



wwPDB X-ray Structure Validation Summary Report ⓘ

Aug 5, 2026 – 09:17 PM EDT

PDB ID : 7MD7 / pdb_00007md7
Title : Crystal structure of the *Thermus thermophilus* 70S ribosome in complex with triphenylphosphonium analog of chloramphenicol CAM-C4-TPP and protein Y (YfiA) at 2.80Å resolution
Authors : Chen, C.-W.; Pavlova, J.A.; Lukianov, D.A.; Tereshchenkov, A.G.; Makarov, G.I.; Khairullina, Z.Z.; Tashlitsky, V.N.; Paleskava, A.; Konevega, A.L.; Bogdanov, A.A.; Osterman, I.A.; Sumbatyan, N.V.; Polikanov, Y.S.
Deposited on : 2021-04-03
Resolution : 2.80 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<https://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)

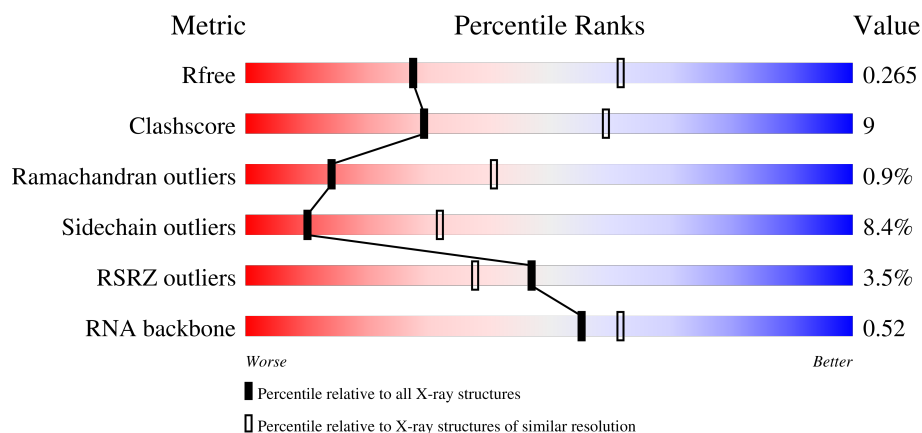
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 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	3866 (2.80-2.80)
Clashscore	190562	4276 (2.80-2.80)
Ramachandran outliers	187476	4196 (2.80-2.80)
Sidechain outliers	187428	4198 (2.80-2.80)
RSRZ outliers	180081	3869 (2.80-2.80)
RNA backbone	3983	1114 (3.00-2.60)

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

Mol	Chain	Length	Quality of chain
1	1A	2915	
1	2A	2915	

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Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.50

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

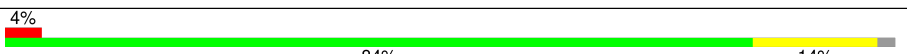
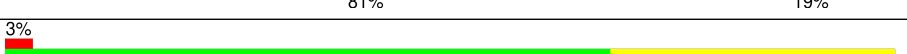
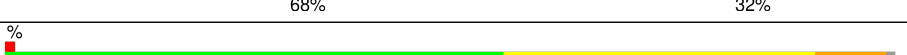
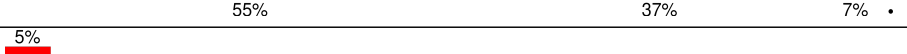
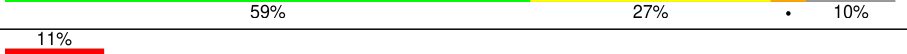
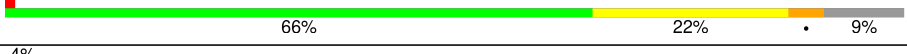
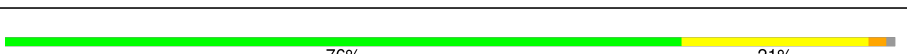
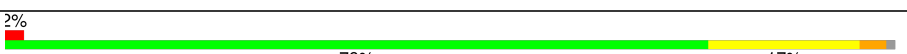
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Mol	Chain	Length	Quality of chain
14	2S	112	
15	1T	146	
15	2T	146	
16	1U	118	
16	2U	118	
17	1V	101	
17	2V	101	
18	1W	113	
18	2W	113	
19	1X	96	
19	2X	96	
20	1Y	110	
20	2Y	110	
21	1Z	206	
21	2Z	206	
22	10	85	
22	20	85	
23	11	98	
23	21	98	
24	12	72	
24	22	72	
25	13	60	
25	23	60	
26	14	71	
26	24	71	

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Mol	Chain	Length	Quality of chain
27	15	60	
27	25	60	
28	16	54	
28	26	54	
29	17	49	
29	27	49	
30	18	65	
30	28	65	
31	19	37	
31	29	37	
32	1a	1521	
32	2a	1521	
33	1b	256	
33	2b	256	
34	1c	239	
34	2c	239	
35	1d	209	
35	2d	209	
36	1e	162	
36	2e	162	
37	1f	101	
37	2f	101	
38	1g	156	
38	2g	156	
39	1h	138	

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Mol	Chain	Length	Quality of chain
39	2h	138	
40	1i	128	
40	2i	128	
41	1j	105	
41	2j	105	
42	1k	129	
42	2k	129	
43	1l	132	
43	2l	132	
44	1m	126	
44	2m	126	
45	1n	61	
45	2n	61	
46	1o	89	
46	2o	89	
47	1p	88	
47	2p	88	
48	1q	105	
48	2q	105	
49	1r	88	
49	2r	88	
50	1s	93	
50	2s	93	
51	1t	106	
51	2t	106	

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Mol	Chain	Length	Quality of chain
52	1u	27	
52	2u	27	
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	1P	203	-	-	-	X
54	MG	2A	3730	-	-	-	X
54	MG	2a	3129	-	-	-	X

2 Entry composition

There are 60 unique types of molecules in this entry. The entry contains 298171 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	1054	Total	Mg	0	0
			1054	1054		
54	1B	27	Total	Mg	0	0
			27	27		
54	1D	17	Total	Mg	0	0
			17	17		
54	1E	6	Total	Mg	0	0
			6	6		
54	1F	15	Total	Mg	0	0
			15	15		
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	6	Total	Mg	0	0
			6	6		
54	1S	1	Total	Mg	0	0
			1	1		
54	1T	6	Total	Mg	0	0
			6	6		
54	1U	8	Total	Mg	0	0
			8	8		
54	1V	5	Total	Mg	0	0
			5	5		
54	1W	4	Total	Mg	0	0
			4	4		
54	1Z	1	Total	Mg	0	0
			1	1		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
54	10	7	Total 7	Mg 7	0	0
54	11	5	Total 5	Mg 5	0	0
54	13	5	Total 5	Mg 5	0	0
54	14	1	Total 1	Mg 1	0	0
54	15	7	Total 7	Mg 7	0	0
54	16	1	Total 1	Mg 1	0	0
54	17	4	Total 4	Mg 4	0	0
54	18	1	Total 1	Mg 1	0	0
54	19	3	Total 3	Mg 3	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	2	Total 2	Mg 2	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	1	Total 1	Mg 1	0	0
54	1n	3	Total 3	Mg 3	0	0

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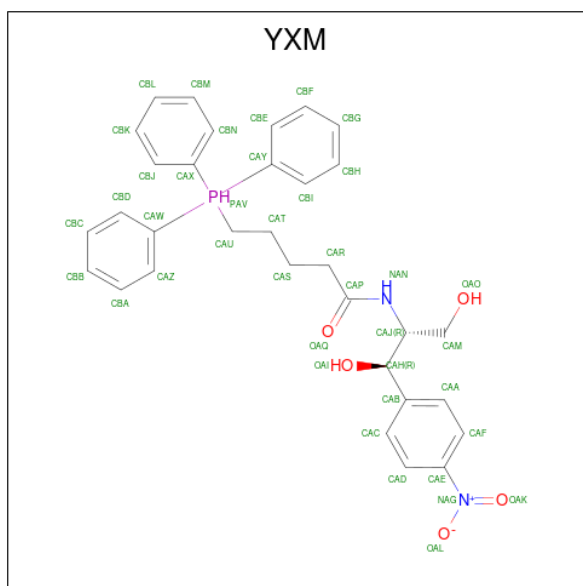
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
54	1o	2	Total 2	Mg 2	0	0
54	1t	1	Total 1	Mg 1	0	0
54	1y	4	Total 4	Mg 4	0	0
54	2A	757	Total 757	Mg 757	0	0
54	2B	19	Total 19	Mg 19	0	0
54	2D	12	Total 12	Mg 12	0	0
54	2E	6	Total 6	Mg 6	0	0
54	2F	3	Total 3	Mg 3	0	0
54	2G	3	Total 3	Mg 3	0	0
54	2I	1	Total 1	Mg 1	0	0
54	2N	1	Total 1	Mg 1	0	0
54	2O	2	Total 2	Mg 2	0	0
54	2P	2	Total 2	Mg 2	0	0
54	2Q	3	Total 3	Mg 3	0	0
54	2R	3	Total 3	Mg 3	0	0
54	2T	3	Total 3	Mg 3	0	0
54	2V	3	Total 3	Mg 3	0	0
54	2W	2	Total 2	Mg 2	0	0
54	2X	2	Total 2	Mg 2	0	0
54	2Y	1	Total 1	Mg 1	0	0
54	20	2	Total 2	Mg 2	0	0

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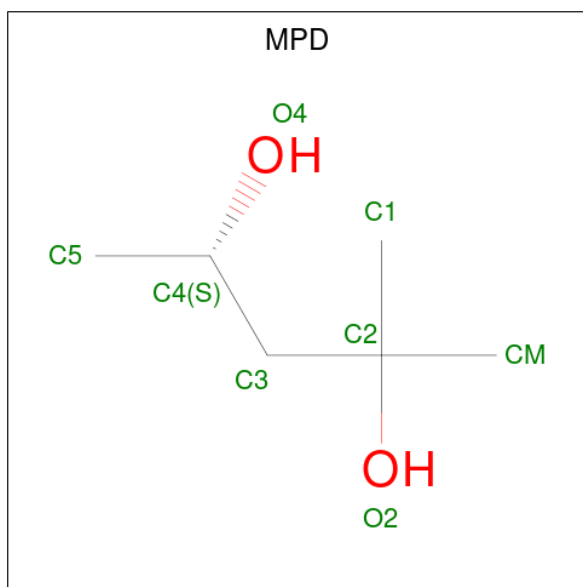
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
54	21	2	Total Mg 2 2	0	0
54	23	2	Total Mg 2 2	0	0
54	25	1	Total Mg 1 1	0	0
54	27	2	Total Mg 2 2	0	0
54	28	2	Total Mg 2 2	0	0
54	2a	200	Total Mg 200 200	0	0
54	2e	2	Total Mg 2 2	0	0
54	2f	1	Total Mg 1 1	0	0
54	2j	1	Total Mg 1 1	0	0
54	2n	1	Total Mg 1 1	0	0
54	2t	1	Total Mg 1 1	0	0

- Molecule 55 is N-[(1R,2R)-1,3-dihydroxy-1-(4-nitrophenyl)propan-2-yl]-5-(triphenyl-lambda 5 -phosphanyl)pentanamide (CCD ID: YXM) (formula: C₃₂H₃₅N₂O₅P).



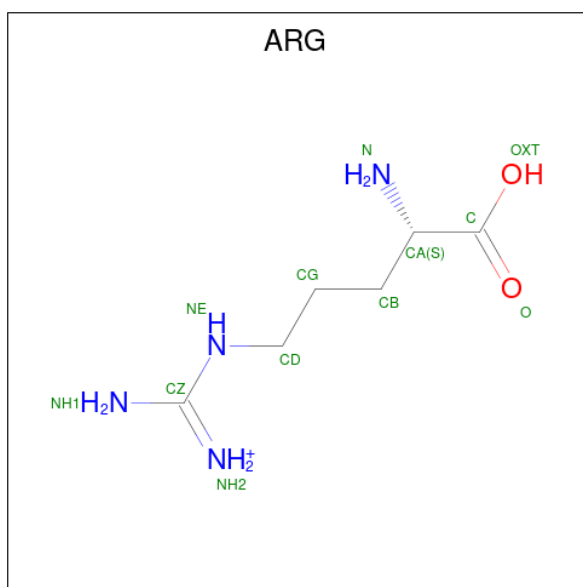
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
55	1A	1	Total	C	N	O	P	0	0
			40	32	2	5	1		
55	2A	1	Total	C	N	O	P	0	0
			40	32	2	5	1		

- Molecule 56 is (4S)-2-METHYL-2,4-PENTANEDIOL (CCD ID: MPD) (formula: C₆H₁₄O₂).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
56	1A	1	Total	C	O	0	0
			8	6	2		
56	1T	1	Total	C	O	0	0
			8	6	2		
56	18	1	Total	C	O	0	0
			8	6	2		
56	1a	1	Total	C	O	0	0
			8	6	2		
56	2A	1	Total	C	O	0	0
			8	6	2		
56	2A	1	Total	C	O	0	0
			8	6	2		
56	2B	1	Total	C	O	0	0
			8	6	2		

- Molecule 57 is ARGinine (CCD ID: ARG) (formula: C₆H₁₅N₄O₂).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
57	1B	1	Total	C	N	O	0	0
			12	6	4	2		
57	1F	1	Total	C	N	O	0	0
			12	6	4	2		

- Molecule 58 is ZINC ION (CCD ID: ZN) (formula: Zn).

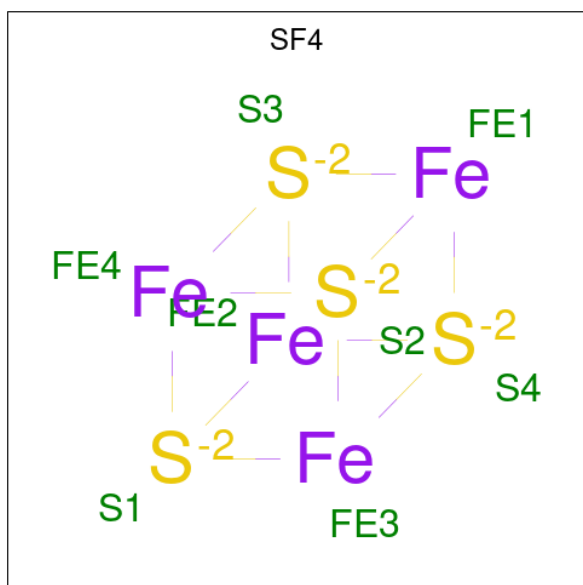
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
58	1Y	1	Total	Zn	0	0
			1	1		
58	14	1	Total	Zn	0	0
			1	1		
58	15	1	Total	Zn	0	0
			1	1		
58	16	1	Total	Zn	0	0
			1	1		
58	19	1	Total	Zn	0	0
			1	1		
58	1n	1	Total	Zn	0	0
			1	1		
58	2Y	1	Total	Zn	0	0
			1	1		
58	24	1	Total	Zn	0	0
			1	1		
58	25	1	Total	Zn	0	0
			1	1		
58	26	1	Total	Zn	0	0
			1	1		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
58	29	1	Total	Zn	0	0
			1	1		
58	2n	1	Total	Zn	0	0
			1	1		

- Molecule 59 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe_4S_4).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
59	1d	1	Total	Fe	S	0	0
			8	4	4		
59	2d	1	Total	Fe	S	0	0
			8	4	4		

- Molecule 60 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
60	1A	4016	Total	O	0	0
			4016	4016		
60	1B	110	Total	O	0	0
			110	110		
60	1D	117	Total	O	0	0
			117	117		
60	1E	85	Total	O	0	0
			85	85		
60	1F	70	Total	O	0	0
			70	70		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
60	1G	17	Total	O	0	0
			17	17		
60	1H	14	Total	O	0	0
			14	14		
60	1I	9	Total	O	0	0
			9	9		
60	1N	54	Total	O	0	0
			54	54		
60	1O	21	Total	O	0	0
			21	21		
60	1P	70	Total	O	0	0
			70	70		
60	1Q	40	Total	O	0	0
			40	40		
60	1R	34	Total	O	0	0
			34	34		
60	1S	10	Total	O	0	0
			10	10		
60	1T	36	Total	O	0	0
			36	36		
60	1U	47	Total	O	0	0
			47	47		
60	1V	39	Total	O	0	0
			39	39		
60	1W	23	Total	O	0	0
			23	23		
60	1X	23	Total	O	0	0
			23	23		
60	1Y	17	Total	O	0	0
			17	17		
60	1Z	18	Total	O	0	0
			18	18		
60	10	29	Total	O	0	0
			29	29		
60	11	24	Total	O	0	0
			24	24		
60	12	17	Total	O	0	0
			17	17		
60	13	27	Total	O	0	0
			27	27		
60	14	4	Total	O	0	0
			4	4		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
60	15	27	Total 27	O 27	0	0
60	16	18	Total 18	O 18	0	0
60	17	18	Total 18	O 18	0	0
60	18	29	Total 29	O 29	0	0
60	19	8	Total 8	O 8	0	0
60	1a	579	Total 579	O 579	0	0
60	1b	1	Total 1	O 1	0	0
60	1c	1	Total 1	O 1	0	0
60	1d	9	Total 9	O 9	0	0
60	1e	5	Total 5	O 5	0	0
60	1f	1	Total 1	O 1	0	0
60	1h	2	Total 2	O 2	0	0
60	1j	1	Total 1	O 1	0	0
60	1k	1	Total 1	O 1	0	0
60	1l	7	Total 7	O 7	0	0
60	1m	1	Total 1	O 1	0	0
60	1o	5	Total 5	O 5	0	0
60	1p	5	Total 5	O 5	0	0
60	1t	1	Total 1	O 1	0	0
60	1u	1	Total 1	O 1	0	0
60	1y	5	Total 5	O 5	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
60	2A	2486	Total 2486	O 2486	0	0
60	2B	64	Total 64	O 64	0	0
60	2D	49	Total 49	O 49	0	0
60	2E	33	Total 33	O 33	0	0
60	2F	19	Total 19	O 19	0	0
60	2G	7	Total 7	O 7	0	0
60	2H	3	Total 3	O 3	0	0
60	2I	4	Total 4	O 4	0	0
60	2N	4	Total 4	O 4	0	0
60	2O	20	Total 20	O 20	0	0
60	2P	29	Total 29	O 29	0	0
60	2Q	29	Total 29	O 29	0	0
60	2R	19	Total 19	O 19	0	0
60	2S	5	Total 5	O 5	0	0
60	2T	12	Total 12	O 12	0	0
60	2U	12	Total 12	O 12	0	0
60	2V	9	Total 9	O 9	0	0
60	2W	16	Total 16	O 16	0	0
60	2X	8	Total 8	O 8	0	0
60	2Y	3	Total 3	O 3	0	0
60	2Z	10	Total 10	O 10	0	0

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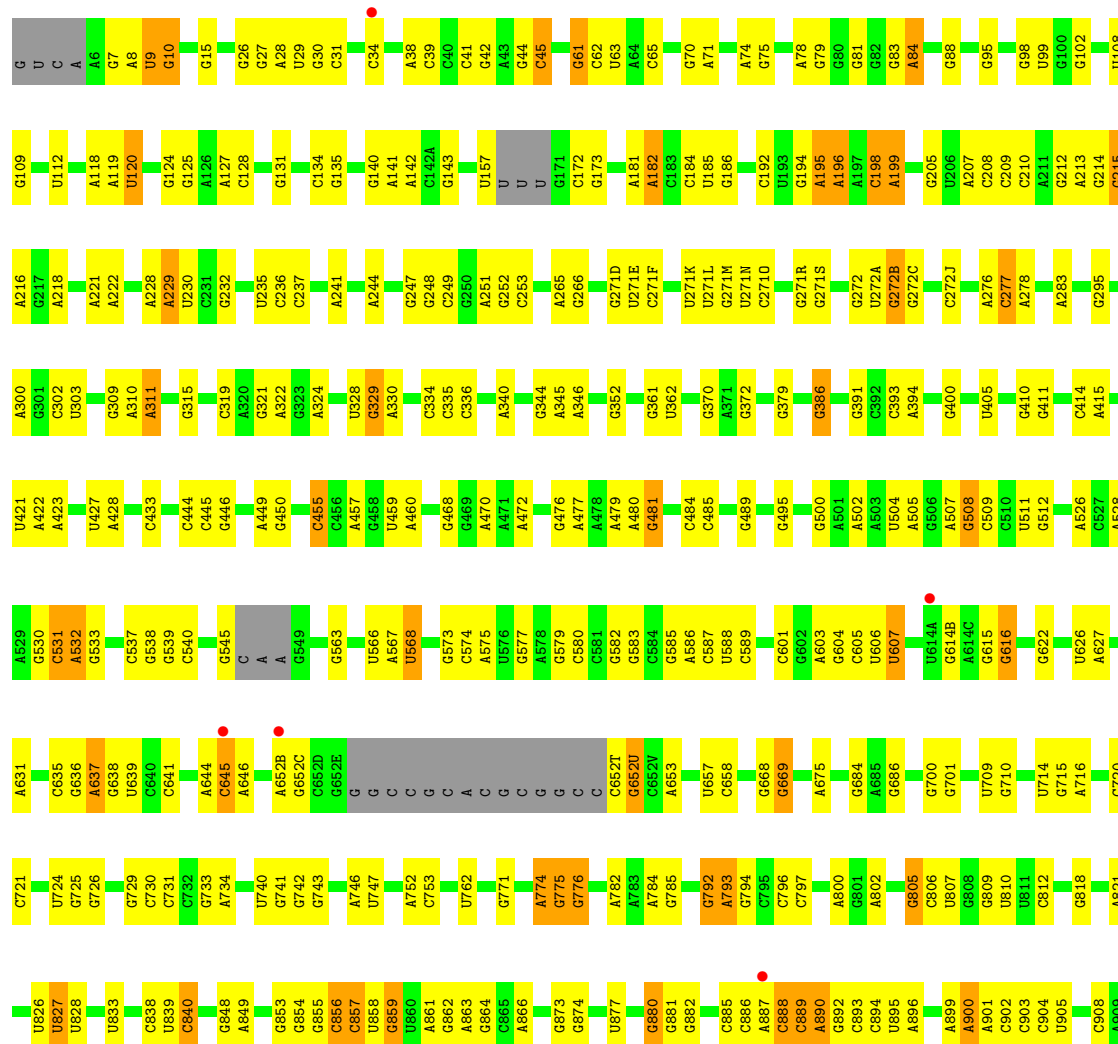
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
60	20	13	Total 13	O 13	0	0
60	21	23	Total 23	O 23	0	0
60	22	3	Total 3	O 3	0	0
60	23	4	Total 4	O 4	0	0
60	24	2	Total 2	O 2	0	0
60	25	7	Total 7	O 7	0	0
60	26	5	Total 5	O 5	0	0
60	27	11	Total 11	O 11	0	0
60	28	11	Total 11	O 11	0	0
60	29	1	Total 1	O 1	0	0
60	2a	420	Total 420	O 420	0	0
60	2d	8	Total 8	O 8	0	0
60	2e	1	Total 1	O 1	0	0
60	2f	3	Total 3	O 3	0	0
60	2j	1	Total 1	O 1	0	0
60	2l	1	Total 1	O 1	0	0
60	2m	1	Total 1	O 1	0	0
60	2o	4	Total 4	O 4	0	0
60	2p	3	Total 3	O 3	0	0
60	2q	1	Total 1	O 1	0	0
60	2r	3	Total 3	O 3	0	0

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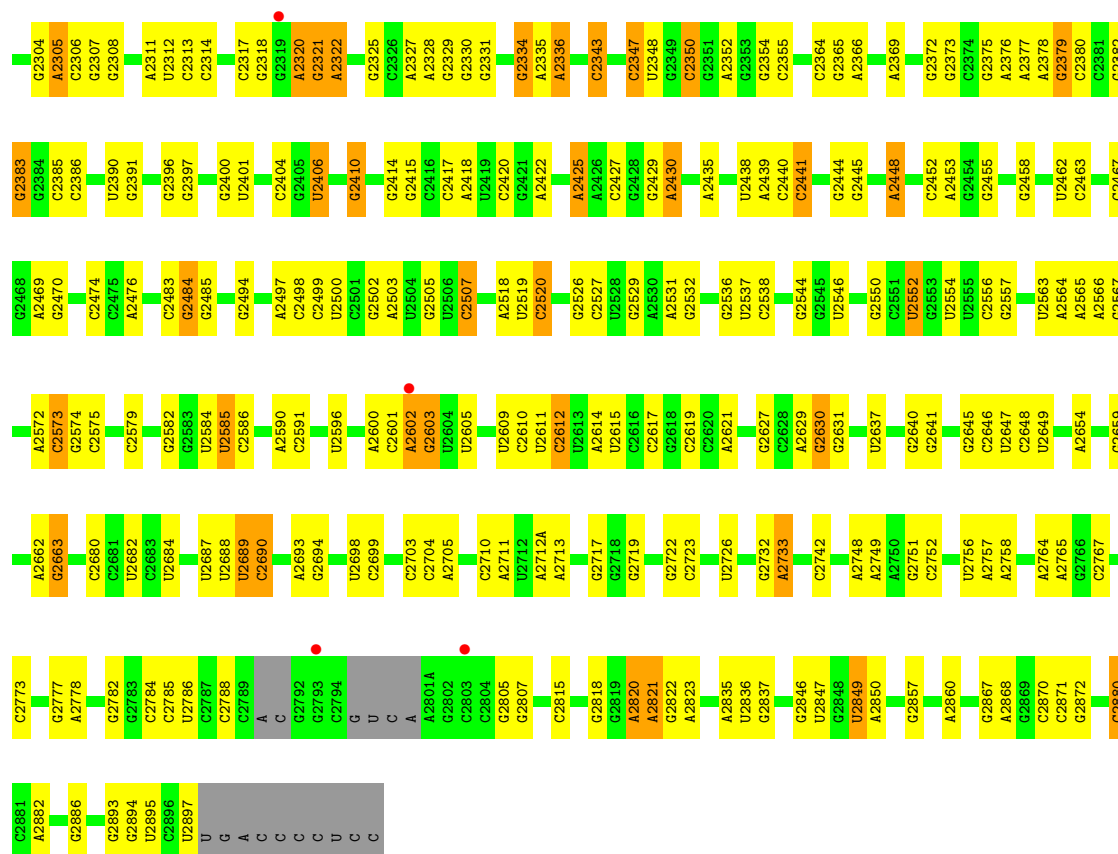
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
60	2t	2	Total	O	0	0
			2	2		
60	2y	3	Total	O	0	0
			3	3		

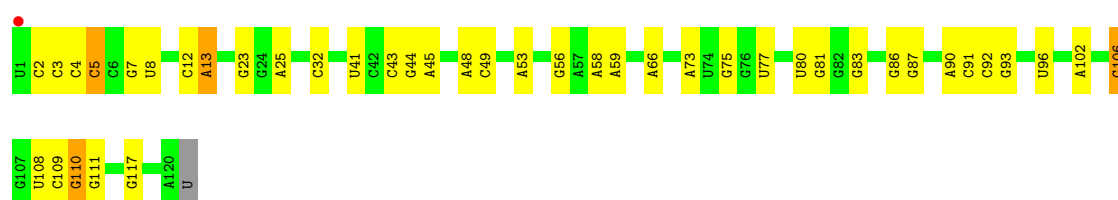
A2426	A2427	G2428	G2429	A2430	A2434	A2435	A2438	A2439	C2440	C2441	C2442	C2443	G2447	A2448	G2454	G2458	C2461	U2462	C2467	G2468	G2470	C2471	C2472	A2476	G2494	G2495	C2496	A2497	C2498	C2499	U2500	C2501	G2502	A2503	G2504	G2505	U2506	C2507	A2518	U2519	C2520	G2521	U2522	G2529	A2530	G2535																																																																
A2327	A2328	G2329	G2330	G2331	G2334	A2335	A2336	G2345	A2346	G2347	U2348	G2349	G2350	G2351	A2352	G2353	U2357	C2364	G2365	G2372	A2377	A2378	C2381	G2382	G2383	G2384	C2385	A2386	A2387	A2388	G2389	A2390	A2391	A2392	A2393	C2394	G2400	U2401	G2404	G2405	U2406	G2407	U2410	A2411	A2418	U2419	A2422	U2423	A2424	A2425	G2426																																																											
C2143	U2144	C2145	C2146	C2147	G2148	C2149	U2150	C2151	C2152	C2153	G2154	C2157	A2158	C2159	C2160	C2161	G2162	C2166	U2167	C2168	A2169	U2170	A2171	U2172	A2173	C2177	C2178	C2179	U2180	C2181	G2182	C2185	U2186	C2187	C2188	U2189	C2190	G2191	C2192	C2193	C2198	A2199	C2202	C2203	C2204	C2205	C2206	C2207	A2208	G2319	A2320	G2325	C2326																																																									
G2072	C2073	U2074	U2075	U2076	C2077	C2078	U2079	U2086	C2087	U1993	C1996	G1997	G2090	G2093	U2096	C2097	U2098	U2099	G2100	G2101	U2102	C2103	G2104	C2105	G2106	C2107	C2108	U2109	G2110	C2111	A2114	G2115	G2116	C2117	C2118	U2119	C2120	G2121	G2124	G2125	U2126	G2127	U2130	G2131	U2132	C2133	C2134	C2135	G2206	G2207	C2208	C2213	C2214	C2215	C2216	G2319	A2320	G2325	C2326																																																			
A1847	A1848	A1849	A1850	A1851	A1852	A1853	A1859	G1862	G1863	G1864	A1865	A1866	A1867	A1868	A1869	A1870	A1871	A1872	A1873	A1874	A1875	A1876	A1877	A1878	A1879	A1880	A1881	A1882	A1883	A1884	A1885	A1886	A1887	A1888	A1889	A1890	A1891	A1892	A1893	A1894	A1895	A1896	A1897	A1898	A1899	A1900	A1901	A1902	A1903	A1904	A1905	A1906	A1907	A1908	A1909	A1910	A1911	A1912	A1913	A1914	A1915	A1916	A1917	A1918	A1919	A1920	A1921	A1922	A1923	A1924	A1925	A1926	A1927	A1928	A1929	A1930	A1931	A1932	A1933	A1934	A1935	A1936	A1937	A1938	A1939	A1940	A1941	A1942	A1943	A1944	A1945	A1946	A1947	A1948	A1949	A1950	A1951	A1952	A1953	A1954	A1955	A1956	A1957	A1958	A1959	A1960	A1961	A1962	A1963	A1964
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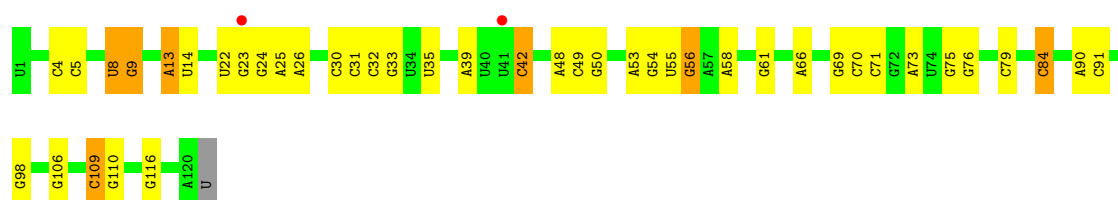
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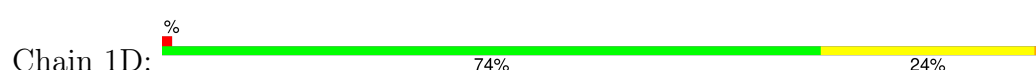
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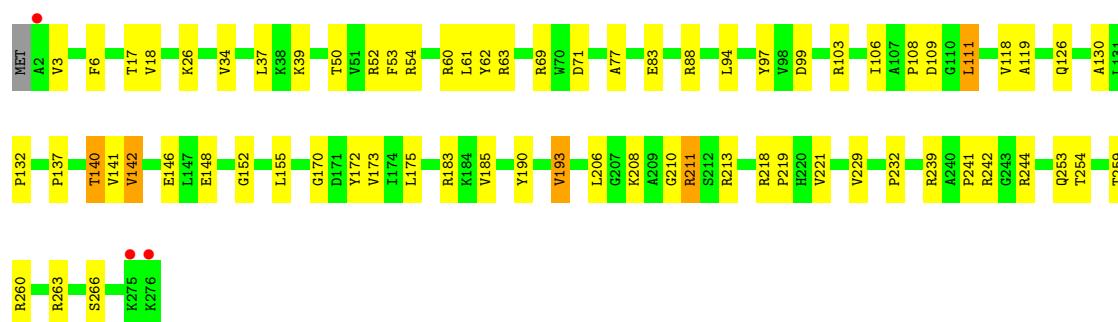


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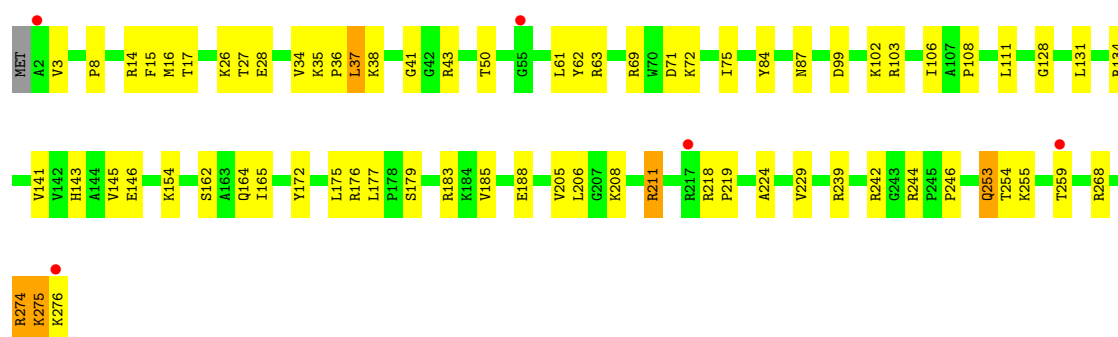
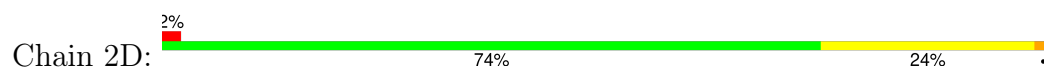


- Molecule 3: 50S ribosomal protein L2

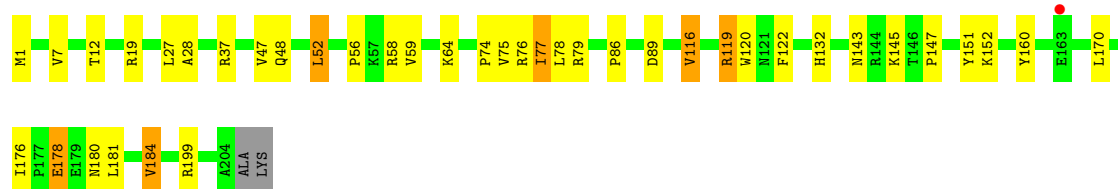
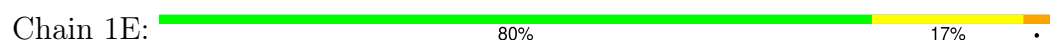




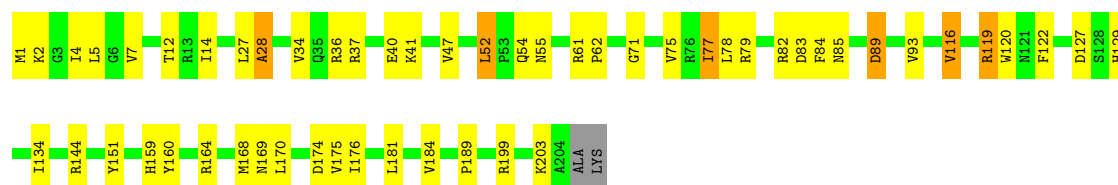
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• Molecule 4: 50S ribosomal protein L3

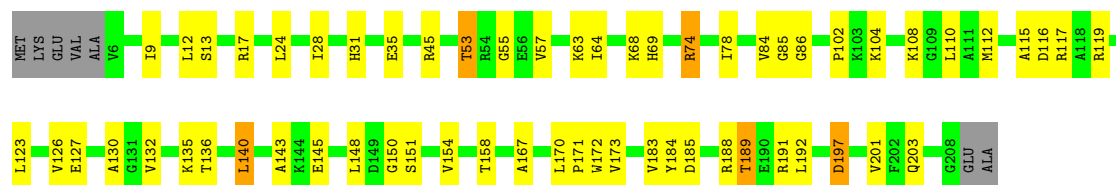


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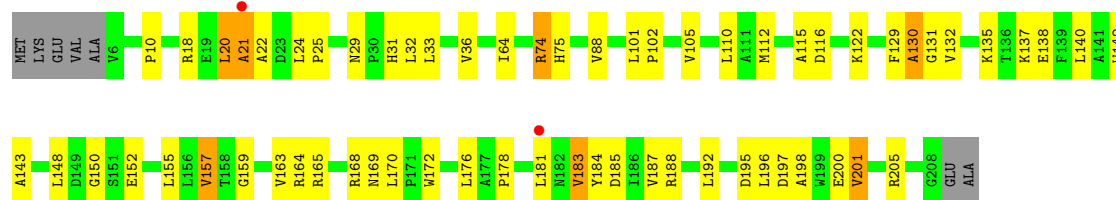


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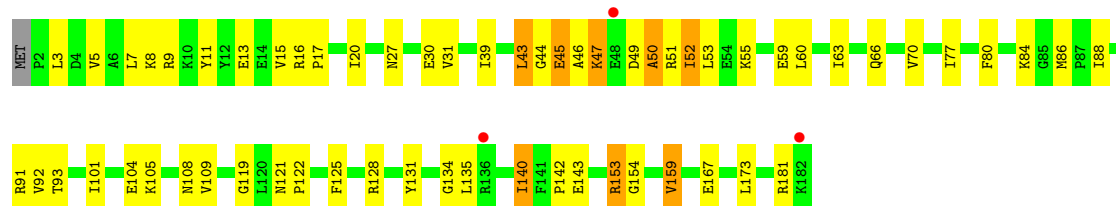




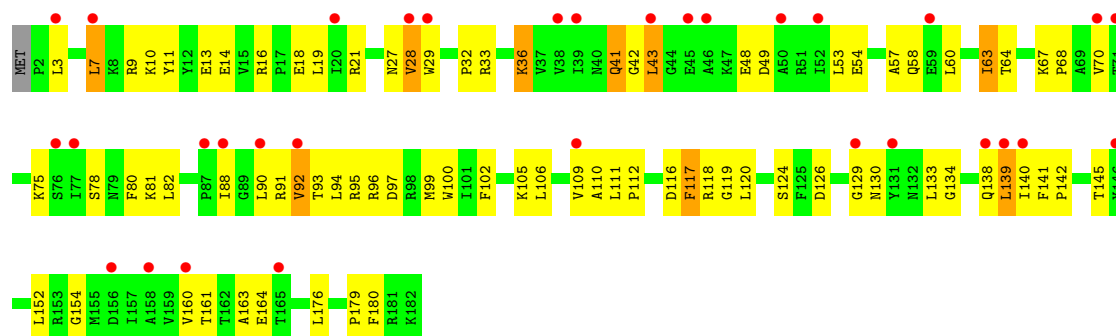
• Molecule 5: 50S ribosomal protein L4



• Molecule 6: 50S ribosomal protein L5



• Molecule 6: 50S ribosomal protein L5

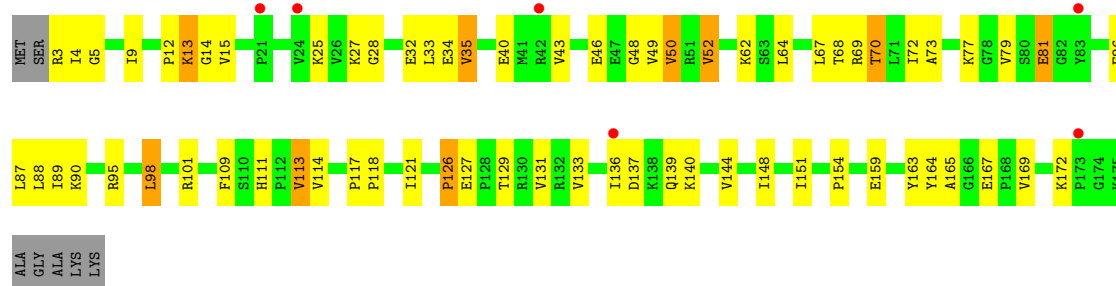


• Molecule 7: 50S ribosomal protein L6

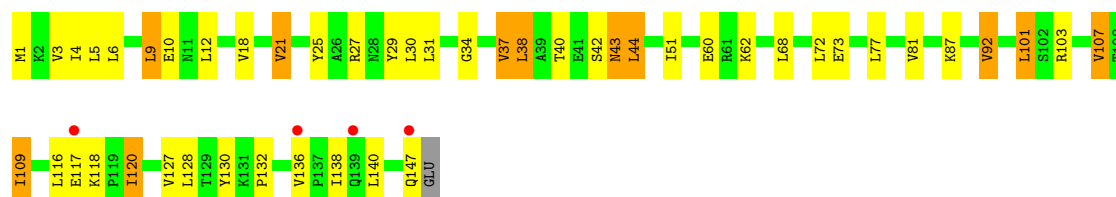




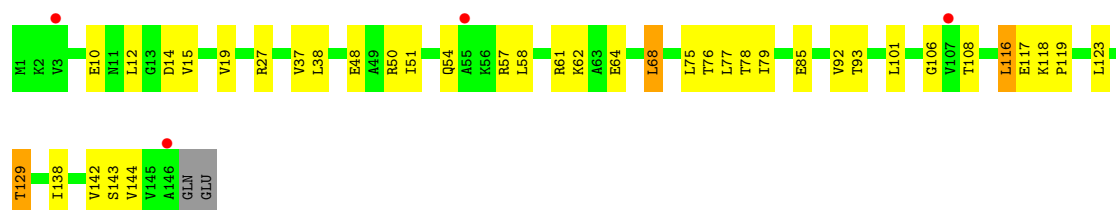
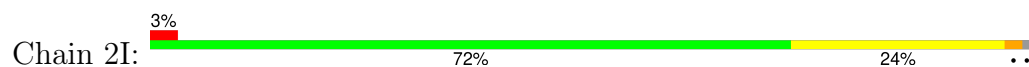
• Molecule 7: 50S ribosomal protein L6



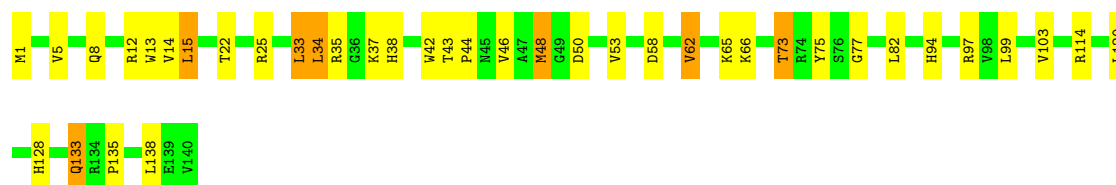
• Molecule 8: 50S ribosomal protein L9



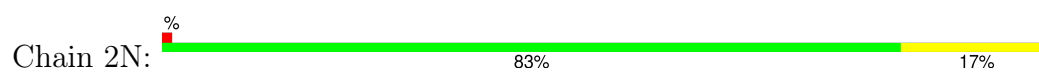
• Molecule 8: 50S ribosomal protein L9



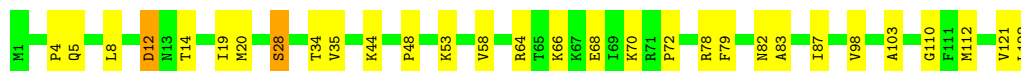
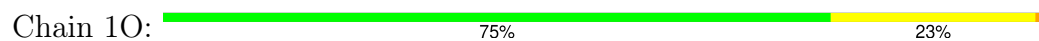
• Molecule 9: 50S ribosomal protein L13



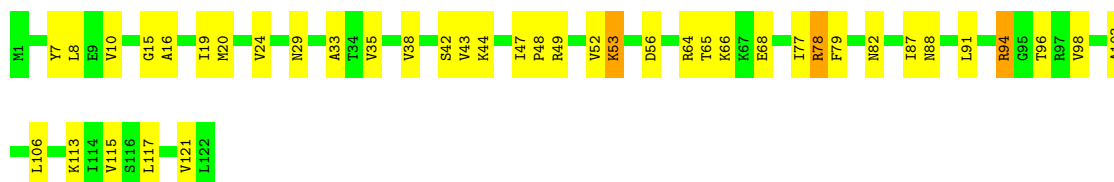
• Molecule 9: 50S ribosomal protein L13



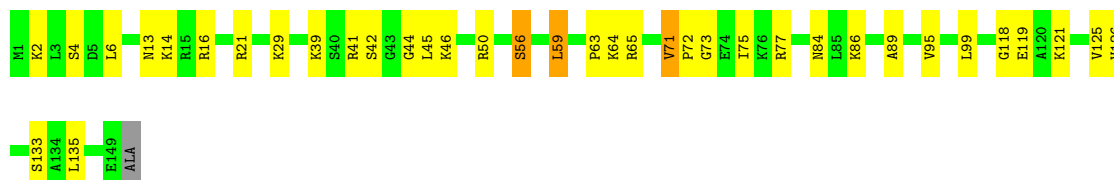
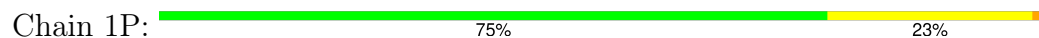
- Molecule 10: 50S ribosomal protein L14



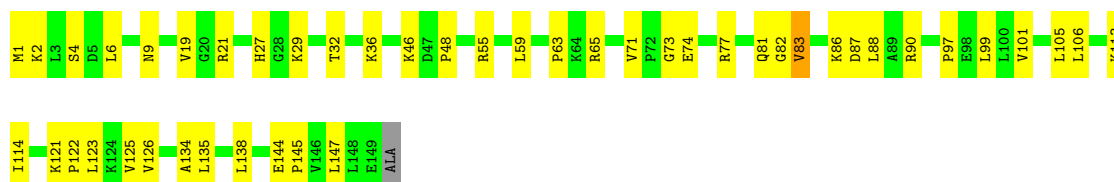
- Molecule 10: 50S ribosomal protein L14



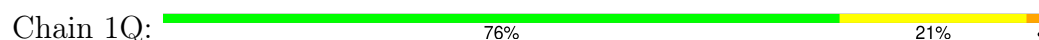
- Molecule 11: 50S ribosomal protein L15



- Molecule 11: 50S ribosomal protein L15

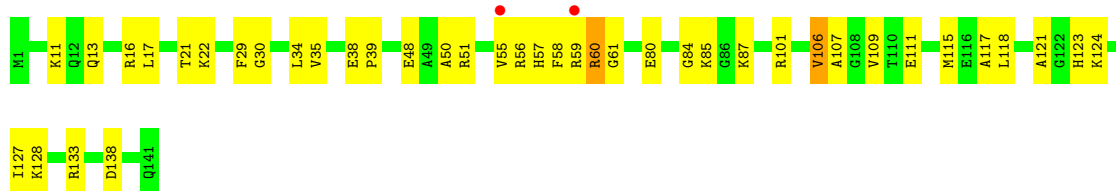


- Molecule 12: 50S ribosomal protein L16

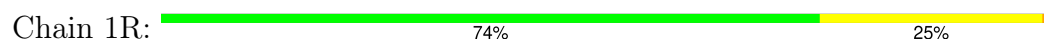




- Molecule 12: 50S ribosomal protein L16



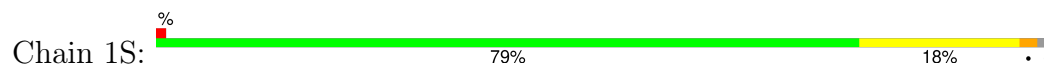
- Molecule 13: 50S ribosomal protein L17



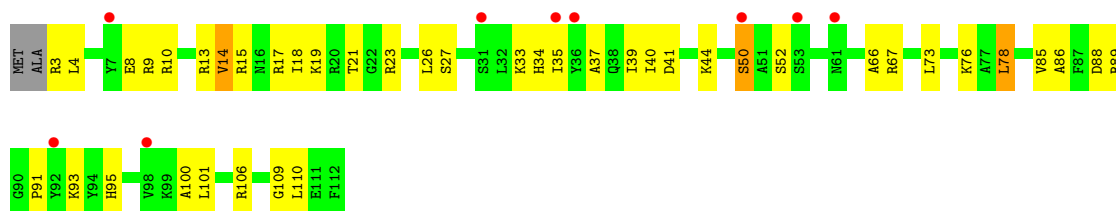
- Molecule 13: 50S ribosomal protein L17



- Molecule 14: 50S ribosomal protein L18

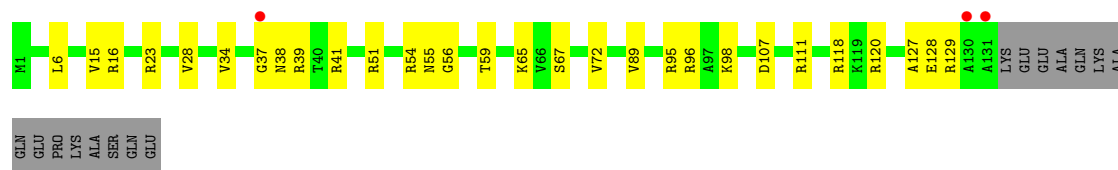


- Molecule 14: 50S ribosomal protein L18

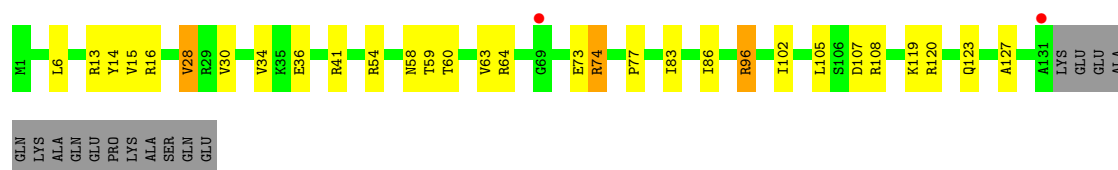


- Molecule 15: 50S ribosomal protein L19

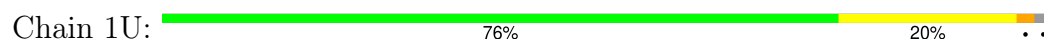




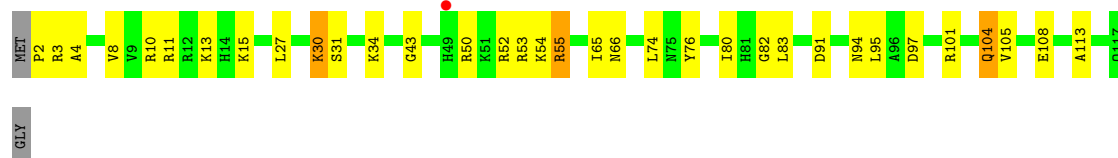
- Molecule 15: 50S ribosomal protein L19



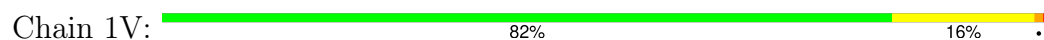
- Molecule 16: 50S ribosomal protein L20



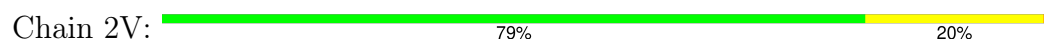
- Molecule 16: 50S ribosomal protein L20



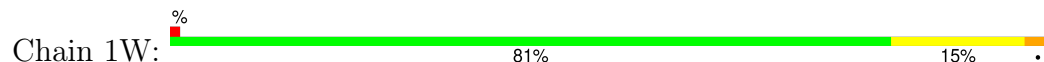
- Molecule 17: 50S ribosomal protein L21

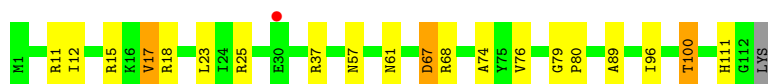


- Molecule 17: 50S ribosomal protein L21



- Molecule 18: 50S ribosomal protein L22

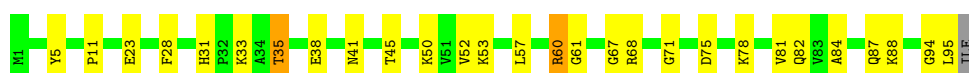




- Molecule 18: 50S ribosomal protein L22



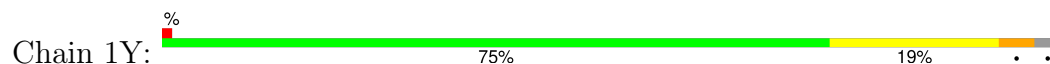
- Molecule 19: 50S ribosomal protein L23



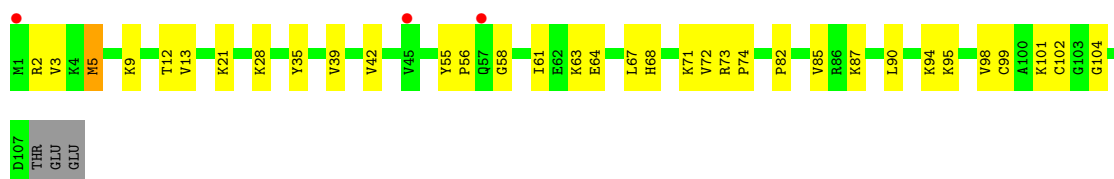
- Molecule 19: 50S ribosomal protein L23



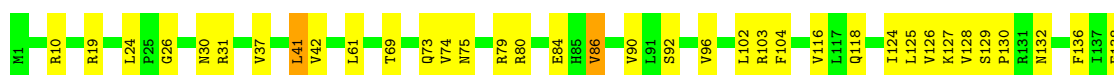
- Molecule 20: 50S ribosomal protein L24



- Molecule 20: 50S ribosomal protein L24



- Molecule 21: 50S ribosomal protein L25

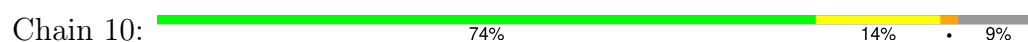




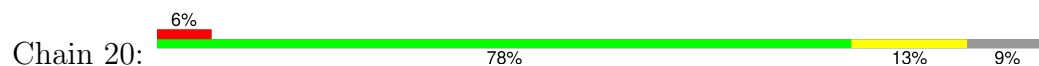
- Molecule 21: 50S ribosomal protein L25



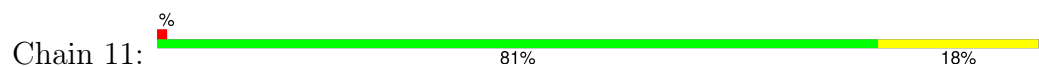
- Molecule 22: 50S ribosomal protein L27



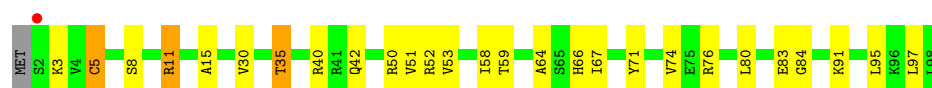
- Molecule 22: 50S ribosomal protein L27



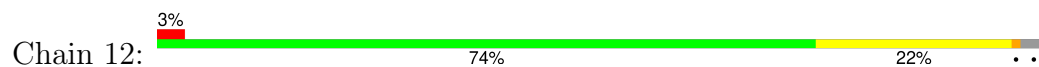
- Molecule 23: 50S ribosomal protein L28



- Molecule 23: 50S ribosomal protein L28



- Molecule 24: 50S ribosomal protein L29

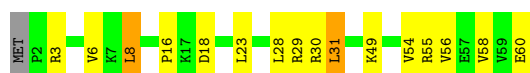




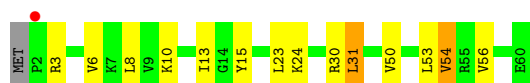
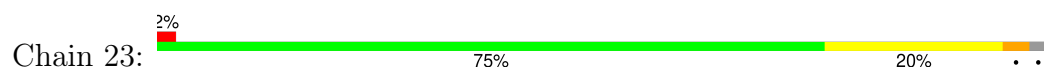
- Molecule 24: 50S ribosomal protein L29



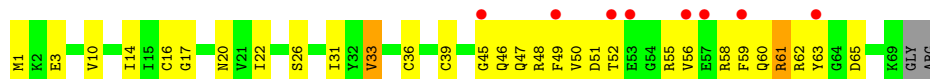
- Molecule 25: 50S ribosomal protein L30



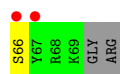
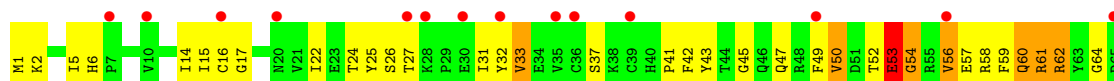
- Molecule 25: 50S ribosomal protein L30



- Molecule 26: 50S ribosomal protein L31



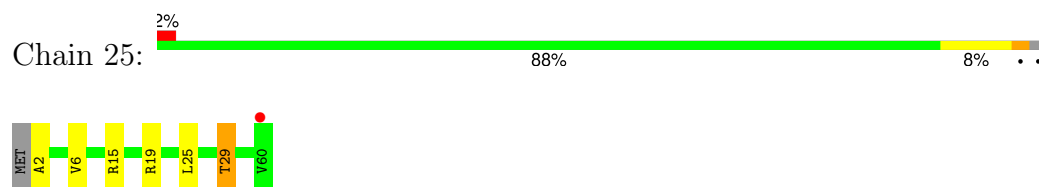
- Molecule 26: 50S ribosomal protein L31



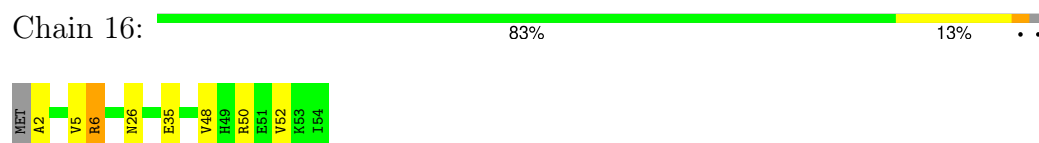
- Molecule 27: 50S ribosomal protein L32



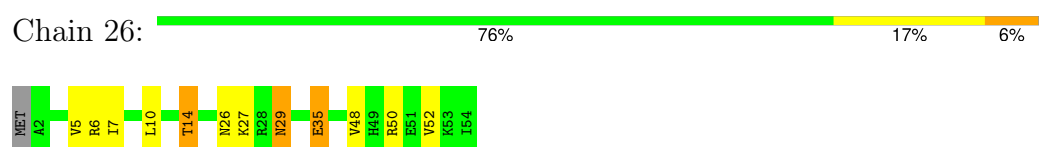
• Molecule 27: 50S ribosomal protein L32



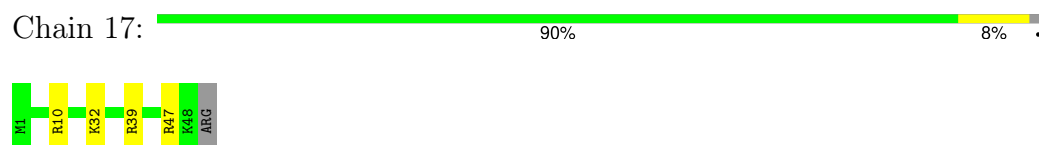
• Molecule 28: 50S ribosomal protein L33



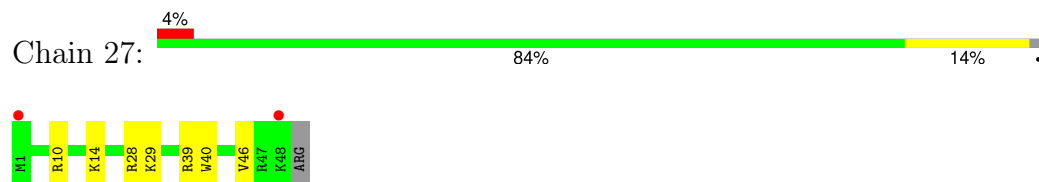
• Molecule 28: 50S ribosomal protein L33



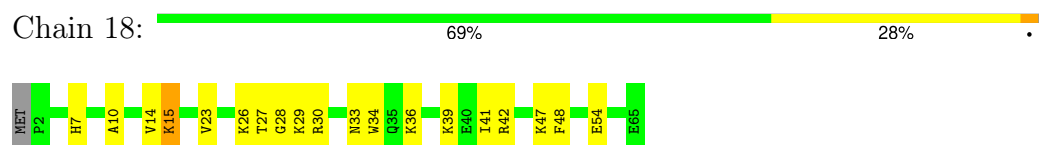
• Molecule 29: 50S ribosomal protein L34



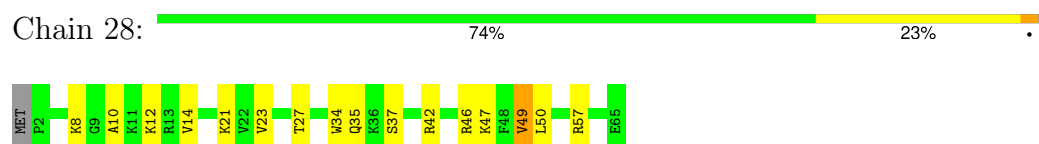
• Molecule 29: 50S ribosomal protein L34



• Molecule 30: 50S ribosomal protein L35



• Molecule 30: 50S ribosomal protein L35



- Molecule 31: 50S ribosomal protein L36

Chain 19:  81% 19%



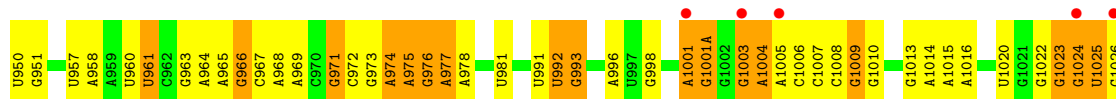
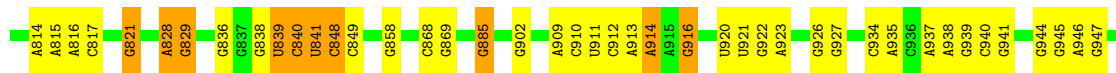
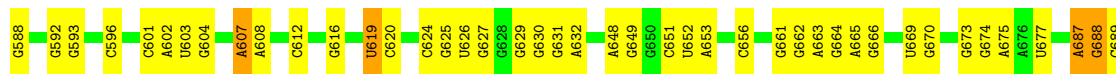
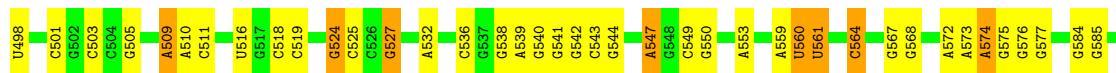
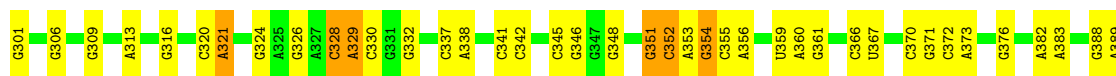
- Molecule 31: 50S ribosomal protein L36

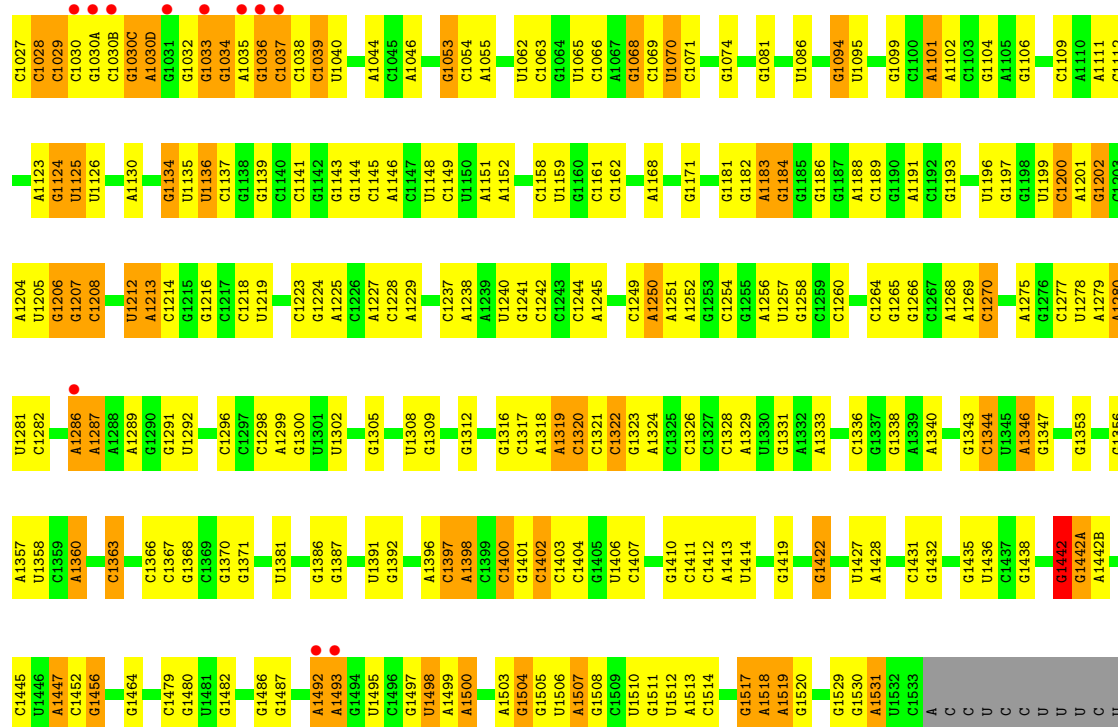
Chain 29:  3% 68% 32%



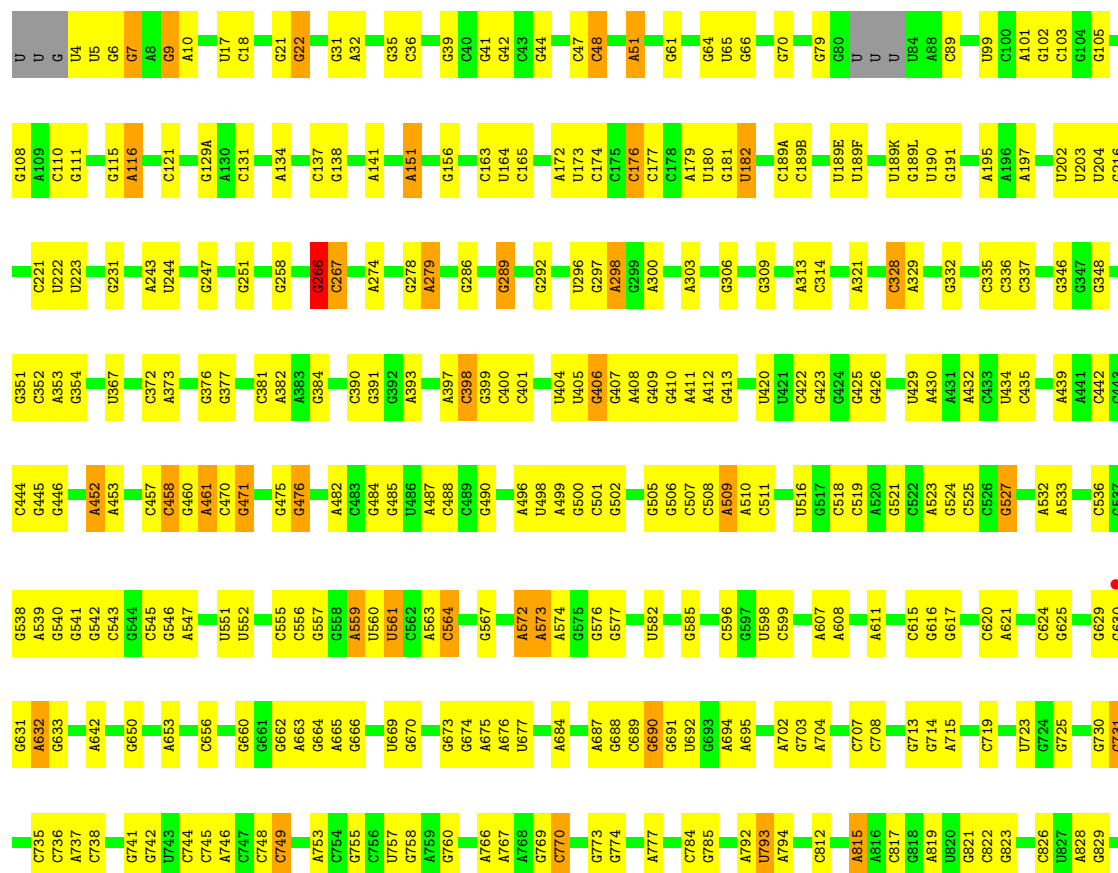
- Molecule 32: 16S Ribosomal RNA

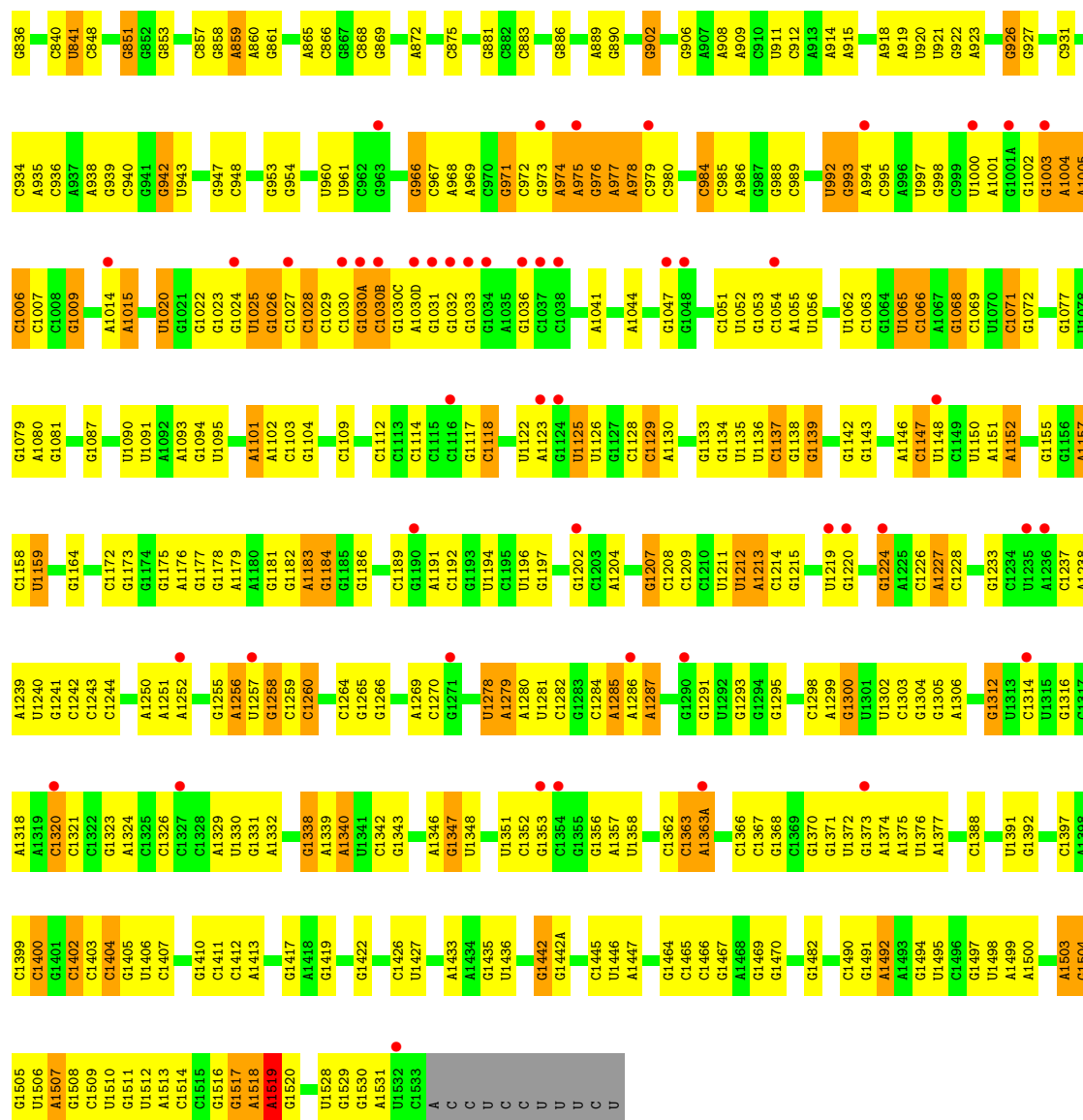
Chain 1a:  56% 35% 8%



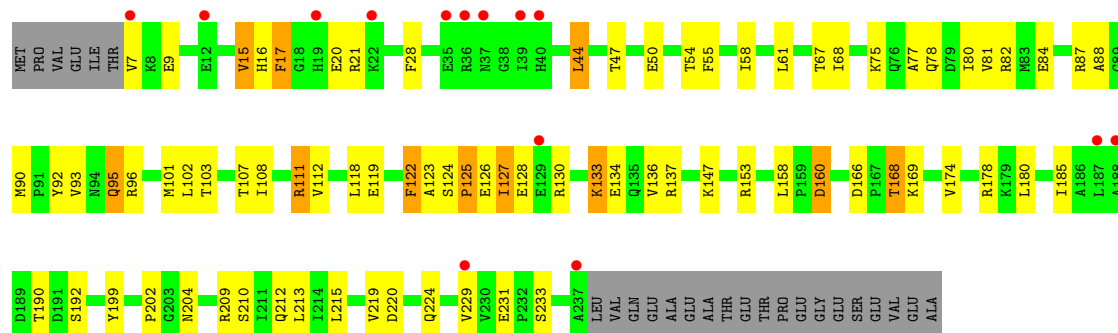


• Molecule 32: 16S Ribosomal RNA

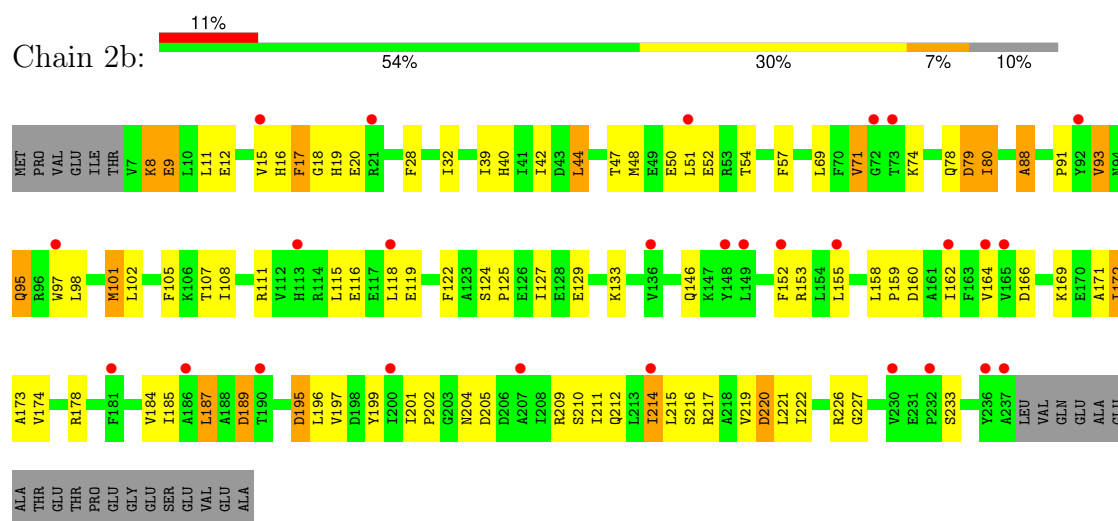




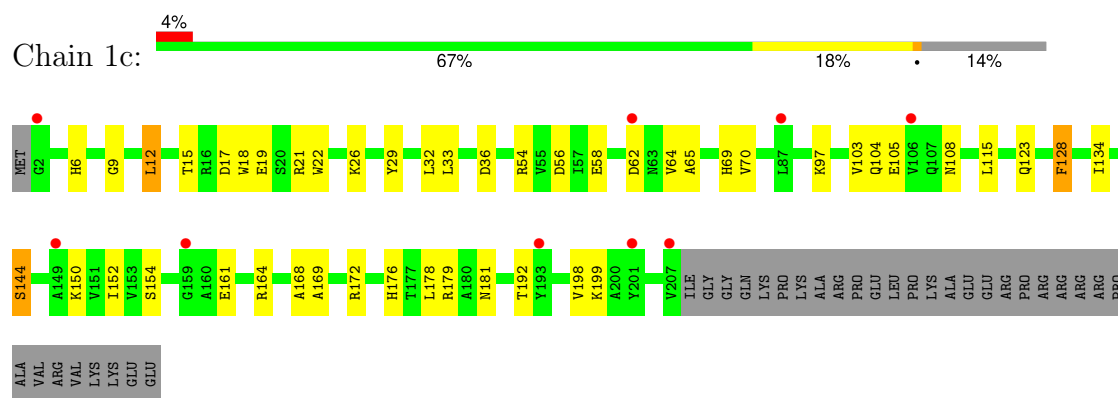
• Molecule 33: 30S ribosomal protein S2



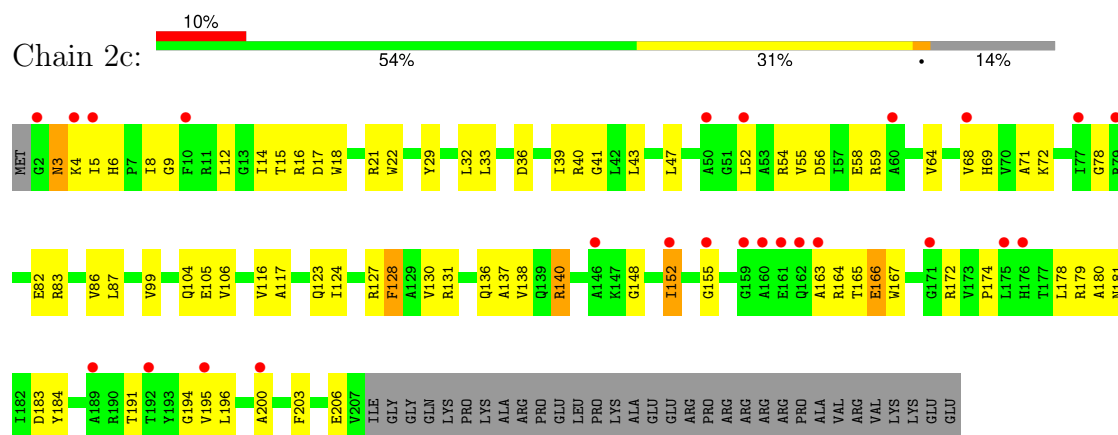
• Molecule 33: 30S ribosomal protein S2



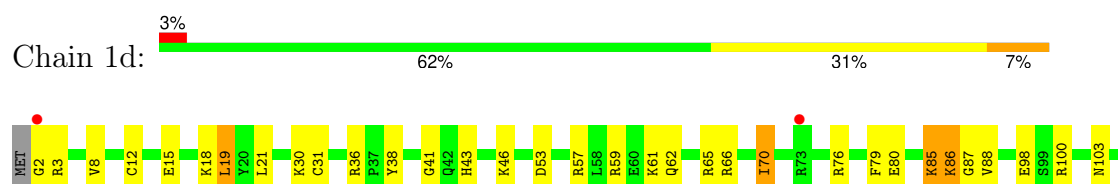
- Molecule 34: 30S ribosomal protein S3

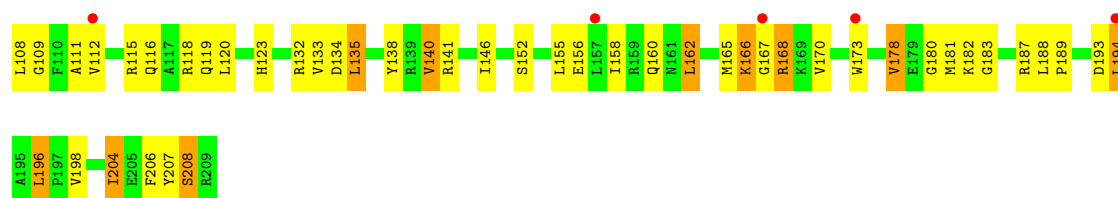


- Molecule 34: 30S ribosomal protein S3

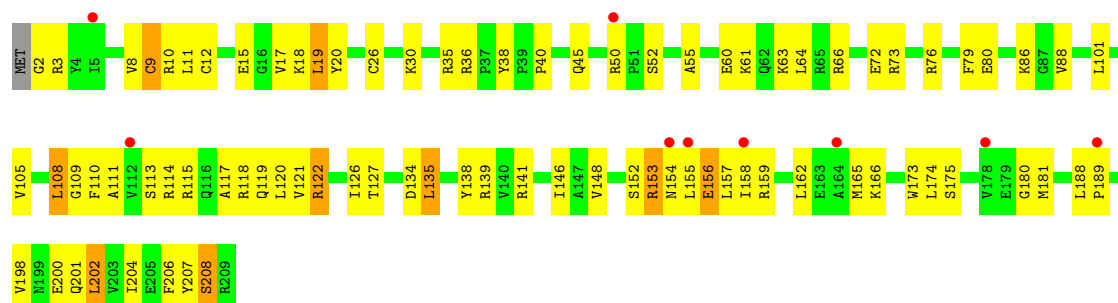


- Molecule 35: 30S ribosomal protein S4

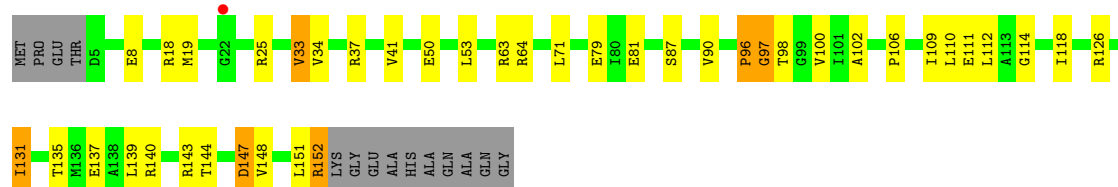




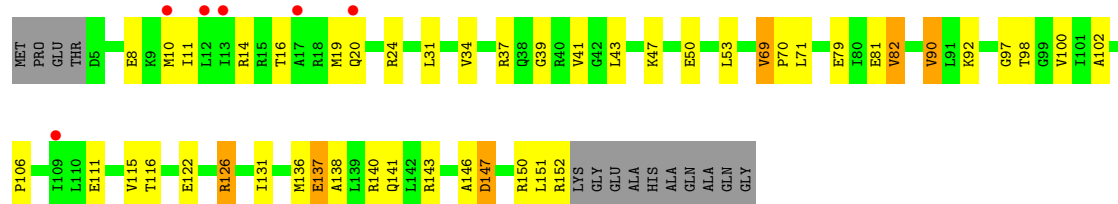
- Molecule 35: 30S ribosomal protein S4



- Molecule 36: 30S ribosomal protein S5



- Molecule 36: 30S ribosomal protein S5

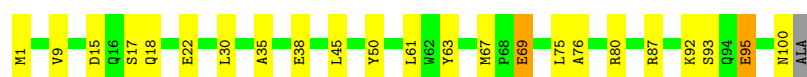


- Molecule 37: 30S ribosomal protein S6



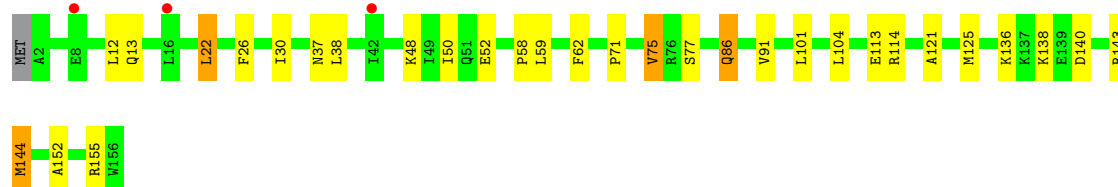
- Molecule 37: 30S ribosomal protein S6

Chain 2f:  76% 21% ..



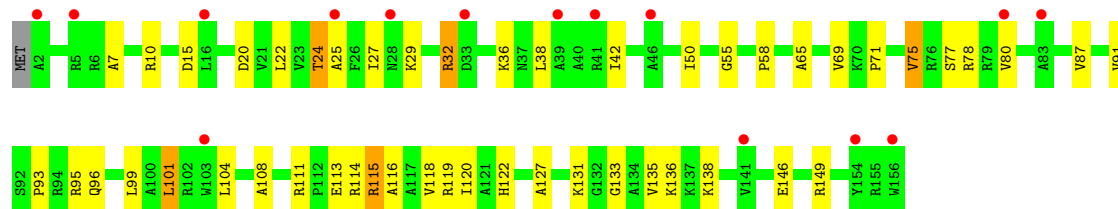
• Molecule 38: 30S ribosomal protein S7

Chain 1g:  2% 79% 17% ..



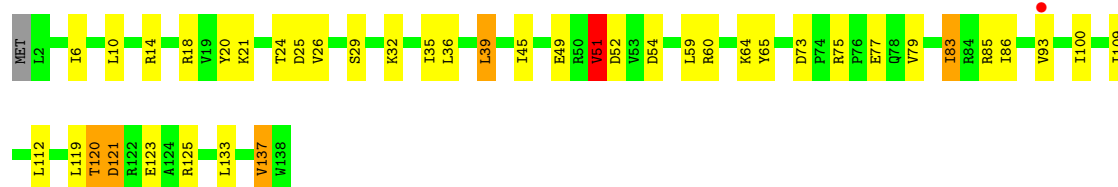
• Molecule 38: 30S ribosomal protein S7

Chain 2g:  10% 68% 28% ..



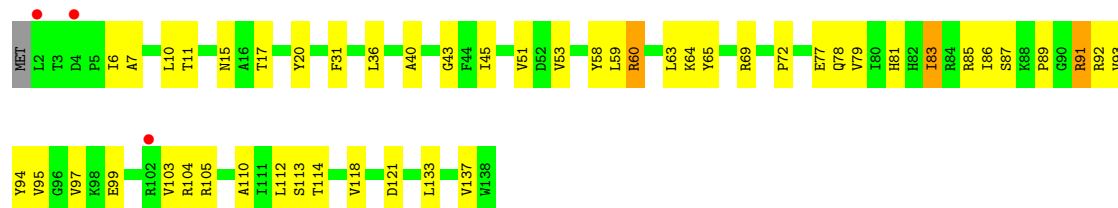
• Molecule 39: 30S ribosomal protein S8

Chain 1h:  0% 70% 25% ..

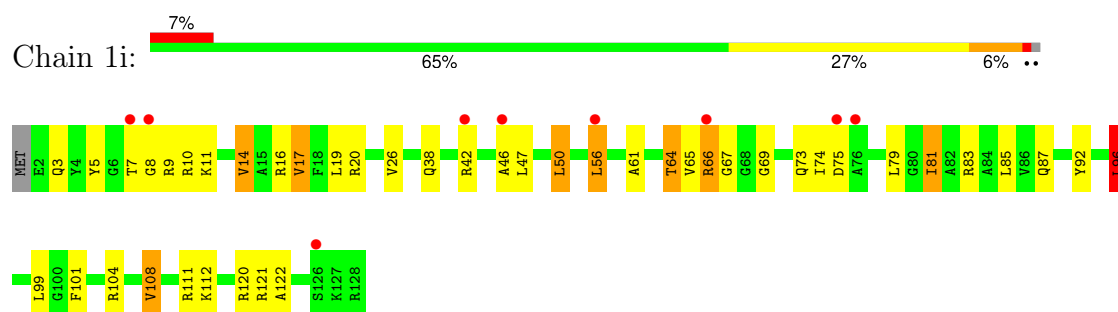


• Molecule 39: 30S ribosomal protein S8

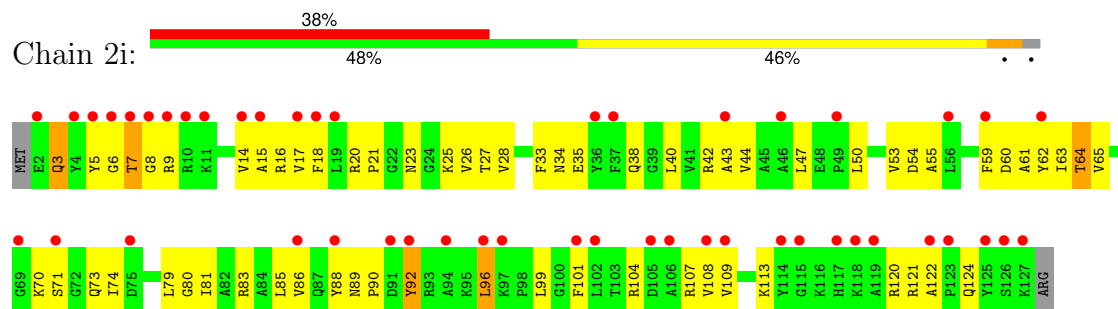
Chain 2h:  2% 64% 33% ..



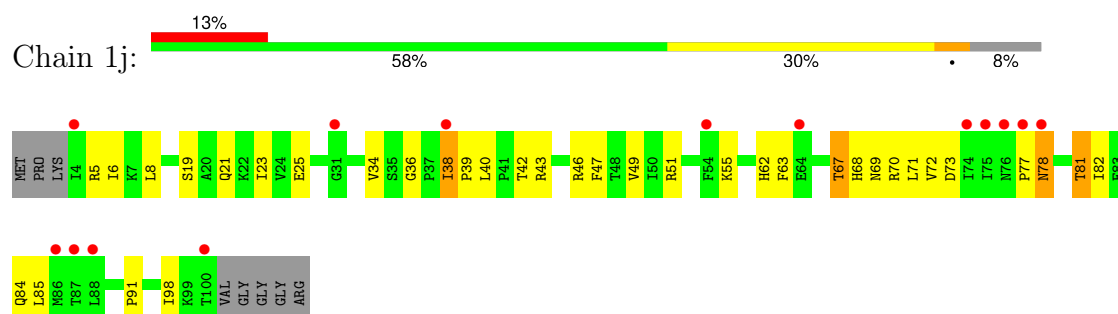
• Molecule 40: 30S ribosomal protein S9



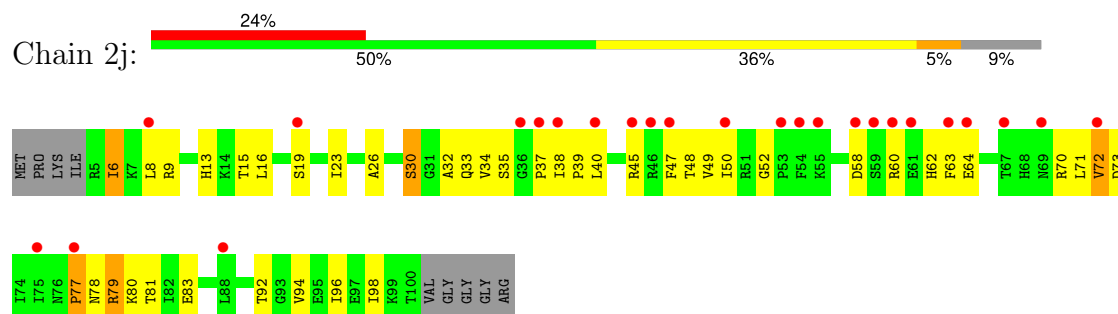
- Molecule 40: 30S ribosomal protein S9



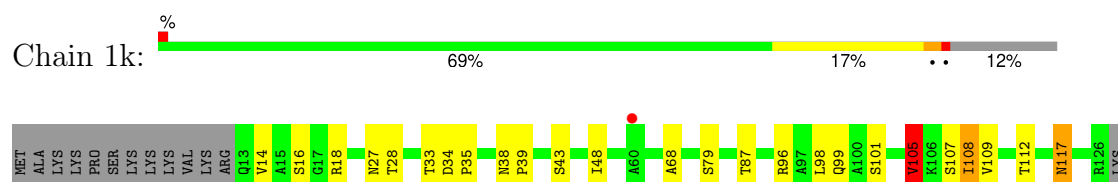
- Molecule 41: 30S ribosomal protein S10



- Molecule 41: 30S ribosomal protein S10



- Molecule 42: 30S ribosomal protein S11



ALA
SER

- Molecule 42: 30S ribosomal protein S11

Chain 2k: 

MET ALA ALA LYS LYS PRO SER LYS LYS VAL VAL ARG Q13 V14 A15 R18 Y25 N26 N27 T28 I29 V30 T31 I32 P39 I40 T41 A68 K71 D81 V82 I83 V84 T87 G88 A89 I95 L98 Q99 L103 Q104 V105 K106 S107 D110 P115 H116 N117

R126
LYS
ALA
SER

- Molecule 43: 30S ribosomal protein S12

Chain 1l: 

MET F5 T6 I7 V11 V24 R34 V39 K47 P48 S50 R53 A56 R59 L60 Y64 E65 Y69 I70 I76 V83 L84 R89 V90 K91 QTD92 V104 Y105 D112 R113 K114 K115 S116 R117 K126 GLU ALA ALA LYS THR ALA LYS

- Molecule 43: 30S ribosomal protein S12

Chain 2l: 

MET F5 N8 R12 K13 G14 E16 K47 P48 S50 K57 Y64 E65 Y69 I70 P71 S81 V82 V83 L84 QTD92 H99 I100 V101 R102 G103 V104 A107 K114 R117 S118 K123 K126 GUJ ALA ALA LYS THR ALA LYS

- Molecule 44: 30S ribosomal protein S13

Chain 1m: 

MET A2 R3 R4 A5 E8 R11 N12 K13 R14 V15 L19 G24 A28 T37 R44 V45 L48 T49 E50 A51 E52 V53 V54 R55 E56 R57 K65 G68 E69 L70 R71 A76 K79 R80 R81 G100 Q101 R102 P113 V117 ALA GLY LYS

LYS
LYS
ALA
PRO
ARG
LYS

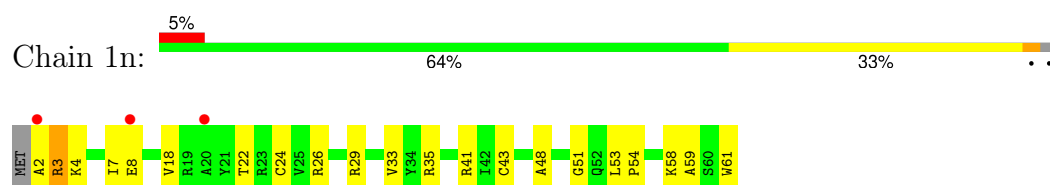
- Molecule 44: 30S ribosomal protein S13

Chain 2m: 

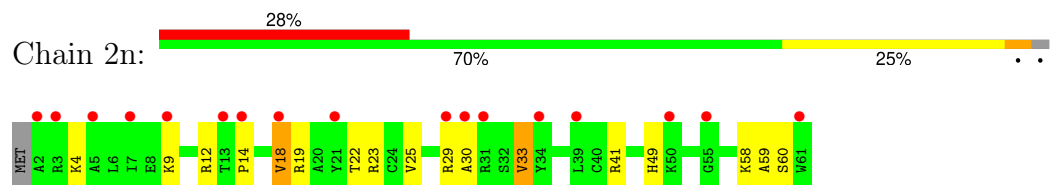
MET ALA R3 I4 A5 G6 W7 E8 K13 R14 V15 D16 V17 L19 Y23 G28 A33 T39 N40 T43 T44 V45 T49 E50 A51 V54 R55 L56 R57 E58 Y59 V60 E61 N62 T63 W64 K65 L66 E69 L70 R71 A72 A75 A76 H77 I78 L81

C86 Y87 R91 H92 R93 R94 G95 P97 V98 H99 G100 Q101 R102 T103 R104 T105 N106 A107 H108 T109 R110 K111 G112 P113 K115 T116 VAL ALA GLY LYS LYS LYS LYS LYS LYS LYS LYS LYS LYS

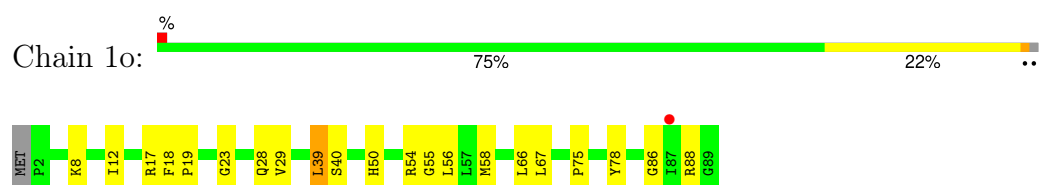
- Molecule 45: 30S ribosomal protein S14 type Z



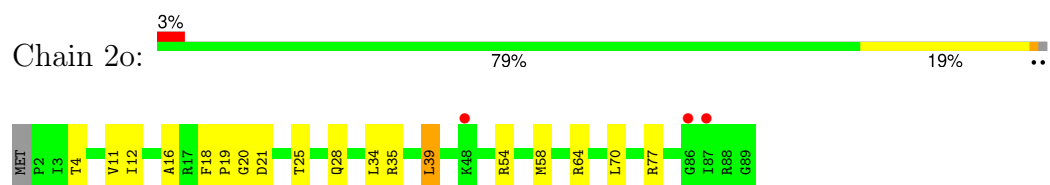
- Molecule 45: 30S ribosomal protein S14 type Z



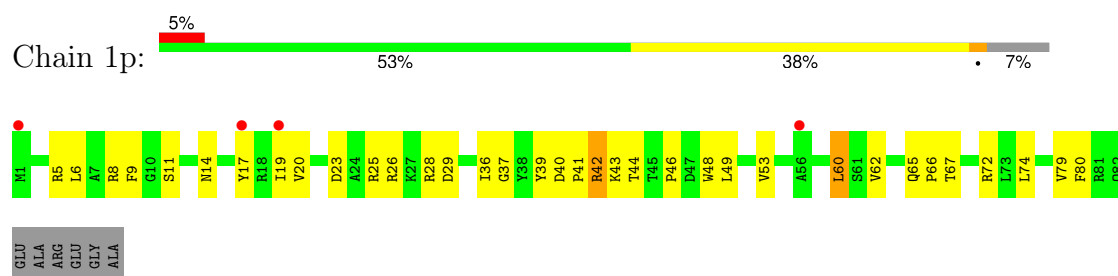
- Molecule 46: 30S ribosomal protein S15



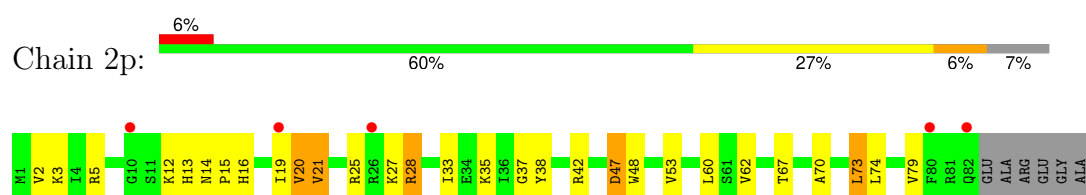
- Molecule 46: 30S ribosomal protein S15



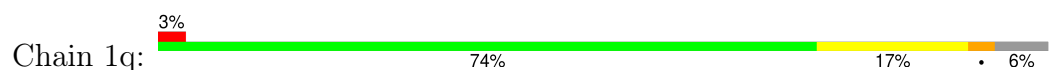
- Molecule 47: 30S ribosomal protein S16



- Molecule 47: 30S ribosomal protein S16

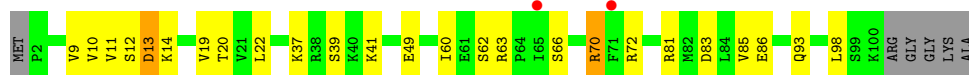


- Molecule 48: 30S ribosomal protein S17

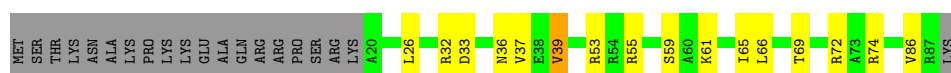




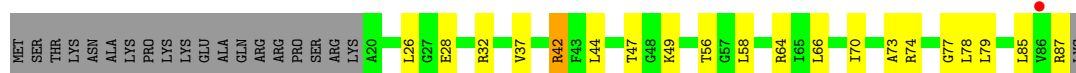
- Molecule 48: 30S ribosomal protein S17



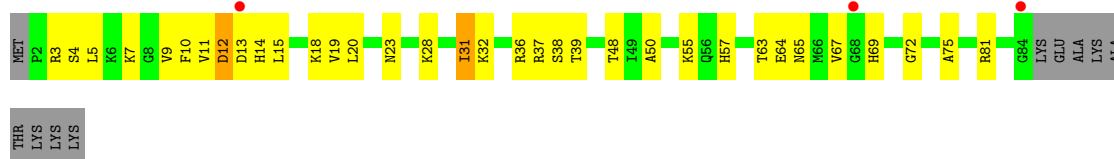
- Molecule 49: 30S ribosomal protein S18



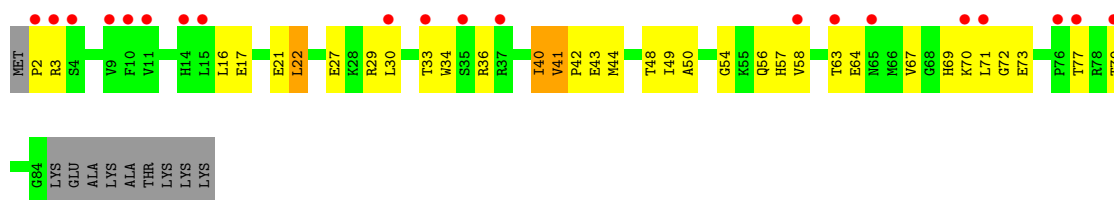
- Molecule 49: 30S ribosomal protein S18



- Molecule 50: 30S ribosomal protein S19



- Molecule 50: 30S ribosomal protein S19



- Molecule 51: 30S ribosomal protein S20

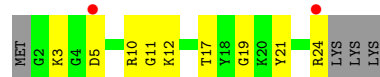




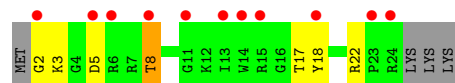
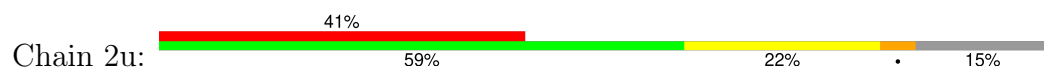
- Molecule 51: 30S ribosomal protein S20



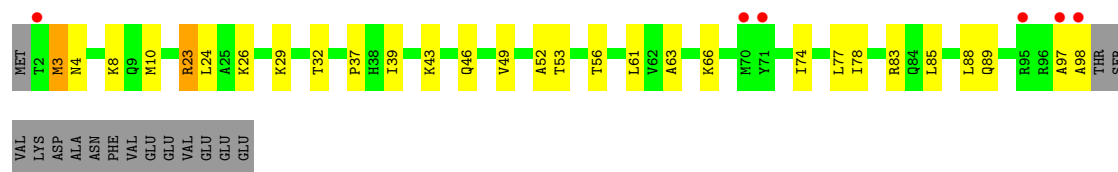
- Molecule 52: 30S ribosomal protein Thx



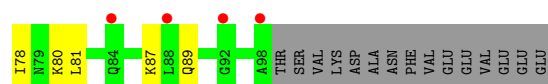
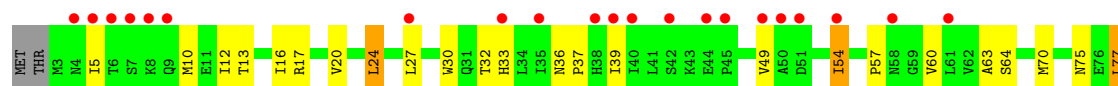
- Molecule 52: 30S ribosomal protein Thx



- 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	209.50Å 448.64Å 621.27Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	152.16 – 2.80 152.16 – 2.80	Depositor EDS
% Data completeness (in resolution range)	97.4 (152.16-2.80) 97.4 (152.16-2.80)	Depositor EDS
R_{merge}	0.20	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.24 (at 2.82Å)	Xtriage
Refinement program	PHENIX 1.8.2	Depositor
R, R_{free}	0.218 , 0.268 0.216 , 0.265	Depositor DCC
R_{free} test set	69237 reflections (4.88%)	wwPDB-VP
Wilson B-factor (Å ²)	51.8	Xtriage
Anisotropy	0.248	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 71.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.42$, $\langle L^2 \rangle = 0.24$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	298171	wwPDB-VP
Average B, all atoms (Å ²)	53.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.78% 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: 5MU, 2MG, M2G, 4OC, 2MA, SF4, OMG, 7MG, UR3, MA6, MPD, ZN, PSU, 5MC, MG, 0TD, 2MU, YXM

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	0.18	0/69029	0.36	2/107746 (0.0%)
1	2A	0.16	0/68901	0.34	0/107544
2	1B	0.16	0/2876	0.33	0/4486
2	2B	0.13	0/2878	0.31	0/4490
3	1D	0.18	0/2181	0.42	0/2940
3	2D	0.16	0/2186	0.41	0/2944
4	1E	0.18	0/1592	0.41	0/2149
4	2E	0.17	0/1592	0.38	0/2149
5	1F	0.17	0/1619	0.39	0/2193
5	2F	0.15	0/1615	0.41	2/2188 (0.1%)
6	1G	0.14	0/1451	0.36	0/1961
6	2G	0.16	0/1449	0.37	0/1957
7	1H	0.14	0/1356	0.33	0/1834
7	2H	0.15	0/1350	0.38	0/1826
8	1I	0.17	0/1109	0.41	0/1512
8	2I	0.13	0/1091	0.33	0/1490
9	1N	0.17	0/1148	0.37	0/1547
9	2N	0.13	0/1144	0.33	0/1543
10	1O	0.19	0/943	0.41	0/1269
10	2O	0.15	0/943	0.35	0/1269
11	1P	0.17	0/1152	0.42	0/1533
11	2P	0.15	0/1152	0.40	0/1533
12	1Q	0.17	0/1143	0.38	0/1527
12	2Q	0.15	0/1143	0.35	0/1527
13	1R	0.17	0/982	0.41	0/1312
13	2R	0.16	0/982	0.39	0/1312
14	1S	0.15	0/887	0.40	0/1180
14	2S	0.13	0/880	0.39	0/1172
15	1T	0.19	0/1105	0.41	0/1477
15	2T	0.15	0/1097	0.37	0/1468
16	1U	0.18	0/977	0.41	0/1301

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
16	2U	0.13	0/977	0.34	0/1301
17	1V	0.16	0/786	0.37	0/1053
17	2V	0.14	0/782	0.37	0/1049
18	1W	0.17	0/897	0.38	0/1205
18	2W	0.15	0/897	0.35	0/1205
19	1X	0.18	0/764	0.40	0/1025
19	2X	0.15	0/764	0.41	0/1025
20	1Y	0.16	0/823	0.41	0/1099
20	2Y	0.13	0/823	0.36	0/1100
21	1Z	0.15	0/1620	0.37	0/2200
21	2Z	0.14	0/1590	0.37	0/2162
22	10	0.18	0/616	0.45	0/821
22	20	0.14	0/616	0.38	0/821
23	11	0.18	0/761	0.38	0/1013
23	21	0.16	0/766	0.36	0/1018
24	12	0.16	0/590	0.37	0/781
24	22	0.14	0/594	0.36	0/785
25	13	0.17	0/474	0.39	0/635
25	23	0.13	0/469	0.33	0/630
26	14	0.17	0/559	0.46	0/754
26	24	0.21	0/549	0.59	0/741
27	15	0.17	0/473	0.39	0/639
27	25	0.16	0/469	0.41	0/635
28	16	0.17	0/460	0.41	0/613
28	26	0.16	0/456	0.37	0/608
29	17	0.19	0/426	0.42	0/561
29	27	0.17	0/426	0.43	0/561
30	18	0.18	0/525	0.40	0/691
30	28	0.16	0/525	0.35	0/691
31	19	0.16	0/310	0.38	0/407
31	29	0.14	0/310	0.38	0/407
32	1a	0.14	0/35795	0.32	2/55864 (0.0%)
32	2a	0.14	0/35890	0.32	1/56012 (0.0%)
33	1b	0.17	0/1876	0.41	0/2533
33	2b	0.20	0/1860	0.45	0/2518
34	1c	0.14	0/1582	0.35	0/2137
34	2c	0.15	0/1566	0.40	0/2119
35	1d	0.15	0/1695	0.38	0/2274
35	2d	0.15	0/1698	0.39	0/2277
36	1e	0.15	0/1149	0.37	0/1548
36	2e	0.15	0/1149	0.37	0/1548
37	1f	0.14	0/827	0.35	0/1120
37	2f	0.13	0/829	0.35	0/1123

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
38	1g	0.14	0/1254	0.35	0/1683
38	2g	0.14	0/1248	0.34	0/1676
39	1h	0.14	0/1118	0.36	0/1506
39	2h	0.13	0/1108	0.36	0/1494
40	1i	0.16	0/1005	0.44	1/1351 (0.1%)
40	2i	0.15	0/985	0.41	0/1329
41	1j	0.15	0/732	0.37	0/993
41	2j	0.15	0/723	0.40	0/984
42	1k	0.15	0/849	0.38	0/1150
42	2k	0.14	0/848	0.41	0/1149
43	1l	0.14	0/937	0.37	0/1260
43	2l	0.14	0/937	0.34	0/1260
44	1m	0.15	0/924	0.41	0/1242
44	2m	0.18	0/905	0.44	0/1217
45	1n	0.14	0/501	0.38	0/664
45	2n	0.15	0/501	0.35	0/664
46	1o	0.15	0/739	0.35	0/985
46	2o	0.13	0/739	0.31	0/985
47	1p	0.15	0/697	0.43	0/939
47	2p	0.14	0/693	0.40	0/935
48	1q	0.13	0/836	0.40	0/1117
48	2q	0.14	0/836	0.38	0/1117
49	1r	0.15	0/560	0.34	0/746
49	2r	0.13	0/560	0.34	0/746
50	1s	0.12	0/663	0.37	0/895
50	2s	0.15	0/660	0.34	0/893
51	1t	0.15	0/734	0.37	0/969
51	2t	0.14	0/736	0.36	0/976
52	1u	0.18	0/203	0.44	0/266
52	2u	0.17	0/203	0.44	0/266
53	1y	0.14	0/776	0.33	0/1048
53	2y	0.14	0/761	0.35	0/1030
All	All	0.16	0/309937	0.35	8/463223 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
21	2Z	0	1
33	1b	0	2
All	All	0	3

There are no bond length outliers.

The worst 5 of 8 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1A	1042	G	OP1-P-O3'	-9.46	79.62	108.00
1	1A	1042	G	OP2-P-O3'	-6.91	87.26	108.00
40	1i	96	LEU	N-CA-C	-6.05	107.72	114.62
32	1a	1442	G	P-O3'-C3'	5.55	126.36	119.70
32	2a	266	G	C2'-C3'-O3'	5.27	117.41	109.50

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
33	1b	123	ALA	Peptide
33	1b	124	SER	Peptide
21	2Z	136	PHE	Peptide

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	1A	61869	0	31198	661	0
1	2A	61758	0	31146	773	0
2	1B	2572	0	1305	33	0
2	2B	2573	0	1306	36	0
3	1D	2131	0	2207	49	0
3	2D	2136	0	2218	58	0
4	1E	1559	0	1618	29	0
4	2E	1559	0	1618	33	0
5	1F	1584	0	1624	36	0
5	2F	1580	0	1619	41	0
6	1G	1426	0	1445	39	0
6	2G	1424	0	1441	51	0
7	1H	1330	0	1407	29	0
7	2H	1324	0	1402	34	0
8	1I	1094	0	1127	26	0
8	2I	1076	0	1094	16	0
9	1N	1121	0	1195	26	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
9	2N	1117	0	1184	16	0
10	1O	933	0	996	18	0
10	2O	933	0	996	26	0
11	1P	1135	0	1212	34	0
11	2P	1135	0	1212	34	0
12	1Q	1122	0	1179	21	0
12	2Q	1122	0	1179	28	0
13	1R	968	0	1033	16	0
13	2R	968	0	1033	20	0
14	1S	877	0	938	13	0
14	2S	870	0	923	28	0
15	1T	1091	0	1151	21	0
15	2T	1083	0	1136	15	0
16	1U	959	0	1018	17	0
16	2U	959	0	1019	26	0
17	1V	775	0	841	9	0
17	2V	771	0	830	9	0
18	1W	886	0	940	11	0
18	2W	886	0	940	18	0
19	1X	750	0	814	16	0
19	2X	750	0	814	19	0
20	1Y	810	0	892	16	0
20	2Y	810	0	887	17	0
21	1Z	1587	0	1598	40	0
21	2Z	1557	0	1564	50	0
22	10	608	0	622	11	0
22	20	608	0	622	9	0
23	11	754	0	823	11	0
23	21	759	0	837	23	0
24	12	588	0	643	11	0
24	22	592	0	654	17	0
25	13	469	0	518	8	0
25	23	464	0	514	8	0
26	14	546	0	522	15	0
26	24	536	0	514	27	0
27	15	459	0	476	10	0
27	25	455	0	465	6	0
28	16	453	0	473	4	0
28	26	449	0	469	6	0
29	17	418	0	467	5	0
29	27	418	0	467	7	0
30	18	517	0	582	17	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
30	28	517	0	582	13	0
31	19	307	0	335	4	0
31	29	307	0	335	6	0
32	1a	32246	0	16295	411	0
32	2a	32331	0	16339	441	0
33	1b	1842	0	1862	40	0
33	2b	1825	0	1828	70	0
34	1c	1558	0	1557	31	0
34	2c	1542	0	1517	46	0
35	1d	1665	0	1687	53	0
35	2d	1668	0	1703	61	0
36	1e	1133	0	1191	26	0
36	2e	1133	0	1191	30	0
37	1f	814	0	808	19	0
37	2f	816	0	808	12	0
38	1g	1235	0	1249	18	0
38	2g	1229	0	1238	26	0
39	1h	1098	0	1143	25	0
39	2h	1088	0	1126	30	0
40	1i	986	0	990	31	0
40	2i	966	0	953	44	0
41	1j	719	0	672	19	0
41	2j	710	0	661	27	0
42	1k	834	0	838	15	0
42	2k	833	0	836	14	0
43	1l	932	0	981	16	0
43	2l	932	0	981	17	0
44	1m	914	0	954	20	0
44	2m	895	0	920	26	0
45	1n	492	0	529	17	0
45	2n	492	0	529	16	0
46	1o	728	0	760	14	0
46	2o	728	0	760	11	0
47	1p	681	0	697	24	0
47	2p	677	0	686	21	0
48	1q	823	0	891	17	0
48	2q	823	0	891	13	0
49	1r	555	0	618	11	0
49	2r	555	0	618	14	0
50	1s	648	0	658	21	0
50	2s	645	0	635	20	0
51	1t	732	0	809	10	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
51	2t	733	0	795	13	0
52	1u	199	0	208	9	0
52	2u	199	0	208	5	0
53	1y	764	0	786	22	0
53	2y	749	0	757	16	0
54	10	7	0	0	0	0
54	11	5	0	0	0	0
54	13	5	0	0	0	0
54	14	1	0	0	0	0
54	15	7	0	0	0	0
54	16	1	0	0	0	0
54	17	4	0	0	0	0
54	18	1	0	0	0	0
54	19	3	0	0	0	0
54	1A	1054	0	0	0	0
54	1B	27	0	0	0	0
54	1D	17	0	0	0	0
54	1E	6	0	0	0	0
54	1F	15	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	6	0	0	0	0
54	1S	1	0	0	0	0
54	1T	6	0	0	0	0
54	1U	8	0	0	0	0
54	1V	5	0	0	0	0
54	1W	4	0	0	0	0
54	1Z	1	0	0	0	0
54	1a	279	0	0	0	0
54	1b	1	0	0	0	0
54	1d	5	0	0	0	0
54	1e	2	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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
54	1m	1	0	0	0	0
54	1n	3	0	0	0	0
54	1o	2	0	0	0	0
54	1t	1	0	0	0	0
54	1y	4	0	0	0	0
54	20	2	0	0	0	0
54	21	2	0	0	0	0
54	23	2	0	0	0	0
54	25	1	0	0	0	0
54	27	2	0	0	0	0
54	28	2	0	0	0	0
54	2A	757	0	0	0	0
54	2B	19	0	0	0	0
54	2D	12	0	0	0	0
54	2E	6	0	0	0	0
54	2F	3	0	0	0	0
54	2G	3	0	0	0	0
54	2I	1	0	0	0	0
54	2N	1	0	0	0	0
54	2O	2	0	0	0	0
54	2P	2	0	0	0	0
54	2Q	3	0	0	0	0
54	2R	3	0	0	0	0
54	2T	3	0	0	0	0
54	2V	3	0	0	0	0
54	2W	2	0	0	0	0
54	2X	2	0	0	0	0
54	2Y	1	0	0	0	0
54	2a	200	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	2n	1	0	0	0	0
54	2t	1	0	0	0	0
55	1A	40	0	0	0	0
55	2A	40	0	0	0	0
56	18	8	0	14	1	0
56	1A	8	0	14	0	0
56	1T	8	0	14	0	0
56	1a	8	0	14	4	0
56	2A	16	0	28	2	0
56	2B	8	0	14	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
57	1B	12	0	12	3	0
57	1F	12	0	12	1	0
58	14	1	0	0	0	0
58	15	1	0	0	0	0
58	16	1	0	0	0	0
58	19	1	0	0	0	0
58	1Y	1	0	0	0	0
58	1n	1	0	0	0	0
58	24	1	0	0	0	0
58	25	1	0	0	0	0
58	26	1	0	0	0	0
58	29	1	0	0	0	0
58	2Y	1	0	0	0	0
58	2n	1	0	0	0	0
59	1d	8	0	0	0	0
59	2d	8	0	0	1	0
60	10	29	0	0	0	0
60	11	24	0	0	1	0
60	12	17	0	0	3	0
60	13	27	0	0	2	0
60	14	4	0	0	0	0
60	15	27	0	0	0	0
60	16	18	0	0	1	0
60	17	18	0	0	0	0
60	18	29	0	0	6	0
60	19	8	0	0	0	0
60	1A	4016	0	0	176	0
60	1B	110	0	0	12	0
60	1D	117	0	0	5	0
60	1E	85	0	0	5	0
60	1F	70	0	0	6	0
60	1G	17	0	0	0	0
60	1H	14	0	0	1	0
60	1I	9	0	0	0	0
60	1N	54	0	0	0	0
60	1O	21	0	0	1	0
60	1P	70	0	0	8	0
60	1Q	40	0	0	1	0
60	1R	34	0	0	2	0
60	1S	10	0	0	0	0
60	1T	36	0	0	1	0
60	1U	47	0	0	6	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
60	1V	39	0	0	1	0
60	1W	23	0	0	1	0
60	1X	23	0	0	0	0
60	1Y	17	0	0	1	0
60	1Z	18	0	0	2	0
60	1a	579	0	0	31	0
60	1b	1	0	0	0	0
60	1c	1	0	0	0	0
60	1d	9	0	0	2	0
60	1e	5	0	0	0	0
60	1f	1	0	0	0	0
60	1h	2	0	0	0	0
60	1j	1	0	0	0	0
60	1k	1	0	0	0	0
60	1l	7	0	0	0	0
60	1m	1	0	0	0	0
60	1o	5	0	0	1	0
60	1p	5	0	0	0	0
60	1t	1	0	0	0	0
60	1u	1	0	0	1	0
60	1y	5	0	0	1	0
60	20	13	0	0	0	0
60	21	23	0	0	3	0
60	22	3	0	0	0	0
60	23	4	0	0	1	0
60	24	2	0	0	0	0
60	25	7	0	0	1	0
60	26	5	0	0	0	0
60	27	11	0	0	0	0
60	28	11	0	0	0	0
60	29	1	0	0	0	0
60	2A	2486	0	0	159	0
60	2B	64	0	0	12	0
60	2D	49	0	0	5	0
60	2E	33	0	0	2	0
60	2F	19	0	0	0	0
60	2G	7	0	0	0	0
60	2H	3	0	0	0	0
60	2I	4	0	0	0	0
60	2N	4	0	0	1	0
60	2O	20	0	0	3	0
60	2P	29	0	0	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
60	2Q	29	0	0	2	0
60	2R	19	0	0	2	0
60	2S	5	0	0	0	0
60	2T	12	0	0	0	0
60	2U	12	0	0	1	0
60	2V	9	0	0	1	0
60	2W	16	0	0	0	0
60	2X	8	0	0	1	0
60	2Y	3	0	0	0	0
60	2Z	10	0	0	0	0
60	2a	420	0	0	25	0
60	2d	8	0	0	1	0
60	2e	1	0	0	0	0
60	2f	3	0	0	0	0
60	2j	1	0	0	0	0
60	2l	1	0	0	0	0
60	2m	1	0	0	0	0
60	2o	4	0	0	0	0
60	2p	3	0	0	0	0
60	2q	1	0	0	0	0
60	2r	3	0	0	0	0
60	2t	2	0	0	0	0
60	2y	3	0	0	0	0
All	All	298171	0	194504	3981	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 3981 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	1.37	1.20
1:1A:2137:C:N4	1:1A:2154:G:H1	1.48	1.12
1:2A:2139:C:N4	1:2A:2152:G:H1	1.55	1.05
1:2A:2128:C:H42	1:2A:2160:G:H1	1.05	1.01
1:2A:2122:U:H3	1:2A:2176:A:N6	1.58	1.00

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%)	257 (94%)	16 (6%)	0	100	100
3	2D	273/276 (99%)	252 (92%)	21 (8%)	0	100	100
4	1E	202/206 (98%)	192 (95%)	8 (4%)	2 (1%)	12	38
4	2E	202/206 (98%)	187 (93%)	12 (6%)	3 (2%)	8	28
5	1F	201/210 (96%)	196 (98%)	4 (2%)	1 (0%)	24	55
5	2F	201/210 (96%)	194 (96%)	6 (3%)	1 (0%)	24	55
6	1G	179/182 (98%)	157 (88%)	19 (11%)	3 (2%)	7	25
6	2G	179/182 (98%)	155 (87%)	20 (11%)	4 (2%)	5	19
7	1H	172/180 (96%)	166 (96%)	4 (2%)	2 (1%)	10	34
7	2H	171/180 (95%)	149 (87%)	20 (12%)	2 (1%)	10	34
8	1I	145/148 (98%)	124 (86%)	21 (14%)	0	100	100
8	2I	144/148 (97%)	133 (92%)	9 (6%)	2 (1%)	9	30
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%)	112 (93%)	8 (7%)	0	100	100
10	2O	120/122 (98%)	110 (92%)	10 (8%)	0	100	100
11	1P	147/150 (98%)	141 (96%)	6 (4%)	0	100	100
11	2P	147/150 (98%)	135 (92%)	10 (7%)	2 (1%)	9	30
12	1Q	139/141 (99%)	130 (94%)	8 (6%)	1 (1%)	18	47
12	2Q	139/141 (99%)	131 (94%)	7 (5%)	1 (1%)	18	47
13	1R	116/118 (98%)	110 (95%)	6 (5%)	0	100	100
13	2R	116/118 (98%)	111 (96%)	5 (4%)	0	100	100
14	1S	108/112 (96%)	101 (94%)	5 (5%)	2 (2%)	6	22
14	2S	108/112 (96%)	101 (94%)	7 (6%)	0	100	100
15	1T	129/146 (88%)	120 (93%)	9 (7%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
15	2T	129/146 (88%)	118 (92%)	10 (8%)	1 (1%)	16	44
16	1U	114/118 (97%)	113 (99%)	1 (1%)	0	100	100
16	2U	114/118 (97%)	113 (99%)	1 (1%)	0	100	100
17	1V	99/101 (98%)	92 (93%)	6 (6%)	1 (1%)	12	38
17	2V	99/101 (98%)	89 (90%)	10 (10%)	0	100	100
18	1W	110/113 (97%)	109 (99%)	1 (1%)	0	100	100
18	2W	110/113 (97%)	108 (98%)	2 (2%)	0	100	100
19	1X	93/96 (97%)	88 (95%)	3 (3%)	2 (2%)	5	19
19	2X	93/96 (97%)	86 (92%)	6 (6%)	1 (1%)	11	36
20	1Y	105/110 (96%)	93 (89%)	11 (10%)	1 (1%)	12	38
20	2Y	105/110 (96%)	98 (93%)	7 (7%)	0	100	100
21	1Z	201/206 (98%)	188 (94%)	13 (6%)	0	100	100
21	2Z	199/206 (97%)	175 (88%)	21 (11%)	3 (2%)	8	28
22	10	75/85 (88%)	72 (96%)	3 (4%)	0	100	100
22	20	75/85 (88%)	72 (96%)	3 (4%)	0	100	100
23	11	95/98 (97%)	94 (99%)	1 (1%)	0	100	100
23	21	95/98 (97%)	91 (96%)	4 (4%)	0	100	100
24	12	68/72 (94%)	67 (98%)	1 (2%)	0	100	100
24	22	68/72 (94%)	66 (97%)	2 (3%)	0	100	100
25	13	57/60 (95%)	54 (95%)	3 (5%)	0	100	100
25	23	57/60 (95%)	54 (95%)	3 (5%)	0	100	100
26	14	67/71 (94%)	51 (76%)	12 (18%)	4 (6%)	1	3
26	24	67/71 (94%)	45 (67%)	18 (27%)	4 (6%)	1	3
27	15	57/60 (95%)	55 (96%)	2 (4%)	0	100	100
27	25	57/60 (95%)	53 (93%)	4 (7%)	0	100	100
28	16	51/54 (94%)	49 (96%)	2 (4%)	0	100	100
28	26	51/54 (94%)	49 (96%)	2 (4%)	0	100	100
29	17	46/49 (94%)	45 (98%)	1 (2%)	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%)	59 (95%)	3 (5%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
31	19	35/37 (95%)	34 (97%)	1 (3%)	0	100	100
31	29	35/37 (95%)	35 (100%)	0	0	100	100
33	1b	229/256 (90%)	202 (88%)	19 (8%)	8 (4%)	3	10
33	2b	229/256 (90%)	191 (83%)	31 (14%)	7 (3%)	3	12
34	1c	204/239 (85%)	188 (92%)	16 (8%)	0	100	100
34	2c	204/239 (85%)	170 (83%)	30 (15%)	4 (2%)	6	21
35	1d	206/209 (99%)	191 (93%)	14 (7%)	1 (0%)	24	55
35	2d	206/209 (99%)	183 (89%)	22 (11%)	1 (0%)	24	55
36	1e	146/162 (90%)	140 (96%)	4 (3%)	2 (1%)	9	30
36	2e	146/162 (90%)	136 (93%)	9 (6%)	1 (1%)	18	47
37	1f	98/101 (97%)	94 (96%)	4 (4%)	0	100	100
37	2f	98/101 (97%)	93 (95%)	4 (4%)	1 (1%)	12	38
38	1g	153/156 (98%)	144 (94%)	9 (6%)	0	100	100
38	2g	153/156 (98%)	136 (89%)	13 (8%)	4 (3%)	4	15
39	1h	135/138 (98%)	126 (93%)	7 (5%)	2 (2%)	8	28
39	2h	135/138 (98%)	125 (93%)	10 (7%)	0	100	100
40	1i	125/128 (98%)	111 (89%)	14 (11%)	0	100	100
40	2i	124/128 (97%)	107 (86%)	13 (10%)	4 (3%)	3	11
41	1j	95/105 (90%)	81 (85%)	9 (10%)	5 (5%)	1	5
41	2j	94/105 (90%)	81 (86%)	10 (11%)	3 (3%)	3	11
42	1k	112/129 (87%)	97 (87%)	14 (12%)	1 (1%)	14	41
42	2k	112/129 (87%)	99 (88%)	11 (10%)	2 (2%)	6	23
43	1l	119/132 (90%)	111 (93%)	8 (7%)	0	100	100
43	2l	119/132 (90%)	110 (92%)	9 (8%)	0	100	100
44	1m	114/126 (90%)	101 (89%)	13 (11%)	0	100	100
44	2m	112/126 (89%)	99 (88%)	11 (10%)	2 (2%)	6	23
45	1n	58/61 (95%)	53 (91%)	5 (9%)	0	100	100
45	2n	58/61 (95%)	51 (88%)	5 (9%)	2 (3%)	3	11
46	1o	86/89 (97%)	81 (94%)	4 (5%)	1 (1%)	10	34
46	2o	86/89 (97%)	81 (94%)	4 (5%)	1 (1%)	10	34
47	1p	80/88 (91%)	70 (88%)	8 (10%)	2 (2%)	4	16

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
47	2p	80/88 (91%)	72 (90%)	8 (10%)	0	100	100
48	1q	97/105 (92%)	87 (90%)	8 (8%)	2 (2%)	5	20
48	2q	97/105 (92%)	88 (91%)	8 (8%)	1 (1%)	12	38
49	1r	66/88 (75%)	62 (94%)	4 (6%)	0	100	100
49	2r	66/88 (75%)	64 (97%)	2 (3%)	0	100	100
50	1s	81/93 (87%)	68 (84%)	12 (15%)	1 (1%)	10	34
50	2s	81/93 (87%)	70 (86%)	10 (12%)	1 (1%)	10	34
51	1t	94/106 (89%)	86 (92%)	5 (5%)	3 (3%)	3	11
51	2t	96/106 (91%)	89 (93%)	5 (5%)	2 (2%)	5	20
52	1u	21/27 (78%)	20 (95%)	1 (5%)	0	100	100
52	2u	21/27 (78%)	17 (81%)	4 (19%)	0	100	100
53	1y	95/113 (84%)	94 (99%)	1 (1%)	0	100	100
53	2y	94/113 (83%)	85 (90%)	7 (7%)	2 (2%)	5	20
All	All	11629/12354 (94%)	10708 (92%)	812 (7%)	109 (1%)	14	41

5 of 109 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
5	1F	130	ALA
6	1G	47	LYS
6	1G	50	ALA
26	14	47	GLN
33	1b	126	GLU

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%)	197 (92%)	17 (8%)	11	35
3	2D	215/218 (99%)	201 (94%)	14 (6%)	15	43
4	1E	164/166 (99%)	156 (95%)	8 (5%)	22	55

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	2E	164/166 (99%)	154 (94%)	10 (6%)	17	46
5	1F	160/166 (96%)	141 (88%)	19 (12%)	5	17
5	2F	159/166 (96%)	147 (92%)	12 (8%)	12	37
6	1G	144/156 (92%)	133 (92%)	11 (8%)	12	36
6	2G	142/156 (91%)	120 (84%)	22 (16%)	2	9
7	1H	144/148 (97%)	133 (92%)	11 (8%)	12	36
7	2H	143/148 (97%)	124 (87%)	19 (13%)	4	14
8	1I	111/124 (90%)	91 (82%)	20 (18%)	2	6
8	2I	108/124 (87%)	95 (88%)	13 (12%)	5	17
9	1N	119/119 (100%)	106 (89%)	13 (11%)	6	21
9	2N	118/119 (99%)	113 (96%)	5 (4%)	26	61
10	1O	100/100 (100%)	94 (94%)	6 (6%)	17	47
10	2O	100/100 (100%)	94 (94%)	6 (6%)	17	47
11	1P	115/116 (99%)	107 (93%)	8 (7%)	14	40
11	2P	115/116 (99%)	109 (95%)	6 (5%)	21	53
12	1Q	111/111 (100%)	102 (92%)	9 (8%)	11	33
12	2Q	111/111 (100%)	105 (95%)	6 (5%)	20	51
13	1R	101/101 (100%)	91 (90%)	10 (10%)	7	24
13	2R	101/101 (100%)	94 (93%)	7 (7%)	14	41
14	1S	87/88 (99%)	82 (94%)	5 (6%)	18	49
14	2S	85/88 (97%)	75 (88%)	10 (12%)	5	17
15	1T	115/127 (91%)	109 (95%)	6 (5%)	21	53
15	2T	113/127 (89%)	103 (91%)	10 (9%)	9	29
16	1U	93/94 (99%)	84 (90%)	9 (10%)	8	25
16	2U	93/94 (99%)	86 (92%)	7 (8%)	12	37
17	1V	81/82 (99%)	73 (90%)	8 (10%)	7	24
17	2V	80/82 (98%)	71 (89%)	9 (11%)	5	19
18	1W	90/92 (98%)	84 (93%)	6 (7%)	15	42
18	2W	90/92 (98%)	86 (96%)	4 (4%)	25	59
19	1X	77/78 (99%)	69 (90%)	8 (10%)	7	22
19	2X	77/78 (99%)	71 (92%)	6 (8%)	11	35

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
20	1Y	86/91 (94%)	80 (93%)	6 (7%)	14	40
20	2Y	86/91 (94%)	78 (91%)	8 (9%)	8	27
21	1Z	169/179 (94%)	155 (92%)	14 (8%)	10	32
21	2Z	165/179 (92%)	156 (94%)	9 (6%)	19	51
22	10	61/67 (91%)	57 (93%)	4 (7%)	15	43
22	20	61/67 (91%)	60 (98%)	1 (2%)	55	83
23	11	79/83 (95%)	75 (95%)	4 (5%)	21	54
23	21	81/83 (98%)	75 (93%)	6 (7%)	13	37
24	12	65/67 (97%)	60 (92%)	5 (8%)	12	36
24	22	66/67 (98%)	60 (91%)	6 (9%)	9	28
25	13	51/52 (98%)	44 (86%)	7 (14%)	3	13
25	23	50/52 (96%)	44 (88%)	6 (12%)	5	17
26	14	58/63 (92%)	49 (84%)	9 (16%)	2	9
26	24	54/63 (86%)	47 (87%)	7 (13%)	4	14
27	15	51/52 (98%)	47 (92%)	4 (8%)	11	35
27	25	50/52 (96%)	48 (96%)	2 (4%)	28	63
28	16	51/52 (98%)	47 (92%)	4 (8%)	11	35
28	26	50/52 (96%)	46 (92%)	4 (8%)	11	34
29	17	41/42 (98%)	41 (100%)	0	100	100
29	27	41/42 (98%)	40 (98%)	1 (2%)	43	77
30	18	54/55 (98%)	52 (96%)	2 (4%)	30	65
30	28	54/55 (98%)	51 (94%)	3 (6%)	19	50
31	19	34/34 (100%)	33 (97%)	1 (3%)	37	73
31	29	34/34 (100%)	30 (88%)	4 (12%)	5	17
33	1b	191/220 (87%)	172 (90%)	19 (10%)	7	24
33	2b	187/220 (85%)	162 (87%)	25 (13%)	4	13
34	1c	144/188 (77%)	132 (92%)	12 (8%)	10	32
34	2c	140/188 (74%)	129 (92%)	11 (8%)	11	35
35	1d	171/181 (94%)	152 (89%)	19 (11%)	6	20
35	2d	172/181 (95%)	155 (90%)	17 (10%)	7	24
36	1e	114/123 (93%)	105 (92%)	9 (8%)	11	35

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
36	2e	114/123 (93%)	101 (89%)	13 (11%)	5	19
37	1f	85/90 (94%)	76 (89%)	9 (11%)	6	22
37	2f	85/90 (94%)	79 (93%)	6 (7%)	13	39
38	1g	120/127 (94%)	110 (92%)	10 (8%)	10	32
38	2g	119/127 (94%)	112 (94%)	7 (6%)	18	48
39	1h	116/119 (98%)	106 (91%)	10 (9%)	10	31
39	2h	114/119 (96%)	106 (93%)	8 (7%)	14	40
40	1i	91/99 (92%)	80 (88%)	11 (12%)	5	16
40	2i	88/99 (89%)	78 (89%)	10 (11%)	5	19
41	1j	68/92 (74%)	60 (88%)	8 (12%)	5	17
41	2j	68/92 (74%)	58 (85%)	10 (15%)	3	10
42	1k	83/99 (84%)	75 (90%)	8 (10%)	8	26
42	2k	83/99 (84%)	76 (92%)	7 (8%)	10	32
43	1l	96/108 (89%)	92 (96%)	4 (4%)	26	61
43	2l	96/108 (89%)	94 (98%)	2 (2%)	47	79
44	1m	90/101 (89%)	87 (97%)	3 (3%)	33	69
44	2m	87/101 (86%)	81 (93%)	6 (7%)	14	41
45	1n	49/50 (98%)	45 (92%)	4 (8%)	10	33
45	2n	49/50 (98%)	46 (94%)	3 (6%)	17	46
46	1o	78/80 (98%)	76 (97%)	2 (3%)	40	75
46	2o	78/80 (98%)	74 (95%)	4 (5%)	21	54
47	1p	69/74 (93%)	62 (90%)	7 (10%)	7	23
47	2p	68/74 (92%)	57 (84%)	11 (16%)	2	8
48	1q	94/97 (97%)	91 (97%)	3 (3%)	34	70
48	2q	94/97 (97%)	87 (93%)	7 (7%)	13	37
49	1r	59/77 (77%)	54 (92%)	5 (8%)	10	31
49	2r	59/77 (77%)	57 (97%)	2 (3%)	32	68
50	1s	68/80 (85%)	61 (90%)	7 (10%)	7	23
50	2s	67/80 (84%)	55 (82%)	12 (18%)	2	6
51	1t	71/82 (87%)	64 (90%)	7 (10%)	7	24
51	2t	70/82 (85%)	62 (89%)	8 (11%)	5	19

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
52	1u	18/22 (82%)	17 (94%)	1 (6%)	19	50
52	2u	18/22 (82%)	17 (94%)	1 (6%)	19	50
53	1y	82/98 (84%)	79 (96%)	3 (4%)	30	65
53	2y	79/98 (81%)	72 (91%)	7 (9%)	9	29
All	All	9524/10260 (93%)	8729 (92%)	795 (8%)	10	32

5 of 795 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
7	2H	95	ARG
21	2Z	74	VAL
8	2I	68	LEU
7	2H	88	LEU
14	2S	40	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 132 such sidechains are listed below:

Mol	Chain	Res	Type
38	2g	64	GLN
42	2k	22	HIS
51	2t	90	GLN
38	1g	64	GLN
38	1g	28	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	1A	2865/2915 (98%)	420 (14%)	24 (0%)
1	2A	2858/2915 (98%)	467 (16%)	29 (1%)
2	1B	119/121 (98%)	10 (8%)	0
2	2B	119/121 (98%)	13 (10%)	0
32	1a	1497/1521 (98%)	258 (17%)	0
32	2a	1501/1521 (98%)	259 (17%)	0
All	All	8959/9114 (98%)	1427 (15%)	53 (0%)

5 of 1427 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	1A	15	G
1	1A	27	G
1	1A	34	C
1	1A	45	C
1	1A	71	A

5 of 53 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	2A	271(M)	G
1	2A	1053	C
1	2A	2406	U
1	2A	277	C
1	2A	840	C

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
32	5MC	1a	1407	32	19,22,23	1.75	3 (15%)	26,32,35	1.18	4 (15%)
32	UR3	2a	1498	32	19,22,23	0.99	2 (10%)	26,32,35	1.68	2 (7%)
1	PSU	1A	2605	1,54	18,21,22	1.35	3 (16%)	21,30,33	2.01	5 (23%)
32	PSU	2a	516	32,54	18,21,22	1.37	2 (11%)	21,30,33	2.03	5 (23%)
32	2MG	1a	1207	32	23,26,27	1.23	2 (8%)	33,38,41	2.26	8 (24%)
1	PSU	1A	1917	1,54	18,21,22	1.38	2 (11%)	21,30,33	1.94	3 (14%)
1	5MC	2A	1942	1	19,22,23	1.66	3 (15%)	26,32,35	1.18	2 (7%)
32	4OC	2a	1402	32	20,23,24	0.77	0	25,32,35	0.94	1 (4%)
1	PSU	1A	1911	1	18,21,22	1.36	2 (11%)	21,30,33	2.06	4 (19%)
32	PSU	1a	516	32,54	18,21,22	1.40	2 (11%)	21,30,33	2.00	4 (19%)
32	MA6	1a	1519	32	23,26,27	0.42	0	33,38,41	2.08	9 (27%)
32	M2G	1a	966	32	24,27,28	1.27	4 (16%)	33,40,43	1.91	6 (18%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
43	0TD	2l	92	43	8,9,10	4.46	1 (12%)	6,11,13	4.98	3 (50%)
32	5MC	1a	967	32	19,22,23	1.60	3 (15%)	26,32,35	1.06	2 (7%)
1	5MU	2A	1939	1	19,22,23	1.46	6 (31%)	27,32,35	2.17	6 (22%)
32	2MG	2a	1207	32	23,26,27	1.24	4 (17%)	33,38,41	2.15	8 (24%)
1	5MU	2A	1915	1	19,22,23	1.41	5 (26%)	27,32,35	2.20	9 (33%)
32	4OC	1a	1402	32	20,23,24	0.74	0	25,32,35	0.92	1 (4%)
1	PSU	2A	1917	1	18,21,22	1.34	2 (11%)	21,30,33	2.02	3 (14%)
1	2MA	2A	2503	1,54	22,25,26	1.51	5 (22%)	32,37,40	2.27	8 (25%)
1	5MU	1A	1939	1	19,22,23	1.44	6 (31%)	27,32,35	2.12	6 (22%)
1	2MA	1A	2503	1,54	22,25,26	1.50	4 (18%)	32,37,40	2.41	8 (25%)
32	7MG	1a	527	32,54	23,26,27	1.35	3 (13%)	27,39,42	2.56	7 (25%)
32	5MC	2a	1400	32	19,22,23	1.60	3 (15%)	26,32,35	1.16	2 (7%)
1	PSU	2A	1911	1	18,21,22	1.36	2 (11%)	21,30,33	1.98	3 (14%)
1	5MU	1A	1915	1,54	19,22,23	1.44	5 (26%)	27,32,35	2.19	8 (29%)
32	5MC	2a	967	32	19,22,23	1.69	3 (15%)	26,32,35	1.07	2 (7%)
32	MA6	2a	1519	32	23,26,27	0.43	0	33,38,41	2.12	9 (27%)
1	4OC	2A	1920	1	19,22,24	0.80	0	25,31,35	0.95	1 (4%)
32	5MC	1a	1400	32	19,22,23	1.69	3 (15%)	26,32,35	1.12	2 (7%)
32	MA6	2a	1518	32	23,26,27	0.39	0	33,38,41	2.08	9 (27%)
32	UR3	1a	1498	32	19,22,23	0.97	1 (5%)	26,32,35	1.73	3 (11%)
43	0TD	1l	92	43	8,9,10	4.58	1 (12%)	6,11,13	3.84	3 (50%)
32	M2G	2a	966	32,54	24,27,28	1.31	4 (16%)	33,40,43	1.85	5 (15%)
1	4OC	1A	1920	1	19,22,24	0.79	0	25,31,35	0.88	1 (4%)
32	5MC	2a	1404	32	19,22,23	1.69	3 (15%)	26,32,35	1.13	2 (7%)
1	2MU	2A	2552	1,54	19,22,24	1.26	3 (15%)	25,31,36	1.93	6 (24%)
1	PSU	2A	2605	1	18,21,22	1.37	3 (16%)	21,30,33	1.89	4 (19%)
32	5MC	1a	1404	32	19,22,23	1.62	3 (15%)	26,32,35	1.09	2 (7%)
1	OMG	2A	2251	1,54	23,26,27	1.19	3 (13%)	32,38,41	2.00	6 (18%)
1	OMG	1A	2251	1,54	23,26,27	1.20	3 (13%)	32,38,41	2.05	7 (21%)
32	MA6	1a	1518	32	23,26,27	0.42	0	33,38,41	1.97	9 (27%)
1	5MC	2A	1962	1,54	19,22,23	1.55	3 (15%)	26,32,35	1.10	2 (7%)
1	2MU	1A	2552	1,54	19,22,24	1.28	3 (15%)	25,31,36	1.86	6 (24%)
1	5MC	1A	1942	1	19,22,23	1.53	3 (15%)	26,32,35	1.13	3 (11%)
32	7MG	2a	527	32,54	23,26,27	1.34	3 (13%)	27,39,42	2.58	7 (25%)
32	5MC	2a	1407	32	19,22,23	1.66	3 (15%)	26,32,35	1.13	3 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	5MC	1A	1962	1,54	19,22,23	1.73	3 (15%)	26,32,35	1.16	3 (11%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
32	5MC	1a	1407	32	-	0/7/25/26	0/2/2/2
32	UR3	2a	1498	32	-	0/7/25/26	0/2/2/2
1	PSU	1A	2605	1,54	-	0/7/25/26	0/2/2/2
32	PSU	2a	516	32,54	-	0/7/25/26	0/2/2/2
32	2MG	1a	1207	32	-	0/9/27/28	0/3/3/3
1	PSU	1A	1917	1,54	-	0/7/25/26	0/2/2/2
1	5MC	2A	1942	1	-	0/7/25/26	0/2/2/2
32	4OC	2a	1402	32	-	3/9/29/30	0/2/2/2
1	PSU	1A	1911	1	-	0/7/25/26	0/2/2/2
32	PSU	1a	516	32,54	-	0/7/25/26	0/2/2/2
32	MA6	1a	1519	32	-	1/11/29/30	0/3/3/3
32	M2G	1a	966	32	-	1/11/29/30	0/3/3/3
43	0TD	2l	92	43	-	2/7/12/14	-
32	5MC	1a	967	32	-	1/7/25/26	0/2/2/2
1	5MU	2A	1939	1	-	0/7/25/26	0/2/2/2
32	2MG	2a	1207	32	-	0/9/27/28	0/3/3/3
1	5MU	2A	1915	1	-	2/7/25/26	0/2/2/2
32	4OC	1a	1402	32	-	2/9/29/30	0/2/2/2
1	PSU	2A	1917	1	-	0/7/25/26	0/2/2/2
1	2MA	2A	2503	1,54	-	1/7/25/26	0/3/3/3
1	5MU	1A	1939	1	-	0/7/25/26	0/2/2/2
1	2MA	1A	2503	1,54	-	1/7/25/26	0/3/3/3
32	7MG	1a	527	32,54	-	1/7/37/38	0/3/3/3
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	5MU	1A	1915	1,54	-	2/7/25/26	0/2/2/2
32	5MC	2a	967	32	-	0/7/25/26	0/2/2/2
32	MA6	2a	1519	32	-	3/11/29/30	0/3/3/3
1	4OC	2A	1920	1	-	1/9/27/30	0/2/2/2
32	5MC	1a	1400	32	-	2/7/25/26	0/2/2/2
32	MA6	2a	1518	32	-	0/11/29/30	0/3/3/3
32	UR3	1a	1498	32	-	0/7/25/26	0/2/2/2
43	0TD	1l	92	43	-	1/7/12/14	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
32	M2G	2a	966	32,54	-	0/11/29/30	0/3/3/3
1	4OC	1A	1920	1	-	0/9/27/30	0/2/2/2
32	5MC	2a	1404	32	-	0/7/25/26	0/2/2/2
1	2MU	2A	2552	1,54	-	0/9/27/28	0/2/2/2
1	PSU	2A	2605	1	-	0/7/25/26	0/2/2/2
32	5MC	1a	1404	32	-	0/7/25/26	0/2/2/2
1	OMG	2A	2251	1,54	-	1/9/27/28	0/3/3/3
1	OMG	1A	2251	1,54	-	1/9/27/28	0/3/3/3
32	MA6	1a	1518	32	-	0/11/29/30	0/3/3/3
1	5MC	2A	1962	1,54	-	0/7/25/26	0/2/2/2
1	2MU	1A	2552	1,54	-	1/9/27/28	0/2/2/2
1	5MC	1A	1942	1	-	0/7/25/26	0/2/2/2
32	7MG	2a	527	32,54	-	2/7/37/38	0/3/3/3
32	5MC	2a	1407	32	-	0/7/25/26	0/2/2/2
1	5MC	1A	1962	1,54	-	0/7/25/26	0/2/2/2

The worst 5 of 122 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
43	1l	92	0TD	CB-SB	-12.59	1.69	1.82
43	2l	92	0TD	CB-SB	-12.32	1.69	1.82
32	1a	1407	5MC	C5-C4	6.59	1.49	1.44
1	1A	1962	5MC	C5-C4	6.34	1.48	1.44
32	2a	967	5MC	C5-C4	6.25	1.48	1.44

The worst 5 of 222 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
43	2l	92	0TD	CSB-SB-CB	-11.44	81.80	102.36
32	1a	527	7MG	N9-C4-N3	8.84	138.42	125.46
32	2a	527	7MG	N9-C4-N3	8.80	138.35	125.46
1	1A	2503	2MA	C5-C4-N3	-8.61	118.11	127.18
43	1l	92	0TD	CSB-SB-CB	-8.34	87.38	102.36

There are no chirality outliers.

5 of 29 torsion outliers are listed below:

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

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Mol	Chain	Res	Type	Atoms
1	2A	1915	5MU	O4'-C1'-N1-C6
1	2A	2251	OMG	C1'-C2'-O2'-CM2

There are no ring outliers.

25 monomers are involved in 34 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
32	1a	1207	2MG	2	0
32	2a	1402	4OC	1	0
32	1a	1519	MA6	3	0
32	1a	966	M2G	1	0
43	2l	92	0TD	1	0
32	2a	1207	2MG	5	0
1	2A	1915	5MU	1	0
32	1a	1402	4OC	1	0
1	2A	1917	PSU	1	0
1	1A	1939	5MU	2	0
32	1a	527	7MG	1	0
32	2a	1400	5MC	2	0
1	2A	1911	PSU	1	0
32	2a	1519	MA6	1	0
1	2A	1920	4OC	1	0
32	1a	1400	5MC	2	0
32	2a	1518	MA6	2	0
32	1a	1498	UR3	1	0
1	1A	1920	4OC	1	0
32	2a	1404	5MC	1	0
1	2A	2552	2MU	1	0
1	2A	2251	OMG	2	0
32	1a	1518	MA6	2	0
1	1A	2552	2MU	1	0
1	1A	1942	5MC	1	0

5.5 Carbohydrates

There are no oligosaccharides in this entry.

5.6 Ligand geometry

Of 2579 ligands modelled in this entry, 2566 are monoatomic - leaving 13 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
56	MPD	1a	3280	-	7,7,7	0.37	0	9,10,10	0.34	0
57	ARG	1F	316	-	10,11,11	0.75	1 (10%)	9,13,13	0.97	1 (11%)
56	MPD	2A	3760	-	7,7,7	0.32	0	9,10,10	0.30	0
56	MPD	1T	207	-	7,7,7	0.30	0	9,10,10	0.22	0
59	SF4	1d	306	35	0,12,12	-	-	-	-	-
55	YXM	2A	3758	-	43,43,43	2.75	7 (16%)	55,58,58	1.49	8 (14%)
56	MPD	18	102	-	7,7,7	0.26	0	9,10,10	0.23	0
56	MPD	1A	4056	-	7,7,7	0.33	0	9,10,10	0.25	0
56	MPD	2A	3759	-	7,7,7	0.30	0	9,10,10	0.25	0
56	MPD	2B	220	-	7,7,7	0.31	0	9,10,10	0.20	0
55	YXM	1A	4055	-	43,43,43	2.93	6 (13%)	55,58,58	1.31	5 (9%)
57	ARG	1B	228	-	10,11,11	0.74	1 (10%)	9,13,13	1.00	1 (11%)
59	SF4	2d	501	35	0,12,12	-	-	-	-	-

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
56	MPD	1a	3280	-	-	4/5/5/5	-
57	ARG	1F	316	-	-	4/11/11/11	-
56	MPD	2A	3760	-	-	3/5/5/5	-
56	MPD	1T	207	-	-	0/5/5/5	-
59	SF4	1d	306	35	-	-	0/6/5/5
55	YXM	2A	3758	-	-	3/42/44/44	0/4/4/4
56	MPD	18	102	-	-	2/5/5/5	-
56	MPD	1A	4056	-	-	2/5/5/5	-
56	MPD	2A	3759	-	-	0/5/5/5	-
56	MPD	2B	220	-	-	4/5/5/5	-
55	YXM	1A	4055	-	-	3/42/44/44	0/4/4/4
57	ARG	1B	228	-	-	2/11/11/11	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
59	SF4	2d	501	35	-	-	0/6/5/5

The worst 5 of 15 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
55	1A	4055	YXM	OAK-NAG	14.28	1.47	1.22
55	2A	3758	YXM	OAK-NAG	13.62	1.46	1.22
55	2A	3758	YXM	CAB-CAH	-8.17	1.39	1.51
55	1A	4055	YXM	CAB-CAH	-7.61	1.40	1.51
55	1A	4055	YXM	PAV-CAY	-6.30	1.68	1.79

The worst 5 of 15 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
55	2A	3758	YXM	CAY-PAV-CAX	5.67	120.00	109.28
55	1A	4055	YXM	CAU-PAV-CAW	-4.76	99.65	109.60
55	1A	4055	YXM	CAY-PAV-CAX	4.27	117.35	109.28
55	2A	3758	YXM	CAU-PAV-CAY	-4.22	100.77	109.60
55	2A	3758	YXM	CAU-PAV-CAW	-4.04	101.15	109.60

There are no chirality outliers.

5 of 27 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
55	2A	3758	YXM	NAN-CAJ-CAM-OAO
56	1a	3280	MPD	C2-C3-C4-O4
56	1a	3280	MPD	C2-C3-C4-C5
56	2B	220	MPD	C2-C3-C4-C5
57	1F	316	ARG	N-CA-CB-CG

There are no ring outliers.

8 monomers are involved in 13 short contacts:

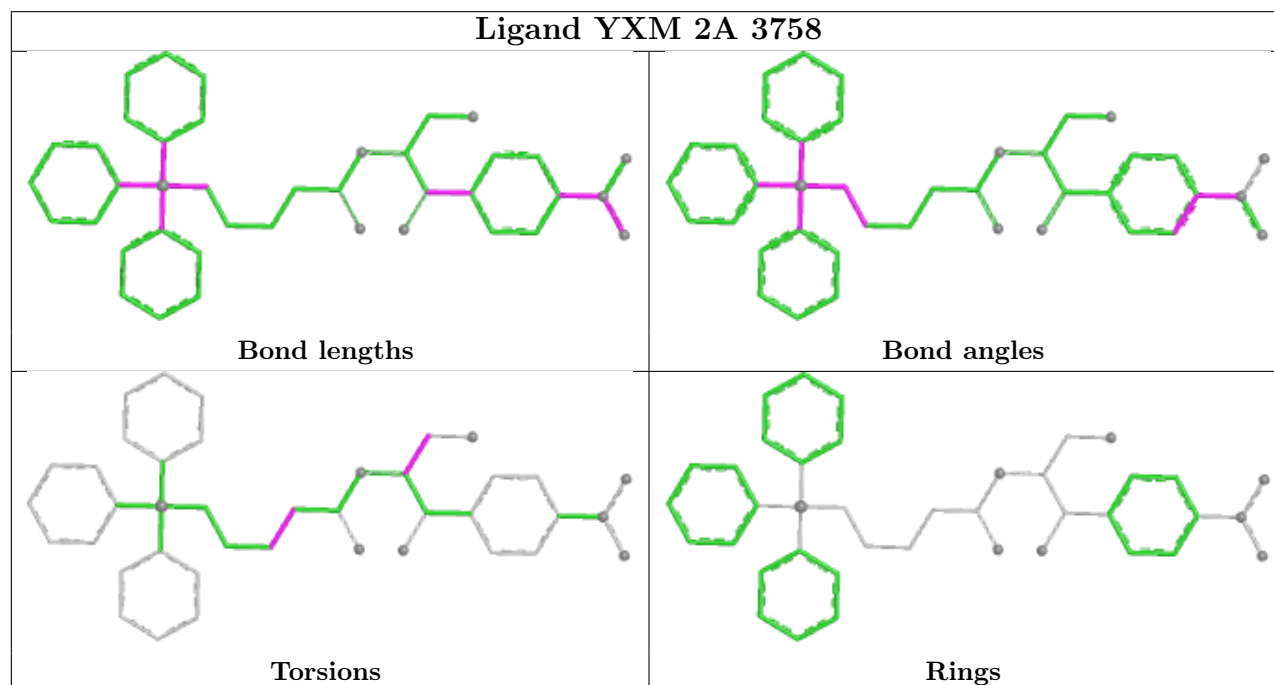
Mol	Chain	Res	Type	Clashes	Symm-Clashes
56	1a	3280	MPD	4	0
57	1F	316	ARG	1	0
56	2A	3760	MPD	1	0
56	18	102	MPD	1	0
56	2A	3759	MPD	1	0
56	2B	220	MPD	1	0
57	1B	228	ARG	3	0

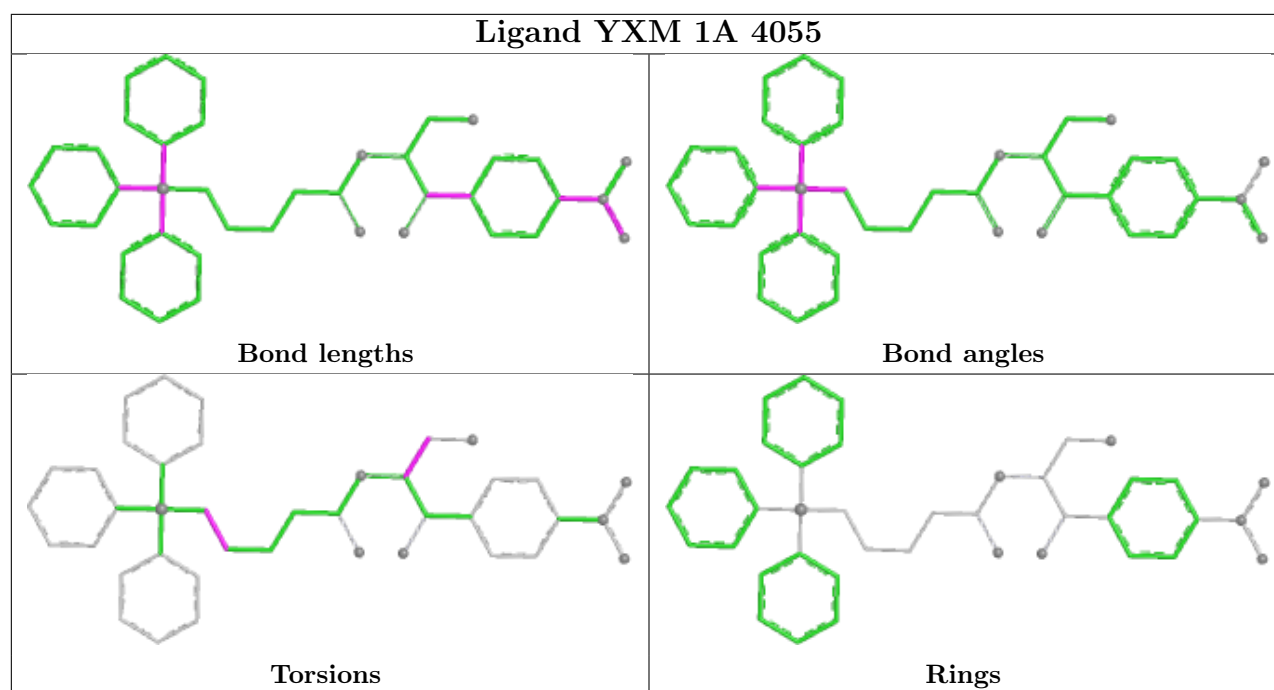
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Mol	Chain	Res	Type	Clashes	Symm-Clashes
59	2d	501	SF4	1	0

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.





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%)	-0.44	65 (2%) 61 51	12, 31, 88, 103	0
1	2A	2856/2915 (97%)	-0.05	87 (3%) 52 42	25, 50, 91, 104	0
2	1B	120/121 (99%)	-0.42	1 (0%) 82 75	22, 45, 60, 81	0
2	2B	120/121 (99%)	0.62	2 (1%) 69 60	52, 73, 84, 92	0
3	1D	275/276 (99%)	-0.14	3 (1%) 78 70	16, 30, 44, 66	0
3	2D	275/276 (99%)	0.20	5 (1%) 67 58	25, 45, 59, 74	0
4	1E	204/206 (99%)	-0.13	1 (0%) 87 82	16, 37, 55, 71	0
4	2E	204/206 (99%)	0.05	0 100 100	27, 50, 65, 77	0
5	1F	203/210 (96%)	-0.14	0 100 100	15, 36, 59, 73	0
5	2F	203/210 (96%)	0.31	2 (0%) 79 72	27, 60, 73, 83	0
6	1G	181/182 (99%)	0.40	3 (1%) 69 60	39, 59, 72, 82	0
6	2G	181/182 (99%)	1.36	32 (17%) 4 3	68, 78, 84, 88	0
7	1H	174/180 (96%)	0.03	1 (0%) 85 80	36, 49, 62, 66	0
7	2H	173/180 (96%)	0.85	6 (3%) 47 38	61, 75, 82, 87	0
8	1I	147/148 (99%)	0.55	4 (2%) 56 46	38, 66, 77, 80	0
8	2I	146/148 (98%)	0.59	4 (2%) 56 46	50, 67, 78, 82	0
9	1N	140/140 (100%)	-0.21	0 100 100	24, 34, 55, 67	0
9	2N	140/140 (100%)	0.50	2 (1%) 73 64	39, 57, 70, 76	0
10	1O	122/122 (100%)	-0.14	0 100 100	22, 35, 50, 59	0
10	2O	122/122 (100%)	0.23	0 100 100	36, 49, 62, 67	0
11	1P	149/150 (99%)	-0.04	0 100 100	16, 41, 61, 71	0
11	2P	149/150 (99%)	0.31	0 100 100	29, 59, 75, 80	0
12	1Q	141/141 (100%)	-0.29	0 100 100	20, 34, 47, 60	0
12	2Q	141/141 (100%)	0.55	2 (1%) 73 64	39, 58, 68, 75	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
13	1R	118/118 (100%)	-0.21	0 100 100	21, 31, 44, 55	0
13	2R	118/118 (100%)	0.03	0 100 100	33, 44, 56, 64	0
14	1S	110/112 (98%)	-0.07	1 (0%) 81 74	32, 44, 56, 60	0
14	2S	110/112 (98%)	1.05	9 (8%) 17 13	55, 68, 76, 78	0
15	1T	131/146 (89%)	0.12	3 (2%) 61 51	28, 42, 64, 76	0
15	2T	131/146 (89%)	0.15	2 (1%) 72 63	39, 51, 69, 74	0
16	1U	116/118 (98%)	-0.35	0 100 100	19, 27, 43, 54	0
16	2U	116/118 (98%)	0.26	1 (0%) 81 74	36, 54, 68, 72	0
17	1V	101/101 (100%)	-0.25	0 100 100	18, 37, 53, 64	0
17	2V	101/101 (100%)	0.40	0 100 100	35, 63, 73, 76	0
18	1W	112/113 (99%)	-0.22	1 (0%) 81 74	18, 27, 52, 79	0
18	2W	112/113 (99%)	0.15	0 100 100	30, 43, 60, 78	0
19	1X	95/96 (98%)	-0.19	0 100 100	18, 32, 52, 67	0
19	2X	95/96 (98%)	0.30	0 100 100	41, 53, 63, 70	0
20	1Y	107/110 (97%)	0.08	1 (0%) 81 74	31, 44, 64, 70	0
20	2Y	107/110 (97%)	0.74	3 (2%) 55 45	52, 64, 75, 79	0
21	1Z	203/206 (98%)	0.15	1 (0%) 87 82	32, 51, 65, 75	0
21	2Z	201/206 (97%)	0.78	6 (2%) 52 42	58, 70, 78, 86	0
22	10	77/85 (90%)	-0.09	0 100 100	21, 32, 46, 51	0
22	20	77/85 (90%)	0.62	5 (6%) 25 18	38, 56, 66, 70	0
23	11	97/98 (98%)	-0.05	1 (1%) 79 72	21, 37, 60, 68	0
23	21	97/98 (98%)	0.44	1 (1%) 79 72	30, 49, 67, 75	0
24	12	70/72 (97%)	0.12	2 (2%) 53 43	29, 43, 56, 78	0
24	22	70/72 (97%)	0.27	0 100 100	50, 63, 70, 73	0
25	13	59/60 (98%)	-0.24	0 100 100	25, 34, 55, 62	0
25	23	59/60 (98%)	0.27	1 (1%) 69 60	42, 55, 69, 82	0
26	14	69/71 (97%)	0.87	8 (11%) 9 7	55, 74, 83, 85	0
26	24	69/71 (97%)	1.56	16 (23%) 2 1	74, 85, 92, 99	0
27	15	59/60 (98%)	-0.25	0 100 100	17, 31, 53, 61	0
27	25	59/60 (98%)	-0.04	1 (1%) 69 60	29, 45, 60, 73	0
28	16	53/54 (98%)	-0.22	0 100 100	28, 36, 50, 57	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
28	26	53/54 (98%)	0.34	0 100 100	46, 54, 64, 66	0
29	17	48/49 (97%)	-0.27	0 100 100	15, 22, 48, 58	0
29	27	48/49 (97%)	0.10	2 (4%) 40 32	25, 34, 61, 69	0
30	18	64/65 (98%)	-0.38	0 100 100	22, 29, 38, 53	0
30	28	64/65 (98%)	0.33	0 100 100	40, 48, 55, 66	0
31	19	37/37 (100%)	-0.06	0 100 100	26, 36, 53, 56	0
31	29	37/37 (100%)	0.93	1 (2%) 56 46	54, 61, 75, 80	0
32	1a	1488/1521 (97%)	0.13	17 (1%) 78 70	30, 63, 88, 104	0
32	2a	1492/1521 (98%)	0.48	50 (3%) 48 39	42, 71, 91, 103	0
33	1b	231/256 (90%)	0.79	14 (6%) 27 20	60, 73, 81, 85	0
33	2b	231/256 (90%)	1.12	27 (11%) 9 7	67, 80, 86, 90	0
34	1c	206/239 (86%)	0.72	9 (4%) 39 31	52, 67, 75, 79	0
34	2c	206/239 (86%)	1.14	25 (12%) 8 6	65, 78, 85, 89	0
35	1d	208/209 (99%)	0.54	7 (3%) 48 39	51, 63, 73, 80	0
35	2d	208/209 (99%)	0.77	9 (4%) 40 31	58, 67, 76, 80	0
36	1e	148/162 (91%)	0.43	1 (0%) 84 77	42, 59, 69, 74	0
36	2e	148/162 (91%)	0.82	6 (4%) 41 33	58, 69, 76, 87	0
37	1f	100/101 (99%)	0.25	0 100 100	49, 59, 69, 72	0
37	2f	100/101 (99%)	0.42	0 100 100	55, 65, 72, 79	0
38	1g	155/156 (99%)	0.51	3 (1%) 66 57	58, 66, 73, 81	0
38	2g	155/156 (99%)	1.09	15 (9%) 13 10	69, 76, 82, 89	0
39	1h	137/138 (99%)	0.43	1 (0%) 84 77	51, 61, 69, 74	0
39	2h	137/138 (99%)	0.63	3 (2%) 62 52	61, 71, 76, 81	0
40	1i	127/128 (99%)	0.96	9 (7%) 22 16	56, 71, 79, 82	0
40	2i	126/128 (98%)	1.81	48 (38%) 1 0	70, 80, 85, 90	0
41	1j	97/105 (92%)	1.18	14 (14%) 6 5	54, 72, 82, 84	0
41	2j	96/105 (91%)	1.48	25 (26%) 1 1	69, 81, 86, 88	0
42	1k	114/129 (88%)	0.32	1 (0%) 81 74	37, 57, 69, 71	0
42	2k	114/129 (88%)	0.63	4 (3%) 47 38	55, 68, 74, 78	0
43	1l	121/132 (91%)	0.37	2 (1%) 69 60	40, 53, 63, 77	0
43	2l	121/132 (91%)	0.58	3 (2%) 58 48	49, 61, 70, 71	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
44	1m	116/126 (92%)	0.62	6 (5%) 33 25	56, 68, 75, 80	0
44	2m	114/126 (90%)	1.45	27 (23%) 2 1	71, 79, 86, 88	0
45	1n	60/61 (98%)	0.73	3 (5%) 34 26	57, 65, 72, 76	0
45	2n	60/61 (98%)	1.66	17 (28%) 1 1	70, 80, 88, 89	0
46	1o	88/89 (98%)	0.43	1 (1%) 78 70	43, 59, 71, 78	0
46	2o	88/89 (98%)	0.68	3 (3%) 48 39	57, 68, 77, 83	0
47	1p	82/88 (93%)	0.94	4 (4%) 35 27	53, 65, 74, 81	0
47	2p	82/88 (93%)	0.91	5 (6%) 27 20	54, 63, 74, 76	0
48	1q	99/105 (94%)	0.51	3 (3%) 52 42	50, 61, 69, 75	0
48	2q	99/105 (94%)	0.55	2 (2%) 65 56	55, 62, 72, 76	0
49	1r	68/88 (77%)	0.07	0 100 100	50, 58, 72, 81	0
49	2r	68/88 (77%)	0.47	1 (1%) 72 63	62, 69, 77, 81	0
50	1s	83/93 (89%)	0.72	3 (3%) 46 37	60, 70, 77, 80	0
50	2s	83/93 (89%)	1.47	20 (24%) 2 1	70, 82, 87, 88	0
51	1t	96/106 (90%)	0.75	5 (5%) 33 25	55, 65, 74, 79	0
51	2t	98/106 (92%)	0.65	4 (4%) 41 33	48, 62, 73, 78	0
52	1u	23/27 (85%)	1.22	2 (8%) 16 11	65, 68, 73, 75	0
52	2u	23/27 (85%)	2.06	11 (47%) 0 0	72, 79, 82, 85	0
53	1y	97/113 (85%)	0.58	6 (6%) 26 20	47, 57, 69, 78	0
53	2y	96/113 (84%)	1.54	25 (26%) 1 1	63, 74, 81, 83	0
All	All	20766/21468 (96%)	0.24	727 (3%) 47 38	12, 57, 84, 104	0

The worst 5 of 727 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	1A	1087	G	8.0
34	1c	2	GLY	7.2
45	2n	2	ALA	7.0
23	21	2	SER	6.1
7	1H	2	SER	5.1

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

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

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
1	PSU	2A	1917	20/21	0.83	0.11	67,77,94,97	0
1	5MU	2A	1915	21/22	0.84	0.11	74,82,85,99	0
1	PSU	2A	1911	20/21	0.85	0.09	64,70,80,82	0
43	0TD	2l	92	10/11	0.85	0.15	52,59,64,79	0
1	5MU	1A	1915	21/22	0.86	0.11	64,70,80,81	0
32	PSU	2a	516	20/21	0.86	0.11	71,75,83,83	0
43	0TD	1l	92	10/11	0.86	0.14	43,54,57,67	0
32	2MG	2a	1207	24/25	0.87	0.14	80,85,90,95	0
32	M2G	2a	966	25/26	0.88	0.15	64,73,81,89	0
32	7MG	2a	527	24/25	0.89	0.13	53,61,67,69	0
32	5MC	2a	967	21/22	0.89	0.12	71,75,79,86	0
1	PSU	1A	1917	20/21	0.90	0.10	59,64,70,76	0
32	2MG	1a	1207	24/25	0.90	0.11	60,70,74,76	0
32	5MC	2a	1404	21/22	0.91	0.12	59,64,70,78	0
1	PSU	1A	1911	20/21	0.92	0.09	50,59,63,64	0
32	4OC	2a	1402	22/23	0.92	0.13	53,63,68,75	0
32	5MC	2a	1400	21/22	0.93	0.12	66,71,75,80	0
32	5MC	2a	1407	21/22	0.93	0.10	54,62,65,77	0
32	MA6	2a	1518	24/25	0.93	0.10	53,63,66,68	0
32	PSU	1a	516	20/21	0.93	0.10	51,60,64,64	0
1	4OC	2A	1920	21/23	0.94	0.08	58,66,69,71	0
32	UR3	2a	1498	21/22	0.94	0.10	54,58,66,67	0
32	5MC	1a	967	21/22	0.94	0.10	55,62,70,73	0
32	MA6	2a	1519	24/25	0.94	0.13	54,60,64,66	0
32	7MG	1a	527	24/25	0.94	0.10	39,47,53,55	0
32	M2G	1a	966	25/26	0.95	0.10	51,56,62,65	0
1	5MC	2A	1942	21/22	0.95	0.09	41,48,53,59	0
32	5MC	1a	1407	21/22	0.95	0.11	34,42,49,50	0
32	4OC	1a	1402	22/23	0.96	0.10	40,46,48,58	0
1	5MC	2A	1962	21/22	0.96	0.09	36,40,49,56	0
1	PSU	2A	2605	20/21	0.96	0.08	28,33,39,44	0
32	5MC	1a	1404	21/22	0.96	0.09	39,42,49,50	0
1	4OC	1A	1920	21/23	0.96	0.10	35,54,58,62	0
32	MA6	1a	1518	24/25	0.96	0.10	33,40,46,51	0
32	MA6	1a	1519	24/25	0.96	0.10	35,41,48,53	0
1	5MU	2A	1939	21/22	0.96	0.08	28,34,36,37	0
1	2MA	2A	2503	23/24	0.97	0.08	24,29,34,35	0
1	2MU	2A	2552	21/23	0.97	0.07	28,33,36,40	0
32	5MC	1a	1400	21/22	0.97	0.08	34,48,52,54	0
1	5MC	1A	1962	21/22	0.97	0.07	27,33,36,40	0
1	5MU	1A	1939	21/22	0.97	0.07	17,23,25,27	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
1	5MC	1A	1942	21/22	0.97	0.07	24,30,34,37	0
32	UR3	1a	1498	21/22	0.97	0.09	36,42,45,55	0
1	OMG	2A	2251	24/25	0.97	0.08	28,34,39,40	0
1	2MA	1A	2503	23/24	0.98	0.06	11,15,18,19	0
1	2MU	1A	2552	21/23	0.98	0.06	24,27,31,32	0
1	PSU	1A	2605	20/21	0.98	0.06	20,25,28,30	0
1	OMG	1A	2251	24/25	0.98	0.06	14,19,20,20	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	2B	211	1/1	0.43	0.24	78,78,78,78	0
54	MG	1a	3203	1/1	0.48	0.22	69,69,69,69	0
54	MG	1A	4003	1/1	0.49	0.19	31,31,31,31	0
54	MG	1B	225	1/1	0.53	0.15	53,53,53,53	0
54	MG	2A	3574	1/1	0.55	0.17	71,71,71,71	0
54	MG	2a	3025	1/1	0.56	0.25	74,74,74,74	0
54	MG	2A	3646	1/1	0.57	0.24	76,76,76,76	0
54	MG	2A	3726	1/1	0.57	0.18	55,55,55,55	0
54	MG	1A	3936	1/1	0.59	0.20	30,30,30,30	0
54	MG	1g	202	1/1	0.60	0.16	78,78,78,78	0
54	MG	2A	3394	1/1	0.61	0.22	47,47,47,47	0
54	MG	2A	3428	1/1	0.63	0.14	81,81,81,81	0
54	MG	1P	203	1/1	0.63	0.47	49,49,49,49	0
57	ARG	1F	316	12/12	0.63	0.20	54,60,69,71	0
54	MG	1A	3872	1/1	0.64	0.17	72,72,72,72	0
54	MG	1a	3156	1/1	0.64	0.15	60,60,60,60	0
56	MPD	2B	220	8/8	0.64	0.24	60,65,71,80	0
54	MG	1B	226	1/1	0.64	0.16	60,60,60,60	0
54	MG	1A	3308	1/1	0.65	0.22	82,82,82,82	0
54	MG	2a	3105	1/1	0.65	0.28	80,80,80,80	0
54	MG	2a	3099	1/1	0.66	0.24	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	2V	201	1/1	0.66	0.17	70,70,70,70	0
54	MG	2a	3183	1/1	0.67	0.13	88,88,88,88	0
54	MG	1A	3380	1/1	0.67	0.15	31,31,31,31	0
54	MG	2A	3449	1/1	0.67	0.22	64,64,64,64	0
54	MG	1B	210	1/1	0.68	0.13	49,49,49,49	0
54	MG	2B	206	1/1	0.68	0.21	78,78,78,78	0
54	MG	1A	3534	1/1	0.68	0.16	53,53,53,53	0
54	MG	2a	3100	1/1	0.68	0.20	80,80,80,80	0
54	MG	1a	3001	1/1	0.69	0.26	77,77,77,77	0
54	MG	1D	310	1/1	0.69	0.24	33,33,33,33	0
54	MG	2A	3456	1/1	0.69	0.17	62,62,62,62	0
54	MG	1a	3192	1/1	0.69	0.25	68,68,68,68	0
54	MG	2a	3051	1/1	0.70	0.17	79,79,79,79	0
54	MG	2a	3061	1/1	0.70	0.26	75,75,75,75	0
54	MG	2A	3488	1/1	0.70	0.17	65,65,65,65	0
54	MG	1A	3714	1/1	0.70	0.17	50,50,50,50	0
54	MG	1a	3022	1/1	0.71	0.23	59,59,59,59	0
54	MG	2A	3279	1/1	0.71	0.27	71,71,71,71	0
54	MG	1A	3517	1/1	0.71	0.11	35,35,35,35	0
54	MG	1A	3354	1/1	0.71	0.15	52,52,52,52	0
54	MG	1A	3448	1/1	0.71	0.16	28,28,28,28	0
54	MG	2A	3746	1/1	0.71	0.11	71,71,71,71	0
54	MG	2A	3289	1/1	0.72	0.20	75,75,75,75	0
54	MG	1A	3041	1/1	0.72	0.20	57,57,57,57	0
54	MG	2a	3020	1/1	0.72	0.27	72,72,72,72	0
54	MG	2A	3475	1/1	0.72	0.21	57,57,57,57	0
54	MG	1A	3887	1/1	0.72	0.17	61,61,61,61	0
54	MG	2A	3524	1/1	0.72	0.21	43,43,43,43	0
54	MG	2A	3581	1/1	0.73	0.16	36,36,36,36	0
54	MG	2A	3629	1/1	0.73	0.19	43,43,43,43	0
54	MG	1A	3034	1/1	0.73	0.33	57,57,57,57	0
54	MG	2A	3228	1/1	0.73	0.14	52,52,52,52	0
54	MG	2A	3509	1/1	0.73	0.16	51,51,51,51	0
54	MG	2A	3512	1/1	0.73	0.16	72,72,72,72	0
54	MG	1a	3195	1/1	0.73	0.15	62,62,62,62	0
54	MG	2G	201	1/1	0.73	0.15	78,78,78,78	0
54	MG	2O	202	1/1	0.73	0.13	63,63,63,63	0
54	MG	1A	4021	1/1	0.73	0.20	43,43,43,43	0
54	MG	1A	3604	1/1	0.74	0.14	25,25,25,25	0
54	MG	1A	3321	1/1	0.74	0.26	63,63,63,63	0
54	MG	1A	3984	1/1	0.74	0.12	51,51,51,51	0
54	MG	2A	3464	1/1	0.74	0.16	44,44,44,44	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	1A	3458	1/1	0.74	0.14	47,47,47,47	0
54	MG	1a	3225	1/1	0.74	0.26	67,67,67,67	0
54	MG	2A	3724	1/1	0.74	0.12	58,58,58,58	0
54	MG	2A	3397	1/1	0.74	0.16	40,40,40,40	0
54	MG	1a	3165	1/1	0.75	0.23	59,59,59,59	0
54	MG	1a	3242	1/1	0.75	0.22	70,70,70,70	0
54	MG	1A	3698	1/1	0.75	0.11	76,76,76,76	0
54	MG	1a	3119	1/1	0.75	0.15	49,49,49,49	0
54	MG	1A	3697	1/1	0.75	0.12	64,64,64,64	0
54	MG	2a	3064	1/1	0.75	0.28	73,73,73,73	0
54	MG	2B	202	1/1	0.75	0.14	70,70,70,70	0
54	MG	2A	3533	1/1	0.75	0.29	65,65,65,65	0
54	MG	1a	3224	1/1	0.75	0.13	64,64,64,64	0
54	MG	2E	304	1/1	0.75	0.16	26,26,26,26	0
54	MG	2a	3196	1/1	0.75	0.17	68,68,68,68	0
54	MG	2j	201	1/1	0.75	0.11	65,65,65,65	0
54	MG	2A	3577	1/1	0.75	0.17	30,30,30,30	0
54	MG	2A	3474	1/1	0.75	0.13	60,60,60,60	0
54	MG	1a	3201	1/1	0.76	0.12	73,73,73,73	0
54	MG	2A	3627	1/1	0.76	0.15	34,34,34,34	0
54	MG	2A	3050	1/1	0.76	0.16	58,58,58,58	0
54	MG	1A	4051	1/1	0.76	0.21	38,38,38,38	0
54	MG	2G	203	1/1	0.76	0.18	72,72,72,72	0
54	MG	2A	3709	1/1	0.76	0.27	70,70,70,70	0
54	MG	1A	4015	1/1	0.76	0.38	47,47,47,47	0
54	MG	2A	3286	1/1	0.76	0.15	54,54,54,54	0
54	MG	1A	3658	1/1	0.76	0.10	56,56,56,56	0
54	MG	1a	3120	1/1	0.76	0.15	82,82,82,82	0
58	ZN	14	102	1/1	0.76	0.19	139,139,139,139	0
54	MG	2A	3565	1/1	0.77	0.23	60,60,60,60	0
54	MG	2A	3566	1/1	0.77	0.21	84,84,84,84	0
54	MG	1A	3781	1/1	0.77	0.15	22,22,22,22	0
54	MG	2A	3423	1/1	0.77	0.40	69,69,69,69	0
54	MG	1a	3189	1/1	0.77	0.11	64,64,64,64	0
54	MG	2a	3028	1/1	0.77	0.20	71,71,71,71	0
54	MG	2A	3033	1/1	0.77	0.13	58,58,58,58	0
54	MG	1a	3057	1/1	0.77	0.17	75,75,75,75	0
54	MG	2A	3114	1/1	0.77	0.13	60,60,60,60	0
54	MG	1a	3068	1/1	0.77	0.20	64,64,64,64	0
54	MG	2A	3242	1/1	0.77	0.29	66,66,66,66	0
54	MG	2A	3247	1/1	0.77	0.15	64,64,64,64	0
54	MG	2a	3129	1/1	0.77	0.45	79,79,79,79	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	1A	3843	1/1	0.77	0.13	31,31,31,31	0
54	MG	1A	3176	1/1	0.77	0.15	59,59,59,59	0
54	MG	2A	3518	1/1	0.77	0.13	67,67,67,67	0
54	MG	1A	3741	1/1	0.77	0.13	36,36,36,36	0
54	MG	1a	3162	1/1	0.77	0.23	64,64,64,64	0
54	MG	2A	3538	1/1	0.77	0.24	67,67,67,67	0
54	MG	2A	3429	1/1	0.78	0.19	44,44,44,44	0
54	MG	1A	3636	1/1	0.78	0.11	25,25,25,25	0
54	MG	1T	201	1/1	0.78	0.24	55,55,55,55	0
54	MG	2A	3346	1/1	0.78	0.14	52,52,52,52	0
54	MG	1a	3247	1/1	0.78	0.13	62,62,62,62	0
54	MG	1a	3276	1/1	0.78	0.10	68,68,68,68	0
54	MG	1a	3138	1/1	0.78	0.19	52,52,52,52	0
54	MG	2a	3096	1/1	0.78	0.21	71,71,71,71	0
54	MG	1A	3383	1/1	0.78	0.11	28,28,28,28	0
54	MG	1a	3042	1/1	0.79	0.21	62,62,62,62	0
54	MG	1a	3151	1/1	0.79	0.22	73,73,73,73	0
54	MG	2A	3525	1/1	0.79	0.17	62,62,62,62	0
54	MG	2G	202	1/1	0.79	0.23	67,67,67,67	0
54	MG	2A	3528	1/1	0.79	0.15	39,39,39,39	0
54	MG	2a	3107	1/1	0.79	0.13	69,69,69,69	0
54	MG	2a	3111	1/1	0.79	0.26	55,55,55,55	0
54	MG	2a	3122	1/1	0.79	0.09	67,67,67,67	0
54	MG	2A	3691	1/1	0.79	0.13	63,63,63,63	0
54	MG	2a	3133	1/1	0.79	0.19	60,60,60,60	0
54	MG	2a	3182	1/1	0.79	0.18	74,74,74,74	0
54	MG	2A	3377	1/1	0.79	0.13	63,63,63,63	0
54	MG	1A	3569	1/1	0.79	0.21	34,34,34,34	0
54	MG	14	101	1/1	0.79	0.10	71,71,71,71	0
54	MG	2A	3256	1/1	0.79	0.10	61,61,61,61	0
54	MG	1A	3723	1/1	0.79	0.14	54,54,54,54	0
54	MG	1A	3533	1/1	0.79	0.14	19,19,19,19	0
54	MG	2A	3458	1/1	0.80	0.26	55,55,55,55	0
54	MG	1y	201	1/1	0.80	0.12	62,62,62,62	0
54	MG	2A	3471	1/1	0.80	0.14	68,68,68,68	0
54	MG	1A	3716	1/1	0.80	0.21	42,42,42,42	0
54	MG	1G	201	1/1	0.80	0.12	70,70,70,70	0
54	MG	2a	3072	1/1	0.80	0.10	61,61,61,61	0
54	MG	1A	3417	1/1	0.80	0.17	20,20,20,20	0
54	MG	2A	3349	1/1	0.80	0.24	57,57,57,57	0
54	MG	2A	3127	1/1	0.80	0.18	60,60,60,60	0
54	MG	2A	3730	1/1	0.80	0.45	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	3146	1/1	0.80	0.18	52,52,52,52	0
54	MG	2A	3203	1/1	0.80	0.12	59,59,59,59	0
54	MG	2a	3119	1/1	0.80	0.17	61,61,61,61	0
54	MG	2A	3401	1/1	0.80	0.19	74,74,74,74	0
54	MG	1A	3421	1/1	0.80	0.22	43,43,43,43	0
54	MG	1a	3271	1/1	0.80	0.10	60,60,60,60	0
54	MG	1A	3594	1/1	0.80	0.11	31,31,31,31	0
54	MG	2A	3548	1/1	0.80	0.14	34,34,34,34	0
54	MG	2A	3431	1/1	0.80	0.11	74,74,74,74	0
54	MG	2A	3441	1/1	0.80	0.18	51,51,51,51	0
54	MG	1a	3095	1/1	0.80	0.14	60,60,60,60	0
54	MG	2X	101	1/1	0.80	0.14	59,59,59,59	0
54	MG	2A	3265	1/1	0.80	0.11	66,66,66,66	0
54	MG	1A	3592	1/1	0.81	0.12	52,52,52,52	0
54	MG	1A	3499	1/1	0.81	0.13	37,37,37,37	0
54	MG	1A	3927	1/1	0.81	0.09	15,15,15,15	0
54	MG	1a	3107	1/1	0.81	0.19	63,63,63,63	0
54	MG	2a	3073	1/1	0.81	0.14	67,67,67,67	0
54	MG	2a	3091	1/1	0.81	0.25	59,59,59,59	0
54	MG	1a	3116	1/1	0.81	0.18	54,54,54,54	0
54	MG	1A	3598	1/1	0.81	0.35	34,34,34,34	0
54	MG	1A	3970	1/1	0.81	0.12	43,43,43,43	0
54	MG	1A	3721	1/1	0.81	0.26	41,41,41,41	0
54	MG	2B	204	1/1	0.81	0.17	76,76,76,76	0
54	MG	1A	3326	1/1	0.81	0.10	48,48,48,48	0
54	MG	1A	4007	1/1	0.81	0.14	73,73,73,73	0
54	MG	2A	3285	1/1	0.81	0.13	50,50,50,50	0
54	MG	1A	3330	1/1	0.81	0.11	34,34,34,34	0
54	MG	2A	3459	1/1	0.81	0.14	53,53,53,53	0
54	MG	2a	3177	1/1	0.81	0.12	69,69,69,69	0
54	MG	1A	3183	1/1	0.81	0.28	32,32,32,32	0
54	MG	1a	3175	1/1	0.81	0.16	54,54,54,54	0
54	MG	2A	3602	1/1	0.81	0.12	38,38,38,38	0
54	MG	2a	3199	1/1	0.81	0.10	73,73,73,73	0
54	MG	2A	3618	1/1	0.81	0.12	64,64,64,64	0
54	MG	2A	3620	1/1	0.81	0.10	28,28,28,28	0
54	MG	1A	3496	1/1	0.81	0.12	22,22,22,22	0
54	MG	2A	3352	1/1	0.81	0.14	33,33,33,33	0
54	MG	2A	3532	1/1	0.82	0.10	56,56,56,56	0
54	MG	1A	3953	1/1	0.82	0.12	52,52,52,52	0
54	MG	2A	3409	1/1	0.82	0.11	62,62,62,62	0
54	MG	2A	3169	1/1	0.82	0.17	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	2A	3559	1/1	0.82	0.11	57,57,57,57	0
54	MG	1A	3780	1/1	0.82	0.15	42,42,42,42	0
54	MG	23	101	1/1	0.82	0.26	57,57,57,57	0
54	MG	2a	3003	1/1	0.82	0.08	51,51,51,51	0
54	MG	2a	3011	1/1	0.82	0.20	73,73,73,73	0
54	MG	1A	3982	1/1	0.82	0.16	40,40,40,40	0
54	MG	1G	202	1/1	0.82	0.09	61,61,61,61	0
54	MG	1A	3027	1/1	0.82	0.15	64,64,64,64	0
54	MG	1a	3137	1/1	0.82	0.27	64,64,64,64	0
54	MG	2A	3584	1/1	0.82	0.19	57,57,57,57	0
54	MG	1A	3688	1/1	0.82	0.15	45,45,45,45	0
54	MG	1a	3143	1/1	0.82	0.11	49,49,49,49	0
54	MG	1A	3851	1/1	0.82	0.12	24,24,24,24	0
54	MG	2A	3621	1/1	0.82	0.17	47,47,47,47	0
54	MG	2A	3463	1/1	0.82	0.14	64,64,64,64	0
54	MG	1A	3864	1/1	0.82	0.17	38,38,38,38	0
54	MG	2A	3635	1/1	0.82	0.18	40,40,40,40	0
54	MG	2A	3467	1/1	0.82	0.14	38,38,38,38	0
54	MG	2A	3675	1/1	0.82	0.13	49,49,49,49	0
54	MG	1a	3161	1/1	0.82	0.15	70,70,70,70	0
54	MG	2A	3313	1/1	0.82	0.10	53,53,53,53	0
54	MG	2A	3341	1/1	0.82	0.13	36,36,36,36	0
54	MG	1A	3689	1/1	0.82	0.30	31,31,31,31	0
54	MG	2A	3503	1/1	0.82	0.22	76,76,76,76	0
54	MG	2A	3736	1/1	0.82	0.21	65,65,65,65	0
54	MG	1A	3632	1/1	0.82	0.12	52,52,52,52	0
54	MG	1A	3075	1/1	0.82	0.41	49,49,49,49	0
54	MG	2A	3368	1/1	0.82	0.17	63,63,63,63	0
54	MG	2A	3065	1/1	0.82	0.09	41,41,41,41	0
54	MG	2B	207	1/1	0.82	0.19	63,63,63,63	0
54	MG	1a	3183	1/1	0.82	0.10	65,65,65,65	0
54	MG	2B	215	1/1	0.82	0.12	74,74,74,74	0
54	MG	1A	3762	1/1	0.82	0.13	51,51,51,51	0
54	MG	1a	3149	1/1	0.83	0.18	64,64,64,64	0
54	MG	1A	3609	1/1	0.83	0.11	26,26,26,26	0
54	MG	1a	3272	1/1	0.83	0.15	60,60,60,60	0
54	MG	1a	3274	1/1	0.83	0.12	58,58,58,58	0
54	MG	1A	3545	1/1	0.83	0.14	50,50,50,50	0
54	MG	1A	3694	1/1	0.83	0.14	59,59,59,59	0
54	MG	2A	3492	1/1	0.83	0.10	23,23,23,23	0
54	MG	1A	3846	1/1	0.83	0.15	39,39,39,39	0
54	MG	1y	202	1/1	0.83	0.12	53,53,53,53	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	1A	3572	1/1	0.83	0.14	43,43,43,43	0
54	MG	1a	3098	1/1	0.83	0.18	43,43,43,43	0
54	MG	2A	3064	1/1	0.83	0.15	69,69,69,69	0
54	MG	1A	3852	1/1	0.83	0.12	42,42,42,42	0
54	MG	2A	3733	1/1	0.83	0.13	82,82,82,82	0
54	MG	1a	3109	1/1	0.83	0.13	41,41,41,41	0
54	MG	1A	3562	1/1	0.83	0.11	22,22,22,22	0
54	MG	1A	3752	1/1	0.83	0.17	53,53,53,53	0
54	MG	2a	3109	1/1	0.83	0.19	63,63,63,63	0
54	MG	2A	3537	1/1	0.83	0.25	65,65,65,65	0
54	MG	2A	3157	1/1	0.83	0.12	40,40,40,40	0
54	MG	1a	3198	1/1	0.83	0.14	73,73,73,73	0
54	MG	1A	3875	1/1	0.83	0.11	47,47,47,47	0
54	MG	1a	3127	1/1	0.83	0.16	65,65,65,65	0
54	MG	2a	3172	1/1	0.83	0.12	68,68,68,68	0
54	MG	2D	309	1/1	0.83	0.10	58,58,58,58	0
54	MG	1A	3706	1/1	0.83	0.14	62,62,62,62	0
54	MG	2A	3452	1/1	0.83	0.14	74,74,74,74	0
54	MG	1A	4048	1/1	0.83	0.28	58,58,58,58	0
54	MG	1a	3228	1/1	0.83	0.13	75,75,75,75	0
54	MG	1a	3240	1/1	0.83	0.28	70,70,70,70	0
54	MG	2A	3591	1/1	0.83	0.22	65,65,65,65	0
54	MG	1a	3013	1/1	0.83	0.11	69,69,69,69	0
54	MG	2I	102	1/1	0.83	0.09	63,63,63,63	0
54	MG	2A	3380	1/1	0.84	0.12	28,28,28,28	0
54	MG	2I	201	1/1	0.84	0.14	66,66,66,66	0
54	MG	2A	3385	1/1	0.84	0.10	70,70,70,70	0
54	MG	2A	3039	1/1	0.84	0.35	66,66,66,66	0
54	MG	1A	3995	1/1	0.84	0.15	44,44,44,44	0
54	MG	1A	4000	1/1	0.84	0.20	67,67,67,67	0
54	MG	2A	3405	1/1	0.84	0.12	54,54,54,54	0
54	MG	1a	3193	1/1	0.84	0.16	72,72,72,72	0
54	MG	1A	3530	1/1	0.84	0.13	14,14,14,14	0
54	MG	1a	3118	1/1	0.84	0.16	55,55,55,55	0
54	MG	1A	3898	1/1	0.84	0.14	33,33,33,33	0
54	MG	2A	3150	1/1	0.84	0.25	66,66,66,66	0
54	MG	2a	3041	1/1	0.84	0.13	60,60,60,60	0
54	MG	2A	3607	1/1	0.84	0.12	56,56,56,56	0
54	MG	2a	3055	1/1	0.84	0.25	68,68,68,68	0
54	MG	2A	3154	1/1	0.84	0.22	64,64,64,64	0
54	MG	2A	3448	1/1	0.84	0.16	46,46,46,46	0
54	MG	2a	3070	1/1	0.84	0.19	63,63,63,63	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	1A	3922	1/1	0.84	0.10	19,19,19,19	0
54	MG	2A	3163	1/1	0.84	0.26	68,68,68,68	0
54	MG	2a	3074	1/1	0.84	0.18	66,66,66,66	0
54	MG	1A	3692	1/1	0.84	0.13	46,46,46,46	0
54	MG	1A	4029	1/1	0.84	0.20	43,43,43,43	0
54	MG	2A	3205	1/1	0.84	0.11	56,56,56,56	0
54	MG	2A	3460	1/1	0.84	0.23	55,55,55,55	0
54	MG	2A	3213	1/1	0.84	0.36	65,65,65,65	0
54	MG	2A	3227	1/1	0.84	0.10	52,52,52,52	0
54	MG	1A	4032	1/1	0.84	0.22	58,58,58,58	0
54	MG	1a	3017	1/1	0.84	0.11	60,60,60,60	0
54	MG	1A	4035	1/1	0.84	0.14	43,43,43,43	0
54	MG	1A	3642	1/1	0.84	0.13	55,55,55,55	0
54	MG	1a	3153	1/1	0.84	0.13	60,60,60,60	0
54	MG	2a	3132	1/1	0.84	0.11	53,53,53,53	0
54	MG	1A	3861	1/1	0.84	0.10	50,50,50,50	0
54	MG	2a	3137	1/1	0.84	0.12	46,46,46,46	0
54	MG	1a	3065	1/1	0.84	0.20	60,60,60,60	0
54	MG	1A	3387	1/1	0.84	0.16	42,42,42,42	0
54	MG	1a	3071	1/1	0.84	0.17	62,62,62,62	0
54	MG	1l	202	1/1	0.84	0.12	59,59,59,59	0
54	MG	1t	201	1/1	0.84	0.15	67,67,67,67	0
54	MG	1a	3172	1/1	0.84	0.15	66,66,66,66	0
54	MG	1A	3551	1/1	0.84	0.12	48,48,48,48	0
56	MPD	2A	3759	8/8	0.84	0.25	37,46,50,56	0
54	MG	2A	3025	1/1	0.84	0.14	58,58,58,58	0
54	MG	2A	3032	1/1	0.84	0.15	28,28,28,28	0
54	MG	1A	3735	1/1	0.84	0.10	23,23,23,23	0
58	ZN	24	501	1/1	0.84	0.22	156,156,156,156	0
54	MG	1A	3946	1/1	0.85	0.11	45,45,45,45	0
54	MG	1n	102	1/1	0.85	0.11	49,49,49,49	0
54	MG	1A	3238	1/1	0.85	0.14	69,69,69,69	0
54	MG	1A	3968	1/1	0.85	0.14	25,25,25,25	0
54	MG	1A	3791	1/1	0.85	0.13	20,20,20,20	0
54	MG	1A	3977	1/1	0.85	0.10	48,48,48,48	0
54	MG	1A	3978	1/1	0.85	0.11	53,53,53,53	0
54	MG	2A	3544	1/1	0.85	0.15	58,58,58,58	0
54	MG	2A	3547	1/1	0.85	0.20	56,56,56,56	0
54	MG	19	103	1/1	0.85	0.17	82,82,82,82	0
54	MG	2A	3381	1/1	0.85	0.15	58,58,58,58	0
54	MG	1A	3841	1/1	0.85	0.34	43,43,43,43	0
54	MG	2A	3393	1/1	0.85	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	3168	1/1	0.85	0.23	68,68,68,68	0
54	MG	2a	3035	1/1	0.85	0.17	50,50,50,50	0
54	MG	2a	3040	1/1	0.85	0.17	50,50,50,50	0
54	MG	1A	3069	1/1	0.85	0.34	25,25,25,25	0
54	MG	1A	3985	1/1	0.85	0.10	28,28,28,28	0
54	MG	1A	3318	1/1	0.85	0.13	36,36,36,36	0
54	MG	2A	3585	1/1	0.85	0.15	46,46,46,46	0
54	MG	1a	3186	1/1	0.85	0.12	64,64,64,64	0
54	MG	2a	3068	1/1	0.85	0.20	72,72,72,72	0
54	MG	2A	3415	1/1	0.85	0.11	63,63,63,63	0
54	MG	2A	3131	1/1	0.85	0.34	61,61,61,61	0
54	MG	1A	3480	1/1	0.85	0.12	37,37,37,37	0
54	MG	1A	3623	1/1	0.85	0.22	33,33,33,33	0
54	MG	2a	3082	1/1	0.85	0.09	68,68,68,68	0
54	MG	2a	3087	1/1	0.85	0.18	57,57,57,57	0
54	MG	2A	3430	1/1	0.85	0.15	51,51,51,51	0
54	MG	1a	3062	1/1	0.85	0.23	71,71,71,71	0
54	MG	1A	3484	1/1	0.85	0.14	48,48,48,48	0
54	MG	1A	3319	1/1	0.85	0.10	63,63,63,63	0
54	MG	1A	3871	1/1	0.85	0.14	19,19,19,19	0
54	MG	2A	3171	1/1	0.85	0.13	50,50,50,50	0
54	MG	1A	3056	1/1	0.85	0.15	55,55,55,55	0
54	MG	2A	3705	1/1	0.85	0.12	39,39,39,39	0
54	MG	1A	3648	1/1	0.85	0.09	33,33,33,33	0
54	MG	1a	3102	1/1	0.85	0.22	66,66,66,66	0
54	MG	1A	3503	1/1	0.85	0.14	15,15,15,15	0
54	MG	1a	3235	1/1	0.85	0.12	57,57,57,57	0
54	MG	2A	3235	1/1	0.85	0.18	50,50,50,50	0
54	MG	1A	3662	1/1	0.85	0.11	27,27,27,27	0
54	MG	2a	3165	1/1	0.85	0.15	76,76,76,76	0
54	MG	1A	3674	1/1	0.85	0.11	25,25,25,25	0
54	MG	1B	202	1/1	0.85	0.18	58,58,58,58	0
54	MG	1B	207	1/1	0.85	0.08	51,51,51,51	0
54	MG	2B	205	1/1	0.85	0.14	59,59,59,59	0
54	MG	2a	3191	1/1	0.85	0.11	75,75,75,75	0
54	MG	2a	3195	1/1	0.85	0.10	71,71,71,71	0
54	MG	1A	3576	1/1	0.85	0.11	53,53,53,53	0
54	MG	1B	224	1/1	0.85	0.10	64,64,64,64	0
54	MG	1A	3930	1/1	0.85	0.14	39,39,39,39	0
54	MG	1A	3217	1/1	0.85	0.31	57,57,57,57	0
56	MPD	2A	3760	8/8	0.85	0.20	54,60,63,69	0
54	MG	2D	301	1/1	0.85	0.25	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	2D	303	1/1	0.85	0.19	48,48,48,48	0
54	MG	2A	3294	1/1	0.85	0.20	24,24,24,24	0
54	MG	2A	3310	1/1	0.85	0.11	37,37,37,37	0
54	MG	1a	3131	1/1	0.86	0.13	62,62,62,62	0
54	MG	20	102	1/1	0.86	0.12	54,54,54,54	0
54	MG	1A	3247	1/1	0.86	0.11	35,35,35,35	0
54	MG	2A	3424	1/1	0.86	0.12	61,61,61,61	0
54	MG	1a	3007	1/1	0.86	0.14	55,55,55,55	0
54	MG	1A	3942	1/1	0.86	0.15	52,52,52,52	0
54	MG	2a	3019	1/1	0.86	0.12	51,51,51,51	0
54	MG	1A	3429	1/1	0.86	0.14	58,58,58,58	0
54	MG	2a	3022	1/1	0.86	0.24	52,52,52,52	0
54	MG	1A	3438	1/1	0.86	0.14	21,21,21,21	0
54	MG	1a	3025	1/1	0.86	0.13	44,44,44,44	0
54	MG	1A	3067	1/1	0.86	0.17	35,35,35,35	0
54	MG	1d	304	1/1	0.86	0.15	46,46,46,46	0
54	MG	1a	3159	1/1	0.86	0.20	64,64,64,64	0
54	MG	2a	3043	1/1	0.86	0.17	59,59,59,59	0
54	MG	2a	3046	1/1	0.86	0.11	62,62,62,62	0
54	MG	2A	3250	1/1	0.86	0.08	49,49,49,49	0
54	MG	1B	201	1/1	0.86	0.14	59,59,59,59	0
54	MG	1A	3634	1/1	0.86	0.11	58,58,58,58	0
54	MG	2A	3634	1/1	0.86	0.14	27,27,27,27	0
54	MG	2a	3065	1/1	0.86	0.23	58,58,58,58	0
54	MG	1A	3751	1/1	0.86	0.14	43,43,43,43	0
54	MG	1A	3154	1/1	0.86	0.24	35,35,35,35	0
54	MG	2A	3667	1/1	0.86	0.11	58,58,58,58	0
54	MG	2A	3669	1/1	0.86	0.09	44,44,44,44	0
54	MG	1A	3476	1/1	0.86	0.12	12,12,12,12	0
54	MG	2A	3678	1/1	0.86	0.13	29,29,29,29	0
54	MG	1a	3082	1/1	0.86	0.33	63,63,63,63	0
54	MG	2A	3695	1/1	0.86	0.12	59,59,59,59	0
54	MG	2A	3290	1/1	0.86	0.17	36,36,36,36	0
54	MG	2A	3027	1/1	0.86	0.17	46,46,46,46	0
54	MG	2A	3716	1/1	0.86	0.15	61,61,61,61	0
54	MG	2A	3296	1/1	0.86	0.16	40,40,40,40	0
54	MG	2A	3479	1/1	0.86	0.16	47,47,47,47	0
54	MG	1a	3088	1/1	0.86	0.11	58,58,58,58	0
54	MG	1A	3773	1/1	0.86	0.15	64,64,64,64	0
54	MG	2A	3332	1/1	0.86	0.12	48,48,48,48	0
54	MG	1A	3412	1/1	0.86	0.12	40,40,40,40	0
54	MG	2A	3749	1/1	0.86	0.13	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	3879	1/1	0.86	0.17	31,31,31,31	0
54	MG	1a	3103	1/1	0.86	0.12	57,57,57,57	0
54	MG	1A	3652	1/1	0.86	0.36	40,40,40,40	0
54	MG	2A	3107	1/1	0.86	0.14	58,58,58,58	0
54	MG	2A	3526	1/1	0.86	0.14	45,45,45,45	0
54	MG	1A	4001	1/1	0.86	0.11	67,67,67,67	0
54	MG	1A	3788	1/1	0.86	0.11	37,37,37,37	0
54	MG	1a	3202	1/1	0.86	0.07	70,70,70,70	0
54	MG	1A	3239	1/1	0.86	0.23	56,56,56,56	0
54	MG	1a	3222	1/1	0.86	0.16	51,51,51,51	0
54	MG	2D	310	1/1	0.86	0.17	41,41,41,41	0
54	MG	2D	311	1/1	0.86	0.10	33,33,33,33	0
54	MG	2A	3152	1/1	0.86	0.18	55,55,55,55	0
56	MPD	1T	207	8/8	0.86	0.24	69,71,74,77	0
54	MG	1A	3812	1/1	0.86	0.16	59,59,59,59	0
54	MG	19	101	1/1	0.86	0.12	57,57,57,57	0
54	MG	2A	3558	1/1	0.86	0.09	56,56,56,56	0
54	MG	1A	3814	1/1	0.86	0.10	36,36,36,36	0
54	MG	2A	3560	1/1	0.86	0.09	66,66,66,66	0
54	MG	2A	3167	1/1	0.86	0.32	56,56,56,56	0
54	MG	1A	3807	1/1	0.87	0.08	29,29,29,29	0
54	MG	2a	3010	1/1	0.87	0.28	66,66,66,66	0
54	MG	2A	3257	1/1	0.87	0.10	54,54,54,54	0
54	MG	1A	3904	1/1	0.87	0.14	49,49,49,49	0
54	MG	2A	3002	1/1	0.87	0.15	44,44,44,44	0
54	MG	1a	3072	1/1	0.87	0.24	64,64,64,64	0
54	MG	1A	3725	1/1	0.87	0.15	69,69,69,69	0
54	MG	1A	3391	1/1	0.87	0.10	31,31,31,31	0
54	MG	1A	3825	1/1	0.87	0.26	25,25,25,25	0
54	MG	2A	3647	1/1	0.87	0.10	65,65,65,65	0
54	MG	10	102	1/1	0.87	0.09	38,38,38,38	0
54	MG	10	103	1/1	0.87	0.12	50,50,50,50	0
54	MG	2A	3671	1/1	0.87	0.10	72,72,72,72	0
54	MG	11	105	1/1	0.87	0.13	46,46,46,46	0
54	MG	2A	3676	1/1	0.87	0.10	72,72,72,72	0
54	MG	1A	3737	1/1	0.87	0.09	36,36,36,36	0
54	MG	2A	3682	1/1	0.87	0.08	21,21,21,21	0
54	MG	2A	3485	1/1	0.87	0.08	62,62,62,62	0
54	MG	2A	3074	1/1	0.87	0.07	51,51,51,51	0
54	MG	2a	3069	1/1	0.87	0.11	74,74,74,74	0
54	MG	2A	3084	1/1	0.87	0.13	67,67,67,67	0
54	MG	15	101	1/1	0.87	0.18	34,34,34,34	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	1a	3112	1/1	0.87	0.13	69,69,69,69	0
54	MG	15	107	1/1	0.87	0.14	63,63,63,63	0
54	MG	2A	3513	1/1	0.87	0.08	40,40,40,40	0
54	MG	1A	3322	1/1	0.87	0.24	51,51,51,51	0
54	MG	2A	3519	1/1	0.87	0.15	55,55,55,55	0
54	MG	1A	3645	1/1	0.87	0.09	30,30,30,30	0
54	MG	2a	3097	1/1	0.87	0.22	71,71,71,71	0
54	MG	2A	3743	1/1	0.87	0.10	54,54,54,54	0
54	MG	1A	3646	1/1	0.87	0.13	21,21,21,21	0
54	MG	1a	3004	1/1	0.87	0.13	58,58,58,58	0
54	MG	1a	3232	1/1	0.87	0.15	31,31,31,31	0
54	MG	1A	3754	1/1	0.87	0.11	49,49,49,49	0
54	MG	1a	3136	1/1	0.87	0.20	54,54,54,54	0
54	MG	2a	3116	1/1	0.87	0.15	73,73,73,73	0
54	MG	1A	3442	1/1	0.87	0.16	21,21,21,21	0
54	MG	2a	3120	1/1	0.87	0.10	55,55,55,55	0
54	MG	2A	3400	1/1	0.87	0.10	46,46,46,46	0
54	MG	2A	3540	1/1	0.87	0.19	75,75,75,75	0
54	MG	1A	3611	1/1	0.87	0.11	53,53,53,53	0
54	MG	1A	3447	1/1	0.87	0.12	48,48,48,48	0
54	MG	2a	3135	1/1	0.87	0.18	62,62,62,62	0
54	MG	2A	3179	1/1	0.87	0.19	52,52,52,52	0
54	MG	1A	3631	1/1	0.87	0.19	45,45,45,45	0
54	MG	1a	3027	1/1	0.87	0.21	64,64,64,64	0
54	MG	2A	3206	1/1	0.87	0.15	52,52,52,52	0
54	MG	2a	3180	1/1	0.87	0.09	58,58,58,58	0
54	MG	2a	3181	1/1	0.87	0.13	53,53,53,53	0
54	MG	1a	3040	1/1	0.87	0.12	68,68,68,68	0
54	MG	1a	3279	1/1	0.87	0.25	68,68,68,68	0
54	MG	1A	3333	1/1	0.87	0.13	45,45,45,45	0
54	MG	1A	3102	1/1	0.87	0.08	48,48,48,48	0
54	MG	2A	3432	1/1	0.87	0.11	39,39,39,39	0
54	MG	2A	3435	1/1	0.87	0.18	65,65,65,65	0
54	MG	2A	3436	1/1	0.87	0.16	70,70,70,70	0
54	MG	1A	3992	1/1	0.87	0.29	46,46,46,46	0
54	MG	2A	3592	1/1	0.87	0.09	30,30,30,30	0
54	MG	1A	3795	1/1	0.87	0.17	37,37,37,37	0
54	MG	1a	3067	1/1	0.87	0.13	67,67,67,67	0
54	MG	27	102	1/1	0.87	0.29	36,36,36,36	0
54	MG	28	102	1/1	0.87	0.16	52,52,52,52	0
54	MG	2a	3002	1/1	0.87	0.12	54,54,54,54	0
54	MG	2B	217	1/1	0.88	0.10	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	3500	1/1	0.88	0.17	65,65,65,65	0
54	MG	2A	3246	1/1	0.88	0.16	51,51,51,51	0
54	MG	15	102	1/1	0.88	0.31	31,31,31,31	0
54	MG	1A	3143	1/1	0.88	0.22	57,57,57,57	0
54	MG	1A	3886	1/1	0.88	0.11	33,33,33,33	0
54	MG	2A	3514	1/1	0.88	0.09	64,64,64,64	0
54	MG	1a	3129	1/1	0.88	0.15	44,44,44,44	0
54	MG	1b	301	1/1	0.88	0.23	64,64,64,64	0
54	MG	2A	3274	1/1	0.88	0.14	63,63,63,63	0
54	MG	2A	3277	1/1	0.88	0.12	49,49,49,49	0
54	MG	1A	3377	1/1	0.88	0.08	43,43,43,43	0
54	MG	1a	3133	1/1	0.88	0.13	67,67,67,67	0
54	MG	2A	3529	1/1	0.88	0.44	45,45,45,45	0
54	MG	1A	4023	1/1	0.88	0.08	85,85,85,85	0
54	MG	1A	3494	1/1	0.88	0.10	25,25,25,25	0
54	MG	1A	3255	1/1	0.88	0.11	39,39,39,39	0
54	MG	1A	3266	1/1	0.88	0.19	62,62,62,62	0
54	MG	1a	3016	1/1	0.88	0.12	68,68,68,68	0
54	MG	2A	3543	1/1	0.88	0.12	63,63,63,63	0
54	MG	1A	4044	1/1	0.88	0.08	35,35,35,35	0
54	MG	1a	3020	1/1	0.88	0.13	61,61,61,61	0
54	MG	2A	3319	1/1	0.88	0.18	50,50,50,50	0
54	MG	2A	3549	1/1	0.88	0.10	44,44,44,44	0
54	MG	2A	3321	1/1	0.88	0.11	57,57,57,57	0
54	MG	1A	3925	1/1	0.88	0.11	35,35,35,35	0
54	MG	2a	3024	1/1	0.88	0.10	43,43,43,43	0
54	MG	1a	3023	1/1	0.88	0.26	64,64,64,64	0
54	MG	1A	3701	1/1	0.88	0.14	20,20,20,20	0
54	MG	2a	3032	1/1	0.88	0.16	66,66,66,66	0
54	MG	2a	3033	1/1	0.88	0.25	57,57,57,57	0
54	MG	2A	3036	1/1	0.88	0.13	70,70,70,70	0
54	MG	1A	3276	1/1	0.88	0.17	51,51,51,51	0
54	MG	2A	3360	1/1	0.88	0.18	39,39,39,39	0
54	MG	1a	3029	1/1	0.88	0.24	59,59,59,59	0
54	MG	1a	3038	1/1	0.88	0.18	63,63,63,63	0
54	MG	1A	3711	1/1	0.88	0.13	60,60,60,60	0
54	MG	2a	3052	1/1	0.88	0.18	54,54,54,54	0
54	MG	1A	3329	1/1	0.88	0.22	69,69,69,69	0
54	MG	1A	3820	1/1	0.88	0.11	58,58,58,58	0
54	MG	2A	3600	1/1	0.88	0.09	51,51,51,51	0
54	MG	2A	3386	1/1	0.88	0.11	47,47,47,47	0
54	MG	2A	3605	1/1	0.88	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	2A	3092	1/1	0.88	0.08	66,66,66,66	0
54	MG	2A	3093	1/1	0.88	0.29	64,64,64,64	0
54	MG	2A	3104	1/1	0.88	0.24	55,55,55,55	0
54	MG	1B	213	1/1	0.88	0.10	59,59,59,59	0
54	MG	2A	3111	1/1	0.88	0.12	41,41,41,41	0
54	MG	1A	3520	1/1	0.88	0.09	31,31,31,31	0
54	MG	2A	3631	1/1	0.88	0.09	74,74,74,74	0
54	MG	2A	3115	1/1	0.88	0.16	69,69,69,69	0
54	MG	2A	3410	1/1	0.88	0.17	31,31,31,31	0
54	MG	2A	3642	1/1	0.88	0.15	51,51,51,51	0
54	MG	1A	3840	1/1	0.88	0.11	21,21,21,21	0
54	MG	1A	3108	1/1	0.88	0.28	35,35,35,35	0
54	MG	2A	3665	1/1	0.88	0.11	42,42,42,42	0
54	MG	2A	3134	1/1	0.88	0.08	47,47,47,47	0
54	MG	1A	3464	1/1	0.88	0.08	45,45,45,45	0
54	MG	1A	3606	1/1	0.88	0.07	33,33,33,33	0
54	MG	2a	3115	1/1	0.88	0.18	72,72,72,72	0
54	MG	1a	3075	1/1	0.88	0.22	50,50,50,50	0
54	MG	1A	3661	1/1	0.88	0.10	45,45,45,45	0
54	MG	1H	201	1/1	0.88	0.26	62,62,62,62	0
54	MG	1a	3204	1/1	0.88	0.11	47,47,47,47	0
54	MG	1a	3209	1/1	0.88	0.17	57,57,57,57	0
54	MG	1a	3219	1/1	0.88	0.18	70,70,70,70	0
54	MG	2A	3170	1/1	0.88	0.18	59,59,59,59	0
54	MG	1A	3207	1/1	0.88	0.28	39,39,39,39	0
54	MG	1a	3097	1/1	0.88	0.21	55,55,55,55	0
54	MG	2A	3186	1/1	0.88	0.20	57,57,57,57	0
54	MG	2A	3193	1/1	0.88	0.12	59,59,59,59	0
54	MG	2A	3200	1/1	0.88	0.19	50,50,50,50	0
54	MG	1R	204	1/1	0.88	0.14	38,38,38,38	0
54	MG	1A	3855	1/1	0.88	0.09	39,39,39,39	0
54	MG	1T	206	1/1	0.88	0.20	48,48,48,48	0
54	MG	2A	3212	1/1	0.88	0.08	45,45,45,45	0
54	MG	2a	3184	1/1	0.88	0.09	58,58,58,58	0
54	MG	1A	3544	1/1	0.88	0.61	27,27,27,27	0
54	MG	2A	3750	1/1	0.88	0.12	45,45,45,45	0
54	MG	2A	3751	1/1	0.88	0.11	57,57,57,57	0
54	MG	2A	3754	1/1	0.88	0.13	47,47,47,47	0
54	MG	2B	201	1/1	0.88	0.16	73,73,73,73	0
54	MG	1A	3677	1/1	0.88	0.10	36,36,36,36	0
54	MG	1A	3680	1/1	0.88	0.15	63,63,63,63	0
54	MG	1A	3681	1/1	0.88	0.18	25,25,25,25	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	2A	3240	1/1	0.88	0.09	65,65,65,65	0
54	MG	2A	3241	1/1	0.88	0.08	53,53,53,53	0
54	MG	2A	3491	1/1	0.88	0.12	63,63,63,63	0
54	MG	1A	3617	1/1	0.88	0.11	36,36,36,36	0
54	MG	2A	3732	1/1	0.89	0.15	61,61,61,61	0
54	MG	1A	3973	1/1	0.89	0.10	50,50,50,50	0
54	MG	2A	3734	1/1	0.89	0.14	67,67,67,67	0
54	MG	1A	3976	1/1	0.89	0.11	61,61,61,61	0
54	MG	1A	3148	1/1	0.89	0.08	50,50,50,50	0
54	MG	2A	3744	1/1	0.89	0.08	54,54,54,54	0
54	MG	1A	3389	1/1	0.89	0.14	36,36,36,36	0
54	MG	2A	3748	1/1	0.89	0.11	53,53,53,53	0
54	MG	1A	3065	1/1	0.89	0.09	44,44,44,44	0
54	MG	1A	3822	1/1	0.89	0.13	54,54,54,54	0
54	MG	1a	3178	1/1	0.89	0.13	47,47,47,47	0
54	MG	2A	3753	1/1	0.89	0.12	57,57,57,57	0
54	MG	2A	3451	1/1	0.89	0.08	50,50,50,50	0
54	MG	2A	3757	1/1	0.89	0.10	46,46,46,46	0
54	MG	1A	3405	1/1	0.89	0.11	36,36,36,36	0
54	MG	1A	3519	1/1	0.89	0.14	32,32,32,32	0
54	MG	2B	203	1/1	0.89	0.12	61,61,61,61	0
54	MG	1A	3618	1/1	0.89	0.10	28,28,28,28	0
54	MG	2A	3172	1/1	0.89	0.08	53,53,53,53	0
54	MG	1A	3074	1/1	0.89	0.06	37,37,37,37	0
54	MG	2A	3180	1/1	0.89	0.08	58,58,58,58	0
54	MG	1A	3704	1/1	0.89	0.12	52,52,52,52	0
54	MG	2B	212	1/1	0.89	0.10	53,53,53,53	0
54	MG	2B	214	1/1	0.89	0.09	60,60,60,60	0
54	MG	2A	3465	1/1	0.89	0.11	60,60,60,60	0
54	MG	1A	3628	1/1	0.89	0.15	35,35,35,35	0
54	MG	2B	218	1/1	0.89	0.09	56,56,56,56	0
54	MG	2A	3468	1/1	0.89	0.13	65,65,65,65	0
54	MG	2D	302	1/1	0.89	0.39	42,42,42,42	0
54	MG	2A	3196	1/1	0.89	0.20	47,47,47,47	0
54	MG	2A	3197	1/1	0.89	0.19	60,60,60,60	0
54	MG	2A	3199	1/1	0.89	0.09	56,56,56,56	0
54	MG	1a	3196	1/1	0.89	0.09	49,49,49,49	0
54	MG	2D	312	1/1	0.89	0.21	46,46,46,46	0
54	MG	2A	3482	1/1	0.89	0.09	38,38,38,38	0
54	MG	2F	301	1/1	0.89	0.06	40,40,40,40	0
54	MG	1a	3197	1/1	0.89	0.14	60,60,60,60	0
54	MG	1A	3120	1/1	0.89	0.17	31,31,31,31	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	1A	3191	1/1	0.89	0.13	45,45,45,45	0
54	MG	1A	3860	1/1	0.89	0.14	34,34,34,34	0
54	MG	1A	3274	1/1	0.89	0.16	51,51,51,51	0
54	MG	2Q	202	1/1	0.89	0.26	44,44,44,44	0
54	MG	2A	3215	1/1	0.89	0.25	60,60,60,60	0
54	MG	2A	3505	1/1	0.89	0.08	41,41,41,41	0
54	MG	2A	3220	1/1	0.89	0.24	54,54,54,54	0
54	MG	2A	3226	1/1	0.89	0.29	62,62,62,62	0
54	MG	1A	4027	1/1	0.89	0.12	42,42,42,42	0
54	MG	1a	3034	1/1	0.89	0.12	47,47,47,47	0
54	MG	2A	3230	1/1	0.89	0.16	59,59,59,59	0
54	MG	1a	3217	1/1	0.89	0.29	72,72,72,72	0
54	MG	2A	3521	1/1	0.89	0.12	53,53,53,53	0
54	MG	2a	3006	1/1	0.89	0.28	67,67,67,67	0
54	MG	1A	3539	1/1	0.89	0.15	55,55,55,55	0
54	MG	1A	3124	1/1	0.89	0.16	50,50,50,50	0
54	MG	1A	3724	1/1	0.89	0.09	32,32,32,32	0
54	MG	1A	3287	1/1	0.89	0.14	62,62,62,62	0
54	MG	1A	3878	1/1	0.89	0.11	41,41,41,41	0
54	MG	2A	3249	1/1	0.89	0.31	46,46,46,46	0
54	MG	1A	3550	1/1	0.89	0.08	24,24,24,24	0
54	MG	2A	3255	1/1	0.89	0.25	57,57,57,57	0
54	MG	1a	3234	1/1	0.89	0.17	64,64,64,64	0
54	MG	1a	3066	1/1	0.89	0.09	66,66,66,66	0
54	MG	1A	3882	1/1	0.89	0.09	34,34,34,34	0
54	MG	2a	3039	1/1	0.89	0.18	77,77,77,77	0
54	MG	1A	3361	1/1	0.89	0.09	45,45,45,45	0
54	MG	1B	205	1/1	0.89	0.07	40,40,40,40	0
54	MG	1a	3267	1/1	0.89	0.15	54,54,54,54	0
54	MG	1B	206	1/1	0.89	0.24	43,43,43,43	0
54	MG	1A	3739	1/1	0.89	0.10	40,40,40,40	0
54	MG	1a	3078	1/1	0.89	0.15	62,62,62,62	0
54	MG	1B	209	1/1	0.89	0.07	55,55,55,55	0
54	MG	2A	3563	1/1	0.89	0.27	61,61,61,61	0
54	MG	2a	3063	1/1	0.89	0.21	77,77,77,77	0
54	MG	1a	3083	1/1	0.89	0.10	69,69,69,69	0
54	MG	1A	3894	1/1	0.89	0.10	31,31,31,31	0
54	MG	2a	3066	1/1	0.89	0.26	59,59,59,59	0
54	MG	2A	3298	1/1	0.89	0.12	48,48,48,48	0
54	MG	2A	3303	1/1	0.89	0.16	49,49,49,49	0
54	MG	2A	3578	1/1	0.89	0.13	32,32,32,32	0
54	MG	1a	3089	1/1	0.89	0.25	66,66,66,66	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	1a	3093	1/1	0.89	0.13	43,43,43,43	0
54	MG	1A	3364	1/1	0.89	0.09	45,45,45,45	0
54	MG	1A	3374	1/1	0.89	0.12	21,21,21,21	0
54	MG	2A	3326	1/1	0.89	0.11	51,51,51,51	0
54	MG	2a	3089	1/1	0.89	0.19	71,71,71,71	0
54	MG	2A	3597	1/1	0.89	0.09	66,66,66,66	0
54	MG	2A	3329	1/1	0.89	0.13	35,35,35,35	0
54	MG	1o	102	1/1	0.89	0.14	48,48,48,48	0
54	MG	1A	3917	1/1	0.89	0.11	58,58,58,58	0
54	MG	2A	3344	1/1	0.89	0.13	35,35,35,35	0
54	MG	2A	3611	1/1	0.89	0.12	32,32,32,32	0
54	MG	2A	3614	1/1	0.89	0.17	47,47,47,47	0
54	MG	1a	3101	1/1	0.89	0.12	48,48,48,48	0
54	MG	1A	3659	1/1	0.89	0.09	49,49,49,49	0
54	MG	1A	3376	1/1	0.89	0.11	42,42,42,42	0
54	MG	2A	3622	1/1	0.89	0.08	66,66,66,66	0
54	MG	2A	3356	1/1	0.89	0.11	59,59,59,59	0
54	MG	1D	316	1/1	0.89	0.15	41,41,41,41	0
54	MG	2a	3121	1/1	0.89	0.21	68,68,68,68	0
54	MG	2A	3362	1/1	0.89	0.09	30,30,30,30	0
54	MG	1E	306	1/1	0.89	0.11	39,39,39,39	0
54	MG	1F	313	1/1	0.89	0.13	58,58,58,58	0
54	MG	2A	3636	1/1	0.89	0.12	57,57,57,57	0
54	MG	1F	315	1/1	0.89	0.14	60,60,60,60	0
54	MG	1A	3289	1/1	0.89	0.19	64,64,64,64	0
54	MG	2a	3148	1/1	0.89	0.11	63,63,63,63	0
54	MG	2a	3151	1/1	0.89	0.18	74,74,74,74	0
54	MG	1A	3673	1/1	0.89	0.09	40,40,40,40	0
54	MG	2a	3168	1/1	0.89	0.11	49,49,49,49	0
54	MG	2a	3169	1/1	0.89	0.11	45,45,45,45	0
54	MG	1A	3214	1/1	0.89	0.07	37,37,37,37	0
54	MG	2a	3174	1/1	0.89	0.09	59,59,59,59	0
54	MG	1a	3124	1/1	0.89	0.14	64,64,64,64	0
54	MG	1A	3940	1/1	0.89	0.10	50,50,50,50	0
54	MG	1P	205	1/1	0.89	0.10	59,59,59,59	0
54	MG	1R	202	1/1	0.89	0.18	29,29,29,29	0
54	MG	1A	3676	1/1	0.89	0.10	14,14,14,14	0
54	MG	2A	3402	1/1	0.89	0.21	62,62,62,62	0
54	MG	2A	3679	1/1	0.89	0.12	30,30,30,30	0
54	MG	2A	3680	1/1	0.89	0.09	29,29,29,29	0
54	MG	1S	201	1/1	0.89	0.10	54,54,54,54	0
54	MG	2A	3687	1/1	0.89	0.10	66,66,66,66	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	1A	3381	1/1	0.89	0.15	15,15,15,15	0
54	MG	1T	203	1/1	0.89	0.08	55,55,55,55	0
56	MPD	1a	3280	8/8	0.89	0.16	47,64,65,66	0
54	MG	1A	3597	1/1	0.89	0.22	43,43,43,43	0
54	MG	1U	208	1/1	0.89	0.25	36,36,36,36	0
54	MG	1A	3954	1/1	0.89	0.13	50,50,50,50	0
57	ARG	1B	228	12/12	0.89	0.11	22,42,59,67	0
54	MG	1A	3962	1/1	0.89	0.07	32,32,32,32	0
54	MG	1A	3035	1/1	0.89	0.10	41,41,41,41	0
54	MG	1A	3683	1/1	0.89	0.14	45,45,45,45	0
54	MG	13	103	1/1	0.90	0.12	37,37,37,37	0
54	MG	1A	3555	1/1	0.90	0.13	58,58,58,58	0
54	MG	2A	3508	1/1	0.90	0.16	61,61,61,61	0
54	MG	1A	3199	1/1	0.90	0.12	33,33,33,33	0
54	MG	2A	3244	1/1	0.90	0.10	45,45,45,45	0
54	MG	1A	3358	1/1	0.90	0.09	26,26,26,26	0
54	MG	1A	3883	1/1	0.90	0.11	48,48,48,48	0
54	MG	1A	3122	1/1	0.90	0.20	33,33,33,33	0
54	MG	1d	301	1/1	0.90	0.14	54,54,54,54	0
54	MG	1A	3212	1/1	0.90	0.18	41,41,41,41	0
54	MG	2E	303	1/1	0.90	0.09	51,51,51,51	0
54	MG	1a	3122	1/1	0.90	0.10	75,75,75,75	0
54	MG	1h	202	1/1	0.90	0.17	61,61,61,61	0
54	MG	1A	3583	1/1	0.90	0.14	36,36,36,36	0
54	MG	1n	101	1/1	0.90	0.16	52,52,52,52	0
54	MG	1a	3002	1/1	0.90	0.14	61,61,61,61	0
54	MG	2A	3530	1/1	0.90	0.20	62,62,62,62	0
54	MG	2A	3278	1/1	0.90	0.12	44,44,44,44	0
54	MG	1A	3756	1/1	0.90	0.10	47,47,47,47	0
54	MG	2R	202	1/1	0.90	0.12	30,30,30,30	0
54	MG	1A	3902	1/1	0.90	0.12	32,32,32,32	0
54	MG	2V	203	1/1	0.90	0.10	54,54,54,54	0
54	MG	1A	3587	1/1	0.90	0.09	63,63,63,63	0
54	MG	2Y	201	1/1	0.90	0.13	54,54,54,54	0
54	MG	2A	3288	1/1	0.90	0.14	48,48,48,48	0
54	MG	1a	3014	1/1	0.90	0.07	55,55,55,55	0
54	MG	1A	3368	1/1	0.90	0.12	51,51,51,51	0
54	MG	2A	3024	1/1	0.90	0.28	51,51,51,51	0
54	MG	1A	3159	1/1	0.90	0.13	33,33,33,33	0
54	MG	2A	3026	1/1	0.90	0.09	43,43,43,43	0
54	MG	2A	3299	1/1	0.90	0.20	53,53,53,53	0
54	MG	1a	3019	1/1	0.90	0.08	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	3030	1/1	0.90	0.12	44,44,44,44	0
54	MG	1A	3014	1/1	0.90	0.16	46,46,46,46	0
54	MG	2a	3014	1/1	0.90	0.19	71,71,71,71	0
54	MG	1A	3306	1/1	0.90	0.15	65,65,65,65	0
54	MG	1A	3220	1/1	0.90	0.28	34,34,34,34	0
54	MG	2A	3567	1/1	0.90	0.12	41,41,41,41	0
54	MG	2a	3023	1/1	0.90	0.06	51,51,51,51	0
54	MG	2A	3569	1/1	0.90	0.10	26,26,26,26	0
54	MG	2A	3570	1/1	0.90	0.08	51,51,51,51	0
54	MG	1A	3933	1/1	0.90	0.16	26,26,26,26	0
54	MG	2A	3043	1/1	0.90	0.09	42,42,42,42	0
54	MG	1A	3223	1/1	0.90	0.11	27,27,27,27	0
54	MG	2A	3056	1/1	0.90	0.14	64,64,64,64	0
54	MG	2A	3062	1/1	0.90	0.08	41,41,41,41	0
54	MG	1a	3028	1/1	0.90	0.26	49,49,49,49	0
54	MG	1A	3801	1/1	0.90	0.16	50,50,50,50	0
54	MG	2a	3042	1/1	0.90	0.18	49,49,49,49	0
54	MG	2A	3066	1/1	0.90	0.31	52,52,52,52	0
54	MG	2A	3353	1/1	0.90	0.11	69,69,69,69	0
54	MG	1A	3806	1/1	0.90	0.12	41,41,41,41	0
54	MG	2A	3357	1/1	0.90	0.09	30,30,30,30	0
54	MG	1a	3035	1/1	0.90	0.19	57,57,57,57	0
54	MG	1a	3037	1/1	0.90	0.20	38,38,38,38	0
54	MG	1A	3232	1/1	0.90	0.33	39,39,39,39	0
54	MG	2A	3097	1/1	0.90	0.18	44,44,44,44	0
54	MG	2A	3101	1/1	0.90	0.18	48,48,48,48	0
54	MG	1A	3384	1/1	0.90	0.08	26,26,26,26	0
54	MG	1a	3182	1/1	0.90	0.08	52,52,52,52	0
54	MG	1a	3041	1/1	0.90	0.11	68,68,68,68	0
54	MG	2A	3392	1/1	0.90	0.12	67,67,67,67	0
54	MG	1a	3184	1/1	0.90	0.10	63,63,63,63	0
54	MG	1A	3320	1/1	0.90	0.12	52,52,52,52	0
54	MG	2A	3395	1/1	0.90	0.13	35,35,35,35	0
54	MG	1A	3955	1/1	0.90	0.07	47,47,47,47	0
54	MG	2a	3083	1/1	0.90	0.15	48,48,48,48	0
54	MG	2A	3398	1/1	0.90	0.10	56,56,56,56	0
54	MG	1a	3191	1/1	0.90	0.09	58,58,58,58	0
54	MG	1A	3235	1/1	0.90	0.18	29,29,29,29	0
54	MG	1A	3078	1/1	0.90	0.10	27,27,27,27	0
54	MG	1A	3624	1/1	0.90	0.13	74,74,74,74	0
54	MG	1A	3323	1/1	0.90	0.25	40,40,40,40	0
54	MG	1A	3532	1/1	0.90	0.19	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	3708	1/1	0.90	0.07	28,28,28,28	0
54	MG	2A	3421	1/1	0.90	0.24	48,48,48,48	0
54	MG	1a	3199	1/1	0.90	0.10	66,66,66,66	0
54	MG	1P	204	1/1	0.90	0.16	47,47,47,47	0
54	MG	2A	3425	1/1	0.90	0.17	45,45,45,45	0
54	MG	1A	3844	1/1	0.90	0.10	43,43,43,43	0
54	MG	1a	3076	1/1	0.90	0.11	56,56,56,56	0
54	MG	1A	3407	1/1	0.90	0.12	22,22,22,22	0
54	MG	1a	3207	1/1	0.90	0.13	56,56,56,56	0
54	MG	1A	3190	1/1	0.90	0.23	56,56,56,56	0
54	MG	1a	3210	1/1	0.90	0.21	58,58,58,58	0
54	MG	2A	3185	1/1	0.90	0.13	57,57,57,57	0
54	MG	2A	3715	1/1	0.90	0.12	43,43,43,43	0
54	MG	2A	3440	1/1	0.90	0.13	50,50,50,50	0
54	MG	1A	3715	1/1	0.90	0.19	48,48,48,48	0
54	MG	2a	3147	1/1	0.90	0.11	69,69,69,69	0
54	MG	2A	3447	1/1	0.90	0.12	49,49,49,49	0
54	MG	1A	3086	1/1	0.90	0.12	56,56,56,56	0
54	MG	2a	3156	1/1	0.90	0.07	45,45,45,45	0
54	MG	2a	3158	1/1	0.90	0.11	81,81,81,81	0
54	MG	2a	3163	1/1	0.90	0.11	70,70,70,70	0
54	MG	1a	3220	1/1	0.90	0.11	63,63,63,63	0
54	MG	1A	3641	1/1	0.90	0.15	15,15,15,15	0
54	MG	1a	3090	1/1	0.90	0.12	50,50,50,50	0
54	MG	2a	3170	1/1	0.90	0.08	74,74,74,74	0
54	MG	1a	3092	1/1	0.90	0.18	50,50,50,50	0
54	MG	1A	3248	1/1	0.90	0.53	36,36,36,36	0
54	MG	1U	201	1/1	0.90	0.27	26,26,26,26	0
54	MG	1a	3233	1/1	0.90	0.09	65,65,65,65	0
54	MG	2A	3461	1/1	0.90	0.17	44,44,44,44	0
54	MG	2A	3462	1/1	0.90	0.10	37,37,37,37	0
54	MG	2A	3208	1/1	0.90	0.24	70,70,70,70	0
54	MG	1A	3196	1/1	0.90	0.18	28,28,28,28	0
54	MG	1W	201	1/1	0.90	0.11	34,34,34,34	0
54	MG	1a	3100	1/1	0.90	0.23	54,54,54,54	0
54	MG	1A	3432	1/1	0.90	0.08	21,21,21,21	0
54	MG	2A	3221	1/1	0.90	0.13	50,50,50,50	0
54	MG	2e	201	1/1	0.90	0.27	63,63,63,63	0
54	MG	2A	3222	1/1	0.90	0.10	50,50,50,50	0
54	MG	2A	3224	1/1	0.90	0.19	48,48,48,48	0
54	MG	1A	3733	1/1	0.90	0.40	32,32,32,32	0
54	MG	1a	3248	1/1	0.90	0.15	69,69,69,69	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	1a	3260	1/1	0.90	0.20	56,56,56,56	0
54	MG	1a	3262	1/1	0.90	0.10	52,52,52,52	0
54	MG	2B	208	1/1	0.90	0.21	57,57,57,57	0
54	MG	2A	3233	1/1	0.90	0.09	49,49,49,49	0
54	MG	1A	3353	1/1	0.90	0.14	27,27,27,27	0
54	MG	2A	3236	1/1	0.90	0.16	35,35,35,35	0
54	MG	1A	3732	1/1	0.91	0.13	38,38,38,38	0
54	MG	1A	3974	1/1	0.91	0.10	60,60,60,60	0
54	MG	1a	3064	1/1	0.91	0.14	71,71,71,71	0
54	MG	1A	3433	1/1	0.91	0.12	19,19,19,19	0
54	MG	2A	3260	1/1	0.91	0.12	50,50,50,50	0
54	MG	2E	301	1/1	0.91	0.12	35,35,35,35	0
54	MG	2A	3264	1/1	0.91	0.07	57,57,57,57	0
54	MG	1a	3185	1/1	0.91	0.12	44,44,44,44	0
54	MG	2E	306	1/1	0.91	0.14	52,52,52,52	0
54	MG	2A	3270	1/1	0.91	0.25	50,50,50,50	0
54	MG	2A	3527	1/1	0.91	0.10	22,22,22,22	0
54	MG	2A	3037	1/1	0.91	0.18	50,50,50,50	0
54	MG	1A	3436	1/1	0.91	0.08	18,18,18,18	0
54	MG	1a	3187	1/1	0.91	0.07	71,71,71,71	0
54	MG	2O	201	1/1	0.91	0.11	53,53,53,53	0
54	MG	2A	3045	1/1	0.91	0.14	45,45,45,45	0
54	MG	1A	3529	1/1	0.91	0.11	16,16,16,16	0
54	MG	2A	3535	1/1	0.91	0.12	43,43,43,43	0
54	MG	2T	201	1/1	0.91	0.12	63,63,63,63	0
54	MG	2A	3536	1/1	0.91	0.07	46,46,46,46	0
54	MG	2A	3052	1/1	0.91	0.15	53,53,53,53	0
54	MG	1A	3738	1/1	0.91	0.07	23,23,23,23	0
54	MG	2A	3058	1/1	0.91	0.22	60,60,60,60	0
54	MG	2A	3061	1/1	0.91	0.23	43,43,43,43	0
54	MG	1A	3273	1/1	0.91	0.29	61,61,61,61	0
54	MG	1A	3200	1/1	0.91	0.22	47,47,47,47	0
54	MG	1A	3867	1/1	0.91	0.10	38,38,38,38	0
54	MG	1A	3204	1/1	0.91	0.22	30,30,30,30	0
54	MG	2A	3069	1/1	0.91	0.09	55,55,55,55	0
54	MG	2A	3304	1/1	0.91	0.17	52,52,52,52	0
54	MG	1A	3997	1/1	0.91	0.14	45,45,45,45	0
54	MG	2a	3007	1/1	0.91	0.08	62,62,62,62	0
54	MG	2A	3080	1/1	0.91	0.17	57,57,57,57	0
54	MG	2A	3081	1/1	0.91	0.10	47,47,47,47	0
54	MG	2A	3320	1/1	0.91	0.12	38,38,38,38	0
54	MG	2A	3083	1/1	0.91	0.12	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	3104	1/1	0.91	0.23	27,27,27,27	0
54	MG	2A	3087	1/1	0.91	0.31	55,55,55,55	0
54	MG	1A	3684	1/1	0.91	0.09	48,48,48,48	0
54	MG	1a	3085	1/1	0.91	0.10	52,52,52,52	0
54	MG	2A	3096	1/1	0.91	0.15	77,77,77,77	0
54	MG	1A	3451	1/1	0.91	0.12	51,51,51,51	0
54	MG	2A	3100	1/1	0.91	0.07	53,53,53,53	0
54	MG	1Z	301	1/1	0.91	0.08	62,62,62,62	0
54	MG	1A	3185	1/1	0.91	0.16	52,52,52,52	0
54	MG	2a	3036	1/1	0.91	0.13	50,50,50,50	0
54	MG	2A	3354	1/1	0.91	0.10	40,40,40,40	0
54	MG	2A	3596	1/1	0.91	0.08	51,51,51,51	0
54	MG	1a	3091	1/1	0.91	0.10	56,56,56,56	0
54	MG	1A	4011	1/1	0.91	0.12	34,34,34,34	0
54	MG	2A	3113	1/1	0.91	0.08	42,42,42,42	0
54	MG	1A	4013	1/1	0.91	0.17	27,27,27,27	0
54	MG	1A	3767	1/1	0.91	0.20	52,52,52,52	0
54	MG	13	105	1/1	0.91	0.11	41,41,41,41	0
54	MG	2a	3053	1/1	0.91	0.19	54,54,54,54	0
54	MG	2A	3128	1/1	0.91	0.34	42,42,42,42	0
54	MG	2a	3056	1/1	0.91	0.18	47,47,47,47	0
54	MG	2A	3130	1/1	0.91	0.17	52,52,52,52	0
54	MG	1A	3392	1/1	0.91	0.09	56,56,56,56	0
54	MG	1A	3472	1/1	0.91	0.07	42,42,42,42	0
54	MG	2A	3391	1/1	0.91	0.11	46,46,46,46	0
54	MG	2A	3140	1/1	0.91	0.17	45,45,45,45	0
54	MG	2a	3067	1/1	0.91	0.20	52,52,52,52	0
54	MG	2A	3142	1/1	0.91	0.11	58,58,58,58	0
54	MG	1A	3695	1/1	0.91	0.12	36,36,36,36	0
54	MG	2A	3633	1/1	0.91	0.08	74,74,74,74	0
54	MG	1A	3890	1/1	0.91	0.18	23,23,23,23	0
54	MG	1A	3402	1/1	0.91	0.10	25,25,25,25	0
54	MG	1a	3229	1/1	0.91	0.09	65,65,65,65	0
54	MG	2a	3076	1/1	0.91	0.12	68,68,68,68	0
54	MG	2a	3079	1/1	0.91	0.20	50,50,50,50	0
54	MG	1A	3477	1/1	0.91	0.09	44,44,44,44	0
54	MG	1A	3900	1/1	0.91	0.08	28,28,28,28	0
54	MG	2A	3166	1/1	0.91	0.12	40,40,40,40	0
54	MG	2A	3663	1/1	0.91	0.12	45,45,45,45	0
54	MG	1A	4045	1/1	0.91	0.21	46,46,46,46	0
54	MG	2A	3168	1/1	0.91	0.18	54,54,54,54	0
54	MG	1A	3794	1/1	0.91	0.11	19,19,19,19	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	1A	3556	1/1	0.91	0.22	27,27,27,27	0
54	MG	1A	3371	1/1	0.91	0.07	27,27,27,27	0
54	MG	2a	3101	1/1	0.91	0.16	63,63,63,63	0
54	MG	2A	3422	1/1	0.91	0.08	42,42,42,42	0
54	MG	1a	3243	1/1	0.91	0.23	51,51,51,51	0
54	MG	1A	3921	1/1	0.91	0.09	16,16,16,16	0
54	MG	1A	3803	1/1	0.91	0.11	39,39,39,39	0
54	MG	1a	3258	1/1	0.91	0.11	55,55,55,55	0
54	MG	2A	3685	1/1	0.91	0.08	50,50,50,50	0
54	MG	2a	3118	1/1	0.91	0.07	48,48,48,48	0
54	MG	1A	3804	1/1	0.91	0.14	55,55,55,55	0
54	MG	2A	3188	1/1	0.91	0.18	56,56,56,56	0
54	MG	2A	3190	1/1	0.91	0.09	47,47,47,47	0
54	MG	2A	3192	1/1	0.91	0.36	73,73,73,73	0
54	MG	2a	3125	1/1	0.91	0.10	66,66,66,66	0
54	MG	2A	3707	1/1	0.91	0.10	52,52,52,52	0
54	MG	1A	3036	1/1	0.91	0.13	44,44,44,44	0
54	MG	2A	3194	1/1	0.91	0.10	57,57,57,57	0
54	MG	2A	3195	1/1	0.91	0.23	66,66,66,66	0
54	MG	2A	3720	1/1	0.91	0.16	54,54,54,54	0
54	MG	2a	3138	1/1	0.91	0.17	59,59,59,59	0
54	MG	1a	3264	1/1	0.91	0.14	50,50,50,50	0
54	MG	1A	3493	1/1	0.91	0.09	14,14,14,14	0
54	MG	1a	3270	1/1	0.91	0.08	56,56,56,56	0
54	MG	1A	3375	1/1	0.91	0.10	42,42,42,42	0
54	MG	1A	3813	1/1	0.91	0.08	69,69,69,69	0
54	MG	2a	3162	1/1	0.91	0.11	58,58,58,58	0
54	MG	1a	3024	1/1	0.91	0.15	55,55,55,55	0
54	MG	1B	216	1/1	0.91	0.10	35,35,35,35	0
54	MG	1A	3579	1/1	0.91	0.09	48,48,48,48	0
54	MG	2A	3209	1/1	0.91	0.09	49,49,49,49	0
54	MG	1a	3139	1/1	0.91	0.07	47,47,47,47	0
54	MG	1A	3816	1/1	0.91	0.17	47,47,47,47	0
54	MG	1d	302	1/1	0.91	0.17	48,48,48,48	0
54	MG	1A	3581	1/1	0.91	0.08	42,42,42,42	0
54	MG	1f	202	1/1	0.91	0.11	36,36,36,36	0
54	MG	1A	3128	1/1	0.91	0.21	27,27,27,27	0
54	MG	1A	3039	1/1	0.91	0.08	34,34,34,34	0
54	MG	1E	305	1/1	0.91	0.09	45,45,45,45	0
54	MG	1a	3158	1/1	0.91	0.14	47,47,47,47	0
54	MG	1A	3722	1/1	0.91	0.13	47,47,47,47	0
54	MG	1A	3588	1/1	0.91	0.08	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	3231	1/1	0.91	0.09	44,44,44,44	0
54	MG	1A	3343	1/1	0.91	0.11	22,22,22,22	0
54	MG	1a	3163	1/1	0.91	0.15	59,59,59,59	0
54	MG	1a	3164	1/1	0.91	0.13	39,39,39,39	0
54	MG	1A	3177	1/1	0.91	0.23	38,38,38,38	0
54	MG	2A	3009	1/1	0.91	0.12	36,36,36,36	0
54	MG	2A	3497	1/1	0.91	0.07	65,65,65,65	0
54	MG	2A	3012	1/1	0.91	0.10	54,54,54,54	0
54	MG	2A	3021	1/1	0.91	0.14	42,42,42,42	0
54	MG	1a	3044	1/1	0.91	0.12	57,57,57,57	0
54	MG	1a	3049	1/1	0.91	0.12	38,38,38,38	0
54	MG	2A	3248	1/1	0.91	0.30	40,40,40,40	0
54	MG	1a	3052	1/1	0.91	0.18	57,57,57,57	0
54	MG	2A	3487	1/1	0.92	0.12	52,52,52,52	0
54	MG	1T	205	1/1	0.92	0.10	59,59,59,59	0
54	MG	1a	3121	1/1	0.92	0.12	62,62,62,62	0
54	MG	1A	3952	1/1	0.92	0.07	34,34,34,34	0
54	MG	2A	3494	1/1	0.92	0.19	55,55,55,55	0
54	MG	1A	3046	1/1	0.92	0.10	34,34,34,34	0
54	MG	1A	3431	1/1	0.92	0.09	23,23,23,23	0
54	MG	2A	3001	1/1	0.92	0.26	51,51,51,51	0
54	MG	1A	3345	1/1	0.92	0.09	21,21,21,21	0
54	MG	1A	3270	1/1	0.92	0.13	47,47,47,47	0
54	MG	1A	3798	1/1	0.92	0.12	27,27,27,27	0
54	MG	1a	3134	1/1	0.92	0.15	38,38,38,38	0
54	MG	1A	3071	1/1	0.92	0.08	34,34,34,34	0
54	MG	1A	3802	1/1	0.92	0.08	39,39,39,39	0
54	MG	2A	3517	1/1	0.92	0.09	69,69,69,69	0
54	MG	1A	3675	1/1	0.92	0.14	46,46,46,46	0
54	MG	1A	3356	1/1	0.92	0.08	33,33,33,33	0
54	MG	2N	3801	1/1	0.92	0.06	54,54,54,54	0
54	MG	1A	3805	1/1	0.92	0.06	26,26,26,26	0
54	MG	1a	3145	1/1	0.92	0.20	57,57,57,57	0
54	MG	2A	3253	1/1	0.92	0.15	52,52,52,52	0
54	MG	1A	3439	1/1	0.92	0.09	19,19,19,19	0
54	MG	1A	3571	1/1	0.92	0.09	44,44,44,44	0
54	MG	2T	203	1/1	0.92	0.07	46,46,46,46	0
54	MG	1A	3811	1/1	0.92	0.17	54,54,54,54	0
54	MG	1a	3154	1/1	0.92	0.12	40,40,40,40	0
54	MG	17	103	1/1	0.92	0.31	30,30,30,30	0
54	MG	1A	3180	1/1	0.92	0.43	34,34,34,34	0
54	MG	1A	3574	1/1	0.92	0.08	34,34,34,34	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	1A	3575	1/1	0.92	0.10	46,46,46,46	0
54	MG	1A	3686	1/1	0.92	0.10	50,50,50,50	0
54	MG	1A	3999	1/1	0.92	0.09	55,55,55,55	0
54	MG	1a	3005	1/1	0.92	0.12	44,44,44,44	0
54	MG	1A	3445	1/1	0.92	0.09	20,20,20,20	0
54	MG	1a	3010	1/1	0.92	0.21	47,47,47,47	0
54	MG	1a	3011	1/1	0.92	0.27	73,73,73,73	0
54	MG	1A	3578	1/1	0.92	0.08	31,31,31,31	0
54	MG	1A	3359	1/1	0.92	0.08	31,31,31,31	0
54	MG	2A	3291	1/1	0.92	0.18	51,51,51,51	0
54	MG	2A	3070	1/1	0.92	0.11	45,45,45,45	0
54	MG	2a	3016	1/1	0.92	0.12	65,65,65,65	0
54	MG	1A	4006	1/1	0.92	0.10	33,33,33,33	0
54	MG	2A	3075	1/1	0.92	0.12	24,24,24,24	0
54	MG	2a	3021	1/1	0.92	0.16	60,60,60,60	0
54	MG	2A	3079	1/1	0.92	0.15	54,54,54,54	0
54	MG	1A	3835	1/1	0.92	0.23	36,36,36,36	0
54	MG	1A	4008	1/1	0.92	0.08	55,55,55,55	0
54	MG	1A	3129	1/1	0.92	0.13	27,27,27,27	0
54	MG	2a	3026	1/1	0.92	0.14	43,43,43,43	0
54	MG	1A	3218	1/1	0.92	0.34	20,20,20,20	0
54	MG	1A	3454	1/1	0.92	0.15	48,48,48,48	0
54	MG	2A	3571	1/1	0.92	0.07	38,38,38,38	0
54	MG	2A	3572	1/1	0.92	0.09	62,62,62,62	0
54	MG	1a	3188	1/1	0.92	0.12	60,60,60,60	0
54	MG	1A	3219	1/1	0.92	0.13	43,43,43,43	0
54	MG	2A	3095	1/1	0.92	0.19	60,60,60,60	0
54	MG	2A	3328	1/1	0.92	0.10	33,33,33,33	0
54	MG	1A	4022	1/1	0.92	0.13	51,51,51,51	0
54	MG	1A	3294	1/1	0.92	0.11	44,44,44,44	0
54	MG	2a	3044	1/1	0.92	0.20	55,55,55,55	0
54	MG	2A	3587	1/1	0.92	0.11	70,70,70,70	0
54	MG	2a	3048	1/1	0.92	0.15	70,70,70,70	0
54	MG	2A	3098	1/1	0.92	0.10	47,47,47,47	0
54	MG	1A	4024	1/1	0.92	0.09	48,48,48,48	0
54	MG	1A	3593	1/1	0.92	0.09	22,22,22,22	0
54	MG	1A	4028	1/1	0.92	0.07	29,29,29,29	0
54	MG	1A	3296	1/1	0.92	0.17	27,27,27,27	0
54	MG	2a	3058	1/1	0.92	0.22	52,52,52,52	0
54	MG	1A	3304	1/1	0.92	0.07	39,39,39,39	0
54	MG	1A	3083	1/1	0.92	0.20	25,25,25,25	0
54	MG	2A	3606	1/1	0.92	0.08	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	3200	1/1	0.92	0.08	55,55,55,55	0
54	MG	1A	3600	1/1	0.92	0.09	41,41,41,41	0
54	MG	2A	3120	1/1	0.92	0.14	46,46,46,46	0
54	MG	1A	3603	1/1	0.92	0.07	28,28,28,28	0
54	MG	2A	3363	1/1	0.92	0.11	37,37,37,37	0
54	MG	2A	3365	1/1	0.92	0.20	48,48,48,48	0
54	MG	1A	3189	1/1	0.92	0.34	44,44,44,44	0
54	MG	2A	3623	1/1	0.92	0.08	39,39,39,39	0
54	MG	1A	3317	1/1	0.92	0.07	47,47,47,47	0
54	MG	1a	3047	1/1	0.92	0.17	59,59,59,59	0
54	MG	2A	3132	1/1	0.92	0.20	47,47,47,47	0
54	MG	1A	3491	1/1	0.92	0.12	12,12,12,12	0
54	MG	2A	3135	1/1	0.92	0.16	72,72,72,72	0
54	MG	2A	3138	1/1	0.92	0.12	59,59,59,59	0
54	MG	1a	3051	1/1	0.92	0.11	42,42,42,42	0
54	MG	1A	3227	1/1	0.92	0.22	37,37,37,37	0
54	MG	2a	3095	1/1	0.92	0.17	62,62,62,62	0
54	MG	2A	3643	1/1	0.92	0.13	54,54,54,54	0
54	MG	1B	203	1/1	0.92	0.21	58,58,58,58	0
54	MG	1A	3145	1/1	0.92	0.34	28,28,28,28	0
54	MG	1A	3147	1/1	0.92	0.10	28,28,28,28	0
54	MG	1a	3223	1/1	0.92	0.12	55,55,55,55	0
54	MG	2A	3156	1/1	0.92	0.24	48,48,48,48	0
54	MG	2a	3106	1/1	0.92	0.10	46,46,46,46	0
54	MG	1A	3193	1/1	0.92	0.12	68,68,68,68	0
54	MG	2A	3158	1/1	0.92	0.18	47,47,47,47	0
54	MG	1A	3500	1/1	0.92	0.09	28,28,28,28	0
54	MG	1A	3626	1/1	0.92	0.49	30,30,30,30	0
54	MG	2A	3677	1/1	0.92	0.10	53,53,53,53	0
54	MG	1A	3119	1/1	0.92	0.20	43,43,43,43	0
54	MG	1a	3231	1/1	0.92	0.11	43,43,43,43	0
54	MG	2A	3416	1/1	0.92	0.10	38,38,38,38	0
54	MG	1a	3070	1/1	0.92	0.09	60,60,60,60	0
54	MG	1A	3240	1/1	0.92	0.21	56,56,56,56	0
54	MG	1B	217	1/1	0.92	0.08	37,37,37,37	0
54	MG	1A	3892	1/1	0.92	0.12	55,55,55,55	0
54	MG	1A	3244	1/1	0.92	0.22	32,32,32,32	0
54	MG	2A	3427	1/1	0.92	0.24	40,40,40,40	0
54	MG	1A	3896	1/1	0.92	0.11	45,45,45,45	0
54	MG	2A	3181	1/1	0.92	0.09	45,45,45,45	0
54	MG	1A	3328	1/1	0.92	0.08	54,54,54,54	0
54	MG	2a	3139	1/1	0.92	0.08	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	3523	1/1	0.92	0.10	22,22,22,22	0
54	MG	2A	3718	1/1	0.92	0.12	51,51,51,51	0
54	MG	2A	3187	1/1	0.92	0.14	55,55,55,55	0
54	MG	1E	301	1/1	0.92	0.41	42,42,42,42	0
54	MG	1a	3249	1/1	0.92	0.10	74,74,74,74	0
54	MG	2a	3159	1/1	0.92	0.10	61,61,61,61	0
54	MG	1a	3086	1/1	0.92	0.15	47,47,47,47	0
54	MG	1a	3259	1/1	0.92	0.07	48,48,48,48	0
54	MG	2a	3164	1/1	0.92	0.10	61,61,61,61	0
54	MG	2A	3444	1/1	0.92	0.24	46,46,46,46	0
54	MG	1A	3012	1/1	0.92	0.20	33,33,33,33	0
54	MG	1A	3753	1/1	0.92	0.06	27,27,27,27	0
54	MG	1F	302	1/1	0.92	0.09	22,22,22,22	0
54	MG	1F	312	1/1	0.92	0.36	39,39,39,39	0
54	MG	1A	3406	1/1	0.92	0.10	39,39,39,39	0
54	MG	1A	3096	1/1	0.92	0.20	42,42,42,42	0
54	MG	2A	3201	1/1	0.92	0.20	53,53,53,53	0
54	MG	2A	3202	1/1	0.92	0.16	40,40,40,40	0
54	MG	1A	3760	1/1	0.92	0.07	62,62,62,62	0
54	MG	1A	3923	1/1	0.92	0.10	32,32,32,32	0
54	MG	1A	3409	1/1	0.92	0.08	18,18,18,18	0
54	MG	2a	3186	1/1	0.92	0.20	58,58,58,58	0
54	MG	2a	3187	1/1	0.92	0.08	62,62,62,62	0
54	MG	2A	3756	1/1	0.92	0.07	53,53,53,53	0
54	MG	2a	3194	1/1	0.92	0.08	72,72,72,72	0
54	MG	1O	201	1/1	0.92	0.12	43,43,43,43	0
54	MG	1A	3766	1/1	0.92	0.08	20,20,20,20	0
54	MG	2a	3198	1/1	0.92	0.14	72,72,72,72	0
54	MG	1A	3929	1/1	0.92	0.09	22,22,22,22	0
54	MG	1A	3331	1/1	0.92	0.11	48,48,48,48	0
54	MG	2f	201	1/1	0.92	0.16	53,53,53,53	0
54	MG	1A	3772	1/1	0.92	0.09	42,42,42,42	0
54	MG	2n	101	1/1	0.92	0.13	65,65,65,65	0
54	MG	2A	3218	1/1	0.92	0.11	63,63,63,63	0
54	MG	1A	3172	1/1	0.92	0.19	25,25,25,25	0
54	MG	1R	206	1/1	0.92	0.11	37,37,37,37	0
54	MG	2A	3477	1/1	0.92	0.13	58,58,58,58	0
54	MG	2A	3478	1/1	0.92	0.08	52,52,52,52	0
54	MG	1A	3656	1/1	0.92	0.24	32,32,32,32	0
54	MG	1A	3339	1/1	0.92	0.07	28,28,28,28	0
54	MG	1A	3785	1/1	0.92	0.11	20,20,20,20	0
54	MG	2A	3486	1/1	0.92	0.07	50,50,50,50	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	1a	3032	1/1	0.93	0.10	58,58,58,58	0
54	MG	1a	3033	1/1	0.93	0.11	26,26,26,26	0
54	MG	2A	3725	1/1	0.93	0.08	59,59,59,59	0
54	MG	2A	3123	1/1	0.93	0.07	41,41,41,41	0
54	MG	2A	3396	1/1	0.93	0.08	37,37,37,37	0
54	MG	1A	3082	1/1	0.93	0.06	34,34,34,34	0
54	MG	1A	3777	1/1	0.93	0.12	41,41,41,41	0
54	MG	2A	3399	1/1	0.93	0.16	50,50,50,50	0
54	MG	1A	3279	1/1	0.93	0.20	48,48,48,48	0
54	MG	2A	3739	1/1	0.93	0.11	40,40,40,40	0
54	MG	1A	3903	1/1	0.93	0.14	41,41,41,41	0
54	MG	1a	3039	1/1	0.93	0.24	54,54,54,54	0
54	MG	1A	3284	1/1	0.93	0.11	53,53,53,53	0
54	MG	1a	3206	1/1	0.93	0.13	64,64,64,64	0
54	MG	1A	3784	1/1	0.93	0.09	45,45,45,45	0
54	MG	1B	208	1/1	0.93	0.10	45,45,45,45	0
54	MG	1A	3682	1/1	0.93	0.06	33,33,33,33	0
54	MG	1a	3045	1/1	0.93	0.18	41,41,41,41	0
54	MG	2A	3148	1/1	0.93	0.33	46,46,46,46	0
54	MG	2A	3755	1/1	0.93	0.20	50,50,50,50	0
54	MG	1a	3218	1/1	0.93	0.11	54,54,54,54	0
54	MG	1A	3787	1/1	0.93	0.09	32,32,32,32	0
54	MG	1A	3285	1/1	0.93	0.12	39,39,39,39	0
54	MG	2A	3426	1/1	0.93	0.12	57,57,57,57	0
54	MG	1B	214	1/1	0.93	0.07	30,30,30,30	0
54	MG	1A	3789	1/1	0.93	0.11	37,37,37,37	0
54	MG	1a	3056	1/1	0.93	0.17	38,38,38,38	0
54	MG	2A	3159	1/1	0.93	0.10	55,55,55,55	0
54	MG	2A	3161	1/1	0.93	0.07	42,42,42,42	0
54	MG	1A	3926	1/1	0.93	0.07	29,29,29,29	0
54	MG	1a	3058	1/1	0.93	0.11	57,57,57,57	0
54	MG	1B	218	1/1	0.93	0.07	31,31,31,31	0
54	MG	2A	3437	1/1	0.93	0.06	45,45,45,45	0
54	MG	2A	3438	1/1	0.93	0.21	48,48,48,48	0
54	MG	1a	3230	1/1	0.93	0.09	48,48,48,48	0
54	MG	1B	223	1/1	0.93	0.11	47,47,47,47	0
54	MG	1A	3109	1/1	0.93	0.14	60,60,60,60	0
54	MG	1A	3928	1/1	0.93	0.11	37,37,37,37	0
54	MG	1A	3531	1/1	0.93	0.08	32,32,32,32	0
54	MG	2D	304	1/1	0.93	0.39	44,44,44,44	0
54	MG	2A	3173	1/1	0.93	0.12	45,45,45,45	0
54	MG	2A	3178	1/1	0.93	0.14	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	1D	305	1/1	0.93	0.08	31,31,31,31	0
54	MG	2A	3454	1/1	0.93	0.15	42,42,42,42	0
54	MG	1a	3236	1/1	0.93	0.09	52,52,52,52	0
54	MG	1a	3237	1/1	0.93	0.07	62,62,62,62	0
54	MG	1D	306	1/1	0.93	0.16	39,39,39,39	0
54	MG	1A	3288	1/1	0.93	0.12	32,32,32,32	0
54	MG	1A	3335	1/1	0.93	0.09	57,57,57,57	0
54	MG	1a	3074	1/1	0.93	0.16	55,55,55,55	0
54	MG	1A	3337	1/1	0.93	0.08	44,44,44,44	0
54	MG	1A	3693	1/1	0.93	0.08	51,51,51,51	0
54	MG	1a	3255	1/1	0.93	0.07	43,43,43,43	0
54	MG	1a	3257	1/1	0.93	0.07	64,64,64,64	0
54	MG	1A	3536	1/1	0.93	0.10	43,43,43,43	0
54	MG	1A	3945	1/1	0.93	0.06	41,41,41,41	0
54	MG	2A	3473	1/1	0.93	0.08	42,42,42,42	0
54	MG	1F	308	1/1	0.93	0.13	19,19,19,19	0
54	MG	1A	3615	1/1	0.93	0.08	52,52,52,52	0
54	MG	2A	3476	1/1	0.93	0.10	50,50,50,50	0
54	MG	1A	3950	1/1	0.93	0.08	48,48,48,48	0
54	MG	1A	3616	1/1	0.93	0.11	38,38,38,38	0
54	MG	1a	3269	1/1	0.93	0.13	70,70,70,70	0
54	MG	1A	3179	1/1	0.93	0.12	27,27,27,27	0
54	MG	2A	3484	1/1	0.93	0.19	69,69,69,69	0
54	MG	2I	101	1/1	0.93	0.13	49,49,49,49	0
54	MG	1A	3126	1/1	0.93	0.13	23,23,23,23	0
54	MG	1A	3393	1/1	0.93	0.10	52,52,52,52	0
54	MG	1a	3273	1/1	0.93	0.06	72,72,72,72	0
54	MG	1A	3957	1/1	0.93	0.10	39,39,39,39	0
54	MG	1A	3548	1/1	0.93	0.07	43,43,43,43	0
54	MG	1a	3094	1/1	0.93	0.13	56,56,56,56	0
54	MG	1A	3963	1/1	0.93	0.15	56,56,56,56	0
54	MG	2A	3496	1/1	0.93	0.10	50,50,50,50	0
54	MG	1A	3964	1/1	0.93	0.09	68,68,68,68	0
54	MG	1A	3206	1/1	0.93	0.08	32,32,32,32	0
54	MG	2a	3012	1/1	0.93	0.14	49,49,49,49	0
54	MG	1A	3709	1/1	0.93	0.07	47,47,47,47	0
54	MG	1d	305	1/1	0.93	0.07	82,82,82,82	0
54	MG	2a	3017	1/1	0.93	0.14	51,51,51,51	0
54	MG	1A	3475	1/1	0.93	0.07	28,28,28,28	0
54	MG	1g	201	1/1	0.93	0.25	50,50,50,50	0
54	MG	1A	3629	1/1	0.93	0.25	34,34,34,34	0
54	MG	1A	3975	1/1	0.93	0.07	50,50,50,50	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	1a	3106	1/1	0.93	0.10	44,44,44,44	0
54	MG	1A	3064	1/1	0.93	0.07	42,42,42,42	0
54	MG	1T	204	1/1	0.93	0.08	48,48,48,48	0
54	MG	1o	101	1/1	0.93	0.11	49,49,49,49	0
54	MG	1a	3111	1/1	0.93	0.10	29,29,29,29	0
54	MG	2a	3029	1/1	0.93	0.12	63,63,63,63	0
54	MG	2A	3522	1/1	0.93	0.11	59,59,59,59	0
54	MG	1A	3016	1/1	0.93	0.31	33,33,33,33	0
54	MG	2a	3034	1/1	0.93	0.24	52,52,52,52	0
54	MG	1A	3719	1/1	0.93	0.25	34,34,34,34	0
54	MG	1A	3981	1/1	0.93	0.14	66,66,66,66	0
54	MG	2A	3243	1/1	0.93	0.11	43,43,43,43	0
54	MG	1U	203	1/1	0.93	0.22	28,28,28,28	0
54	MG	2A	3245	1/1	0.93	0.25	42,42,42,42	0
54	MG	1U	207	1/1	0.93	0.13	42,42,42,42	0
54	MG	2A	3003	1/1	0.93	0.07	47,47,47,47	0
54	MG	2A	3005	1/1	0.93	0.17	51,51,51,51	0
54	MG	2a	3045	1/1	0.93	0.17	62,62,62,62	0
54	MG	2A	3534	1/1	0.93	0.14	50,50,50,50	0
54	MG	2A	3006	1/1	0.93	0.23	52,52,52,52	0
54	MG	1A	3839	1/1	0.93	0.09	52,52,52,52	0
54	MG	2A	3251	1/1	0.93	0.29	41,41,41,41	0
54	MG	1V	205	1/1	0.93	0.05	67,67,67,67	0
54	MG	2A	3539	1/1	0.93	0.09	68,68,68,68	0
54	MG	2A	3254	1/1	0.93	0.27	59,59,59,59	0
54	MG	2A	3015	1/1	0.93	0.28	36,36,36,36	0
54	MG	1A	3559	1/1	0.93	0.06	29,29,29,29	0
54	MG	2a	3062	1/1	0.93	0.12	62,62,62,62	0
54	MG	1A	3561	1/1	0.93	0.08	27,27,27,27	0
54	MG	1A	3991	1/1	0.93	0.10	43,43,43,43	0
54	MG	1A	3638	1/1	0.93	0.08	25,25,25,25	0
54	MG	2A	3551	1/1	0.93	0.12	30,30,30,30	0
54	MG	2A	3556	1/1	0.93	0.07	62,62,62,62	0
54	MG	2A	3557	1/1	0.93	0.07	52,52,52,52	0
54	MG	10	107	1/1	0.93	0.08	45,45,45,45	0
54	MG	2A	3267	1/1	0.93	0.11	47,47,47,47	0
54	MG	11	101	1/1	0.93	0.07	36,36,36,36	0
54	MG	2A	3272	1/1	0.93	0.13	26,26,26,26	0
54	MG	11	102	1/1	0.93	0.19	48,48,48,48	0
54	MG	2A	3275	1/1	0.93	0.10	39,39,39,39	0
54	MG	2a	3077	1/1	0.93	0.21	58,58,58,58	0
54	MG	1A	3186	1/1	0.93	0.10	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	3845	1/1	0.93	0.09	42,42,42,42	0
54	MG	1A	3998	1/1	0.93	0.08	42,42,42,42	0
54	MG	2A	3281	1/1	0.93	0.17	60,60,60,60	0
54	MG	2A	3282	1/1	0.93	0.08	49,49,49,49	0
54	MG	2A	3573	1/1	0.93	0.06	59,59,59,59	0
54	MG	2a	3094	1/1	0.93	0.15	38,38,38,38	0
54	MG	2A	3283	1/1	0.93	0.15	34,34,34,34	0
54	MG	1a	3142	1/1	0.93	0.09	57,57,57,57	0
54	MG	1A	3316	1/1	0.93	0.19	31,31,31,31	0
54	MG	2a	3098	1/1	0.93	0.07	62,62,62,62	0
54	MG	2A	3580	1/1	0.93	0.09	45,45,45,45	0
54	MG	2A	3044	1/1	0.93	0.08	27,27,27,27	0
54	MG	2A	3582	1/1	0.93	0.06	48,48,48,48	0
54	MG	2a	3103	1/1	0.93	0.10	67,67,67,67	0
54	MG	1A	3849	1/1	0.93	0.09	43,43,43,43	0
54	MG	2A	3046	1/1	0.93	0.12	55,55,55,55	0
54	MG	2A	3047	1/1	0.93	0.11	49,49,49,49	0
54	MG	2A	3590	1/1	0.93	0.07	45,45,45,45	0
54	MG	1a	3147	1/1	0.93	0.18	52,52,52,52	0
54	MG	2a	3113	1/1	0.93	0.10	53,53,53,53	0
54	MG	2A	3051	1/1	0.93	0.16	53,53,53,53	0
54	MG	1A	3726	1/1	0.93	0.10	45,45,45,45	0
54	MG	2a	3117	1/1	0.93	0.10	45,45,45,45	0
54	MG	1A	3728	1/1	0.93	0.08	33,33,33,33	0
54	MG	2A	3302	1/1	0.93	0.11	42,42,42,42	0
54	MG	2A	3057	1/1	0.93	0.09	53,53,53,53	0
54	MG	1A	3643	1/1	0.93	0.07	40,40,40,40	0
54	MG	2A	3306	1/1	0.93	0.07	36,36,36,36	0
54	MG	2a	3124	1/1	0.93	0.12	56,56,56,56	0
54	MG	1A	3570	1/1	0.93	0.09	23,23,23,23	0
54	MG	2a	3127	1/1	0.93	0.15	57,57,57,57	0
54	MG	2A	3608	1/1	0.93	0.12	52,52,52,52	0
54	MG	2a	3131	1/1	0.93	0.08	67,67,67,67	0
54	MG	1A	3489	1/1	0.93	0.09	44,44,44,44	0
54	MG	2A	3612	1/1	0.93	0.07	48,48,48,48	0
54	MG	2a	3134	1/1	0.93	0.12	64,64,64,64	0
54	MG	2A	3315	1/1	0.93	0.09	45,45,45,45	0
54	MG	2A	3318	1/1	0.93	0.13	64,64,64,64	0
54	MG	1A	4010	1/1	0.93	0.34	34,34,34,34	0
54	MG	1A	3647	1/1	0.93	0.11	51,51,51,51	0
54	MG	2a	3140	1/1	0.93	0.08	53,53,53,53	0
54	MG	2a	3141	1/1	0.93	0.16	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	2a	3145	1/1	0.93	0.06	56,56,56,56	0
54	MG	1a	3003	1/1	0.93	0.25	61,61,61,61	0
54	MG	2A	3323	1/1	0.93	0.12	55,55,55,55	0
54	MG	2A	3625	1/1	0.93	0.08	53,53,53,53	0
54	MG	2a	3152	1/1	0.93	0.09	77,77,77,77	0
54	MG	1A	3158	1/1	0.93	0.34	29,29,29,29	0
54	MG	1A	3131	1/1	0.93	0.12	48,48,48,48	0
54	MG	1A	4020	1/1	0.93	0.13	53,53,53,53	0
54	MG	1A	3262	1/1	0.93	0.17	37,37,37,37	0
54	MG	2A	3335	1/1	0.93	0.09	38,38,38,38	0
54	MG	2A	3337	1/1	0.93	0.11	21,21,21,21	0
54	MG	1A	3657	1/1	0.93	0.08	68,68,68,68	0
54	MG	2A	3342	1/1	0.93	0.09	35,35,35,35	0
54	MG	2A	3343	1/1	0.93	0.07	27,27,27,27	0
54	MG	1a	3012	1/1	0.93	0.14	24,24,24,24	0
54	MG	1A	3136	1/1	0.93	0.07	40,40,40,40	0
54	MG	2A	3652	1/1	0.93	0.07	58,58,58,58	0
54	MG	1A	3497	1/1	0.93	0.08	24,24,24,24	0
54	MG	2a	3178	1/1	0.93	0.11	47,47,47,47	0
54	MG	1a	3179	1/1	0.93	0.08	64,64,64,64	0
54	MG	1a	3181	1/1	0.93	0.06	60,60,60,60	0
54	MG	2A	3089	1/1	0.93	0.27	43,43,43,43	0
54	MG	2A	3355	1/1	0.93	0.09	28,28,28,28	0
54	MG	2A	3090	1/1	0.93	0.10	33,33,33,33	0
54	MG	1A	3498	1/1	0.93	0.10	37,37,37,37	0
54	MG	1A	3175	1/1	0.93	0.22	31,31,31,31	0
54	MG	2A	3361	1/1	0.93	0.06	35,35,35,35	0
54	MG	2a	3192	1/1	0.93	0.12	56,56,56,56	0
54	MG	1A	3667	1/1	0.93	0.09	47,47,47,47	0
54	MG	1A	3222	1/1	0.93	0.41	33,33,33,33	0
54	MG	1A	3888	1/1	0.93	0.08	22,22,22,22	0
54	MG	1A	4039	1/1	0.93	0.15	34,34,34,34	0
54	MG	2A	3686	1/1	0.93	0.08	64,64,64,64	0
54	MG	1A	3501	1/1	0.93	0.09	29,29,29,29	0
54	MG	1A	3194	1/1	0.93	0.12	49,49,49,49	0
54	MG	1a	3026	1/1	0.93	0.08	50,50,50,50	0
54	MG	2A	3698	1/1	0.93	0.10	58,58,58,58	0
56	MPD	1A	4056	8/8	0.93	0.16	39,46,54,57	0
54	MG	2A	3382	1/1	0.93	0.09	48,48,48,48	0
54	MG	1A	4046	1/1	0.93	0.08	56,56,56,56	0
54	MG	1A	3769	1/1	0.93	0.16	46,46,46,46	0
54	MG	2A	3710	1/1	0.93	0.07	50,50,50,50	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	2A	3712	1/1	0.93	0.07	45,45,45,45	0
54	MG	2A	3390	1/1	0.93	0.10	23,23,23,23	0
54	MG	1A	3435	1/1	0.93	0.09	50,50,50,50	0
54	MG	2A	3717	1/1	0.93	0.12	38,38,38,38	0
54	MG	1a	3030	1/1	0.93	0.19	47,47,47,47	0
54	MG	1A	3396	1/1	0.94	0.07	37,37,37,37	0
54	MG	1A	3770	1/1	0.94	0.13	44,44,44,44	0
54	MG	1A	3397	1/1	0.94	0.09	34,34,34,34	0
54	MG	1A	3949	1/1	0.94	0.08	31,31,31,31	0
54	MG	1A	3399	1/1	0.94	0.09	42,42,42,42	0
54	MG	1e	202	1/1	0.94	0.14	55,55,55,55	0
54	MG	2A	3211	1/1	0.94	0.06	41,41,41,41	0
54	MG	1f	201	1/1	0.94	0.19	61,61,61,61	0
54	MG	1A	3062	1/1	0.94	0.11	33,33,33,33	0
54	MG	2B	209	1/1	0.94	0.10	57,57,57,57	0
54	MG	2A	3214	1/1	0.94	0.21	45,45,45,45	0
54	MG	1a	3104	1/1	0.94	0.15	61,61,61,61	0
54	MG	2B	213	1/1	0.94	0.07	77,77,77,77	0
54	MG	1A	3403	1/1	0.94	0.07	15,15,15,15	0
54	MG	2A	3469	1/1	0.94	0.07	43,43,43,43	0
54	MG	2A	3219	1/1	0.94	0.18	50,50,50,50	0
54	MG	1h	201	1/1	0.94	0.13	29,29,29,29	0
54	MG	1A	3123	1/1	0.94	0.10	21,21,21,21	0
54	MG	1l	201	1/1	0.94	0.15	55,55,55,55	0
54	MG	1A	3649	1/1	0.94	0.16	57,57,57,57	0
54	MG	1A	3026	1/1	0.94	0.30	27,27,27,27	0
54	MG	1A	3960	1/1	0.94	0.17	40,40,40,40	0
54	MG	1A	3654	1/1	0.94	0.20	20,20,20,20	0
54	MG	1A	3541	1/1	0.94	0.09	52,52,52,52	0
54	MG	2A	3483	1/1	0.94	0.07	48,48,48,48	0
54	MG	1A	3038	1/1	0.94	0.10	28,28,28,28	0
54	MG	1A	3967	1/1	0.94	0.06	14,14,14,14	0
54	MG	1U	206	1/1	0.94	0.32	33,33,33,33	0
54	MG	1y	203	1/1	0.94	0.08	59,59,59,59	0
54	MG	1A	3127	1/1	0.94	0.10	42,42,42,42	0
54	MG	2F	302	1/1	0.94	0.10	60,60,60,60	0
54	MG	2F	303	1/1	0.94	0.19	49,49,49,49	0
54	MG	2A	3490	1/1	0.94	0.11	62,62,62,62	0
54	MG	1A	3181	1/1	0.94	0.16	51,51,51,51	0
54	MG	1V	201	1/1	0.94	0.19	29,29,29,29	0
54	MG	2A	3493	1/1	0.94	0.11	35,35,35,35	0
54	MG	1A	3971	1/1	0.94	0.14	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	1a	3130	1/1	0.94	0.07	53,53,53,53	0
54	MG	2A	3007	1/1	0.94	0.06	37,37,37,37	0
54	MG	2P	201	1/1	0.94	0.09	51,51,51,51	0
54	MG	1A	3972	1/1	0.94	0.09	53,53,53,53	0
54	MG	2Q	203	1/1	0.94	0.07	51,51,51,51	0
54	MG	1A	3231	1/1	0.94	0.21	24,24,24,24	0
54	MG	1A	3182	1/1	0.94	0.17	53,53,53,53	0
54	MG	2A	3020	1/1	0.94	0.19	31,31,31,31	0
54	MG	1A	3324	1/1	0.94	0.10	53,53,53,53	0
54	MG	2A	3510	1/1	0.94	0.16	42,42,42,42	0
54	MG	2W	201	1/1	0.94	0.17	41,41,41,41	0
54	MG	10	105	1/1	0.94	0.10	54,54,54,54	0
54	MG	2X	102	1/1	0.94	0.12	58,58,58,58	0
54	MG	1A	3668	1/1	0.94	0.15	51,51,51,51	0
54	MG	1A	3430	1/1	0.94	0.07	26,26,26,26	0
54	MG	2A	3515	1/1	0.94	0.08	60,60,60,60	0
54	MG	2A	3516	1/1	0.94	0.08	46,46,46,46	0
54	MG	1A	3233	1/1	0.94	0.14	28,28,28,28	0
54	MG	2A	3028	1/1	0.94	0.11	41,41,41,41	0
54	MG	1A	3092	1/1	0.94	0.30	32,32,32,32	0
54	MG	1A	3184	1/1	0.94	0.06	43,43,43,43	0
54	MG	2A	3262	1/1	0.94	0.18	50,50,50,50	0
54	MG	2a	3005	1/1	0.94	0.09	50,50,50,50	0
54	MG	1A	3094	1/1	0.94	0.12	27,27,27,27	0
54	MG	1A	3678	1/1	0.94	0.11	14,14,14,14	0
54	MG	1A	3986	1/1	0.94	0.08	24,24,24,24	0
54	MG	2A	3038	1/1	0.94	0.14	50,50,50,50	0
54	MG	1a	3152	1/1	0.94	0.13	47,47,47,47	0
54	MG	1A	3988	1/1	0.94	0.11	57,57,57,57	0
54	MG	1A	3010	1/1	0.94	0.15	39,39,39,39	0
54	MG	17	101	1/1	0.94	0.11	37,37,37,37	0
54	MG	17	102	1/1	0.94	0.10	32,32,32,32	0
54	MG	1A	3187	1/1	0.94	0.13	25,25,25,25	0
54	MG	1a	3160	1/1	0.94	0.09	48,48,48,48	0
54	MG	18	101	1/1	0.94	0.15	25,25,25,25	0
54	MG	1A	3334	1/1	0.94	0.16	55,55,55,55	0
54	MG	1A	3440	1/1	0.94	0.10	48,48,48,48	0
54	MG	1A	3100	1/1	0.94	0.18	34,34,34,34	0
54	MG	1A	3821	1/1	0.94	0.10	48,48,48,48	0
54	MG	2a	3027	1/1	0.94	0.23	64,64,64,64	0
54	MG	2A	3541	1/1	0.94	0.10	33,33,33,33	0
54	MG	2A	3542	1/1	0.94	0.06	42,42,42,42	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	2A	3059	1/1	0.94	0.22	45,45,45,45	0
54	MG	1A	3138	1/1	0.94	0.08	34,34,34,34	0
54	MG	1a	3170	1/1	0.94	0.06	64,64,64,64	0
54	MG	2A	3293	1/1	0.94	0.08	39,39,39,39	0
54	MG	1A	3824	1/1	0.94	0.11	51,51,51,51	0
54	MG	2a	3038	1/1	0.94	0.05	70,70,70,70	0
54	MG	1a	3173	1/1	0.94	0.13	54,54,54,54	0
54	MG	1a	3174	1/1	0.94	0.12	60,60,60,60	0
54	MG	1A	3251	1/1	0.94	0.11	34,34,34,34	0
54	MG	2A	3300	1/1	0.94	0.09	71,71,71,71	0
54	MG	1a	3177	1/1	0.94	0.07	57,57,57,57	0
54	MG	2A	3071	1/1	0.94	0.13	34,34,34,34	0
54	MG	1A	4004	1/1	0.94	0.09	36,36,36,36	0
54	MG	2A	3564	1/1	0.94	0.08	55,55,55,55	0
54	MG	1A	3833	1/1	0.94	0.09	46,46,46,46	0
54	MG	2a	3049	1/1	0.94	0.19	44,44,44,44	0
54	MG	2A	3076	1/1	0.94	0.08	44,44,44,44	0
54	MG	2A	3311	1/1	0.94	0.16	49,49,49,49	0
54	MG	2A	3312	1/1	0.94	0.13	42,42,42,42	0
54	MG	1a	3180	1/1	0.94	0.07	63,63,63,63	0
54	MG	2A	3314	1/1	0.94	0.12	47,47,47,47	0
54	MG	1A	3834	1/1	0.94	0.09	21,21,21,21	0
54	MG	2A	3316	1/1	0.94	0.07	19,19,19,19	0
54	MG	1A	3139	1/1	0.94	0.12	21,21,21,21	0
54	MG	1A	3031	1/1	0.94	0.11	17,17,17,17	0
54	MG	1A	3582	1/1	0.94	0.08	48,48,48,48	0
54	MG	1a	3015	1/1	0.94	0.15	63,63,63,63	0
54	MG	1A	3346	1/1	0.94	0.15	12,12,12,12	0
54	MG	1A	3263	1/1	0.94	0.14	34,34,34,34	0
54	MG	1A	4016	1/1	0.94	0.12	25,25,25,25	0
54	MG	1A	4018	1/1	0.94	0.22	53,53,53,53	0
54	MG	1A	3463	1/1	0.94	0.13	55,55,55,55	0
54	MG	2a	3071	1/1	0.94	0.14	61,61,61,61	0
54	MG	2A	3334	1/1	0.94	0.07	34,34,34,34	0
54	MG	1A	3589	1/1	0.94	0.13	45,45,45,45	0
54	MG	1A	3590	1/1	0.94	0.12	33,33,33,33	0
54	MG	1A	3591	1/1	0.94	0.15	50,50,50,50	0
54	MG	2A	3099	1/1	0.94	0.12	59,59,59,59	0
54	MG	2A	3598	1/1	0.94	0.06	57,57,57,57	0
54	MG	1A	3705	1/1	0.94	0.07	52,52,52,52	0
54	MG	1A	3002	1/1	0.94	0.07	38,38,38,38	0
54	MG	1A	3268	1/1	0.94	0.25	24,24,24,24	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	2A	3347	1/1	0.94	0.10	31,31,31,31	0
54	MG	2A	3105	1/1	0.94	0.30	45,45,45,45	0
54	MG	2A	3350	1/1	0.94	0.11	50,50,50,50	0
54	MG	1A	3146	1/1	0.94	0.08	39,39,39,39	0
54	MG	2A	3108	1/1	0.94	0.12	46,46,46,46	0
54	MG	1A	3595	1/1	0.94	0.09	18,18,18,18	0
54	MG	1A	4033	1/1	0.94	0.06	29,29,29,29	0
54	MG	1A	3863	1/1	0.94	0.07	39,39,39,39	0
54	MG	1A	3712	1/1	0.94	0.11	39,39,39,39	0
54	MG	2A	3359	1/1	0.94	0.10	26,26,26,26	0
54	MG	2A	3116	1/1	0.94	0.19	61,61,61,61	0
54	MG	2A	3118	1/1	0.94	0.19	39,39,39,39	0
54	MG	1A	3866	1/1	0.94	0.10	41,41,41,41	0
54	MG	2A	3121	1/1	0.94	0.07	38,38,38,38	0
54	MG	2A	3630	1/1	0.94	0.13	49,49,49,49	0
54	MG	1A	3596	1/1	0.94	0.17	35,35,35,35	0
54	MG	1A	3868	1/1	0.94	0.09	40,40,40,40	0
54	MG	2a	3114	1/1	0.94	0.17	51,51,51,51	0
54	MG	2A	3370	1/1	0.94	0.06	44,44,44,44	0
54	MG	1A	3198	1/1	0.94	0.16	50,50,50,50	0
54	MG	1A	3052	1/1	0.94	0.13	11,11,11,11	0
54	MG	2A	3641	1/1	0.94	0.09	74,74,74,74	0
54	MG	1a	3212	1/1	0.94	0.06	60,60,60,60	0
54	MG	1A	4052	1/1	0.94	0.09	45,45,45,45	0
54	MG	2A	3645	1/1	0.94	0.16	48,48,48,48	0
54	MG	2A	3384	1/1	0.94	0.10	61,61,61,61	0
54	MG	2a	3123	1/1	0.94	0.16	63,63,63,63	0
54	MG	2A	3133	1/1	0.94	0.27	61,61,61,61	0
54	MG	2A	3650	1/1	0.94	0.07	52,52,52,52	0
54	MG	2A	3651	1/1	0.94	0.07	72,72,72,72	0
54	MG	1A	3363	1/1	0.94	0.11	17,17,17,17	0
54	MG	2A	3655	1/1	0.94	0.10	52,52,52,52	0
54	MG	2A	3388	1/1	0.94	0.06	49,49,49,49	0
54	MG	1a	3043	1/1	0.94	0.09	47,47,47,47	0
54	MG	1A	3275	1/1	0.94	0.09	49,49,49,49	0
54	MG	1A	3367	1/1	0.94	0.07	28,28,28,28	0
54	MG	1A	3881	1/1	0.94	0.08	30,30,30,30	0
54	MG	1A	3020	1/1	0.94	0.35	33,33,33,33	0
54	MG	1A	3201	1/1	0.94	0.29	39,39,39,39	0
54	MG	1A	3202	1/1	0.94	0.17	47,47,47,47	0
54	MG	1a	3055	1/1	0.94	0.16	41,41,41,41	0
54	MG	2a	3144	1/1	0.94	0.08	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	3613	1/1	0.94	0.08	39,39,39,39	0
54	MG	2a	3146	1/1	0.94	0.08	70,70,70,70	0
54	MG	1A	3151	1/1	0.94	0.12	36,36,36,36	0
54	MG	1A	3730	1/1	0.94	0.33	30,30,30,30	0
54	MG	2a	3150	1/1	0.94	0.11	64,64,64,64	0
54	MG	1A	3205	1/1	0.94	0.17	38,38,38,38	0
54	MG	1a	3063	1/1	0.94	0.10	53,53,53,53	0
54	MG	1B	215	1/1	0.94	0.11	50,50,50,50	0
54	MG	2A	3408	1/1	0.94	0.13	41,41,41,41	0
54	MG	1A	3110	1/1	0.94	0.25	27,27,27,27	0
54	MG	2a	3161	1/1	0.94	0.08	66,66,66,66	0
54	MG	1A	3895	1/1	0.94	0.08	17,17,17,17	0
54	MG	2A	3702	1/1	0.94	0.09	66,66,66,66	0
54	MG	1a	3239	1/1	0.94	0.12	47,47,47,47	0
54	MG	1A	3734	1/1	0.94	0.14	33,33,33,33	0
54	MG	2A	3708	1/1	0.94	0.08	49,49,49,49	0
54	MG	2A	3417	1/1	0.94	0.07	33,33,33,33	0
54	MG	2A	3420	1/1	0.94	0.10	59,59,59,59	0
54	MG	2a	3171	1/1	0.94	0.10	68,68,68,68	0
54	MG	1A	3115	1/1	0.94	0.29	24,24,24,24	0
54	MG	2A	3714	1/1	0.94	0.14	39,39,39,39	0
54	MG	2a	3176	1/1	0.94	0.13	63,63,63,63	0
54	MG	1a	3069	1/1	0.94	0.19	40,40,40,40	0
54	MG	1A	3619	1/1	0.94	0.08	33,33,33,33	0
54	MG	1A	3290	1/1	0.94	0.15	43,43,43,43	0
54	MG	1A	3209	1/1	0.94	0.10	34,34,34,34	0
54	MG	2A	3719	1/1	0.94	0.10	61,61,61,61	0
54	MG	1D	301	1/1	0.94	0.39	28,28,28,28	0
54	MG	1A	3502	1/1	0.94	0.12	15,15,15,15	0
54	MG	1A	3908	1/1	0.94	0.07	37,37,37,37	0
54	MG	1A	3745	1/1	0.94	0.08	48,48,48,48	0
54	MG	2a	3190	1/1	0.94	0.09	60,60,60,60	0
54	MG	2A	3183	1/1	0.94	0.11	51,51,51,51	0
54	MG	2A	3731	1/1	0.94	0.06	70,70,70,70	0
54	MG	1A	3747	1/1	0.94	0.08	32,32,32,32	0
54	MG	1A	3748	1/1	0.94	0.17	61,61,61,61	0
54	MG	1A	3061	1/1	0.94	0.10	40,40,40,40	0
54	MG	1A	3509	1/1	0.94	0.05	26,26,26,26	0
54	MG	2A	3737	1/1	0.94	0.05	67,67,67,67	0
54	MG	1A	3511	1/1	0.94	0.10	26,26,26,26	0
54	MG	2e	202	1/1	0.94	0.07	66,66,66,66	0
54	MG	2A	3740	1/1	0.94	0.13	48,48,48,48	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	1A	3300	1/1	0.94	0.08	46,46,46,46	0
54	MG	1A	3755	1/1	0.94	0.06	30,30,30,30	0
54	MG	2A	3745	1/1	0.94	0.16	50,50,50,50	0
54	MG	1A	3633	1/1	0.94	0.07	26,26,26,26	0
54	MG	2A	3442	1/1	0.94	0.07	38,38,38,38	0
54	MG	1A	3168	1/1	0.94	0.07	36,36,36,36	0
54	MG	1A	3216	1/1	0.94	0.15	43,43,43,43	0
54	MG	1A	3079	1/1	0.94	0.14	29,29,29,29	0
54	MG	1a	3277	1/1	0.94	0.10	65,65,65,65	0
54	MG	1a	3278	1/1	0.94	0.20	66,66,66,66	0
54	MG	1A	3310	1/1	0.94	0.08	45,45,45,45	0
54	MG	2A	3453	1/1	0.94	0.09	54,54,54,54	0
54	MG	1a	3105	1/1	0.95	0.19	46,46,46,46	0
54	MG	1A	3192	1/1	0.95	0.15	44,44,44,44	0
54	MG	1A	3817	1/1	0.95	0.06	38,38,38,38	0
54	MG	1T	202	1/1	0.95	0.08	47,47,47,47	0
54	MG	1A	3149	1/1	0.95	0.16	36,36,36,36	0
54	MG	1A	3121	1/1	0.95	0.21	39,39,39,39	0
54	MG	1A	3699	1/1	0.95	0.08	16,16,16,16	0
54	MG	1A	3243	1/1	0.95	0.12	60,60,60,60	0
54	MG	1A	3495	1/1	0.95	0.07	24,24,24,24	0
54	MG	1A	3979	1/1	0.95	0.09	51,51,51,51	0
54	MG	2A	3216	1/1	0.95	0.09	49,49,49,49	0
54	MG	2A	3466	1/1	0.95	0.08	58,58,58,58	0
54	MG	2A	3217	1/1	0.95	0.12	34,34,34,34	0
54	MG	1A	3826	1/1	0.95	0.12	39,39,39,39	0
54	MG	1n	103	1/1	0.95	0.20	54,54,54,54	0
54	MG	1A	3830	1/1	0.95	0.08	44,44,44,44	0
54	MG	1A	3831	1/1	0.95	0.07	39,39,39,39	0
54	MG	1A	3390	1/1	0.95	0.06	28,28,28,28	0
54	MG	2A	3223	1/1	0.95	0.16	48,48,48,48	0
54	MG	1a	3128	1/1	0.95	0.10	54,54,54,54	0
54	MG	2A	3225	1/1	0.95	0.10	45,45,45,45	0
54	MG	1A	3599	1/1	0.95	0.20	39,39,39,39	0
54	MG	1A	3987	1/1	0.95	0.07	39,39,39,39	0
54	MG	1y	204	1/1	0.95	0.06	63,63,63,63	0
54	MG	1A	3093	1/1	0.95	0.06	29,29,29,29	0
54	MG	1A	3836	1/1	0.95	0.16	28,28,28,28	0
54	MG	2A	3232	1/1	0.95	0.11	50,50,50,50	0
54	MG	1A	3837	1/1	0.95	0.14	26,26,26,26	0
54	MG	1a	3135	1/1	0.95	0.09	41,41,41,41	0
54	MG	1A	3156	1/1	0.95	0.17	23,23,23,23	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	2A	3238	1/1	0.95	0.16	35,35,35,35	0
54	MG	1A	3058	1/1	0.95	0.04	39,39,39,39	0
54	MG	1A	3060	1/1	0.95	0.14	27,27,27,27	0
54	MG	2A	3010	1/1	0.95	0.23	58,58,58,58	0
54	MG	1A	3842	1/1	0.95	0.06	24,24,24,24	0
54	MG	2A	3013	1/1	0.95	0.07	24,24,24,24	0
54	MG	1a	3141	1/1	0.95	0.18	64,64,64,64	0
54	MG	2A	3498	1/1	0.95	0.07	38,38,38,38	0
54	MG	11	104	1/1	0.95	0.06	33,33,33,33	0
54	MG	1A	3607	1/1	0.95	0.15	53,53,53,53	0
54	MG	2P	202	1/1	0.95	0.07	48,48,48,48	0
54	MG	1A	3252	1/1	0.95	0.18	37,37,37,37	0
54	MG	13	104	1/1	0.95	0.06	46,46,46,46	0
54	MG	1A	3163	1/1	0.95	0.07	45,45,45,45	0
54	MG	1A	3257	1/1	0.95	0.09	37,37,37,37	0
54	MG	2A	3511	1/1	0.95	0.10	66,66,66,66	0
54	MG	1A	4005	1/1	0.95	0.07	61,61,61,61	0
54	MG	1A	3166	1/1	0.95	0.23	40,40,40,40	0
54	MG	15	103	1/1	0.95	0.26	32,32,32,32	0
54	MG	1a	3155	1/1	0.95	0.08	61,61,61,61	0
54	MG	2A	3034	1/1	0.95	0.24	53,53,53,53	0
54	MG	2A	3258	1/1	0.95	0.24	59,59,59,59	0
54	MG	20	101	1/1	0.95	0.15	41,41,41,41	0
54	MG	2A	3259	1/1	0.95	0.06	48,48,48,48	0
54	MG	1A	3099	1/1	0.95	0.17	37,37,37,37	0
54	MG	1A	3514	1/1	0.95	0.10	13,13,13,13	0
54	MG	1A	3265	1/1	0.95	0.14	40,40,40,40	0
54	MG	23	102	1/1	0.95	0.07	35,35,35,35	0
54	MG	25	101	1/1	0.95	0.34	36,36,36,36	0
54	MG	1A	3858	1/1	0.95	0.06	48,48,48,48	0
54	MG	2A	3266	1/1	0.95	0.16	35,35,35,35	0
54	MG	2A	3040	1/1	0.95	0.15	48,48,48,48	0
54	MG	2A	3268	1/1	0.95	0.15	44,44,44,44	0
54	MG	2a	3004	1/1	0.95	0.06	41,41,41,41	0
54	MG	2A	3042	1/1	0.95	0.12	43,43,43,43	0
54	MG	17	104	1/1	0.95	0.10	36,36,36,36	0
54	MG	1A	3169	1/1	0.95	0.07	36,36,36,36	0
54	MG	1A	3620	1/1	0.95	0.07	36,36,36,36	0
54	MG	1A	3408	1/1	0.95	0.08	26,26,26,26	0
54	MG	1A	3267	1/1	0.95	0.26	34,34,34,34	0
54	MG	2A	3048	1/1	0.95	0.12	54,54,54,54	0
54	MG	2A	3280	1/1	0.95	0.07	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	3049	1/1	0.95	0.12	54,54,54,54	0
54	MG	2a	3018	1/1	0.95	0.07	40,40,40,40	0
54	MG	1a	3167	1/1	0.95	0.12	56,56,56,56	0
54	MG	1A	4019	1/1	0.95	0.10	54,54,54,54	0
54	MG	1A	3410	1/1	0.95	0.07	17,17,17,17	0
54	MG	2A	3055	1/1	0.95	0.11	41,41,41,41	0
54	MG	2A	3287	1/1	0.95	0.09	33,33,33,33	0
54	MG	1a	3171	1/1	0.95	0.06	72,72,72,72	0
54	MG	1A	3008	1/1	0.95	0.09	31,31,31,31	0
54	MG	2A	3545	1/1	0.95	0.07	47,47,47,47	0
54	MG	1A	3018	1/1	0.95	0.13	23,23,23,23	0
54	MG	1a	3006	1/1	0.95	0.07	57,57,57,57	0
54	MG	1A	3630	1/1	0.95	0.10	45,45,45,45	0
54	MG	2A	3550	1/1	0.95	0.09	25,25,25,25	0
54	MG	1a	3176	1/1	0.95	0.10	45,45,45,45	0
54	MG	2A	3552	1/1	0.95	0.06	47,47,47,47	0
54	MG	2A	3553	1/1	0.95	0.07	47,47,47,47	0
54	MG	2A	3555	1/1	0.95	0.05	47,47,47,47	0
54	MG	2a	3037	1/1	0.95	0.11	55,55,55,55	0
54	MG	2A	3063	1/1	0.95	0.08	46,46,46,46	0
54	MG	1a	3008	1/1	0.95	0.07	46,46,46,46	0
54	MG	1A	3419	1/1	0.95	0.07	19,19,19,19	0
54	MG	1A	3873	1/1	0.95	0.07	24,24,24,24	0
54	MG	2A	3301	1/1	0.95	0.10	27,27,27,27	0
54	MG	1A	3420	1/1	0.95	0.09	19,19,19,19	0
54	MG	1A	3063	1/1	0.95	0.06	24,24,24,24	0
54	MG	1A	4030	1/1	0.95	0.07	36,36,36,36	0
54	MG	1A	3535	1/1	0.95	0.06	40,40,40,40	0
54	MG	2a	3047	1/1	0.95	0.12	53,53,53,53	0
54	MG	2A	3307	1/1	0.95	0.06	28,28,28,28	0
54	MG	1A	3743	1/1	0.95	0.10	55,55,55,55	0
54	MG	1A	3427	1/1	0.95	0.11	50,50,50,50	0
54	MG	2A	3077	1/1	0.95	0.19	51,51,51,51	0
54	MG	1A	3537	1/1	0.95	0.09	23,23,23,23	0
54	MG	1A	4040	1/1	0.95	0.07	55,55,55,55	0
54	MG	1A	4042	1/1	0.95	0.28	40,40,40,40	0
54	MG	1A	4043	1/1	0.95	0.21	43,43,43,43	0
54	MG	1A	3639	1/1	0.95	0.10	45,45,45,45	0
54	MG	2A	3086	1/1	0.95	0.10	43,43,43,43	0
54	MG	1A	3340	1/1	0.95	0.07	29,29,29,29	0
54	MG	1A	3342	1/1	0.95	0.14	54,54,54,54	0
54	MG	2A	3322	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	1A	3211	1/1	0.95	0.12	27,27,27,27	0
54	MG	2A	3325	1/1	0.95	0.09	35,35,35,35	0
54	MG	1A	3106	1/1	0.95	0.12	18,18,18,18	0
54	MG	1A	3178	1/1	0.95	0.11	25,25,25,25	0
54	MG	1A	3549	1/1	0.95	0.06	57,57,57,57	0
54	MG	2A	3593	1/1	0.95	0.11	45,45,45,45	0
54	MG	2A	3594	1/1	0.95	0.11	49,49,49,49	0
54	MG	1A	3133	1/1	0.95	0.16	21,21,21,21	0
54	MG	2A	3333	1/1	0.95	0.09	50,50,50,50	0
54	MG	2a	3075	1/1	0.95	0.05	51,51,51,51	0
54	MG	1A	3761	1/1	0.95	0.13	38,38,38,38	0
54	MG	1B	204	1/1	0.95	0.08	40,40,40,40	0
54	MG	1A	3135	1/1	0.95	0.06	42,42,42,42	0
54	MG	2a	3081	1/1	0.95	0.17	60,60,60,60	0
54	MG	1A	3651	1/1	0.95	0.08	32,32,32,32	0
54	MG	1A	3554	1/1	0.95	0.07	44,44,44,44	0
54	MG	1A	3355	1/1	0.95	0.05	28,28,28,28	0
54	MG	1A	3007	1/1	0.95	0.12	41,41,41,41	0
54	MG	2a	3090	1/1	0.95	0.10	63,63,63,63	0
54	MG	2A	3106	1/1	0.95	0.10	37,37,37,37	0
54	MG	1A	3912	1/1	0.95	0.11	35,35,35,35	0
54	MG	1A	3557	1/1	0.95	0.07	48,48,48,48	0
54	MG	1A	3137	1/1	0.95	0.23	36,36,36,36	0
54	MG	1a	3215	1/1	0.95	0.07	73,73,73,73	0
54	MG	1A	3053	1/1	0.95	0.20	24,24,24,24	0
54	MG	1A	3778	1/1	0.95	0.13	28,28,28,28	0
54	MG	1a	3046	1/1	0.95	0.19	41,41,41,41	0
54	MG	1A	3660	1/1	0.95	0.20	28,28,28,28	0
54	MG	1a	3221	1/1	0.95	0.06	35,35,35,35	0
54	MG	2A	3358	1/1	0.95	0.10	49,49,49,49	0
54	MG	1A	3360	1/1	0.95	0.11	34,34,34,34	0
54	MG	1B	220	1/1	0.95	0.11	40,40,40,40	0
54	MG	2A	3126	1/1	0.95	0.13	40,40,40,40	0
54	MG	1B	221	1/1	0.95	0.10	38,38,38,38	0
54	MG	1B	222	1/1	0.95	0.12	45,45,45,45	0
54	MG	1A	3783	1/1	0.95	0.09	51,51,51,51	0
54	MG	1A	3564	1/1	0.95	0.07	20,20,20,20	0
54	MG	1A	3568	1/1	0.95	0.11	42,42,42,42	0
54	MG	1a	3059	1/1	0.95	0.14	48,48,48,48	0
54	MG	2A	3378	1/1	0.95	0.10	73,73,73,73	0
54	MG	1A	3085	1/1	0.95	0.39	37,37,37,37	0
54	MG	1A	3142	1/1	0.95	0.07	26,26,26,26	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	1D	304	1/1	0.95	0.08	19,19,19,19	0
54	MG	1A	3450	1/1	0.95	0.07	30,30,30,30	0
54	MG	1A	3790	1/1	0.95	0.07	28,28,28,28	0
54	MG	2A	3653	1/1	0.95	0.08	55,55,55,55	0
54	MG	2A	3144	1/1	0.95	0.04	41,41,41,41	0
54	MG	1D	307	1/1	0.95	0.12	10,10,10,10	0
54	MG	2A	3147	1/1	0.95	0.07	27,27,27,27	0
54	MG	2a	3130	1/1	0.95	0.11	61,61,61,61	0
54	MG	2A	3666	1/1	0.95	0.08	54,54,54,54	0
54	MG	1A	3291	1/1	0.95	0.08	18,18,18,18	0
54	MG	1D	312	1/1	0.95	0.08	32,32,32,32	0
54	MG	1D	313	1/1	0.95	0.09	43,43,43,43	0
54	MG	2A	3674	1/1	0.95	0.07	42,42,42,42	0
54	MG	1D	314	1/1	0.95	0.08	44,44,44,44	0
54	MG	2A	3155	1/1	0.95	0.06	46,46,46,46	0
54	MG	1a	3244	1/1	0.95	0.07	47,47,47,47	0
54	MG	1a	3245	1/1	0.95	0.06	31,31,31,31	0
54	MG	1a	3246	1/1	0.95	0.09	47,47,47,47	0
54	MG	1A	3365	1/1	0.95	0.09	40,40,40,40	0
54	MG	2A	3681	1/1	0.95	0.09	36,36,36,36	0
54	MG	2A	3160	1/1	0.95	0.15	49,49,49,49	0
54	MG	1a	3073	1/1	0.95	0.21	52,52,52,52	0
54	MG	1D	317	1/1	0.95	0.06	43,43,43,43	0
54	MG	2A	3164	1/1	0.95	0.23	45,45,45,45	0
54	MG	2A	3688	1/1	0.95	0.07	42,42,42,42	0
54	MG	2A	3406	1/1	0.95	0.12	49,49,49,49	0
54	MG	1A	3455	1/1	0.95	0.06	16,16,16,16	0
54	MG	1a	3256	1/1	0.95	0.06	39,39,39,39	0
54	MG	1E	304	1/1	0.95	0.08	15,15,15,15	0
54	MG	2a	3160	1/1	0.95	0.07	57,57,57,57	0
54	MG	2A	3703	1/1	0.95	0.07	55,55,55,55	0
54	MG	2A	3411	1/1	0.95	0.08	54,54,54,54	0
54	MG	2A	3412	1/1	0.95	0.06	27,27,27,27	0
54	MG	1A	3796	1/1	0.95	0.24	39,39,39,39	0
54	MG	1A	3797	1/1	0.95	0.07	45,45,45,45	0
54	MG	1A	3225	1/1	0.95	0.13	28,28,28,28	0
54	MG	2A	3419	1/1	0.95	0.10	37,37,37,37	0
54	MG	1a	3261	1/1	0.95	0.05	55,55,55,55	0
54	MG	1F	303	1/1	0.95	0.19	30,30,30,30	0
54	MG	2A	3174	1/1	0.95	0.23	45,45,45,45	0
54	MG	1a	3263	1/1	0.95	0.10	38,38,38,38	0
54	MG	1A	3799	1/1	0.95	0.09	32,32,32,32	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	1a	3087	1/1	0.95	0.18	48,48,48,48	0
54	MG	1A	3113	1/1	0.95	0.27	37,37,37,37	0
54	MG	2A	3182	1/1	0.95	0.15	39,39,39,39	0
54	MG	1A	3114	1/1	0.95	0.15	28,28,28,28	0
54	MG	1A	3466	1/1	0.95	0.10	37,37,37,37	0
54	MG	2A	3727	1/1	0.95	0.09	50,50,50,50	0
54	MG	2A	3728	1/1	0.95	0.07	40,40,40,40	0
54	MG	1A	3958	1/1	0.95	0.08	29,29,29,29	0
54	MG	1A	3301	1/1	0.95	0.08	35,35,35,35	0
54	MG	2a	3188	1/1	0.95	0.08	77,77,77,77	0
54	MG	1G	203	1/1	0.95	0.07	52,52,52,52	0
54	MG	2A	3433	1/1	0.95	0.09	39,39,39,39	0
54	MG	2A	3434	1/1	0.95	0.10	55,55,55,55	0
54	MG	2A	3735	1/1	0.95	0.14	46,46,46,46	0
54	MG	2A	3189	1/1	0.95	0.12	62,62,62,62	0
54	MG	1A	3054	1/1	0.95	0.07	23,23,23,23	0
54	MG	2A	3738	1/1	0.95	0.10	51,51,51,51	0
54	MG	1H	202	1/1	0.95	0.09	38,38,38,38	0
54	MG	1A	3087	1/1	0.95	0.12	34,34,34,34	0
54	MG	1A	3023	1/1	0.95	0.07	22,22,22,22	0
54	MG	1A	3478	1/1	0.95	0.13	61,61,61,61	0
54	MG	1A	3309	1/1	0.95	0.29	31,31,31,31	0
54	MG	1A	3969	1/1	0.95	0.07	51,51,51,51	0
54	MG	2t	3100	1/1	0.95	0.10	48,48,48,48	0
55	YXM	1A	4055	40/40	0.95	0.10	16,31,46,48	0
54	MG	2A	3747	1/1	0.95	0.09	54,54,54,54	0
54	MG	2A	3445	1/1	0.95	0.09	58,58,58,58	0
54	MG	2A	3446	1/1	0.95	0.07	37,37,37,37	0
54	MG	2A	3198	1/1	0.95	0.18	38,38,38,38	0
54	MG	1d	303	1/1	0.95	0.11	45,45,45,45	0
54	MG	2A	3752	1/1	0.95	0.12	51,51,51,51	0
54	MG	1A	3482	1/1	0.95	0.08	51,51,51,51	0
54	MG	2A	3450	1/1	0.95	0.08	48,48,48,48	0
54	MG	1A	3236	1/1	0.95	0.16	25,25,25,25	0
54	MG	1e	201	1/1	0.95	0.12	44,44,44,44	0
58	ZN	2n	102	1/1	0.95	0.09	93,93,93,93	0
54	MG	1a	3009	1/1	0.96	0.21	44,44,44,44	0
54	MG	1A	3171	1/1	0.96	0.09	47,47,47,47	0
54	MG	2A	3741	1/1	0.96	0.09	40,40,40,40	0
54	MG	1A	3044	1/1	0.96	0.09	22,22,22,22	0
54	MG	1A	3664	1/1	0.96	0.06	28,28,28,28	0
54	MG	1A	3665	1/1	0.96	0.07	48,48,48,48	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	1A	4012	1/1	0.96	0.32	35,35,35,35	0
54	MG	1A	3425	1/1	0.96	0.07	21,21,21,21	0
54	MG	2A	3162	1/1	0.96	0.12	48,48,48,48	0
54	MG	1A	3336	1/1	0.96	0.06	47,47,47,47	0
54	MG	1A	3669	1/1	0.96	0.11	45,45,45,45	0
54	MG	2A	3165	1/1	0.96	0.11	54,54,54,54	0
54	MG	1A	4017	1/1	0.96	0.05	60,60,60,60	0
54	MG	1A	3829	1/1	0.96	0.07	40,40,40,40	0
54	MG	1A	3547	1/1	0.96	0.12	22,22,22,22	0
54	MG	1A	3174	1/1	0.96	0.10	35,35,35,35	0
54	MG	1A	3832	1/1	0.96	0.08	54,54,54,54	0
54	MG	1A	3338	1/1	0.96	0.07	21,21,21,21	0
54	MG	1A	3045	1/1	0.96	0.08	33,33,33,33	0
54	MG	1A	3084	1/1	0.96	0.20	34,34,34,34	0
54	MG	1A	4026	1/1	0.96	0.19	10,10,10,10	0
54	MG	2A	3439	1/1	0.96	0.07	38,38,38,38	0
54	MG	2A	3176	1/1	0.96	0.08	33,33,33,33	0
54	MG	1A	3552	1/1	0.96	0.05	35,35,35,35	0
54	MG	1A	3679	1/1	0.96	0.07	41,41,41,41	0
54	MG	1A	3838	1/1	0.96	0.37	28,28,28,28	0
54	MG	1A	3111	1/1	0.96	0.10	21,21,21,21	0
54	MG	1A	3434	1/1	0.96	0.09	12,12,12,12	0
54	MG	1A	3215	1/1	0.96	0.19	23,23,23,23	0
54	MG	2A	3184	1/1	0.96	0.21	38,38,38,38	0
54	MG	1A	4034	1/1	0.96	0.06	50,50,50,50	0
54	MG	1A	3272	1/1	0.96	0.18	27,27,27,27	0
54	MG	2B	216	1/1	0.96	0.06	53,53,53,53	0
54	MG	1A	3437	1/1	0.96	0.06	48,48,48,48	0
54	MG	1A	3560	1/1	0.96	0.09	35,35,35,35	0
54	MG	1A	4041	1/1	0.96	0.06	41,41,41,41	0
54	MG	1a	3253	1/1	0.96	0.05	61,61,61,61	0
54	MG	2A	3455	1/1	0.96	0.07	51,51,51,51	0
54	MG	2A	3191	1/1	0.96	0.10	61,61,61,61	0
54	MG	2D	307	1/1	0.96	0.10	63,63,63,63	0
54	MG	1A	3687	1/1	0.96	0.06	38,38,38,38	0
54	MG	1A	3022	1/1	0.96	0.06	29,29,29,29	0
54	MG	1A	3347	1/1	0.96	0.15	33,33,33,33	0
54	MG	1A	3690	1/1	0.96	0.08	50,50,50,50	0
54	MG	1A	3349	1/1	0.96	0.08	14,14,14,14	0
54	MG	1A	3565	1/1	0.96	0.04	29,29,29,29	0
54	MG	1A	4049	1/1	0.96	0.09	52,52,52,52	0
54	MG	1A	3856	1/1	0.96	0.07	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	1A	3566	1/1	0.96	0.14	27,27,27,27	0
54	MG	1a	3053	1/1	0.96	0.19	61,61,61,61	0
54	MG	1A	4053	1/1	0.96	0.14	56,56,56,56	0
54	MG	1A	3567	1/1	0.96	0.04	36,36,36,36	0
54	MG	1A	3441	1/1	0.96	0.08	35,35,35,35	0
54	MG	1A	3351	1/1	0.96	0.13	9,9,9,9	0
54	MG	2A	3207	1/1	0.96	0.09	42,42,42,42	0
54	MG	1A	3443	1/1	0.96	0.06	18,18,18,18	0
54	MG	1a	3060	1/1	0.96	0.21	57,57,57,57	0
54	MG	1a	3061	1/1	0.96	0.16	59,59,59,59	0
54	MG	1A	3444	1/1	0.96	0.10	13,13,13,13	0
54	MG	1A	3050	1/1	0.96	0.20	30,30,30,30	0
54	MG	2Q	201	1/1	0.96	0.06	60,60,60,60	0
54	MG	2A	3481	1/1	0.96	0.12	19,19,19,19	0
54	MG	1A	3446	1/1	0.96	0.14	32,32,32,32	0
54	MG	2R	201	1/1	0.96	0.15	47,47,47,47	0
54	MG	1A	3051	1/1	0.96	0.17	36,36,36,36	0
54	MG	2R	203	1/1	0.96	0.05	19,19,19,19	0
54	MG	1A	3707	1/1	0.96	0.06	26,26,26,26	0
54	MG	1A	3144	1/1	0.96	0.06	20,20,20,20	0
54	MG	1A	3577	1/1	0.96	0.05	35,35,35,35	0
54	MG	1A	3278	1/1	0.96	0.07	26,26,26,26	0
54	MG	1A	3117	1/1	0.96	0.10	24,24,24,24	0
54	MG	2W	202	1/1	0.96	0.13	53,53,53,53	0
54	MG	1A	3713	1/1	0.96	0.21	24,24,24,24	0
54	MG	1A	3580	1/1	0.96	0.06	46,46,46,46	0
54	MG	1A	3453	1/1	0.96	0.05	39,39,39,39	0
54	MG	1A	3884	1/1	0.96	0.08	56,56,56,56	0
54	MG	1A	3281	1/1	0.96	0.16	22,22,22,22	0
54	MG	1A	3283	1/1	0.96	0.26	40,40,40,40	0
54	MG	1a	3077	1/1	0.96	0.13	39,39,39,39	0
54	MG	1g	203	1/1	0.96	0.14	57,57,57,57	0
54	MG	2A	3499	1/1	0.96	0.08	25,25,25,25	0
54	MG	1A	3221	1/1	0.96	0.10	40,40,40,40	0
54	MG	27	101	1/1	0.96	0.19	38,38,38,38	0
54	MG	1a	3080	1/1	0.96	0.13	37,37,37,37	0
54	MG	28	101	1/1	0.96	0.08	54,54,54,54	0
54	MG	1k	201	1/1	0.96	0.17	36,36,36,36	0
54	MG	2a	3001	1/1	0.96	0.06	31,31,31,31	0
54	MG	2A	3507	1/1	0.96	0.09	53,53,53,53	0
54	MG	1a	3081	1/1	0.96	0.13	53,53,53,53	0
54	MG	2A	3234	1/1	0.96	0.36	45,45,45,45	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	1A	3889	1/1	0.96	0.07	45,45,45,45	0
54	MG	1A	3459	1/1	0.96	0.08	45,45,45,45	0
54	MG	2A	3237	1/1	0.96	0.08	43,43,43,43	0
54	MG	2a	3008	1/1	0.96	0.09	36,36,36,36	0
54	MG	2a	3009	1/1	0.96	0.05	67,67,67,67	0
54	MG	1a	3084	1/1	0.96	0.13	70,70,70,70	0
54	MG	2A	3239	1/1	0.96	0.23	40,40,40,40	0
54	MG	1A	3462	1/1	0.96	0.07	45,45,45,45	0
54	MG	1A	3001	1/1	0.96	0.04	26,26,26,26	0
54	MG	1D	302	1/1	0.96	0.18	23,23,23,23	0
54	MG	1D	303	1/1	0.96	0.07	46,46,46,46	0
54	MG	1A	3068	1/1	0.96	0.15	30,30,30,30	0
54	MG	1A	3465	1/1	0.96	0.08	35,35,35,35	0
54	MG	1A	3224	1/1	0.96	0.26	32,32,32,32	0
54	MG	2A	3523	1/1	0.96	0.08	38,38,38,38	0
54	MG	1A	3729	1/1	0.96	0.11	33,33,33,33	0
54	MG	1D	308	1/1	0.96	0.07	45,45,45,45	0
54	MG	1D	309	1/1	0.96	0.14	25,25,25,25	0
54	MG	1A	3901	1/1	0.96	0.06	24,24,24,24	0
54	MG	1a	3096	1/1	0.96	0.23	43,43,43,43	0
54	MG	1A	3471	1/1	0.96	0.05	35,35,35,35	0
54	MG	1A	3024	1/1	0.96	0.10	12,12,12,12	0
54	MG	1a	3099	1/1	0.96	0.09	54,54,54,54	0
54	MG	2a	3030	1/1	0.96	0.19	53,53,53,53	0
54	MG	2a	3031	1/1	0.96	0.13	56,56,56,56	0
54	MG	1A	3473	1/1	0.96	0.10	44,44,44,44	0
54	MG	1A	3905	1/1	0.96	0.06	41,41,41,41	0
54	MG	1A	3907	1/1	0.96	0.12	18,18,18,18	0
54	MG	2A	3014	1/1	0.96	0.06	44,44,44,44	0
54	MG	1A	3025	1/1	0.96	0.15	40,40,40,40	0
54	MG	2A	3261	1/1	0.96	0.27	58,58,58,58	0
54	MG	2A	3018	1/1	0.96	0.07	36,36,36,36	0
54	MG	2A	3263	1/1	0.96	0.13	44,44,44,44	0
54	MG	1A	3369	1/1	0.96	0.06	19,19,19,19	0
54	MG	1A	3916	1/1	0.96	0.06	56,56,56,56	0
54	MG	2A	3022	1/1	0.96	0.07	31,31,31,31	0
54	MG	2A	3023	1/1	0.96	0.16	40,40,40,40	0
54	MG	1A	3736	1/1	0.96	0.06	15,15,15,15	0
54	MG	1A	3919	1/1	0.96	0.09	44,44,44,44	0
54	MG	1A	3230	1/1	0.96	0.20	32,32,32,32	0
54	MG	2A	3273	1/1	0.96	0.32	48,48,48,48	0
54	MG	1F	304	1/1	0.96	0.17	26,26,26,26	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	1F	305	1/1	0.96	0.17	25,25,25,25	0
54	MG	2a	3050	1/1	0.96	0.18	55,55,55,55	0
54	MG	2A	3276	1/1	0.96	0.07	29,29,29,29	0
54	MG	1a	3115	1/1	0.96	0.06	44,44,44,44	0
54	MG	2A	3554	1/1	0.96	0.06	60,60,60,60	0
54	MG	2a	3054	1/1	0.96	0.21	50,50,50,50	0
54	MG	1A	3293	1/1	0.96	0.23	44,44,44,44	0
54	MG	1a	3117	1/1	0.96	0.07	68,68,68,68	0
54	MG	1A	3601	1/1	0.96	0.06	33,33,33,33	0
54	MG	2a	3059	1/1	0.96	0.10	53,53,53,53	0
54	MG	1A	3602	1/1	0.96	0.06	44,44,44,44	0
54	MG	1A	3479	1/1	0.96	0.06	36,36,36,36	0
54	MG	1A	3150	1/1	0.96	0.33	35,35,35,35	0
54	MG	2A	3284	1/1	0.96	0.06	45,45,45,45	0
54	MG	1A	3481	1/1	0.96	0.08	46,46,46,46	0
54	MG	1A	3097	1/1	0.96	0.10	49,49,49,49	0
54	MG	1a	3126	1/1	0.96	0.08	50,50,50,50	0
54	MG	1G	204	1/1	0.96	0.11	37,37,37,37	0
54	MG	1A	3750	1/1	0.96	0.12	28,28,28,28	0
54	MG	1A	3608	1/1	0.96	0.16	51,51,51,51	0
54	MG	1N	201	1/1	0.96	0.12	40,40,40,40	0
54	MG	1N	202	1/1	0.96	0.14	40,40,40,40	0
54	MG	1a	3132	1/1	0.96	0.06	53,53,53,53	0
54	MG	1N	203	1/1	0.96	0.09	58,58,58,58	0
54	MG	1A	3152	1/1	0.96	0.10	40,40,40,40	0
54	MG	1P	201	1/1	0.96	0.40	34,34,34,34	0
54	MG	1A	3937	1/1	0.96	0.06	39,39,39,39	0
54	MG	2a	3078	1/1	0.96	0.16	33,33,33,33	0
54	MG	2A	3054	1/1	0.96	0.09	37,37,37,37	0
54	MG	2a	3080	1/1	0.96	0.14	49,49,49,49	0
54	MG	1A	3488	1/1	0.96	0.12	47,47,47,47	0
54	MG	1A	3234	1/1	0.96	0.15	33,33,33,33	0
54	MG	1Q	201	1/1	0.96	0.08	26,26,26,26	0
54	MG	2a	3085	1/1	0.96	0.25	53,53,53,53	0
54	MG	2a	3086	1/1	0.96	0.36	45,45,45,45	0
54	MG	1a	3140	1/1	0.96	0.07	49,49,49,49	0
54	MG	1Q	204	1/1	0.96	0.10	37,37,37,37	0
54	MG	2A	3060	1/1	0.96	0.09	27,27,27,27	0
54	MG	1R	201	1/1	0.96	0.14	26,26,26,26	0
54	MG	2a	3093	1/1	0.96	0.11	60,60,60,60	0
54	MG	1A	3614	1/1	0.96	0.06	46,46,46,46	0
54	MG	1R	203	1/1	0.96	0.23	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	3490	1/1	0.96	0.08	40,40,40,40	0
54	MG	1a	3148	1/1	0.96	0.06	48,48,48,48	0
54	MG	1A	3947	1/1	0.96	0.08	39,39,39,39	0
54	MG	2A	3317	1/1	0.96	0.08	53,53,53,53	0
54	MG	2A	3068	1/1	0.96	0.05	35,35,35,35	0
54	MG	1A	3759	1/1	0.96	0.14	31,31,31,31	0
54	MG	2a	3102	1/1	0.96	0.05	56,56,56,56	0
54	MG	1A	3153	1/1	0.96	0.28	33,33,33,33	0
54	MG	1A	3382	1/1	0.96	0.16	51,51,51,51	0
54	MG	2A	3072	1/1	0.96	0.14	52,52,52,52	0
54	MG	2A	3073	1/1	0.96	0.19	33,33,33,33	0
54	MG	2A	3324	1/1	0.96	0.12	38,38,38,38	0
54	MG	2a	3110	1/1	0.96	0.08	54,54,54,54	0
54	MG	1A	3098	1/1	0.96	0.05	26,26,26,26	0
54	MG	1A	3019	1/1	0.96	0.19	22,22,22,22	0
54	MG	1A	3157	1/1	0.96	0.16	29,29,29,29	0
54	MG	1a	3157	1/1	0.96	0.06	46,46,46,46	0
54	MG	2A	3331	1/1	0.96	0.09	42,42,42,42	0
54	MG	1A	3621	1/1	0.96	0.09	39,39,39,39	0
54	MG	1A	3388	1/1	0.96	0.06	36,36,36,36	0
54	MG	1A	3959	1/1	0.96	0.07	42,42,42,42	0
54	MG	2A	3628	1/1	0.96	0.05	58,58,58,58	0
54	MG	2A	3082	1/1	0.96	0.25	56,56,56,56	0
54	MG	1A	3057	1/1	0.96	0.12	17,17,17,17	0
54	MG	2A	3339	1/1	0.96	0.07	31,31,31,31	0
54	MG	1A	3961	1/1	0.96	0.06	38,38,38,38	0
54	MG	1A	3625	1/1	0.96	0.28	28,28,28,28	0
54	MG	2a	3126	1/1	0.96	0.11	48,48,48,48	0
54	MG	1A	3311	1/1	0.96	0.12	30,30,30,30	0
54	MG	2A	3088	1/1	0.96	0.09	34,34,34,34	0
54	MG	2A	3637	1/1	0.96	0.04	52,52,52,52	0
54	MG	2A	3639	1/1	0.96	0.07	40,40,40,40	0
54	MG	2A	3345	1/1	0.96	0.12	50,50,50,50	0
54	MG	1V	202	1/1	0.96	0.15	43,43,43,43	0
54	MG	1V	204	1/1	0.96	0.09	40,40,40,40	0
54	MG	2A	3644	1/1	0.96	0.06	57,57,57,57	0
54	MG	2a	3136	1/1	0.96	0.04	47,47,47,47	0
54	MG	2A	3348	1/1	0.96	0.06	24,24,24,24	0
54	MG	1A	3314	1/1	0.96	0.16	31,31,31,31	0
54	MG	1A	3779	1/1	0.96	0.15	38,38,38,38	0
54	MG	2A	3351	1/1	0.96	0.09	21,21,21,21	0
54	MG	1A	3241	1/1	0.96	0.20	36,36,36,36	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	2a	3142	1/1	0.96	0.07	62,62,62,62	0
54	MG	10	101	1/1	0.96	0.11	32,32,32,32	0
54	MG	1A	3242	1/1	0.96	0.12	32,32,32,32	0
54	MG	2A	3654	1/1	0.96	0.06	63,63,63,63	0
54	MG	1A	3782	1/1	0.96	0.08	19,19,19,19	0
54	MG	2A	3662	1/1	0.96	0.05	64,64,64,64	0
54	MG	10	104	1/1	0.96	0.08	44,44,44,44	0
54	MG	1A	3077	1/1	0.96	0.10	22,22,22,22	0
54	MG	1A	3504	1/1	0.96	0.07	51,51,51,51	0
54	MG	2a	3154	1/1	0.96	0.06	50,50,50,50	0
54	MG	1A	3505	1/1	0.96	0.08	16,16,16,16	0
54	MG	2A	3668	1/1	0.96	0.09	49,49,49,49	0
54	MG	1A	3506	1/1	0.96	0.07	15,15,15,15	0
54	MG	1A	3508	1/1	0.96	0.07	59,59,59,59	0
54	MG	1A	3161	1/1	0.96	0.17	40,40,40,40	0
54	MG	1A	3245	1/1	0.96	0.12	32,32,32,32	0
54	MG	2A	3364	1/1	0.96	0.11	70,70,70,70	0
54	MG	1A	3640	1/1	0.96	0.11	46,46,46,46	0
54	MG	2A	3366	1/1	0.96	0.08	42,42,42,42	0
54	MG	2a	3167	1/1	0.96	0.12	65,65,65,65	0
54	MG	1A	3792	1/1	0.96	0.13	38,38,38,38	0
54	MG	2A	3369	1/1	0.96	0.06	44,44,44,44	0
54	MG	1A	3246	1/1	0.96	0.13	26,26,26,26	0
54	MG	2A	3373	1/1	0.96	0.08	53,53,53,53	0
54	MG	1A	3515	1/1	0.96	0.05	53,53,53,53	0
54	MG	2a	3173	1/1	0.96	0.07	47,47,47,47	0
54	MG	1A	3009	1/1	0.96	0.17	25,25,25,25	0
54	MG	1A	3404	1/1	0.96	0.06	20,20,20,20	0
54	MG	15	104	1/1	0.96	0.10	29,29,29,29	0
54	MG	15	105	1/1	0.96	0.25	18,18,18,18	0
54	MG	15	106	1/1	0.96	0.08	41,41,41,41	0
54	MG	2A	3125	1/1	0.96	0.09	34,34,34,34	0
54	MG	2A	3700	1/1	0.96	0.09	56,56,56,56	0
54	MG	1A	3164	1/1	0.96	0.05	23,23,23,23	0
54	MG	16	101	1/1	0.96	0.07	39,39,39,39	0
54	MG	2a	3185	1/1	0.96	0.07	45,45,45,45	0
54	MG	2A	3704	1/1	0.96	0.07	55,55,55,55	0
54	MG	2A	3389	1/1	0.96	0.12	25,25,25,25	0
54	MG	1A	3522	1/1	0.96	0.06	36,36,36,36	0
54	MG	1A	3105	1/1	0.96	0.12	37,37,37,37	0
54	MG	1A	3989	1/1	0.96	0.07	32,32,32,32	0
54	MG	1A	3203	1/1	0.96	0.06	35,35,35,35	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	2a	3193	1/1	0.96	0.07	52,52,52,52	0
54	MG	1A	3030	1/1	0.96	0.04	24,24,24,24	0
54	MG	1A	3134	1/1	0.96	0.25	26,26,26,26	0
54	MG	1A	3653	1/1	0.96	0.07	42,42,42,42	0
54	MG	2a	3197	1/1	0.96	0.10	56,56,56,56	0
54	MG	2A	3136	1/1	0.96	0.18	50,50,50,50	0
54	MG	1A	3258	1/1	0.96	0.19	33,33,33,33	0
54	MG	2a	3200	1/1	0.96	0.12	70,70,70,70	0
54	MG	1A	3655	1/1	0.96	0.13	28,28,28,28	0
54	MG	2A	3141	1/1	0.96	0.14	43,43,43,43	0
54	MG	1a	3205	1/1	0.96	0.09	74,74,74,74	0
54	MG	2A	3722	1/1	0.96	0.11	48,48,48,48	0
54	MG	2A	3143	1/1	0.96	0.13	42,42,42,42	0
54	MG	2A	3403	1/1	0.96	0.07	28,28,28,28	0
54	MG	1A	3808	1/1	0.96	0.09	60,60,60,60	0
55	YXM	2A	3758	40/40	0.96	0.11	28,39,51,52	0
54	MG	2A	3145	1/1	0.96	0.09	28,28,28,28	0
54	MG	1A	3259	1/1	0.96	0.06	65,65,65,65	0
54	MG	1a	3208	1/1	0.96	0.12	53,53,53,53	0
54	MG	1A	3414	1/1	0.96	0.10	15,15,15,15	0
54	MG	2A	3149	1/1	0.96	0.11	48,48,48,48	0
54	MG	1A	3415	1/1	0.96	0.08	19,19,19,19	0
54	MG	2A	3413	1/1	0.96	0.10	56,56,56,56	0
54	MG	2A	3151	1/1	0.96	0.08	50,50,50,50	0
54	MG	1A	3332	1/1	0.96	0.14	46,46,46,46	0
54	MG	1A	3260	1/1	0.96	0.09	39,39,39,39	0
54	MG	2A	3418	1/1	0.96	0.09	28,28,28,28	0
54	MG	1A	3327	1/1	0.97	0.12	42,42,42,42	0
54	MG	1a	3110	1/1	0.97	0.07	20,20,20,20	0
54	MG	1A	3880	1/1	0.97	0.05	47,47,47,47	0
54	MG	2T	202	1/1	0.97	0.11	45,45,45,45	0
54	MG	1W	203	1/1	0.97	0.14	26,26,26,26	0
54	MG	1a	3113	1/1	0.97	0.06	52,52,52,52	0
54	MG	2V	202	1/1	0.97	0.12	42,42,42,42	0
54	MG	1A	3229	1/1	0.97	0.09	40,40,40,40	0
54	MG	1A	3271	1/1	0.97	0.08	36,36,36,36	0
54	MG	1A	3764	1/1	0.97	0.09	24,24,24,24	0
54	MG	1A	3765	1/1	0.97	0.07	30,30,30,30	0
54	MG	1A	3394	1/1	0.97	0.04	24,24,24,24	0
54	MG	2A	3561	1/1	0.97	0.05	43,43,43,43	0
54	MG	2A	3562	1/1	0.97	0.06	60,60,60,60	0
54	MG	1A	3395	1/1	0.97	0.04	34,34,34,34	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	10	106	1/1	0.97	0.08	59,59,59,59	0
54	MG	1A	3768	1/1	0.97	0.06	46,46,46,46	0
54	MG	1a	3123	1/1	0.97	0.06	32,32,32,32	0
54	MG	1A	3011	1/1	0.97	0.12	49,49,49,49	0
54	MG	1A	3162	1/1	0.97	0.12	26,26,26,26	0
54	MG	1i	201	1/1	0.97	0.12	56,56,56,56	0
54	MG	1A	4031	1/1	0.97	0.04	33,33,33,33	0
54	MG	1A	3771	1/1	0.97	0.07	32,32,32,32	0
54	MG	13	101	1/1	0.97	0.10	26,26,26,26	0
54	MG	1m	201	1/1	0.97	0.07	66,66,66,66	0
54	MG	2A	3575	1/1	0.97	0.06	45,45,45,45	0
54	MG	2A	3576	1/1	0.97	0.06	56,56,56,56	0
54	MG	13	102	1/1	0.97	0.07	18,18,18,18	0
54	MG	2A	3175	1/1	0.97	0.07	41,41,41,41	0
54	MG	2A	3579	1/1	0.97	0.06	49,49,49,49	0
54	MG	1A	3037	1/1	0.97	0.15	48,48,48,48	0
54	MG	2A	3177	1/1	0.97	0.05	33,33,33,33	0
54	MG	1A	3400	1/1	0.97	0.14	27,27,27,27	0
54	MG	1A	3776	1/1	0.97	0.06	30,30,30,30	0
54	MG	1A	3897	1/1	0.97	0.06	36,36,36,36	0
54	MG	2A	3372	1/1	0.97	0.04	27,27,27,27	0
54	MG	2A	3589	1/1	0.97	0.15	51,51,51,51	0
54	MG	2a	3015	1/1	0.97	0.15	44,44,44,44	0
54	MG	1A	3066	1/1	0.97	0.06	20,20,20,20	0
54	MG	2A	3374	1/1	0.97	0.09	36,36,36,36	0
54	MG	2A	3376	1/1	0.97	0.05	50,50,50,50	0
54	MG	1A	3197	1/1	0.97	0.07	49,49,49,49	0
54	MG	1A	3277	1/1	0.97	0.19	27,27,27,27	0
54	MG	2A	3379	1/1	0.97	0.09	38,38,38,38	0
54	MG	1A	3672	1/1	0.97	0.10	42,42,42,42	0
54	MG	1A	3165	1/1	0.97	0.14	49,49,49,49	0
54	MG	1A	3088	1/1	0.97	0.05	32,32,32,32	0
54	MG	2A	3601	1/1	0.97	0.07	38,38,38,38	0
54	MG	1A	3237	1/1	0.97	0.17	22,22,22,22	0
54	MG	2A	3603	1/1	0.97	0.06	32,32,32,32	0
54	MG	1A	4047	1/1	0.97	0.10	46,46,46,46	0
54	MG	1A	3167	1/1	0.97	0.10	31,31,31,31	0
54	MG	1A	3089	1/1	0.97	0.08	28,28,28,28	0
54	MG	1A	4050	1/1	0.97	0.10	35,35,35,35	0
54	MG	1A	3091	1/1	0.97	0.18	34,34,34,34	0
54	MG	1A	3286	1/1	0.97	0.09	56,56,56,56	0
54	MG	2A	3613	1/1	0.97	0.07	25,25,25,25	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	1a	3150	1/1	0.97	0.09	56,56,56,56	0
54	MG	1A	3413	1/1	0.97	0.05	24,24,24,24	0
54	MG	1A	3344	1/1	0.97	0.10	37,37,37,37	0
54	MG	1A	3141	1/1	0.97	0.05	28,28,28,28	0
54	MG	2A	3016	1/1	0.97	0.17	47,47,47,47	0
54	MG	2A	3017	1/1	0.97	0.14	45,45,45,45	0
54	MG	1A	3416	1/1	0.97	0.09	10,10,10,10	0
54	MG	2A	3626	1/1	0.97	0.07	30,30,30,30	0
54	MG	2A	3019	1/1	0.97	0.10	54,54,54,54	0
54	MG	1A	3793	1/1	0.97	0.09	39,39,39,39	0
54	MG	1A	3116	1/1	0.97	0.12	27,27,27,27	0
54	MG	2A	3204	1/1	0.97	0.06	41,41,41,41	0
54	MG	1A	3173	1/1	0.97	0.20	29,29,29,29	0
54	MG	2A	3404	1/1	0.97	0.05	29,29,29,29	0
54	MG	1A	3348	1/1	0.97	0.07	14,14,14,14	0
54	MG	1A	3003	1/1	0.97	0.06	24,24,24,24	0
54	MG	2A	3407	1/1	0.97	0.08	23,23,23,23	0
54	MG	1A	3422	1/1	0.97	0.07	31,31,31,31	0
54	MG	1A	3423	1/1	0.97	0.05	21,21,21,21	0
54	MG	2A	3210	1/1	0.97	0.17	33,33,33,33	0
54	MG	1B	212	1/1	0.97	0.05	30,30,30,30	0
54	MG	1A	3932	1/1	0.97	0.06	34,34,34,34	0
54	MG	2a	3057	1/1	0.97	0.10	59,59,59,59	0
54	MG	2A	3029	1/1	0.97	0.08	28,28,28,28	0
54	MG	2A	3414	1/1	0.97	0.05	26,26,26,26	0
54	MG	2a	3060	1/1	0.97	0.08	46,46,46,46	0
54	MG	1A	3424	1/1	0.97	0.11	45,45,45,45	0
54	MG	1A	3935	1/1	0.97	0.10	37,37,37,37	0
54	MG	1a	3166	1/1	0.97	0.07	65,65,65,65	0
54	MG	1A	3118	1/1	0.97	0.06	13,13,13,13	0
54	MG	2A	3035	1/1	0.97	0.15	38,38,38,38	0
54	MG	1A	3004	1/1	0.97	0.08	30,30,30,30	0
54	MG	1A	3512	1/1	0.97	0.07	35,35,35,35	0
54	MG	1A	3941	1/1	0.97	0.05	38,38,38,38	0
54	MG	2A	3656	1/1	0.97	0.06	45,45,45,45	0
54	MG	2A	3658	1/1	0.97	0.05	58,58,58,58	0
54	MG	1a	3018	1/1	0.97	0.06	35,35,35,35	0
54	MG	1A	3040	1/1	0.97	0.09	24,24,24,24	0
54	MG	2A	3664	1/1	0.97	0.06	62,62,62,62	0
54	MG	2A	3041	1/1	0.97	0.13	39,39,39,39	0
54	MG	1A	3944	1/1	0.97	0.08	37,37,37,37	0
54	MG	1a	3021	1/1	0.97	0.09	36,36,36,36	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	1A	3055	1/1	0.97	0.09	45,45,45,45	0
54	MG	1A	3605	1/1	0.97	0.07	35,35,35,35	0
54	MG	2A	3229	1/1	0.97	0.07	53,53,53,53	0
54	MG	1A	3516	1/1	0.97	0.07	25,25,25,25	0
54	MG	1A	3948	1/1	0.97	0.06	27,27,27,27	0
54	MG	1A	3809	1/1	0.97	0.07	41,41,41,41	0
54	MG	1A	3297	1/1	0.97	0.05	40,40,40,40	0
54	MG	1A	3357	1/1	0.97	0.07	31,31,31,31	0
54	MG	1A	3249	1/1	0.97	0.20	27,27,27,27	0
54	MG	1A	3521	1/1	0.97	0.08	35,35,35,35	0
54	MG	2a	3088	1/1	0.97	0.28	50,50,50,50	0
54	MG	2A	3053	1/1	0.97	0.11	42,42,42,42	0
54	MG	1a	3031	1/1	0.97	0.13	45,45,45,45	0
54	MG	1A	3250	1/1	0.97	0.17	32,32,32,32	0
54	MG	2a	3092	1/1	0.97	0.18	53,53,53,53	0
54	MG	1A	3072	1/1	0.97	0.05	24,24,24,24	0
54	MG	1A	3524	1/1	0.97	0.05	49,49,49,49	0
54	MG	2A	3443	1/1	0.97	0.06	47,47,47,47	0
54	MG	2A	3690	1/1	0.97	0.06	59,59,59,59	0
54	MG	1A	3526	1/1	0.97	0.06	34,34,34,34	0
54	MG	2A	3693	1/1	0.97	0.05	38,38,38,38	0
54	MG	1a	3190	1/1	0.97	0.06	50,50,50,50	0
54	MG	2A	3696	1/1	0.97	0.05	45,45,45,45	0
54	MG	2A	3697	1/1	0.97	0.06	48,48,48,48	0
54	MG	1a	3036	1/1	0.97	0.21	50,50,50,50	0
54	MG	2A	3699	1/1	0.97	0.05	44,44,44,44	0
54	MG	2a	3104	1/1	0.97	0.06	61,61,61,61	0
54	MG	1A	3527	1/1	0.97	0.07	13,13,13,13	0
54	MG	2A	3701	1/1	0.97	0.07	30,30,30,30	0
54	MG	1A	3823	1/1	0.97	0.05	37,37,37,37	0
54	MG	2a	3108	1/1	0.97	0.10	48,48,48,48	0
54	MG	1A	3305	1/1	0.97	0.09	40,40,40,40	0
54	MG	1A	3362	1/1	0.97	0.11	45,45,45,45	0
54	MG	1A	3032	1/1	0.97	0.10	36,36,36,36	0
54	MG	2a	3112	1/1	0.97	0.08	47,47,47,47	0
54	MG	1A	3966	1/1	0.97	0.04	17,17,17,17	0
54	MG	2A	3067	1/1	0.97	0.08	37,37,37,37	0
54	MG	1A	3828	1/1	0.97	0.07	40,40,40,40	0
54	MG	1E	302	1/1	0.97	0.06	28,28,28,28	0
54	MG	2A	3711	1/1	0.97	0.06	58,58,58,58	0
54	MG	1A	3717	1/1	0.97	0.13	34,34,34,34	0
54	MG	1A	3307	1/1	0.97	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	1A	3720	1/1	0.97	0.05	30,30,30,30	0
54	MG	1a	3048	1/1	0.97	0.13	40,40,40,40	0
54	MG	1F	301	1/1	0.97	0.10	20,20,20,20	0
54	MG	1A	3622	1/1	0.97	0.09	28,28,28,28	0
54	MG	1A	3253	1/1	0.97	0.08	41,41,41,41	0
54	MG	1A	3366	1/1	0.97	0.06	22,22,22,22	0
54	MG	2A	3078	1/1	0.97	0.13	30,30,30,30	0
54	MG	2A	3723	1/1	0.97	0.06	48,48,48,48	0
54	MG	2a	3128	1/1	0.97	0.08	61,61,61,61	0
54	MG	1A	3254	1/1	0.97	0.27	49,49,49,49	0
54	MG	1F	306	1/1	0.97	0.07	24,24,24,24	0
54	MG	1A	3033	1/1	0.97	0.09	35,35,35,35	0
54	MG	1F	309	1/1	0.97	0.10	29,29,29,29	0
54	MG	1F	311	1/1	0.97	0.12	28,28,28,28	0
54	MG	2A	3729	1/1	0.97	0.09	40,40,40,40	0
54	MG	2A	3269	1/1	0.97	0.16	18,18,18,18	0
54	MG	1A	3627	1/1	0.97	0.28	18,18,18,18	0
54	MG	2A	3271	1/1	0.97	0.07	43,43,43,43	0
54	MG	2A	3085	1/1	0.97	0.22	54,54,54,54	0
54	MG	1A	3125	1/1	0.97	0.04	65,65,65,65	0
54	MG	1F	314	1/1	0.97	0.06	47,47,47,47	0
54	MG	1A	3370	1/1	0.97	0.06	16,16,16,16	0
54	MG	1A	3312	1/1	0.97	0.07	12,12,12,12	0
54	MG	1A	3980	1/1	0.97	0.07	34,34,34,34	0
54	MG	1A	3542	1/1	0.97	0.06	34,34,34,34	0
54	MG	1A	3373	1/1	0.97	0.10	24,24,24,24	0
54	MG	2A	3094	1/1	0.97	0.07	35,35,35,35	0
54	MG	1A	3983	1/1	0.97	0.09	35,35,35,35	0
54	MG	1A	3015	1/1	0.97	0.11	37,37,37,37	0
54	MG	1A	3546	1/1	0.97	0.09	48,48,48,48	0
54	MG	1A	3315	1/1	0.97	0.18	35,35,35,35	0
54	MG	1A	3059	1/1	0.97	0.12	44,44,44,44	0
54	MG	1N	204	1/1	0.97	0.08	47,47,47,47	0
54	MG	1A	3847	1/1	0.97	0.04	31,31,31,31	0
54	MG	2A	3102	1/1	0.97	0.08	27,27,27,27	0
54	MG	2A	3103	1/1	0.97	0.07	49,49,49,49	0
54	MG	1A	3021	1/1	0.97	0.21	32,32,32,32	0
54	MG	1P	202	1/1	0.97	0.26	24,24,24,24	0
54	MG	1A	3990	1/1	0.97	0.15	35,35,35,35	0
54	MG	1a	3238	1/1	0.97	0.07	54,54,54,54	0
54	MG	2A	3501	1/1	0.97	0.09	52,52,52,52	0
54	MG	2a	3166	1/1	0.97	0.06	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	3502	1/1	0.97	0.10	74,74,74,74	0
54	MG	2A	3295	1/1	0.97	0.07	57,57,57,57	0
54	MG	2A	3504	1/1	0.97	0.07	26,26,26,26	0
54	MG	1A	3850	1/1	0.97	0.05	34,34,34,34	0
54	MG	2A	3297	1/1	0.97	0.06	38,38,38,38	0
54	MG	1a	3079	1/1	0.97	0.15	36,36,36,36	0
54	MG	1A	3155	1/1	0.97	0.11	40,40,40,40	0
54	MG	1A	3047	1/1	0.97	0.07	36,36,36,36	0
54	MG	1Q	203	1/1	0.97	0.04	26,26,26,26	0
54	MG	1A	3853	1/1	0.97	0.10	46,46,46,46	0
54	MG	2B	210	1/1	0.97	0.13	56,56,56,56	0
54	MG	2a	3179	1/1	0.97	0.10	59,59,59,59	0
54	MG	2A	3117	1/1	0.97	0.19	39,39,39,39	0
54	MG	1A	3854	1/1	0.97	0.06	31,31,31,31	0
54	MG	1A	3456	1/1	0.97	0.10	43,43,43,43	0
54	MG	1A	3744	1/1	0.97	0.08	29,29,29,29	0
54	MG	2A	3308	1/1	0.97	0.05	27,27,27,27	0
54	MG	2A	3309	1/1	0.97	0.06	25,25,25,25	0
54	MG	2A	3122	1/1	0.97	0.15	42,42,42,42	0
54	MG	2A	3520	1/1	0.97	0.12	46,46,46,46	0
54	MG	1A	3264	1/1	0.97	0.16	15,15,15,15	0
54	MG	1a	3250	1/1	0.97	0.04	37,37,37,37	0
54	MG	1R	205	1/1	0.97	0.03	20,20,20,20	0
54	MG	1A	4002	1/1	0.97	0.04	40,40,40,40	0
54	MG	2D	306	1/1	0.97	0.06	44,44,44,44	0
54	MG	1A	3188	1/1	0.97	0.15	32,32,32,32	0
54	MG	2D	308	1/1	0.97	0.10	55,55,55,55	0
54	MG	1A	3048	1/1	0.97	0.19	49,49,49,49	0
54	MG	1A	3749	1/1	0.97	0.07	50,50,50,50	0
54	MG	1A	3385	1/1	0.97	0.13	40,40,40,40	0
54	MG	1A	3865	1/1	0.97	0.13	31,31,31,31	0
54	MG	1A	3558	1/1	0.97	0.04	12,12,12,12	0
54	MG	2A	3531	1/1	0.97	0.07	51,51,51,51	0
54	MG	1A	3132	1/1	0.97	0.05	29,29,29,29	0
54	MG	1A	3049	1/1	0.97	0.12	28,28,28,28	0
54	MG	2A	3137	1/1	0.97	0.06	21,21,21,21	0
54	MG	1U	202	1/1	0.97	0.06	32,32,32,32	0
54	MG	1a	3266	1/1	0.97	0.07	69,69,69,69	0
54	MG	1A	3325	1/1	0.97	0.07	47,47,47,47	0
54	MG	2A	3327	1/1	0.97	0.05	40,40,40,40	0
54	MG	1a	3268	1/1	0.97	0.07	76,76,76,76	0
54	MG	1U	204	1/1	0.97	0.48	33,33,33,33	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MPD	18	102	8/8	0.97	0.09	28,33,38,41	0
54	MG	1U	205	1/1	0.97	0.07	24,24,24,24	0
54	MG	1A	3469	1/1	0.97	0.07	37,37,37,37	0
54	MG	1A	4014	1/1	0.97	0.07	41,41,41,41	0
54	MG	1A	3470	1/1	0.97	0.07	49,49,49,49	0
54	MG	1A	3874	1/1	0.97	0.05	34,34,34,34	0
54	MG	2A	3336	1/1	0.97	0.11	26,26,26,26	0
54	MG	1A	3757	1/1	0.97	0.08	24,24,24,24	0
58	ZN	2Y	202	1/1	0.97	0.07	101,101,101,101	0
54	MG	1A	3269	1/1	0.97	0.06	39,39,39,39	0
54	MG	1a	3108	1/1	0.97	0.16	63,63,63,63	0
59	SF4	2d	501	8/8	0.97	0.05	56,69,75,79	0
54	MG	1A	3931	1/1	0.98	0.03	12,12,12,12	0
54	MG	1A	3553	1/1	0.98	0.04	39,39,39,39	0
54	MG	1A	3042	1/1	0.98	0.07	24,24,24,24	0
54	MG	2A	3252	1/1	0.98	0.14	44,44,44,44	0
54	MG	2A	3721	1/1	0.98	0.06	42,42,42,42	0
54	MG	2A	3119	1/1	0.98	0.19	49,49,49,49	0
54	MG	1a	3169	1/1	0.98	0.07	44,44,44,44	0
54	MG	1a	3054	1/1	0.98	0.10	32,32,32,32	0
54	MG	2A	3546	1/1	0.98	0.10	53,53,53,53	0
54	MG	1A	3934	1/1	0.98	0.04	33,33,33,33	0
54	MG	1A	4036	1/1	0.98	0.04	47,47,47,47	0
54	MG	2A	3124	1/1	0.98	0.08	33,33,33,33	0
54	MG	1A	4037	1/1	0.98	0.07	26,26,26,26	0
54	MG	1A	4038	1/1	0.98	0.05	51,51,51,51	0
54	MG	1A	3610	1/1	0.98	0.08	34,34,34,34	0
54	MG	1A	3418	1/1	0.98	0.04	14,14,14,14	0
54	MG	1A	3612	1/1	0.98	0.04	32,32,32,32	0
54	MG	1A	3938	1/1	0.98	0.04	52,52,52,52	0
54	MG	1A	3939	1/1	0.98	0.06	42,42,42,42	0
54	MG	1A	3457	1/1	0.98	0.07	44,44,44,44	0
54	MG	1A	3195	1/1	0.98	0.23	36,36,36,36	0
54	MG	1A	3507	1/1	0.98	0.05	24,24,24,24	0
54	MG	1A	3043	1/1	0.98	0.13	10,10,10,10	0
54	MG	1A	3261	1/1	0.98	0.05	33,33,33,33	0
54	MG	1A	3510	1/1	0.98	0.07	16,16,16,16	0
54	MG	2A	3742	1/1	0.98	0.07	59,59,59,59	0
54	MG	2A	3139	1/1	0.98	0.12	45,45,45,45	0
54	MG	2A	3004	1/1	0.98	0.05	28,28,28,28	0
54	MG	1A	3758	1/1	0.98	0.04	31,31,31,31	0
54	MG	1A	3076	1/1	0.98	0.15	23,23,23,23	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	1A	3685	1/1	0.98	0.08	40,40,40,40	0
54	MG	1V	203	1/1	0.98	0.04	43,43,43,43	0
54	MG	1A	3563	1/1	0.98	0.12	25,25,25,25	0
54	MG	2A	3011	1/1	0.98	0.04	25,25,25,25	0
54	MG	2a	3084	1/1	0.98	0.10	50,50,50,50	0
54	MG	1A	4054	1/1	0.98	0.04	34,34,34,34	0
54	MG	1A	3130	1/1	0.98	0.12	28,28,28,28	0
54	MG	1A	3763	1/1	0.98	0.09	30,30,30,30	0
54	MG	1a	3194	1/1	0.98	0.05	56,56,56,56	0
54	MG	1W	204	1/1	0.98	0.05	25,25,25,25	0
54	MG	1A	3513	1/1	0.98	0.10	40,40,40,40	0
54	MG	2A	3153	1/1	0.98	0.09	42,42,42,42	0
54	MG	1A	3006	1/1	0.98	0.13	20,20,20,20	0
54	MG	1A	3101	1/1	0.98	0.16	30,30,30,30	0
54	MG	1A	3691	1/1	0.98	0.04	53,53,53,53	0
54	MG	1A	3426	1/1	0.98	0.04	35,35,35,35	0
54	MG	1A	3013	1/1	0.98	0.07	21,21,21,21	0
54	MG	2A	3292	1/1	0.98	0.04	25,25,25,25	0
54	MG	1A	3518	1/1	0.98	0.07	45,45,45,45	0
54	MG	1A	3292	1/1	0.98	0.09	14,14,14,14	0
54	MG	1B	211	1/1	0.98	0.05	27,27,27,27	0
54	MG	1A	3696	1/1	0.98	0.05	49,49,49,49	0
54	MG	1l	103	1/1	0.98	0.05	39,39,39,39	0
54	MG	1A	3857	1/1	0.98	0.27	39,39,39,39	0
54	MG	1A	3965	1/1	0.98	0.07	17,17,17,17	0
54	MG	2A	3595	1/1	0.98	0.05	50,50,50,50	0
54	MG	1A	3090	1/1	0.98	0.06	25,25,25,25	0
54	MG	1A	3859	1/1	0.98	0.06	14,14,14,14	0
54	MG	1A	3774	1/1	0.98	0.06	33,33,33,33	0
54	MG	1a	3213	1/1	0.98	0.05	54,54,54,54	0
54	MG	1a	3214	1/1	0.98	0.03	56,56,56,56	0
54	MG	2A	3305	1/1	0.98	0.07	53,53,53,53	0
54	MG	1A	3573	1/1	0.98	0.06	34,34,34,34	0
54	MG	1a	3216	1/1	0.98	0.04	58,58,58,58	0
54	MG	2D	305	1/1	0.98	0.04	32,32,32,32	0
54	MG	1B	219	1/1	0.98	0.04	33,33,33,33	0
54	MG	1A	3070	1/1	0.98	0.14	25,25,25,25	0
54	MG	1A	3474	1/1	0.98	0.04	37,37,37,37	0
54	MG	2A	3609	1/1	0.98	0.07	52,52,52,52	0
54	MG	1A	3702	1/1	0.98	0.07	44,44,44,44	0
54	MG	1A	3703	1/1	0.98	0.04	43,43,43,43	0
54	MG	1A	3295	1/1	0.98	0.07	46,46,46,46	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	2A	3457	1/1	0.98	0.04	51,51,51,51	0
54	MG	2E	302	1/1	0.98	0.04	36,36,36,36	0
54	MG	2A	3616	1/1	0.98	0.09	59,59,59,59	0
54	MG	2A	3617	1/1	0.98	0.06	57,57,57,57	0
54	MG	1A	3081	1/1	0.98	0.18	34,34,34,34	0
54	MG	1A	3870	1/1	0.98	0.07	38,38,38,38	0
54	MG	1B	227	1/1	0.98	0.10	65,65,65,65	0
54	MG	1a	3226	1/1	0.98	0.04	55,55,55,55	0
54	MG	1a	3227	1/1	0.98	0.07	43,43,43,43	0
54	MG	1A	3525	1/1	0.98	0.09	51,51,51,51	0
54	MG	1A	3226	1/1	0.98	0.26	28,28,28,28	0
54	MG	1A	3298	1/1	0.98	0.03	29,29,29,29	0
54	MG	1A	3398	1/1	0.98	0.06	32,32,32,32	0
54	MG	1A	3710	1/1	0.98	0.05	22,22,22,22	0
54	MG	1A	3877	1/1	0.98	0.07	38,38,38,38	0
54	MG	1A	3170	1/1	0.98	0.06	29,29,29,29	0
54	MG	2A	3632	1/1	0.98	0.11	40,40,40,40	0
54	MG	2A	3470	1/1	0.98	0.06	36,36,36,36	0
54	MG	1A	3228	1/1	0.98	0.15	28,28,28,28	0
54	MG	2A	3472	1/1	0.98	0.09	44,44,44,44	0
54	MG	1A	3584	1/1	0.98	0.07	42,42,42,42	0
54	MG	2a	3143	1/1	0.98	0.04	57,57,57,57	0
54	MG	1A	3644	1/1	0.98	0.09	18,18,18,18	0
54	MG	2A	3638	1/1	0.98	0.05	43,43,43,43	0
54	MG	1A	3585	1/1	0.98	0.11	31,31,31,31	0
54	MG	2A	3640	1/1	0.98	0.07	49,49,49,49	0
54	MG	2A	3330	1/1	0.98	0.06	35,35,35,35	0
54	MG	2a	3149	1/1	0.98	0.04	64,64,64,64	0
54	MG	1A	3586	1/1	0.98	0.05	12,12,12,12	0
54	MG	1A	3302	1/1	0.98	0.10	20,20,20,20	0
54	MG	1a	3241	1/1	0.98	0.06	56,56,56,56	0
54	MG	2a	3153	1/1	0.98	0.04	67,67,67,67	0
54	MG	2A	3480	1/1	0.98	0.12	63,63,63,63	0
54	MG	2a	3155	1/1	0.98	0.05	64,64,64,64	0
54	MG	1D	315	1/1	0.98	0.05	44,44,44,44	0
54	MG	2a	3157	1/1	0.98	0.08	41,41,41,41	0
54	MG	1A	3885	1/1	0.98	0.04	30,30,30,30	0
54	MG	2A	3649	1/1	0.98	0.06	47,47,47,47	0
54	MG	1A	3718	1/1	0.98	0.05	41,41,41,41	0
54	MG	1A	3303	1/1	0.98	0.12	26,26,26,26	0
54	MG	2A	3338	1/1	0.98	0.10	24,24,24,24	0
54	MG	1A	3993	1/1	0.98	0.09	18,18,18,18	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	2A	3340	1/1	0.98	0.06	27,27,27,27	0
54	MG	1A	3485	1/1	0.98	0.06	38,38,38,38	0
54	MG	1A	3996	1/1	0.98	0.05	44,44,44,44	0
54	MG	2A	3657	1/1	0.98	0.04	65,65,65,65	0
54	MG	1A	3650	1/1	0.98	0.05	27,27,27,27	0
54	MG	1A	3487	1/1	0.98	0.09	28,28,28,28	0
54	MG	1a	3252	1/1	0.98	0.04	56,56,56,56	0
54	MG	1A	3005	1/1	0.98	0.11	19,19,19,19	0
54	MG	1A	3029	1/1	0.98	0.12	38,38,38,38	0
54	MG	1A	3538	1/1	0.98	0.09	24,24,24,24	0
54	MG	1A	3095	1/1	0.98	0.13	16,16,16,16	0
54	MG	1A	3727	1/1	0.98	0.12	33,33,33,33	0
54	MG	1F	307	1/1	0.98	0.04	25,25,25,25	0
54	MG	1A	3540	1/1	0.98	0.12	16,16,16,16	0
54	MG	2A	3672	1/1	0.98	0.05	35,35,35,35	0
54	MG	1A	3899	1/1	0.98	0.09	59,59,59,59	0
54	MG	1A	3140	1/1	0.98	0.07	25,25,25,25	0
54	MG	1A	3073	1/1	0.98	0.07	28,28,28,28	0
54	MG	1A	3810	1/1	0.98	0.04	56,56,56,56	0
54	MG	1a	3265	1/1	0.98	0.04	45,45,45,45	0
54	MG	2a	3013	1/1	0.98	0.07	50,50,50,50	0
54	MG	1A	4009	1/1	0.98	0.06	14,14,14,14	0
54	MG	1A	3543	1/1	0.98	0.05	20,20,20,20	0
54	MG	1A	3213	1/1	0.98	0.19	32,32,32,32	0
54	MG	2a	3189	1/1	0.98	0.05	64,64,64,64	0
54	MG	1A	3256	1/1	0.98	0.19	19,19,19,19	0
54	MG	2A	3683	1/1	0.98	0.03	58,58,58,58	0
54	MG	1a	3144	1/1	0.98	0.04	52,52,52,52	0
54	MG	1A	3906	1/1	0.98	0.10	26,26,26,26	0
54	MG	2A	3091	1/1	0.98	0.06	31,31,31,31	0
54	MG	1a	3146	1/1	0.98	0.04	31,31,31,31	0
54	MG	1A	3341	1/1	0.98	0.06	37,37,37,37	0
54	MG	2A	3367	1/1	0.98	0.04	28,28,28,28	0
54	MG	2A	3692	1/1	0.98	0.04	70,70,70,70	0
54	MG	1A	3815	1/1	0.98	0.07	26,26,26,26	0
54	MG	2A	3694	1/1	0.98	0.03	29,29,29,29	0
54	MG	1a	3275	1/1	0.98	0.04	44,44,44,44	0
54	MG	1A	3663	1/1	0.98	0.09	29,29,29,29	0
54	MG	1A	3915	1/1	0.98	0.05	39,39,39,39	0
54	MG	1A	3449	1/1	0.98	0.07	46,46,46,46	0
54	MG	1A	3818	1/1	0.98	0.04	29,29,29,29	0
54	MG	1A	3280	1/1	0.98	0.07	15,15,15,15	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	1A	3920	1/1	0.98	0.20	19,19,19,19	0
54	MG	1A	3666	1/1	0.98	0.04	34,34,34,34	0
54	MG	1A	3740	1/1	0.98	0.04	61,61,61,61	0
54	MG	1A	3112	1/1	0.98	0.07	41,41,41,41	0
54	MG	1A	4025	1/1	0.98	0.18	30,30,30,30	0
54	MG	2A	3706	1/1	0.98	0.06	36,36,36,36	0
54	MG	1A	3742	1/1	0.98	0.06	39,39,39,39	0
54	MG	1A	3452	1/1	0.98	0.06	42,42,42,42	0
54	MG	1Q	202	1/1	0.98	0.04	29,29,29,29	0
54	MG	1A	3378	1/1	0.98	0.07	13,13,13,13	0
54	MG	2A	3387	1/1	0.98	0.04	54,54,54,54	0
54	MG	2A	3112	1/1	0.98	0.07	50,50,50,50	0
54	MG	2A	3713	1/1	0.98	0.05	35,35,35,35	0
54	MG	1A	3827	1/1	0.98	0.18	27,27,27,27	0
58	ZN	29	501	1/1	0.98	0.04	64,64,64,64	0
54	MG	1A	3313	1/1	0.98	0.30	28,28,28,28	0
54	MG	1A	3746	1/1	0.98	0.05	32,32,32,32	0
54	MG	2A	3624	1/1	0.99	0.04	32,32,32,32	0
54	MG	1A	3775	1/1	0.99	0.10	23,23,23,23	0
54	MG	1a	3114	1/1	0.99	0.06	28,28,28,28	0
54	MG	1A	3918	1/1	0.99	0.04	37,37,37,37	0
54	MG	1A	3492	1/1	0.99	0.06	32,32,32,32	0
54	MG	1A	3876	1/1	0.99	0.04	38,38,38,38	0
54	MG	1A	3372	1/1	0.99	0.03	13,13,13,13	0
54	MG	1A	3386	1/1	0.99	0.10	30,30,30,30	0
54	MG	1A	3401	1/1	0.99	0.06	25,25,25,25	0
54	MG	1A	3924	1/1	0.99	0.03	47,47,47,47	0
54	MG	1F	310	1/1	0.99	0.06	45,45,45,45	0
54	MG	1A	3299	1/1	0.99	0.06	28,28,28,28	0
54	MG	1A	3350	1/1	0.99	0.05	19,19,19,19	0
54	MG	1W	202	1/1	0.99	0.13	36,36,36,36	0
54	MG	1A	3160	1/1	0.99	0.12	28,28,28,28	0
54	MG	1A	3282	1/1	0.99	0.09	18,18,18,18	0
54	MG	2A	3109	1/1	0.99	0.07	23,23,23,23	0
54	MG	2A	3495	1/1	0.99	0.05	39,39,39,39	0
54	MG	2A	3110	1/1	0.99	0.04	50,50,50,50	0
54	MG	1A	3848	1/1	0.99	0.05	33,33,33,33	0
54	MG	1A	3670	1/1	0.99	0.12	40,40,40,40	0
54	MG	1A	3671	1/1	0.99	0.13	47,47,47,47	0
54	MG	2A	3568	1/1	0.99	0.05	52,52,52,52	0
54	MG	1A	3210	1/1	0.99	0.11	29,29,29,29	0
54	MG	2A	3648	1/1	0.99	0.03	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	3819	1/1	0.99	0.14	31,31,31,31	0
54	MG	1A	3700	1/1	0.99	0.08	46,46,46,46	0
54	MG	1A	3080	1/1	0.99	0.12	29,29,29,29	0
54	MG	1A	3891	1/1	0.99	0.07	25,25,25,25	0
54	MG	2A	3371	1/1	0.99	0.03	25,25,25,25	0
54	MG	2A	3506	1/1	0.99	0.04	38,38,38,38	0
54	MG	1A	3379	1/1	0.99	0.07	33,33,33,33	0
54	MG	1A	3893	1/1	0.99	0.04	24,24,24,24	0
54	MG	1A	3731	1/1	0.99	0.04	23,23,23,23	0
54	MG	2A	3375	1/1	0.99	0.04	40,40,40,40	0
54	MG	2A	3659	1/1	0.99	0.05	51,51,51,51	0
54	MG	2A	3660	1/1	0.99	0.07	24,24,24,24	0
54	MG	2A	3661	1/1	0.99	0.03	28,28,28,28	0
54	MG	1a	3251	1/1	0.99	0.04	39,39,39,39	0
54	MG	2a	3175	1/1	0.99	0.04	68,68,68,68	0
54	MG	1A	3028	1/1	0.99	0.23	20,20,20,20	0
54	MG	1A	3460	1/1	0.99	0.02	15,15,15,15	0
54	MG	2A	3583	1/1	0.99	0.07	26,26,26,26	0
54	MG	1a	3254	1/1	0.99	0.07	49,49,49,49	0
54	MG	1A	3528	1/1	0.99	0.05	17,17,17,17	0
54	MG	2A	3586	1/1	0.99	0.04	41,41,41,41	0
54	MG	1A	3943	1/1	0.99	0.04	41,41,41,41	0
54	MG	2A	3670	1/1	0.99	0.07	57,57,57,57	0
54	MG	1A	3461	1/1	0.99	0.04	32,32,32,32	0
54	MG	2A	3383	1/1	0.99	0.04	38,38,38,38	0
54	MG	2A	3673	1/1	0.99	0.03	38,38,38,38	0
54	MG	2A	3129	1/1	0.99	0.16	31,31,31,31	0
54	MG	1A	3483	1/1	0.99	0.04	35,35,35,35	0
54	MG	2A	3008	1/1	0.99	0.05	35,35,35,35	0
54	MG	1A	3862	1/1	0.99	0.05	36,36,36,36	0
54	MG	1A	3107	1/1	0.99	0.03	26,26,26,26	0
54	MG	1A	3994	1/1	0.99	0.04	15,15,15,15	0
54	MG	1A	3411	1/1	0.99	0.10	15,15,15,15	0
54	MG	1Q	205	1/1	0.99	0.04	27,27,27,27	0
54	MG	2A	3599	1/1	0.99	0.04	45,45,45,45	0
54	MG	1A	3486	1/1	0.99	0.04	20,20,20,20	0
54	MG	2A	3684	1/1	0.99	0.04	42,42,42,42	0
54	MG	1A	3800	1/1	0.99	0.06	25,25,25,25	0
54	MG	1D	311	1/1	0.99	0.16	18,18,18,18	0
54	MG	1A	3951	1/1	0.99	0.04	48,48,48,48	0
54	MG	2A	3604	1/1	0.99	0.04	30,30,30,30	0
54	MG	2A	3689	1/1	0.99	0.03	45,45,45,45	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	1A	3428	1/1	0.99	0.03	22,22,22,22	0
54	MG	2B	219	1/1	0.99	0.03	58,58,58,58	0
54	MG	1a	3211	1/1	0.99	0.03	63,63,63,63	0
54	MG	1A	3103	1/1	0.99	0.09	20,20,20,20	0
54	MG	1A	3869	1/1	0.99	0.07	53,53,53,53	0
54	MG	1A	3017	1/1	0.99	0.24	17,17,17,17	0
54	MG	2A	3610	1/1	0.99	0.03	42,42,42,42	0
54	MG	1A	3956	1/1	0.99	0.04	50,50,50,50	0
54	MG	1a	3050	1/1	0.99	0.09	43,43,43,43	0
54	MG	1A	3909	1/1	0.99	0.02	15,15,15,15	0
54	MG	1A	3468	1/1	0.99	0.05	14,14,14,14	0
54	MG	2A	3615	1/1	0.99	0.04	39,39,39,39	0
54	MG	19	102	1/1	0.99	0.10	34,34,34,34	0
54	MG	1E	303	1/1	0.99	0.05	27,27,27,27	0
54	MG	1A	3913	1/1	0.99	0.03	29,29,29,29	0
58	ZN	1Y	501	1/1	0.99	0.03	62,62,62,62	0
54	MG	2A	3619	1/1	0.99	0.07	30,30,30,30	0
58	ZN	15	108	1/1	0.99	0.02	42,42,42,42	0
58	ZN	16	102	1/1	0.99	0.05	36,36,36,36	0
58	ZN	19	104	1/1	0.99	0.06	45,45,45,45	0
58	ZN	1n	104	1/1	0.99	0.04	64,64,64,64	0
54	MG	1A	3914	1/1	0.99	0.05	23,23,23,23	0
54	MG	2A	3031	1/1	0.99	0.04	24,24,24,24	0
58	ZN	25	102	1/1	0.99	0.03	53,53,53,53	0
58	ZN	26	501	1/1	0.99	0.03	58,58,58,58	0
54	MG	2E	305	1/1	0.99	0.07	23,23,23,23	0
54	MG	1A	3208	1/1	0.99	0.09	31,31,31,31	0
59	SF4	1d	306	8/8	0.99	0.04	47,53,61,66	0
54	MG	1A	3635	1/1	0.99	0.06	41,41,41,41	0
54	MG	1A	3786	1/1	1.00	0.02	27,27,27,27	0
54	MG	1A	3352	1/1	1.00	0.02	31,31,31,31	0
54	MG	1A	3637	1/1	1.00	0.05	17,17,17,17	0
54	MG	1A	3467	1/1	1.00	0.06	19,19,19,19	0
54	MG	1a	3125	1/1	1.00	0.07	24,24,24,24	0
54	MG	2A	3489	1/1	1.00	0.05	29,29,29,29	0
54	MG	1A	3910	1/1	1.00	0.02	37,37,37,37	0
54	MG	1A	3911	1/1	1.00	0.06	22,22,22,22	0
54	MG	2A	3588	1/1	1.00	0.02	40,40,40,40	0

6.5 Other polymers ⓘ

There are no such residues in this entry.