MG	2A	3647	1/1	0.98	0.06	89,89,89,89	0
54	MG	2A	3648	1/1	0.98	0.06	48,48,48,48	0
54	MG	2A	3293	1/1	0.98	0.06	68,68,68,68	0
54	MG	2A	3650	1/1	0.98	0.13	62,62,62,62	0
54	MG	2A	3100	1/1	0.98	0.09	56,56,56,56	0
54	MG	1A	3933	1/1	0.98	0.07	53,53,53,53	0
54	MG	2A	3296	1/1	0.98	0.08	46,46,46,46	0
54	MG	2A	3525	1/1	0.98	0.06	62,62,62,62	0
54	MG	1A	3264	1/1	0.98	0.23	36,36,36,36	0
54	MG	1A	3935	1/1	0.98	0.04	52,52,52,52	0
54	MG	1a	1734	1/1	0.98	0.06	46,46,46,46	0
54	MG	1A	3936	1/1	0.98	0.06	63,63,63,63	0
54	MG	1A	3240	1/1	0.98	0.17	33,33,33,33	0
54	MG	2A	3415	1/1	0.98	0.04	43,43,43,43	0
54	MG	1A	3318	1/1	0.98	0.16	44,44,44,44	0
54	MG	1A	3503	1/1	0.98	0.05	29,29,29,29	0
54	MG	1A	3382	1/1	0.98	0.05	31,31,31,31	0
54	MG	2A	3306	1/1	0.98	0.05	43,43,43,43	0
54	MG	1A	4010	1/1	0.98	0.06	57,57,57,57	0
54	MG	1A	3186	1/1	0.98	0.10	38,38,38,38	0
54	MG	1E	302	1/1	0.98	0.13	35,35,35,35	0
54	MG	1A	3078	1/1	0.98	0.26	37,37,37,37	0
54	MG	1A	3145	1/1	0.98	0.12	27,27,27,27	0
54	MG	2a	3123	1/1	0.98	0.06	61,61,61,61	0
54	MG	1A	3602	1/1	0.98	0.06	24,24,24,24	0
54	MG	1A	3421	1/1	0.98	0.07	46,46,46,46	0
54	MG	2A	3315	1/1	0.98	0.05	44,44,44,44	0
54	MG	1A	3876	1/1	0.98	0.04	39,39,39,39	0
54	MG	2A	3429	1/1	0.98	0.04	55,55,55,55	0
54	MG	13	103	1/1	0.98	0.14	45,45,45,45	0
54	MG	1F	302	1/1	0.98	0.11	39,39,39,39	0
54	MG	1F	303	1/1	0.98	0.14	38,38,38,38	0
54	MG	1A	3509	1/1	0.98	0.05	37,37,37,37	0
54	MG	1A	3463	1/1	0.98	0.05	18,18,18,18	0
54	MG	1A	3042	1/1	0.98	0.04	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	1845	1/1	0.98	0.06	70,70,70,70	0
54	MG	1A	4020	1/1	0.98	0.04	42,42,42,42	0
54	MG	1a	1848	1/1	0.98	0.06	62,62,62,62	0
54	MG	2A	3127	1/1	0.98	0.22	47,47,47,47	0
54	MG	1A	4021	1/1	0.98	0.04	54,54,54,54	0
54	MG	2A	3687	1/1	0.98	0.05	52,52,52,52	0
54	MG	1A	3512	1/1	0.98	0.12	28,28,28,28	0
54	MG	1a	1851	1/1	0.98	0.09	65,65,65,65	0
54	MG	2A	3330	1/1	0.98	0.11	63,63,63,63	0
54	MG	1A	4023	1/1	0.98	0.10	46,46,46,46	0
54	MG	1A	3423	1/1	0.98	0.11	29,29,29,29	0
54	MG	2A	3693	1/1	0.98	0.08	49,49,49,49	0
54	MG	2A	3562	1/1	0.98	0.05	30,30,30,30	0
54	MG	1A	3245	1/1	0.98	0.12	36,36,36,36	0
54	MG	2A	3564	1/1	0.98	0.06	64,64,64,64	0
54	MG	2A	3447	1/1	0.98	0.06	47,47,47,47	0
54	MG	1a	1855	1/1	0.98	0.08	39,39,39,39	0
54	MG	1A	3224	1/1	0.98	0.14	29,29,29,29	0
54	MG	1a	1857	1/1	0.98	0.05	58,58,58,58	0
54	MG	2A	3042	1/1	0.98	0.09	40,40,40,40	0
54	MG	1A	3710	1/1	0.98	0.05	51,51,51,51	0
54	MG	1A	3956	1/1	0.98	0.04	62,62,62,62	0
54	MG	1A	3468	1/1	0.98	0.04	27,27,27,27	0
54	MG	1A	3517	1/1	0.98	0.07	32,32,32,32	0
54	MG	1A	3050	1/1	0.98	0.18	39,39,39,39	0
54	MG	1a	1767	1/1	0.98	0.05	80,80,80,80	0
54	MG	1A	3123	1/1	0.98	0.04	22,22,22,22	0
54	MG	2A	3345	1/1	0.98	0.07	58,58,58,58	0
54	MG	1A	3961	1/1	0.98	0.05	48,48,48,48	0
54	MG	2A	3347	1/1	0.98	0.06	35,35,35,35	0
54	MG	2A	3348	1/1	0.98	0.09	38,38,38,38	0
54	MG	1A	3568	1/1	0.98	0.06	35,35,35,35	0
54	MG	1A	3299	1/1	0.98	0.09	22,22,22,22	0
54	MG	2A	3244	1/1	0.98	0.13	56,56,56,56	0
54	MG	1A	3090	1/1	0.98	0.10	47,47,47,47	0
54	MG	1A	3431	1/1	0.98	0.06	33,33,33,33	0
54	MG	1A	3275	1/1	0.98	0.22	41,41,41,41	0
54	MG	1A	3163	1/1	0.98	0.10	39,39,39,39	0
54	MG	2a	3174	1/1	0.98	0.10	68,68,68,68	0
54	MG	1A	3252	1/1	0.98	0.16	32,32,32,32	0
54	MG	1A	3043	1/1	0.98	0.10	22,22,22,22	0
54	MG	2A	3358	1/1	0.98	0.06	39,39,39,39	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	1A	3672	1/1	0.98	0.11	47,47,47,47	0
54	MG	1A	3398	1/1	0.98	0.04	30,30,30,30	0
54	MG	1A	3902	1/1	0.98	0.05	67,67,67,67	0
54	MG	2A	3254	1/1	0.98	0.11	27,27,27,27	0
54	MG	1A	3230	1/1	0.98	0.05	50,50,50,50	0
54	MG	1A	3306	1/1	0.98	0.10	50,50,50,50	0
54	MG	1A	3365	1/1	0.98	0.05	38,38,38,38	0
54	MG	1A	3195	1/1	0.98	0.14	45,45,45,45	0
54	MG	1A	3336	1/1	0.98	0.10	38,38,38,38	0
54	MG	2a	3057	1/1	0.98	0.13	66,66,66,66	0
54	MG	1A	3978	1/1	0.98	0.08	56,56,56,56	0
54	MG	1A	3082	1/1	0.98	0.07	48,48,48,48	0
54	MG	1A	3534	1/1	0.98	0.04	31,31,31,31	0
54	MG	1d	305	1/1	0.98	0.04	74,74,74,74	0
54	MG	2A	3608	1/1	0.98	0.06	54,54,54,54	0
54	MG	2A	3372	1/1	0.98	0.09	35,35,35,35	0
54	MG	1R	201	1/1	0.98	0.10	44,44,44,44	0
54	MG	2A	3611	1/1	0.98	0.04	73,73,73,73	0
54	MG	1a	1621	1/1	0.98	0.04	55,55,55,55	0
54	MG	1B	214	1/1	0.98	0.05	46,46,46,46	0
54	MG	1A	3180	1/1	0.98	0.20	34,34,34,34	0
54	MG	1A	3735	1/1	0.98	0.04	43,43,43,43	0
54	MG	2A	3379	1/1	0.98	0.05	59,59,59,59	0
54	MG	1A	3912	1/1	0.98	0.03	35,35,35,35	0
54	MG	1A	3234	1/1	0.98	0.20	39,39,39,39	0
54	MG	1A	3793	1/1	0.98	0.04	45,45,45,45	0
54	MG	1A	3371	1/1	0.98	0.08	31,31,31,31	0
54	MG	2A	3498	1/1	0.98	0.04	65,65,65,65	0
54	MG	1A	3044	1/1	0.98	0.15	40,40,40,40	0
54	MG	1T	205	1/1	0.98	0.10	54,54,54,54	0
54	MG	1A	3540	1/1	0.98	0.05	27,27,27,27	0
54	MG	1A	3007	1/1	0.98	0.08	42,42,42,42	0
54	MG	1A	3037	1/1	0.98	0.09	47,47,47,47	0
54	MG	1A	3857	1/1	0.98	0.05	42,42,42,42	0
54	MG	1A	3029	1/1	0.98	0.10	48,48,48,48	0
59	ZN	15	109	1/1	0.98	0.03	46,46,46,46	0
59	ZN	2Y	202	1/1	0.98	0.05	94,94,94,94	0
54	MG	1A	3743	1/1	0.98	0.04	35,35,35,35	0
59	ZN	26	501	1/1	0.98	0.05	75,75,75,75	0
54	MG	1a	1807	1/1	0.98	0.04	83,83,83,83	0
54	MG	2A	3509	1/1	0.98	0.07	49,49,49,49	0
54	MG	1A	3926	1/1	0.98	0.04	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	1V	201	1/1	0.98	0.20	35,35,35,35	0
54	MG	1A	3989	1/1	0.99	0.07	40,40,40,40	0
54	MG	1A	3013	1/1	0.99	0.03	23,23,23,23	0
54	MG	2A	3579	1/1	0.99	0.04	59,59,59,59	0
54	MG	2a	3159	1/1	0.99	0.06	51,51,51,51	0
54	MG	1a	1844	1/1	0.99	0.04	61,61,61,61	0
54	MG	1A	3097	1/1	0.99	0.19	38,38,38,38	0
54	MG	2A	3644	1/1	0.99	0.06	49,49,49,49	0
54	MG	2A	3582	1/1	0.99	0.05	56,56,56,56	0
54	MG	1a	1846	1/1	0.99	0.03	61,61,61,61	0
54	MG	1D	306	1/1	0.99	0.04	20,20,20,20	0
54	MG	1A	3549	1/1	0.99	0.03	49,49,49,49	0
54	MG	1A	3914	1/1	0.99	0.08	44,44,44,44	0
54	MG	1A	3550	1/1	0.99	0.06	37,37,37,37	0
54	MG	2A	3304	1/1	0.99	0.05	69,69,69,69	0
54	MG	1A	3916	1/1	0.99	0.03	51,51,51,51	0
54	MG	1A	3917	1/1	0.99	0.07	39,39,39,39	0
54	MG	1A	3046	1/1	0.99	0.05	14,14,14,14	0
54	MG	1A	3789	1/1	0.99	0.03	36,36,36,36	0
54	MG	1A	3009	1/1	0.99	0.10	33,33,33,33	0
54	MG	2A	3594	1/1	0.99	0.05	43,43,43,43	0
54	MG	2A	3310	1/1	0.99	0.10	50,50,50,50	0
54	MG	1A	3851	1/1	0.99	0.05	50,50,50,50	0
54	MG	1A	3711	1/1	0.99	0.03	37,37,37,37	0
54	MG	1A	3475	1/1	0.99	0.04	34,34,34,34	0
54	MG	1A	3688	1/1	0.99	0.03	50,50,50,50	0
54	MG	1A	3794	1/1	0.99	0.06	47,47,47,47	0
54	MG	2a	3182	1/1	0.99	0.03	68,68,68,68	0
54	MG	2A	3601	1/1	0.99	0.04	42,42,42,42	0
54	MG	1A	3493	1/1	0.99	0.02	44,44,44,44	0
54	MG	1A	3494	1/1	0.99	0.04	35,35,35,35	0
54	MG	1E	304	1/1	0.99	0.14	34,34,34,34	0
54	MG	1A	3476	1/1	0.99	0.04	35,35,35,35	0
54	MG	1E	306	1/1	0.99	0.07	50,50,50,50	0
54	MG	1A	3535	1/1	0.99	0.07	28,28,28,28	0
54	MG	1A	3646	1/1	0.99	0.10	38,38,38,38	0
54	MG	2A	3377	1/1	0.99	0.06	46,46,46,46	0
54	MG	1A	3374	1/1	0.99	0.08	34,34,34,34	0
54	MG	2A	3674	1/1	0.99	0.07	62,62,62,62	0
54	MG	1A	3894	1/1	0.99	0.04	36,36,36,36	0
54	MG	2A	3381	1/1	0.99	0.06	45,45,45,45	0
54	MG	1A	3862	1/1	0.99	0.03	27,27,27,27	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	1A	3896	1/1	0.99	0.06	44,44,44,44	0
54	MG	1A	3772	1/1	0.99	0.10	39,39,39,39	0
54	MG	1a	1822	1/1	0.99	0.04	61,61,61,61	0
54	MG	1A	3075	1/1	0.99	0.04	39,39,39,39	0
54	MG	1A	3436	1/1	0.99	0.04	34,34,34,34	0
54	MG	1A	3900	1/1	0.99	0.06	50,50,50,50	0
54	MG	1A	3247	1/1	0.99	0.20	33,33,33,33	0
54	MG	1A	3438	1/1	0.99	0.05	35,35,35,35	0
54	MG	1A	3806	1/1	0.99	0.05	44,44,44,44	0
54	MG	1A	3482	1/1	0.99	0.03	62,62,62,62	0
54	MG	1a	1736	1/1	0.99	0.06	45,45,45,45	0
54	MG	2A	3507	1/1	0.99	0.06	40,40,40,40	0
54	MG	1B	223	1/1	0.99	0.03	55,55,55,55	0
54	MG	1A	3386	1/1	0.99	0.02	19,19,19,19	0
54	MG	1A	3944	1/1	0.99	0.05	56,56,56,56	0
54	MG	1A	4024	1/1	0.99	0.03	69,69,69,69	0
54	MG	1A	3360	1/1	0.99	0.05	43,43,43,43	0
59	ZN	1Y	202	1/1	0.99	0.06	61,61,61,61	0
59	ZN	14	102	1/1	0.99	0.04	94,94,94,94	0
54	MG	1a	1836	1/1	0.99	0.09	67,67,67,67	0
59	ZN	16	501	1/1	0.99	0.05	49,49,49,49	0
59	ZN	19	103	1/1	0.99	0.04	45,45,45,45	0
59	ZN	1n	103	1/1	0.99	0.03	79,79,79,79	0
54	MG	1A	3454	1/1	0.99	0.04	39,39,39,39	0
54	MG	1A	3728	1/1	0.99	0.03	48,48,48,48	0
59	ZN	25	104	1/1	0.99	0.06	68,68,68,68	0
54	MG	2A	3135	1/1	0.99	0.06	38,38,38,38	0
54	MG	1A	3428	1/1	0.99	0.04	28,28,28,28	0
54	MG	1a	1791	1/1	0.99	0.04	77,77,77,77	0
54	MG	1A	3121	1/1	0.99	0.19	38,38,38,38	0
54	MG	2E	304	1/1	0.99	0.05	62,62,62,62	0
54	MG	2A	3642	1/1	1.00	0.03	62,62,62,62	0
54	MG	2A	3492	1/1	1.00	0.06	42,42,42,42	0
54	MG	2A	3380	1/1	1.00	0.04	40,40,40,40	0
54	MG	1A	3500	1/1	1.00	0.09	51,51,51,51	0

6.5 Other polymers

There are no such residues in this entry.