



wwPDB X-ray Structure Validation Summary Report ⓘ

Sep 2, 2026 – 08:27 PM EDT

PDB ID : 9Q6U / pdb_00009q6u
Title : Crystal structure of the wild-type *Thermus thermophilus* 70S ribosome in complex with tiamulin-26 triazole derivative and protein Y at 2.80Å resolution
Authors : Killam, B.Y.; Kopec, I.; Breiner, L.M.; Hoernig, M.; LoPresti, M.; Abdelsattar, A.S.; Abouelkhair, A.A.; Briganti, A.J.; Slowinski, R.P.; Vogelaar, N.J.; Seleem, M.N.; Brown, A.M.; Lowell, A.N.; Polikanov, Y.S.
Deposited on : 2025-08-22
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

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

The following versions of software and data (see [references](#) ①) were used in the production of this report:

MolProbity	:	FAILED
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.015 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.50

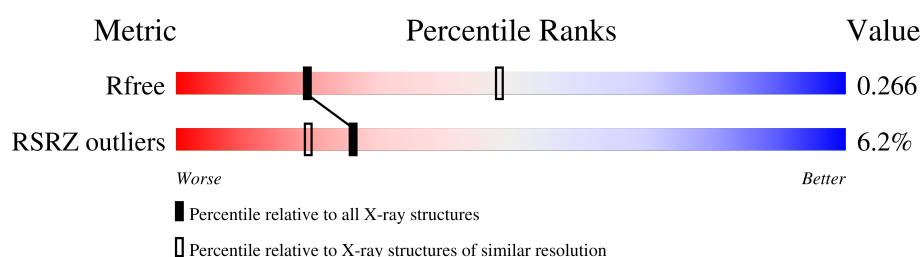
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 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)
RSRZ outliers	180081	3869 (2.80-2.80)

MolProbity failed to run properly - the sequence quality summary graphics cannot be shown.

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	2A	3726	-	-	-	X

2 Entry composition [i](#)

There are 60 unique types of molecules in this entry. The entry contains 297159 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	990	Total	Mg	0	0
			990	990		
54	1B	29	Total	Mg	0	0
			29	29		
54	1D	18	Total	Mg	0	0
			18	18		
54	1E	8	Total	Mg	0	0
			8	8		
54	1F	17	Total	Mg	0	0
			17	17		
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	6	Total	Mg	0	0
			6	6		
54	1Q	8	Total	Mg	0	0
			8	8		
54	1R	4	Total	Mg	0	0
			4	4		
54	1S	1	Total	Mg	0	0
			1	1		
54	1T	5	Total	Mg	0	0
			5	5		
54	1U	6	Total	Mg	0	0
			6	6		
54	1V	6	Total	Mg	0	0
			6	6		
54	1W	2	Total	Mg	0	0
			2	2		
54	1X	1	Total	Mg	0	0
			1	1		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
54	1Y	2	Total 2	Mg 2	0	0
54	1Z	1	Total 1	Mg 1	0	0
54	10	8	Total 8	Mg 8	0	0
54	11	2	Total 2	Mg 2	0	0
54	13	3	Total 3	Mg 3	0	0
54	15	9	Total 9	Mg 9	0	0
54	17	4	Total 4	Mg 4	0	0
54	18	4	Total 4	Mg 4	0	0
54	19	2	Total 2	Mg 2	0	0
54	1a	265	Total 265	Mg 265	0	0
54	1b	1	Total 1	Mg 1	0	0
54	1d	5	Total 5	Mg 5	0	0
54	1e	3	Total 3	Mg 3	0	0
54	1f	2	Total 2	Mg 2	0	0
54	1g	3	Total 3	Mg 3	0	0
54	1h	2	Total 2	Mg 2	0	0
54	1i	1	Total 1	Mg 1	0	0
54	1k	1	Total 1	Mg 1	0	0
54	1l	2	Total 2	Mg 2	0	0
54	1m	1	Total 1	Mg 1	0	0
54	1n	1	Total 1	Mg 1	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
54	1o	2	Total 2	Mg 2	0	0
54	1t	2	Total 2	Mg 2	0	0
54	1y	4	Total 4	Mg 4	0	0
54	2A	737	Total 737	Mg 737	0	0
54	2B	20	Total 20	Mg 20	0	0
54	2D	7	Total 7	Mg 7	0	0
54	2E	8	Total 8	Mg 8	0	0
54	2F	5	Total 5	Mg 5	0	0
54	2G	2	Total 2	Mg 2	0	0
54	2I	1	Total 1	Mg 1	0	0
54	2N	2	Total 2	Mg 2	0	0
54	2O	1	Total 1	Mg 1	0	0
54	2P	3	Total 3	Mg 3	0	0
54	2Q	4	Total 4	Mg 4	0	0
54	2R	1	Total 1	Mg 1	0	0
54	2T	3	Total 3	Mg 3	0	0
54	2U	1	Total 1	Mg 1	0	0
54	2V	2	Total 2	Mg 2	0	0
54	2W	4	Total 4	Mg 4	0	0
54	2X	1	Total 1	Mg 1	0	0
54	2Y	1	Total 1	Mg 1	0	0

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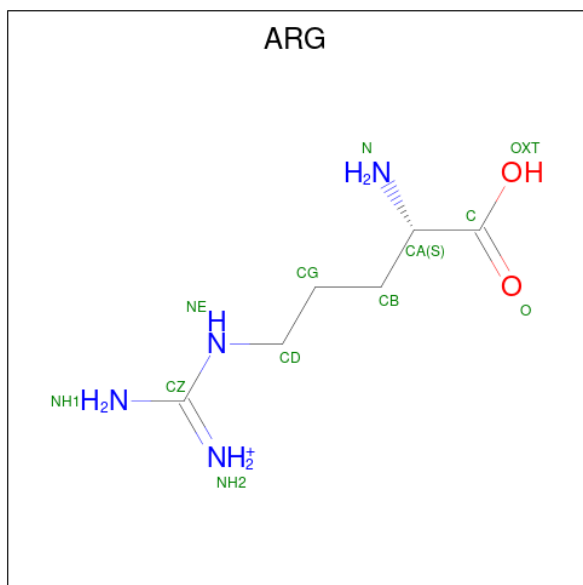
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
54	20	2	Total 2	Mg 2	0	0
54	21	4	Total 4	Mg 4	0	0
54	23	2	Total 2	Mg 2	0	0
54	25	3	Total 3	Mg 3	0	0
54	26	1	Total 1	Mg 1	0	0
54	27	2	Total 2	Mg 2	0	0
54	28	1	Total 1	Mg 1	0	0
54	2a	198	Total 198	Mg 198	0	0
54	2e	2	Total 2	Mg 2	0	0
54	2f	1	Total 1	Mg 1	0	0
54	2j	1	Total 1	Mg 1	0	0
54	2t	1	Total 1	Mg 1	0	0

- Molecule 55 is (3aS,4R,5S,6S,8R,9R,9aR,10R)-6-(2-{4-[(benzyloxy)methyl]-1H-1,2,3-triazol-1-yl}ethyl)-5-hydroxy-4,6,9,10-tetramethyl-1-oxodecahydro-3a,9-propanocyclopenta[8]annulen-8-yl {[2-(diethylamino)ethyl]sulfanyl}acetate (CCD ID: A1CRD) (formula: C₃₈H₅₈N₄O₅S) (labeled as "Ligand of Interest" by depositor).

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
56	18	1	Total	C	O	0	0
			8	6	2		
56	1a	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: $C_6H_{15}N_4O_2$).



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).

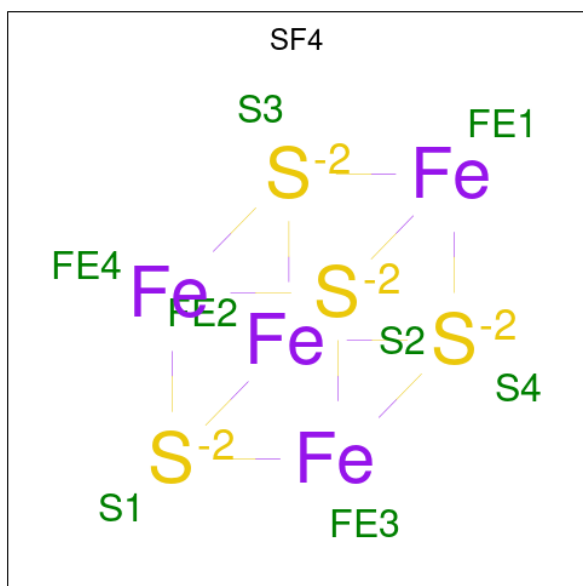
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
58	1Y	1	Total	Zn	0	0
			1	1		
58	14	1	Total	Zn	0	0
			1	1		
58	15	1	Total	Zn	0	0
			1	1		
58	16	1	Total	Zn	0	0
			1	1		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
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		
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	3668	Total 3668	O 3668	0	0
60	1B	89	Total 89	O 89	0	0
60	1D	110	Total 110	O 110	0	0
60	1E	69	Total 69	O 69	0	0
60	1F	59	Total 59	O 59	0	0
60	1G	15	Total 15	O 15	0	0
60	1H	15	Total 15	O 15	0	0
60	1I	4	Total 4	O 4	0	0
60	1N	45	Total 45	O 45	0	0
60	1O	21	Total 21	O 21	0	0
60	1P	67	Total 67	O 67	0	0
60	1Q	32	Total 32	O 32	0	0
60	1R	25	Total 25	O 25	0	0
60	1S	10	Total 10	O 10	0	0
60	1T	33	Total 33	O 33	0	0
60	1U	44	Total 44	O 44	0	0
60	1V	35	Total 35	O 35	0	0
60	1W	30	Total 30	O 30	0	0
60	1X	26	Total 26	O 26	0	0
60	1Y	16	Total 16	O 16	0	0
60	1Z	12	Total 12	O 12	0	0
60	10	23	Total 23	O 23	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
60	11	28	Total 28	O 28	0	0
60	12	10	Total 10	O 10	0	0
60	13	22	Total 22	O 22	0	0
60	14	1	Total 1	O 1	0	0
60	15	23	Total 23	O 23	0	0
60	16	18	Total 18	O 18	0	0
60	17	10	Total 10	O 10	0	0
60	18	22	Total 22	O 22	0	0
60	19	6	Total 6	O 6	0	0
60	1a	444	Total 444	O 444	0	0
60	1b	2	Total 2	O 2	0	0
60	1c	2	Total 2	O 2	0	0
60	1d	9	Total 9	O 9	0	0
60	1e	2	Total 2	O 2	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	1l	4	Total 4	O 4	0	0
60	1m	1	Total 1	O 1	0	0
60	1o	4	Total 4	O 4	0	0
60	1p	1	Total 1	O 1	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
60	1t	1	Total 1	O 1	0	0
60	1u	1	Total 1	O 1	0	0
60	1y	2	Total 2	O 2	0	0
60	2A	2343	Total 2343	O 2343	0	0
60	2B	48	Total 48	O 48	0	0
60	2D	50	Total 50	O 50	0	0
60	2E	29	Total 29	O 29	0	0
60	2F	21	Total 21	O 21	0	0
60	2G	7	Total 7	O 7	0	0
60	2H	2	Total 2	O 2	0	0
60	2I	3	Total 3	O 3	0	0
60	2N	4	Total 4	O 4	0	0
60	2O	20	Total 20	O 20	0	0
60	2P	25	Total 25	O 25	0	0
60	2Q	22	Total 22	O 22	0	0
60	2R	15	Total 15	O 15	0	0
60	2S	5	Total 5	O 5	0	0
60	2T	10	Total 10	O 10	0	0
60	2U	13	Total 13	O 13	0	0
60	2V	7	Total 7	O 7	0	0
60	2W	17	Total 17	O 17	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
60	2X	10	Total 10	O 10	0	0
60	2Y	4	Total 4	O 4	0	0
60	2Z	12	Total 12	O 12	0	0
60	20	9	Total 9	O 9	0	0
60	21	21	Total 21	O 21	0	0
60	22	4	Total 4	O 4	0	0
60	23	4	Total 4	O 4	0	0
60	25	11	Total 11	O 11	0	0
60	26	4	Total 4	O 4	0	0
60	27	12	Total 12	O 12	0	0
60	28	14	Total 14	O 14	0	0
60	29	1	Total 1	O 1	0	0
60	2a	310	Total 310	O 310	0	0
60	2d	3	Total 3	O 3	0	0
60	2f	3	Total 3	O 3	0	0
60	2l	3	Total 3	O 3	0	0
60	2m	1	Total 1	O 1	0	0
60	2n	1	Total 1	O 1	0	0
60	2o	4	Total 4	O 4	0	0
60	2p	2	Total 2	O 2	0	0
60	2q	1	Total 1	O 1	0	0

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

MolProbity failed to run properly - this section is therefore empty.

3 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	211.16Å 452.53Å 626.77Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	366.89 – 2.80 366.89 – 2.80	Depositor EDS
% Data completeness (in resolution range)	99.5 (366.89-2.80) 99.7 (366.89-2.80)	Depositor EDS
R_{merge}	0.32	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.24 (at 2.82Å)	Xtriage
Refinement program	PHENIX 1.17.1	Depositor
R, R_{free}	0.216 , 0.269 0.215 , 0.266	Depositor DCC
R_{free} test set	72766 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	49.0	Xtriage
Anisotropy	0.081	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.40 , 148.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.40$, $\langle L^2 \rangle = 0.23$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.85	EDS
Total number of atoms	297159	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 1.67% 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.

4 Model quality [i](#)

4.1 Standard geometry [i](#)

MolProbity failed to run properly - this section is therefore empty.

4.2 Too-close contacts [i](#)

MolProbity failed to run properly - this section is therefore empty.

4.3 Torsion angles [i](#)

4.3.1 Protein backbone [i](#)

MolProbity failed to run properly - this section is therefore empty.

4.3.2 Protein sidechains [i](#)

MolProbity failed to run properly - this section is therefore empty.

4.3.3 RNA [i](#)

MolProbity failed to run properly - this section is therefore empty.

4.4 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	4OC	1a	1402	32	20,23,24	0.78	0	25,32,35	0.87	1 (4%)
32	MA6	1a	1519	32	23,26,27	0.41	0	33,38,41	2.07	9 (27%)
32	5MC	2a	1400	32	19,22,23	1.69	3 (15%)	26,32,35	1.36	5 (19%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
32	M2G	2a	966	32	24,27,28	1.29	3 (12%)	33,40,43	1.83	6 (18%)
1	OMC	1A	1920	1	19,22,23	0.84	0	25,31,34	1.15	2 (8%)
32	5MC	1a	1400	32	19,22,23	1.57	3 (15%)	26,32,35	1.23	3 (11%)
1	5MC	2A	1942	1	19,22,23	1.49	3 (15%)	26,32,35	1.13	2 (7%)
32	5MC	1a	1407	32	19,22,23	1.71	2 (10%)	26,32,35	1.01	2 (7%)
1	2MA	1A	2503	54,1	22,25,26	1.42	5 (22%)	32,37,40	2.29	10 (31%)
32	2MG	1a	1207	32	23,26,27	1.25	2 (8%)	33,38,41	2.35	9 (27%)
32	UR3	2a	1498	32	19,22,23	0.95	1 (5%)	26,32,35	1.77	3 (11%)
1	5MC	1A	1962	54,1	19,22,23	1.50	3 (15%)	26,32,35	1.26	3 (11%)
32	5MC	1a	1404	32	19,22,23	1.65	3 (15%)	26,32,35	1.20	3 (11%)
32	G7M	1a	527	54,32	23,26,27	1.52	3 (13%)	34,39,42	1.67	5 (14%)
1	2MA	2A	2503	54,1	22,25,26	1.49	5 (22%)	32,37,40	2.32	7 (21%)
32	4OC	2a	1402	32	20,23,24	0.75	0	25,32,35	0.93	1 (4%)
1	PSU	2A	1917	1	18,21,22	1.36	2 (11%)	21,30,33	1.97	3 (14%)
32	MA6	1a	1518	32	23,26,27	0.38	0	33,38,41	2.04	10 (30%)
1	OMU	1A	2552	54,1	19,22,23	1.21	2 (10%)	25,31,34	1.68	4 (16%)
1	5MU	2A	1915	1	19,22,23	1.46	4 (21%)	27,32,35	2.20	9 (33%)
32	MA6	2a	1519	32	23,26,27	0.43	0	33,38,41	2.10	10 (30%)
1	OMG	2A	2251	54,1	23,26,27	1.25	3 (13%)	32,38,41	2.06	6 (18%)
1	PSU	2A	2605	1	18,21,22	1.37	3 (16%)	21,30,33	1.96	3 (14%)
1	5MC	1A	1942	1	19,22,23	1.62	3 (15%)	26,32,35	1.14	2 (7%)
1	5MC	2A	1962	54,1	19,22,23	1.60	3 (15%)	26,32,35	1.14	2 (7%)
32	5MC	2a	1404	32	19,22,23	1.64	3 (15%)	26,32,35	1.25	3 (11%)
1	5MU	2A	1939	54,1	19,22,23	1.43	6 (31%)	27,32,35	2.22	6 (22%)
1	PSU	1A	1911	1	18,21,22	1.38	2 (11%)	21,30,33	1.97	4 (19%)
32	PSU	1a	516	54,32	18,21,22	1.40	2 (11%)	21,30,33	1.95	5 (23%)
32	UR3	1a	1498	32	19,22,23	0.99	1 (5%)	26,32,35	1.74	3 (11%)
43	0TD	1l	92	43	8,9,10	4.62	2 (25%)	6,11,13	9.05	2 (33%)
32	2MG	2a	1207	32	23,26,27	1.28	4 (17%)	33,38,41	2.04	5 (15%)
1	PSU	1A	2605	1	18,21,22	1.40	3 (16%)	21,30,33	2.08	3 (14%)
1	5MU	1A	1939	1	19,22,23	1.36	4 (21%)	27,32,35	2.18	6 (22%)
1	PSU	2A	1911	1	18,21,22	1.34	2 (11%)	21,30,33	2.03	4 (19%)
32	G7M	2a	527	54,32	23,26,27	1.49	3 (13%)	34,39,42	1.67	5 (14%)
1	5MU	1A	1915	1	19,22,23	1.48	5 (26%)	27,32,35	2.33	10 (37%)
1	OMG	1A	2251	54,1	23,26,27	1.22	2 (8%)	32,38,41	2.06	6 (18%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
32	MA6	2a	1518	32	23,26,27	0.42	0	33,38,41	2.04	9 (27%)
32	M2G	1a	966	32	24,27,28	1.26	4 (16%)	33,40,43	1.76	6 (18%)
32	PSU	2a	516	54,32	18,21,22	1.36	2 (11%)	21,30,33	2.10	5 (23%)
32	5MC	2a	967	32	19,22,23	1.70	3 (15%)	26,32,35	1.12	2 (7%)
1	PSU	1A	1917	1	18,21,22	1.34	2 (11%)	21,30,33	2.00	3 (14%)
43	0TD	2l	92	43	8,9,10	4.44	1 (12%)	6,11,13	1.55	1 (16%)
1	OMC	2A	1920	1	19,22,23	0.80	0	25,31,34	0.86	0
32	5MC	2a	1407	32	19,22,23	1.73	3 (15%)	26,32,35	1.23	3 (11%)
32	5MC	1a	967	32	19,22,23	1.80	3 (15%)	26,32,35	1.15	3 (11%)
1	OMU	2A	2552	54,1	19,22,23	1.20	2 (10%)	25,31,34	1.93	6 (24%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
32	4OC	1a	1402	32	-	3/9/29/30	0/2/2/2
32	MA6	1a	1519	32	-	2/11/29/30	0/3/3/3
32	5MC	2a	1400	32	-	6/7/25/26	0/2/2/2
32	M2G	2a	966	32	-	0/11/29/30	0/3/3/3
1	OMC	1A	1920	1	-	1/9/27/28	0/2/2/2
32	5MC	1a	1400	32	-	1/7/25/26	0/2/2/2
1	5MC	2A	1942	1	-	0/7/25/26	0/2/2/2
32	5MC	1a	1407	32	-	0/7/25/26	0/2/2/2
1	2MA	1A	2503	54,1	-	0/7/25/26	0/3/3/3
32	2MG	1a	1207	32	-	3/9/27/28	0/3/3/3
32	UR3	2a	1498	32	-	0/7/25/26	0/2/2/2
1	5MC	1A	1962	54,1	-	2/7/25/26	0/2/2/2
32	5MC	1a	1404	32	-	0/7/25/26	0/2/2/2
32	G7M	1a	527	54,32	-	3/7/25/26	0/3/3/3
1	2MA	2A	2503	54,1	-	3/7/25/26	0/3/3/3
32	4OC	2a	1402	32	-	2/9/29/30	0/2/2/2
1	PSU	2A	1917	1	-	0/7/25/26	0/2/2/2
32	MA6	1a	1518	32	-	0/11/29/30	0/3/3/3
1	OMU	1A	2552	54,1	-	0/9/27/28	0/2/2/2
1	5MU	2A	1915	1	-	2/7/25/26	0/2/2/2
32	MA6	2a	1519	32	-	3/11/29/30	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	OMG	2A	2251	54,1	-	0/9/27/28	0/3/3/3
1	PSU	2A	2605	1	-	0/7/25/26	0/2/2/2
1	5MC	1A	1942	1	-	0/7/25/26	0/2/2/2
1	5MC	2A	1962	54,1	-	0/7/25/26	0/2/2/2
32	5MC	2a	1404	32	-	0/7/25/26	0/2/2/2
1	5MU	2A	1939	54,1	-	0/7/25/26	0/2/2/2
1	PSU	1A	1911	1	-	0/7/25/26	0/2/2/2
32	PSU	1a	516	54,32	-	0/7/25/26	0/2/2/2
32	UR3	1a	1498	32	-	2/7/25/26	0/2/2/2
43	0TD	1l	92	43	-	4/7/12/14	-
32	2MG	2a	1207	32	-	0/9/27/28	0/3/3/3
1	PSU	1A	2605	1	-	0/7/25/26	0/2/2/2
1	5MU	1A	1939	1	-	0/7/25/26	0/2/2/2
1	PSU	2A	1911	1	-	0/7/25/26	0/2/2/2
32	G7M	2a	527	54,32	-	2/7/25/26	0/3/3/3
1	5MU	1A	1915	1	-	2/7/25/26	0/2/2/2
1	OMG	1A	2251	54,1	-	1/9/27/28	0/3/3/3
32	MA6	2a	1518	32	-	0/11/29/30	0/3/3/3
32	M2G	1a	966	32	-	0/11/29/30	0/3/3/3
32	PSU	2a	516	54,32	-	0/7/25/26	0/2/2/2
32	5MC	2a	967	32	-	0/7/25/26	0/2/2/2
1	PSU	1A	1917	1	-	0/7/25/26	0/2/2/2
43	0TD	2l	92	43	-	1/7/12/14	-
1	OMC	2A	1920	1	-	2/9/27/28	0/2/2/2
32	5MC	2a	1407	32	-	0/7/25/26	0/2/2/2
32	5MC	1a	967	32	-	0/7/25/26	0/2/2/2
1	OMU	2A	2552	54,1	-	1/9/27/28	0/2/2/2

The worst 5 of 115 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
43	1l	92	0TD	CB-SB	-12.52	1.69	1.82
43	2l	92	0TD	CB-SB	-12.20	1.70	1.82
32	1a	967	5MC	C5-C4	6.66	1.49	1.44
32	2a	1407	5MC	C5-C4	6.37	1.48	1.44
32	2a	967	5MC	C5-C4	6.31	1.48	1.44

The worst 5 of 220 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
43	1l	92	0TD	CSB-SB-CB	-21.96	62.90	102.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	2A	2503	2MA	C5-C4-N3	-8.38	118.36	127.18
1	1A	2503	2MA	C5-C4-N3	-8.07	118.68	127.18
32	2a	1498	UR3	C4-N3-C2	-7.31	118.69	124.58
32	1a	1207	2MG	C2-N3-C4	7.27	121.09	112.00

There are no chirality outliers.

5 of 46 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
32	1a	1207	2MG	N1-C2-N2-CM2
32	1a	1207	2MG	N3-C2-N2-CM2
43	1l	92	0TD	O-C-CA-CB

There are no ring outliers.

No monomer is involved in short contacts.

4.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

4.6 Ligand geometry [i](#)

Of 2486 ligands modelled in this entry, 2475 are monoatomic - leaving 11 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
56	MPD	1T	206	-	7,7,7	0.40	0	9,10,10	0.42	0
59	SF4	2d	501	35	0,12,12	-	-	-		
56	MPD	1a	1866	-	7,7,7	0.40	0	9,10,10	0.60	0
56	MPD	18	105	-	7,7,7	0.33	0	9,10,10	0.37	0
56	MPD	1A	3992	-	7,7,7	0.36	0	9,10,10	0.30	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
56	MPD	2B	221	-	7,7,7	0.36	0	9,10,10	0.23	0
59	SF4	1d	306	35	0,12,12	-	-	-	-	-
55	A1CRD	1A	3991	-	51,52,52	2.36	13 (25%)	67,76,76	2.28	17 (25%)
55	A1CRD	2A	3738	-	51,52,52	2.27	11 (21%)	67,76,76	2.28	21 (31%)
57	ARG	1F	318	-	10,11,11	0.74	1 (10%)	9,13,13	1.00	1 (11%)
57	ARG	1B	230	54	10,11,11	0.69	0	9,13,13	1.00	1 (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
56	MPD	1T	206	-	-	0/5/5/5	-
59	SF4	2d	501	35	-	-	0/6/5/5
56	MPD	1a	1866	-	-	1/5/5/5	-
56	MPD	18	105	-	-	3/5/5/5	-
56	MPD	1A	3992	-	-	3/5/5/5	-
56	MPD	2B	221	-	-	1/5/5/5	-
59	SF4	1d	306	35	-	-	0/6/5/5
55	A1CRD	1A	3991	-	-	8/26/88/88	0/5/5/5
55	A1CRD	2A	3738	-	-	6/26/88/88	0/5/5/5
57	ARG	1F	318	-	-	2/11/11/11	-
57	ARG	1B	230	54	-	3/11/11/11	-

The worst 5 of 25 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
55	1A	3991	A1CRD	CAA-CAQ	-8.89	1.40	1.53
55	1A	3991	A1CRD	CAT-CAQ	-8.59	1.37	1.51
55	2A	3738	A1CRD	CAA-CAQ	-8.51	1.40	1.53
55	2A	3738	A1CRD	CAT-CAQ	-8.17	1.38	1.51
55	2A	3738	A1CRD	CBI-CBJ	-5.10	1.38	1.50

The worst 5 of 40 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
55	2A	3738	A1CRD	CAK-CAC-CAB	-9.16	106.45	116.28
55	1A	3991	A1CRD	CAK-CAC-CAB	-8.74	106.90	116.28
55	1A	3991	A1CRD	CAC-OAU-CAV	-5.02	108.88	118.03

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
55	1A	3991	A1CRD	CAG-CAB-CAC	4.81	115.39	112.13
55	1A	3991	A1CRD	CBI-OBH-CBG	-4.79	106.87	112.36

There are no chirality outliers.

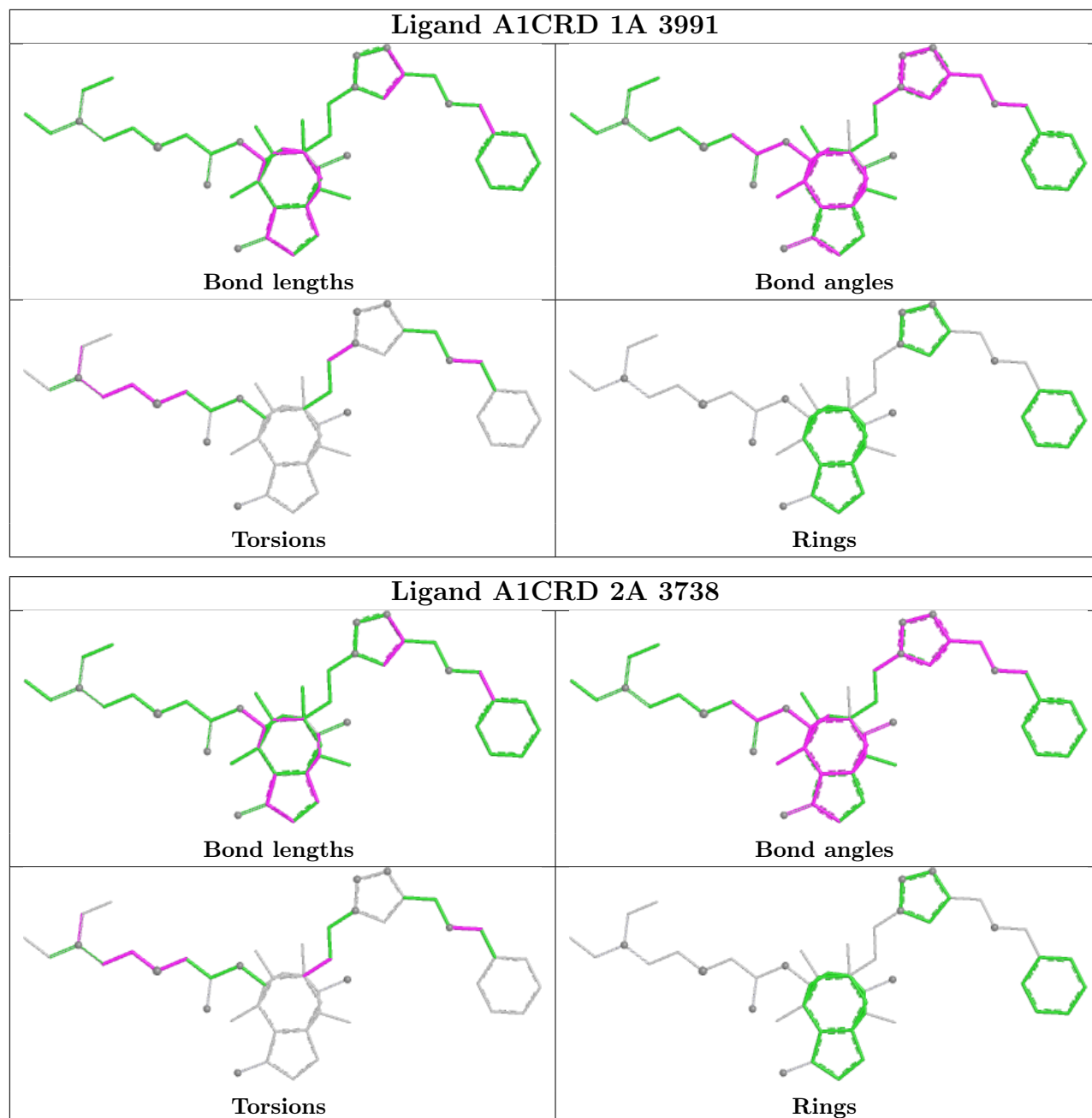
5 of 27 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
55	1A	3991	A1CRD	SAY-CBP-CBQ-NBR
55	1A	3991	A1CRD	CBQ-CBP-SAY-CAW
55	2A	3738	A1CRD	CAK-CAJ-CAN-CBA
56	1A	3992	MPD	O2-C2-C3-C4
56	1A	3992	MPD	CM-C2-C3-C4

There are no ring outliers.

No monomer is involved in short contacts.

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.



4.7 Other polymers [i](#)

There are no such residues in this entry.

4.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

5 Fit of model and data ⓘ

5.1 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%)	-0.40	145 (5%) 33 25	13, 29, 89, 103	0
1	2A	2856/2915 (97%)	0.09	146 (5%) 33 25	26, 49, 91, 105	0
2	1B	120/121 (99%)	-0.25	1 (0%) 82 75	25, 46, 61, 81	0
2	2B	120/121 (99%)	0.63	1 (0%) 82 75	50, 71, 79, 85	0
3	1D	275/276 (99%)	-0.26	2 (0%) 84 77	15, 30, 45, 65	0
3	2D	275/276 (99%)	0.11	1 (0%) 88 84	26, 44, 56, 69	0
4	1E	204/206 (99%)	-0.32	0 100 100	13, 33, 52, 67	0
4	2E	204/206 (99%)	0.22	3 (1%) 72 63	30, 49, 66, 80	0
5	1F	203/210 (96%)	-0.30	2 (0%) 79 72	12, 32, 61, 79	0
5	2F	203/210 (96%)	0.45	4 (1%) 65 56	26, 56, 72, 78	0
6	1G	181/182 (99%)	0.63	9 (4%) 34 26	42, 59, 73, 85	0
6	2G	181/182 (99%)	1.23	31 (17%) 4 3	66, 75, 83, 90	0
7	1H	174/180 (96%)	0.05	1 (0%) 85 80	29, 46, 59, 65	0
7	2H	173/180 (96%)	1.00	9 (5%) 33 25	59, 74, 83, 90	0
8	1I	147/148 (99%)	0.60	6 (4%) 41 33	38, 63, 75, 79	0
8	2I	146/148 (98%)	2.45	82 (56%) 0 0	46, 81, 92, 98	0
9	1N	140/140 (100%)	-0.33	0 100 100	18, 30, 52, 62	0
9	2N	140/140 (100%)	0.29	4 (2%) 53 43	36, 55, 68, 74	0
10	1O	122/122 (100%)	-0.27	1 (0%) 82 75	21, 33, 49, 56	0
10	2O	122/122 (100%)	0.15	0 100 100	37, 47, 59, 67	0
11	1P	149/150 (99%)	-0.16	2 (1%) 75 66	13, 37, 56, 66	0
11	2P	149/150 (99%)	0.35	1 (0%) 84 77	31, 58, 73, 81	0
12	1Q	141/141 (100%)	-0.17	1 (0%) 84 77	18, 34, 48, 64	0
12	2Q	141/141 (100%)	0.37	4 (2%) 55 45	37, 53, 64, 72	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
13	1R	118/118 (100%)	-0.28	0 100 100	19, 30, 44, 53	0
13	2R	118/118 (100%)	0.07	1 (0%) 82 75	34, 45, 56, 66	0
14	1S	110/112 (98%)	0.05	1 (0%) 81 74	32, 46, 58, 67	0
14	2S	110/112 (98%)	0.96	9 (8%) 17 13	58, 67, 75, 85	0
15	1T	131/146 (89%)	-0.03	4 (3%) 51 41	26, 38, 61, 68	0
15	2T	131/146 (89%)	0.22	3 (2%) 61 51	41, 50, 66, 79	0
16	1U	116/118 (98%)	-0.46	0 100 100	16, 24, 39, 52	0
16	2U	116/118 (98%)	0.23	1 (0%) 81 74	33, 51, 65, 71	0
17	1V	101/101 (100%)	-0.31	0 100 100	16, 35, 51, 59	0
17	2V	101/101 (100%)	0.41	2 (1%) 65 56	32, 60, 68, 77	0
18	1W	112/113 (99%)	-0.49	0 100 100	14, 23, 43, 77	0
18	2W	112/113 (99%)	-0.02	0 100 100	26, 41, 58, 79	0
19	1X	95/96 (98%)	-0.26	1 (1%) 78 70	21, 31, 55, 70	0
19	2X	95/96 (98%)	0.44	3 (3%) 50 40	37, 51, 67, 76	0
20	1Y	107/110 (97%)	0.21	4 (3%) 45 36	30, 42, 61, 68	0
20	2Y	107/110 (97%)	1.02	13 (12%) 8 6	50, 64, 78, 86	0
21	1Z	203/206 (98%)	0.46	3 (1%) 72 63	33, 51, 68, 81	0
21	2Z	201/206 (97%)	0.96	9 (4%) 38 30	55, 69, 80, 88	0
22	10	77/85 (90%)	0.04	1 (1%) 75 66	22, 32, 48, 61	0
22	20	77/85 (90%)	0.74	4 (5%) 33 25	38, 53, 66, 72	0
23	11	97/98 (98%)	-0.03	2 (2%) 63 54	21, 37, 59, 65	0
23	21	97/98 (98%)	0.32	2 (2%) 63 54	34, 48, 65, 71	0
24	12	70/72 (97%)	-0.12	1 (1%) 73 64	26, 39, 50, 66	0
24	22	70/72 (97%)	0.71	7 (10%) 12 9	51, 61, 70, 72	0
25	13	59/60 (98%)	-0.02	1 (1%) 69 60	21, 32, 57, 77	0
25	23	59/60 (98%)	0.33	1 (1%) 69 60	43, 51, 68, 73	0
26	14	69/71 (97%)	1.06	11 (15%) 5 4	58, 77, 86, 90	0
26	24	69/71 (97%)	1.57	18 (26%) 1 1	70, 83, 92, 96	0
27	15	59/60 (98%)	-0.25	0 100 100	12, 28, 55, 63	0
27	25	59/60 (98%)	0.28	2 (3%) 48 39	28, 47, 67, 75	0
28	16	53/54 (98%)	-0.16	0 100 100	26, 36, 47, 55	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
28	26	53/54 (98%)	0.29	2 (3%) 44 35	45, 52, 61, 67	0
29	17	48/49 (97%)	-0.28	3 (6%) 26 19	14, 19, 50, 61	0
29	27	48/49 (97%)	0.04	3 (6%) 26 19	29, 35, 59, 62	0
30	18	64/65 (98%)	-0.31	0 100 100	21, 27, 36, 40	0
30	28	64/65 (98%)	0.27	2 (3%) 51 41	39, 46, 55, 61	0
31	19	37/37 (100%)	-0.34	0 100 100	21, 33, 49, 58	0
31	29	37/37 (100%)	0.68	0 100 100	47, 58, 71, 74	0
32	1a	1488/1521 (97%)	0.53	62 (4%) 40 32	30, 67, 90, 104	0
32	2a	1492/1521 (98%)	0.61	93 (6%) 26 20	38, 69, 91, 104	0
33	1b	231/256 (90%)	1.20	32 (13%) 6 5	59, 75, 84, 90	0
33	2b	231/256 (90%)	1.29	39 (16%) 4 3	60, 77, 86, 92	0
34	1c	206/239 (86%)	1.17	21 (10%) 12 9	61, 73, 82, 86	0
34	2c	206/239 (86%)	1.56	54 (26%) 1 1	65, 78, 83, 86	0
35	1d	208/209 (99%)	1.28	37 (17%) 4 3	52, 67, 77, 82	0
35	2d	208/209 (99%)	1.00	21 (10%) 12 9	52, 66, 74, 80	0
36	1e	148/162 (91%)	0.54	3 (2%) 65 56	43, 60, 69, 86	0
36	2e	148/162 (91%)	0.89	9 (6%) 27 20	51, 65, 74, 83	0
37	1f	100/101 (99%)	0.59	2 (2%) 65 56	50, 64, 71, 76	0
37	2f	100/101 (99%)	0.79	7 (7%) 22 16	50, 64, 72, 76	0
38	1g	155/156 (99%)	0.80	5 (3%) 50 40	60, 69, 78, 84	0
38	2g	155/156 (99%)	0.90	17 (10%) 10 8	64, 72, 78, 87	0
39	1h	137/138 (99%)	0.57	3 (2%) 62 52	52, 62, 71, 78	0
39	2h	137/138 (99%)	0.70	4 (2%) 53 43	55, 64, 72, 78	0
40	1i	127/128 (99%)	1.45	27 (21%) 2 2	64, 76, 82, 84	0
40	2i	126/128 (98%)	1.55	28 (22%) 2 1	65, 79, 84, 86	0
41	1j	97/105 (92%)	1.74	25 (25%) 1 1	63, 78, 87, 88	0
41	2j	96/105 (91%)	1.72	36 (37%) 1 0	68, 78, 86, 93	0
42	1k	114/129 (88%)	0.76	9 (7%) 18 13	40, 59, 70, 80	0
42	2k	114/129 (88%)	0.92	10 (8%) 15 11	47, 65, 74, 79	0
43	1l	121/132 (91%)	0.52	3 (2%) 58 48	43, 56, 66, 74	0
43	2l	121/132 (91%)	0.76	9 (7%) 20 15	48, 60, 67, 71	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
44	1m	116/126 (92%)	1.03	12 (10%) 12 9	59, 71, 78, 79	0
44	2m	114/126 (90%)	1.18	12 (10%) 11 8	66, 77, 82, 85	0
45	1n	60/61 (98%)	1.14	5 (8%) 17 12	61, 72, 77, 82	0
45	2n	60/61 (98%)	1.67	18 (30%) 1 1	70, 78, 82, 87	0
46	1o	88/89 (98%)	0.58	3 (3%) 48 39	45, 60, 71, 82	0
46	2o	88/89 (98%)	0.47	0 100 100	52, 64, 72, 79	0
47	1p	82/88 (93%)	0.98	9 (10%) 10 8	55, 67, 77, 82	0
47	2p	82/88 (93%)	0.86	3 (3%) 45 36	54, 62, 70, 77	0
48	1q	99/105 (94%)	0.69	0 100 100	46, 61, 71, 73	0
48	2q	99/105 (94%)	0.58	2 (2%) 65 56	50, 60, 72, 74	0
49	1r	68/88 (77%)	0.59	1 (1%) 72 63	49, 59, 72, 75	0
49	2r	68/88 (77%)	0.73	3 (4%) 39 31	56, 65, 73, 82	0
50	1s	83/93 (89%)	1.28	11 (13%) 7 5	66, 75, 83, 85	0
50	2s	83/93 (89%)	1.50	19 (22%) 2 1	69, 80, 88, 90	0
51	1t	96/106 (90%)	1.01	8 (8%) 17 12	54, 66, 73, 78	0
51	2t	98/106 (92%)	0.56	3 (3%) 51 41	49, 61, 73, 77	0
52	1u	23/27 (85%)	1.40	3 (13%) 7 6	64, 71, 76, 81	0
52	2u	23/27 (85%)	1.59	7 (30%) 1 1	69, 75, 80, 82	0
53	1y	97/113 (85%)	0.56	3 (3%) 51 41	46, 64, 70, 75	0
53	2y	96/113 (84%)	1.97	40 (41%) 0 0	67, 79, 86, 88	0
All	All	20766/21468 (96%)	0.37	1288 (6%) 26 20	12, 57, 84, 105	0

The worst 5 of 1288 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	2A	2119	A	9.0
1	2A	2173	A	8.7
1	2A	2174	C	8.6
1	1A	2117	A	8.2
8	2I	92	VAL	8.1

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

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

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
1	5MU	1A	1915	21/22	0.84	0.15	65,76,83,93	0
32	2MG	2a	1207	24/25	0.85	0.14	79,84,92,97	0
1	5MU	2A	1915	21/22	0.87	0.12	75,80,89,97	0
32	M2G	2a	966	25/26	0.88	0.13	58,67,76,79	0
1	PSU	2A	1911	20/21	0.88	0.11	60,70,79,79	0
32	5MC	2a	967	21/22	0.90	0.12	64,70,77,80	0
32	2MG	1a	1207	24/25	0.90	0.11	70,74,77,82	0
32	M2G	1a	966	25/26	0.91	0.12	53,61,72,73	0
1	PSU	2A	1917	20/21	0.91	0.09	66,73,81,90	0
32	PSU	2a	516	20/21	0.91	0.10	63,76,82,84	0
32	5MC	1a	967	21/22	0.91	0.12	60,64,76,80	0
1	PSU	1A	1911	20/21	0.91	0.11	54,62,66,69	0
1	PSU	1A	1917	20/21	0.91	0.10	61,67,75,82	0
32	5MC	1a	1407	21/22	0.92	0.11	36,51,58,64	0
43	0TD	1l	92	10/11	0.92	0.12	49,51,56,70	0
32	G7M	2a	527	24/25	0.92	0.13	53,61,68,72	0
32	5MC	2a	1400	21/22	0.92	0.12	50,64,69,70	0
1	5MC	2A	1942	21/22	0.93	0.12	41,47,50,53	0
32	MA6	2a	1518	24/25	0.93	0.12	49,58,65,66	0
32	4OC	2a	1402	22/23	0.94	0.12	46,57,66,68	0
32	G7M	1a	527	24/25	0.94	0.09	48,53,59,62	0
32	UR3	1a	1498	21/22	0.95	0.10	42,47,52,60	0
32	5MC	1a	1400	21/22	0.95	0.10	48,53,59,60	0
1	OMC	2A	1920	21/22	0.95	0.09	52,65,68,68	0
32	5MC	2a	1407	21/22	0.95	0.10	54,59,62,63	0
32	UR3	2a	1498	21/22	0.95	0.11	47,54,60,64	0
32	PSU	1a	516	20/21	0.95	0.10	45,61,64,71	0
32	MA6	1a	1518	24/25	0.96	0.09	38,43,46,49	0
32	4OC	1a	1402	22/23	0.96	0.10	44,49,55,63	0
32	5MC	2a	1404	21/22	0.96	0.09	42,51,54,57	0
32	MA6	2a	1519	24/25	0.96	0.10	44,59,65,68	0
43	0TD	2l	92	10/11	0.96	0.08	59,61,62,68	0
32	MA6	1a	1519	24/25	0.97	0.09	34,46,52,52	0
1	5MC	1A	1942	21/22	0.97	0.09	20,29,34,42	0
1	OMC	1A	1920	21/22	0.97	0.08	42,52,57,58	0
1	2MA	2A	2503	23/24	0.97	0.08	22,27,32,33	0
1	OMU	2A	2552	21/22	0.97	0.08	27,35,39,44	0
32	5MC	1a	1404	21/22	0.97	0.08	39,47,52,58	0
1	PSU	2A	2605	20/21	0.98	0.06	29,34,38,38	0
1	5MU	2A	1939	21/22	0.98	0.06	28,33,36,37	0
1	OMG	1A	2251	24/25	0.98	0.06	14,18,21,23	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
1	5MC	2A	1962	21/22	0.98	0.07	33,40,45,52	0
1	OMG	2A	2251	24/25	0.98	0.07	25,32,35,41	0
1	5MU	1A	1939	21/22	0.98	0.06	17,23,28,32	0
1	5MC	1A	1962	21/22	0.98	0.06	25,30,34,42	0
1	OMU	1A	2552	21/22	0.99	0.06	15,20,24,25	0
1	PSU	1A	2605	20/21	0.99	0.06	16,19,22,29	0
1	2MA	1A	2503	23/24	0.99	0.06	9,14,17,19	0

5.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.4 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	1B	228	1/1	0.29	0.17	81,81,81,81	0
54	MG	1a	1672	1/1	0.56	0.33	83,83,83,83	0
54	MG	18	102	1/1	0.61	0.17	59,59,59,59	0
54	MG	2W	203	1/1	0.62	0.17	64,64,64,64	0
54	MG	2a	3094	1/1	0.62	0.21	71,71,71,71	0
54	MG	1A	3628	1/1	0.64	0.14	23,23,23,23	0
54	MG	1A	3262	1/1	0.64	0.20	56,56,56,56	0
54	MG	2A	3698	1/1	0.65	0.25	57,57,57,57	0
54	MG	1a	1660	1/1	0.65	0.24	75,75,75,75	0
54	MG	2A	3341	1/1	0.65	0.17	79,79,79,79	0
54	MG	2A	3450	1/1	0.66	0.23	76,76,76,76	0
54	MG	1A	3647	1/1	0.66	0.15	49,49,49,49	0
54	MG	2A	3295	1/1	0.67	0.16	33,33,33,33	0
54	MG	1a	1761	1/1	0.67	0.25	61,61,61,61	0
54	MG	1a	1770	1/1	0.67	0.17	88,88,88,88	0
54	MG	2A	3408	1/1	0.68	0.18	71,71,71,71	0
54	MG	2A	3726	1/1	0.68	0.76	72,72,72,72	0
54	MG	2a	3012	1/1	0.69	0.22	66,66,66,66	0
54	MG	1A	3638	1/1	0.69	0.24	61,61,61,61	0
54	MG	2A	3558	1/1	0.71	0.17	54,54,54,54	0
54	MG	1A	3172	1/1	0.71	0.19	56,56,56,56	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	1A	3629	1/1	0.71	0.25	48,48,48,48	0
54	MG	2A	3345	1/1	0.71	0.21	71,71,71,71	0
54	MG	1a	1822	1/1	0.71	0.22	80,80,80,80	0
54	MG	2A	3189	1/1	0.71	0.26	58,58,58,58	0
54	MG	1A	3395	1/1	0.72	0.14	72,72,72,72	0
54	MG	1d	304	1/1	0.72	0.14	95,95,95,95	0
54	MG	2a	3108	1/1	0.72	0.27	70,70,70,70	0
54	MG	2a	3125	1/1	0.72	0.19	68,68,68,68	0
54	MG	1a	1733	1/1	0.73	0.17	43,43,43,43	0
54	MG	1G	202	1/1	0.73	0.18	60,60,60,60	0
54	MG	1a	1828	1/1	0.73	0.16	65,65,65,65	0
54	MG	2A	3195	1/1	0.74	0.25	66,66,66,66	0
54	MG	1a	1806	1/1	0.74	0.16	87,87,87,87	0
56	MPD	1T	206	8/8	0.74	0.30	56,70,76,80	0
54	MG	2A	3510	1/1	0.75	0.15	61,61,61,61	0
54	MG	2a	3003	1/1	0.75	0.28	64,64,64,64	0
54	MG	1a	1700	1/1	0.75	0.17	69,69,69,69	0
54	MG	2A	3649	1/1	0.75	0.28	97,97,97,97	0
54	MG	1T	204	1/1	0.75	0.11	63,63,63,63	0
54	MG	1A	3617	1/1	0.75	0.17	69,69,69,69	0
54	MG	2B	201	1/1	0.75	0.15	71,71,71,71	0
54	MG	2a	3068	1/1	0.76	0.13	63,63,63,63	0
54	MG	2a	3069	1/1	0.76	0.16	66,66,66,66	0
54	MG	1a	1780	1/1	0.76	0.17	78,78,78,78	0
54	MG	1A	3131	1/1	0.76	0.17	61,61,61,61	0
54	MG	1A	3838	1/1	0.76	0.14	56,56,56,56	0
54	MG	2a	3134	1/1	0.76	0.18	68,68,68,68	0
54	MG	2a	3189	1/1	0.76	0.21	67,67,67,67	0
54	MG	2a	3065	1/1	0.76	0.16	76,76,76,76	0
54	MG	2A	3672	1/1	0.77	0.29	85,85,85,85	0
54	MG	1A	3917	1/1	0.77	0.12	20,20,20,20	0
54	MG	1a	1863	1/1	0.77	0.27	69,69,69,69	0
54	MG	1A	3219	1/1	0.77	0.21	53,53,53,53	0
54	MG	2A	3056	1/1	0.77	0.16	61,61,61,61	0
54	MG	2A	3614	1/1	0.77	0.13	70,70,70,70	0
54	MG	2A	3123	1/1	0.77	0.20	74,74,74,74	0
54	MG	2A	3658	1/1	0.77	0.18	69,69,69,69	0
54	MG	1a	1609	1/1	0.78	0.15	64,64,64,64	0
54	MG	1A	3986	1/1	0.78	0.23	32,32,32,32	0
54	MG	1A	3753	1/1	0.78	0.15	63,63,63,63	0
54	MG	1a	1687	1/1	0.78	0.15	64,64,64,64	0
54	MG	1a	1854	1/1	0.78	0.10	61,61,61,61	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	2A	3413	1/1	0.78	0.19	67,67,67,67	0
54	MG	2a	3063	1/1	0.78	0.18	70,70,70,70	0
54	MG	1a	1690	1/1	0.78	0.14	63,63,63,63	0
54	MG	2A	3492	1/1	0.78	0.13	78,78,78,78	0
54	MG	1E	304	1/1	0.78	0.19	52,52,52,52	0
54	MG	1d	305	1/1	0.78	0.18	89,89,89,89	0
54	MG	2A	3596	1/1	0.78	0.15	33,33,33,33	0
54	MG	1y	203	1/1	0.78	0.18	75,75,75,75	0
54	MG	1A	3075	1/1	0.78	0.11	56,56,56,56	0
54	MG	1A	3858	1/1	0.78	0.30	26,26,26,26	0
54	MG	1A	3118	1/1	0.78	0.16	54,54,54,54	0
54	MG	1A	3903	1/1	0.79	0.17	41,41,41,41	0
54	MG	1B	207	1/1	0.79	0.22	54,54,54,54	0
54	MG	2A	3512	1/1	0.79	0.34	72,72,72,72	0
54	MG	2A	3114	1/1	0.79	0.07	57,57,57,57	0
54	MG	1T	203	1/1	0.79	0.12	55,55,55,55	0
54	MG	1A	3929	1/1	0.79	0.26	80,80,80,80	0
54	MG	2A	3644	1/1	0.79	0.16	76,76,76,76	0
54	MG	1a	1758	1/1	0.79	0.14	82,82,82,82	0
54	MG	2a	3026	1/1	0.79	0.10	66,66,66,66	0
54	MG	2a	3051	1/1	0.79	0.14	62,62,62,62	0
54	MG	1g	201	1/1	0.80	0.20	62,62,62,62	0
54	MG	1A	3835	1/1	0.80	0.13	64,64,64,64	0
54	MG	2a	3011	1/1	0.80	0.17	68,68,68,68	0
54	MG	1a	1803	1/1	0.80	0.14	83,83,83,83	0
54	MG	2A	3075	1/1	0.80	0.18	60,60,60,60	0
54	MG	1A	3176	1/1	0.80	0.22	68,68,68,68	0
54	MG	1a	1619	1/1	0.80	0.17	71,71,71,71	0
54	MG	1A	3962	1/1	0.80	0.18	51,51,51,51	0
54	MG	1A	3714	1/1	0.80	0.15	57,57,57,57	0
54	MG	1a	1858	1/1	0.80	0.10	54,54,54,54	0
54	MG	1a	1763	1/1	0.80	0.18	67,67,67,67	0
54	MG	1d	301	1/1	0.80	0.20	63,63,63,63	0
54	MG	1A	3261	1/1	0.80	0.12	60,60,60,60	0
54	MG	2A	3723	1/1	0.80	0.20	67,67,67,67	0
54	MG	2A	3410	1/1	0.80	0.13	35,35,35,35	0
54	MG	1a	1771	1/1	0.80	0.15	73,73,73,73	0
54	MG	2A	3095	1/1	0.81	0.16	68,68,68,68	0
54	MG	1A	3384	1/1	0.81	0.16	59,59,59,59	0
54	MG	1A	3746	1/1	0.81	0.10	18,18,18,18	0
54	MG	1A	3663	1/1	0.81	0.19	61,61,61,61	0
54	MG	1a	1612	1/1	0.81	0.20	56,56,56,56	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	2a	3028	1/1	0.81	0.29	68,68,68,68	0
54	MG	2A	3609	1/1	0.81	0.13	54,54,54,54	0
54	MG	2A	3264	1/1	0.81	0.15	54,54,54,54	0
54	MG	1a	1694	1/1	0.81	0.20	73,73,73,73	0
54	MG	1a	1697	1/1	0.81	0.23	65,65,65,65	0
54	MG	1a	1785	1/1	0.81	0.18	66,66,66,66	0
54	MG	1A	3666	1/1	0.81	0.21	46,46,46,46	0
54	MG	1a	1651	1/1	0.81	0.26	59,59,59,59	0
54	MG	1a	1814	1/1	0.81	0.27	61,61,61,61	0
54	MG	1a	1744	1/1	0.81	0.17	58,58,58,58	0
54	MG	2a	3140	1/1	0.81	0.21	73,73,73,73	0
54	MG	2A	3476	1/1	0.81	0.20	56,56,56,56	0
54	MG	2a	3198	1/1	0.81	0.15	56,56,56,56	0
54	MG	2B	215	1/1	0.81	0.14	62,62,62,62	0
54	MG	2I	201	1/1	0.82	0.11	63,63,63,63	0
54	MG	2A	3494	1/1	0.82	0.17	57,57,57,57	0
54	MG	1A	3741	1/1	0.82	0.17	54,54,54,54	0
54	MG	1A	3104	1/1	0.82	0.16	50,50,50,50	0
54	MG	1a	1617	1/1	0.82	0.21	74,74,74,74	0
54	MG	1A	3250	1/1	0.82	0.13	51,51,51,51	0
54	MG	1a	1732	1/1	0.82	0.10	67,67,67,67	0
54	MG	1A	3423	1/1	0.82	0.18	58,58,58,58	0
54	MG	2A	3393	1/1	0.82	0.18	54,54,54,54	0
54	MG	1y	204	1/1	0.82	0.23	62,62,62,62	0
54	MG	1a	1742	1/1	0.82	0.18	57,57,57,57	0
54	MG	1a	1655	1/1	0.82	0.30	70,70,70,70	0
54	MG	2A	3675	1/1	0.82	0.15	56,56,56,56	0
54	MG	2a	3097	1/1	0.82	0.21	60,60,60,60	0
54	MG	2A	3697	1/1	0.82	0.26	66,66,66,66	0
54	MG	1A	3518	1/1	0.82	0.17	35,35,35,35	0
54	MG	2A	3721	1/1	0.82	0.14	52,52,52,52	0
54	MG	2a	3136	1/1	0.82	0.21	55,55,55,55	0
54	MG	2A	3454	1/1	0.82	0.14	59,59,59,59	0
54	MG	2a	3164	1/1	0.82	0.21	62,62,62,62	0
54	MG	1A	3733	1/1	0.82	0.16	51,51,51,51	0
54	MG	2A	3488	1/1	0.82	0.13	51,51,51,51	0
54	MG	1a	1607	1/1	0.82	0.10	54,54,54,54	0
54	MG	1h	201	1/1	0.83	0.09	57,57,57,57	0
54	MG	1A	3188	1/1	0.83	0.10	42,42,42,42	0
54	MG	2E	304	1/1	0.83	0.13	50,50,50,50	0
54	MG	2G	202	1/1	0.83	0.14	62,62,62,62	0
54	MG	1V	205	1/1	0.83	0.21	59,59,59,59	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	2N	202	1/1	0.83	0.10	65,65,65,65	0
54	MG	1a	1802	1/1	0.83	0.19	60,60,60,60	0
54	MG	2A	3062	1/1	0.83	0.12	70,70,70,70	0
54	MG	1A	3653	1/1	0.83	0.10	23,23,23,23	0
54	MG	2A	3508	1/1	0.83	0.23	87,87,87,87	0
54	MG	2a	3021	1/1	0.83	0.19	70,70,70,70	0
54	MG	1A	3956	1/1	0.83	0.18	35,35,35,35	0
54	MG	1A	3959	1/1	0.83	0.10	78,78,78,78	0
54	MG	2A	3518	1/1	0.83	0.14	69,69,69,69	0
54	MG	2a	3062	1/1	0.83	0.22	66,66,66,66	0
54	MG	1A	3627	1/1	0.83	0.15	58,58,58,58	0
54	MG	1A	3775	1/1	0.83	0.12	67,67,67,67	0
54	MG	2a	3066	1/1	0.83	0.15	63,63,63,63	0
54	MG	1a	1833	1/1	0.83	0.10	44,44,44,44	0
54	MG	2A	3201	1/1	0.83	0.16	65,65,65,65	0
54	MG	1a	1851	1/1	0.83	0.18	52,52,52,52	0
54	MG	1A	3200	1/1	0.83	0.11	48,48,48,48	0
54	MG	2A	3651	1/1	0.83	0.12	28,28,28,28	0
54	MG	2a	3118	1/1	0.83	0.18	69,69,69,69	0
54	MG	1a	1757	1/1	0.83	0.11	61,61,61,61	0
54	MG	1A	3692	1/1	0.83	0.14	31,31,31,31	0
54	MG	1A	3548	1/1	0.83	0.14	47,47,47,47	0
54	MG	2A	3397	1/1	0.83	0.14	54,54,54,54	0
54	MG	2a	3159	1/1	0.83	0.14	62,62,62,62	0
54	MG	1A	3550	1/1	0.83	0.13	44,44,44,44	0
54	MG	2a	3169	1/1	0.83	0.16	69,69,69,69	0
54	MG	1T	202	1/1	0.83	0.15	77,77,77,77	0
54	MG	1A	3904	1/1	0.83	0.13	51,51,51,51	0
54	MG	2A	3425	1/1	0.83	0.13	58,58,58,58	0
57	ARG	1F	318	12/12	0.83	0.16	35,55,70,71	0
54	MG	1A	3680	1/1	0.84	0.17	32,32,32,32	0
54	MG	1P	205	1/1	0.84	0.14	69,69,69,69	0
54	MG	1A	3938	1/1	0.84	0.20	58,58,58,58	0
54	MG	2A	3356	1/1	0.84	0.21	61,61,61,61	0
54	MG	2A	3364	1/1	0.84	0.17	83,83,83,83	0
54	MG	2A	3367	1/1	0.84	0.12	29,29,29,29	0
54	MG	2A	3055	1/1	0.84	0.26	72,72,72,72	0
54	MG	1A	3749	1/1	0.84	0.11	43,43,43,43	0
54	MG	1A	3451	1/1	0.84	0.08	16,16,16,16	0
54	MG	1A	3704	1/1	0.84	0.23	44,44,44,44	0
54	MG	1a	1767	1/1	0.84	0.17	75,75,75,75	0
54	MG	2a	3077	1/1	0.84	0.12	61,61,61,61	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	2a	3090	1/1	0.84	0.21	64,64,64,64	0
54	MG	2A	3424	1/1	0.84	0.16	56,56,56,56	0
54	MG	1Z	301	1/1	0.84	0.14	54,54,54,54	0
54	MG	1A	3823	1/1	0.84	0.13	58,58,58,58	0
54	MG	2a	3111	1/1	0.84	0.09	65,65,65,65	0
54	MG	2A	3162	1/1	0.84	0.14	58,58,58,58	0
54	MG	2a	3119	1/1	0.84	0.13	65,65,65,65	0
54	MG	2A	3172	1/1	0.84	0.09	56,56,56,56	0
54	MG	1A	3826	1/1	0.84	0.10	43,43,43,43	0
54	MG	2B	213	1/1	0.84	0.12	59,59,59,59	0
54	MG	2A	3190	1/1	0.84	0.17	58,58,58,58	0
54	MG	1B	218	1/1	0.84	0.15	53,53,53,53	0
54	MG	2A	3498	1/1	0.84	0.22	62,62,62,62	0
54	MG	2A	3500	1/1	0.84	0.13	27,27,27,27	0
54	MG	2a	3183	1/1	0.84	0.12	61,61,61,61	0
54	MG	2A	3504	1/1	0.84	0.18	50,50,50,50	0
54	MG	1A	3921	1/1	0.84	0.15	63,63,63,63	0
54	MG	2A	3248	1/1	0.84	0.14	61,61,61,61	0
54	MG	1A	3926	1/1	0.84	0.17	60,60,60,60	0
54	MG	2a	3013	1/1	0.85	0.16	74,74,74,74	0
54	MG	1A	3841	1/1	0.85	0.40	24,24,24,24	0
54	MG	2A	3520	1/1	0.85	0.09	45,45,45,45	0
54	MG	2A	3532	1/1	0.85	0.12	52,52,52,52	0
54	MG	2a	3050	1/1	0.85	0.14	66,66,66,66	0
54	MG	1A	3554	1/1	0.85	0.25	33,33,33,33	0
54	MG	2a	3059	1/1	0.85	0.10	64,64,64,64	0
54	MG	1f	201	1/1	0.85	0.21	64,64,64,64	0
54	MG	2A	3607	1/1	0.85	0.14	30,30,30,30	0
54	MG	1A	3886	1/1	0.85	0.23	47,47,47,47	0
54	MG	1a	1661	1/1	0.85	0.25	67,67,67,67	0
54	MG	1A	3887	1/1	0.85	0.15	25,25,25,25	0
54	MG	2A	3368	1/1	0.85	0.13	50,50,50,50	0
54	MG	1Y	201	1/1	0.85	0.45	47,47,47,47	0
54	MG	1A	3460	1/1	0.85	0.09	15,15,15,15	0
54	MG	2A	3407	1/1	0.85	0.18	63,63,63,63	0
54	MG	1a	1800	1/1	0.85	0.11	58,58,58,58	0
54	MG	2a	3105	1/1	0.85	0.17	59,59,59,59	0
54	MG	15	107	1/1	0.85	0.14	35,35,35,35	0
54	MG	1a	1696	1/1	0.85	0.29	57,57,57,57	0
54	MG	2A	3082	1/1	0.85	0.18	69,69,69,69	0
54	MG	1A	3782	1/1	0.85	0.15	58,58,58,58	0
54	MG	1a	1698	1/1	0.85	0.15	54,54,54,54	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	1A	3175	1/1	0.85	0.22	55,55,55,55	0
54	MG	1a	1715	1/1	0.85	0.16	73,73,73,73	0
54	MG	1a	1608	1/1	0.85	0.12	64,64,64,64	0
54	MG	1a	1850	1/1	0.85	0.23	81,81,81,81	0
54	MG	2a	3163	1/1	0.85	0.18	68,68,68,68	0
54	MG	1A	3328	1/1	0.85	0.14	65,65,65,65	0
54	MG	1A	3549	1/1	0.85	0.12	20,20,20,20	0
54	MG	2a	3171	1/1	0.85	0.08	62,62,62,62	0
54	MG	1A	3236	1/1	0.85	0.09	55,55,55,55	0
54	MG	1A	3937	1/1	0.85	0.17	65,65,65,65	0
54	MG	2a	3193	1/1	0.85	0.15	68,68,68,68	0
54	MG	1a	1648	1/1	0.85	0.10	39,39,39,39	0
56	MPD	1A	3992	8/8	0.85	0.27	45,52,60,67	0
54	MG	2A	3266	1/1	0.85	0.15	46,46,46,46	0
56	MPD	1a	1866	8/8	0.85	0.18	48,63,68,71	0
54	MG	2A	3292	1/1	0.85	0.09	46,46,46,46	0
54	MG	2A	3375	1/1	0.86	0.11	46,46,46,46	0
54	MG	2A	3727	1/1	0.86	0.17	62,62,62,62	0
54	MG	2A	3729	1/1	0.86	0.15	53,53,53,53	0
54	MG	2A	3732	1/1	0.86	0.29	57,57,57,57	0
54	MG	1A	3822	1/1	0.86	0.12	22,22,22,22	0
54	MG	1t	201	1/1	0.86	0.13	60,60,60,60	0
54	MG	1a	1662	1/1	0.86	0.20	55,55,55,55	0
54	MG	2D	303	1/1	0.86	0.22	37,37,37,37	0
54	MG	1A	3562	1/1	0.86	0.10	46,46,46,46	0
54	MG	2A	3023	1/1	0.86	0.27	70,70,70,70	0
54	MG	2A	3038	1/1	0.86	0.18	64,64,64,64	0
54	MG	2A	3421	1/1	0.86	0.11	66,66,66,66	0
54	MG	2A	3045	1/1	0.86	0.21	40,40,40,40	0
54	MG	1a	1676	1/1	0.86	0.14	56,56,56,56	0
54	MG	2A	3431	1/1	0.86	0.08	59,59,59,59	0
54	MG	2A	3432	1/1	0.86	0.17	63,63,63,63	0
54	MG	2A	3435	1/1	0.86	0.14	48,48,48,48	0
54	MG	2a	3014	1/1	0.86	0.13	55,55,55,55	0
54	MG	1a	1680	1/1	0.86	0.24	59,59,59,59	0
54	MG	2A	3451	1/1	0.86	0.17	61,61,61,61	0
54	MG	1A	3650	1/1	0.86	0.12	57,57,57,57	0
54	MG	2a	3038	1/1	0.86	0.11	65,65,65,65	0
54	MG	2A	3473	1/1	0.86	0.11	62,62,62,62	0
54	MG	1a	1781	1/1	0.86	0.11	58,58,58,58	0
54	MG	1a	1689	1/1	0.86	0.11	56,56,56,56	0
54	MG	2A	3490	1/1	0.86	0.09	62,62,62,62	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	1a	1797	1/1	0.86	0.16	50,50,50,50	0
54	MG	2A	3097	1/1	0.86	0.13	55,55,55,55	0
54	MG	1A	3588	1/1	0.86	0.10	13,13,13,13	0
54	MG	1a	1601	1/1	0.86	0.13	51,51,51,51	0
54	MG	2A	3137	1/1	0.86	0.16	60,60,60,60	0
54	MG	2a	3071	1/1	0.86	0.11	64,64,64,64	0
54	MG	1D	316	1/1	0.86	0.15	69,69,69,69	0
54	MG	2a	3080	1/1	0.86	0.13	61,61,61,61	0
54	MG	1A	3037	1/1	0.86	0.12	51,51,51,51	0
54	MG	1E	306	1/1	0.86	0.10	48,48,48,48	0
54	MG	1F	311	1/1	0.86	0.14	34,34,34,34	0
54	MG	2a	3101	1/1	0.86	0.22	50,50,50,50	0
54	MG	1a	1827	1/1	0.86	0.11	64,64,64,64	0
54	MG	1a	1703	1/1	0.86	0.15	54,54,54,54	0
54	MG	2A	3545	1/1	0.86	0.17	73,73,73,73	0
54	MG	2A	3224	1/1	0.86	0.17	53,53,53,53	0
54	MG	2A	3572	1/1	0.86	0.11	68,68,68,68	0
54	MG	2A	3593	1/1	0.86	0.10	36,36,36,36	0
54	MG	2a	3128	1/1	0.86	0.10	56,56,56,56	0
54	MG	2A	3243	1/1	0.86	0.13	57,57,57,57	0
54	MG	2A	3602	1/1	0.86	0.15	40,40,40,40	0
54	MG	1a	1705	1/1	0.86	0.12	52,52,52,52	0
54	MG	1A	3182	1/1	0.86	0.14	52,52,52,52	0
54	MG	1A	3406	1/1	0.86	0.51	57,57,57,57	0
54	MG	2A	3278	1/1	0.86	0.16	44,44,44,44	0
54	MG	1a	1624	1/1	0.86	0.09	43,43,43,43	0
54	MG	1a	1741	1/1	0.86	0.11	54,54,54,54	0
54	MG	2A	3329	1/1	0.86	0.12	29,29,29,29	0
54	MG	1A	3501	1/1	0.86	0.17	48,48,48,48	0
54	MG	1A	3506	1/1	0.86	0.21	25,25,25,25	0
54	MG	2A	3676	1/1	0.86	0.21	67,67,67,67	0
54	MG	1a	1745	1/1	0.86	0.19	62,62,62,62	0
54	MG	1a	1749	1/1	0.86	0.11	61,61,61,61	0
54	MG	1A	3815	1/1	0.86	0.11	41,41,41,41	0
54	MG	1A	3979	1/1	0.86	0.13	68,68,68,68	0
54	MG	2A	3468	1/1	0.87	0.14	33,33,33,33	0
54	MG	2A	3198	1/1	0.87	0.13	52,52,52,52	0
54	MG	1A	3970	1/1	0.87	0.09	22,22,22,22	0
54	MG	1A	3399	1/1	0.87	0.10	21,21,21,21	0
54	MG	1a	1640	1/1	0.87	0.15	78,78,78,78	0
54	MG	21	103	1/1	0.87	0.11	68,68,68,68	0
54	MG	1a	1647	1/1	0.87	0.21	62,62,62,62	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	2a	3005	1/1	0.87	0.13	58,58,58,58	0
54	MG	1a	1794	1/1	0.87	0.18	73,73,73,73	0
54	MG	1A	3461	1/1	0.87	0.09	13,13,13,13	0
54	MG	2A	3268	1/1	0.87	0.24	77,77,77,77	0
54	MG	1B	201	1/1	0.87	0.12	44,44,44,44	0
54	MG	2A	3291	1/1	0.87	0.14	42,42,42,42	0
54	MG	1A	3491	1/1	0.87	0.11	22,22,22,22	0
54	MG	2A	3024	1/1	0.87	0.13	60,60,60,60	0
54	MG	2a	3037	1/1	0.87	0.18	62,62,62,62	0
54	MG	2A	3304	1/1	0.87	0.18	54,54,54,54	0
54	MG	2A	3035	1/1	0.87	0.13	56,56,56,56	0
54	MG	2A	3525	1/1	0.87	0.18	42,42,42,42	0
54	MG	2A	3336	1/1	0.87	0.09	42,42,42,42	0
54	MG	1a	1657	1/1	0.87	0.14	61,61,61,61	0
54	MG	2A	3554	1/1	0.87	0.11	31,31,31,31	0
54	MG	1A	3633	1/1	0.87	0.32	30,30,30,30	0
54	MG	2A	3355	1/1	0.87	0.16	53,53,53,53	0
54	MG	1a	1809	1/1	0.87	0.10	56,56,56,56	0
54	MG	1B	227	1/1	0.87	0.10	48,48,48,48	0
54	MG	1a	1816	1/1	0.87	0.08	60,60,60,60	0
54	MG	2A	3603	1/1	0.87	0.13	59,59,59,59	0
54	MG	2A	3605	1/1	0.87	0.17	62,62,62,62	0
54	MG	2a	3085	1/1	0.87	0.20	62,62,62,62	0
54	MG	2a	3089	1/1	0.87	0.16	52,52,52,52	0
54	MG	2A	3070	1/1	0.87	0.32	54,54,54,54	0
54	MG	1A	3492	1/1	0.87	0.10	42,42,42,42	0
54	MG	1D	312	1/1	0.87	0.20	44,44,44,44	0
54	MG	2A	3617	1/1	0.87	0.11	56,56,56,56	0
54	MG	2A	3642	1/1	0.87	0.09	45,45,45,45	0
54	MG	1A	3785	1/1	0.87	0.13	62,62,62,62	0
54	MG	2A	3405	1/1	0.87	0.14	56,56,56,56	0
54	MG	1A	3951	1/1	0.87	0.11	51,51,51,51	0
54	MG	2A	3102	1/1	0.87	0.23	44,44,44,44	0
54	MG	2A	3409	1/1	0.87	0.13	55,55,55,55	0
54	MG	2A	3110	1/1	0.87	0.24	48,48,48,48	0
54	MG	2a	3132	1/1	0.87	0.20	70,70,70,70	0
54	MG	1a	1683	1/1	0.87	0.13	53,53,53,53	0
54	MG	2A	3679	1/1	0.87	0.17	58,58,58,58	0
54	MG	1A	3367	1/1	0.87	0.10	22,22,22,22	0
54	MG	2A	3126	1/1	0.87	0.13	69,69,69,69	0
54	MG	2A	3700	1/1	0.87	0.35	50,50,50,50	0
54	MG	1a	1688	1/1	0.87	0.23	55,55,55,55	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	1A	3302	1/1	0.87	0.16	56,56,56,56	0
54	MG	1a	1861	1/1	0.87	0.16	52,52,52,52	0
54	MG	1a	1764	1/1	0.87	0.22	48,48,48,48	0
54	MG	2a	3187	1/1	0.87	0.08	63,63,63,63	0
54	MG	2A	3438	1/1	0.87	0.12	49,49,49,49	0
54	MG	2A	3445	1/1	0.87	0.10	34,34,34,34	0
54	MG	2A	3449	1/1	0.87	0.16	62,62,62,62	0
54	MG	1A	3257	1/1	0.87	0.13	57,57,57,57	0
54	MG	2A	3191	1/1	0.87	0.16	54,54,54,54	0
54	MG	1H	201	1/1	0.87	0.12	51,51,51,51	0
54	MG	2D	306	1/1	0.87	0.10	28,28,28,28	0
54	MG	1A	3316	1/1	0.88	0.09	36,36,36,36	0
54	MG	1a	1702	1/1	0.88	0.11	60,60,60,60	0
54	MG	2B	206	1/1	0.88	0.16	54,54,54,54	0
54	MG	1A	3446	1/1	0.88	0.14	55,55,55,55	0
54	MG	1a	1818	1/1	0.88	0.13	64,64,64,64	0
54	MG	2B	216	1/1	0.88	0.11	68,68,68,68	0
54	MG	1A	3876	1/1	0.88	0.13	32,32,32,32	0
54	MG	2D	305	1/1	0.88	0.11	48,48,48,48	0
54	MG	1A	3879	1/1	0.88	0.11	37,37,37,37	0
54	MG	2A	3147	1/1	0.88	0.09	49,49,49,49	0
54	MG	2G	201	1/1	0.88	0.10	74,74,74,74	0
54	MG	1A	3745	1/1	0.88	0.09	40,40,40,40	0
54	MG	2A	3457	1/1	0.88	0.09	29,29,29,29	0
54	MG	1A	3023	1/1	0.88	0.23	53,53,53,53	0
54	MG	2Q	202	1/1	0.88	0.20	45,45,45,45	0
54	MG	1a	1641	1/1	0.88	0.18	60,60,60,60	0
54	MG	1A	3199	1/1	0.88	0.10	57,57,57,57	0
54	MG	2A	3486	1/1	0.88	0.09	44,44,44,44	0
54	MG	1A	3166	1/1	0.88	0.12	53,53,53,53	0
54	MG	1A	3908	1/1	0.88	0.11	26,26,26,26	0
54	MG	1a	1860	1/1	0.88	0.12	58,58,58,58	0
54	MG	1a	1746	1/1	0.88	0.20	55,55,55,55	0
54	MG	2A	3221	1/1	0.88	0.10	49,49,49,49	0
54	MG	1a	1654	1/1	0.88	0.15	39,39,39,39	0
54	MG	2a	3025	1/1	0.88	0.24	65,65,65,65	0
54	MG	1a	1756	1/1	0.88	0.16	55,55,55,55	0
54	MG	1A	3756	1/1	0.88	0.25	46,46,46,46	0
54	MG	1A	3758	1/1	0.88	0.10	34,34,34,34	0
54	MG	1e	201	1/1	0.88	0.17	44,44,44,44	0
54	MG	2a	3044	1/1	0.88	0.13	65,65,65,65	0
54	MG	2a	3045	1/1	0.88	0.12	61,61,61,61	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	1A	3760	1/1	0.88	0.14	57,57,57,57	0
54	MG	2A	3269	1/1	0.88	0.11	26,26,26,26	0
54	MG	2A	3277	1/1	0.88	0.10	47,47,47,47	0
54	MG	1A	3480	1/1	0.88	0.12	47,47,47,47	0
54	MG	2A	3537	1/1	0.88	0.27	39,39,39,39	0
54	MG	1g	202	1/1	0.88	0.09	50,50,50,50	0
54	MG	2A	3546	1/1	0.88	0.11	57,57,57,57	0
54	MG	1A	3780	1/1	0.88	0.09	30,30,30,30	0
54	MG	1l	202	1/1	0.88	0.10	42,42,42,42	0
54	MG	1o	102	1/1	0.88	0.11	63,63,63,63	0
54	MG	2A	3573	1/1	0.88	0.11	52,52,52,52	0
54	MG	2A	3326	1/1	0.88	0.09	52,52,52,52	0
54	MG	1A	3277	1/1	0.88	0.14	41,41,41,41	0
54	MG	1t	202	1/1	0.88	0.06	69,69,69,69	0
54	MG	1a	1768	1/1	0.88	0.10	61,61,61,61	0
54	MG	1A	3288	1/1	0.88	0.13	36,36,36,36	0
54	MG	2A	3347	1/1	0.88	0.10	61,61,61,61	0
54	MG	2a	3100	1/1	0.88	0.13	64,64,64,64	0
54	MG	2A	3608	1/1	0.88	0.13	38,38,38,38	0
54	MG	2A	3014	1/1	0.88	0.14	52,52,52,52	0
54	MG	2A	3610	1/1	0.88	0.11	63,63,63,63	0
54	MG	2A	3611	1/1	0.88	0.10	67,67,67,67	0
54	MG	1W	201	1/1	0.88	0.15	48,48,48,48	0
54	MG	1a	1778	1/1	0.88	0.17	86,86,86,86	0
54	MG	1A	3803	1/1	0.88	0.08	27,27,27,27	0
54	MG	1A	3251	1/1	0.88	0.11	42,42,42,42	0
54	MG	2A	3372	1/1	0.88	0.12	42,42,42,42	0
54	MG	2A	3040	1/1	0.88	0.11	53,53,53,53	0
54	MG	2A	3652	1/1	0.88	0.11	29,29,29,29	0
54	MG	2A	3379	1/1	0.88	0.15	61,61,61,61	0
54	MG	2a	3148	1/1	0.88	0.08	71,71,71,71	0
54	MG	1a	1782	1/1	0.88	0.15	69,69,69,69	0
54	MG	2A	3049	1/1	0.88	0.17	59,59,59,59	0
54	MG	10	108	1/1	0.88	0.43	42,42,42,42	0
54	MG	1a	1787	1/1	0.88	0.17	68,68,68,68	0
54	MG	2A	3689	1/1	0.88	0.12	59,59,59,59	0
54	MG	2A	3058	1/1	0.88	0.12	60,60,60,60	0
54	MG	2A	3059	1/1	0.88	0.15	52,52,52,52	0
54	MG	15	106	1/1	0.88	0.11	29,29,29,29	0
54	MG	2A	3706	1/1	0.88	0.15	70,70,70,70	0
54	MG	2a	3194	1/1	0.88	0.07	61,61,61,61	0
54	MG	2a	3195	1/1	0.88	0.10	62,62,62,62	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	2a	3196	1/1	0.88	0.15	56,56,56,56	0
54	MG	1A	3700	1/1	0.88	0.15	52,52,52,52	0
54	MG	2t	201	1/1	0.88	0.10	49,49,49,49	0
54	MG	1A	3408	1/1	0.88	0.13	21,21,21,21	0
54	MG	1A	3513	1/1	0.88	0.16	45,45,45,45	0
54	MG	1A	3720	1/1	0.88	0.11	51,51,51,51	0
56	MPD	2B	221	8/8	0.88	0.22	59,68,73,74	0
54	MG	1A	3728	1/1	0.88	0.13	56,56,56,56	0
54	MG	2A	3440	1/1	0.89	0.10	63,63,63,63	0
54	MG	2A	3441	1/1	0.89	0.20	71,71,71,71	0
54	MG	1a	1738	1/1	0.89	0.07	56,56,56,56	0
54	MG	2A	3181	1/1	0.89	0.19	47,47,47,47	0
54	MG	2A	3184	1/1	0.89	0.16	54,54,54,54	0
54	MG	2A	3186	1/1	0.89	0.13	54,54,54,54	0
54	MG	1A	3599	1/1	0.89	0.18	21,21,21,21	0
54	MG	1B	226	1/1	0.89	0.10	59,59,59,59	0
54	MG	2A	3463	1/1	0.89	0.12	55,55,55,55	0
54	MG	1a	1633	1/1	0.89	0.22	54,54,54,54	0
54	MG	1a	1639	1/1	0.89	0.21	67,67,67,67	0
54	MG	2P	201	1/1	0.89	0.15	58,58,58,58	0
54	MG	1A	3610	1/1	0.89	0.11	50,50,50,50	0
54	MG	1A	3899	1/1	0.89	0.16	42,42,42,42	0
54	MG	2A	3212	1/1	0.89	0.11	57,57,57,57	0
54	MG	2A	3214	1/1	0.89	0.23	62,62,62,62	0
54	MG	2a	3004	1/1	0.89	0.26	61,61,61,61	0
54	MG	1A	3247	1/1	0.89	0.18	41,41,41,41	0
54	MG	1A	3151	1/1	0.89	0.11	48,48,48,48	0
54	MG	2A	3495	1/1	0.89	0.23	46,46,46,46	0
54	MG	2A	3231	1/1	0.89	0.10	51,51,51,51	0
54	MG	2A	3233	1/1	0.89	0.20	55,55,55,55	0
54	MG	1e	203	1/1	0.89	0.08	52,52,52,52	0
54	MG	2A	3245	1/1	0.89	0.18	54,54,54,54	0
54	MG	1A	3711	1/1	0.89	0.13	57,57,57,57	0
54	MG	1a	1652	1/1	0.89	0.14	62,62,62,62	0
54	MG	1a	1762	1/1	0.89	0.12	59,59,59,59	0
54	MG	1A	3799	1/1	0.89	0.12	44,44,44,44	0
54	MG	2a	3042	1/1	0.89	0.20	62,62,62,62	0
54	MG	1A	3194	1/1	0.89	0.17	62,62,62,62	0
54	MG	1A	3924	1/1	0.89	0.08	60,60,60,60	0
54	MG	2a	3047	1/1	0.89	0.19	44,44,44,44	0
54	MG	2a	3049	1/1	0.89	0.12	57,57,57,57	0
54	MG	2A	3536	1/1	0.89	0.12	83,83,83,83	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	1A	3256	1/1	0.89	0.31	44,44,44,44	0
54	MG	2a	3054	1/1	0.89	0.23	53,53,53,53	0
54	MG	1A	3049	1/1	0.89	0.07	23,23,23,23	0
54	MG	1A	3934	1/1	0.89	0.10	31,31,31,31	0
54	MG	2A	3551	1/1	0.89	0.13	27,27,27,27	0
54	MG	1a	1669	1/1	0.89	0.12	61,61,61,61	0
54	MG	1A	3935	1/1	0.89	0.19	64,64,64,64	0
54	MG	2A	3560	1/1	0.89	0.15	71,71,71,71	0
54	MG	2A	3310	1/1	0.89	0.10	44,44,44,44	0
54	MG	1a	1675	1/1	0.89	0.11	57,57,57,57	0
54	MG	1A	3634	1/1	0.89	0.16	60,60,60,60	0
54	MG	2A	3330	1/1	0.89	0.11	64,64,64,64	0
54	MG	2A	3601	1/1	0.89	0.10	57,57,57,57	0
54	MG	2A	3334	1/1	0.89	0.10	36,36,36,36	0
54	MG	1A	3490	1/1	0.89	0.10	48,48,48,48	0
54	MG	2a	3093	1/1	0.89	0.15	62,62,62,62	0
54	MG	1A	3942	1/1	0.89	0.15	49,49,49,49	0
54	MG	2a	3096	1/1	0.89	0.17	62,62,62,62	0
54	MG	1A	3553	1/1	0.89	0.12	53,53,53,53	0
54	MG	1A	3953	1/1	0.89	0.11	23,23,23,23	0
54	MG	1A	3246	1/1	0.89	0.11	53,53,53,53	0
54	MG	13	102	1/1	0.89	0.13	63,63,63,63	0
54	MG	2A	3362	1/1	0.89	0.08	54,54,54,54	0
54	MG	1A	3344	1/1	0.89	0.09	36,36,36,36	0
54	MG	1A	3855	1/1	0.89	0.14	43,43,43,43	0
54	MG	1A	3857	1/1	0.89	0.28	38,38,38,38	0
54	MG	2A	3369	1/1	0.89	0.21	63,63,63,63	0
54	MG	1A	3577	1/1	0.89	0.30	35,35,35,35	0
54	MG	1A	3984	1/1	0.89	0.11	50,50,50,50	0
54	MG	1A	3873	1/1	0.89	0.10	14,14,14,14	0
54	MG	2A	3382	1/1	0.89	0.21	66,66,66,66	0
54	MG	1A	3987	1/1	0.89	0.11	51,51,51,51	0
54	MG	1a	1825	1/1	0.89	0.09	65,65,65,65	0
54	MG	1a	1610	1/1	0.89	0.21	60,60,60,60	0
54	MG	1A	3665	1/1	0.89	0.15	43,43,43,43	0
54	MG	1a	1831	1/1	0.89	0.24	72,72,72,72	0
54	MG	1a	1615	1/1	0.89	0.09	60,60,60,60	0
54	MG	1a	1835	1/1	0.89	0.16	70,70,70,70	0
54	MG	2a	3172	1/1	0.89	0.18	44,44,44,44	0
54	MG	2A	3699	1/1	0.89	0.16	51,51,51,51	0
54	MG	2A	3412	1/1	0.89	0.10	58,58,58,58	0
54	MG	1A	3426	1/1	0.89	0.10	39,39,39,39	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	2A	3711	1/1	0.89	0.15	48,48,48,48	0
54	MG	2A	3133	1/1	0.89	0.12	66,66,66,66	0
54	MG	2A	3722	1/1	0.89	0.08	49,49,49,49	0
54	MG	1a	1736	1/1	0.89	0.14	65,65,65,65	0
54	MG	2A	3144	1/1	0.89	0.18	48,48,48,48	0
54	MG	1a	1852	1/1	0.89	0.13	49,49,49,49	0
54	MG	2A	3155	1/1	0.89	0.10	66,66,66,66	0
54	MG	2A	3161	1/1	0.89	0.22	55,55,55,55	0
54	MG	2A	3736	1/1	0.89	0.22	57,57,57,57	0
54	MG	2A	3437	1/1	0.89	0.09	42,42,42,42	0
54	MG	1a	1853	1/1	0.89	0.23	66,66,66,66	0
54	MG	1A	3402	1/1	0.90	0.11	20,20,20,20	0
54	MG	2A	3160	1/1	0.90	0.19	48,48,48,48	0
54	MG	19	101	1/1	0.90	0.11	46,46,46,46	0
54	MG	2A	3737	1/1	0.90	0.16	52,52,52,52	0
54	MG	1A	3279	1/1	0.90	0.11	70,70,70,70	0
54	MG	1A	3066	1/1	0.90	0.17	43,43,43,43	0
54	MG	2B	209	1/1	0.90	0.32	67,67,67,67	0
54	MG	1A	3411	1/1	0.90	0.12	63,63,63,63	0
54	MG	1a	1708	1/1	0.90	0.12	58,58,58,58	0
54	MG	1A	3001	1/1	0.90	0.13	44,44,44,44	0
54	MG	1a	1717	1/1	0.90	0.10	51,51,51,51	0
54	MG	1a	1719	1/1	0.90	0.11	79,79,79,79	0
54	MG	1a	1727	1/1	0.90	0.11	68,68,68,68	0
54	MG	2D	307	1/1	0.90	0.18	50,50,50,50	0
54	MG	1A	3678	1/1	0.90	0.13	25,25,25,25	0
54	MG	2A	3455	1/1	0.90	0.14	57,57,57,57	0
54	MG	1A	3311	1/1	0.90	0.13	8,8,8,8	0
54	MG	2A	3461	1/1	0.90	0.17	52,52,52,52	0
54	MG	2A	3462	1/1	0.90	0.10	53,53,53,53	0
54	MG	1a	1613	1/1	0.90	0.15	62,62,62,62	0
54	MG	2A	3211	1/1	0.90	0.08	67,67,67,67	0
54	MG	1A	3830	1/1	0.90	0.10	22,22,22,22	0
54	MG	2A	3474	1/1	0.90	0.08	45,45,45,45	0
54	MG	26	101	1/1	0.90	0.20	55,55,55,55	0
54	MG	28	101	1/1	0.90	0.13	49,49,49,49	0
54	MG	1A	3683	1/1	0.90	0.16	69,69,69,69	0
54	MG	2A	3479	1/1	0.90	0.12	60,60,60,60	0
54	MG	1a	1865	1/1	0.90	0.15	42,42,42,42	0
54	MG	2a	3006	1/1	0.90	0.14	58,58,58,58	0
54	MG	2a	3010	1/1	0.90	0.09	63,63,63,63	0
54	MG	1A	3836	1/1	0.90	0.08	39,39,39,39	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	2A	3225	1/1	0.90	0.17	59,59,59,59	0
54	MG	1A	3201	1/1	0.90	0.20	32,32,32,32	0
54	MG	1A	3563	1/1	0.90	0.12	64,64,64,64	0
54	MG	2A	3236	1/1	0.90	0.08	49,49,49,49	0
54	MG	2A	3241	1/1	0.90	0.16	47,47,47,47	0
54	MG	1A	3849	1/1	0.90	0.09	15,15,15,15	0
54	MG	2A	3244	1/1	0.90	0.13	49,49,49,49	0
54	MG	1A	3570	1/1	0.90	0.11	37,37,37,37	0
54	MG	1a	1753	1/1	0.90	0.13	55,55,55,55	0
54	MG	2A	3252	1/1	0.90	0.55	39,39,39,39	0
54	MG	2A	3256	1/1	0.90	0.29	49,49,49,49	0
54	MG	2A	3519	1/1	0.90	0.09	47,47,47,47	0
54	MG	1f	202	1/1	0.90	0.15	55,55,55,55	0
54	MG	2A	3522	1/1	0.90	0.09	29,29,29,29	0
54	MG	1A	3574	1/1	0.90	0.13	31,31,31,31	0
54	MG	1A	3165	1/1	0.90	0.18	33,33,33,33	0
54	MG	1A	3718	1/1	0.90	0.09	24,24,24,24	0
54	MG	2a	3055	1/1	0.90	0.21	62,62,62,62	0
54	MG	1a	1649	1/1	0.90	0.18	44,44,44,44	0
54	MG	1o	101	1/1	0.90	0.12	41,41,41,41	0
54	MG	2A	3286	1/1	0.90	0.09	30,30,30,30	0
54	MG	1A	3338	1/1	0.90	0.09	35,35,35,35	0
54	MG	1D	314	1/1	0.90	0.24	34,34,34,34	0
54	MG	1A	3228	1/1	0.90	0.40	41,41,41,41	0
54	MG	2A	3300	1/1	0.90	0.10	44,44,44,44	0
54	MG	1a	1765	1/1	0.90	0.15	55,55,55,55	0
54	MG	2a	3075	1/1	0.90	0.18	70,70,70,70	0
54	MG	2A	3307	1/1	0.90	0.10	39,39,39,39	0
54	MG	1A	3600	1/1	0.90	0.15	58,58,58,58	0
54	MG	2a	3083	1/1	0.90	0.11	60,60,60,60	0
54	MG	2A	3594	1/1	0.90	0.13	42,42,42,42	0
54	MG	1A	3740	1/1	0.90	0.11	28,28,28,28	0
54	MG	2A	3327	1/1	0.90	0.12	48,48,48,48	0
54	MG	1a	1769	1/1	0.90	0.10	78,78,78,78	0
54	MG	1a	1659	1/1	0.90	0.17	63,63,63,63	0
54	MG	2A	3034	1/1	0.90	0.12	47,47,47,47	0
54	MG	1A	3893	1/1	0.90	0.08	39,39,39,39	0
54	MG	1F	314	1/1	0.90	0.29	57,57,57,57	0
54	MG	2A	3039	1/1	0.90	0.15	58,58,58,58	0
54	MG	1A	3608	1/1	0.90	0.48	34,34,34,34	0
54	MG	2A	3044	1/1	0.90	0.23	53,53,53,53	0
54	MG	2a	3110	1/1	0.90	0.12	70,70,70,70	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	2A	3612	1/1	0.90	0.09	46,46,46,46	0
54	MG	1a	1666	1/1	0.90	0.24	57,57,57,57	0
54	MG	2A	3361	1/1	0.90	0.11	60,60,60,60	0
54	MG	2A	3618	1/1	0.90	0.29	56,56,56,56	0
54	MG	2A	3627	1/1	0.90	0.15	77,77,77,77	0
54	MG	2a	3130	1/1	0.90	0.12	50,50,50,50	0
54	MG	2a	3131	1/1	0.90	0.10	69,69,69,69	0
54	MG	1A	3609	1/1	0.90	0.13	51,51,51,51	0
54	MG	1a	1784	1/1	0.90	0.10	53,53,53,53	0
54	MG	1A	3469	1/1	0.90	0.10	25,25,25,25	0
54	MG	2A	3057	1/1	0.90	0.23	56,56,56,56	0
54	MG	1A	3907	1/1	0.90	0.11	77,77,77,77	0
54	MG	1a	1789	1/1	0.90	0.16	62,62,62,62	0
54	MG	2a	3162	1/1	0.90	0.10	48,48,48,48	0
54	MG	1a	1791	1/1	0.90	0.10	62,62,62,62	0
54	MG	1A	3359	1/1	0.90	0.12	53,53,53,53	0
54	MG	1a	1796	1/1	0.90	0.11	71,71,71,71	0
54	MG	2A	3678	1/1	0.90	0.13	72,72,72,72	0
54	MG	2A	3386	1/1	0.90	0.18	45,45,45,45	0
54	MG	2a	3177	1/1	0.90	0.13	54,54,54,54	0
54	MG	1A	3360	1/1	0.90	0.08	30,30,30,30	0
54	MG	1a	1798	1/1	0.90	0.16	83,83,83,83	0
54	MG	2a	3188	1/1	0.90	0.11	63,63,63,63	0
54	MG	1A	3234	1/1	0.90	0.13	36,36,36,36	0
54	MG	1A	3033	1/1	0.90	0.11	42,42,42,42	0
54	MG	1A	3393	1/1	0.90	0.09	17,17,17,17	0
54	MG	1A	3768	1/1	0.90	0.09	49,49,49,49	0
54	MG	1a	1808	1/1	0.90	0.19	49,49,49,49	0
54	MG	2A	3718	1/1	0.90	0.14	38,38,38,38	0
54	MG	1A	3268	1/1	0.90	0.11	63,63,63,63	0
54	MG	1a	1691	1/1	0.90	0.15	57,57,57,57	0
54	MG	1A	3776	1/1	0.90	0.39	28,28,28,28	0
54	MG	2A	3725	1/1	0.90	0.10	49,49,49,49	0
54	MG	1A	3507	1/1	0.90	0.08	43,43,43,43	0
54	MG	1A	3059	1/1	0.90	0.09	45,45,45,45	0
54	MG	1a	1735	1/1	0.91	0.10	47,47,47,47	0
54	MG	2A	3173	1/1	0.91	0.23	54,54,54,54	0
54	MG	2A	3731	1/1	0.91	0.11	51,51,51,51	0
54	MG	2A	3436	1/1	0.91	0.10	54,54,54,54	0
54	MG	2A	3733	1/1	0.91	0.14	45,45,45,45	0
54	MG	2A	3735	1/1	0.91	0.09	46,46,46,46	0
54	MG	1A	3988	1/1	0.91	0.12	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	1A	3145	1/1	0.91	0.12	41,41,41,41	0
54	MG	1a	1623	1/1	0.91	0.10	54,54,54,54	0
54	MG	2A	3187	1/1	0.91	0.28	53,53,53,53	0
54	MG	2B	208	1/1	0.91	0.13	57,57,57,57	0
54	MG	1B	203	1/1	0.91	0.16	38,38,38,38	0
54	MG	1a	1630	1/1	0.91	0.17	60,60,60,60	0
54	MG	2B	214	1/1	0.91	0.15	96,96,96,96	0
54	MG	1A	3578	1/1	0.91	0.12	59,59,59,59	0
54	MG	1B	209	1/1	0.91	0.08	42,42,42,42	0
54	MG	1A	3677	1/1	0.91	0.21	54,54,54,54	0
54	MG	2A	3199	1/1	0.91	0.22	39,39,39,39	0
54	MG	1A	3763	1/1	0.91	0.09	40,40,40,40	0
54	MG	2A	3460	1/1	0.91	0.12	51,51,51,51	0
54	MG	2A	3208	1/1	0.91	0.09	55,55,55,55	0
54	MG	1a	1754	1/1	0.91	0.13	56,56,56,56	0
54	MG	1a	1643	1/1	0.91	0.17	61,61,61,61	0
54	MG	2A	3213	1/1	0.91	0.11	52,52,52,52	0
54	MG	1A	3415	1/1	0.91	0.09	15,15,15,15	0
54	MG	1A	3106	1/1	0.91	0.14	40,40,40,40	0
54	MG	2P	202	1/1	0.91	0.13	56,56,56,56	0
54	MG	1A	3386	1/1	0.91	0.08	36,36,36,36	0
54	MG	2T	201	1/1	0.91	0.13	71,71,71,71	0
54	MG	1a	1650	1/1	0.91	0.09	46,46,46,46	0
54	MG	2W	204	1/1	0.91	0.15	39,39,39,39	0
54	MG	2A	3481	1/1	0.91	0.07	43,43,43,43	0
54	MG	25	103	1/1	0.91	0.11	53,53,53,53	0
54	MG	1A	3436	1/1	0.91	0.14	41,41,41,41	0
54	MG	27	102	1/1	0.91	0.15	42,42,42,42	0
54	MG	1D	315	1/1	0.91	0.19	49,49,49,49	0
54	MG	2A	3489	1/1	0.91	0.11	62,62,62,62	0
54	MG	1a	1653	1/1	0.91	0.12	72,72,72,72	0
54	MG	2A	3238	1/1	0.91	0.23	44,44,44,44	0
54	MG	1g	203	1/1	0.91	0.13	53,53,53,53	0
54	MG	1A	3906	1/1	0.91	0.07	49,49,49,49	0
54	MG	2A	3497	1/1	0.91	0.18	66,66,66,66	0
54	MG	1A	3514	1/1	0.91	0.09	16,16,16,16	0
54	MG	1A	3703	1/1	0.91	0.13	38,38,38,38	0
54	MG	1F	306	1/1	0.91	0.14	25,25,25,25	0
54	MG	2A	3251	1/1	0.91	0.09	41,41,41,41	0
54	MG	1A	3911	1/1	0.91	0.10	44,44,44,44	0
54	MG	1a	1773	1/1	0.91	0.11	59,59,59,59	0
54	MG	2A	3262	1/1	0.91	0.08	41,41,41,41	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	2a	3035	1/1	0.91	0.13	52,52,52,52	0
54	MG	1a	1776	1/1	0.91	0.15	58,58,58,58	0
54	MG	1A	3915	1/1	0.91	0.08	22,22,22,22	0
54	MG	2A	3007	1/1	0.91	0.10	40,40,40,40	0
54	MG	1G	201	1/1	0.91	0.15	64,64,64,64	0
54	MG	2A	3273	1/1	0.91	0.12	17,17,17,17	0
54	MG	1A	3389	1/1	0.91	0.10	48,48,48,48	0
54	MG	1A	3520	1/1	0.91	0.10	33,33,33,33	0
54	MG	1A	3804	1/1	0.91	0.13	43,43,43,43	0
54	MG	1A	3812	1/1	0.91	0.20	54,54,54,54	0
54	MG	2A	3549	1/1	0.91	0.11	61,61,61,61	0
54	MG	1A	3713	1/1	0.91	0.09	52,52,52,52	0
54	MG	1A	3932	1/1	0.91	0.13	64,64,64,64	0
54	MG	1A	3009	1/1	0.91	0.12	43,43,43,43	0
54	MG	1A	3454	1/1	0.91	0.07	18,18,18,18	0
54	MG	2A	3564	1/1	0.91	0.10	60,60,60,60	0
54	MG	2A	3306	1/1	0.91	0.09	28,28,28,28	0
54	MG	2a	3067	1/1	0.91	0.12	57,57,57,57	0
54	MG	1A	3824	1/1	0.91	0.10	32,32,32,32	0
54	MG	2A	3585	1/1	0.91	0.11	54,54,54,54	0
54	MG	2a	3070	1/1	0.91	0.24	54,54,54,54	0
54	MG	2A	3591	1/1	0.91	0.09	43,43,43,43	0
54	MG	2A	3047	1/1	0.91	0.15	49,49,49,49	0
54	MG	2A	3323	1/1	0.91	0.07	41,41,41,41	0
54	MG	2a	3078	1/1	0.91	0.08	55,55,55,55	0
54	MG	1A	3070	1/1	0.91	0.17	59,59,59,59	0
54	MG	10	105	1/1	0.91	0.10	39,39,39,39	0
54	MG	1A	3726	1/1	0.91	0.07	39,39,39,39	0
54	MG	1A	3948	1/1	0.91	0.13	39,39,39,39	0
54	MG	1A	3350	1/1	0.91	0.14	36,36,36,36	0
54	MG	1A	3357	1/1	0.91	0.08	41,41,41,41	0
54	MG	2A	3337	1/1	0.91	0.12	57,57,57,57	0
54	MG	1A	3555	1/1	0.91	0.16	38,38,38,38	0
54	MG	2A	3063	1/1	0.91	0.12	41,41,41,41	0
54	MG	2A	3065	1/1	0.91	0.14	43,43,43,43	0
54	MG	2A	3353	1/1	0.91	0.12	52,52,52,52	0
54	MG	18	103	1/1	0.91	0.32	32,32,32,32	0
54	MG	18	104	1/1	0.91	0.16	46,46,46,46	0
54	MG	2A	3081	1/1	0.91	0.14	45,45,45,45	0
54	MG	1A	3646	1/1	0.91	0.08	52,52,52,52	0
54	MG	2a	3112	1/1	0.91	0.09	55,55,55,55	0
54	MG	2A	3628	1/1	0.91	0.23	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	3630	1/1	0.91	0.10	64,64,64,64	0
54	MG	2A	3638	1/1	0.91	0.21	47,47,47,47	0
54	MG	2A	3084	1/1	0.91	0.22	56,56,56,56	0
54	MG	2A	3092	1/1	0.91	0.12	46,46,46,46	0
54	MG	2A	3646	1/1	0.91	0.14	55,55,55,55	0
54	MG	2A	3647	1/1	0.91	0.09	45,45,45,45	0
54	MG	2A	3094	1/1	0.91	0.09	50,50,50,50	0
54	MG	1A	3847	1/1	0.91	0.14	45,45,45,45	0
54	MG	2a	3137	1/1	0.91	0.09	56,56,56,56	0
54	MG	1A	3742	1/1	0.91	0.06	20,20,20,20	0
54	MG	2A	3653	1/1	0.91	0.09	38,38,38,38	0
54	MG	2A	3099	1/1	0.91	0.25	46,46,46,46	0
54	MG	2a	3160	1/1	0.91	0.13	63,63,63,63	0
54	MG	2A	3659	1/1	0.91	0.07	47,47,47,47	0
54	MG	2A	3669	1/1	0.91	0.09	54,54,54,54	0
54	MG	2A	3671	1/1	0.91	0.08	46,46,46,46	0
54	MG	1A	3978	1/1	0.91	0.10	43,43,43,43	0
54	MG	1A	3168	1/1	0.91	0.27	58,58,58,58	0
54	MG	2A	3383	1/1	0.91	0.10	37,37,37,37	0
54	MG	1A	3983	1/1	0.91	0.14	48,48,48,48	0
54	MG	1a	1830	1/1	0.91	0.12	54,54,54,54	0
54	MG	2A	3683	1/1	0.91	0.11	58,58,58,58	0
54	MG	1A	3487	1/1	0.91	0.09	14,14,14,14	0
54	MG	2A	3130	1/1	0.91	0.18	59,59,59,59	0
54	MG	1A	3248	1/1	0.91	0.15	35,35,35,35	0
54	MG	1a	1834	1/1	0.91	0.10	65,65,65,65	0
54	MG	1A	3409	1/1	0.91	0.08	23,23,23,23	0
54	MG	1a	1839	1/1	0.91	0.09	53,53,53,53	0
54	MG	2A	3154	1/1	0.91	0.12	38,38,38,38	0
54	MG	1a	1843	1/1	0.91	0.15	57,57,57,57	0
54	MG	1a	1845	1/1	0.91	0.10	58,58,58,58	0
54	MG	1a	1846	1/1	0.91	0.16	60,60,60,60	0
54	MG	1a	1848	1/1	0.91	0.07	39,39,39,39	0
54	MG	2A	3430	1/1	0.91	0.10	57,57,57,57	0
54	MG	2A	3166	1/1	0.91	0.13	51,51,51,51	0
54	MG	1B	205	1/1	0.92	0.46	35,35,35,35	0
54	MG	1A	3315	1/1	0.92	0.17	39,39,39,39	0
54	MG	1B	208	1/1	0.92	0.09	52,52,52,52	0
54	MG	2B	204	1/1	0.92	0.12	62,62,62,62	0
54	MG	2B	205	1/1	0.92	0.16	46,46,46,46	0
54	MG	1A	3898	1/1	0.92	0.09	45,45,45,45	0
54	MG	1A	3767	1/1	0.92	0.13	40,40,40,40	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	2A	3470	1/1	0.92	0.14	48,48,48,48	0
54	MG	2B	212	1/1	0.92	0.13	50,50,50,50	0
54	MG	1a	1626	1/1	0.92	0.12	45,45,45,45	0
54	MG	1B	220	1/1	0.92	0.08	35,35,35,35	0
54	MG	1a	1631	1/1	0.92	0.28	52,52,52,52	0
54	MG	1B	221	1/1	0.92	0.07	26,26,26,26	0
54	MG	2A	3232	1/1	0.92	0.08	63,63,63,63	0
54	MG	2A	3483	1/1	0.92	0.08	54,54,54,54	0
54	MG	2A	3484	1/1	0.92	0.14	64,64,64,64	0
54	MG	1a	1635	1/1	0.92	0.12	57,57,57,57	0
54	MG	2A	3487	1/1	0.92	0.14	51,51,51,51	0
54	MG	2E	308	1/1	0.92	0.16	39,39,39,39	0
54	MG	1a	1637	1/1	0.92	0.07	38,38,38,38	0
54	MG	1A	3900	1/1	0.92	0.10	35,35,35,35	0
54	MG	1A	3010	1/1	0.92	0.10	32,32,32,32	0
54	MG	1A	3770	1/1	0.92	0.29	31,31,31,31	0
54	MG	1a	1642	1/1	0.92	0.10	46,46,46,46	0
54	MG	1B	229	1/1	0.92	0.11	41,41,41,41	0
54	MG	1A	3424	1/1	0.92	0.07	51,51,51,51	0
54	MG	1A	3174	1/1	0.92	0.09	44,44,44,44	0
54	MG	2A	3012	1/1	0.92	0.14	51,51,51,51	0
54	MG	1A	3580	1/1	0.92	0.27	27,27,27,27	0
54	MG	2X	101	1/1	0.92	0.10	46,46,46,46	0
54	MG	1A	3584	1/1	0.92	0.10	46,46,46,46	0
54	MG	2A	3509	1/1	0.92	0.18	47,47,47,47	0
54	MG	1A	3912	1/1	0.92	0.12	50,50,50,50	0
54	MG	1A	3336	1/1	0.92	0.11	46,46,46,46	0
54	MG	2A	3515	1/1	0.92	0.10	47,47,47,47	0
54	MG	1A	3791	1/1	0.92	0.11	55,55,55,55	0
54	MG	1a	1779	1/1	0.92	0.14	58,58,58,58	0
54	MG	1A	3696	1/1	0.92	0.09	26,26,26,26	0
54	MG	2A	3275	1/1	0.92	0.14	34,34,34,34	0
54	MG	2a	3007	1/1	0.92	0.12	61,61,61,61	0
54	MG	2a	3008	1/1	0.92	0.09	67,67,67,67	0
54	MG	2a	3009	1/1	0.92	0.10	50,50,50,50	0
54	MG	1F	313	1/1	0.92	0.07	32,32,32,32	0
54	MG	1A	3923	1/1	0.92	0.10	49,49,49,49	0
54	MG	1F	315	1/1	0.92	0.28	40,40,40,40	0
54	MG	2A	3046	1/1	0.92	0.22	58,58,58,58	0
54	MG	1A	3440	1/1	0.92	0.10	39,39,39,39	0
54	MG	1A	3702	1/1	0.92	0.15	38,38,38,38	0
54	MG	2a	3023	1/1	0.92	0.20	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	3052	1/1	0.92	0.06	59,59,59,59	0
54	MG	1A	3212	1/1	0.92	0.66	30,30,30,30	0
54	MG	2A	3553	1/1	0.92	0.10	31,31,31,31	0
54	MG	1N	201	1/1	0.92	0.34	46,46,46,46	0
54	MG	1a	1667	1/1	0.92	0.12	50,50,50,50	0
54	MG	1a	1795	1/1	0.92	0.10	56,56,56,56	0
54	MG	2a	3040	1/1	0.92	0.13	53,53,53,53	0
54	MG	2a	3041	1/1	0.92	0.09	50,50,50,50	0
54	MG	1a	1668	1/1	0.92	0.29	64,64,64,64	0
54	MG	2A	3565	1/1	0.92	0.08	29,29,29,29	0
54	MG	2A	3061	1/1	0.92	0.20	41,41,41,41	0
54	MG	2a	3046	1/1	0.92	0.19	61,61,61,61	0
54	MG	1N	204	1/1	0.92	0.17	57,57,57,57	0
54	MG	2a	3048	1/1	0.92	0.17	59,59,59,59	0
54	MG	1A	3603	1/1	0.92	0.11	36,36,36,36	0
54	MG	1a	1674	1/1	0.92	0.11	61,61,61,61	0
54	MG	2A	3066	1/1	0.92	0.11	51,51,51,51	0
54	MG	2a	3053	1/1	0.92	0.20	38,38,38,38	0
54	MG	2A	3335	1/1	0.92	0.09	44,44,44,44	0
54	MG	1R	203	1/1	0.92	0.12	56,56,56,56	0
54	MG	2a	3056	1/1	0.92	0.10	64,64,64,64	0
54	MG	2A	3599	1/1	0.92	0.09	25,25,25,25	0
54	MG	1A	3819	1/1	0.92	0.10	46,46,46,46	0
54	MG	1A	3517	1/1	0.92	0.10	38,38,38,38	0
54	MG	1a	1682	1/1	0.92	0.13	50,50,50,50	0
54	MG	1A	3189	1/1	0.92	0.30	40,40,40,40	0
54	MG	2A	3606	1/1	0.92	0.15	72,72,72,72	0
54	MG	1a	1813	1/1	0.92	0.07	63,63,63,63	0
54	MG	1a	1684	1/1	0.92	0.17	61,61,61,61	0
54	MG	1T	205	1/1	0.92	0.14	49,49,49,49	0
54	MG	2A	3359	1/1	0.92	0.18	61,61,61,61	0
54	MG	2a	3072	1/1	0.92	0.18	53,53,53,53	0
54	MG	1A	3112	1/1	0.92	0.08	41,41,41,41	0
54	MG	1a	1820	1/1	0.92	0.08	38,38,38,38	0
54	MG	1a	1821	1/1	0.92	0.15	62,62,62,62	0
54	MG	2A	3107	1/1	0.92	0.14	59,59,59,59	0
54	MG	1A	3528	1/1	0.92	0.14	55,55,55,55	0
54	MG	2A	3112	1/1	0.92	0.08	69,69,69,69	0
54	MG	1A	3547	1/1	0.92	0.07	55,55,55,55	0
54	MG	2A	3374	1/1	0.92	0.12	39,39,39,39	0
54	MG	2A	3116	1/1	0.92	0.12	49,49,49,49	0
54	MG	1A	3253	1/1	0.92	0.12	28,28,28,28	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	1A	3290	1/1	0.92	0.12	38,38,38,38	0
54	MG	1a	1829	1/1	0.92	0.13	61,61,61,61	0
54	MG	10	107	1/1	0.92	0.12	60,60,60,60	0
54	MG	2A	3135	1/1	0.92	0.15	47,47,47,47	0
54	MG	2a	3102	1/1	0.92	0.18	61,61,61,61	0
54	MG	1A	3466	1/1	0.92	0.11	49,49,49,49	0
54	MG	1A	3552	1/1	0.92	0.07	28,28,28,28	0
54	MG	1A	3197	1/1	0.92	0.18	24,24,24,24	0
54	MG	2A	3655	1/1	0.92	0.10	25,25,25,25	0
54	MG	1A	3641	1/1	0.92	0.19	27,27,27,27	0
54	MG	1a	1837	1/1	0.92	0.15	44,44,44,44	0
54	MG	15	109	1/1	0.92	0.07	52,52,52,52	0
54	MG	2a	3120	1/1	0.92	0.09	63,63,63,63	0
54	MG	2a	3123	1/1	0.92	0.10	58,58,58,58	0
54	MG	2A	3670	1/1	0.92	0.09	50,50,50,50	0
54	MG	17	104	1/1	0.92	0.10	34,34,34,34	0
54	MG	1A	3976	1/1	0.92	0.23	23,23,23,23	0
54	MG	2A	3414	1/1	0.92	0.09	42,42,42,42	0
54	MG	2A	3415	1/1	0.92	0.11	51,51,51,51	0
54	MG	2A	3419	1/1	0.92	0.08	41,41,41,41	0
54	MG	2A	3164	1/1	0.92	0.10	86,86,86,86	0
54	MG	2A	3682	1/1	0.92	0.08	54,54,54,54	0
54	MG	1a	1709	1/1	0.92	0.10	52,52,52,52	0
54	MG	2A	3687	1/1	0.92	0.16	64,64,64,64	0
54	MG	2a	3151	1/1	0.92	0.20	57,57,57,57	0
54	MG	1a	1714	1/1	0.92	0.10	39,39,39,39	0
54	MG	2A	3696	1/1	0.92	0.15	43,43,43,43	0
54	MG	1A	3645	1/1	0.92	0.07	60,60,60,60	0
54	MG	2A	3180	1/1	0.92	0.18	53,53,53,53	0
54	MG	1A	3473	1/1	0.92	0.08	62,62,62,62	0
54	MG	1A	3410	1/1	0.92	0.18	41,41,41,41	0
54	MG	2A	3703	1/1	0.92	0.11	59,59,59,59	0
54	MG	2A	3185	1/1	0.92	0.12	52,52,52,52	0
54	MG	1a	1725	1/1	0.92	0.15	45,45,45,45	0
54	MG	2a	3180	1/1	0.92	0.15	72,72,72,72	0
54	MG	2A	3714	1/1	0.92	0.16	58,58,58,58	0
54	MG	2A	3717	1/1	0.92	0.19	57,57,57,57	0
54	MG	1A	3864	1/1	0.92	0.09	48,48,48,48	0
54	MG	2A	3720	1/1	0.92	0.07	48,48,48,48	0
54	MG	1A	3008	1/1	0.92	0.08	35,35,35,35	0
54	MG	1a	1859	1/1	0.92	0.17	48,48,48,48	0
54	MG	1A	3414	1/1	0.92	0.12	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	3447	1/1	0.92	0.09	68,68,68,68	0
54	MG	2A	3193	1/1	0.92	0.11	63,63,63,63	0
54	MG	2e	201	1/1	0.92	0.29	56,56,56,56	0
54	MG	1A	3757	1/1	0.92	0.09	24,24,24,24	0
54	MG	1A	3990	1/1	0.92	0.09	44,44,44,44	0
54	MG	1A	3658	1/1	0.92	0.10	59,59,59,59	0
54	MG	1A	3564	1/1	0.92	0.12	21,21,21,21	0
54	MG	2A	3204	1/1	0.92	0.11	55,55,55,55	0
54	MG	2A	3458	1/1	0.92	0.14	56,56,56,56	0
54	MG	1A	3954	1/1	0.93	0.33	37,37,37,37	0
54	MG	1A	3159	1/1	0.93	0.26	33,33,33,33	0
54	MG	1A	3957	1/1	0.93	0.07	42,42,42,42	0
54	MG	2A	3705	1/1	0.93	0.09	49,49,49,49	0
54	MG	1A	3793	1/1	0.93	0.26	36,36,36,36	0
54	MG	2A	3710	1/1	0.93	0.08	39,39,39,39	0
54	MG	1A	3795	1/1	0.93	0.07	16,16,16,16	0
54	MG	2A	3376	1/1	0.93	0.10	35,35,35,35	0
54	MG	2A	3715	1/1	0.93	0.14	57,57,57,57	0
54	MG	1A	3966	1/1	0.93	0.08	58,58,58,58	0
54	MG	2A	3064	1/1	0.93	0.18	56,56,56,56	0
54	MG	1a	1620	1/1	0.93	0.11	61,61,61,61	0
54	MG	1a	1772	1/1	0.93	0.09	53,53,53,53	0
54	MG	2A	3069	1/1	0.93	0.20	46,46,46,46	0
54	MG	2A	3394	1/1	0.93	0.08	34,34,34,34	0
54	MG	2A	3396	1/1	0.93	0.24	43,43,43,43	0
54	MG	1a	1622	1/1	0.93	0.10	33,33,33,33	0
54	MG	1A	3968	1/1	0.93	0.17	33,33,33,33	0
54	MG	2A	3076	1/1	0.93	0.27	45,45,45,45	0
54	MG	1A	3797	1/1	0.93	0.14	36,36,36,36	0
54	MG	1A	3457	1/1	0.93	0.08	25,25,25,25	0
54	MG	1A	3801	1/1	0.93	0.10	45,45,45,45	0
54	MG	2A	3411	1/1	0.93	0.16	48,48,48,48	0
54	MG	2A	3090	1/1	0.93	0.11	64,64,64,64	0
54	MG	1A	3667	1/1	0.93	0.16	51,51,51,51	0
54	MG	1A	3982	1/1	0.93	0.10	43,43,43,43	0
54	MG	2B	203	1/1	0.93	0.11	61,61,61,61	0
54	MG	1A	3672	1/1	0.93	0.21	48,48,48,48	0
54	MG	2A	3096	1/1	0.93	0.10	47,47,47,47	0
54	MG	1a	1636	1/1	0.93	0.20	51,51,51,51	0
54	MG	2B	207	1/1	0.93	0.12	67,67,67,67	0
54	MG	2A	3098	1/1	0.93	0.06	42,42,42,42	0
54	MG	1A	3810	1/1	0.93	0.09	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	2B	211	1/1	0.93	0.10	63,63,63,63	0
54	MG	1A	3673	1/1	0.93	0.08	42,42,42,42	0
54	MG	2A	3103	1/1	0.93	0.17	54,54,54,54	0
54	MG	1A	3675	1/1	0.93	0.08	24,24,24,24	0
54	MG	1a	1793	1/1	0.93	0.15	76,76,76,76	0
54	MG	1A	3084	1/1	0.93	0.13	46,46,46,46	0
54	MG	1A	3401	1/1	0.93	0.15	24,24,24,24	0
54	MG	1A	3463	1/1	0.93	0.12	18,18,18,18	0
54	MG	2A	3119	1/1	0.93	0.10	43,43,43,43	0
54	MG	2A	3120	1/1	0.93	0.25	38,38,38,38	0
54	MG	2E	301	1/1	0.93	0.11	55,55,55,55	0
54	MG	2A	3122	1/1	0.93	0.11	42,42,42,42	0
54	MG	1a	1644	1/1	0.93	0.15	52,52,52,52	0
54	MG	2F	303	1/1	0.93	0.14	38,38,38,38	0
54	MG	1a	1645	1/1	0.93	0.13	41,41,41,41	0
54	MG	2A	3129	1/1	0.93	0.14	58,58,58,58	0
54	MG	1A	3321	1/1	0.93	0.07	47,47,47,47	0
54	MG	2A	3452	1/1	0.93	0.11	51,51,51,51	0
54	MG	1A	3119	1/1	0.93	0.06	26,26,26,26	0
54	MG	1A	3571	1/1	0.93	0.22	27,27,27,27	0
54	MG	1A	3220	1/1	0.93	0.09	39,39,39,39	0
54	MG	2R	201	1/1	0.93	0.07	38,38,38,38	0
54	MG	1a	1807	1/1	0.93	0.08	55,55,55,55	0
54	MG	2U	201	1/1	0.93	0.46	60,60,60,60	0
54	MG	2V	201	1/1	0.93	0.26	41,41,41,41	0
54	MG	2W	202	1/1	0.93	0.19	50,50,50,50	0
54	MG	1A	3575	1/1	0.93	0.10	38,38,38,38	0
54	MG	1B	210	1/1	0.93	0.16	46,46,46,46	0
54	MG	1a	1812	1/1	0.93	0.09	56,56,56,56	0
54	MG	1B	215	1/1	0.93	0.08	44,44,44,44	0
54	MG	2A	3466	1/1	0.93	0.10	51,51,51,51	0
54	MG	1A	3167	1/1	0.93	0.10	45,45,45,45	0
54	MG	1A	3484	1/1	0.93	0.19	40,40,40,40	0
54	MG	1A	3843	1/1	0.93	0.15	43,43,43,43	0
54	MG	1A	3193	1/1	0.93	0.32	23,23,23,23	0
54	MG	1A	3712	1/1	0.93	0.10	57,57,57,57	0
54	MG	2A	3477	1/1	0.93	0.11	54,54,54,54	0
54	MG	2A	3478	1/1	0.93	0.08	66,66,66,66	0
54	MG	1A	3852	1/1	0.93	0.10	47,47,47,47	0
54	MG	1A	3108	1/1	0.93	0.07	41,41,41,41	0
54	MG	1A	3413	1/1	0.93	0.09	50,50,50,50	0
54	MG	1A	3591	1/1	0.93	0.08	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	3594	1/1	0.93	0.11	15,15,15,15	0
54	MG	1A	3870	1/1	0.93	0.06	26,26,26,26	0
54	MG	1a	1671	1/1	0.93	0.13	52,52,52,52	0
54	MG	1E	301	1/1	0.93	0.43	34,34,34,34	0
54	MG	2a	3017	1/1	0.93	0.22	42,42,42,42	0
54	MG	1A	3722	1/1	0.93	0.10	27,27,27,27	0
54	MG	1A	3725	1/1	0.93	0.19	57,57,57,57	0
54	MG	1A	3878	1/1	0.93	0.09	10,10,10,10	0
54	MG	1F	308	1/1	0.93	0.14	35,35,35,35	0
54	MG	1A	3598	1/1	0.93	0.06	25,25,25,25	0
54	MG	2a	3029	1/1	0.93	0.10	42,42,42,42	0
54	MG	1F	312	1/1	0.93	0.30	36,36,36,36	0
54	MG	1A	3278	1/1	0.93	0.10	67,67,67,67	0
54	MG	1A	3498	1/1	0.93	0.17	71,71,71,71	0
54	MG	2A	3206	1/1	0.93	0.08	36,36,36,36	0
54	MG	1A	3735	1/1	0.93	0.09	57,57,57,57	0
54	MG	1F	316	1/1	0.93	0.11	39,39,39,39	0
54	MG	2a	3043	1/1	0.93	0.21	60,60,60,60	0
54	MG	1A	3737	1/1	0.93	0.07	24,24,24,24	0
54	MG	1A	3196	1/1	0.93	0.06	44,44,44,44	0
54	MG	2A	3517	1/1	0.93	0.10	58,58,58,58	0
54	MG	1a	1693	1/1	0.93	0.23	58,58,58,58	0
54	MG	2A	3218	1/1	0.93	0.10	49,49,49,49	0
54	MG	2A	3220	1/1	0.93	0.18	57,57,57,57	0
54	MG	1A	3422	1/1	0.93	0.12	46,46,46,46	0
54	MG	2A	3223	1/1	0.93	0.11	51,51,51,51	0
54	MG	2a	3052	1/1	0.93	0.18	49,49,49,49	0
54	MG	2A	3529	1/1	0.93	0.07	53,53,53,53	0
54	MG	1A	3280	1/1	0.93	0.10	23,23,23,23	0
54	MG	2A	3533	1/1	0.93	0.09	57,57,57,57	0
54	MG	1N	203	1/1	0.93	0.10	49,49,49,49	0
54	MG	1A	3510	1/1	0.93	0.09	33,33,33,33	0
54	MG	2a	3061	1/1	0.93	0.10	56,56,56,56	0
54	MG	2A	3540	1/1	0.93	0.18	67,67,67,67	0
54	MG	1A	3512	1/1	0.93	0.48	25,25,25,25	0
54	MG	1a	1701	1/1	0.93	0.10	59,59,59,59	0
54	MG	2A	3234	1/1	0.93	0.30	41,41,41,41	0
54	MG	1b	301	1/1	0.93	0.06	65,65,65,65	0
54	MG	1A	3364	1/1	0.93	0.07	19,19,19,19	0
54	MG	2A	3239	1/1	0.93	0.21	55,55,55,55	0
54	MG	1A	3110	1/1	0.93	0.10	28,28,28,28	0
54	MG	1A	3755	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	3432	1/1	0.93	0.13	50,50,50,50	0
54	MG	1A	3198	1/1	0.93	0.37	35,35,35,35	0
54	MG	1U	205	1/1	0.93	0.15	28,28,28,28	0
54	MG	1V	203	1/1	0.93	0.23	48,48,48,48	0
54	MG	2a	3079	1/1	0.93	0.12	39,39,39,39	0
54	MG	2A	3578	1/1	0.93	0.09	53,53,53,53	0
54	MG	2A	3579	1/1	0.93	0.10	71,71,71,71	0
54	MG	2a	3084	1/1	0.93	0.09	51,51,51,51	0
54	MG	1A	3437	1/1	0.93	0.15	46,46,46,46	0
54	MG	2A	3589	1/1	0.93	0.12	66,66,66,66	0
54	MG	1a	1718	1/1	0.93	0.14	51,51,51,51	0
54	MG	1V	206	1/1	0.93	0.06	39,39,39,39	0
54	MG	1a	1720	1/1	0.93	0.10	64,64,64,64	0
54	MG	1A	3439	1/1	0.93	0.05	26,26,26,26	0
54	MG	1n	101	1/1	0.93	0.07	53,53,53,53	0
54	MG	1a	1726	1/1	0.93	0.14	68,68,68,68	0
54	MG	2A	3270	1/1	0.93	0.08	48,48,48,48	0
54	MG	1A	3922	1/1	0.93	0.09	65,65,65,65	0
54	MG	2a	3103	1/1	0.93	0.15	55,55,55,55	0
54	MG	1a	1730	1/1	0.93	0.09	48,48,48,48	0
54	MG	2a	3106	1/1	0.93	0.08	62,62,62,62	0
54	MG	1A	3639	1/1	0.93	0.08	25,25,25,25	0
54	MG	1y	201	1/1	0.93	0.10	56,56,56,56	0
54	MG	2A	3281	1/1	0.93	0.19	64,64,64,64	0
54	MG	1A	3764	1/1	0.93	0.09	75,75,75,75	0
54	MG	2A	3288	1/1	0.93	0.07	28,28,28,28	0
54	MG	1A	3529	1/1	0.93	0.09	39,39,39,39	0
54	MG	2A	3002	1/1	0.93	0.09	48,48,48,48	0
54	MG	2a	3122	1/1	0.93	0.09	64,64,64,64	0
54	MG	2A	3293	1/1	0.93	0.14	43,43,43,43	0
54	MG	2a	3124	1/1	0.93	0.08	42,42,42,42	0
54	MG	2A	3616	1/1	0.93	0.13	53,53,53,53	0
54	MG	2A	3006	1/1	0.93	0.09	39,39,39,39	0
54	MG	2A	3298	1/1	0.93	0.14	49,49,49,49	0
54	MG	2A	3623	1/1	0.93	0.24	78,78,78,78	0
54	MG	1A	3927	1/1	0.93	0.07	31,31,31,31	0
54	MG	2A	3011	1/1	0.93	0.15	35,35,35,35	0
54	MG	2a	3135	1/1	0.93	0.16	40,40,40,40	0
54	MG	1A	3928	1/1	0.93	0.12	48,48,48,48	0
54	MG	1A	3534	1/1	0.93	0.12	49,49,49,49	0
54	MG	2A	3017	1/1	0.93	0.09	37,37,37,37	0
54	MG	2A	3018	1/1	0.93	0.24	54,54,54,54	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	2a	3149	1/1	0.93	0.13	56,56,56,56	0
54	MG	1A	3539	1/1	0.93	0.16	61,61,61,61	0
54	MG	2a	3154	1/1	0.93	0.09	38,38,38,38	0
54	MG	1A	3933	1/1	0.93	0.20	38,38,38,38	0
54	MG	2A	3025	1/1	0.93	0.08	50,50,50,50	0
54	MG	2A	3026	1/1	0.93	0.13	43,43,43,43	0
54	MG	2A	3332	1/1	0.93	0.09	37,37,37,37	0
54	MG	2A	3333	1/1	0.93	0.12	56,56,56,56	0
54	MG	17	102	1/1	0.93	0.17	29,29,29,29	0
54	MG	2a	3170	1/1	0.93	0.10	39,39,39,39	0
54	MG	1A	3300	1/1	0.93	0.08	25,25,25,25	0
54	MG	1a	1747	1/1	0.93	0.12	46,46,46,46	0
54	MG	2a	3176	1/1	0.93	0.11	69,69,69,69	0
54	MG	1A	3442	1/1	0.93	0.10	42,42,42,42	0
54	MG	1a	1751	1/1	0.93	0.09	54,54,54,54	0
54	MG	2A	3041	1/1	0.93	0.10	38,38,38,38	0
54	MG	2a	3186	1/1	0.93	0.09	57,57,57,57	0
54	MG	1A	3063	1/1	0.93	0.30	26,26,26,26	0
54	MG	2A	3350	1/1	0.93	0.06	58,58,58,58	0
54	MG	1A	3449	1/1	0.93	0.11	12,12,12,12	0
54	MG	2A	3354	1/1	0.93	0.12	51,51,51,51	0
54	MG	1A	3783	1/1	0.93	0.07	33,33,33,33	0
54	MG	2A	3681	1/1	0.93	0.06	49,49,49,49	0
54	MG	1A	3946	1/1	0.93	0.07	45,45,45,45	0
54	MG	2a	3197	1/1	0.93	0.08	56,56,56,56	0
54	MG	2A	3048	1/1	0.93	0.12	55,55,55,55	0
54	MG	2A	3686	1/1	0.93	0.11	42,42,42,42	0
54	MG	2j	201	1/1	0.93	0.22	52,52,52,52	0
54	MG	1a	1604	1/1	0.93	0.11	67,67,67,67	0
55	A1CRD	2A	3738	48/48	0.93	0.15	33,44,68,73	0
54	MG	2A	3688	1/1	0.93	0.11	46,46,46,46	0
54	MG	1A	3154	1/1	0.93	0.14	43,43,43,43	0
54	MG	1A	3787	1/1	0.93	0.14	26,26,26,26	0
54	MG	2A	3366	1/1	0.93	0.08	23,23,23,23	0
54	MG	1A	3788	1/1	0.93	0.17	36,36,36,36	0
54	MG	1y	202	1/1	0.94	0.09	61,61,61,61	0
54	MG	1A	3204	1/1	0.94	0.14	32,32,32,32	0
54	MG	1A	3148	1/1	0.94	0.31	33,33,33,33	0
54	MG	1a	1759	1/1	0.94	0.08	40,40,40,40	0
54	MG	2A	3475	1/1	0.94	0.09	29,29,29,29	0
54	MG	2D	304	1/1	0.94	0.07	45,45,45,45	0
54	MG	1D	313	1/1	0.94	0.30	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	1638	1/1	0.94	0.09	61,61,61,61	0
54	MG	1A	3012	1/1	0.94	0.07	28,28,28,28	0
54	MG	2A	3229	1/1	0.94	0.26	39,39,39,39	0
54	MG	2A	3230	1/1	0.94	0.14	61,61,61,61	0
54	MG	1A	3566	1/1	0.94	0.10	41,41,41,41	0
54	MG	1A	3670	1/1	0.94	0.31	35,35,35,35	0
54	MG	1a	1766	1/1	0.94	0.16	58,58,58,58	0
54	MG	1A	3778	1/1	0.94	0.17	25,25,25,25	0
54	MG	2A	3235	1/1	0.94	0.10	52,52,52,52	0
54	MG	2N	201	1/1	0.94	0.05	49,49,49,49	0
54	MG	2A	3022	1/1	0.94	0.18	46,46,46,46	0
54	MG	1A	3779	1/1	0.94	0.13	46,46,46,46	0
54	MG	1A	3483	1/1	0.94	0.07	38,38,38,38	0
54	MG	2P	203	1/1	0.94	0.09	54,54,54,54	0
54	MG	1A	3265	1/1	0.94	0.19	40,40,40,40	0
54	MG	1A	3920	1/1	0.94	0.08	54,54,54,54	0
54	MG	2A	3032	1/1	0.94	0.10	46,46,46,46	0
54	MG	2T	202	1/1	0.94	0.06	42,42,42,42	0
54	MG	2T	203	1/1	0.94	0.05	47,47,47,47	0
54	MG	1A	3341	1/1	0.94	0.08	15,15,15,15	0
54	MG	2A	3246	1/1	0.94	0.09	35,35,35,35	0
54	MG	1A	3186	1/1	0.94	0.31	35,35,35,35	0
54	MG	2A	3250	1/1	0.94	0.26	30,30,30,30	0
54	MG	1A	3271	1/1	0.94	0.38	36,36,36,36	0
54	MG	1A	3416	1/1	0.94	0.11	44,44,44,44	0
54	MG	2A	3254	1/1	0.94	0.07	35,35,35,35	0
54	MG	1A	3352	1/1	0.94	0.08	33,33,33,33	0
54	MG	2A	3261	1/1	0.94	0.18	56,56,56,56	0
54	MG	1A	3582	1/1	0.94	0.22	28,28,28,28	0
54	MG	1A	3694	1/1	0.94	0.08	32,32,32,32	0
54	MG	2a	3002	1/1	0.94	0.07	36,36,36,36	0
54	MG	1A	3071	1/1	0.94	0.27	31,31,31,31	0
54	MG	2A	3267	1/1	0.94	0.13	46,46,46,46	0
54	MG	1a	1656	1/1	0.94	0.13	65,65,65,65	0
54	MG	1A	3699	1/1	0.94	0.20	27,27,27,27	0
54	MG	2A	3530	1/1	0.94	0.09	75,75,75,75	0
54	MG	1A	3585	1/1	0.94	0.23	24,24,24,24	0
54	MG	1A	3158	1/1	0.94	0.08	41,41,41,41	0
54	MG	2A	3535	1/1	0.94	0.16	71,71,71,71	0
54	MG	1A	3073	1/1	0.94	0.10	39,39,39,39	0
54	MG	1a	1792	1/1	0.94	0.10	58,58,58,58	0
54	MG	1A	3239	1/1	0.94	0.15	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	3708	1/1	0.94	0.07	34,34,34,34	0
54	MG	2a	3015	1/1	0.94	0.14	52,52,52,52	0
54	MG	2A	3282	1/1	0.94	0.08	54,54,54,54	0
54	MG	2A	3283	1/1	0.94	0.15	47,47,47,47	0
54	MG	1R	204	1/1	0.94	0.13	44,44,44,44	0
54	MG	1S	201	1/1	0.94	0.09	51,51,51,51	0
54	MG	2A	3290	1/1	0.94	0.09	52,52,52,52	0
54	MG	2a	3027	1/1	0.94	0.22	51,51,51,51	0
54	MG	2A	3557	1/1	0.94	0.08	41,41,41,41	0
54	MG	1A	3710	1/1	0.94	0.13	32,32,32,32	0
54	MG	2a	3031	1/1	0.94	0.09	51,51,51,51	0
54	MG	2a	3033	1/1	0.94	0.13	54,54,54,54	0
54	MG	1A	3596	1/1	0.94	0.07	28,28,28,28	0
54	MG	1A	3434	1/1	0.94	0.14	37,37,37,37	0
54	MG	1A	3949	1/1	0.94	0.06	54,54,54,54	0
54	MG	2A	3566	1/1	0.94	0.13	63,63,63,63	0
54	MG	2A	3568	1/1	0.94	0.10	55,55,55,55	0
54	MG	2A	3570	1/1	0.94	0.16	75,75,75,75	0
54	MG	1A	3950	1/1	0.94	0.14	42,42,42,42	0
54	MG	1A	3435	1/1	0.94	0.06	12,12,12,12	0
54	MG	1a	1677	1/1	0.94	0.07	55,55,55,55	0
54	MG	1V	204	1/1	0.94	0.08	39,39,39,39	0
54	MG	1a	1681	1/1	0.94	0.26	62,62,62,62	0
54	MG	1a	1810	1/1	0.94	0.19	61,61,61,61	0
54	MG	2A	3318	1/1	0.94	0.09	31,31,31,31	0
54	MG	1A	3365	1/1	0.94	0.12	34,34,34,34	0
54	MG	1A	3716	1/1	0.94	0.10	29,29,29,29	0
54	MG	2A	3595	1/1	0.94	0.18	68,68,68,68	0
54	MG	1A	3281	1/1	0.94	0.13	33,33,33,33	0
54	MG	2A	3088	1/1	0.94	0.08	73,73,73,73	0
54	MG	1a	1686	1/1	0.94	0.07	54,54,54,54	0
54	MG	2A	3091	1/1	0.94	0.19	57,57,57,57	0
54	MG	1A	3833	1/1	0.94	0.06	29,29,29,29	0
54	MG	2a	3060	1/1	0.94	0.19	58,58,58,58	0
54	MG	1a	1819	1/1	0.94	0.10	47,47,47,47	0
54	MG	1A	3376	1/1	0.94	0.07	18,18,18,18	0
54	MG	10	101	1/1	0.94	0.09	37,37,37,37	0
54	MG	10	103	1/1	0.94	0.10	38,38,38,38	0
54	MG	1A	3961	1/1	0.94	0.09	60,60,60,60	0
54	MG	2A	3342	1/1	0.94	0.25	39,39,39,39	0
54	MG	1a	1826	1/1	0.94	0.07	52,52,52,52	0
54	MG	1a	1692	1/1	0.94	0.14	57,57,57,57	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	1A	3382	1/1	0.94	0.13	31,31,31,31	0
54	MG	1A	3074	1/1	0.94	0.15	28,28,28,28	0
54	MG	1A	3035	1/1	0.94	0.13	41,41,41,41	0
54	MG	1A	3625	1/1	0.94	0.07	30,30,30,30	0
54	MG	2A	3619	1/1	0.94	0.09	71,71,71,71	0
54	MG	2A	3113	1/1	0.94	0.07	60,60,60,60	0
54	MG	2A	3358	1/1	0.94	0.09	54,54,54,54	0
54	MG	1A	3530	1/1	0.94	0.06	29,29,29,29	0
54	MG	1A	3028	1/1	0.94	0.10	14,14,14,14	0
54	MG	1A	3851	1/1	0.94	0.07	19,19,19,19	0
54	MG	1a	1836	1/1	0.94	0.08	57,57,57,57	0
54	MG	2a	3088	1/1	0.94	0.09	49,49,49,49	0
54	MG	1A	3538	1/1	0.94	0.08	44,44,44,44	0
54	MG	18	101	1/1	0.94	0.09	34,34,34,34	0
54	MG	2a	3092	1/1	0.94	0.21	47,47,47,47	0
54	MG	2A	3124	1/1	0.94	0.45	43,43,43,43	0
54	MG	1A	3632	1/1	0.94	0.20	52,52,52,52	0
54	MG	1a	1844	1/1	0.94	0.09	58,58,58,58	0
54	MG	1a	1707	1/1	0.94	0.20	54,54,54,54	0
54	MG	1A	3856	1/1	0.94	0.14	41,41,41,41	0
54	MG	1A	3985	1/1	0.94	0.13	48,48,48,48	0
54	MG	2A	3377	1/1	0.94	0.08	37,37,37,37	0
54	MG	1a	1712	1/1	0.94	0.13	52,52,52,52	0
54	MG	2A	3664	1/1	0.94	0.07	51,51,51,51	0
54	MG	2A	3139	1/1	0.94	0.10	52,52,52,52	0
54	MG	2A	3143	1/1	0.94	0.09	46,46,46,46	0
54	MG	1A	3128	1/1	0.94	0.21	23,23,23,23	0
54	MG	1A	3452	1/1	0.94	0.08	21,21,21,21	0
54	MG	2A	3148	1/1	0.94	0.13	52,52,52,52	0
54	MG	2A	3149	1/1	0.94	0.11	57,57,57,57	0
54	MG	1a	1603	1/1	0.94	0.10	54,54,54,54	0
54	MG	2A	3401	1/1	0.94	0.09	47,47,47,47	0
54	MG	2a	3121	1/1	0.94	0.09	51,51,51,51	0
54	MG	1A	3304	1/1	0.94	0.24	56,56,56,56	0
54	MG	1a	1606	1/1	0.94	0.08	55,55,55,55	0
54	MG	1A	3129	1/1	0.94	0.09	43,43,43,43	0
54	MG	1A	3871	1/1	0.94	0.16	18,18,18,18	0
54	MG	2A	3163	1/1	0.94	0.07	41,41,41,41	0
54	MG	1A	3872	1/1	0.94	0.10	10,10,10,10	0
54	MG	1A	3091	1/1	0.94	0.17	27,27,27,27	0
54	MG	2A	3695	1/1	0.94	0.10	54,54,54,54	0
54	MG	2A	3169	1/1	0.94	0.10	47,47,47,47	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	1a	1611	1/1	0.94	0.09	44,44,44,44	0
54	MG	1A	3551	1/1	0.94	0.13	22,22,22,22	0
54	MG	2A	3418	1/1	0.94	0.11	48,48,48,48	0
54	MG	2A	3174	1/1	0.94	0.10	60,60,60,60	0
54	MG	2a	3142	1/1	0.94	0.12	63,63,63,63	0
54	MG	2a	3143	1/1	0.94	0.06	61,61,61,61	0
54	MG	2A	3175	1/1	0.94	0.07	40,40,40,40	0
54	MG	2A	3176	1/1	0.94	0.11	37,37,37,37	0
54	MG	1A	3039	1/1	0.94	0.19	11,11,11,11	0
54	MG	2a	3153	1/1	0.94	0.07	73,73,73,73	0
54	MG	2A	3426	1/1	0.94	0.09	67,67,67,67	0
54	MG	1d	302	1/1	0.94	0.23	57,57,57,57	0
54	MG	2A	3182	1/1	0.94	0.06	51,51,51,51	0
54	MG	1A	3462	1/1	0.94	0.06	45,45,45,45	0
54	MG	1a	1616	1/1	0.94	0.09	54,54,54,54	0
54	MG	1a	1737	1/1	0.94	0.14	52,52,52,52	0
54	MG	2a	3168	1/1	0.94	0.16	63,63,63,63	0
54	MG	2A	3719	1/1	0.94	0.09	44,44,44,44	0
54	MG	1A	3404	1/1	0.94	0.06	18,18,18,18	0
54	MG	2A	3188	1/1	0.94	0.12	50,50,50,50	0
54	MG	1A	3320	1/1	0.94	0.09	38,38,38,38	0
54	MG	1A	3888	1/1	0.94	0.17	33,33,33,33	0
54	MG	2A	3724	1/1	0.94	0.11	48,48,48,48	0
54	MG	2A	3443	1/1	0.94	0.07	69,69,69,69	0
54	MG	2a	3181	1/1	0.94	0.09	53,53,53,53	0
54	MG	1A	3556	1/1	0.94	0.16	45,45,45,45	0
54	MG	2a	3185	1/1	0.94	0.14	61,61,61,61	0
54	MG	2A	3446	1/1	0.94	0.13	56,56,56,56	0
54	MG	2A	3192	1/1	0.94	0.09	48,48,48,48	0
54	MG	2A	3730	1/1	0.94	0.12	57,57,57,57	0
54	MG	1A	3895	1/1	0.94	0.30	53,53,53,53	0
54	MG	2a	3191	1/1	0.94	0.14	46,46,46,46	0
54	MG	1B	222	1/1	0.94	0.08	39,39,39,39	0
54	MG	2A	3196	1/1	0.94	0.08	48,48,48,48	0
54	MG	1B	225	1/1	0.94	0.11	43,43,43,43	0
54	MG	2A	3453	1/1	0.94	0.08	39,39,39,39	0
54	MG	1i	201	1/1	0.94	0.13	50,50,50,50	0
54	MG	1a	1627	1/1	0.94	0.06	61,61,61,61	0
54	MG	1A	3659	1/1	0.94	0.09	44,44,44,44	0
54	MG	1a	1752	1/1	0.94	0.10	38,38,38,38	0
54	MG	1A	3662	1/1	0.94	0.07	59,59,59,59	0
55	A1CRD	1A	3991	48/48	0.94	0.13	20,27,51,61	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	2A	3209	1/1	0.94	0.10	50,50,50,50	0
54	MG	1A	3765	1/1	0.94	0.07	32,32,32,32	0
54	MG	1a	1755	1/1	0.94	0.10	50,50,50,50	0
54	MG	2A	3464	1/1	0.94	0.09	37,37,37,37	0
54	MG	1a	1634	1/1	0.94	0.09	38,38,38,38	0
54	MG	2A	3467	1/1	0.94	0.13	60,60,60,60	0
54	MG	1a	1823	1/1	0.95	0.09	66,66,66,66	0
54	MG	1a	1824	1/1	0.95	0.10	61,61,61,61	0
54	MG	1A	3561	1/1	0.95	0.09	37,37,37,37	0
54	MG	1A	3054	1/1	0.95	0.12	53,53,53,53	0
54	MG	1A	3115	1/1	0.95	0.08	30,30,30,30	0
54	MG	1A	3272	1/1	0.95	0.31	29,29,29,29	0
54	MG	1E	307	1/1	0.95	0.08	19,19,19,19	0
54	MG	2A	3152	1/1	0.95	0.06	58,58,58,58	0
54	MG	2A	3728	1/1	0.95	0.09	59,59,59,59	0
54	MG	2A	3416	1/1	0.95	0.10	35,35,35,35	0
54	MG	1A	3565	1/1	0.95	0.11	41,41,41,41	0
54	MG	1A	3274	1/1	0.95	0.10	19,19,19,19	0
54	MG	2A	3420	1/1	0.95	0.27	33,33,33,33	0
54	MG	1A	3368	1/1	0.95	0.07	17,17,17,17	0
54	MG	1a	1678	1/1	0.95	0.14	50,50,50,50	0
54	MG	1A	3370	1/1	0.95	0.06	14,14,14,14	0
54	MG	1A	3087	1/1	0.95	0.20	22,22,22,22	0
54	MG	2A	3428	1/1	0.95	0.07	44,44,44,44	0
54	MG	2B	202	1/1	0.95	0.18	62,62,62,62	0
54	MG	1A	3884	1/1	0.95	0.38	27,27,27,27	0
54	MG	2A	3165	1/1	0.95	0.09	52,52,52,52	0
54	MG	1A	3090	1/1	0.95	0.11	25,25,25,25	0
54	MG	2A	3433	1/1	0.95	0.05	48,48,48,48	0
54	MG	2A	3434	1/1	0.95	0.12	59,59,59,59	0
54	MG	2A	3167	1/1	0.95	0.27	39,39,39,39	0
54	MG	1a	1841	1/1	0.95	0.13	77,77,77,77	0
54	MG	1A	3026	1/1	0.95	0.10	29,29,29,29	0
54	MG	1a	1685	1/1	0.95	0.07	47,47,47,47	0
54	MG	1A	3095	1/1	0.95	0.10	33,33,33,33	0
54	MG	1A	3892	1/1	0.95	0.07	43,43,43,43	0
54	MG	1A	3579	1/1	0.95	0.12	52,52,52,52	0
54	MG	2A	3444	1/1	0.95	0.06	57,57,57,57	0
54	MG	2B	219	1/1	0.95	0.07	62,62,62,62	0
54	MG	2D	302	1/1	0.95	0.09	50,50,50,50	0
54	MG	2A	3179	1/1	0.95	0.08	65,65,65,65	0
54	MG	1A	3719	1/1	0.95	0.33	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	3387	1/1	0.95	0.12	37,37,37,37	0
54	MG	1A	3096	1/1	0.95	0.14	32,32,32,32	0
54	MG	1A	3724	1/1	0.95	0.09	44,44,44,44	0
54	MG	1Q	204	1/1	0.95	0.08	24,24,24,24	0
54	MG	2E	302	1/1	0.95	0.20	34,34,34,34	0
54	MG	1A	3901	1/1	0.95	0.07	43,43,43,43	0
54	MG	1a	1695	1/1	0.95	0.06	34,34,34,34	0
54	MG	1A	3475	1/1	0.95	0.10	28,28,28,28	0
54	MG	1A	3287	1/1	0.95	0.17	22,22,22,22	0
54	MG	2A	3456	1/1	0.95	0.08	44,44,44,44	0
54	MG	1T	201	1/1	0.95	0.10	48,48,48,48	0
54	MG	1A	3587	1/1	0.95	0.09	31,31,31,31	0
54	MG	1A	3394	1/1	0.95	0.08	15,15,15,15	0
54	MG	1A	3231	1/1	0.95	0.08	46,46,46,46	0
54	MG	1A	3592	1/1	0.95	0.09	51,51,51,51	0
54	MG	1d	303	1/1	0.95	0.07	85,85,85,85	0
54	MG	1A	3593	1/1	0.95	0.10	35,35,35,35	0
54	MG	2Q	204	1/1	0.95	0.10	78,78,78,78	0
54	MG	1a	1706	1/1	0.95	0.07	43,43,43,43	0
54	MG	1A	3913	1/1	0.95	0.10	71,71,71,71	0
54	MG	2A	3203	1/1	0.95	0.15	31,31,31,31	0
54	MG	2A	3469	1/1	0.95	0.09	34,34,34,34	0
54	MG	1A	3132	1/1	0.95	0.12	33,33,33,33	0
54	MG	2A	3205	1/1	0.95	0.08	43,43,43,43	0
54	MG	1A	3595	1/1	0.95	0.07	41,41,41,41	0
54	MG	1A	3488	1/1	0.95	0.06	11,11,11,11	0
54	MG	1A	3489	1/1	0.95	0.07	38,38,38,38	0
54	MG	1A	3400	1/1	0.95	0.09	30,30,30,30	0
54	MG	20	101	1/1	0.95	0.11	41,41,41,41	0
54	MG	21	101	1/1	0.95	0.10	43,43,43,43	0
54	MG	1A	3750	1/1	0.95	0.16	27,27,27,27	0
54	MG	25	101	1/1	0.95	0.26	47,47,47,47	0
54	MG	1A	3299	1/1	0.95	0.07	29,29,29,29	0
54	MG	1h	202	1/1	0.95	0.06	46,46,46,46	0
54	MG	27	101	1/1	0.95	0.11	44,44,44,44	0
54	MG	2A	3216	1/1	0.95	0.12	46,46,46,46	0
54	MG	2A	3217	1/1	0.95	0.07	49,49,49,49	0
54	MG	2a	3001	1/1	0.95	0.08	52,52,52,52	0
54	MG	1A	3135	1/1	0.95	0.14	39,39,39,39	0
54	MG	2A	3219	1/1	0.95	0.10	50,50,50,50	0
54	MG	1A	3605	1/1	0.95	0.37	24,24,24,24	0
54	MG	1A	3607	1/1	0.95	0.28	22,22,22,22	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	1A	3185	1/1	0.95	0.08	36,36,36,36	0
54	MG	2A	3491	1/1	0.95	0.08	45,45,45,45	0
54	MG	1A	3499	1/1	0.95	0.13	40,40,40,40	0
54	MG	2A	3493	1/1	0.95	0.10	46,46,46,46	0
54	MG	1a	1729	1/1	0.95	0.17	45,45,45,45	0
54	MG	15	102	1/1	0.95	0.14	33,33,33,33	0
54	MG	15	104	1/1	0.95	0.21	25,25,25,25	0
54	MG	15	105	1/1	0.95	0.29	22,22,22,22	0
54	MG	1A	3303	1/1	0.95	0.10	16,16,16,16	0
54	MG	1A	3614	1/1	0.95	0.06	22,22,22,22	0
54	MG	1A	3616	1/1	0.95	0.07	39,39,39,39	0
54	MG	2a	3020	1/1	0.95	0.08	46,46,46,46	0
54	MG	2A	3005	1/1	0.95	0.22	46,46,46,46	0
54	MG	1A	3504	1/1	0.95	0.11	28,28,28,28	0
54	MG	1a	1740	1/1	0.95	0.12	51,51,51,51	0
54	MG	2A	3513	1/1	0.95	0.07	49,49,49,49	0
54	MG	2A	3514	1/1	0.95	0.13	57,57,57,57	0
54	MG	1A	3620	1/1	0.95	0.07	40,40,40,40	0
54	MG	1A	3407	1/1	0.95	0.10	39,39,39,39	0
54	MG	2A	3242	1/1	0.95	0.13	47,47,47,47	0
54	MG	1a	1743	1/1	0.95	0.07	60,60,60,60	0
54	MG	2A	3016	1/1	0.95	0.14	50,50,50,50	0
54	MG	1A	3943	1/1	0.95	0.15	36,36,36,36	0
54	MG	1A	3626	1/1	0.95	0.09	16,16,16,16	0
54	MG	2A	3247	1/1	0.95	0.15	51,51,51,51	0
54	MG	1A	3947	1/1	0.95	0.06	19,19,19,19	0
54	MG	1A	3241	1/1	0.95	0.23	19,19,19,19	0
54	MG	1a	1748	1/1	0.95	0.08	49,49,49,49	0
54	MG	1A	3305	1/1	0.95	0.11	15,15,15,15	0
54	MG	1A	3511	1/1	0.95	0.09	49,49,49,49	0
54	MG	2A	3027	1/1	0.95	0.06	41,41,41,41	0
54	MG	2A	3259	1/1	0.95	0.32	42,42,42,42	0
54	MG	2A	3541	1/1	0.95	0.07	67,67,67,67	0
54	MG	2A	3260	1/1	0.95	0.08	50,50,50,50	0
54	MG	2A	3029	1/1	0.95	0.13	44,44,44,44	0
54	MG	2A	3547	1/1	0.95	0.07	57,57,57,57	0
54	MG	1A	3306	1/1	0.95	0.05	17,17,17,17	0
54	MG	1A	3242	1/1	0.95	0.09	40,40,40,40	0
54	MG	1A	3412	1/1	0.95	0.12	37,37,37,37	0
54	MG	2A	3037	1/1	0.95	0.07	42,42,42,42	0
54	MG	1A	3515	1/1	0.95	0.07	30,30,30,30	0
54	MG	2a	3058	1/1	0.95	0.07	49,49,49,49	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	1A	3313	1/1	0.95	0.08	24,24,24,24	0
54	MG	1A	3097	1/1	0.95	0.20	26,26,26,26	0
54	MG	2A	3271	1/1	0.95	0.07	31,31,31,31	0
54	MG	2A	3272	1/1	0.95	0.09	40,40,40,40	0
54	MG	1A	3960	1/1	0.95	0.09	58,58,58,58	0
54	MG	2a	3064	1/1	0.95	0.06	63,63,63,63	0
54	MG	2A	3042	1/1	0.95	0.11	45,45,45,45	0
54	MG	1A	3790	1/1	0.95	0.22	24,24,24,24	0
54	MG	1a	1760	1/1	0.95	0.14	40,40,40,40	0
54	MG	1A	3644	1/1	0.95	0.07	43,43,43,43	0
54	MG	2A	3574	1/1	0.95	0.07	31,31,31,31	0
54	MG	1A	3964	1/1	0.95	0.06	72,72,72,72	0
54	MG	1A	3187	1/1	0.95	0.12	32,32,32,32	0
54	MG	2A	3580	1/1	0.95	0.11	62,62,62,62	0
54	MG	2A	3584	1/1	0.95	0.05	32,32,32,32	0
54	MG	2a	3076	1/1	0.95	0.11	55,55,55,55	0
54	MG	1A	3967	1/1	0.95	0.07	17,17,17,17	0
54	MG	2A	3587	1/1	0.95	0.09	36,36,36,36	0
54	MG	2A	3050	1/1	0.95	0.08	46,46,46,46	0
54	MG	1A	3527	1/1	0.95	0.09	25,25,25,25	0
54	MG	1A	3034	1/1	0.95	0.18	41,41,41,41	0
54	MG	1a	1621	1/1	0.95	0.07	61,61,61,61	0
54	MG	1A	3972	1/1	0.95	0.07	38,38,38,38	0
54	MG	2a	3086	1/1	0.95	0.14	57,57,57,57	0
54	MG	2A	3294	1/1	0.95	0.10	39,39,39,39	0
54	MG	1A	3421	1/1	0.95	0.12	47,47,47,47	0
54	MG	2A	3600	1/1	0.95	0.09	33,33,33,33	0
54	MG	2A	3296	1/1	0.95	0.10	51,51,51,51	0
54	MG	1A	3105	1/1	0.95	0.13	33,33,33,33	0
54	MG	1A	3531	1/1	0.95	0.09	42,42,42,42	0
54	MG	2a	3095	1/1	0.95	0.14	46,46,46,46	0
54	MG	1A	3191	1/1	0.95	0.20	27,27,27,27	0
54	MG	1a	1628	1/1	0.95	0.10	42,42,42,42	0
54	MG	1a	1775	1/1	0.95	0.15	63,63,63,63	0
54	MG	1A	3807	1/1	0.95	0.05	19,19,19,19	0
54	MG	2A	3311	1/1	0.95	0.11	59,59,59,59	0
54	MG	2A	3312	1/1	0.95	0.07	37,37,37,37	0
54	MG	1A	3536	1/1	0.95	0.08	38,38,38,38	0
54	MG	1a	1632	1/1	0.95	0.10	49,49,49,49	0
54	MG	1A	3152	1/1	0.95	0.07	35,35,35,35	0
54	MG	2a	3109	1/1	0.95	0.09	36,36,36,36	0
54	MG	2A	3072	1/1	0.95	0.24	37,37,37,37	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	2A	3073	1/1	0.95	0.07	26,26,26,26	0
54	MG	2A	3074	1/1	0.95	0.09	44,44,44,44	0
54	MG	1A	3425	1/1	0.95	0.12	34,34,34,34	0
54	MG	2A	3620	1/1	0.95	0.20	80,80,80,80	0
54	MG	1A	3816	1/1	0.95	0.12	20,20,20,20	0
54	MG	2A	3080	1/1	0.95	0.12	62,62,62,62	0
54	MG	1A	3818	1/1	0.95	0.10	54,54,54,54	0
54	MG	2A	3629	1/1	0.95	0.08	49,49,49,49	0
54	MG	1A	3540	1/1	0.95	0.20	29,29,29,29	0
54	MG	1A	3545	1/1	0.95	0.22	47,47,47,47	0
54	MG	2A	3640	1/1	0.95	0.13	79,79,79,79	0
54	MG	2A	3641	1/1	0.95	0.07	43,43,43,43	0
54	MG	2A	3340	1/1	0.95	0.08	31,31,31,31	0
54	MG	1A	3064	1/1	0.95	0.05	28,28,28,28	0
54	MG	2a	3133	1/1	0.95	0.11	42,42,42,42	0
54	MG	1A	3157	1/1	0.95	0.10	25,25,25,25	0
54	MG	1A	3342	1/1	0.95	0.09	12,12,12,12	0
54	MG	2A	3648	1/1	0.95	0.07	46,46,46,46	0
54	MG	1A	3260	1/1	0.95	0.07	35,35,35,35	0
54	MG	2A	3093	1/1	0.95	0.24	40,40,40,40	0
54	MG	1A	3831	1/1	0.95	0.07	60,60,60,60	0
54	MG	1A	3832	1/1	0.95	0.07	26,26,26,26	0
54	MG	1B	212	1/1	0.95	0.06	41,41,41,41	0
54	MG	1A	3346	1/1	0.95	0.08	30,30,30,30	0
54	MG	2A	3357	1/1	0.95	0.05	29,29,29,29	0
54	MG	1B	217	1/1	0.95	0.11	53,53,53,53	0
54	MG	1A	3051	1/1	0.95	0.13	51,51,51,51	0
54	MG	1a	1801	1/1	0.95	0.17	55,55,55,55	0
54	MG	1A	3679	1/1	0.95	0.05	19,19,19,19	0
54	MG	2A	3105	1/1	0.95	0.14	42,42,42,42	0
54	MG	2A	3673	1/1	0.95	0.06	58,58,58,58	0
54	MG	2A	3674	1/1	0.95	0.06	44,44,44,44	0
54	MG	2a	3165	1/1	0.95	0.08	53,53,53,53	0
54	MG	1A	3076	1/1	0.95	0.10	31,31,31,31	0
54	MG	2A	3108	1/1	0.95	0.07	35,35,35,35	0
54	MG	1A	3681	1/1	0.95	0.35	23,23,23,23	0
54	MG	1A	3682	1/1	0.95	0.10	37,37,37,37	0
54	MG	2A	3370	1/1	0.95	0.07	39,39,39,39	0
54	MG	2A	3371	1/1	0.95	0.09	49,49,49,49	0
54	MG	1A	3354	1/1	0.95	0.05	39,39,39,39	0
54	MG	1A	3684	1/1	0.95	0.12	21,21,21,21	0
54	MG	1A	3686	1/1	0.95	0.05	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	1a	1811	1/1	0.95	0.08	57,57,57,57	0
54	MG	1A	3688	1/1	0.95	0.09	47,47,47,47	0
54	MG	2A	3693	1/1	0.95	0.12	65,65,65,65	0
54	MG	2A	3694	1/1	0.95	0.09	48,48,48,48	0
54	MG	2A	3378	1/1	0.95	0.07	54,54,54,54	0
54	MG	1a	1658	1/1	0.95	0.12	66,66,66,66	0
54	MG	2a	3190	1/1	0.95	0.06	57,57,57,57	0
54	MG	1D	308	1/1	0.95	0.11	32,32,32,32	0
54	MG	1D	311	1/1	0.95	0.10	24,24,24,24	0
54	MG	1A	3854	1/1	0.95	0.18	30,30,30,30	0
54	MG	2A	3387	1/1	0.95	0.08	35,35,35,35	0
54	MG	2A	3702	1/1	0.95	0.10	44,44,44,44	0
54	MG	2A	3388	1/1	0.95	0.08	39,39,39,39	0
54	MG	1A	3264	1/1	0.95	0.11	11,11,11,11	0
54	MG	1a	1663	1/1	0.95	0.10	57,57,57,57	0
54	MG	2e	202	1/1	0.95	0.14	55,55,55,55	0
54	MG	2f	201	1/1	0.95	0.12	49,49,49,49	0
54	MG	2A	3709	1/1	0.95	0.14	48,48,48,48	0
54	MG	2A	3131	1/1	0.95	0.12	41,41,41,41	0
54	MG	2A	3132	1/1	0.95	0.07	31,31,31,31	0
54	MG	2A	3398	1/1	0.95	0.07	44,44,44,44	0
54	MG	1A	3163	1/1	0.95	0.06	33,33,33,33	0
54	MG	2A	3716	1/1	0.95	0.08	39,39,39,39	0
54	MG	2A	3403	1/1	0.95	0.10	44,44,44,44	0
54	MG	2A	3134	1/1	0.95	0.12	63,63,63,63	0
54	MG	1A	3558	1/1	0.95	0.09	45,45,45,45	0
58	ZN	24	501	1/1	0.95	0.13	145,145,145,145	0
54	MG	1A	3945	1/1	0.96	0.09	51,51,51,51	0
54	MG	2A	3701	1/1	0.96	0.10	64,64,64,64	0
54	MG	1A	3493	1/1	0.96	0.07	46,46,46,46	0
54	MG	1A	3761	1/1	0.96	0.06	69,69,69,69	0
54	MG	2A	3704	1/1	0.96	0.07	65,65,65,65	0
54	MG	1A	3762	1/1	0.96	0.14	46,46,46,46	0
54	MG	1A	3495	1/1	0.96	0.04	18,18,18,18	0
54	MG	2A	3111	1/1	0.96	0.05	42,42,42,42	0
54	MG	1A	3497	1/1	0.96	0.10	47,47,47,47	0
54	MG	2A	3381	1/1	0.96	0.06	27,27,27,27	0
54	MG	1a	1618	1/1	0.96	0.08	67,67,67,67	0
54	MG	1A	3050	1/1	0.96	0.09	36,36,36,36	0
54	MG	2A	3385	1/1	0.96	0.07	42,42,42,42	0
54	MG	2A	3115	1/1	0.96	0.13	39,39,39,39	0
54	MG	1A	3952	1/1	0.96	0.05	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	3117	1/1	0.96	0.07	41,41,41,41	0
54	MG	2A	3390	1/1	0.96	0.09	42,42,42,42	0
54	MG	2A	3392	1/1	0.96	0.07	43,43,43,43	0
54	MG	1A	3031	1/1	0.96	0.07	37,37,37,37	0
54	MG	1A	3397	1/1	0.96	0.05	45,45,45,45	0
54	MG	2A	3121	1/1	0.96	0.06	44,44,44,44	0
54	MG	1A	3502	1/1	0.96	0.11	43,43,43,43	0
54	MG	1A	3773	1/1	0.96	0.14	45,45,45,45	0
54	MG	1a	1805	1/1	0.96	0.07	49,49,49,49	0
54	MG	2A	3125	1/1	0.96	0.34	38,38,38,38	0
54	MG	1A	3618	1/1	0.96	0.07	28,28,28,28	0
54	MG	2A	3128	1/1	0.96	0.19	41,41,41,41	0
54	MG	1A	3292	1/1	0.96	0.07	34,34,34,34	0
54	MG	1A	3623	1/1	0.96	0.12	40,40,40,40	0
54	MG	1a	1629	1/1	0.96	0.16	52,52,52,52	0
54	MG	1A	3624	1/1	0.96	0.09	34,34,34,34	0
54	MG	1A	3505	1/1	0.96	0.06	57,57,57,57	0
54	MG	1A	3965	1/1	0.96	0.14	11,11,11,11	0
54	MG	1A	3293	1/1	0.96	0.06	24,24,24,24	0
54	MG	1A	3296	1/1	0.96	0.07	39,39,39,39	0
54	MG	1A	3509	1/1	0.96	0.12	55,55,55,55	0
54	MG	2A	3140	1/1	0.96	0.06	29,29,29,29	0
54	MG	1a	1817	1/1	0.96	0.12	53,53,53,53	0
54	MG	1A	3786	1/1	0.96	0.07	13,13,13,13	0
54	MG	2A	3145	1/1	0.96	0.05	40,40,40,40	0
54	MG	2A	3423	1/1	0.96	0.17	52,52,52,52	0
54	MG	1A	3971	1/1	0.96	0.08	32,32,32,32	0
54	MG	1A	3227	1/1	0.96	0.19	27,27,27,27	0
54	MG	1A	3973	1/1	0.96	0.10	31,31,31,31	0
54	MG	2A	3427	1/1	0.96	0.05	46,46,46,46	0
54	MG	2A	3150	1/1	0.96	0.14	50,50,50,50	0
54	MG	1A	3630	1/1	0.96	0.09	16,16,16,16	0
54	MG	1A	3173	1/1	0.96	0.06	35,35,35,35	0
54	MG	1A	3041	1/1	0.96	0.12	33,33,33,33	0
54	MG	2A	3156	1/1	0.96	0.15	45,45,45,45	0
54	MG	2A	3158	1/1	0.96	0.10	38,38,38,38	0
54	MG	1A	3980	1/1	0.96	0.11	41,41,41,41	0
54	MG	1A	3981	1/1	0.96	0.05	32,32,32,32	0
54	MG	1A	3232	1/1	0.96	0.06	29,29,29,29	0
54	MG	1A	3133	1/1	0.96	0.36	31,31,31,31	0
54	MG	1A	3056	1/1	0.96	0.07	32,32,32,32	0
54	MG	1A	3516	1/1	0.96	0.08	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	1A	3177	1/1	0.96	0.18	35,35,35,35	0
54	MG	2E	305	1/1	0.96	0.06	36,36,36,36	0
54	MG	2E	307	1/1	0.96	0.06	24,24,24,24	0
54	MG	1A	3802	1/1	0.96	0.07	41,41,41,41	0
54	MG	2F	301	1/1	0.96	0.08	44,44,44,44	0
54	MG	2F	302	1/1	0.96	0.08	32,32,32,32	0
54	MG	1A	3178	1/1	0.96	0.15	42,42,42,42	0
54	MG	2A	3170	1/1	0.96	0.09	44,44,44,44	0
54	MG	2A	3171	1/1	0.96	0.09	44,44,44,44	0
54	MG	1A	3179	1/1	0.96	0.06	25,25,25,25	0
54	MG	1A	3522	1/1	0.96	0.10	43,43,43,43	0
54	MG	1B	202	1/1	0.96	0.10	50,50,50,50	0
54	MG	1A	3808	1/1	0.96	0.06	39,39,39,39	0
54	MG	1A	3524	1/1	0.96	0.17	33,33,33,33	0
54	MG	2A	3177	1/1	0.96	0.16	49,49,49,49	0
54	MG	2A	3178	1/1	0.96	0.11	49,49,49,49	0
54	MG	1a	1842	1/1	0.96	0.09	44,44,44,44	0
54	MG	1B	206	1/1	0.96	0.14	52,52,52,52	0
54	MG	1A	3525	1/1	0.96	0.07	22,22,22,22	0
54	MG	1A	3656	1/1	0.96	0.10	55,55,55,55	0
54	MG	1A	3657	1/1	0.96	0.06	42,42,42,42	0
54	MG	1A	3137	1/1	0.96	0.06	24,24,24,24	0
54	MG	1A	3183	1/1	0.96	0.32	35,35,35,35	0
54	MG	1A	3143	1/1	0.96	0.07	38,38,38,38	0
54	MG	1A	3109	1/1	0.96	0.05	56,56,56,56	0
54	MG	1A	3664	1/1	0.96	0.31	27,27,27,27	0
54	MG	1B	219	1/1	0.96	0.09	53,53,53,53	0
54	MG	1a	1857	1/1	0.96	0.20	61,61,61,61	0
54	MG	20	102	1/1	0.96	0.10	55,55,55,55	0
54	MG	1A	3825	1/1	0.96	0.08	30,30,30,30	0
54	MG	21	102	1/1	0.96	0.07	46,46,46,46	0
54	MG	1A	3417	1/1	0.96	0.16	29,29,29,29	0
54	MG	23	101	1/1	0.96	0.18	53,53,53,53	0
54	MG	2A	3194	1/1	0.96	0.12	48,48,48,48	0
54	MG	25	102	1/1	0.96	0.06	53,53,53,53	0
54	MG	1A	3829	1/1	0.96	0.06	25,25,25,25	0
54	MG	1A	3419	1/1	0.96	0.10	46,46,46,46	0
54	MG	2A	3197	1/1	0.96	0.08	37,37,37,37	0
54	MG	1a	1862	1/1	0.96	0.13	47,47,47,47	0
54	MG	1A	3323	1/1	0.96	0.06	17,17,17,17	0
54	MG	1a	1864	1/1	0.96	0.06	49,49,49,49	0
54	MG	2A	3202	1/1	0.96	0.07	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	3072	1/1	0.96	0.18	34,34,34,34	0
54	MG	1A	3329	1/1	0.96	0.05	17,17,17,17	0
54	MG	1A	3331	1/1	0.96	0.07	17,17,17,17	0
54	MG	1D	301	1/1	0.96	0.38	28,28,28,28	0
54	MG	2A	3207	1/1	0.96	0.07	45,45,45,45	0
54	MG	1D	303	1/1	0.96	0.08	39,39,39,39	0
54	MG	1D	304	1/1	0.96	0.10	39,39,39,39	0
54	MG	1D	306	1/1	0.96	0.08	48,48,48,48	0
54	MG	1D	307	1/1	0.96	0.11	45,45,45,45	0
54	MG	1e	202	1/1	0.96	0.16	60,60,60,60	0
54	MG	1A	3674	1/1	0.96	0.06	36,36,36,36	0
54	MG	2A	3496	1/1	0.96	0.09	55,55,55,55	0
54	MG	1A	3544	1/1	0.96	0.15	25,25,25,25	0
54	MG	2a	3016	1/1	0.96	0.16	49,49,49,49	0
54	MG	1A	3676	1/1	0.96	0.21	60,60,60,60	0
54	MG	2A	3499	1/1	0.96	0.11	51,51,51,51	0
54	MG	1A	3333	1/1	0.96	0.05	20,20,20,20	0
54	MG	2A	3502	1/1	0.96	0.05	41,41,41,41	0
54	MG	2a	3024	1/1	0.96	0.16	42,42,42,42	0
54	MG	2A	3503	1/1	0.96	0.10	17,17,17,17	0
54	MG	1A	3546	1/1	0.96	0.07	26,26,26,26	0
54	MG	2A	3505	1/1	0.96	0.17	37,37,37,37	0
54	MG	2A	3507	1/1	0.96	0.06	36,36,36,36	0
54	MG	1A	3149	1/1	0.96	0.29	39,39,39,39	0
54	MG	1A	3850	1/1	0.96	0.12	57,57,57,57	0
54	MG	2a	3032	1/1	0.96	0.13	66,66,66,66	0
54	MG	1D	318	1/1	0.96	0.11	43,43,43,43	0
54	MG	1A	3431	1/1	0.96	0.09	38,38,38,38	0
54	MG	2a	3036	1/1	0.96	0.08	38,38,38,38	0
54	MG	1k	201	1/1	0.96	0.14	39,39,39,39	0
54	MG	2A	3227	1/1	0.96	0.23	48,48,48,48	0
54	MG	2a	3039	1/1	0.96	0.12	57,57,57,57	0
54	MG	1l	201	1/1	0.96	0.10	40,40,40,40	0
54	MG	1A	3337	1/1	0.96	0.07	41,41,41,41	0
54	MG	1m	201	1/1	0.96	0.05	62,62,62,62	0
54	MG	1A	3150	1/1	0.96	0.04	25,25,25,25	0
54	MG	1A	3190	1/1	0.96	0.23	32,32,32,32	0
54	MG	1F	302	1/1	0.96	0.24	28,28,28,28	0
54	MG	2A	3524	1/1	0.96	0.09	20,20,20,20	0
54	MG	1A	3259	1/1	0.96	0.07	61,61,61,61	0
54	MG	2A	3526	1/1	0.96	0.06	46,46,46,46	0
54	MG	1A	3111	1/1	0.96	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	3438	1/1	0.96	0.13	43,43,43,43	0
54	MG	1A	3863	1/1	0.96	0.09	46,46,46,46	0
54	MG	2A	3240	1/1	0.96	0.10	34,34,34,34	0
54	MG	1A	3192	1/1	0.96	0.22	32,32,32,32	0
54	MG	1A	3693	1/1	0.96	0.12	35,35,35,35	0
54	MG	1A	3349	1/1	0.96	0.06	35,35,35,35	0
54	MG	2A	3538	1/1	0.96	0.09	60,60,60,60	0
54	MG	2a	3057	1/1	0.96	0.11	47,47,47,47	0
54	MG	2A	3539	1/1	0.96	0.10	57,57,57,57	0
54	MG	2A	3003	1/1	0.96	0.17	42,42,42,42	0
54	MG	1A	3092	1/1	0.96	0.17	16,16,16,16	0
54	MG	1A	3351	1/1	0.96	0.08	22,22,22,22	0
54	MG	1A	3448	1/1	0.96	0.09	33,33,33,33	0
54	MG	1a	1713	1/1	0.96	0.06	46,46,46,46	0
54	MG	2A	3548	1/1	0.96	0.09	72,72,72,72	0
54	MG	2A	3249	1/1	0.96	0.05	53,53,53,53	0
54	MG	2A	3550	1/1	0.96	0.06	32,32,32,32	0
54	MG	1G	204	1/1	0.96	0.11	44,44,44,44	0
54	MG	1A	3701	1/1	0.96	0.06	49,49,49,49	0
54	MG	1H	202	1/1	0.96	0.11	37,37,37,37	0
54	MG	2A	3253	1/1	0.96	0.23	40,40,40,40	0
54	MG	1A	3093	1/1	0.96	0.31	29,29,29,29	0
54	MG	1N	202	1/1	0.96	0.29	44,44,44,44	0
54	MG	2a	3073	1/1	0.96	0.11	33,33,33,33	0
54	MG	2A	3562	1/1	0.96	0.06	49,49,49,49	0
54	MG	2A	3019	1/1	0.96	0.27	36,36,36,36	0
54	MG	2A	3021	1/1	0.96	0.09	36,36,36,36	0
54	MG	1A	3117	1/1	0.96	0.32	22,22,22,22	0
54	MG	1a	1721	1/1	0.96	0.08	45,45,45,45	0
54	MG	2A	3569	1/1	0.96	0.07	41,41,41,41	0
54	MG	1A	3355	1/1	0.96	0.05	19,19,19,19	0
54	MG	2A	3265	1/1	0.96	0.11	55,55,55,55	0
54	MG	1P	203	1/1	0.96	0.28	24,24,24,24	0
54	MG	1A	3707	1/1	0.96	0.05	25,25,25,25	0
54	MG	2A	3575	1/1	0.96	0.08	32,32,32,32	0
54	MG	1A	3453	1/1	0.96	0.05	18,18,18,18	0
54	MG	1Q	207	1/1	0.96	0.05	30,30,30,30	0
54	MG	2A	3031	1/1	0.96	0.09	25,25,25,25	0
54	MG	2A	3581	1/1	0.96	0.09	54,54,54,54	0
54	MG	1Q	208	1/1	0.96	0.12	43,43,43,43	0
54	MG	2A	3033	1/1	0.96	0.10	44,44,44,44	0
54	MG	1A	3889	1/1	0.96	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	3891	1/1	0.96	0.10	45,45,45,45	0
54	MG	2a	3098	1/1	0.96	0.19	52,52,52,52	0
54	MG	2a	3099	1/1	0.96	0.08	41,41,41,41	0
54	MG	2A	3276	1/1	0.96	0.08	39,39,39,39	0
54	MG	1A	3568	1/1	0.96	0.08	27,27,27,27	0
54	MG	1A	3569	1/1	0.96	0.09	49,49,49,49	0
54	MG	2A	3279	1/1	0.96	0.10	56,56,56,56	0
54	MG	1A	3267	1/1	0.96	0.24	28,28,28,28	0
54	MG	1A	3896	1/1	0.96	0.13	35,35,35,35	0
54	MG	2a	3107	1/1	0.96	0.18	52,52,52,52	0
54	MG	1A	3455	1/1	0.96	0.08	21,21,21,21	0
54	MG	1A	3047	1/1	0.96	0.13	27,27,27,27	0
54	MG	1U	201	1/1	0.96	0.05	17,17,17,17	0
54	MG	1U	203	1/1	0.96	0.18	21,21,21,21	0
54	MG	2A	3604	1/1	0.96	0.09	66,66,66,66	0
54	MG	1A	3062	1/1	0.96	0.07	41,41,41,41	0
54	MG	1A	3576	1/1	0.96	0.16	37,37,37,37	0
54	MG	1A	3362	1/1	0.96	0.06	15,15,15,15	0
54	MG	1A	3120	1/1	0.96	0.26	36,36,36,36	0
54	MG	1A	3273	1/1	0.96	0.13	41,41,41,41	0
54	MG	2A	3051	1/1	0.96	0.19	43,43,43,43	0
54	MG	2A	3297	1/1	0.96	0.12	50,50,50,50	0
54	MG	1a	1750	1/1	0.96	0.06	64,64,64,64	0
54	MG	2A	3613	1/1	0.96	0.13	57,57,57,57	0
54	MG	2a	3129	1/1	0.96	0.08	51,51,51,51	0
54	MG	2A	3053	1/1	0.96	0.11	41,41,41,41	0
54	MG	2A	3301	1/1	0.96	0.12	41,41,41,41	0
54	MG	2A	3054	1/1	0.96	0.20	42,42,42,42	0
54	MG	2A	3305	1/1	0.96	0.10	36,36,36,36	0
54	MG	1A	3723	1/1	0.96	0.06	36,36,36,36	0
54	MG	1A	3164	1/1	0.96	0.08	29,29,29,29	0
54	MG	1Y	202	1/1	0.96	0.10	74,74,74,74	0
54	MG	2A	3625	1/1	0.96	0.06	38,38,38,38	0
54	MG	2a	3138	1/1	0.96	0.07	52,52,52,52	0
54	MG	2a	3139	1/1	0.96	0.09	53,53,53,53	0
54	MG	1A	3468	1/1	0.96	0.06	17,17,17,17	0
54	MG	1A	3276	1/1	0.96	0.04	28,28,28,28	0
54	MG	2A	3313	1/1	0.96	0.07	37,37,37,37	0
54	MG	2a	3144	1/1	0.96	0.07	58,58,58,58	0
54	MG	2A	3315	1/1	0.96	0.08	32,32,32,32	0
54	MG	2A	3637	1/1	0.96	0.06	66,66,66,66	0
54	MG	2A	3060	1/1	0.96	0.06	34,34,34,34	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	2A	3321	1/1	0.96	0.10	37,37,37,37	0
54	MG	2A	3322	1/1	0.96	0.08	39,39,39,39	0
54	MG	2a	3157	1/1	0.96	0.07	68,68,68,68	0
54	MG	1A	3470	1/1	0.96	0.07	37,37,37,37	0
54	MG	1A	3914	1/1	0.96	0.10	19,19,19,19	0
54	MG	2a	3161	1/1	0.96	0.07	33,33,33,33	0
54	MG	2A	3645	1/1	0.96	0.09	45,45,45,45	0
54	MG	10	106	1/1	0.96	0.07	35,35,35,35	0
54	MG	1A	3730	1/1	0.96	0.07	33,33,33,33	0
54	MG	1A	3732	1/1	0.96	0.09	41,41,41,41	0
54	MG	2a	3166	1/1	0.96	0.09	57,57,57,57	0
54	MG	2A	3331	1/1	0.96	0.07	35,35,35,35	0
54	MG	11	102	1/1	0.96	0.10	24,24,24,24	0
54	MG	2A	3068	1/1	0.96	0.23	38,38,38,38	0
54	MG	1A	3918	1/1	0.96	0.06	37,37,37,37	0
54	MG	1A	3919	1/1	0.96	0.12	36,36,36,36	0
54	MG	2a	3174	1/1	0.96	0.07	53,53,53,53	0
54	MG	1A	3121	1/1	0.96	0.05	25,25,25,25	0
54	MG	1A	3474	1/1	0.96	0.09	21,21,21,21	0
54	MG	2a	3178	1/1	0.96	0.12	41,41,41,41	0
54	MG	1A	3372	1/1	0.96	0.07	24,24,24,24	0
54	MG	2A	3665	1/1	0.96	0.05	49,49,49,49	0
54	MG	1A	3124	1/1	0.96	0.15	24,24,24,24	0
54	MG	1A	3482	1/1	0.96	0.08	50,50,50,50	0
54	MG	2A	3343	1/1	0.96	0.09	48,48,48,48	0
54	MG	2A	3079	1/1	0.96	0.08	38,38,38,38	0
54	MG	2A	3346	1/1	0.96	0.05	49,49,49,49	0
54	MG	1A	3925	1/1	0.96	0.08	58,58,58,58	0
54	MG	1A	3377	1/1	0.96	0.07	11,11,11,11	0
54	MG	1A	3211	1/1	0.96	0.08	35,35,35,35	0
54	MG	2A	3083	1/1	0.96	0.07	49,49,49,49	0
54	MG	1A	3383	1/1	0.96	0.07	16,16,16,16	0
54	MG	2A	3680	1/1	0.96	0.07	40,40,40,40	0
54	MG	2A	3087	1/1	0.96	0.09	33,33,33,33	0
54	MG	1A	3748	1/1	0.96	0.08	39,39,39,39	0
54	MG	1a	1774	1/1	0.96	0.06	55,55,55,55	0
54	MG	1A	3930	1/1	0.96	0.13	35,35,35,35	0
54	MG	1A	3038	1/1	0.96	0.05	27,27,27,27	0
54	MG	1A	3213	1/1	0.96	0.47	31,31,31,31	0
54	MG	1A	3284	1/1	0.96	0.09	31,31,31,31	0
54	MG	2A	3691	1/1	0.96	0.07	59,59,59,59	0
54	MG	2A	3692	1/1	0.96	0.07	55,55,55,55	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	2A	3365	1/1	0.96	0.07	46,46,46,46	0
54	MG	1A	3754	1/1	0.96	0.07	17,17,17,17	0
54	MG	1A	3286	1/1	0.96	0.19	29,29,29,29	0
56	MPD	18	105	8/8	0.96	0.12	17,24,28,31	0
54	MG	1A	3604	1/1	0.96	0.11	19,19,19,19	0
54	MG	1A	3941	1/1	0.96	0.10	31,31,31,31	0
54	MG	1A	3214	1/1	0.96	0.13	32,32,32,32	0
58	ZN	14	501	1/1	0.96	0.13	124,124,124,124	0
54	MG	1A	3606	1/1	0.96	0.07	29,29,29,29	0
54	MG	1A	3485	1/1	0.97	0.07	13,13,13,13	0
54	MG	1A	3116	1/1	0.97	0.12	34,34,34,34	0
54	MG	1A	3202	1/1	0.97	0.07	29,29,29,29	0
54	MG	1A	3601	1/1	0.97	0.06	28,28,28,28	0
54	MG	1A	3602	1/1	0.97	0.12	34,34,34,34	0
54	MG	1A	3371	1/1	0.97	0.04	14,14,14,14	0
54	MG	1A	3015	1/1	0.97	0.20	15,15,15,15	0
54	MG	2A	3151	1/1	0.97	0.07	28,28,28,28	0
54	MG	1A	3208	1/1	0.97	0.14	24,24,24,24	0
54	MG	2A	3153	1/1	0.97	0.07	38,38,38,38	0
54	MG	1a	1614	1/1	0.97	0.12	20,20,20,20	0
54	MG	2A	3422	1/1	0.97	0.05	45,45,45,45	0
54	MG	1A	3161	1/1	0.97	0.11	22,22,22,22	0
54	MG	1A	3381	1/1	0.97	0.11	36,36,36,36	0
54	MG	1A	3494	1/1	0.97	0.07	35,35,35,35	0
54	MG	1A	3089	1/1	0.97	0.25	37,37,37,37	0
54	MG	1A	3496	1/1	0.97	0.10	23,23,23,23	0
54	MG	1A	3612	1/1	0.97	0.17	26,26,26,26	0
54	MG	1A	3283	1/1	0.97	0.26	35,35,35,35	0
54	MG	1A	3766	1/1	0.97	0.04	22,22,22,22	0
54	MG	1A	3615	1/1	0.97	0.07	28,28,28,28	0
54	MG	1A	3060	1/1	0.97	0.05	35,35,35,35	0
54	MG	1a	1625	1/1	0.97	0.11	38,38,38,38	0
54	MG	1A	3285	1/1	0.97	0.11	38,38,38,38	0
54	MG	1A	3027	1/1	0.97	0.04	23,23,23,23	0
54	MG	1A	3963	1/1	0.97	0.07	38,38,38,38	0
54	MG	1A	3619	1/1	0.97	0.11	42,42,42,42	0
54	MG	2A	3439	1/1	0.97	0.17	40,40,40,40	0
54	MG	1A	3216	1/1	0.97	0.09	21,21,21,21	0
54	MG	2B	210	1/1	0.97	0.12	41,41,41,41	0
54	MG	1A	3777	1/1	0.97	0.08	30,30,30,30	0
54	MG	2A	3442	1/1	0.97	0.05	30,30,30,30	0
54	MG	1A	3621	1/1	0.97	0.08	54,54,54,54	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	1A	3391	1/1	0.97	0.08	45,45,45,45	0
54	MG	1A	3969	1/1	0.97	0.11	42,42,42,42	0
54	MG	1A	3218	1/1	0.97	0.07	54,54,54,54	0
54	MG	2B	217	1/1	0.97	0.06	56,56,56,56	0
54	MG	2B	218	1/1	0.97	0.07	68,68,68,68	0
54	MG	1A	3289	1/1	0.97	0.04	24,24,24,24	0
54	MG	2B	220	1/1	0.97	0.05	36,36,36,36	0
54	MG	2D	301	1/1	0.97	0.17	31,31,31,31	0
54	MG	2A	3448	1/1	0.97	0.09	56,56,56,56	0
54	MG	1A	3018	1/1	0.97	0.19	32,32,32,32	0
54	MG	1A	3508	1/1	0.97	0.09	35,35,35,35	0
54	MG	1A	3974	1/1	0.97	0.11	61,61,61,61	0
54	MG	1A	3045	1/1	0.97	0.31	21,21,21,21	0
54	MG	1a	1849	1/1	0.97	0.07	58,58,58,58	0
54	MG	1A	3977	1/1	0.97	0.10	61,61,61,61	0
54	MG	1A	3221	1/1	0.97	0.20	27,27,27,27	0
54	MG	1A	3294	1/1	0.97	0.15	27,27,27,27	0
54	MG	1A	3789	1/1	0.97	0.14	29,29,29,29	0
54	MG	1A	3223	1/1	0.97	0.12	24,24,24,24	0
54	MG	1a	1856	1/1	0.97	0.05	52,52,52,52	0
54	MG	1a	1646	1/1	0.97	0.09	47,47,47,47	0
54	MG	1A	3297	1/1	0.97	0.04	20,20,20,20	0
54	MG	1A	3224	1/1	0.97	0.32	24,24,24,24	0
54	MG	2F	304	1/1	0.97	0.05	43,43,43,43	0
54	MG	1A	3635	1/1	0.97	0.05	38,38,38,38	0
54	MG	1A	3636	1/1	0.97	0.06	43,43,43,43	0
54	MG	1A	3798	1/1	0.97	0.06	31,31,31,31	0
54	MG	1A	3637	1/1	0.97	0.09	39,39,39,39	0
54	MG	1A	3405	1/1	0.97	0.06	11,11,11,11	0
54	MG	2A	3200	1/1	0.97	0.07	43,43,43,43	0
54	MG	1A	3989	1/1	0.97	0.12	51,51,51,51	0
54	MG	1A	3125	1/1	0.97	0.16	27,27,27,27	0
54	MG	1A	3126	1/1	0.97	0.10	47,47,47,47	0
54	MG	1A	3642	1/1	0.97	0.06	51,51,51,51	0
54	MG	1A	3805	1/1	0.97	0.04	31,31,31,31	0
54	MG	1A	3643	1/1	0.97	0.08	54,54,54,54	0
54	MG	1A	3229	1/1	0.97	0.08	31,31,31,31	0
54	MG	2A	3480	1/1	0.97	0.07	31,31,31,31	0
54	MG	1A	3519	1/1	0.97	0.10	31,31,31,31	0
54	MG	1A	3094	1/1	0.97	0.21	38,38,38,38	0
54	MG	2V	202	1/1	0.97	0.07	51,51,51,51	0
54	MG	2W	201	1/1	0.97	0.39	40,40,40,40	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	1A	3814	1/1	0.97	0.13	41,41,41,41	0
54	MG	2A	3485	1/1	0.97	0.05	56,56,56,56	0
54	MG	1a	1664	1/1	0.97	0.12	49,49,49,49	0
54	MG	1A	3521	1/1	0.97	0.07	24,24,24,24	0
54	MG	2Y	201	1/1	0.97	0.10	46,46,46,46	0
54	MG	1B	211	1/1	0.97	0.05	28,28,28,28	0
54	MG	1A	3648	1/1	0.97	0.11	63,63,63,63	0
54	MG	1B	214	1/1	0.97	0.06	32,32,32,32	0
54	MG	1a	1670	1/1	0.97	0.06	36,36,36,36	0
54	MG	1A	3817	1/1	0.97	0.21	38,38,38,38	0
54	MG	2I	104	1/1	0.97	0.07	55,55,55,55	0
54	MG	1B	216	1/1	0.97	0.09	39,39,39,39	0
54	MG	23	102	1/1	0.97	0.07	52,52,52,52	0
54	MG	1a	1673	1/1	0.97	0.05	45,45,45,45	0
54	MG	1A	3649	1/1	0.97	0.05	55,55,55,55	0
54	MG	1A	3030	1/1	0.97	0.06	42,42,42,42	0
54	MG	1A	3233	1/1	0.97	0.21	23,23,23,23	0
54	MG	2A	3226	1/1	0.97	0.07	37,37,37,37	0
54	MG	1A	3309	1/1	0.97	0.05	17,17,17,17	0
54	MG	2A	3228	1/1	0.97	0.26	44,44,44,44	0
54	MG	2A	3501	1/1	0.97	0.08	47,47,47,47	0
54	MG	1A	3526	1/1	0.97	0.06	45,45,45,45	0
54	MG	1a	1679	1/1	0.97	0.10	44,44,44,44	0
54	MG	1A	3130	1/1	0.97	0.08	21,21,21,21	0
54	MG	1A	3235	1/1	0.97	0.20	21,21,21,21	0
54	MG	1A	3827	1/1	0.97	0.10	46,46,46,46	0
54	MG	1A	3661	1/1	0.97	0.12	27,27,27,27	0
54	MG	1A	3314	1/1	0.97	0.07	32,32,32,32	0
54	MG	1A	3067	1/1	0.97	0.41	35,35,35,35	0
54	MG	1A	3069	1/1	0.97	0.28	29,29,29,29	0
54	MG	1D	302	1/1	0.97	0.31	22,22,22,22	0
54	MG	1A	3532	1/1	0.97	0.10	27,27,27,27	0
54	MG	1A	3834	1/1	0.97	0.11	36,36,36,36	0
54	MG	2A	3516	1/1	0.97	0.08	39,39,39,39	0
54	MG	1A	3317	1/1	0.97	0.07	23,23,23,23	0
54	MG	2A	3008	1/1	0.97	0.06	31,31,31,31	0
54	MG	2A	3009	1/1	0.97	0.08	41,41,41,41	0
54	MG	2a	3018	1/1	0.97	0.10	45,45,45,45	0
54	MG	2a	3019	1/1	0.97	0.06	46,46,46,46	0
54	MG	2A	3010	1/1	0.97	0.05	45,45,45,45	0
54	MG	2A	3521	1/1	0.97	0.05	42,42,42,42	0
54	MG	2a	3022	1/1	0.97	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	1A	3319	1/1	0.97	0.06	31,31,31,31	0
54	MG	1A	3837	1/1	0.97	0.07	33,33,33,33	0
54	MG	1D	310	1/1	0.97	0.07	41,41,41,41	0
54	MG	2A	3015	1/1	0.97	0.10	39,39,39,39	0
54	MG	2A	3528	1/1	0.97	0.07	69,69,69,69	0
54	MG	1A	3668	1/1	0.97	0.15	25,25,25,25	0
54	MG	1A	3839	1/1	0.97	0.04	24,24,24,24	0
54	MG	2a	3030	1/1	0.97	0.14	48,48,48,48	0
54	MG	2A	3531	1/1	0.97	0.07	52,52,52,52	0
54	MG	1A	3537	1/1	0.97	0.08	46,46,46,46	0
54	MG	1A	3098	1/1	0.97	0.05	31,31,31,31	0
54	MG	2a	3034	1/1	0.97	0.21	52,52,52,52	0
54	MG	2A	3534	1/1	0.97	0.06	63,63,63,63	0
54	MG	2A	3020	1/1	0.97	0.12	34,34,34,34	0
54	MG	1A	3845	1/1	0.97	0.05	23,23,23,23	0
54	MG	2A	3258	1/1	0.97	0.06	33,33,33,33	0
54	MG	1A	3134	1/1	0.97	0.13	26,26,26,26	0
54	MG	1A	3244	1/1	0.97	0.28	24,24,24,24	0
54	MG	1A	3541	1/1	0.97	0.09	14,14,14,14	0
54	MG	1E	302	1/1	0.97	0.21	26,26,26,26	0
54	MG	2A	3542	1/1	0.97	0.06	22,22,22,22	0
54	MG	1a	1704	1/1	0.97	0.19	48,48,48,48	0
54	MG	1A	3543	1/1	0.97	0.13	39,39,39,39	0
54	MG	1E	305	1/1	0.97	0.09	15,15,15,15	0
54	MG	2A	3030	1/1	0.97	0.07	42,42,42,42	0
54	MG	1A	3326	1/1	0.97	0.04	20,20,20,20	0
54	MG	1A	3245	1/1	0.97	0.29	20,20,20,20	0
54	MG	1A	3180	1/1	0.97	0.14	38,38,38,38	0
54	MG	1F	303	1/1	0.97	0.40	30,30,30,30	0
54	MG	1F	304	1/1	0.97	0.25	26,26,26,26	0
54	MG	2A	3556	1/1	0.97	0.06	17,17,17,17	0
54	MG	2A	3036	1/1	0.97	0.16	52,52,52,52	0
54	MG	1A	3181	1/1	0.97	0.07	38,38,38,38	0
54	MG	1A	3332	1/1	0.97	0.06	11,11,11,11	0
54	MG	1F	309	1/1	0.97	0.07	27,27,27,27	0
54	MG	2A	3563	1/1	0.97	0.05	39,39,39,39	0
54	MG	1F	310	1/1	0.97	0.10	17,17,17,17	0
54	MG	1A	3019	1/1	0.97	0.18	28,28,28,28	0
54	MG	1A	3859	1/1	0.97	0.04	32,32,32,32	0
54	MG	2A	3043	1/1	0.97	0.07	19,19,19,19	0
54	MG	1A	3334	1/1	0.97	0.06	18,18,18,18	0
54	MG	2A	3284	1/1	0.97	0.13	58,58,58,58	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	1A	3021	1/1	0.97	0.29	34,34,34,34	0
54	MG	1A	3867	1/1	0.97	0.08	41,41,41,41	0
54	MG	1A	3868	1/1	0.97	0.12	62,62,62,62	0
54	MG	1a	1728	1/1	0.97	0.05	33,33,33,33	0
54	MG	1F	317	1/1	0.97	0.10	26,26,26,26	0
54	MG	1A	3869	1/1	0.97	0.10	47,47,47,47	0
54	MG	1a	1731	1/1	0.97	0.06	45,45,45,45	0
54	MG	1A	3685	1/1	0.97	0.15	32,32,32,32	0
54	MG	2A	3582	1/1	0.97	0.03	69,69,69,69	0
54	MG	2a	3074	1/1	0.97	0.19	50,50,50,50	0
54	MG	1A	3184	1/1	0.97	0.18	35,35,35,35	0
54	MG	1a	1734	1/1	0.97	0.06	49,49,49,49	0
54	MG	2A	3586	1/1	0.97	0.06	23,23,23,23	0
54	MG	1A	3252	1/1	0.97	0.30	32,32,32,32	0
54	MG	1A	3138	1/1	0.97	0.15	24,24,24,24	0
54	MG	2A	3590	1/1	0.97	0.05	48,48,48,48	0
54	MG	2a	3082	1/1	0.97	0.20	42,42,42,42	0
54	MG	1A	3140	1/1	0.97	0.27	23,23,23,23	0
54	MG	2A	3592	1/1	0.97	0.05	25,25,25,25	0
54	MG	2A	3302	1/1	0.97	0.08	47,47,47,47	0
54	MG	1A	3443	1/1	0.97	0.05	48,48,48,48	0
54	MG	2a	3087	1/1	0.97	0.08	60,60,60,60	0
54	MG	1A	3343	1/1	0.97	0.06	44,44,44,44	0
54	MG	1A	3880	1/1	0.97	0.08	19,19,19,19	0
54	MG	1P	201	1/1	0.97	0.24	19,19,19,19	0
54	MG	2a	3091	1/1	0.97	0.23	48,48,48,48	0
54	MG	1A	3881	1/1	0.97	0.10	44,44,44,44	0
54	MG	1P	204	1/1	0.97	0.13	17,17,17,17	0
54	MG	1A	3697	1/1	0.97	0.10	48,48,48,48	0
54	MG	1Q	201	1/1	0.97	0.19	24,24,24,24	0
54	MG	1A	3559	1/1	0.97	0.05	25,25,25,25	0
54	MG	2A	3316	1/1	0.97	0.08	28,28,28,28	0
54	MG	2A	3317	1/1	0.97	0.09	38,38,38,38	0
54	MG	1Q	205	1/1	0.97	0.06	25,25,25,25	0
54	MG	2A	3319	1/1	0.97	0.08	36,36,36,36	0
54	MG	1A	3142	1/1	0.97	0.14	27,27,27,27	0
54	MG	1A	3345	1/1	0.97	0.06	24,24,24,24	0
54	MG	1R	201	1/1	0.97	0.23	37,37,37,37	0
54	MG	2a	3104	1/1	0.97	0.18	51,51,51,51	0
54	MG	1A	3258	1/1	0.97	0.15	47,47,47,47	0
54	MG	1A	3890	1/1	0.97	0.07	48,48,48,48	0
54	MG	2A	3328	1/1	0.97	0.07	33,33,33,33	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	1A	3347	1/1	0.97	0.03	25,25,25,25	0
54	MG	1A	3348	1/1	0.97	0.06	27,27,27,27	0
54	MG	2A	3078	1/1	0.97	0.22	43,43,43,43	0
54	MG	1A	3705	1/1	0.97	0.04	19,19,19,19	0
54	MG	1A	3706	1/1	0.97	0.10	39,39,39,39	0
54	MG	2a	3113	1/1	0.97	0.12	41,41,41,41	0
54	MG	2a	3114	1/1	0.97	0.05	53,53,53,53	0
54	MG	2a	3116	1/1	0.97	0.07	51,51,51,51	0
54	MG	2a	3117	1/1	0.97	0.09	45,45,45,45	0
54	MG	2A	3621	1/1	0.97	0.07	50,50,50,50	0
54	MG	1A	3006	1/1	0.97	0.05	36,36,36,36	0
54	MG	1A	3144	1/1	0.97	0.11	30,30,30,30	0
54	MG	1A	3709	1/1	0.97	0.09	39,39,39,39	0
54	MG	1U	202	1/1	0.97	0.24	24,24,24,24	0
54	MG	2A	3339	1/1	0.97	0.07	22,22,22,22	0
54	MG	2A	3085	1/1	0.97	0.40	45,45,45,45	0
54	MG	2A	3631	1/1	0.97	0.07	77,77,77,77	0
54	MG	2a	3126	1/1	0.97	0.09	54,54,54,54	0
54	MG	2A	3635	1/1	0.97	0.05	58,58,58,58	0
54	MG	2A	3086	1/1	0.97	0.35	45,45,45,45	0
54	MG	1A	3107	1/1	0.97	0.05	29,29,29,29	0
54	MG	1U	204	1/1	0.97	0.20	20,20,20,20	0
54	MG	1A	3458	1/1	0.97	0.08	17,17,17,17	0
54	MG	1A	3902	1/1	0.97	0.07	57,57,57,57	0
54	MG	2A	3643	1/1	0.97	0.07	63,63,63,63	0
54	MG	1A	3147	1/1	0.97	0.04	37,37,37,37	0
54	MG	1A	3573	1/1	0.97	0.04	18,18,18,18	0
54	MG	2A	3351	1/1	0.97	0.10	31,31,31,31	0
54	MG	2A	3352	1/1	0.97	0.08	42,42,42,42	0
54	MG	1A	3905	1/1	0.97	0.06	48,48,48,48	0
54	MG	1A	3353	1/1	0.97	0.06	62,62,62,62	0
54	MG	1A	3715	1/1	0.97	0.09	37,37,37,37	0
54	MG	1A	3052	1/1	0.97	0.08	18,18,18,18	0
54	MG	1A	3053	1/1	0.97	0.07	40,40,40,40	0
54	MG	2a	3145	1/1	0.97	0.07	58,58,58,58	0
54	MG	1A	3356	1/1	0.97	0.05	33,33,33,33	0
54	MG	2A	3656	1/1	0.97	0.04	66,66,66,66	0
54	MG	2a	3150	1/1	0.97	0.12	59,59,59,59	0
54	MG	1A	3467	1/1	0.97	0.06	29,29,29,29	0
54	MG	1A	3721	1/1	0.97	0.05	43,43,43,43	0
54	MG	2A	3660	1/1	0.97	0.05	63,63,63,63	0
54	MG	2a	3156	1/1	0.97	0.06	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	2A	3661	1/1	0.97	0.10	55,55,55,55	0
54	MG	1A	3024	1/1	0.97	0.12	20,20,20,20	0
54	MG	2A	3363	1/1	0.97	0.10	60,60,60,60	0
54	MG	2A	3666	1/1	0.97	0.07	65,65,65,65	0
54	MG	2A	3668	1/1	0.97	0.05	31,31,31,31	0
54	MG	1a	1777	1/1	0.97	0.05	48,48,48,48	0
54	MG	1A	3358	1/1	0.97	0.09	48,48,48,48	0
54	MG	2A	3109	1/1	0.97	0.08	41,41,41,41	0
54	MG	1A	3581	1/1	0.97	0.23	29,29,29,29	0
54	MG	1A	3025	1/1	0.97	0.20	28,28,28,28	0
54	MG	1A	3583	1/1	0.97	0.15	18,18,18,18	0
54	MG	13	103	1/1	0.97	0.22	37,37,37,37	0
54	MG	1A	3727	1/1	0.97	0.05	43,43,43,43	0
54	MG	15	103	1/1	0.97	0.22	25,25,25,25	0
54	MG	2A	3373	1/1	0.97	0.05	40,40,40,40	0
54	MG	2a	3175	1/1	0.97	0.07	42,42,42,42	0
54	MG	1A	3471	1/1	0.97	0.10	44,44,44,44	0
54	MG	1a	1788	1/1	0.97	0.11	43,43,43,43	0
54	MG	2A	3118	1/1	0.97	0.07	37,37,37,37	0
54	MG	1A	3472	1/1	0.97	0.04	13,13,13,13	0
54	MG	1a	1790	1/1	0.97	0.08	51,51,51,51	0
54	MG	1A	3586	1/1	0.97	0.08	24,24,24,24	0
54	MG	1A	3270	1/1	0.97	0.12	43,43,43,43	0
54	MG	1A	3361	1/1	0.97	0.05	17,17,17,17	0
54	MG	2A	3690	1/1	0.97	0.07	61,61,61,61	0
54	MG	17	101	1/1	0.97	0.11	23,23,23,23	0
54	MG	1A	3079	1/1	0.97	0.24	23,23,23,23	0
54	MG	1A	3479	1/1	0.97	0.06	28,28,28,28	0
54	MG	2A	3127	1/1	0.97	0.11	46,46,46,46	0
54	MG	2a	3192	1/1	0.97	0.05	49,49,49,49	0
54	MG	1A	3363	1/1	0.97	0.05	10,10,10,10	0
54	MG	2A	3389	1/1	0.97	0.07	44,44,44,44	0
54	MG	1A	3114	1/1	0.97	0.21	30,30,30,30	0
54	MG	1a	1799	1/1	0.97	0.07	47,47,47,47	0
54	MG	1A	3743	1/1	0.97	0.10	15,15,15,15	0
54	MG	1A	3744	1/1	0.97	0.09	29,29,29,29	0
54	MG	2A	3395	1/1	0.97	0.05	30,30,30,30	0
54	MG	1A	3156	1/1	0.97	0.26	21,21,21,21	0
54	MG	19	102	1/1	0.97	0.05	37,37,37,37	0
54	MG	1A	3057	1/1	0.97	0.12	29,29,29,29	0
54	MG	2A	3136	1/1	0.97	0.08	45,45,45,45	0
54	MG	2A	3402	1/1	0.97	0.08	31,31,31,31	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	2A	3707	1/1	0.97	0.06	50,50,50,50	0
54	MG	2A	3708	1/1	0.97	0.07	34,34,34,34	0
54	MG	1A	3936	1/1	0.97	0.10	30,30,30,30	0
54	MG	1A	3747	1/1	0.97	0.19	24,24,24,24	0
54	MG	2A	3406	1/1	0.97	0.06	49,49,49,49	0
54	MG	2A	3713	1/1	0.97	0.10	39,39,39,39	0
57	ARG	1B	230	12/12	0.97	0.08	26,31,42,44	0
54	MG	1a	1605	1/1	0.97	0.14	58,58,58,58	0
58	ZN	1Y	203	1/1	0.97	0.05	73,73,73,73	0
54	MG	2A	3141	1/1	0.97	0.06	32,32,32,32	0
54	MG	2A	3142	1/1	0.97	0.12	33,33,33,33	0
58	ZN	2n	501	1/1	0.97	0.07	90,90,90,90	0
54	MG	1a	1855	1/1	0.98	0.09	49,49,49,49	0
54	MG	2A	3552	1/1	0.98	0.05	70,70,70,70	0
54	MG	2A	3338	1/1	0.98	0.04	21,21,21,21	0
54	MG	2A	3138	1/1	0.98	0.09	38,38,38,38	0
54	MG	2A	3555	1/1	0.98	0.04	40,40,40,40	0
54	MG	1A	3774	1/1	0.98	0.05	33,33,33,33	0
54	MG	1A	3557	1/1	0.98	0.05	37,37,37,37	0
54	MG	1A	3385	1/1	0.98	0.05	13,13,13,13	0
54	MG	2A	3559	1/1	0.98	0.06	49,49,49,49	0
54	MG	1A	3032	1/1	0.98	0.08	25,25,25,25	0
54	MG	2A	3561	1/1	0.98	0.07	62,62,62,62	0
54	MG	1A	3560	1/1	0.98	0.04	33,33,33,33	0
54	MG	1P	202	1/1	0.98	0.21	23,23,23,23	0
54	MG	1A	3061	1/1	0.98	0.06	19,19,19,19	0
54	MG	1A	3388	1/1	0.98	0.04	19,19,19,19	0
54	MG	1A	3781	1/1	0.98	0.05	31,31,31,31	0
54	MG	2A	3567	1/1	0.98	0.11	40,40,40,40	0
54	MG	1P	206	1/1	0.98	0.04	28,28,28,28	0
54	MG	1A	3206	1/1	0.98	0.21	22,22,22,22	0
54	MG	1Q	202	1/1	0.98	0.16	29,29,29,29	0
54	MG	2A	3571	1/1	0.98	0.10	58,58,58,58	0
54	MG	1A	3390	1/1	0.98	0.06	27,27,27,27	0
54	MG	1A	3784	1/1	0.98	0.07	48,48,48,48	0
54	MG	1Q	206	1/1	0.98	0.20	40,40,40,40	0
54	MG	1a	1699	1/1	0.98	0.05	59,59,59,59	0
54	MG	2A	3576	1/1	0.98	0.04	43,43,43,43	0
54	MG	1A	3477	1/1	0.98	0.03	30,30,30,30	0
54	MG	2A	3157	1/1	0.98	0.06	48,48,48,48	0
54	MG	1A	3478	1/1	0.98	0.09	32,32,32,32	0
54	MG	1A	3567	1/1	0.98	0.06	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	1R	202	1/1	0.98	0.23	21,21,21,21	0
54	MG	1A	3669	1/1	0.98	0.09	37,37,37,37	0
54	MG	1A	3207	1/1	0.98	0.33	25,25,25,25	0
54	MG	1A	3077	1/1	0.98	0.09	32,32,32,32	0
54	MG	1A	3481	1/1	0.98	0.05	13,13,13,13	0
54	MG	1A	3792	1/1	0.98	0.05	11,11,11,11	0
54	MG	1A	3209	1/1	0.98	0.13	23,23,23,23	0
54	MG	2A	3168	1/1	0.98	0.18	37,37,37,37	0
54	MG	1A	3794	1/1	0.98	0.07	16,16,16,16	0
54	MG	1A	3572	1/1	0.98	0.04	27,27,27,27	0
54	MG	1A	3796	1/1	0.98	0.10	40,40,40,40	0
54	MG	1A	3944	1/1	0.98	0.06	27,27,27,27	0
54	MG	1a	1716	1/1	0.98	0.06	31,31,31,31	0
54	MG	2A	3598	1/1	0.98	0.05	44,44,44,44	0
54	MG	1A	3210	1/1	0.98	0.26	32,32,32,32	0
54	MG	1A	3396	1/1	0.98	0.05	21,21,21,21	0
54	MG	1A	3322	1/1	0.98	0.06	34,34,34,34	0
54	MG	2A	3380	1/1	0.98	0.05	27,27,27,27	0
54	MG	1U	206	1/1	0.98	0.04	39,39,39,39	0
54	MG	1V	201	1/1	0.98	0.22	18,18,18,18	0
54	MG	1a	1723	1/1	0.98	0.15	65,65,65,65	0
54	MG	2A	3384	1/1	0.98	0.04	28,28,28,28	0
54	MG	1A	3800	1/1	0.98	0.05	36,36,36,36	0
54	MG	1A	3398	1/1	0.98	0.08	16,16,16,16	0
54	MG	1A	3263	1/1	0.98	0.10	15,15,15,15	0
54	MG	2A	3183	1/1	0.98	0.21	37,37,37,37	0
54	MG	2A	3001	1/1	0.98	0.12	44,44,44,44	0
54	MG	1A	3324	1/1	0.98	0.03	28,28,28,28	0
54	MG	1A	3170	1/1	0.98	0.12	39,39,39,39	0
54	MG	2A	3004	1/1	0.98	0.05	30,30,30,30	0
54	MG	2A	3615	1/1	0.98	0.05	40,40,40,40	0
54	MG	1W	202	1/1	0.98	0.06	31,31,31,31	0
54	MG	1A	3327	1/1	0.98	0.04	18,18,18,18	0
54	MG	1A	3403	1/1	0.98	0.08	14,14,14,14	0
54	MG	1A	3955	1/1	0.98	0.22	31,31,31,31	0
54	MG	1A	3171	1/1	0.98	0.10	33,33,33,33	0
54	MG	2A	3400	1/1	0.98	0.12	42,42,42,42	0
54	MG	10	102	1/1	0.98	0.14	43,43,43,43	0
54	MG	2A	3624	1/1	0.98	0.11	59,59,59,59	0
54	MG	1A	3809	1/1	0.98	0.14	24,24,24,24	0
54	MG	1A	3958	1/1	0.98	0.11	37,37,37,37	0
54	MG	2A	3404	1/1	0.98	0.10	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	2A	3013	1/1	0.98	0.07	22,22,22,22	0
54	MG	1A	3078	1/1	0.98	0.05	32,32,32,32	0
54	MG	1a	1739	1/1	0.98	0.04	51,51,51,51	0
54	MG	2A	3632	1/1	0.98	0.07	50,50,50,50	0
54	MG	1A	3136	1/1	0.98	0.15	33,33,33,33	0
54	MG	2A	3636	1/1	0.98	0.06	43,43,43,43	0
54	MG	1A	3813	1/1	0.98	0.10	31,31,31,31	0
54	MG	11	101	1/1	0.98	0.05	37,37,37,37	0
54	MG	1A	3689	1/1	0.98	0.08	19,19,19,19	0
54	MG	1A	3691	1/1	0.98	0.07	70,70,70,70	0
54	MG	1A	3269	1/1	0.98	0.04	34,34,34,34	0
54	MG	15	101	1/1	0.98	0.11	21,21,21,21	0
54	MG	1A	3215	1/1	0.98	0.18	25,25,25,25	0
54	MG	1A	3048	1/1	0.98	0.22	26,26,26,26	0
54	MG	2A	3417	1/1	0.98	0.06	40,40,40,40	0
54	MG	1A	3695	1/1	0.98	0.08	44,44,44,44	0
54	MG	1A	3820	1/1	0.98	0.11	37,37,37,37	0
54	MG	2A	3210	1/1	0.98	0.08	36,36,36,36	0
54	MG	2A	3650	1/1	0.98	0.06	33,33,33,33	0
54	MG	1A	3821	1/1	0.98	0.16	34,34,34,34	0
54	MG	1A	3335	1/1	0.98	0.06	31,31,31,31	0
54	MG	15	108	1/1	0.98	0.04	38,38,38,38	0
54	MG	2A	3654	1/1	0.98	0.05	27,27,27,27	0
54	MG	1A	3589	1/1	0.98	0.06	13,13,13,13	0
54	MG	2A	3215	1/1	0.98	0.04	39,39,39,39	0
54	MG	2A	3657	1/1	0.98	0.05	56,56,56,56	0
54	MG	1A	3698	1/1	0.98	0.05	20,20,20,20	0
54	MG	1A	3590	1/1	0.98	0.04	18,18,18,18	0
54	MG	1A	3500	1/1	0.98	0.05	17,17,17,17	0
54	MG	2A	3429	1/1	0.98	0.08	52,52,52,52	0
54	MG	2A	3662	1/1	0.98	0.05	57,57,57,57	0
54	MG	2A	3663	1/1	0.98	0.06	38,38,38,38	0
54	MG	1A	3217	1/1	0.98	0.16	20,20,20,20	0
54	MG	1A	3080	1/1	0.98	0.18	12,12,12,12	0
54	MG	1A	3503	1/1	0.98	0.06	21,21,21,21	0
54	MG	2a	3081	1/1	0.98	0.18	34,34,34,34	0
54	MG	2A	3222	1/1	0.98	0.08	44,44,44,44	0
54	MG	1A	3081	1/1	0.98	0.07	29,29,29,29	0
54	MG	1A	3275	1/1	0.98	0.16	24,24,24,24	0
54	MG	1A	3141	1/1	0.98	0.07	29,29,29,29	0
54	MG	1A	3016	1/1	0.98	0.24	17,17,17,17	0
54	MG	1a	1602	1/1	0.98	0.07	55,55,55,55	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	1A	3085	1/1	0.98	0.12	30,30,30,30	0
54	MG	1A	3418	1/1	0.98	0.08	32,32,32,32	0
54	MG	1A	3113	1/1	0.98	0.17	30,30,30,30	0
54	MG	2A	3677	1/1	0.98	0.08	66,66,66,66	0
54	MG	1A	3225	1/1	0.98	0.06	32,32,32,32	0
54	MG	1A	3086	1/1	0.98	0.11	29,29,29,29	0
54	MG	1A	3840	1/1	0.98	0.09	41,41,41,41	0
54	MG	1A	3282	1/1	0.98	0.07	12,12,12,12	0
54	MG	1A	3146	1/1	0.98	0.05	28,28,28,28	0
54	MG	1A	3017	1/1	0.98	0.17	31,31,31,31	0
54	MG	2A	3684	1/1	0.98	0.04	35,35,35,35	0
54	MG	1A	3846	1/1	0.98	0.07	10,10,10,10	0
54	MG	1A	3230	1/1	0.98	0.13	36,36,36,36	0
54	MG	1B	204	1/1	0.98	0.06	41,41,41,41	0
54	MG	1A	3429	1/1	0.98	0.05	33,33,33,33	0
54	MG	1A	3430	1/1	0.98	0.04	37,37,37,37	0
54	MG	1A	3065	1/1	0.98	0.12	21,21,21,21	0
54	MG	1A	3613	1/1	0.98	0.06	36,36,36,36	0
54	MG	1A	3853	1/1	0.98	0.04	36,36,36,36	0
54	MG	1A	3003	1/1	0.98	0.04	20,20,20,20	0
54	MG	1A	3013	1/1	0.98	0.21	28,28,28,28	0
54	MG	1A	3068	1/1	0.98	0.30	22,22,22,22	0
54	MG	2A	3459	1/1	0.98	0.04	57,57,57,57	0
54	MG	1A	3523	1/1	0.98	0.09	39,39,39,39	0
54	MG	1A	3014	1/1	0.98	0.18	21,21,21,21	0
54	MG	1A	3291	1/1	0.98	0.13	13,13,13,13	0
54	MG	1A	3861	1/1	0.98	0.04	27,27,27,27	0
54	MG	2a	3115	1/1	0.98	0.08	47,47,47,47	0
54	MG	2A	3067	1/1	0.98	0.12	36,36,36,36	0
54	MG	1A	3153	1/1	0.98	0.21	28,28,28,28	0
54	MG	2A	3255	1/1	0.98	0.06	17,17,17,17	0
54	MG	1A	3729	1/1	0.98	0.11	42,42,42,42	0
54	MG	1A	3029	1/1	0.98	0.11	49,49,49,49	0
54	MG	2A	3071	1/1	0.98	0.15	30,30,30,30	0
54	MG	2A	3472	1/1	0.98	0.04	36,36,36,36	0
54	MG	1A	3731	1/1	0.98	0.07	26,26,26,26	0
54	MG	1A	3155	1/1	0.98	0.34	24,24,24,24	0
54	MG	1B	223	1/1	0.98	0.07	54,54,54,54	0
54	MG	2A	3712	1/1	0.98	0.05	37,37,37,37	0
54	MG	2a	3127	1/1	0.98	0.05	66,66,66,66	0
54	MG	2A	3263	1/1	0.98	0.05	52,52,52,52	0
54	MG	1A	3295	1/1	0.98	0.04	17,17,17,17	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	0.98	0.11	19,19,19,19	0
54	MG	2A	3077	1/1	0.98	0.07	42,42,42,42	0
54	MG	1A	3736	1/1	0.98	0.04	44,44,44,44	0
54	MG	1A	3445	1/1	0.98	0.06	30,30,30,30	0
54	MG	2A	3482	1/1	0.98	0.04	29,29,29,29	0
54	MG	1A	3739	1/1	0.98	0.04	29,29,29,29	0
54	MG	1A	3877	1/1	0.98	0.04	20,20,20,20	0
54	MG	1a	1804	1/1	0.98	0.04	53,53,53,53	0
54	MG	1A	3022	1/1	0.98	0.26	23,23,23,23	0
54	MG	1A	3533	1/1	0.98	0.04	25,25,25,25	0
54	MG	1A	3447	1/1	0.98	0.06	41,41,41,41	0
54	MG	2a	3141	1/1	0.98	0.07	51,51,51,51	0
54	MG	1A	3535	1/1	0.98	0.05	43,43,43,43	0
54	MG	1A	3882	1/1	0.98	0.05	11,11,11,11	0
54	MG	1A	3883	1/1	0.98	0.10	47,47,47,47	0
54	MG	1A	3298	1/1	0.98	0.04	17,17,17,17	0
54	MG	2a	3147	1/1	0.98	0.07	60,60,60,60	0
54	MG	1A	3005	1/1	0.98	0.04	23,23,23,23	0
54	MG	1A	3195	1/1	0.98	0.12	26,26,26,26	0
54	MG	1A	3301	1/1	0.98	0.08	44,44,44,44	0
54	MG	1a	1815	1/1	0.98	0.05	68,68,68,68	0
54	MG	2A	3734	1/1	0.98	0.05	28,28,28,28	0
54	MG	2A	3285	1/1	0.98	0.05	32,32,32,32	0
54	MG	2a	3155	1/1	0.98	0.07	30,30,30,30	0
54	MG	1A	3369	1/1	0.98	0.04	11,11,11,11	0
54	MG	1A	3127	1/1	0.98	0.09	25,25,25,25	0
54	MG	2a	3158	1/1	0.98	0.09	55,55,55,55	0
54	MG	2A	3289	1/1	0.98	0.05	41,41,41,41	0
54	MG	1A	3046	1/1	0.98	0.11	24,24,24,24	0
54	MG	1D	317	1/1	0.98	0.11	46,46,46,46	0
54	MG	1A	3751	1/1	0.98	0.09	34,34,34,34	0
54	MG	2A	3101	1/1	0.98	0.13	40,40,40,40	0
54	MG	1A	3752	1/1	0.98	0.06	31,31,31,31	0
54	MG	2A	3506	1/1	0.98	0.10	41,41,41,41	0
54	MG	1A	3894	1/1	0.98	0.04	41,41,41,41	0
54	MG	2a	3167	1/1	0.98	0.04	57,57,57,57	0
54	MG	2A	3104	1/1	0.98	0.04	46,46,46,46	0
54	MG	1A	3249	1/1	0.98	0.18	25,25,25,25	0
54	MG	2A	3106	1/1	0.98	0.04	20,20,20,20	0
54	MG	2A	3511	1/1	0.98	0.04	39,39,39,39	0
54	MG	2A	3299	1/1	0.98	0.12	35,35,35,35	0
54	MG	2a	3173	1/1	0.98	0.05	73,73,73,73	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	1A	3640	1/1	0.98	0.06	30,30,30,30	0
54	MG	1A	3897	1/1	0.98	0.10	45,45,45,45	0
54	MG	1A	3374	1/1	0.98	0.09	12,12,12,12	0
54	MG	2A	3303	1/1	0.98	0.04	37,37,37,37	0
54	MG	1F	301	1/1	0.98	0.17	26,26,26,26	0
54	MG	2a	3179	1/1	0.98	0.08	59,59,59,59	0
54	MG	1A	3459	1/1	0.98	0.05	21,21,21,21	0
54	MG	1A	3162	1/1	0.98	0.33	24,24,24,24	0
54	MG	2a	3182	1/1	0.98	0.04	50,50,50,50	0
54	MG	1A	3100	1/1	0.98	0.06	25,25,25,25	0
54	MG	2a	3184	1/1	0.98	0.08	48,48,48,48	0
54	MG	2A	3309	1/1	0.98	0.04	32,32,32,32	0
54	MG	1F	305	1/1	0.98	0.05	35,35,35,35	0
54	MG	2A	3523	1/1	0.98	0.04	34,34,34,34	0
54	MG	1a	1832	1/1	0.98	0.04	36,36,36,36	0
54	MG	1a	1665	1/1	0.98	0.09	51,51,51,51	0
54	MG	1A	3759	1/1	0.98	0.24	58,58,58,58	0
54	MG	1F	307	1/1	0.98	0.16	24,24,24,24	0
54	MG	1A	3379	1/1	0.98	0.05	15,15,15,15	0
54	MG	2E	303	1/1	0.98	0.04	43,43,43,43	0
54	MG	1A	3380	1/1	0.98	0.04	26,26,26,26	0
54	MG	1a	1838	1/1	0.98	0.05	49,49,49,49	0
54	MG	1A	3464	1/1	0.98	0.07	10,10,10,10	0
54	MG	2A	3320	1/1	0.98	0.07	20,20,20,20	0
54	MG	1A	3465	1/1	0.98	0.04	21,21,21,21	0
54	MG	1A	3101	1/1	0.98	0.10	20,20,20,20	0
54	MG	1A	3310	1/1	0.98	0.05	25,25,25,25	0
54	MG	2A	3325	1/1	0.98	0.05	25,25,25,25	0
54	MG	2F	305	1/1	0.98	0.08	43,43,43,43	0
54	MG	1A	3909	1/1	0.98	0.05	27,27,27,27	0
54	MG	1A	3910	1/1	0.98	0.06	46,46,46,46	0
54	MG	1A	3652	1/1	0.98	0.07	37,37,37,37	0
54	MG	1a	1847	1/1	0.98	0.07	34,34,34,34	0
54	MG	1A	3103	1/1	0.98	0.12	26,26,26,26	0
54	MG	2O	201	1/1	0.98	0.05	31,31,31,31	0
54	MG	1A	3654	1/1	0.98	0.05	32,32,32,32	0
54	MG	1A	3655	1/1	0.98	0.08	39,39,39,39	0
54	MG	1G	203	1/1	0.98	0.07	41,41,41,41	0
54	MG	2Q	201	1/1	0.98	0.09	45,45,45,45	0
54	MG	1A	3772	1/1	0.98	0.12	64,64,64,64	0
54	MG	2Q	203	1/1	0.98	0.06	45,45,45,45	0
58	ZN	2Y	202	1/1	0.98	0.05	95,95,95,95	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	1A	3916	1/1	0.98	0.12	16,16,16,16	0
54	MG	1A	3255	1/1	0.98	0.21	30,30,30,30	0
59	SF4	1d	306	8/8	0.98	0.04	57,63,70,75	0
59	SF4	2d	501	8/8	0.98	0.05	60,72,75,76	0
54	MG	2A	3667	1/1	0.99	0.05	30,30,30,30	0
54	MG	2A	3543	1/1	0.99	0.04	41,41,41,41	0
54	MG	2A	3544	1/1	0.99	0.04	43,43,43,43	0
54	MG	1A	3169	1/1	0.99	0.19	23,23,23,23	0
54	MG	1A	3420	1/1	0.99	0.03	12,12,12,12	0
54	MG	1A	3240	1/1	0.99	0.03	21,21,21,21	0
54	MG	1A	3874	1/1	0.99	0.03	24,24,24,24	0
54	MG	1A	3378	1/1	0.99	0.04	12,12,12,12	0
54	MG	1V	202	1/1	0.99	0.10	23,23,23,23	0
54	MG	2A	3324	1/1	0.99	0.08	23,23,23,23	0
54	MG	1D	305	1/1	0.99	0.03	24,24,24,24	0
54	MG	1A	3082	1/1	0.99	0.06	20,20,20,20	0
54	MG	1A	3083	1/1	0.99	0.13	12,12,12,12	0
54	MG	2A	3028	1/1	0.99	0.06	25,25,25,25	0
54	MG	1A	3806	1/1	0.99	0.04	18,18,18,18	0
54	MG	1D	309	1/1	0.99	0.04	15,15,15,15	0
54	MG	1A	3476	1/1	0.99	0.05	41,41,41,41	0
54	MG	1X	101	1/1	0.99	0.05	20,20,20,20	0
54	MG	2A	3685	1/1	0.99	0.14	34,34,34,34	0
54	MG	1A	3339	1/1	0.99	0.04	9,9,9,9	0
54	MG	1A	3687	1/1	0.99	0.03	12,12,12,12	0
54	MG	1A	3631	1/1	0.99	0.03	35,35,35,35	0
54	MG	1A	3340	1/1	0.99	0.03	29,29,29,29	0
54	MG	1A	3885	1/1	0.99	0.08	40,40,40,40	0
54	MG	1A	3690	1/1	0.99	0.04	35,35,35,35	0
54	MG	1a	1840	1/1	0.99	0.04	55,55,55,55	0
54	MG	10	104	1/1	0.99	0.04	32,32,32,32	0
54	MG	1A	3428	1/1	0.99	0.04	15,15,15,15	0
54	MG	1A	3243	1/1	0.99	0.09	36,36,36,36	0
54	MG	2A	3237	1/1	0.99	0.12	41,41,41,41	0
54	MG	1A	3007	1/1	0.99	0.08	18,18,18,18	0
54	MG	1A	3099	1/1	0.99	0.11	23,23,23,23	0
54	MG	1E	303	1/1	0.99	0.06	37,37,37,37	0
54	MG	2A	3348	1/1	0.99	0.03	28,28,28,28	0
54	MG	2A	3349	1/1	0.99	0.05	27,27,27,27	0
54	MG	1A	3040	1/1	0.99	0.08	7,7,7,7	0
54	MG	13	101	1/1	0.99	0.14	24,24,24,24	0
54	MG	1A	3307	1/1	0.99	0.12	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	3308	1/1	0.99	0.06	11,11,11,11	0
54	MG	2A	3465	1/1	0.99	0.06	26,26,26,26	0
54	MG	2A	3146	1/1	0.99	0.06	50,50,50,50	0
54	MG	1A	3011	1/1	0.99	0.04	22,22,22,22	0
54	MG	1E	308	1/1	0.99	0.06	45,45,45,45	0
54	MG	1A	3102	1/1	0.99	0.06	19,19,19,19	0
54	MG	1A	3042	1/1	0.99	0.03	19,19,19,19	0
54	MG	2A	3588	1/1	0.99	0.04	38,38,38,38	0
54	MG	2A	3471	1/1	0.99	0.03	33,33,33,33	0
54	MG	1A	3392	1/1	0.99	0.03	17,17,17,17	0
54	MG	2A	3360	1/1	0.99	0.08	37,37,37,37	0
54	MG	1A	3312	1/1	0.99	0.04	23,23,23,23	0
54	MG	1A	3441	1/1	0.99	0.05	30,30,30,30	0
54	MG	2a	3146	1/1	0.99	0.09	54,54,54,54	0
54	MG	1A	3542	1/1	0.99	0.04	28,28,28,28	0
54	MG	1A	3828	1/1	0.99	0.09	41,41,41,41	0
54	MG	1A	3222	1/1	0.99	0.19	30,30,30,30	0
54	MG	1A	3975	1/1	0.99	0.04	21,21,21,21	0
54	MG	2A	3257	1/1	0.99	0.06	20,20,20,20	0
54	MG	17	103	1/1	0.99	0.16	48,48,48,48	0
54	MG	2A	3159	1/1	0.99	0.10	37,37,37,37	0
54	MG	1A	3088	1/1	0.99	0.32	21,21,21,21	0
54	MG	1A	3444	1/1	0.99	0.05	19,19,19,19	0
54	MG	1A	3139	1/1	0.99	0.10	21,21,21,21	0
54	MG	1A	3769	1/1	0.99	0.05	31,31,31,31	0
54	MG	1A	3597	1/1	0.99	0.04	17,17,17,17	0
54	MG	1A	3771	1/1	0.99	0.10	44,44,44,44	0
54	MG	1A	3043	1/1	0.99	0.23	29,29,29,29	0
54	MG	1A	3254	1/1	0.99	0.04	19,19,19,19	0
54	MG	1A	3318	1/1	0.99	0.04	24,24,24,24	0
54	MG	1A	3226	1/1	0.99	0.19	27,27,27,27	0
54	MG	1A	3160	1/1	0.99	0.09	27,27,27,27	0
54	MG	1A	3203	1/1	0.99	0.11	30,30,30,30	0
54	MG	1A	3122	1/1	0.99	0.08	17,17,17,17	0
54	MG	1a	1783	1/1	0.99	0.06	52,52,52,52	0
54	MG	2A	3274	1/1	0.99	0.04	59,59,59,59	0
54	MG	1A	3717	1/1	0.99	0.03	26,26,26,26	0
54	MG	1A	3660	1/1	0.99	0.06	32,32,32,32	0
54	MG	1a	1786	1/1	0.99	0.04	55,55,55,55	0
54	MG	1A	3123	1/1	0.99	0.04	24,24,24,24	0
54	MG	1A	3848	1/1	0.99	0.03	36,36,36,36	0
54	MG	2A	3622	1/1	0.99	0.04	56,56,56,56	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	2A	3280	1/1	0.99	0.07	37,37,37,37	0
54	MG	1A	3044	1/1	0.99	0.12	24,24,24,24	0
54	MG	1O	201	1/1	0.99	0.03	28,28,28,28	0
54	MG	2A	3626	1/1	0.99	0.03	47,47,47,47	0
54	MG	1A	3456	1/1	0.99	0.05	27,27,27,27	0
54	MG	1A	3325	1/1	0.99	0.04	37,37,37,37	0
54	MG	1A	3020	1/1	0.99	0.14	12,12,12,12	0
54	MG	1A	3036	1/1	0.99	0.11	22,22,22,22	0
54	MG	2A	3287	1/1	0.99	0.04	34,34,34,34	0
54	MG	2A	3399	1/1	0.99	0.03	40,40,40,40	0
54	MG	2A	3633	1/1	0.99	0.02	27,27,27,27	0
54	MG	1A	3611	1/1	0.99	0.05	41,41,41,41	0
54	MG	1A	3366	1/1	0.99	0.05	25,25,25,25	0
54	MG	2A	3089	1/1	0.99	0.06	27,27,27,27	0
54	MG	1A	3002	1/1	0.99	0.07	16,16,16,16	0
54	MG	2A	3639	1/1	0.99	0.03	41,41,41,41	0
54	MG	1A	3058	1/1	0.99	0.05	26,26,26,26	0
54	MG	1Q	203	1/1	0.99	0.11	38,38,38,38	0
54	MG	1A	3671	1/1	0.99	0.04	36,36,36,36	0
54	MG	1B	213	1/1	0.99	0.09	51,51,51,51	0
54	MG	1a	1710	1/1	0.99	0.04	32,32,32,32	0
54	MG	1a	1711	1/1	0.99	0.06	33,33,33,33	0
54	MG	1A	3330	1/1	0.99	0.04	13,13,13,13	0
54	MG	1A	3931	1/1	0.99	0.06	52,52,52,52	0
54	MG	2E	306	1/1	0.99	0.06	55,55,55,55	0
54	MG	1A	3004	1/1	0.99	0.06	17,17,17,17	0
54	MG	2A	3100	1/1	0.99	0.08	36,36,36,36	0
54	MG	1A	3862	1/1	0.99	0.04	26,26,26,26	0
54	MG	2A	3527	1/1	0.99	0.06	39,39,39,39	0
54	MG	1A	3266	1/1	0.99	0.23	25,25,25,25	0
54	MG	1A	3237	1/1	0.99	0.07	30,30,30,30	0
54	MG	1A	3865	1/1	0.99	0.03	17,17,17,17	0
54	MG	1A	3866	1/1	0.99	0.05	29,29,29,29	0
54	MG	1A	3373	1/1	0.99	0.04	31,31,31,31	0
54	MG	2A	3308	1/1	0.99	0.05	39,39,39,39	0
54	MG	1A	3939	1/1	0.99	0.07	10,10,10,10	0
54	MG	1a	1722	1/1	0.99	0.04	26,26,26,26	0
54	MG	1B	224	1/1	0.99	0.03	32,32,32,32	0
54	MG	1a	1724	1/1	0.99	0.03	31,31,31,31	0
58	ZN	15	110	1/1	0.99	0.03	49,49,49,49	0
58	ZN	1n	102	1/1	0.99	0.03	74,74,74,74	0
54	MG	1A	3940	1/1	0.99	0.04	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	2A	3314	1/1	0.99	0.08	24,24,24,24	0
58	ZN	25	104	1/1	0.99	0.03	86,86,86,86	0
58	ZN	29	501	1/1	0.99	0.03	60,60,60,60	0
54	MG	1A	3238	1/1	0.99	0.06	30,30,30,30	0
54	MG	1A	3375	1/1	0.99	0.10	10,10,10,10	0
54	MG	1A	3738	1/1	0.99	0.03	26,26,26,26	0
54	MG	1A	3205	1/1	1.00	0.04	28,28,28,28	0
54	MG	1A	3433	1/1	1.00	0.03	43,43,43,43	0
54	MG	1A	3842	1/1	1.00	0.03	25,25,25,25	0
54	MG	1A	3734	1/1	1.00	0.02	20,20,20,20	0
54	MG	2A	3391	1/1	1.00	0.03	20,20,20,20	0
54	MG	1A	3844	1/1	1.00	0.02	22,22,22,22	0
54	MG	1A	3427	1/1	1.00	0.04	14,14,14,14	0
54	MG	1A	3651	1/1	1.00	0.03	11,11,11,11	0
54	MG	2a	3152	1/1	1.00	0.04	50,50,50,50	0
54	MG	1A	3486	1/1	1.00	0.03	9,9,9,9	0
54	MG	1A	3622	1/1	1.00	0.11	33,33,33,33	0
54	MG	2A	3577	1/1	1.00	0.05	28,28,28,28	0
58	ZN	16	501	1/1	1.00	0.05	38,38,38,38	0
58	ZN	19	103	1/1	1.00	0.02	43,43,43,43	0
54	MG	1A	3860	1/1	1.00	0.03	18,18,18,18	0
54	MG	1A	3811	1/1	1.00	0.02	14,14,14,14	0
54	MG	2A	3597	1/1	1.00	0.04	33,33,33,33	0
54	MG	2A	3634	1/1	1.00	0.03	31,31,31,31	0
58	ZN	26	102	1/1	1.00	0.02	49,49,49,49	0
54	MG	1A	3450	1/1	1.00	0.03	33,33,33,33	0
54	MG	1A	3875	1/1	1.00	0.03	44,44,44,44	0
54	MG	2A	3344	1/1	1.00	0.03	22,22,22,22	0
54	MG	2A	3583	1/1	1.00	0.06	29,29,29,29	0

5.5 Other polymers ⓘ

There are no such residues in this entry.