



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 17, 2026 – 03:44 PM UTC

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

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity	: FAILED
Mogul	: 2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	: 2.0
EDS	: 3.0
buster-report	: 1.1.7 (2018)
Percentile statistics	: 20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	: 9.0.010 (Gargrove)
Density-Fitness	: 1.0.12
Ideal geometry (proteins)	: Engh & Huber (2001)

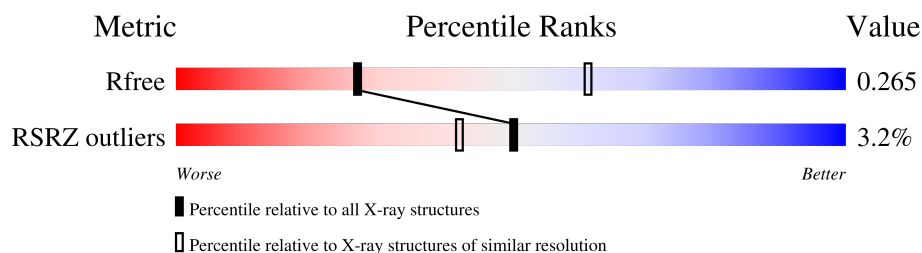
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	164625	3657 (2.80-2.80)
RSRZ outliers	164620	3659 (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	1P	203	-	-	-	X
54	MG	2A	3730	-	-	-	X
54	MG	2a	3129	-	-	-	X

Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.48.1

2 Entry composition [i](#)

There are 60 unique types of molecules in this entry. The entry contains 298171 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a RNA chain called 23S Ribosomal RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	1A	2872	Total	C	N	O	P	0	0	0
			61869	27540	11574	19884	2871			
1	2A	2867	Total	C	N	O	P	0	0	0
			61758	27491	11552	19850	2865			

- Molecule 2 is a RNA chain called 5S Ribosomal RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	1B	120	Total	C	N	O	P	0	0	0
			2572	1145	476	832	119			
2	2B	120	Total	C	N	O	P	0	0	0
			2573	1146	476	832	119			

- Molecule 3 is a protein called 50S ribosomal protein L2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	1D	275	Total	C	N	O	S	0	0	0
			2131	1346	422	360	3			
3	2D	275	Total	C	N	O	S	0	0	0
			2136	1349	423	361	3			

- Molecule 4 is a protein called 50S ribosomal protein L3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	1E	204	Total	C	N	O	S	0	0	0
			1559	985	298	270	6			
4	2E	204	Total	C	N	O	S	0	0	0
			1559	985	298	270	6			

- Molecule 5 is a protein called 50S ribosomal protein L4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	1F	203	Total	C	N	O	S	0	0	1
			1584	1009	298	275	2			
5	2F	203	Total	C	N	O	S	0	0	1
			1580	1007	297	274	2			

- Molecule 6 is a protein called 50S ribosomal protein L5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	1G	181	Total	C	N	O	S	0	0	0
			1426	916	253	253	4			
6	2G	181	Total	C	N	O	S	0	0	0
			1424	912	259	249	4			

- Molecule 7 is a protein called 50S ribosomal protein L6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	1H	174	Total	C	N	O	S	0	0	0
			1330	845	248	236	1			
7	2H	173	Total	C	N	O	S	0	0	0
			1324	842	247	234	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	1I	147	Total	C	N	O	S	0	0	0
			1094	699	191	203	1			
8	2I	146	Total	C	N	O	S	0	0	0
			1076	687	186	202	1			

- Molecule 9 is a protein called 50S ribosomal protein L13.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	1N	140	Total	C	N	O	S	0	0	0
			1121	722	208	187	4			
9	2N	140	Total	C	N	O	S	0	0	0
			1117	719	207	187	4			

- Molecule 10 is a protein called 50S ribosomal protein L14.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	1O	122	Total	C	N	O	S	0	0	0
			933	588	171	170	4			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	2O	122	Total	C	N	O	S	0	0	0
			933	588	171	170	4			

- Molecule 11 is a protein called 50S ribosomal protein L15.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	1P	149	Total	C	N	O	S	0	0	0
			1135	706	230	196	3			
11	2P	149	Total	C	N	O	S	0	0	0
			1135	706	230	196	3			

- Molecule 12 is a protein called 50S ribosomal protein L16.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	1Q	141	Total	C	N	O	S	0	0	0
			1122	715	212	188	7			
12	2Q	141	Total	C	N	O	S	0	0	0
			1122	715	212	188	7			

- Molecule 13 is a protein called 50S ribosomal protein L17.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	1R	118	Total	C	N	O	S	0	0	0
			968	604	203	160	1			
13	2R	118	Total	C	N	O	S	0	0	0
			968	604	203	160	1			

- Molecule 14 is a protein called 50S ribosomal protein L18.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
14	1S	110	Total	C	N	O	0	0	0
			877	553	175	149			
14	2S	110	Total	C	N	O	0	0	0
			870	549	173	148			

- Molecule 15 is a protein called 50S ribosomal protein L19.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
15	1T	131	Total	C	N	O	S	0	0	0
			1091	680	225	185	1			
15	2T	131	Total	C	N	O	S	0	0	0
			1083	675	224	183	1			

- Molecule 16 is a protein called 50S ribosomal protein L20.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
16	1U	116	Total	C	N	O	S	0	0	0
			959	608	201	149	1			
16	2U	116	Total	C	N	O	S	0	0	0
			959	608	201	149	1			

- Molecule 17 is a protein called 50S ribosomal protein L21.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
17	1V	101	Total	C	N	O	S	0	0	0
			775	498	141	135	1			
17	2V	101	Total	C	N	O	S	0	0	0
			771	495	140	135	1			

- Molecule 18 is a protein called 50S ribosomal protein L22.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
18	1W	112	Total	C	N	O	S	0	0	0
			886	557	174	153	2			
18	2W	112	Total	C	N	O	S	0	0	0
			886	557	174	153	2			

- Molecule 19 is a protein called 50S ribosomal protein L23.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
19	1X	95	Total	C	N	O	S	0	0	0
			750	488	135	126	1			
19	2X	95	Total	C	N	O	S	0	0	0
			750	488	135	126	1			

- Molecule 20 is a protein called 50S ribosomal protein L24.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
20	1Y	107	Total	C	N	O	S	0	0	0
			810	520	153	131	6			
20	2Y	107	Total	C	N	O	S	0	0	0
			810	519	153	132	6			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
21	1Z	203	Total	C	N	O	S	0	0	0
			1587	1011	282	292	2			
21	2Z	201	Total	C	N	O	S	0	0	0
			1557	995	274	286	2			

- Molecule 22 is a protein called 50S ribosomal protein L27.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
22	10	77	Total	C	N	O	S	0	0	0
			608	375	129	103	1			
22	20	77	Total	C	N	O	S	0	0	0
			608	375	129	103	1			

- Molecule 23 is a protein called 50S ribosomal protein L28.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
23	11	97	Total	C	N	O	S	0	0	0
			754	475	148	130	1			
23	21	97	Total	C	N	O	S	0	0	0
			759	478	149	131	1			

- Molecule 24 is a protein called 50S ribosomal protein L29.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
24	12	70	Total	C	N	O	S	0	0	0
			588	365	118	103	2			
24	22	70	Total	C	N	O	S	0	0	0
			592	368	119	103	2			

- Molecule 25 is a protein called 50S ribosomal protein L30.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
25	13	59	Total	C	N	O	0	0	0
			469	298	90	81			
25	23	59	Total	C	N	O	0	0	0
			464	296	90	78			

- Molecule 26 is a protein called 50S ribosomal protein L31.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
26	14	69	Total	C	N	O	S	0	0	0
			546	346	96	99	5			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
26	24	69	Total	C	N	O	S	0	0	0
			536	342	98	91	5			

- Molecule 27 is a protein called 50S ribosomal protein L32.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
27	15	59	Total	C	N	O	S	0	0	0
			459	288	90	76	5			
27	25	59	Total	C	N	O	S	0	0	0
			455	285	89	76	5			

- Molecule 28 is a protein called 50S ribosomal protein L33.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
28	16	53	Total	C	N	O	S	0	0	0
			453	281	91	77	4			
28	26	53	Total	C	N	O	S	0	0	0
			449	279	91	75	4			

- Molecule 29 is a protein called 50S ribosomal protein L34.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
29	17	48	Total	C	N	O	S	0	0	0
			418	257	104	55	2			
29	27	48	Total	C	N	O	S	0	0	0
			418	257	104	55	2			

- Molecule 30 is a protein called 50S ribosomal protein L35.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
30	18	64	Total	C	N	O	S	0	0	0
			517	331	102	82	2			
30	28	64	Total	C	N	O	S	0	0	0
			517	331	102	82	2			

- Molecule 31 is a protein called 50S ribosomal protein L36.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
31	19	37	Total	C	N	O	S	0	0	0
			307	188	68	47	4			
31	29	37	Total	C	N	O	S	0	0	0
			307	188	68	47	4			

- Molecule 32 is a RNA chain called 16S Ribosomal RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
32	1a	1500	Total	C	N	O	P	0	0	0
			32246	14358	5975	10413	1500			
32	2a	1504	Total	C	N	O	P	0	0	0
			32331	14396	5990	10441	1504			

- Molecule 33 is a protein called 30S ribosomal protein S2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
33	1b	231	Total	C	N	O	S	0	0	0
			1842	1175	330	332	5			
33	2b	231	Total	C	N	O	S	0	0	0
			1825	1167	326	327	5			

- Molecule 34 is a protein called 30S ribosomal protein S3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
34	1c	206	Total	C	N	O	S	0	0	0
			1558	979	305	273	1			
34	2c	206	Total	C	N	O	S	0	0	0
			1542	968	300	273	1			

- Molecule 35 is a protein called 30S ribosomal protein S4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
35	1d	208	Total	C	N	O	S	0	0	0
			1665	1043	329	286	7			
35	2d	208	Total	C	N	O	S	0	0	0
			1668	1047	330	284	7			

- Molecule 36 is a protein called 30S ribosomal protein S5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
36	1e	148	Total	C	N	O	S	0	0	0
			1133	716	214	199	4			
36	2e	148	Total	C	N	O	S	0	0	0
			1133	716	214	199	4			

- Molecule 37 is a protein called 30S ribosomal protein S6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
37	1f	100	Total	C	N	O	S	0	0	0
			814	516	144	151	3			
37	2f	100	Total	C	N	O	S	0	0	0
			816	516	146	151	3			

- Molecule 38 is a protein called 30S ribosomal protein S7.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
38	1g	155	Total	C	N	O	S	0	0	0
			1235	769	244	216	6			
38	2g	155	Total	C	N	O	S	0	0	0
			1229	766	241	216	6			

- Molecule 39 is a protein called 30S ribosomal protein S8.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
39	1h	137	Total	C	N	O	S	0	0	0
			1098	694	210	192	2			
39	2h	137	Total	C	N	O	S	0	0	0
			1088	689	206	191	2			

- Molecule 40 is a protein called 30S ribosomal protein S9.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
40	1i	127	Total	C	N	O	0	0	0
			986	625	193	168			
40	2i	126	Total	C	N	O	0	0	0
			966	613	186	167			

- Molecule 41 is a protein called 30S ribosomal protein S10.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
41	1j	97	Total	C	N	O	0	0	0
			719	446	142	131			
41	2j	96	Total	C	N	O	0	0	0
			710	442	137	131			

- Molecule 42 is a protein called 30S ribosomal protein S11.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
42	1k	114	Total	C	N	O	S	0	0	0
			834	520	156	155	3			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
42	2k	114	Total	C	N	O	S	0	0	0
			833	519	156	155	3			

- Molecule 43 is a protein called 30S ribosomal protein S12.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
43	1l	122	Total	C	N	O	S	0	0	0
			932	586	185	159	2			
43	2l	122	Total	C	N	O	S	0	0	0
			932	586	185	159	2			

- Molecule 44 is a protein called 30S ribosomal protein S13.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
44	1m	116	Total	C	N	O	S	0	0	0
			914	564	189	159	2			
44	2m	114	Total	C	N	O	S	0	0	0
			895	550	186	157	2			

- Molecule 45 is a protein called 30S ribosomal protein S14 type Z.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
45	1n	60	Total	C	N	O	S	0	0	0
			492	312	104	72	4			
45	2n	60	Total	C	N	O	S	0	0	0
			492	312	104	72	4			

- Molecule 46 is a protein called 30S ribosomal protein S15.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
46	1o	88	Total	C	N	O	S	0	0	0
			728	456	144	126	2			
46	2o	88	Total	C	N	O	S	0	0	0
			728	456	144	126	2			

- Molecule 47 is a protein called 30S ribosomal protein S16.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
47	1p	82	Total	C	N	O	S	0	0	0
			681	433	134	113	1			
47	2p	82	Total	C	N	O	S	0	0	0
			677	430	133	113	1			

- Molecule 48 is a protein called 30S ribosomal protein S17.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
48	1q	99	Total	C	N	O	S	0	0	0
			823	528	151	142	2			
48	2q	99	Total	C	N	O	S	0	0	0
			823	528	151	142	2			

- Molecule 49 is a protein called 30S ribosomal protein S18.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
49	1r	68	Total	C	N	O		0	0	0
			555	355	108	92				
49	2r	68	Total	C	N	O		0	0	0
			555	355	108	92				

- Molecule 50 is a protein called 30S ribosomal protein S19.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
50	1s	83	Total	C	N	O	S	0	0	0
			648	415	120	111	2			
50	2s	83	Total	C	N	O	S	0	0	0
			645	410	118	115	2			

- Molecule 51 is a protein called 30S ribosomal protein S20.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
51	1t	96	Total	C	N	O	S	0	0	0
			732	449	157	124	2			
51	2t	98	Total	C	N	O	S	0	0	0
			733	451	154	126	2			

- Molecule 52 is a protein called 30S ribosomal protein Thx.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
52	1u	23	Total	C	N	O	0	0	0
			199	122	48	29			
52	2u	23	Total	C	N	O	0	0	0
			199	122	48	29			

- Molecule 53 is a protein called Ribosome-associated inhibitor A.

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

- Molecule 54 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
54	1A	1054	Total	Mg	0	0
			1054	1054		
54	1B	27	Total	Mg	0	0
			27	27		
54	1D	17	Total	Mg	0	0
			17	17		
54	1E	6	Total	Mg	0	0
			6	6		
54	1F	15	Total	Mg	0	0
			15	15		
54	1G	4	Total	Mg	0	0
			4	4		
54	1H	2	Total	Mg	0	0
			2	2		
54	1N	4	Total	Mg	0	0
			4	4		
54	1O	1	Total	Mg	0	0
			1	1		
54	1P	5	Total	Mg	0	0
			5	5		
54	1Q	5	Total	Mg	0	0
			5	5		
54	1R	6	Total	Mg	0	0
			6	6		
54	1S	1	Total	Mg	0	0
			1	1		
54	1T	6	Total	Mg	0	0
			6	6		
54	1U	8	Total	Mg	0	0
			8	8		
54	1V	5	Total	Mg	0	0
			5	5		
54	1W	4	Total	Mg	0	0
			4	4		
54	1Z	1	Total	Mg	0	0
			1	1		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
54	10	7	Total 7	Mg 7	0	0
54	11	5	Total 5	Mg 5	0	0
54	13	5	Total 5	Mg 5	0	0
54	14	1	Total 1	Mg 1	0	0
54	15	7	Total 7	Mg 7	0	0
54	16	1	Total 1	Mg 1	0	0
54	17	4	Total 4	Mg 4	0	0
54	18	1	Total 1	Mg 1	0	0
54	19	3	Total 3	Mg 3	0	0
54	1a	279	Total 279	Mg 279	0	0
54	1b	1	Total 1	Mg 1	0	0
54	1d	5	Total 5	Mg 5	0	0
54	1e	2	Total 2	Mg 2	0	0
54	1f	2	Total 2	Mg 2	0	0
54	1g	3	Total 3	Mg 3	0	0
54	1h	2	Total 2	Mg 2	0	0
54	1i	1	Total 1	Mg 1	0	0
54	1k	1	Total 1	Mg 1	0	0
54	1l	2	Total 2	Mg 2	0	0
54	1m	1	Total 1	Mg 1	0	0
54	1n	3	Total 3	Mg 3	0	0

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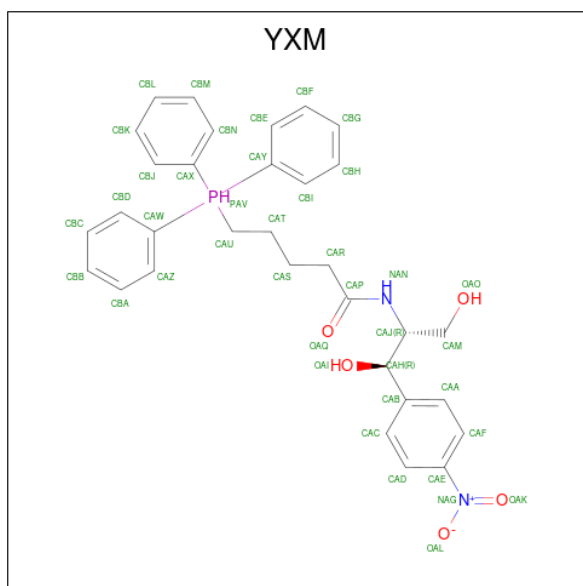
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
54	1o	2	Total 2	Mg 2	0	0
54	1t	1	Total 1	Mg 1	0	0
54	1y	4	Total 4	Mg 4	0	0
54	2A	757	Total 757	Mg 757	0	0
54	2B	19	Total 19	Mg 19	0	0
54	2D	12	Total 12	Mg 12	0	0
54	2E	6	Total 6	Mg 6	0	0
54	2F	3	Total 3	Mg 3	0	0
54	2G	3	Total 3	Mg 3	0	0
54	2I	1	Total 1	Mg 1	0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

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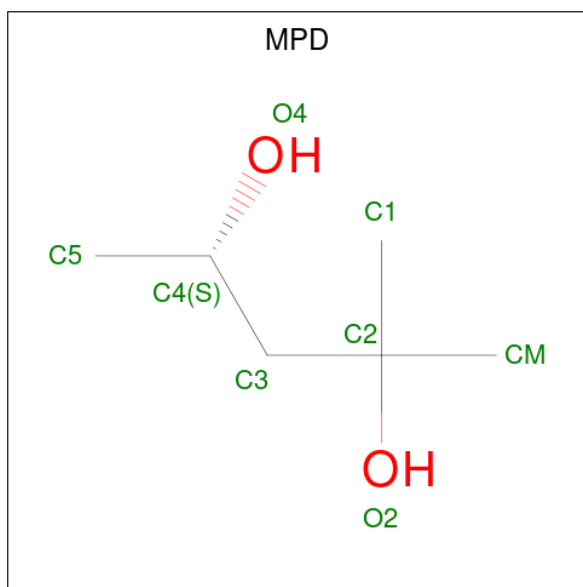
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
54	21	2	Total Mg 2 2	0	0
54	23	2	Total Mg 2 2	0	0
54	25	1	Total Mg 1 1	0	0
54	27	2	Total Mg 2 2	0	0
54	28	2	Total Mg 2 2	0	0
54	2a	200	Total Mg 200 200	0	0
54	2e	2	Total Mg 2 2	0	0
54	2f	1	Total Mg 1 1	0	0
54	2j	1	Total Mg 1 1	0	0
54	2n	1	Total Mg 1 1	0	0
54	2t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

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



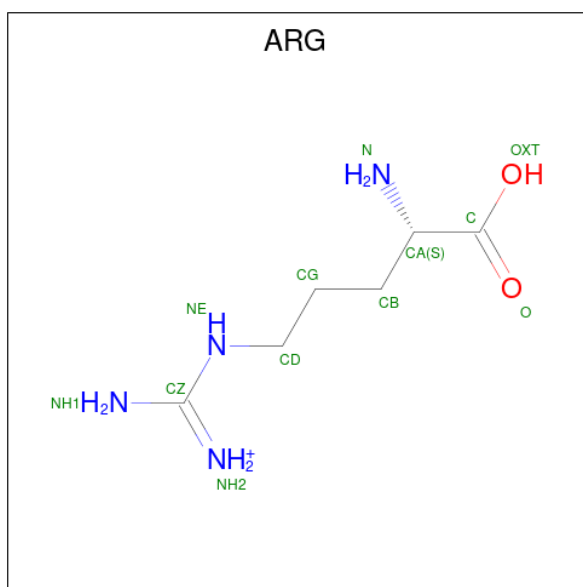
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
55	1A	1	Total	C	N	O	P	0	0
			40	32	2	5	1		
55	2A	1	Total	C	N	O	P	0	0
			40	32	2	5	1		

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



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

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



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

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

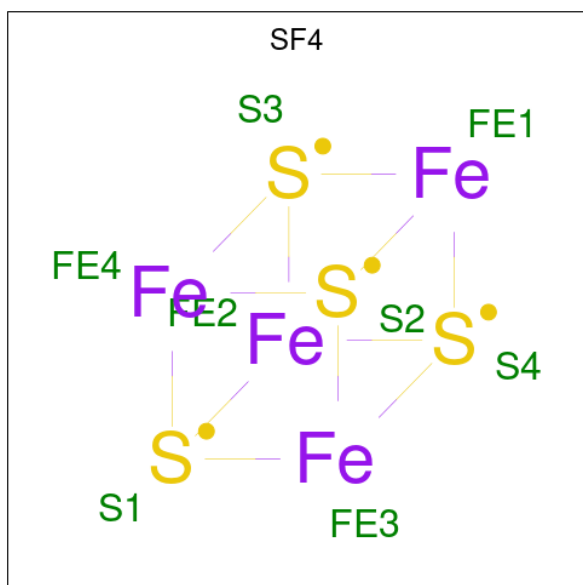
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
58	1Y	1	Total	Zn	0	0
			1	1		
58	14	1	Total	Zn	0	0
			1	1		
58	15	1	Total	Zn	0	0
			1	1		
58	16	1	Total	Zn	0	0
			1	1		
58	19	1	Total	Zn	0	0
			1	1		
58	1n	1	Total	Zn	0	0
			1	1		
58	2Y	1	Total	Zn	0	0
			1	1		
58	24	1	Total	Zn	0	0
			1	1		
58	25	1	Total	Zn	0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

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

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



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

- Molecule 60 is water.

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

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

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

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

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

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

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

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.78% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

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	$\# Z > 2$
1	5MU	2A	1915	1	19,22,23	1.41	5 (26%)	27,32,35	2.20	9 (33%)
1	5MC	1A	1942	1	19,22,23	1.53	3 (15%)	26,32,35	1.13	3 (11%)
32	5MC	1a	1407	32	19,22,23	1.75	3 (15%)	26,32,35	1.18	4 (15%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	5MC	2A	1942	1	19,22,23	1.66	3 (15%)	26,32,35	1.18	2 (7%)
1	PSU	2A	2605	1	18,21,22	1.37	3 (16%)	21,30,33	1.89	4 (19%)
32	MA6	1a	1519	32	19,26,27	1.04	2 (10%)	18,38,41	1.83	3 (16%)
32	5MC	1a	967	32	19,22,23	1.60	3 (15%)	26,32,35	1.06	2 (7%)
43	0TD	1l	92	43	8,9,10	4.58	1 (12%)	6,11,13	3.84	3 (50%)
1	4OC	2A	1920	1	19,22,24	0.80	0	25,31,35	0.95	1 (4%)
32	5MC	1a	1404	32	19,22,23	1.62	3 (15%)	26,32,35	1.09	2 (7%)
32	7MG	2a	527	54,32	23,26,27	1.34	3 (13%)	27,39,42	2.58	7 (25%)
1	PSU	1A	1917	54,1	18,21,22	1.38	2 (11%)	21,30,33	1.94	3 (14%)
1	5MU	1A	1939	1	19,22,23	1.44	6 (31%)	27,32,35	2.12	6 (22%)
32	UR3	1a	1498	32	19,22,23	0.97	1 (5%)	26,32,35	1.73	3 (11%)
32	MA6	2a	1519	32	19,26,27	1.03	2 (10%)	18,38,41	1.96	3 (16%)
32	PSU	1a	516	54,32	18,21,22	1.40	2 (11%)	21,30,33	2.00	4 (19%)
1	5MC	2A	1962	54,1	19,22,23	1.55	3 (15%)	26,32,35	1.10	2 (7%)
1	5MC	1A	1962	54,1	19,22,23	1.73	3 (15%)	26,32,35	1.16	3 (11%)
32	5MC	2a	1400	32	19,22,23	1.60	3 (15%)	26,32,35	1.16	2 (7%)
43	0TD	2l	92	43	8,9,10	4.46	1 (12%)	6,11,13	4.98	3 (50%)
32	5MC	2a	1407	32	19,22,23	1.66	3 (15%)	26,32,35	1.13	3 (11%)
1	4OC	1A	1920	1	19,22,24	0.79	0	25,31,35	0.88	1 (4%)
1	5MU	2A	1939	1	19,22,23	1.46	6 (31%)	27,32,35	2.17	6 (22%)
32	M2G	1a	966	32	20,27,28	1.29	3 (15%)	19,40,43	1.08	2 (10%)
1	PSU	1A	1911	1	18,21,22	1.36	2 (11%)	21,30,33	2.06	4 (19%)
32	2MG	1a	1207	32	18,26,27	0.93	1 (5%)	16,38,41	1.61	4 (25%)
32	UR3	2a	1498	32	19,22,23	0.99	2 (10%)	26,32,35	1.68	2 (7%)
32	MA6	1a	1518	32	19,26,27	1.02	2 (10%)	18,38,41	1.93	3 (16%)
32	5MC	2a	1404	32	19,22,23	1.69	3 (15%)	26,32,35	1.13	2 (7%)
1	2MA	1A	2503	54,1	18,25,26	0.71	0	20,37,40	1.96	4 (20%)
1	OMG	1A	2251	54,1	19,26,27	0.90	1 (5%)	21,38,41	1.12	2 (9%)
32	4OC	1a	1402	32	20,23,24	0.74	0	25,32,35	0.92	1 (4%)
1	PSU	2A	1911	1	18,21,22	1.36	2 (11%)	21,30,33	1.98	3 (14%)
1	OMG	2A	2251	54,1	19,26,27	0.88	1 (5%)	21,38,41	1.03	2 (9%)
1	PSU	2A	1917	1	18,21,22	1.34	2 (11%)	21,30,33	2.02	3 (14%)
1	2MU	1A	2552	54,1	19,22,24	1.28	3 (15%)	25,31,36	1.86	6 (24%)
32	5MC	1a	1400	32	19,22,23	1.69	3 (15%)	26,32,35	1.12	2 (7%)
32	5MC	2a	967	32	19,22,23	1.69	3 (15%)	26,32,35	1.07	2 (7%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	5MU	1A	1915	54,1	19,22,23	1.44	5 (26%)	27,32,35	2.19	8 (29%)
1	2MU	2A	2552	54,1	19,22,24	1.26	3 (15%)	25,31,36	1.93	6 (24%)
1	2MA	2A	2503	54,1	18,25,26	0.72	0	20,37,40	1.81	4 (20%)
32	M2G	2a	966	54,32	20,27,28	1.37	3 (15%)	19,40,43	0.98	1 (5%)
32	7MG	1a	527	54,32	23,26,27	1.35	3 (13%)	27,39,42	2.56	7 (25%)
1	PSU	1A	2605	54,1	18,21,22	1.35	3 (16%)	21,30,33	2.01	5 (23%)
32	MA6	2a	1518	32	19,26,27	1.01	2 (10%)	18,38,41	1.94	3 (16%)
32	PSU	2a	516	54,32	18,21,22	1.37	2 (11%)	21,30,33	2.03	5 (23%)
32	4OC	2a	1402	32	20,23,24	0.77	0	25,32,35	0.94	1 (4%)
32	2MG	2a	1207	32	18,26,27	0.86	1 (5%)	16,38,41	1.34	3 (18%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	5MU	2A	1915	1	-	2/7/25/26	0/2/2/2
1	5MC	1A	1942	1	-	0/7/25/26	0/2/2/2
32	5MC	1a	1407	32	-	0/7/25/26	0/2/2/2
1	5MC	2A	1942	1	-	0/7/25/26	0/2/2/2
1	PSU	2A	2605	1	-	0/7/25/26	0/2/2/2
32	MA6	1a	1519	32	-	1/7/29/30	0/3/3/3
32	5MC	1a	967	32	-	1/7/25/26	0/2/2/2
43	0TD	1l	92	43	-	1/7/12/14	-
1	4OC	2A	1920	1	-	1/9/27/30	0/2/2/2
32	5MC	1a	1404	32	-	0/7/25/26	0/2/2/2
32	7MG	2a	527	54,32	-	2/7/37/38	0/3/3/3
1	PSU	1A	1917	54,1	-	0/7/25/26	0/2/2/2
1	5MU	1A	1939	1	-	0/7/25/26	0/2/2/2
32	UR3	1a	1498	32	-	0/7/25/26	0/2/2/2
32	MA6	2a	1519	32	-	3/7/29/30	0/3/3/3
32	PSU	1a	516	54,32	-	0/7/25/26	0/2/2/2
1	5MC	2A	1962	54,1	-	0/7/25/26	0/2/2/2
1	5MC	1A	1962	54,1	-	0/7/25/26	0/2/2/2
32	5MC	2a	1400	32	-	0/7/25/26	0/2/2/2
43	0TD	2l	92	43	-	2/7/12/14	-
32	5MC	2a	1407	32	-	0/7/25/26	0/2/2/2
1	4OC	1A	1920	1	-	0/9/27/30	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	5MU	2A	1939	1	-	0/7/25/26	0/2/2/2
32	M2G	1a	966	32	-	1/7/29/30	0/3/3/3
1	PSU	1A	1911	1	-	0/7/25/26	0/2/2/2
32	2MG	1a	1207	32	-	0/5/27/28	0/3/3/3
32	UR3	2a	1498	32	-	0/7/25/26	0/2/2/2
32	MA6	1a	1518	32	-	0/7/29/30	0/3/3/3
32	5MC	2a	1404	32	-	0/7/25/26	0/2/2/2
1	2MA	1A	2503	54,1	-	1/3/25/26	0/3/3/3
1	OMG	1A	2251	54,1	-	1/5/27/28	0/3/3/3
32	4OC	1a	1402	32	-	2/9/29/30	0/2/2/2
1	PSU	2A	1911	1	-	0/7/25/26	0/2/2/2
1	OMG	2A	2251	54,1	-	1/5/27/28	0/3/3/3
1	PSU	2A	1917	1	-	0/7/25/26	0/2/2/2
1	2MU	1A	2552	54,1	-	1/9/27/28	0/2/2/2
32	5MC	1a	1400	32	-	2/7/25/26	0/2/2/2
32	5MC	2a	967	32	-	0/7/25/26	0/2/2/2
1	5MU	1A	1915	54,1	-	2/7/25/26	0/2/2/2
1	2MU	2A	2552	54,1	-	0/9/27/28	0/2/2/2
1	2MA	2A	2503	54,1	-	1/3/25/26	0/3/3/3
32	M2G	2a	966	54,32	-	0/7/29/30	0/3/3/3
32	7MG	1a	527	54,32	-	1/7/37/38	0/3/3/3
1	PSU	1A	2605	54,1	-	0/7/25/26	0/2/2/2
32	MA6	2a	1518	32	-	0/7/29/30	0/3/3/3
32	PSU	2a	516	54,32	-	0/7/25/26	0/2/2/2
32	4OC	2a	1402	32	-	3/9/29/30	0/2/2/2
32	2MG	2a	1207	32	-	0/5/27/28	0/3/3/3

All (111) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
43	1l	92	0TD	CB-SB	-12.59	1.69	1.82
43	2l	92	0TD	CB-SB	-12.32	1.69	1.82
32	1a	1407	5MC	C5-C4	6.59	1.49	1.44
1	1A	1962	5MC	C5-C4	6.34	1.48	1.44
32	2a	967	5MC	C5-C4	6.25	1.48	1.44
32	2a	1404	5MC	C5-C4	6.18	1.48	1.44
32	1a	1400	5MC	C5-C4	6.14	1.48	1.44
1	2A	1942	5MC	C5-C4	6.00	1.48	1.44
32	2a	1407	5MC	C5-C4	5.91	1.48	1.44
32	1a	1404	5MC	C5-C4	5.83	1.48	1.44
32	2a	1400	5MC	C5-C4	5.75	1.48	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	1a	967	5MC	C5-C4	5.68	1.48	1.44
1	2A	1962	5MC	C5-C4	5.51	1.48	1.44
1	1A	1942	5MC	C5-C4	5.34	1.48	1.44
32	2a	966	M2G	C2-N3	4.04	1.36	1.30
32	1a	966	M2G	C2-N3	3.74	1.35	1.30
32	1a	516	PSU	C6-C5	3.57	1.39	1.35
1	1A	1917	PSU	C6-C5	3.52	1.39	1.35
1	2A	1911	PSU	C6-C5	3.50	1.39	1.35
32	2a	516	PSU	C6-C5	3.49	1.39	1.35
1	1A	1911	PSU	C6-C5	3.39	1.39	1.35
32	1a	527	7MG	C5-C4	3.38	1.48	1.37
1	2A	1917	PSU	C6-C5	3.37	1.39	1.35
32	2a	527	7MG	C5-C4	3.26	1.47	1.37
32	1a	527	7MG	C4-N9	-3.23	1.33	1.37
1	2A	2605	PSU	C6-C5	3.16	1.38	1.35
1	2A	1939	5MU	C6-C5	3.08	1.39	1.34
32	2a	527	7MG	C4-N9	-3.06	1.34	1.37
1	1A	2605	PSU	C6-C5	2.98	1.38	1.35
32	2a	1407	5MC	C6-C5	2.95	1.39	1.34
1	2A	1939	5MU	C4-C5	2.92	1.49	1.44
1	1A	1915	5MU	C2-N1	2.89	1.43	1.38
32	2a	966	M2G	C2-N2	2.88	1.40	1.35
1	1A	2552	2MU	C4-N3	-2.88	1.33	1.38
32	1a	966	M2G	C2-N2	2.87	1.40	1.35
1	1A	2605	PSU	C4-N3	-2.87	1.33	1.38
32	1a	967	5MC	C6-C5	2.85	1.39	1.34
1	2A	2552	2MU	C4-N3	-2.83	1.33	1.38
1	1A	1939	5MU	C6-C5	2.83	1.39	1.34
32	1a	1400	5MC	C6-C5	2.81	1.39	1.34
32	1a	1404	5MC	C6-C5	2.78	1.39	1.34
1	1A	1915	5MU	C6-C5	2.78	1.39	1.34
32	2a	967	5MC	C6-C5	2.77	1.39	1.34
1	2A	1915	5MU	C6-C5	2.76	1.39	1.34
1	2A	1962	5MC	C6-C5	2.76	1.39	1.34
32	2a	1404	5MC	C6-C5	2.76	1.39	1.34
1	2A	1915	5MU	C2-N1	2.75	1.42	1.38
1	1A	1939	5MU	C4-N3	-2.72	1.33	1.38
1	2A	2605	PSU	C4-N3	-2.71	1.33	1.38
1	1A	1962	5MC	C6-C5	2.70	1.39	1.34
32	2a	1400	5MC	C6-C5	2.66	1.38	1.34
1	1A	1942	5MC	C6-C5	2.64	1.38	1.34
1	2A	1942	5MC	C6-C5	2.64	1.38	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	1A	1915	5MU	C4-N3	-2.61	1.34	1.38
32	1a	1407	5MC	C6-C5	2.60	1.38	1.34
1	1A	1962	5MC	C6-N1	-2.53	1.33	1.38
1	2A	1915	5MU	C4-N3	-2.52	1.34	1.38
1	2A	1911	PSU	C4-N3	-2.51	1.34	1.38
32	1a	516	PSU	C4-N3	-2.50	1.34	1.38
32	2a	516	PSU	C4-N3	-2.50	1.34	1.38
1	1A	1911	PSU	C4-N3	-2.50	1.34	1.38
1	2A	1917	PSU	C4-N3	-2.50	1.34	1.38
1	2A	1939	5MU	C4-N3	-2.49	1.34	1.38
1	1A	1917	PSU	C4-N3	-2.44	1.34	1.38
32	1a	1518	MA6	C6-C5	-2.43	1.41	1.44
32	2a	527	7MG	C6-N1	-2.40	1.34	1.38
1	2A	1942	5MC	C6-N1	-2.40	1.33	1.38
1	1A	1939	5MU	C4-C5	2.37	1.48	1.44
1	1A	1942	5MC	C6-N1	-2.36	1.34	1.38
1	2A	2552	2MU	C5-C4	2.36	1.48	1.43
32	2a	1519	MA6	C6-C5	-2.35	1.41	1.44
32	2a	1518	MA6	C6-C5	-2.35	1.41	1.44
32	1a	1519	MA6	C6-C5	-2.33	1.41	1.44
1	1A	2251	OMG	C6-N1	-2.31	1.34	1.37
32	2a	966	M2G	C6-N1	-2.29	1.34	1.37
32	1a	1400	5MC	C6-N1	-2.29	1.34	1.38
32	1a	1207	2MG	C6-N1	-2.26	1.34	1.37
1	1A	1915	5MU	C4-C5	2.25	1.48	1.44
1	1A	2552	2MU	C5-C4	2.25	1.48	1.43
1	2A	2251	OMG	C6-N1	-2.25	1.34	1.37
1	1A	2605	PSU	C2-N3	-2.24	1.33	1.37
1	2A	1915	5MU	C4-C5	2.23	1.48	1.44
1	1A	1939	5MU	C6-N1	-2.23	1.34	1.38
1	2A	2605	PSU	C2-N3	-2.23	1.33	1.37
1	1A	1939	5MU	C2-N1	2.23	1.41	1.38
32	1a	527	7MG	C6-N1	-2.22	1.34	1.38
32	2a	1400	5MC	C6-N1	-2.22	1.34	1.38
32	2a	1404	5MC	C6-N1	-2.21	1.34	1.38
1	1A	2552	2MU	C2-N3	-2.18	1.34	1.38
1	2A	1962	5MC	C6-N1	-2.18	1.34	1.38
1	2A	1939	5MU	C2-N1	2.18	1.41	1.38
32	1a	1404	5MC	C6-N1	-2.16	1.34	1.38
1	2A	2552	2MU	C2-N3	-2.16	1.34	1.38
32	2a	1519	MA6	C6-N1	2.13	1.35	1.32
32	1a	1498	UR3	C6-C5	2.13	1.40	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	2a	1518	MA6	C6-N1	2.12	1.35	1.32
32	1a	1407	5MC	C6-N1	-2.11	1.34	1.38
32	1a	967	5MC	C6-N1	-2.10	1.34	1.38
32	1a	966	M2G	C6-N1	-2.10	1.34	1.37
32	1a	1519	MA6	C6-N1	2.09	1.35	1.32
1	1A	1939	5MU	C2-N3	-2.07	1.34	1.38
1	2A	1915	5MU	C6-N1	-2.07	1.34	1.38
32	2a	967	5MC	C6-N1	-2.06	1.34	1.38
32	2a	1207	2MG	C6-N1	-2.06	1.34	1.37
1	2A	1939	5MU	C6-N1	-2.05	1.34	1.38
1	2A	1939	5MU	C2-N3	-2.04	1.34	1.38
32	1a	1518	MA6	C6-N1	2.04	1.35	1.32
32	2a	1498	UR3	C2-N1	2.03	1.41	1.38
32	2a	1407	5MC	C6-N1	-2.02	1.34	1.38
1	1A	1915	5MU	C2-N3	-2.02	1.34	1.38
32	2a	1498	UR3	C6-C5	2.01	1.39	1.35

All (164) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
43	2l	92	0TD	CSB-SB-CB	-11.44	81.80	102.36
32	1a	527	7MG	N9-C4-N3	8.84	138.42	125.46
32	2a	527	7MG	N9-C4-N3	8.80	138.35	125.46
43	1l	92	0TD	CSB-SB-CB	-8.34	87.38	102.36
1	1A	2503	2MA	C2-N3-C4	6.98	121.10	115.46
32	1a	1498	UR3	C4-N3-C2	-6.86	119.06	124.58
32	2a	1498	UR3	C4-N3-C2	-6.67	119.21	124.58
1	1A	1911	PSU	N1-C2-N3	6.28	121.80	115.17
32	2a	516	PSU	N1-C2-N3	6.28	121.79	115.17
1	2A	1917	PSU	N1-C2-N3	6.19	121.70	115.17
1	2A	1911	PSU	N1-C2-N3	6.18	121.69	115.17
32	1a	516	PSU	N1-C2-N3	6.17	121.68	115.17
1	1A	2605	PSU	N1-C2-N3	6.14	121.65	115.17
1	1A	1917	PSU	N1-C2-N3	6.00	121.50	115.17
1	2A	2503	2MA	C2-N3-C4	5.90	120.22	115.46
1	2A	2605	PSU	N1-C2-N3	5.75	121.24	115.17
1	2A	1939	5MU	N3-C2-N1	5.74	122.37	114.89
32	2a	1518	MA6	N3-C2-N1	-5.60	121.07	128.67
32	2a	1519	MA6	N3-C2-N1	-5.49	121.22	128.67
1	2A	2552	2MU	N3-C2-N1	5.43	121.95	114.89
1	2A	1939	5MU	C4-N3-C2	-5.41	120.25	127.34
32	1a	1518	MA6	N3-C2-N1	-5.36	121.40	128.67

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	2a	527	7MG	N9-C8-N7	-5.34	95.82	103.37
32	2a	527	7MG	C5-C4-N3	-5.31	118.17	128.13
1	1A	1939	5MU	C4-N3-C2	-5.22	120.50	127.34
32	1a	527	7MG	C5-C4-N3	-5.21	118.34	128.13
1	1A	2552	2MU	N3-C2-N1	5.19	121.65	114.89
32	1a	527	7MG	N9-C8-N7	-5.14	96.10	103.37
32	1a	1519	MA6	N3-C2-N1	-5.10	121.75	128.67
32	1a	1518	MA6	C2-N1-C6	5.01	121.75	116.84
32	2a	1518	MA6	C2-N1-C6	4.89	121.63	116.84
1	2A	1915	5MU	N3-C2-N1	4.88	121.24	114.89
1	1A	1939	5MU	N3-C2-N1	4.84	121.20	114.89
1	1A	1915	5MU	N3-C2-N1	4.83	121.18	114.89
32	2a	1519	MA6	C2-N1-C6	4.75	121.50	116.84
1	2A	2552	2MU	C4-N3-C2	-4.72	120.75	126.61
1	1A	1939	5MU	C5-C4-N3	4.66	119.37	115.32
1	2A	1915	5MU	C4-N3-C2	-4.61	121.29	127.34
1	1A	2552	2MU	C4-N3-C2	-4.61	120.89	126.61
32	1a	1519	MA6	C2-N1-C6	4.47	121.22	116.84
1	1A	1915	5MU	C4-N3-C2	-4.44	121.52	127.34
1	1A	2605	PSU	C4-N3-C2	-4.38	120.34	126.37
32	2a	527	7MG	C2-N3-C4	4.31	119.73	112.30
1	1A	1915	5MU	C1'-N1-C2	4.22	125.17	117.59
1	1A	1911	PSU	C4-N3-C2	-4.18	120.61	126.37
1	1A	1939	5MU	C5-C6-N1	-4.10	118.86	123.31
1	1A	1939	5MU	O4-C4-C5	-4.09	120.23	124.92
1	1A	1915	5MU	C5-C4-N3	4.09	118.88	115.32
32	2a	516	PSU	C4-N3-C2	-4.09	120.74	126.37
32	1a	527	7MG	C2-N3-C4	4.06	119.29	112.30
1	2A	1917	PSU	C4-N3-C2	-4.03	120.82	126.37
1	2A	1915	5MU	C5-C4-N3	4.02	118.82	115.32
1	2A	1917	PSU	O2-C2-N1	-4.00	118.66	122.79
1	2A	1915	5MU	C1'-N1-C2	4.00	124.78	117.59
1	1A	1911	PSU	O2-C2-N1	-4.00	118.67	122.79
1	2A	1939	5MU	C5-C4-N3	3.99	118.79	115.32
1	2A	2605	PSU	C4-N3-C2	-3.91	120.99	126.37
32	1a	516	PSU	C4-N3-C2	-3.90	121.00	126.37
1	2A	1911	PSU	C4-N3-C2	-3.90	121.00	126.37
1	2A	1939	5MU	C5-C6-N1	-3.86	119.12	123.31
1	2A	1915	5MU	O4-C4-C5	-3.83	120.54	124.92
1	1A	1917	PSU	C4-N3-C2	-3.82	121.11	126.37
1	1A	1915	5MU	O4-C4-C5	-3.78	120.60	124.92
32	1a	516	PSU	O2-C2-N1	-3.73	118.94	122.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	2A	1962	5MC	C5-C6-N1	-3.56	119.45	123.31
1	2A	1942	5MC	C5-C6-N1	-3.54	119.47	123.31
1	2A	1911	PSU	O2-C2-N1	-3.54	119.14	122.79
32	1a	1400	5MC	C5-C6-N1	-3.53	119.48	123.31
1	1A	1917	PSU	O2-C2-N1	-3.53	119.15	122.79
1	1A	1915	5MU	C1'-N1-C6	-3.50	115.39	121.15
1	1A	1962	5MC	C5-C6-N1	-3.48	119.53	123.31
32	2a	516	PSU	O2-C2-N1	-3.46	119.22	122.79
32	2a	1400	5MC	C5-C6-N1	-3.42	119.60	123.31
1	2A	1915	5MU	C1'-N1-C6	-3.40	115.54	121.15
1	1A	1942	5MC	C5-C6-N1	-3.37	119.65	123.31
32	2a	1404	5MC	C5-C6-N1	-3.36	119.67	123.31
43	1l	92	0TD	OD2-CG-CB	3.35	120.38	113.15
32	2a	1498	UR3	C5-C4-N3	3.31	119.39	115.04
32	1a	1407	5MC	C5-C6-N1	-3.26	119.78	123.31
1	2A	1939	5MU	O4-C4-C5	-3.23	121.22	124.92
32	2a	1519	MA6	C4-C5-N7	-3.20	105.96	109.34
43	2l	92	0TD	OD2-CG-CB	3.19	120.04	113.15
32	1a	1404	5MC	C5-C6-N1	-3.18	119.86	123.31
1	2A	1939	5MU	O2-C2-N1	-3.17	118.67	122.80
1	1A	2251	OMG	C8-N7-C5	3.17	107.94	102.55
32	1a	1498	UR3	C5-C4-N3	3.06	119.08	115.04
32	2a	967	5MC	C5-C6-N1	-3.06	119.99	123.31
1	2A	2552	2MU	O2-C2-N1	-3.04	118.84	122.80
32	1a	967	5MC	C5-C6-N1	-3.00	120.05	123.31
1	2A	2552	2MU	C2'-C1'-N1	-2.96	108.63	114.24
1	1A	2552	2MU	C5-C4-N3	2.96	118.94	114.80
32	2a	1404	5MC	C5-C4-N3	-2.95	118.73	121.75
1	2A	2552	2MU	C5-C4-N3	2.92	118.88	114.80
32	1a	1404	5MC	C5-C4-N3	-2.87	118.81	121.75
32	1a	966	M2G	C8-N7-C5	2.87	107.44	102.55
32	1a	1518	MA6	C4-C5-N7	-2.86	106.31	109.34
32	2a	1407	5MC	C5-C6-N1	-2.84	120.23	123.31
32	2a	1207	2MG	C8-N7-C5	2.83	107.36	102.55
1	2A	1942	5MC	C5-C4-N3	-2.83	118.86	121.75
32	1a	1207	2MG	C8-N7-C5	2.82	107.36	102.55
32	1a	1519	MA6	C4-C5-N7	-2.80	106.38	109.34
32	2a	1407	5MC	C5-C4-N3	-2.79	118.89	121.75
32	2a	966	M2G	C8-N7-C5	2.78	107.29	102.55
1	2A	2503	2MA	C2-N1-C6	2.78	122.38	118.10
32	2a	1518	MA6	C4-C5-N7	-2.78	106.40	109.34
32	1a	1207	2MG	N1-C2-N2	2.77	119.39	116.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	2A	2251	OMG	C8-N7-C5	2.72	107.18	102.55
32	2a	527	7MG	C5-C6-N1	2.70	115.69	110.94
1	1A	2503	2MA	C4-C5-N7	-2.68	106.50	109.34
32	1a	1400	5MC	C5-C4-N3	-2.68	119.01	121.75
1	2A	2503	2MA	C5-C6-N1	-2.67	117.68	120.84
32	1a	1407	5MC	C5-C4-N3	-2.63	119.06	121.75
1	1A	1962	5MC	C5-C4-N3	-2.63	119.06	121.75
32	2a	967	5MC	C5-C4-N3	-2.60	119.09	121.75
1	1A	2605	PSU	O2-C2-N1	-2.59	120.12	122.79
32	1a	967	5MC	C5-C4-N3	-2.56	119.13	121.75
1	1A	1915	5MU	O2-C2-N3	-2.55	116.78	121.49
1	1A	1942	5MC	C5-C4-N3	-2.55	119.14	121.75
1	1A	2552	2MU	O4-C4-C5	-2.51	120.84	125.16
1	1A	2503	2MA	C2-N1-C6	2.50	121.94	118.10
1	1A	1939	5MU	O2-C2-N1	-2.49	119.55	122.80
32	1a	1498	UR3	C6-N1-C2	-2.47	119.78	121.80
1	2A	1915	5MU	C5-C6-N1	-2.46	120.65	123.31
32	1a	527	7MG	C5-C6-N1	2.45	115.25	110.94
32	1a	527	7MG	C5-C4-N9	-2.42	103.23	106.33
1	1A	2552	2MU	C2'-C1'-N1	-2.38	109.73	114.24
1	2A	2503	2MA	C4-C5-N7	-2.38	106.83	109.34
1	1A	2552	2MU	O2-C2-N1	-2.36	119.72	122.80
32	2a	1407	5MC	O2-C2-N3	-2.36	118.62	122.33
1	1A	2605	PSU	C5-C6-N1	-2.36	118.87	122.14
32	2a	1400	5MC	C5-C4-N3	-2.35	119.34	121.75
43	2l	92	0TD	OD1-CG-CB	-2.34	117.54	122.44
32	1a	1402	4OC	C6-C5-C4	2.33	119.80	117.00
1	2A	2605	PSU	O2-C2-N1	-2.30	120.42	122.79
1	1A	1962	5MC	CM5-C5-C6	-2.28	119.77	122.85
32	1a	527	7MG	O6-C6-C5	-2.28	122.03	127.62
32	1a	1407	5MC	CM5-C5-C6	-2.27	119.78	122.85
1	1A	2503	2MA	C5-C6-N1	-2.27	118.16	120.84
32	2a	1402	4OC	C6-C5-C4	2.26	119.72	117.00
1	1A	1942	5MC	O2-C2-N3	-2.26	118.77	122.33
32	2a	1207	2MG	N1-C2-N2	2.26	118.86	116.56
43	1l	92	0TD	OD1-CG-CB	-2.24	117.75	122.44
32	2a	527	7MG	C5-C4-N9	-2.24	103.47	106.33
1	1A	1915	5MU	C5-C6-N1	-2.24	120.89	123.31
1	2A	2552	2MU	O4-C4-C5	-2.23	121.31	125.16
32	1a	1207	2MG	O3'-C3'-C2'	2.22	118.92	111.82
32	1a	966	M2G	C5-C6-N1	2.20	118.27	114.07
1	2A	1962	5MC	C5-C4-N3	-2.19	119.51	121.75

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	2a	516	PSU	O4'-C1'-C2'	2.19	108.18	105.15
32	1a	1207	2MG	N2-C2-N3	-2.18	117.73	120.51
1	2A	1915	5MU	O2-C2-N3	-2.17	117.48	121.49
1	2A	1920	4OC	O2-C2-N3	-2.15	118.94	122.33
1	1A	1920	4OC	O2-C2-N3	-2.15	118.95	122.33
32	1a	1407	5MC	O2-C2-N3	-2.12	118.99	122.33
32	2a	527	7MG	O6-C6-C5	-2.11	122.45	127.62
1	1A	2251	OMG	C5-C6-N1	2.11	118.09	114.07
32	2a	516	PSU	C5-C6-N1	-2.07	119.27	122.14
1	2A	1915	5MU	C5M-C5-C4	2.05	120.97	118.78
1	1A	2605	PSU	O2-C2-N3	-2.05	118.23	121.86
32	2a	1207	2MG	N2-C2-N3	-2.04	117.91	120.51
1	1A	1911	PSU	O4'-C1'-C2'	2.03	107.97	105.15
1	2A	2605	PSU	C5-C6-N1	-2.02	119.33	122.14
32	1a	516	PSU	O4'-C1'-C2'	2.02	107.94	105.15
1	2A	2251	OMG	O6-C6-C5	-2.00	120.35	124.32

There are no chirality outliers.

All (29) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	1A	1915	5MU	O4'-C1'-N1-C2
1	1A	1915	5MU	O4'-C1'-N1-C6
1	2A	1915	5MU	O4'-C1'-N1-C2
1	2A	1915	5MU	O4'-C1'-N1-C6
1	2A	2251	OMG	C1'-C2'-O2'-CM2
32	2a	1519	MA6	O4'-C4'-C5'-O5'
32	2a	527	7MG	C3'-C4'-C5'-O5'
32	2a	1402	4OC	O4'-C4'-C5'-O5'
32	2a	1519	MA6	C3'-C4'-C5'-O5'
32	2a	527	7MG	O4'-C4'-C5'-O5'
32	1a	1400	5MC	O4'-C4'-C5'-O5'
32	2a	1402	4OC	C3'-C4'-C5'-O5'
32	1a	1402	4OC	O4'-C4'-C5'-O5'
43	2l	92	0TD	CG-CB-SB-CSB
32	2a	1519	MA6	C4'-C5'-O5'-P
32	1a	1519	MA6	O4'-C4'-C5'-O5'
1	1A	2552	2MU	O4'-C4'-C5'-O5'
32	1a	967	5MC	O4'-C4'-C5'-O5'
1	2A	2503	2MA	O4'-C4'-C5'-O5'
43	2l	92	0TD	CA-CB-SB-CSB
1	1A	2251	OMG	C4'-C5'-O5'-P

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Mol	Chain	Res	Type	Atoms
32	1a	527	7MG	C3'-C4'-C5'-O5'
32	1a	1400	5MC	C3'-C4'-C5'-O5'
1	2A	1920	4OC	C3'-C2'-O2'-CM2
32	2a	1402	4OC	C3'-C2'-O2'-CM2
43	1l	92	0TD	CG-CB-SB-CSB
1	1A	2503	2MA	C4'-C5'-O5'-P
32	1a	966	M2G	C4'-C5'-O5'-P
32	1a	1402	4OC	C3'-C4'-C5'-O5'

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
56	MPD	2A	3759	-	7,7,7	0.30	0	9,10,10	0.25	0
56	MPD	2A	3760	-	7,7,7	0.32	0	9,10,10	0.30	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
59	SF4	1d	306	35	-	-	0/6/5/5
55	YXM	2A	3758	-	-	3/42/44/44	0/4/4/4
56	MPD	2B	220	-	-	4/5/5/5	-
59	SF4	2d	501	35	-	-	0/6/5/5
57	ARG	1F	316	-	-	4/11/11/11	-
56	MPD	1A	4056	-	-	2/5/5/5	-
55	YXM	1A	4055	-	-	3/42/44/44	0/4/4/4
57	ARG	1B	228	-	-	2/11/11/11	-
56	MPD	1T	207	-	-	0/5/5/5	-
56	MPD	18	102	-	-	2/5/5/5	-
56	MPD	1a	3280	-	-	4/5/5/5	-
56	MPD	2A	3759	-	-	0/5/5/5	-
56	MPD	2A	3760	-	-	3/5/5/5	-

All (15) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
55	1A	4055	YXM	OAK-NAG	14.28	1.47	1.22
55	2A	3758	YXM	OAK-NAG	13.62	1.46	1.22
55	2A	3758	YXM	CAB-CAH	-8.17	1.39	1.51
55	1A	4055	YXM	CAB-CAH	-7.61	1.40	1.51
55	1A	4055	YXM	PAV-CAY	-6.30	1.68	1.79
55	2A	3758	YXM	PAV-CAY	-5.39	1.70	1.79
55	1A	4055	YXM	PAV-CAX	-4.99	1.70	1.79
55	1A	4055	YXM	CAE-NAG	-4.82	1.33	1.45
55	2A	3758	YXM	CAE-NAG	-4.57	1.34	1.45
55	1A	4055	YXM	PAV-CAW	-3.51	1.73	1.79
55	2A	3758	YXM	PAV-CAX	-2.68	1.75	1.79
55	2A	3758	YXM	PAV-CAU	-2.26	1.75	1.80
57	1F	316	ARG	OXT-C	-2.16	1.23	1.30
57	1B	228	ARG	OXT-C	-2.15	1.23	1.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
55	2A	3758	YXM	PAV-CAW	-2.09	1.76	1.79

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
55	2A	3758	YXM	CAY-PAV-CAX	5.67	120.00	109.28
55	1A	4055	YXM	CAU-PAV-CAW	-4.76	99.65	109.60
55	1A	4055	YXM	CAY-PAV-CAX	4.27	117.35	109.28
55	2A	3758	YXM	CAU-PAV-CAY	-4.22	100.77	109.60
55	2A	3758	YXM	CAU-PAV-CAW	-4.04	101.15	109.60
55	1A	4055	YXM	CAU-PAV-CAY	-4.02	101.19	109.60
55	2A	3758	YXM	CAF-CAE-NAG	3.00	121.96	119.34
57	1F	316	ARG	OXT-C-O	-2.83	117.65	124.08
57	1B	228	ARG	OXT-C-O	-2.83	117.67	124.08
55	1A	4055	YXM	CAY-PAV-CAW	2.75	114.48	109.28
55	1A	4055	YXM	CAX-PAV-CAW	2.62	114.23	109.28
55	2A	3758	YXM	PAV-CAU-CAT	-2.62	107.81	114.41
55	2A	3758	YXM	CAU-PAV-CAX	-2.28	104.83	109.60
55	2A	3758	YXM	CAY-PAV-CAW	2.24	113.51	109.28
55	2A	3758	YXM	CAX-PAV-CAW	2.10	113.26	109.28

There are no chirality outliers.

All (27) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
55	2A	3758	YXM	NAN-CAJ-CAM-OAO
56	1a	3280	MPD	C2-C3-C4-O4
56	1a	3280	MPD	C2-C3-C4-C5
56	2B	220	MPD	C2-C3-C4-C5
57	1F	316	ARG	N-CA-CB-CG
57	1F	316	ARG	C-CA-CB-CG
57	1F	316	ARG	NE-CD-CG-CB
55	2A	3758	YXM	CAH-CAJ-CAM-OAO
57	1F	316	ARG	CA-CB-CG-CD
55	1A	4055	YXM	CAH-CAJ-CAM-OAO
55	2A	3758	YXM	CAP-CAR-CAS-CAT
56	2A	3760	MPD	C2-C3-C4-O4
56	1a	3280	MPD	C1-C2-C3-C4
56	2A	3760	MPD	CM-C2-C3-C4
56	18	102	MPD	C2-C3-C4-C5
55	1A	4055	YXM	NAN-CAJ-CAM-OAO
57	1B	228	ARG	NE-CD-CG-CB

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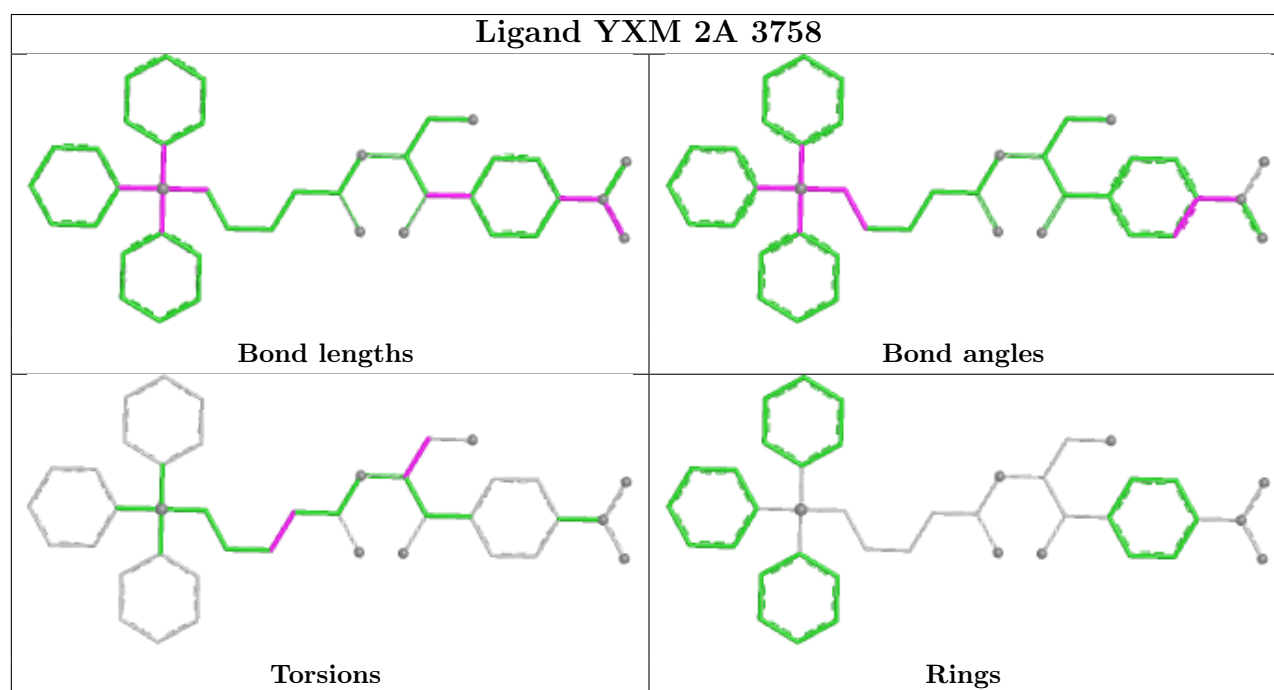
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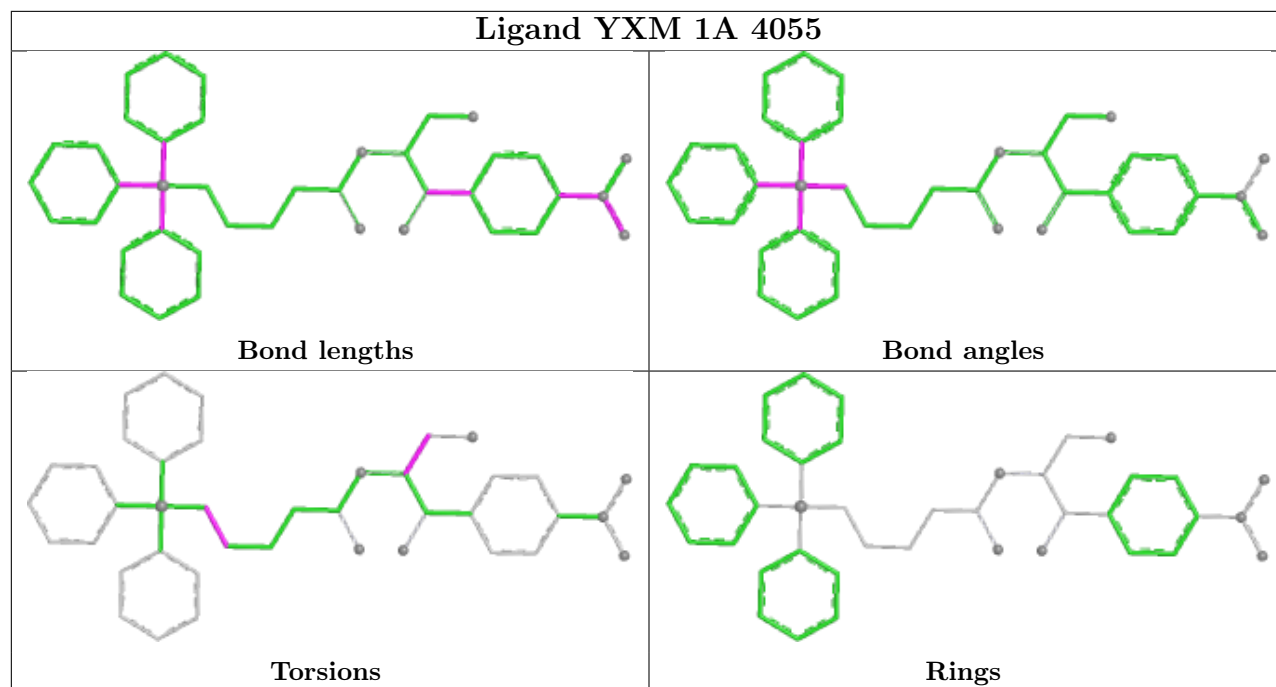
Mol	Chain	Res	Type	Atoms
55	1A	4055	YXM	CAS-CAT-CAU-PAV
56	2B	220	MPD	O2-C2-C3-C4
56	18	102	MPD	C2-C3-C4-O4
56	2B	220	MPD	C2-C3-C4-O4
56	1A	4056	MPD	C1-C2-C3-C4
56	1A	4056	MPD	CM-C2-C3-C4
56	1a	3280	MPD	CM-C2-C3-C4
56	2A	3760	MPD	C1-C2-C3-C4
56	2B	220	MPD	C1-C2-C3-C4
57	1B	228	ARG	OXT-C-CA-N

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	70 (2%) 59 51	12, 31, 88, 103	0
1	2A	2856/2915 (97%)	-0.00	97 (3%) 48 40	25, 50, 91, 104	0
2	1B	120/121 (99%)	-0.38	1 (0%) 82 77	22, 45, 60, 81	0
2	2B	120/121 (99%)	0.68	4 (3%) 49 41	52, 73, 84, 92	0
3	1D	275/276 (99%)	-0.29	3 (1%) 77 71	16, 30, 44, 66	0
3	2D	275/276 (99%)	0.06	3 (1%) 77 71	25, 45, 59, 74	0
4	1E	204/206 (99%)	-0.27	1 (0%) 87 83	16, 37, 55, 71	0
4	2E	204/206 (99%)	-0.09	0 100 100	27, 50, 65, 77	0
5	1F	203/210 (96%)	-0.29	0 100 100	15, 36, 59, 73	0
5	2F	203/210 (96%)	0.17	2 (0%) 79 73	27, 60, 73, 83	0
6	1G	181/182 (99%)	0.26	2 (1%) 77 71	39, 59, 72, 82	0
6	2G	181/182 (99%)	1.24	25 (13%) 8 7	68, 78, 84, 88	0
7	1H	174/180 (96%)	-0.11	1 (0%) 85 81	36, 49, 62, 66	0
7	2H	173/180 (96%)	0.72	4 (2%) 61 52	61, 75, 82, 87	0
8	1I	147/148 (99%)	0.42	4 (2%) 56 47	38, 66, 77, 80	0
8	2I	146/148 (98%)	0.46	3 (2%) 63 55	50, 67, 78, 82	0
9	1N	140/140 (100%)	-0.36	0 100 100	24, 34, 55, 67	0
9	2N	140/140 (100%)	0.37	1 (0%) 84 79	39, 57, 70, 76	0
10	1O	122/122 (100%)	-0.29	0 100 100	22, 35, 50, 59	0
10	2O	122/122 (100%)	0.09	0 100 100	36, 49, 62, 67	0
11	1P	149/150 (99%)	-0.18	0 100 100	16, 41, 61, 71	0
11	2P	149/150 (99%)	0.17	0 100 100	29, 59, 75, 80	0
12	1Q	141/141 (100%)	-0.44	0 100 100	20, 34, 47, 60	0
12	2Q	141/141 (100%)	0.42	2 (1%) 73 66	39, 58, 68, 75	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
13	1R	118/118 (100%)	-0.36	0 100 100	21, 31, 44, 55	0
13	2R	118/118 (100%)	-0.12	0 100 100	33, 44, 56, 64	0
14	1S	110/112 (98%)	-0.22	0 100 100	32, 44, 56, 60	0
14	2S	110/112 (98%)	0.92	8 (7%) 22 17	55, 68, 76, 78	0
15	1T	131/146 (89%)	-0.03	3 (2%) 61 52	28, 42, 64, 76	0
15	2T	131/146 (89%)	0.01	2 (1%) 71 64	39, 51, 69, 74	0
16	1U	116/118 (98%)	-0.51	0 100 100	19, 27, 43, 54	0
16	2U	116/118 (98%)	0.12	1 (0%) 81 75	36, 54, 68, 72	0
17	1V	101/101 (100%)	-0.40	0 100 100	18, 37, 53, 64	0
17	2V	101/101 (100%)	0.25	0 100 100	35, 63, 73, 76	0
18	1W	112/113 (99%)	-0.37	1 (0%) 81 75	18, 27, 52, 79	0
18	2W	112/113 (99%)	0.01	0 100 100	30, 43, 60, 78	0
19	1X	95/96 (98%)	-0.34	0 100 100	18, 32, 52, 67	0
19	2X	95/96 (98%)	0.16	0 100 100	41, 53, 63, 70	0
20	1Y	107/110 (97%)	-0.06	1 (0%) 81 75	31, 44, 64, 70	0
20	2Y	107/110 (97%)	0.61	3 (2%) 55 46	52, 64, 75, 79	0
21	1Z	203/206 (98%)	0.01	1 (0%) 87 83	32, 51, 65, 75	0
21	2Z	201/206 (97%)	0.64	5 (2%) 58 49	58, 70, 78, 86	0
22	10	77/85 (90%)	-0.23	0 100 100	21, 32, 46, 51	0
22	20	77/85 (90%)	0.49	3 (3%) 44 36	38, 56, 66, 70	0
23	11	97/98 (98%)	-0.19	1 (1%) 79 73	21, 37, 60, 68	0
23	21	97/98 (98%)	0.30	1 (1%) 79 73	30, 49, 67, 75	0
24	12	70/72 (97%)	-0.02	1 (1%) 73 66	29, 43, 56, 78	0
24	22	70/72 (97%)	0.13	0 100 100	50, 63, 70, 73	0
25	13	59/60 (98%)	-0.39	0 100 100	25, 34, 55, 62	0
25	23	59/60 (98%)	0.13	1 (1%) 69 61	42, 55, 69, 82	0
26	14	69/71 (97%)	0.73	8 (11%) 11 9	55, 74, 83, 85	0
26	24	69/71 (97%)	1.44	13 (18%) 4 4	74, 85, 92, 99	0
27	15	59/60 (98%)	-0.40	0 100 100	17, 31, 53, 61	0
27	25	59/60 (98%)	-0.19	1 (1%) 69 61	29, 45, 60, 73	0
28	16	53/54 (98%)	-0.37	0 100 100	28, 36, 50, 57	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
28	26	53/54 (98%)	0.20	0 100 100	46, 54, 64, 66	0
29	17	48/49 (97%)	-0.42	0 100 100	15, 22, 48, 58	0
29	27	48/49 (97%)	-0.05	2 (4%) 41 33	25, 34, 61, 69	0
30	18	64/65 (98%)	-0.53	0 100 100	22, 29, 38, 53	0
30	28	64/65 (98%)	0.19	0 100 100	40, 48, 55, 66	0
31	19	37/37 (100%)	-0.21	0 100 100	26, 36, 53, 56	0
31	29	37/37 (100%)	0.80	0 100 100	54, 61, 75, 80	0
32	1a	1488/1521 (97%)	0.19	20 (1%) 74 67	30, 63, 88, 104	0
32	2a	1492/1521 (98%)	0.54	56 (3%) 44 36	42, 71, 91, 103	0
33	1b	231/256 (90%)	0.66	12 (5%) 34 26	60, 73, 81, 85	0
33	2b	231/256 (90%)	0.99	20 (8%) 17 13	67, 80, 86, 90	0
34	1c	206/239 (86%)	0.59	7 (3%) 48 40	52, 67, 75, 79	0
34	2c	206/239 (86%)	1.01	22 (10%) 12 10	65, 78, 85, 89	0
35	1d	208/209 (99%)	0.40	6 (2%) 54 45	51, 63, 73, 80	0
35	2d	208/209 (99%)	0.64	6 (2%) 54 45	58, 67, 76, 80	0
36	1e	148/162 (91%)	0.29	1 (0%) 84 79	42, 59, 69, 74	0
36	2e	148/162 (91%)	0.68	5 (3%) 48 40	58, 69, 76, 87	0
37	1f	100/101 (99%)	0.10	0 100 100	49, 59, 69, 72	0
37	2f	100/101 (99%)	0.28	0 100 100	55, 65, 72, 79	0
38	1g	155/156 (99%)	0.37	2 (1%) 74 67	58, 66, 73, 81	0
38	2g	155/156 (99%)	0.97	11 (7%) 23 18	69, 76, 82, 89	0
39	1h	137/138 (99%)	0.30	1 (0%) 84 79	51, 61, 69, 74	0
39	2h	137/138 (99%)	0.49	2 (1%) 71 64	61, 71, 76, 81	0
40	1i	127/128 (99%)	0.82	8 (6%) 27 21	56, 71, 79, 82	0
40	2i	126/128 (98%)	1.69	42 (33%) 1 1	70, 80, 85, 90	0
41	1j	97/105 (92%)	1.06	13 (13%) 8 7	54, 72, 82, 84	0
41	2j	96/105 (91%)	1.36	19 (19%) 3 3	69, 81, 86, 88	0
42	1k	114/129 (88%)	0.18	1 (0%) 81 75	37, 57, 69, 71	0
42	2k	114/129 (88%)	0.49	4 (3%) 47 39	55, 68, 74, 78	0
43	1l	121/132 (91%)	0.23	0 100 100	40, 53, 63, 77	0
43	2l	121/132 (91%)	0.45	2 (1%) 69 61	49, 61, 70, 71	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
44	1m	116/126 (92%)	0.48	6 (5%) 34 26	56, 68, 75, 80	0
44	2m	114/126 (90%)	1.33	23 (20%) 3 3	71, 79, 86, 88	0
45	1n	60/61 (98%)	0.60	3 (5%) 35 28	57, 65, 72, 76	0
45	2n	60/61 (98%)	1.54	16 (26%) 2 2	70, 80, 88, 89	0
46	1o	88/89 (98%)	0.29	1 (1%) 77 71	43, 59, 71, 78	0
46	2o	88/89 (98%)	0.54	2 (2%) 61 52	57, 68, 77, 83	0
47	1p	82/88 (93%)	0.81	3 (3%) 45 37	53, 65, 74, 81	0
47	2p	82/88 (93%)	0.77	4 (4%) 36 28	54, 63, 74, 76	0
48	1q	99/105 (94%)	0.37	3 (3%) 52 44	50, 61, 69, 75	0
48	2q	99/105 (94%)	0.41	0 100 100	55, 62, 72, 76	0
49	1r	68/88 (77%)	-0.08	0 100 100	50, 58, 72, 81	0
49	2r	68/88 (77%)	0.34	0 100 100	62, 69, 77, 81	0
50	1s	83/93 (89%)	0.58	2 (2%) 59 51	60, 70, 77, 80	0
50	2s	83/93 (89%)	1.35	18 (21%) 3 3	70, 82, 87, 88	0
51	1t	96/106 (90%)	0.62	4 (4%) 41 33	55, 65, 74, 79	0
51	2t	98/106 (92%)	0.52	4 (4%) 42 34	48, 62, 73, 78	0
52	1u	23/27 (85%)	1.10	2 (8%) 17 13	65, 68, 73, 75	0
52	2u	23/27 (85%)	1.95	8 (34%) 1 1	72, 79, 82, 85	0
53	1y	97/113 (85%)	0.45	5 (5%) 34 26	47, 57, 69, 78	0
53	2y	96/113 (84%)	1.42	22 (22%) 2 3	63, 74, 81, 83	0
All	All	20766/21468 (96%)	0.18	665 (3%) 50 42	12, 57, 84, 104	0

All (665) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	1A	1087	G	8.2
34	1c	2	GLY	7.1
45	2n	2	ALA	6.9
23	2l	2	SER	6.1
1	1A	1089	G	5.2
7	1H	2	SER	5.0
1	1A	1064	C	5.0
53	2y	98	ALA	4.8
52	2u	14	TRP	4.6
40	2i	125	TYR	4.6

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Mol	Chain	Res	Type	RSRZ
1	1A	1076	C	4.5
1	2A	2162	G	4.5
44	2m	116	THR	4.4
1	2A	2153	G	4.3
32	1a	1036	G	4.3
52	2u	11	GLY	4.3
40	1i	75	ASP	4.2
53	2y	40	ILE	4.2
1	2A	2106	G	4.1
29	27	48	LYS	4.1
33	2b	152	PHE	4.1
45	2n	18	VAL	4.1
1	1A	1176	G	4.1
1	2A	2138	C	4.0
40	2i	10	ARG	4.0
40	2i	127	LYS	4.0
1	1A	1086	A	4.0
50	2s	9	VAL	3.9
1	1A	1077	A	3.9
1	1A	2147	G	3.9
32	2a	1030(A)	G	3.9
1	1A	1088	A	3.9
51	1t	103	GLY	3.9
40	1i	66	ARG	3.8
40	2i	109	VAL	3.8
1	1A	1090	U	3.8
1	1A	1091	G	3.8
26	24	39	CYS	3.8
1	1A	1104	C	3.8
6	2G	160	VAL	3.8
1	1A	1102	C	3.7
12	2Q	59	ARG	3.7
1	2A	1076	C	3.7
1	2A	2174	C	3.7
1	2A	2152	G	3.7
21	2Z	191	VAL	3.7
41	2j	55	LYS	3.7
44	2m	102	ARG	3.7
53	1y	98	ALA	3.7
1	2A	1075	C	3.7
26	24	49	PHE	3.6
32	2a	1030(B)	C	3.6

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Mol	Chain	Res	Type	RSRZ
40	2i	7	THR	3.6
6	2G	39	ILE	3.6
1	1A	1067	A	3.6
1	1A	888	C	3.6
1	2A	2147	G	3.6
38	2g	2	ALA	3.6
45	1n	2	ALA	3.6
45	2n	29	ARG	3.5
39	2h	2	LEU	3.5
26	24	56	VAL	3.5
1	2A	1083	U	3.5
2	1B	1	U	3.5
53	2y	8	LYS	3.5
1	1A	1072	C	3.5
1	2A	1064	C	3.5
1	1A	1103	A	3.5
1	2A	2125	G	3.5
1	1A	1063	G	3.4
1	2A	2116	G	3.4
6	2G	28	VAL	3.4
53	1y	95	ARG	3.4
1	1A	1057	A	3.4
53	2y	38	HIS	3.4
34	2c	2	GLY	3.4
1	2A	2124	G	3.3
1	2A	2133	G	3.3
1	2A	2159	G	3.3
1	1A	1078	U	3.3
52	2u	2	GLY	3.3
51	2t	6	PRO	3.3
1	2A	1085	A	3.3
1	1A	2139	C	3.3
1	2A	2136	C	3.3
6	2G	76	SER	3.3
26	24	66	SER	3.3
41	2j	54	PHE	3.3
53	2y	33	HIS	3.3
46	2o	86	GLY	3.3
15	1T	130	ALA	3.3
32	1a	1001	A	3.3
40	2i	114	TYR	3.2
8	2I	146	ALA	3.2

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Mol	Chain	Res	Type	RSRZ
1	1A	1058	G	3.2
1	1A	2153	G	3.2
40	2i	102	LEU	3.2
45	2n	55	GLY	3.2
41	2j	37	PRO	3.2
40	2i	43	ALA	3.2
53	2y	9	GLN	3.2
1	1A	1080	C	3.2
20	1Y	1	MET	3.2
1	2A	2127	G	3.2
40	2i	119	ALA	3.2
1	1A	1065	U	3.2
32	2a	1235	U	3.2
24	12	70	GLN	3.2
50	2s	30	LEU	3.2
40	2i	115	GLY	3.2
6	1G	48	GLU	3.2
41	1j	78	ASN	3.2
32	2a	1036	G	3.2
1	1A	2143	C	3.2
33	1b	7	VAL	3.1
1	2A	1067	A	3.1
1	1A	1081	U	3.1
32	2a	1257	U	3.1
44	1m	2	ALA	3.1
1	2A	1536	C	3.1
41	2j	59	SER	3.1
52	1u	5	ASP	3.1
1	2A	2319	G	3.1
32	2a	973	G	3.1
32	2a	1202	G	3.1
45	2n	30	ALA	3.1
40	2i	11	LYS	3.1
32	1a	1492	A	3.1
53	2y	35	ILE	3.1
34	2c	162	GLN	3.1
40	2i	6	GLY	3.1
23	1l	2	SER	3.1
1	2A	2135	A	3.1
53	2y	61	LEU	3.0
33	2b	136	VAL	3.0
32	2a	630	G	3.0

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Mol	Chain	Res	Type	RSRZ
48	1q	99	SER	3.0
1	1A	2107	C	3.0
44	2m	9	ILE	3.0
1	1A	1084	A	3.0
1	1A	1085	A	3.0
33	1b	36	ARG	3.0
40	2i	15	ALA	3.0
1	1A	1026	U	3.0
1	2A	2137	C	3.0
1	2A	2134	A	3.0
44	2m	3	ARG	3.0
44	2m	113	PRO	3.0
14	2S	31	SER	3.0
40	2i	126	SER	3.0
1	1A	1082	U	3.0
32	1a	1026	G	3.0
40	2i	123	PRO	3.0
41	2j	38	ILE	3.0
40	2i	75	ASP	2.9
1	2A	2148	G	2.9
1	2A	2157	G	2.9
6	2G	38	VAL	2.9
38	2g	33	ASP	2.9
1	2A	2176	A	2.9
32	1a	1003	G	2.9
33	2b	164	VAL	2.9
15	1T	37	GLY	2.9
34	1c	62	ASP	2.9
38	2g	16	LEU	2.9
40	2i	46	ALA	2.9
32	1a	1030	C	2.9
1	1A	1071	G	2.9
32	2a	1124	G	2.9
50	2s	35	SER	2.9
40	2i	69	GLY	2.9
53	2y	54	ILE	2.9
33	1b	237	ALA	2.9
45	2n	5	ALA	2.9
29	27	1	MET	2.9
1	2A	652(B)	A	2.8
1	2A	1046	A	2.8
1	2A	2107	C	2.8

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Mol	Chain	Res	Type	RSRZ
1	2A	2146	C	2.8
1	2A	2169	A	2.8
3	2D	55	GLY	2.8
34	2c	152	ILE	2.8
48	1q	100	LYS	2.8
14	2S	92	TYR	2.8
50	2s	58	VAL	2.8
34	2c	175	LEU	2.8
1	2A	2139	C	2.8
1	1A	1083	U	2.8
35	2d	164	ALA	2.8
1	2A	2123	G	2.8
1	2A	2165	G	2.8
36	2e	109	ILE	2.8
41	1j	76	ASN	2.8
26	14	45	GLY	2.8
50	2s	2	PRO	2.8
1	2A	34	C	2.8
32	1a	1037	C	2.8
33	2b	165	VAL	2.8
40	2i	14	VAL	2.8
40	2i	108	VAL	2.8
52	1u	24	ARG	2.8
40	2i	36	TYR	2.8
6	2G	90	LEU	2.8
1	2A	1074	G	2.8
44	2m	6	GLY	2.8
36	2e	17	ALA	2.8
41	2j	19	SER	2.8
8	2I	3	VAL	2.8
14	2S	98	VAL	2.8
42	1k	60	ALA	2.8
53	2y	50	ALA	2.8
51	2t	7	LYS	2.8
34	2c	5	ILE	2.8
41	1j	31	GLY	2.8
44	2m	100	GLY	2.8
1	1A	2116	G	2.7
20	2Y	45	VAL	2.7
26	14	56	VAL	2.7
5	2F	181	LEU	2.7
44	2m	66	LEU	2.7

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Mol	Chain	Res	Type	RSRZ
41	1j	4	ILE	2.7
1	1A	1079	C	2.7
1	1A	2138	C	2.7
1	2A	2140	C	2.7
40	2i	86	VAL	2.7
40	1i	126	SER	2.7
1	2A	1089	G	2.7
1	2A	2154	G	2.7
50	2s	15	LEU	2.7
52	2u	5	ASP	2.7
43	2l	16	GLU	2.7
34	2c	192	THR	2.7
32	2a	1236	A	2.7
33	2b	148	TYR	2.7
1	2A	2151	G	2.7
1	2A	2793	G	2.7
38	2g	5	ARG	2.7
40	2i	94	ALA	2.7
1	1A	34	C	2.7
1	2A	2143	C	2.7
1	2A	2145	C	2.7
20	2Y	57	GLN	2.7
41	2j	64	GLU	2.7
1	1A	1066	U	2.7
44	2m	60	VAL	2.6
1	2A	2141	G	2.6
32	2a	1001(A)	G	2.6
32	2a	1031	G	2.6
50	2s	71	LEU	2.6
4	1E	163	GLU	2.6
40	2i	49	PRO	2.6
52	2u	15	ARG	2.6
14	2S	61	ASN	2.6
1	1A	1073	A	2.6
1	2A	2173	A	2.6
26	14	49	PHE	2.6
35	2d	158	ILE	2.6
1	2A	2155	G	2.6
45	1n	8	GLU	2.6
1	2A	2129	C	2.6
1	2A	2179	C	2.6
3	2D	259	THR	2.6

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Mol	Chain	Res	Type	RSRZ
44	1m	102	ARG	2.6
50	1s	13	ASP	2.6
35	2d	112	VAL	2.6
38	2g	80	VAL	2.6
42	2k	89	ALA	2.6
41	2j	50	ILE	2.6
53	2y	5	ILE	2.6
32	2a	1286	A	2.6
1	1A	1074	G	2.6
7	2H	24	VAL	2.6
33	1b	229	VAL	2.6
21	1Z	192	ALA	2.6
33	2b	149	LEU	2.6
34	2c	163	ALA	2.6
53	1y	97	ALA	2.6
6	2G	20	ILE	2.6
7	2H	42	ARG	2.6
1	2A	887	A	2.6
53	2y	7	SER	2.6
40	2i	106	ALA	2.5
1	2A	1091	G	2.5
1	2A	1104	C	2.5
32	2a	1027	C	2.5
6	2G	88	ILE	2.5
40	2i	18	PHE	2.5
38	2g	41	ARG	2.5
41	2j	53	PRO	2.5
40	1i	8	GLY	2.5
33	2b	15	VAL	2.5
38	2g	154	TYR	2.5
1	2A	2602	A	2.5
1	1A	2115	G	2.5
1	1A	2132	U	2.5
1	2A	2144	U	2.5
1	2A	2168	G	2.5
32	2a	1224	G	2.5
32	2a	1373	G	2.5
26	24	7	PRO	2.5
41	2j	60	ARG	2.5
35	1d	167	GLY	2.5
33	1b	187	LEU	2.5
44	2m	87	TYR	2.5

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Mol	Chain	Res	Type	RSRZ
41	2j	75	ILE	2.5
50	2s	4	SER	2.5
1	1A	2117	A	2.5
36	2e	20	GLN	2.5
47	2p	26	ARG	2.5
50	2s	37	ARG	2.5
1	1A	1075	C	2.5
32	2a	1030	C	2.5
40	2i	8	GLY	2.5
1	2A	2121	G	2.5
6	2G	3	LEU	2.5
32	1a	1024	G	2.5
32	2a	1003	G	2.5
32	2a	1220	G	2.5
32	2a	1290	G	2.5
40	2i	96	LEU	2.5
38	2g	25	ALA	2.5
7	2H	136	ILE	2.5
41	1j	77	PRO	2.5
35	1d	2	GLY	2.5
53	2y	44	GLU	2.5
32	1a	1030(B)	C	2.5
52	2u	13	ILE	2.5
26	14	59	PHE	2.5
1	2A	2160	G	2.4
32	2a	1048	G	2.4
32	2a	1190	G	2.4
52	2u	6	ARG	2.4
26	14	57	GLU	2.4
34	2c	161	GLU	2.4
48	1q	98	LEU	2.4
32	2a	1148	U	2.4
41	1j	86	MET	2.4
44	2m	54	VAL	2.4
3	1D	275	LYS	2.4
8	1I	147	GLN	2.4
1	1A	2106	G	2.4
1	2A	2131	G	2.4
33	2b	97	TRP	2.4
1	1A	2158	A	2.4
32	1a	1035	A	2.4
41	1j	75	ILE	2.4

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Mol	Chain	Res	Type	RSRZ
3	1D	276	LYS	2.4
33	2b	237	ALA	2.4
34	2c	146	ALA	2.4
26	14	52	THR	2.4
6	2G	146	TYR	2.4
34	2c	79	ARG	2.4
32	2a	1354	C	2.4
22	20	84	LEU	2.4
38	1g	16	LEU	2.4
6	2G	70	VAL	2.4
38	1g	8	GLU	2.4
1	2A	1059	G	2.4
1	2A	2120	G	2.4
32	2a	1033	G	2.4
32	2a	1219	U	2.4
45	2n	34	TYR	2.4
33	2b	232	PRO	2.4
51	1t	99	LEU	2.4
1	1A	2145	C	2.4
1	1A	2146	C	2.4
1	2A	2142	C	2.4
32	2a	1037	C	2.4
44	2m	39	ILE	2.4
1	1A	1420	U	2.4
1	1A	2119	A	2.4
1	1A	2602	A	2.4
1	2A	2114	A	2.4
32	1a	1030(A)	G	2.4
32	2a	1047	G	2.4
33	2b	21	ARG	2.4
44	2m	106	ASN	2.4
53	2y	4	ASN	2.4
6	2G	7	LEU	2.3
6	2G	87	PRO	2.3
34	2c	68	VAL	2.3
40	2i	17	VAL	2.3
44	2m	78	ILE	2.3
5	2F	21	ALA	2.3
33	1b	188	ALA	2.3
42	2k	15	ALA	2.3
44	2m	5	ALA	2.3
52	2u	8	THR	2.3

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Mol	Chain	Res	Type	RSRZ
1	2A	2130	U	2.3
1	2A	2150	U	2.3
32	2a	994	A	2.3
1	1A	1051	G	2.3
44	2m	101	GLN	2.3
43	2l	14	GLY	2.3
50	2s	70	LYS	2.3
6	2G	59	GLU	2.3
26	14	53	GLU	2.3
39	2h	4	ASP	2.3
15	2T	131	ALA	2.3
51	1t	76	ALA	2.3
1	2A	645	C	2.3
1	2A	2803	C	2.3
53	1y	2	THR	2.3
7	2H	21	PRO	2.3
25	23	2	PRO	2.3
26	24	67	TYR	2.3
6	2G	109	VAL	2.3
32	1a	1286	A	2.3
1	1A	1068	G	2.3
1	2A	2104	G	2.3
32	2a	1024	G	2.3
41	2j	40	LEU	2.3
1	1A	1092	C	2.3
1	2A	2111	C	2.3
1	2A	2175	C	2.3
32	1a	63	C	2.3
38	2g	28	ASN	2.3
45	2n	21	TYR	2.3
34	2c	176	HIS	2.3
32	1a	1493	A	2.3
3	1D	2	ALA	2.3
6	2G	158	ALA	2.3
33	1b	35	GLU	2.3
1	1A	2166	G	2.3
21	2Z	125	LEU	2.3
32	2a	1032	G	2.3
32	2a	1271	G	2.3
34	2c	52	LEU	2.3
41	2j	88	LEU	2.3
21	2Z	99	TYR	2.2

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Mol	Chain	Res	Type	RSRZ
33	2b	236	TYR	2.2
1	2A	2132	U	2.2
32	2a	979	C	2.2
35	1d	112	VAL	2.2
41	1j	38	ILE	2.2
44	1m	24	GLY	2.2
53	2y	49	VAL	2.2
53	2y	84	GLN	2.2
41	2j	63	PHE	2.2
34	2c	160	ALA	2.2
1	2A	1048	A	2.2
32	2a	1123	A	2.2
53	1y	70	MET	2.2
41	2j	8	LEU	2.2
42	2k	98	LEU	2.2
53	2y	42	SER	2.2
40	2i	97	LYS	2.2
35	2d	189	PRO	2.2
2	2B	23	G	2.2
8	1I	139	GLN	2.2
8	2I	107	VAL	2.2
32	1a	1031	G	2.2
34	1c	193	TYR	2.2
36	1e	22	GLY	2.2
45	2n	7	ILE	2.2
47	2p	19	ILE	2.2
47	2p	82	GLN	2.2
50	1s	84	GLY	2.2
26	24	16	CYS	2.2
1	1A	2150	U	2.2
40	2i	59	PHE	2.2
1	1A	2161	C	2.2
1	2A	1079	C	2.2
1	2A	2161	C	2.2
32	2a	1327	C	2.2
6	2G	45	GLU	2.2
9	2N	68	GLU	2.2
33	2b	186	ALA	2.2
34	2c	50	ALA	2.2
40	1i	46	ALA	2.2
40	2i	118	LYS	2.2
46	2o	48	LYS	2.2

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Mol	Chain	Res	Type	RSRZ
1	2A	1070	A	2.2
32	1a	1005	A	2.2
32	2a	1363(A)	A	2.2
45	2n	14	PRO	2.2
50	2s	76	PRO	2.2
51	2t	98	PRO	2.2
33	2b	73	THR	2.2
33	2b	190	THR	2.2
33	2b	214	ILE	2.2
40	2i	88	TYR	2.2
40	2i	92	TYR	2.2
6	1G	136	ARG	2.2
26	24	36	CYS	2.2
40	2i	9	ARG	2.2
41	2j	45	ARG	2.2
1	1A	1056	G	2.2
1	2A	2110	G	2.2
2	2B	41	U	2.2
21	2Z	188	ALA	2.2
26	24	30	GLU	2.2
32	2a	963	G	2.2
32	2a	1000	U	2.2
32	2a	1353	G	2.2
44	2m	70	LEU	2.2
1	2A	2105	C	2.2
32	2a	1320	C	2.2
12	2Q	55	VAL	2.2
40	1i	7	THR	2.2
41	1j	74	ILE	2.2
41	2j	72	VAL	2.2
6	2G	138	GLN	2.2
53	2y	58	ASN	2.2
15	1T	131	ALA	2.2
33	1b	129	GLU	2.2
44	1m	56	LEU	2.2
32	1a	1033	G	2.2
32	2a	1054	C	2.2
32	2a	1314	C	2.2
6	2G	165	THR	2.1
22	20	76	GLY	2.1
26	24	27	THR	2.1
41	1j	87	THR	2.1

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Mol	Chain	Res	Type	RSRZ
41	2j	67	THR	2.1
32	2a	1014	A	2.1
32	2a	1252	A	2.1
45	2n	3	ARG	2.1
14	2S	7	TYR	2.1
42	2k	25	TYR	2.1
50	2s	65	ASN	2.1
1	2A	614(A)	U	2.1
32	2a	1532	U	2.1
6	2G	140	ILE	2.1
46	1o	87	ILE	2.1
14	2S	53	SER	2.1
34	2c	155	GLY	2.1
1	1A	2186	G	2.1
1	2A	1039	G	2.1
1	2A	1049	C	2.1
1	2A	1118	C	2.1
3	2D	217	ARG	2.1
32	2a	1034	G	2.1
32	2a	1038	C	2.1
32	2a	1116	C	2.1
40	1i	42	ARG	2.1
41	1j	100	THR	2.1
50	2s	79	THR	2.1
33	2b	92	TYR	2.1
35	1d	157	LEU	2.1
40	2i	19	LEU	2.1
45	2n	50	LYS	2.1
45	1n	20	ALA	2.1
53	2y	27	LEU	2.1
1	2A	1073	A	2.1
32	2a	1030(D)	A	2.1
18	1W	30	GLU	2.1
40	2i	2	GLU	2.1
1	2A	2167	U	2.1
1	2A	2172	U	2.1
44	1m	113	PRO	2.1
14	2S	35	ILE	2.1
8	1I	136	VAL	2.1
39	1h	93	VAL	2.1
22	20	8	GLY	2.1
34	1c	159	GLY	2.1

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Mol	Chain	Res	Type	RSRZ
40	2i	105	ASP	2.1
50	2s	3	ARG	2.1
33	1b	19	HIS	2.1
34	2c	10	PHE	2.1
50	2s	33	THR	2.1
53	2y	6	THR	2.1
51	1t	10	LEU	2.1
53	2y	88	LEU	2.1
1	1A	1053	C	2.1
1	1A	2108	C	2.1
1	1A	2137	C	2.1
6	2G	50	ALA	2.1
1	1A	1093	G	2.1
8	1I	117	GLU	2.1
1	1A	2790	A	2.1
1	2A	1077	A	2.1
1	2A	2126	A	2.1
32	2a	975	A	2.1
53	2y	45	PRO	2.1
33	2b	200	ILE	2.1
36	2e	13	ILE	2.1
1	2A	2118	U	2.1
6	2G	156	ASP	2.1
16	2U	49	HIS	2.1
33	1b	22	LYS	2.1
33	1b	40	HIS	2.1
41	1j	54	PHE	2.1
44	2m	65	LYS	2.1
50	2s	14	HIS	2.1
6	2G	139	LEU	2.1
34	1c	87	LEU	2.1
21	2Z	173	ALA	2.1
34	2c	200	ALA	2.1
44	2m	18	ALA	2.1
44	2m	51	ALA	2.1
40	2i	4	TYR	2.1
47	1p	17	TYR	2.1
1	1A	886	C	2.1
1	2A	2164	C	2.1
33	1b	12	GLU	2.1
41	1j	64	GLU	2.1
41	2j	61	GLU	2.1

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Mol	Chain	Res	Type	RSRZ
35	2d	154	ASN	2.1
1	1A	2141	G	2.1
1	2A	1047	G	2.1
1	2A	1062	G	2.1
1	2A	2158	A	2.1
32	2a	1004	A	2.1
38	2g	156	TRP	2.1
44	2m	15	VAL	2.1
50	2s	11	VAL	2.1
20	2Y	1	MET	2.1
32	2a	1364	U	2.1
45	2n	31	ARG	2.1
15	2T	69	GLY	2.1
34	2c	4	LYS	2.1
45	2n	9	LYS	2.1
47	2p	10	GLY	2.1
51	2t	103	GLY	2.1
33	2b	118	LEU	2.0
35	2d	155	LEU	2.0
45	2n	39	LEU	2.0
6	2G	71	THR	2.0
26	24	65	ASP	2.0
45	2n	13	THR	2.0
34	2c	189	ALA	2.0
38	2g	83	ALA	2.0
44	2m	76	ALA	2.0
14	2S	36	TYR	2.0
6	2G	77	ILE	2.0
33	2b	162	ILE	2.0
1	1A	2129	C	2.0
1	2A	2128	C	2.0
1	2A	2178	C	2.0
27	25	60	VAL	2.0
32	1a	1027	C	2.0
32	2a	1066	C	2.0
32	2a	1234	C	2.0
34	1c	207	VAL	2.0
35	1d	73	ARG	2.0
44	2m	17	VAL	2.0
26	24	28	LYS	2.0
1	2A	229	A	2.0
2	2B	58	A	2.0

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Mol	Chain	Res	Type	RSRZ
32	2a	1044	A	2.0
44	1m	100	GLY	2.0
1	1A	2130	U	2.0
1	2A	271(K)	U	2.0
35	1d	194	LEU	2.0
40	1i	56	LEU	2.0
1	2A	2166	G	2.0
32	1a	1001(A)	G	2.0
32	1a	1002	G	2.0
32	2a	1002	G	2.0
40	2i	117	HIS	2.0
50	2s	63	THR	2.0
34	2c	60	ALA	2.0
40	2i	122	ALA	2.0
26	14	63	TYR	2.0
34	1c	201	TYR	2.0
40	2i	62	TYR	2.0
34	2c	77	ILE	2.0
47	1p	19	ILE	2.0
36	2e	10	MET	2.0
47	1p	1	MET	2.0
26	24	10	VAL	2.0
1	1A	889	C	2.0
1	2A	2108	C	2.0
2	2B	4	C	2.0

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

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
1	PSU	2A	1917	20/21	0.83	0.11	67,77,94,97	0
1	5MU	2A	1915	21/22	0.84	0.11	74,82,85,99	0
1	PSU	2A	1911	20/21	0.85	0.09	64,70,80,82	0
43	0TD	2l	92	10/11	0.85	0.15	52,59,64,79	0
1	5MU	1A	1915	21/22	0.86	0.11	64,70,80,81	0
32	PSU	2a	516	20/21	0.86	0.11	71,75,83,83	0
43	0TD	1l	92	10/11	0.86	0.14	43,54,57,67	0
32	2MG	2a	1207	24/25	0.87	0.14	80,85,90,95	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
32	M2G	2a	966	25/26	0.88	0.15	64,73,81,89	0
32	7MG	2a	527	24/25	0.89	0.13	53,61,67,69	0
32	5MC	2a	967	21/22	0.89	0.12	71,75,79,86	0
1	PSU	1A	1917	20/21	0.90	0.10	59,64,70,76	0
32	2MG	1a	1207	24/25	0.90	0.11	60,70,74,76	0
32	5MC	2a	1404	21/22	0.91	0.12	59,64,70,78	0
1	PSU	1A	1911	20/21	0.92	0.09	50,59,63,64	0
32	4OC	2a	1402	22/23	0.92	0.13	53,63,68,75	0
32	5MC	2a	1400	21/22	0.93	0.12	66,71,75,80	0
32	5MC	2a	1407	21/22	0.93	0.10	54,62,65,77	0
32	MA6	2a	1518	24/25	0.93	0.10	53,63,66,68	0
32	PSU	1a	516	20/21	0.93	0.10	51,60,64,64	0
1	4OC	2A	1920	21/23	0.94	0.08	58,66,69,71	0
32	UR3	2a	1498	21/22	0.94	0.10	54,58,66,67	0
32	5MC	1a	967	21/22	0.94	0.10	55,62,70,73	0
32	MA6	2a	1519	24/25	0.94	0.13	54,60,64,66	0
32	7MG	1a	527	24/25	0.94	0.10	39,47,53,55	0
32	M2G	1a	966	25/26	0.95	0.10	51,56,62,65	0
1	5MC	2A	1942	21/22	0.95	0.09	41,48,53,59	0
32	5MC	1a	1407	21/22	0.95	0.11	34,42,49,50	0
32	4OC	1a	1402	22/23	0.96	0.10	40,46,48,58	0
1	5MC	2A	1962	21/22	0.96	0.09	36,40,49,56	0
1	PSU	2A	2605	20/21	0.96	0.08	28,33,39,44	0
32	5MC	1a	1404	21/22	0.96	0.09	39,42,49,50	0
1	4OC	1A	1920	21/23	0.96	0.10	35,54,58,62	0
32	MA6	1a	1518	24/25	0.96	0.10	33,40,46,51	0
32	MA6	1a	1519	24/25	0.96	0.10	35,41,48,53	0
1	5MU	2A	1939	21/22	0.96	0.08	28,34,36,37	0
1	2MA	2A	2503	23/24	0.97	0.08	24,29,34,35	0
1	2MU	2A	2552	21/23	0.97	0.07	28,33,36,40	0
32	5MC	1a	1400	21/22	0.97	0.08	34,48,52,54	0
1	5MC	1A	1962	21/22	0.97	0.07	27,33,36,40	0
1	5MU	1A	1939	21/22	0.97	0.07	17,23,25,27	0
1	5MC	1A	1942	21/22	0.97	0.07	24,30,34,37	0
32	UR3	1a	1498	21/22	0.97	0.09	36,42,45,55	0
1	OMG	2A	2251	24/25	0.97	0.08	28,34,39,40	0
1	2MA	1A	2503	23/24	0.98	0.06	11,15,18,19	0
1	2MU	1A	2552	21/23	0.98	0.06	24,27,31,32	0
1	PSU	1A	2605	20/21	0.98	0.06	20,25,28,30	0
1	OMG	1A	2251	24/25	0.98	0.06	14,19,20,20	0

5.3 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.4 Ligands ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
54	MG	2B	211	1/1	0.43	0.24	78,78,78,78	0
54	MG	1a	3203	1/1	0.48	0.22	69,69,69,69	0
54	MG	1A	4003	1/1	0.49	0.19	31,31,31,31	0
54	MG	1B	225	1/1	0.53	0.15	53,53,53,53	0
54	MG	2A	3574	1/1	0.55	0.17	71,71,71,71	0
54	MG	2a	3025	1/1	0.56	0.25	74,74,74,74	0
54	MG	2A	3646	1/1	0.57	0.24	76,76,76,76	0
54	MG	2A	3726	1/1	0.57	0.18	55,55,55,55	0
54	MG	1A	3936	1/1	0.59	0.20	30,30,30,30	0
54	MG	1g	202	1/1	0.60	0.16	78,78,78,78	0
54	MG	2A	3394	1/1	0.61	0.22	47,47,47,47	0
54	MG	2A	3428	1/1	0.63	0.14	81,81,81,81	0
54	MG	1P	203	1/1	0.63	0.47	49,49,49,49	0
57	ARG	1F	316	12/12	0.63	0.20	54,60,69,71	0
54	MG	1A	3872	1/1	0.64	0.17	72,72,72,72	0
54	MG	1a	3156	1/1	0.64	0.15	60,60,60,60	0
56	MPD	2B	220	8/8	0.64	0.24	60,65,71,80	0
54	MG	1B	226	1/1	0.64	0.16	60,60,60,60	0
54	MG	1A	3308	1/1	0.65	0.22	82,82,82,82	0
54	MG	2a	3105	1/1	0.65	0.28	80,80,80,80	0
54	MG	2a	3099	1/1	0.66	0.24	76,76,76,76	0
54	MG	2V	201	1/1	0.66	0.17	70,70,70,70	0
54	MG	2a	3183	1/1	0.67	0.13	88,88,88,88	0
54	MG	1A	3380	1/1	0.67	0.15	31,31,31,31	0
54	MG	2A	3449	1/1	0.67	0.22	64,64,64,64	0
54	MG	1B	210	1/1	0.68	0.13	49,49,49,49	0
54	MG	2B	206	1/1	0.68	0.21	78,78,78,78	0
54	MG	1A	3534	1/1	0.68	0.16	53,53,53,53	0
54	MG	2a	3100	1/1	0.68	0.20	80,80,80,80	0
54	MG	1a	3001	1/1	0.69	0.26	77,77,77,77	0
54	MG	1D	310	1/1	0.69	0.24	33,33,33,33	0
54	MG	2A	3456	1/1	0.69	0.17	62,62,62,62	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	1a	3192	1/1	0.69	0.25	68,68,68,68	0
54	MG	2a	3051	1/1	0.70	0.17	79,79,79,79	0
54	MG	2a	3061	1/1	0.70	0.26	75,75,75,75	0
54	MG	2A	3488	1/1	0.70	0.17	65,65,65,65	0
54	MG	1A	3714	1/1	0.70	0.17	50,50,50,50	0
54	MG	1a	3022	1/1	0.71	0.23	59,59,59,59	0
54	MG	2A	3279	1/1	0.71	0.27	71,71,71,71	0
54	MG	1A	3517	1/1	0.71	0.11	35,35,35,35	0
54	MG	1A	3354	1/1	0.71	0.15	52,52,52,52	0
54	MG	1A	3448	1/1	0.71	0.16	28,28,28,28	0
54	MG	2A	3746	1/1	0.71	0.11	71,71,71,71	0
54	MG	2A	3289	1/1	0.72	0.20	75,75,75,75	0
54	MG	1A	3041	1/1	0.72	0.20	57,57,57,57	0
54	MG	2a	3020	1/1	0.72	0.27	72,72,72,72	0
54	MG	2A	3475	1/1	0.72	0.21	57,57,57,57	0
54	MG	1A	3887	1/1	0.72	0.17	61,61,61,61	0
54	MG	2A	3524	1/1	0.72	0.21	43,43,43,43	0
54	MG	2A	3581	1/1	0.73	0.16	36,36,36,36	0
54	MG	2A	3629	1/1	0.73	0.19	43,43,43,43	0
54	MG	1A	3034	1/1	0.73	0.33	57,57,57,57	0
54	MG	2A	3228	1/1	0.73	0.14	52,52,52,52	0
54	MG	2A	3509	1/1	0.73	0.16	51,51,51,51	0
54	MG	2A	3512	1/1	0.73	0.16	72,72,72,72	0
54	MG	1a	3195	1/1	0.73	0.15	62,62,62,62	0
54	MG	2G	201	1/1	0.73	0.15	78,78,78,78	0
54	MG	2O	202	1/1	0.73	0.13	63,63,63,63	0
54	MG	1A	4021	1/1	0.73	0.20	43,43,43,43	0
54	MG	1A	3604	1/1	0.74	0.14	25,25,25,25	0
54	MG	1A	3321	1/1	0.74	0.26	63,63,63,63	0
54	MG	1A	3984	1/1	0.74	0.12	51,51,51,51	0
54	MG	2A	3464	1/1	0.74	0.16	44,44,44,44	0
54	MG	1A	3458	1/1	0.74	0.14	47,47,47,47	0
54	MG	1a	3225	1/1	0.74	0.26	67,67,67,67	0
54	MG	2A	3724	1/1	0.74	0.12	58,58,58,58	0
54	MG	2A	3397	1/1	0.74	0.16	40,40,40,40	0
54	MG	1a	3165	1/1	0.75	0.23	59,59,59,59	0
54	MG	1a	3242	1/1	0.75	0.22	70,70,70,70	0
54	MG	1A	3698	1/1	0.75	0.11	76,76,76,76	0
54	MG	1a	3119	1/1	0.75	0.15	49,49,49,49	0
54	MG	1A	3697	1/1	0.75	0.12	64,64,64,64	0
54	MG	2a	3064	1/1	0.75	0.28	73,73,73,73	0
54	MG	2B	202	1/1	0.75	0.14	70,70,70,70	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	2A	3533	1/1	0.75	0.29	65,65,65,65	0
54	MG	1a	3224	1/1	0.75	0.13	64,64,64,64	0
54	MG	2E	304	1/1	0.75	0.16	26,26,26,26	0
54	MG	2a	3196	1/1	0.75	0.17	68,68,68,68	0
54	MG	2j	201	1/1	0.75	0.11	65,65,65,65	0
54	MG	2A	3577	1/1	0.75	0.17	30,30,30,30	0
54	MG	2A	3474	1/1	0.75	0.13	60,60,60,60	0
54	MG	1a	3201	1/1	0.76	0.12	73,73,73,73	0
54	MG	2A	3627	1/1	0.76	0.15	34,34,34,34	0
54	MG	2A	3050	1/1	0.76	0.16	58,58,58,58	0
54	MG	1A	4051	1/1	0.76	0.21	38,38,38,38	0
54	MG	2G	203	1/1	0.76	0.18	72,72,72,72	0
54	MG	2A	3709	1/1	0.76	0.27	70,70,70,70	0
54	MG	1A	4015	1/1	0.76	0.38	47,47,47,47	0
54	MG	2A	3286	1/1	0.76	0.15	54,54,54,54	0
54	MG	1A	3658	1/1	0.76	0.10	56,56,56,56	0
54	MG	1a	3120	1/1	0.76	0.15	82,82,82,82	0
58	ZN	14	102	1/1	0.76	0.19	139,139,139,139	0
54	MG	2A	3565	1/1	0.77	0.23	60,60,60,60	0
54	MG	2A	3566	1/1	0.77	0.21	84,84,84,84	0
54	MG	1A	3781	1/1	0.77	0.15	22,22,22,22	0
54	MG	2A	3423	1/1	0.77	0.40	69,69,69,69	0
54	MG	1a	3189	1/1	0.77	0.11	64,64,64,64	0
54	MG	2a	3028	1/1	0.77	0.20	71,71,71,71	0
54	MG	2A	3033	1/1	0.77	0.13	58,58,58,58	0
54	MG	1a	3057	1/1	0.77	0.17	75,75,75,75	0
54	MG	2A	3114	1/1	0.77	0.13	60,60,60,60	0
54	MG	1a	3068	1/1	0.77	0.20	64,64,64,64	0
54	MG	2A	3242	1/1	0.77	0.29	66,66,66,66	0
54	MG	2A	3247	1/1	0.77	0.15	64,64,64,64	0
54	MG	2a	3129	1/1	0.77	0.45	79,79,79,79	0
54	MG	1A	3843	1/1	0.77	0.13	31,31,31,31	0
54	MG	1A	3176	1/1	0.77	0.15	59,59,59,59	0
54	MG	2A	3518	1/1	0.77	0.13	67,67,67,67	0
54	MG	1A	3741	1/1	0.77	0.13	36,36,36,36	0
54	MG	1a	3162	1/1	0.77	0.23	64,64,64,64	0
54	MG	2A	3538	1/1	0.77	0.24	67,67,67,67	0
54	MG	2A	3429	1/1	0.78	0.19	44,44,44,44	0
54	MG	1A	3636	1/1	0.78	0.11	25,25,25,25	0
54	MG	1T	201	1/1	0.78	0.24	55,55,55,55	0
54	MG	2A	3346	1/1	0.78	0.14	52,52,52,52	0
54	MG	1a	3247	1/1	0.78	0.13	62,62,62,62	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	1a	3276	1/1	0.78	0.10	68,68,68,68	0
54	MG	1a	3138	1/1	0.78	0.19	52,52,52,52	0
54	MG	2a	3096	1/1	0.78	0.21	71,71,71,71	0
54	MG	1A	3383	1/1	0.78	0.11	28,28,28,28	0
54	MG	1a	3042	1/1	0.79	0.21	62,62,62,62	0
54	MG	1a	3151	1/1	0.79	0.22	73,73,73,73	0
54	MG	2A	3525	1/1	0.79	0.17	62,62,62,62	0
54	MG	2G	202	1/1	0.79	0.23	67,67,67,67	0
54	MG	2A	3528	1/1	0.79	0.15	39,39,39,39	0
54	MG	2a	3107	1/1	0.79	0.13	69,69,69,69	0
54	MG	2a	3111	1/1	0.79	0.26	55,55,55,55	0
54	MG	2a	3122	1/1	0.79	0.09	67,67,67,67	0
54	MG	2A	3691	1/1	0.79	0.13	63,63,63,63	0
54	MG	2a	3133	1/1	0.79	0.19	60,60,60,60	0
54	MG	2a	3182	1/1	0.79	0.18	74,74,74,74	0
54	MG	2A	3377	1/1	0.79	0.13	63,63,63,63	0
54	MG	1A	3569	1/1	0.79	0.21	34,34,34,34	0
54	MG	14	101	1/1	0.79	0.10	71,71,71,71	0
54	MG	2A	3256	1/1	0.79	0.10	61,61,61,61	0
54	MG	1A	3723	1/1	0.79	0.14	54,54,54,54	0
54	MG	1A	3533	1/1	0.79	0.14	19,19,19,19	0
54	MG	2A	3458	1/1	0.80	0.26	55,55,55,55	0
54	MG	1y	201	1/1	0.80	0.12	62,62,62,62	0
54	MG	2A	3471	1/1	0.80	0.14	68,68,68,68	0
54	MG	1A	3716	1/1	0.80	0.21	42,42,42,42	0
54	MG	1G	201	1/1	0.80	0.12	70,70,70,70	0
54	MG	2a	3072	1/1	0.80	0.10	61,61,61,61	0
54	MG	1A	3417	1/1	0.80	0.17	20,20,20,20	0
54	MG	2A	3349	1/1	0.80	0.24	57,57,57,57	0
54	MG	2A	3127	1/1	0.80	0.18	60,60,60,60	0
54	MG	2A	3730	1/1	0.80	0.45	57,57,57,57	0
54	MG	2A	3146	1/1	0.80	0.18	52,52,52,52	0
54	MG	2A	3203	1/1	0.80	0.12	59,59,59,59	0
54	MG	2a	3119	1/1	0.80	0.17	61,61,61,61	0
54	MG	2A	3401	1/1	0.80	0.19	74,74,74,74	0
54	MG	1A	3421	1/1	0.80	0.22	43,43,43,43	0
54	MG	1a	3271	1/1	0.80	0.10	60,60,60,60	0
54	MG	1A	3594	1/1	0.80	0.11	31,31,31,31	0
54	MG	2A	3548	1/1	0.80	0.14	34,34,34,34	0
54	MG	2A	3431	1/1	0.80	0.11	74,74,74,74	0
54	MG	2A	3441	1/1	0.80	0.18	51,51,51,51	0
54	MG	1a	3095	1/1	0.80	0.14	60,60,60,60	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	2X	101	1/1	0.80	0.14	59,59,59,59	0
54	MG	2A	3265	1/1	0.80	0.11	66,66,66,66	0
54	MG	1A	3592	1/1	0.81	0.12	52,52,52,52	0
54	MG	1A	3499	1/1	0.81	0.13	37,37,37,37	0
54	MG	1A	3927	1/1	0.81	0.09	15,15,15,15	0
54	MG	1a	3107	1/1	0.81	0.19	63,63,63,63	0
54	MG	2a	3073	1/1	0.81	0.14	67,67,67,67	0
54	MG	2a	3091	1/1	0.81	0.25	59,59,59,59	0
54	MG	1a	3116	1/1	0.81	0.18	54,54,54,54	0
54	MG	1A	3598	1/1	0.81	0.35	34,34,34,34	0
54	MG	1A	3970	1/1	0.81	0.12	43,43,43,43	0
54	MG	1A	3721	1/1	0.81	0.26	41,41,41,41	0
54	MG	2B	204	1/1	0.81	0.17	76,76,76,76	0
54	MG	1A	3326	1/1	0.81	0.10	48,48,48,48	0
54	MG	1A	4007	1/1	0.81	0.14	73,73,73,73	0
54	MG	2A	3285	1/1	0.81	0.13	50,50,50,50	0
54	MG	1A	3330	1/1	0.81	0.11	34,34,34,34	0
54	MG	2A	3459	1/1	0.81	0.14	53,53,53,53	0
54	MG	2a	3177	1/1	0.81	0.12	69,69,69,69	0
54	MG	1A	3183	1/1	0.81	0.28	32,32,32,32	0
54	MG	1a	3175	1/1	0.81	0.16	54,54,54,54	0
54	MG	2A	3602	1/1	0.81	0.12	38,38,38,38	0
54	MG	2a	3199	1/1	0.81	0.10	73,73,73,73	0
54	MG	2A	3618	1/1	0.81	0.12	64,64,64,64	0
54	MG	2A	3620	1/1	0.81	0.10	28,28,28,28	0
54	MG	1A	3496	1/1	0.81	0.12	22,22,22,22	0
54	MG	2A	3352	1/1	0.81	0.14	33,33,33,33	0
54	MG	2A	3532	1/1	0.82	0.10	56,56,56,56	0
54	MG	1A	3953	1/1	0.82	0.12	52,52,52,52	0
54	MG	2A	3409	1/1	0.82	0.11	62,62,62,62	0
54	MG	2A	3169	1/1	0.82	0.17	68,68,68,68	0
54	MG	2A	3559	1/1	0.82	0.11	57,57,57,57	0
54	MG	1A	3780	1/1	0.82	0.15	42,42,42,42	0
54	MG	23	101	1/1	0.82	0.26	57,57,57,57	0
54	MG	2a	3003	1/1	0.82	0.08	51,51,51,51	0
54	MG	2a	3011	1/1	0.82	0.20	73,73,73,73	0
54	MG	1A	3982	1/1	0.82	0.16	40,40,40,40	0
54	MG	1G	202	1/1	0.82	0.09	61,61,61,61	0
54	MG	1A	3027	1/1	0.82	0.15	64,64,64,64	0
54	MG	1a	3137	1/1	0.82	0.27	64,64,64,64	0
54	MG	2A	3584	1/1	0.82	0.19	57,57,57,57	0
54	MG	1A	3688	1/1	0.82	0.15	45,45,45,45	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	1a	3143	1/1	0.82	0.11	49,49,49,49	0
54	MG	1A	3851	1/1	0.82	0.12	24,24,24,24	0
54	MG	2A	3621	1/1	0.82	0.17	47,47,47,47	0
54	MG	2A	3463	1/1	0.82	0.14	64,64,64,64	0
54	MG	1A	3864	1/1	0.82	0.17	38,38,38,38	0
54	MG	2A	3635	1/1	0.82	0.18	40,40,40,40	0
54	MG	2A	3467	1/1	0.82	0.14	38,38,38,38	0
54	MG	2A	3675	1/1	0.82	0.13	49,49,49,49	0
54	MG	1a	3161	1/1	0.82	0.15	70,70,70,70	0
54	MG	2A	3313	1/1	0.82	0.10	53,53,53,53	0
54	MG	2A	3341	1/1	0.82	0.13	36,36,36,36	0
54	MG	1A	3689	1/1	0.82	0.30	31,31,31,31	0
54	MG	2A	3503	1/1	0.82	0.22	76,76,76,76	0
54	MG	2A	3736	1/1	0.82	0.21	65,65,65,65	0
54	MG	1A	3632	1/1	0.82	0.12	52,52,52,52	0
54	MG	1A	3075	1/1	0.82	0.41	49,49,49,49	0
54	MG	2A	3368	1/1	0.82	0.17	63,63,63,63	0
54	MG	2A	3065	1/1	0.82	0.09	41,41,41,41	0
54	MG	2B	207	1/1	0.82	0.19	63,63,63,63	0
54	MG	1a	3183	1/1	0.82	0.10	65,65,65,65	0
54	MG	2B	215	1/1	0.82	0.12	74,74,74,74	0
54	MG	1A	3762	1/1	0.82	0.13	51,51,51,51	0
54	MG	1a	3149	1/1	0.83	0.18	64,64,64,64	0
54	MG	1A	3609	1/1	0.83	0.11	26,26,26,26	0
54	MG	1a	3272	1/1	0.83	0.15	60,60,60,60	0
54	MG	1a	3274	1/1	0.83	0.12	58,58,58,58	0
54	MG	1A	3545	1/1	0.83	0.14	50,50,50,50	0
54	MG	1A	3694	1/1	0.83	0.14	59,59,59,59	0
54	MG	2A	3492	1/1	0.83	0.10	23,23,23,23	0
54	MG	1A	3846	1/1	0.83	0.15	39,39,39,39	0
54	MG	1y	202	1/1	0.83	0.12	53,53,53,53	0
54	MG	1A	3572	1/1	0.83	0.14	43,43,43,43	0
54	MG	1a	3098	1/1	0.83	0.18	43,43,43,43	0
54	MG	2A	3064	1/1	0.83	0.15	69,69,69,69	0
54	MG	1A	3852	1/1	0.83	0.12	42,42,42,42	0
54	MG	2A	3733	1/1	0.83	0.13	82,82,82,82	0
54	MG	1a	3109	1/1	0.83	0.13	41,41,41,41	0
54	MG	1A	3562	1/1	0.83	0.11	22,22,22,22	0
54	MG	1A	3752	1/1	0.83	0.17	53,53,53,53	0
54	MG	2a	3109	1/1	0.83	0.19	63,63,63,63	0
54	MG	2A	3537	1/1	0.83	0.25	65,65,65,65	0
54	MG	2A	3157	1/1	0.83	0.12	40,40,40,40	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	1a	3198	1/1	0.83	0.14	73,73,73,73	0
54	MG	1A	3875	1/1	0.83	0.11	47,47,47,47	0
54	MG	1a	3127	1/1	0.83	0.16	65,65,65,65	0
54	MG	2a	3172	1/1	0.83	0.12	68,68,68,68	0
54	MG	2D	309	1/1	0.83	0.10	58,58,58,58	0
54	MG	1A	3706	1/1	0.83	0.14	62,62,62,62	0
54	MG	2A	3452	1/1	0.83	0.14	74,74,74,74	0
54	MG	1A	4048	1/1	0.83	0.28	58,58,58,58	0
54	MG	1a	3228	1/1	0.83	0.13	75,75,75,75	0
54	MG	1a	3240	1/1	0.83	0.28	70,70,70,70	0
54	MG	2A	3591	1/1	0.83	0.22	65,65,65,65	0
54	MG	1a	3013	1/1	0.83	0.11	69,69,69,69	0
54	MG	2I	102	1/1	0.83	0.09	63,63,63,63	0
54	MG	2A	3380	1/1	0.84	0.12	28,28,28,28	0
54	MG	2I	201	1/1	0.84	0.14	66,66,66,66	0
54	MG	2A	3385	1/1	0.84	0.10	70,70,70,70	0
54	MG	2A	3039	1/1	0.84	0.35	66,66,66,66	0
54	MG	1A	3995	1/1	0.84	0.15	44,44,44,44	0
54	MG	1A	4000	1/1	0.84	0.20	67,67,67,67	0
54	MG	2A	3405	1/1	0.84	0.12	54,54,54,54	0
54	MG	1a	3193	1/1	0.84	0.16	72,72,72,72	0
54	MG	1A	3530	1/1	0.84	0.13	14,14,14,14	0
54	MG	1a	3118	1/1	0.84	0.16	55,55,55,55	0
54	MG	1A	3898	1/1	0.84	0.14	33,33,33,33	0
54	MG	2A	3150	1/1	0.84	0.25	66,66,66,66	0
54	MG	2a	3041	1/1	0.84	0.13	60,60,60,60	0
54	MG	2A	3607	1/1	0.84	0.12	56,56,56,56	0
54	MG	2a	3055	1/1	0.84	0.25	68,68,68,68	0
54	MG	2A	3154	1/1	0.84	0.22	64,64,64,64	0
54	MG	2A	3448	1/1	0.84	0.16	46,46,46,46	0
54	MG	2a	3070	1/1	0.84	0.19	63,63,63,63	0
54	MG	1A	3922	1/1	0.84	0.10	19,19,19,19	0
54	MG	2A	3163	1/1	0.84	0.26	68,68,68,68	0
54	MG	2a	3074	1/1	0.84	0.18	66,66,66,66	0
54	MG	1A	3692	1/1	0.84	0.13	46,46,46,46	0
54	MG	1A	4029	1/1	0.84	0.20	43,43,43,43	0
54	MG	2A	3205	1/1	0.84	0.11	56,56,56,56	0
54	MG	2A	3460	1/1	0.84	0.23	55,55,55,55	0
54	MG	2A	3213	1/1	0.84	0.36	65,65,65,65	0
54	MG	2A	3227	1/1	0.84	0.10	52,52,52,52	0
54	MG	1A	4032	1/1	0.84	0.22	58,58,58,58	0
54	MG	1a	3017	1/1	0.84	0.11	60,60,60,60	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	1A	4035	1/1	0.84	0.14	43,43,43,43	0
54	MG	1A	3642	1/1	0.84	0.13	55,55,55,55	0
54	MG	1a	3153	1/1	0.84	0.13	60,60,60,60	0
54	MG	2a	3132	1/1	0.84	0.11	53,53,53,53	0
54	MG	1A	3861	1/1	0.84	0.10	50,50,50,50	0
54	MG	2a	3137	1/1	0.84	0.12	46,46,46,46	0
54	MG	1a	3065	1/1	0.84	0.20	60,60,60,60	0
54	MG	1A	3387	1/1	0.84	0.16	42,42,42,42	0
54	MG	1a	3071	1/1	0.84	0.17	62,62,62,62	0
54	MG	1l	202	1/1	0.84	0.12	59,59,59,59	0
54	MG	1t	201	1/1	0.84	0.15	67,67,67,67	0
54	MG	1a	3172	1/1	0.84	0.15	66,66,66,66	0
54	MG	1A	3551	1/1	0.84	0.12	48,48,48,48	0
56	MPD	2A	3759	8/8	0.84	0.25	37,46,50,56	0
54	MG	2A	3025	1/1	0.84	0.14	58,58,58,58	0
54	MG	2A	3032	1/1	0.84	0.15	28,28,28,28	0
54	MG	1A	3735	1/1	0.84	0.10	23,23,23,23	0
58	ZN	24	501	1/1	0.84	0.22	156,156,156,156	0
54	MG	1A	3946	1/1	0.85	0.11	45,45,45,45	0
54	MG	1n	102	1/1	0.85	0.11	49,49,49,49	0
54	MG	1A	3238	1/1	0.85	0.14	69,69,69,69	0
54	MG	1A	3968	1/1	0.85	0.14	25,25,25,25	0
54	MG	1A	3791	1/1	0.85	0.13	20,20,20,20	0
54	MG	1A	3977	1/1	0.85	0.10	48,48,48,48	0
54	MG	1A	3978	1/1	0.85	0.11	53,53,53,53	0
54	MG	2A	3544	1/1	0.85	0.15	58,58,58,58	0
54	MG	2A	3547	1/1	0.85	0.20	56,56,56,56	0
54	MG	19	103	1/1	0.85	0.17	82,82,82,82	0
54	MG	2A	3381	1/1	0.85	0.15	58,58,58,58	0
54	MG	1A	3841	1/1	0.85	0.34	43,43,43,43	0
54	MG	2A	3393	1/1	0.85	0.17	44,44,44,44	0
54	MG	1a	3168	1/1	0.85	0.23	68,68,68,68	0
54	MG	2a	3035	1/1	0.85	0.17	50,50,50,50	0
54	MG	2a	3040	1/1	0.85	0.17	50,50,50,50	0
54	MG	1A	3069	1/1	0.85	0.34	25,25,25,25	0
54	MG	1A	3985	1/1	0.85	0.10	28,28,28,28	0
54	MG	1A	3318	1/1	0.85	0.13	36,36,36,36	0
54	MG	2A	3585	1/1	0.85	0.15	46,46,46,46	0
54	MG	1a	3186	1/1	0.85	0.12	64,64,64,64	0
54	MG	2a	3068	1/1	0.85	0.20	72,72,72,72	0
54	MG	2A	3415	1/1	0.85	0.11	63,63,63,63	0
54	MG	2A	3131	1/1	0.85	0.34	61,61,61,61	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	1A	3480	1/1	0.85	0.12	37,37,37,37	0
54	MG	1A	3623	1/1	0.85	0.22	33,33,33,33	0
54	MG	2a	3082	1/1	0.85	0.09	68,68,68,68	0
54	MG	2a	3087	1/1	0.85	0.18	57,57,57,57	0
54	MG	2A	3430	1/1	0.85	0.15	51,51,51,51	0
54	MG	1a	3062	1/1	0.85	0.23	71,71,71,71	0
54	MG	1A	3484	1/1	0.85	0.14	48,48,48,48	0
54	MG	1A	3319	1/1	0.85	0.10	63,63,63,63	0
54	MG	1A	3871	1/1	0.85	0.14	19,19,19,19	0
54	MG	2A	3171	1/1	0.85	0.13	50,50,50,50	0
54	MG	1A	3056	1/1	0.85	0.15	55,55,55,55	0
54	MG	2A	3705	1/1	0.85	0.12	39,39,39,39	0
54	MG	1A	3648	1/1	0.85	0.09	33,33,33,33	0
54	MG	1a	3102	1/1	0.85	0.22	66,66,66,66	0
54	MG	1A	3503	1/1	0.85	0.14	15,15,15,15	0
54	MG	1a	3235	1/1	0.85	0.12	57,57,57,57	0
54	MG	2A	3235	1/1	0.85	0.18	50,50,50,50	0
54	MG	1A	3662	1/1	0.85	0.11	27,27,27,27	0
54	MG	2a	3165	1/1	0.85	0.15	76,76,76,76	0
54	MG	1A	3674	1/1	0.85	0.11	25,25,25,25	0
54	MG	1B	202	1/1	0.85	0.18	58,58,58,58	0
54	MG	1B	207	1/1	0.85	0.08	51,51,51,51	0
54	MG	2B	205	1/1	0.85	0.14	59,59,59,59	0
54	MG	2a	3191	1/1	0.85	0.11	75,75,75,75	0
54	MG	2a	3195	1/1	0.85	0.10	71,71,71,71	0
54	MG	1A	3576	1/1	0.85	0.11	53,53,53,53	0
54	MG	1B	224	1/1	0.85	0.10	64,64,64,64	0
54	MG	1A	3930	1/1	0.85	0.14	39,39,39,39	0
54	MG	1A	3217	1/1	0.85	0.31	57,57,57,57	0
56	MPD	2A	3760	8/8	0.85	0.20	54,60,63,69	0
54	MG	2D	301	1/1	0.85	0.25	40,40,40,40	0
54	MG	2D	303	1/1	0.85	0.19	48,48,48,48	0
54	MG	2A	3294	1/1	0.85	0.20	24,24,24,24	0
54	MG	2A	3310	1/1	0.85	0.11	37,37,37,37	0
54	MG	1a	3131	1/1	0.86	0.13	62,62,62,62	0
54	MG	20	102	1/1	0.86	0.12	54,54,54,54	0
54	MG	1A	3247	1/1	0.86	0.11	35,35,35,35	0
54	MG	2A	3424	1/1	0.86	0.12	61,61,61,61	0
54	MG	1a	3007	1/1	0.86	0.14	55,55,55,55	0
54	MG	1A	3942	1/1	0.86	0.15	52,52,52,52	0
54	MG	2a	3019	1/1	0.86	0.12	51,51,51,51	0
54	MG	1A	3429	1/1	0.86	0.14	58,58,58,58	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	2a	3022	1/1	0.86	0.24	52,52,52,52	0
54	MG	1A	3438	1/1	0.86	0.14	21,21,21,21	0
54	MG	1a	3025	1/1	0.86	0.13	44,44,44,44	0
54	MG	1A	3067	1/1	0.86	0.17	35,35,35,35	0
54	MG	1d	304	1/1	0.86	0.15	46,46,46,46	0
54	MG	1a	3159	1/1	0.86	0.20	64,64,64,64	0
54	MG	2a	3043	1/1	0.86	0.17	59,59,59,59	0
54	MG	2a	3046	1/1	0.86	0.11	62,62,62,62	0
54	MG	2A	3250	1/1	0.86	0.08	49,49,49,49	0
54	MG	1B	201	1/1	0.86	0.14	59,59,59,59	0
54	MG	1A	3634	1/1	0.86	0.11	58,58,58,58	0
54	MG	2A	3634	1/1	0.86	0.14	27,27,27,27	0
54	MG	2a	3065	1/1	0.86	0.23	58,58,58,58	0
54	MG	1A	3751	1/1	0.86	0.14	43,43,43,43	0
54	MG	1A	3154	1/1	0.86	0.24	35,35,35,35	0
54	MG	2A	3667	1/1	0.86	0.11	58,58,58,58	0
54	MG	2A	3669	1/1	0.86	0.09	44,44,44,44	0
54	MG	1A	3476	1/1	0.86	0.12	12,12,12,12	0
54	MG	2A	3678	1/1	0.86	0.13	29,29,29,29	0
54	MG	1a	3082	1/1	0.86	0.33	63,63,63,63	0
54	MG	2A	3695	1/1	0.86	0.12	59,59,59,59	0
54	MG	2A	3290	1/1	0.86	0.17	36,36,36,36	0
54	MG	2A	3027	1/1	0.86	0.17	46,46,46,46	0
54	MG	2A	3716	1/1	0.86	0.15	61,61,61,61	0
54	MG	2A	3296	1/1	0.86	0.16	40,40,40,40	0
54	MG	2A	3479	1/1	0.86	0.16	47,47,47,47	0
54	MG	1a	3088	1/1	0.86	0.11	58,58,58,58	0
54	MG	1A	3773	1/1	0.86	0.15	64,64,64,64	0
54	MG	2A	3332	1/1	0.86	0.12	48,48,48,48	0
54	MG	1A	3412	1/1	0.86	0.12	40,40,40,40	0
54	MG	2A	3749	1/1	0.86	0.13	53,53,53,53	0
54	MG	1A	3879	1/1	0.86	0.17	31,31,31,31	0
54	MG	1a	3103	1/1	0.86	0.12	57,57,57,57	0
54	MG	1A	3652	1/1	0.86	0.36	40,40,40,40	0
54	MG	2A	3107	1/1	0.86	0.14	58,58,58,58	0
54	MG	2A	3526	1/1	0.86	0.14	45,45,45,45	0
54	MG	1A	4001	1/1	0.86	0.11	67,67,67,67	0
54	MG	1A	3788	1/1	0.86	0.11	37,37,37,37	0
54	MG	1a	3202	1/1	0.86	0.07	70,70,70,70	0
54	MG	1A	3239	1/1	0.86	0.23	56,56,56,56	0
54	MG	1a	3222	1/1	0.86	0.16	51,51,51,51	0
54	MG	2D	310	1/1	0.86	0.17	41,41,41,41	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	2D	311	1/1	0.86	0.10	33,33,33,33	0
54	MG	2A	3152	1/1	0.86	0.18	55,55,55,55	0
56	MPD	1T	207	8/8	0.86	0.24	69,71,74,77	0
54	MG	1A	3812	1/1	0.86	0.16	59,59,59,59	0
54	MG	19	101	1/1	0.86	0.12	57,57,57,57	0
54	MG	2A	3558	1/1	0.86	0.09	56,56,56,56	0
54	MG	1A	3814	1/1	0.86	0.10	36,36,36,36	0
54	MG	2A	3560	1/1	0.86	0.09	66,66,66,66	0
54	MG	2A	3167	1/1	0.86	0.32	56,56,56,56	0
54	MG	1A	3807	1/1	0.87	0.08	29,29,29,29	0
54	MG	2a	3010	1/1	0.87	0.28	66,66,66,66	0
54	MG	2A	3257	1/1	0.87	0.10	54,54,54,54	0
54	MG	1A	3904	1/1	0.87	0.14	49,49,49,49	0
54	MG	2A	3002	1/1	0.87	0.15	44,44,44,44	0
54	MG	1a	3072	1/1	0.87	0.24	64,64,64,64	0
54	MG	1A	3725	1/1	0.87	0.15	69,69,69,69	0
54	MG	1A	3391	1/1	0.87	0.10	31,31,31,31	0
54	MG	1A	3825	1/1	0.87	0.26	25,25,25,25	0
54	MG	2A	3647	1/1	0.87	0.10	65,65,65,65	0
54	MG	10	102	1/1	0.87	0.09	38,38,38,38	0
54	MG	10	103	1/1	0.87	0.12	50,50,50,50	0
54	MG	2A	3671	1/1	0.87	0.10	72,72,72,72	0
54	MG	11	105	1/1	0.87	0.13	46,46,46,46	0
54	MG	2A	3676	1/1	0.87	0.10	72,72,72,72	0
54	MG	1A	3737	1/1	0.87	0.09	36,36,36,36	0
54	MG	2A	3682	1/1	0.87	0.08	21,21,21,21	0
54	MG	2A	3485	1/1	0.87	0.08	62,62,62,62	0
54	MG	2A	3074	1/1	0.87	0.07	51,51,51,51	0
54	MG	2a	3069	1/1	0.87	0.11	74,74,74,74	0
54	MG	2A	3084	1/1	0.87	0.13	67,67,67,67	0
54	MG	15	101	1/1	0.87	0.18	34,34,34,34	0
54	MG	1a	3112	1/1	0.87	0.13	69,69,69,69	0
54	MG	15	107	1/1	0.87	0.14	63,63,63,63	0
54	MG	2A	3513	1/1	0.87	0.08	40,40,40,40	0
54	MG	1A	3322	1/1	0.87	0.24	51,51,51,51	0
54	MG	2A	3519	1/1	0.87	0.15	55,55,55,55	0
54	MG	1A	3645	1/1	0.87	0.09	30,30,30,30	0
54	MG	2a	3097	1/1	0.87	0.22	71,71,71,71	0
54	MG	2A	3743	1/1	0.87	0.10	54,54,54,54	0
54	MG	1A	3646	1/1	0.87	0.13	21,21,21,21	0
54	MG	1a	3004	1/1	0.87	0.13	58,58,58,58	0
54	MG	1a	3232	1/1	0.87	0.15	31,31,31,31	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	1A	3754	1/1	0.87	0.11	49,49,49,49	0
54	MG	1a	3136	1/1	0.87	0.20	54,54,54,54	0
54	MG	2a	3116	1/1	0.87	0.15	73,73,73,73	0
54	MG	1A	3442	1/1	0.87	0.16	21,21,21,21	0
54	MG	2a	3120	1/1	0.87	0.10	55,55,55,55	0
54	MG	2A	3400	1/1	0.87	0.10	46,46,46,46	0
54	MG	2A	3540	1/1	0.87	0.19	75,75,75,75	0
54	MG	1A	3611	1/1	0.87	0.11	53,53,53,53	0
54	MG	1A	3447	1/1	0.87	0.12	48,48,48,48	0
54	MG	2a	3135	1/1	0.87	0.18	62,62,62,62	0
54	MG	2A	3179	1/1	0.87	0.19	52,52,52,52	0
54	MG	1A	3631	1/1	0.87	0.19	45,45,45,45	0
54	MG	1a	3027	1/1	0.87	0.21	64,64,64,64	0
54	MG	2A	3206	1/1	0.87	0.15	52,52,52,52	0
54	MG	2a	3180	1/1	0.87	0.09	58,58,58,58	0
54	MG	2a	3181	1/1	0.87	0.13	53,53,53,53	0
54	MG	1a	3040	1/1	0.87	0.12	68,68,68,68	0
54	MG	1a	3279	1/1	0.87	0.25	68,68,68,68	0
54	MG	1A	3333	1/1	0.87	0.13	45,45,45,45	0
54	MG	1A	3102	1/1	0.87	0.08	48,48,48,48	0
54	MG	2A	3432	1/1	0.87	0.11	39,39,39,39	0
54	MG	2A	3435	1/1	0.87	0.18	65,65,65,65	0
54	MG	2A	3436	1/1	0.87	0.16	70,70,70,70	0
54	MG	1A	3992	1/1	0.87	0.29	46,46,46,46	0
54	MG	2A	3592	1/1	0.87	0.09	30,30,30,30	0
54	MG	1A	3795	1/1	0.87	0.17	37,37,37,37	0
54	MG	1a	3067	1/1	0.87	0.13	67,67,67,67	0
54	MG	27	102	1/1	0.87	0.29	36,36,36,36	0
54	MG	28	102	1/1	0.87	0.16	52,52,52,52	0
54	MG	2a	3002	1/1	0.87	0.12	54,54,54,54	0
54	MG	2B	217	1/1	0.88	0.10	71,71,71,71	0
54	MG	2A	3500	1/1	0.88	0.17	65,65,65,65	0
54	MG	2A	3246	1/1	0.88	0.16	51,51,51,51	0
54	MG	15	102	1/1	0.88	0.31	31,31,31,31	0
54	MG	1A	3143	1/1	0.88	0.22	57,57,57,57	0
54	MG	1A	3886	1/1	0.88	0.11	33,33,33,33	0
54	MG	2A	3514	1/1	0.88	0.09	64,64,64,64	0
54	MG	1a	3129	1/1	0.88	0.15	44,44,44,44	0
54	MG	1b	301	1/1	0.88	0.23	64,64,64,64	0
54	MG	2A	3274	1/1	0.88	0.14	63,63,63,63	0
54	MG	2A	3277	1/1	0.88	0.12	49,49,49,49	0
54	MG	1A	3377	1/1	0.88	0.08	43,43,43,43	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	1a	3133	1/1	0.88	0.13	67,67,67,67	0
54	MG	2A	3529	1/1	0.88	0.44	45,45,45,45	0
54	MG	1A	4023	1/1	0.88	0.08	85,85,85,85	0
54	MG	1A	3494	1/1	0.88	0.10	25,25,25,25	0
54	MG	1A	3255	1/1	0.88	0.11	39,39,39,39	0
54	MG	1A	3266	1/1	0.88	0.19	62,62,62,62	0
54	MG	1a	3016	1/1	0.88	0.12	68,68,68,68	0
54	MG	2A	3543	1/1	0.88	0.12	63,63,63,63	0
54	MG	1A	4044	1/1	0.88	0.08	35,35,35,35	0
54	MG	1a	3020	1/1	0.88	0.13	61,61,61,61	0
54	MG	2A	3319	1/1	0.88	0.18	50,50,50,50	0
54	MG	2A	3549	1/1	0.88	0.10	44,44,44,44	0
54	MG	2A	3321	1/1	0.88	0.11	57,57,57,57	0
54	MG	1A	3925	1/1	0.88	0.11	35,35,35,35	0
54	MG	2a	3024	1/1	0.88	0.10	43,43,43,43	0
54	MG	1a	3023	1/1	0.88	0.26	64,64,64,64	0
54	MG	1A	3701	1/1	0.88	0.14	20,20,20,20	0
54	MG	2a	3032	1/1	0.88	0.16	66,66,66,66	0
54	MG	2a	3033	1/1	0.88	0.25	57,57,57,57	0
54	MG	2A	3036	1/1	0.88	0.13	70,70,70,70	0
54	MG	1A	3276	1/1	0.88	0.17	51,51,51,51	0
54	MG	2A	3360	1/1	0.88	0.18	39,39,39,39	0
54	MG	1a	3029	1/1	0.88	0.24	59,59,59,59	0
54	MG	1a	3038	1/1	0.88	0.18	63,63,63,63	0
54	MG	1A	3711	1/1	0.88	0.13	60,60,60,60	0
54	MG	2a	3052	1/1	0.88	0.18	54,54,54,54	0
54	MG	1A	3329	1/1	0.88	0.22	69,69,69,69	0
54	MG	1A	3820	1/1	0.88	0.11	58,58,58,58	0
54	MG	2A	3600	1/1	0.88	0.09	51,51,51,51	0
54	MG	2A	3386	1/1	0.88	0.11	47,47,47,47	0
54	MG	2A	3605	1/1	0.88	0.10	55,55,55,55	0
54	MG	2A	3092	1/1	0.88	0.08	66,66,66,66	0
54	MG	2A	3093	1/1	0.88	0.29	64,64,64,64	0
54	MG	2A	3104	1/1	0.88	0.24	55,55,55,55	0
54	MG	1B	213	1/1	0.88	0.10	59,59,59,59	0
54	MG	2A	3111	1/1	0.88	0.12	41,41,41,41	0
54	MG	1A	3520	1/1	0.88	0.09	31,31,31,31	0
54	MG	2A	3631	1/1	0.88	0.09	74,74,74,74	0
54	MG	2A	3115	1/1	0.88	0.16	69,69,69,69	0
54	MG	2A	3410	1/1	0.88	0.17	31,31,31,31	0
54	MG	2A	3642	1/1	0.88	0.15	51,51,51,51	0
54	MG	1A	3840	1/1	0.88	0.11	21,21,21,21	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	1A	3108	1/1	0.88	0.28	35,35,35,35	0
54	MG	2A	3665	1/1	0.88	0.11	42,42,42,42	0
54	MG	2A	3134	1/1	0.88	0.08	47,47,47,47	0
54	MG	1A	3464	1/1	0.88	0.08	45,45,45,45	0
54	MG	1A	3606	1/1	0.88	0.07	33,33,33,33	0
54	MG	2a	3115	1/1	0.88	0.18	72,72,72,72	0
54	MG	1a	3075	1/1	0.88	0.22	50,50,50,50	0
54	MG	1A	3661	1/1	0.88	0.10	45,45,45,45	0
54	MG	1H	201	1/1	0.88	0.26	62,62,62,62	0
54	MG	1a	3204	1/1	0.88	0.11	47,47,47,47	0
54	MG	1a	3209	1/1	0.88	0.17	57,57,57,57	0
54	MG	1a	3219	1/1	0.88	0.18	70,70,70,70	0
54	MG	2A	3170	1/1	0.88	0.18	59,59,59,59	0
54	MG	1A	3207	1/1	0.88	0.28	39,39,39,39	0
54	MG	1a	3097	1/1	0.88	0.21	55,55,55,55	0
54	MG	2A	3186	1/1	0.88	0.20	57,57,57,57	0
54	MG	2A	3193	1/1	0.88	0.12	59,59,59,59	0
54	MG	2A	3200	1/1	0.88	0.19	50,50,50,50	0
54	MG	1R	204	1/1	0.88	0.14	38,38,38,38	0
54	MG	1A	3855	1/1	0.88	0.09	39,39,39,39	0
54	MG	1T	206	1/1	0.88	0.20	48,48,48,48	0
54	MG	2A	3212	1/1	0.88	0.08	45,45,45,45	0
54	MG	2a	3184	1/1	0.88	0.09	58,58,58,58	0
54	MG	1A	3544	1/1	0.88	0.61	27,27,27,27	0
54	MG	2A	3750	1/1	0.88	0.12	45,45,45,45	0
54	MG	2A	3751	1/1	0.88	0.11	57,57,57,57	0
54	MG	2A	3754	1/1	0.88	0.13	47,47,47,47	0
54	MG	2B	201	1/1	0.88	0.16	73,73,73,73	0
54	MG	1A	3677	1/1	0.88	0.10	36,36,36,36	0
54	MG	1A	3680	1/1	0.88	0.15	63,63,63,63	0
54	MG	1A	3681	1/1	0.88	0.18	25,25,25,25	0
54	MG	2A	3240	1/1	0.88	0.09	65,65,65,65	0
54	MG	2A	3241	1/1	0.88	0.08	53,53,53,53	0
54	MG	2A	3491	1/1	0.88	0.12	63,63,63,63	0
54	MG	1A	3617	1/1	0.88	0.11	36,36,36,36	0
54	MG	2A	3732	1/1	0.89	0.15	61,61,61,61	0
54	MG	1A	3973	1/1	0.89	0.10	50,50,50,50	0
54	MG	2A	3734	1/1	0.89	0.14	67,67,67,67	0
54	MG	1A	3976	1/1	0.89	0.11	61,61,61,61	0
54	MG	1A	3148	1/1	0.89	0.08	50,50,50,50	0
54	MG	2A	3744	1/1	0.89	0.08	54,54,54,54	0
54	MG	1A	3389	1/1	0.89	0.14	36,36,36,36	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	2A	3748	1/1	0.89	0.11	53,53,53,53	0
54	MG	1A	3065	1/1	0.89	0.09	44,44,44,44	0
54	MG	1A	3822	1/1	0.89	0.13	54,54,54,54	0
54	MG	1a	3178	1/1	0.89	0.13	47,47,47,47	0
54	MG	2A	3753	1/1	0.89	0.12	57,57,57,57	0
54	MG	2A	3451	1/1	0.89	0.08	50,50,50,50	0
54	MG	2A	3757	1/1	0.89	0.10	46,46,46,46	0
54	MG	1A	3405	1/1	0.89	0.11	36,36,36,36	0
54	MG	1A	3519	1/1	0.89	0.14	32,32,32,32	0
54	MG	2B	203	1/1	0.89	0.12	61,61,61,61	0
54	MG	1A	3618	1/1	0.89	0.10	28,28,28,28	0
54	MG	2A	3172	1/1	0.89	0.08	53,53,53,53	0
54	MG	1A	3074	1/1	0.89	0.06	37,37,37,37	0
54	MG	2A	3180	1/1	0.89	0.08	58,58,58,58	0
54	MG	1A	3704	1/1	0.89	0.12	52,52,52,52	0
54	MG	2B	212	1/1	0.89	0.10	53,53,53,53	0
54	MG	2B	214	1/1	0.89	0.09	60,60,60,60	0
54	MG	2A	3465	1/1	0.89	0.11	60,60,60,60	0
54	MG	1A	3628	1/1	0.89	0.15	35,35,35,35	0
54	MG	2B	218	1/1	0.89	0.09	56,56,56,56	0
54	MG	2A	3468	1/1	0.89	0.13	65,65,65,65	0
54	MG	2D	302	1/1	0.89	0.39	42,42,42,42	0
54	MG	2A	3196	1/1	0.89	0.20	47,47,47,47	0
54	MG	2A	3197	1/1	0.89	0.19	60,60,60,60	0
54	MG	2A	3199	1/1	0.89	0.09	56,56,56,56	0
54	MG	1a	3196	1/1	0.89	0.09	49,49,49,49	0
54	MG	2D	312	1/1	0.89	0.21	46,46,46,46	0
54	MG	2A	3482	1/1	0.89	0.09	38,38,38,38	0
54	MG	2F	301	1/1	0.89	0.06	40,40,40,40	0
54	MG	1a	3197	1/1	0.89	0.14	60,60,60,60	0
54	MG	1A	3120	1/1	0.89	0.17	31,31,31,31	0
54	MG	1A	3191	1/1	0.89	0.13	45,45,45,45	0
54	MG	1A	3860	1/1	0.89	0.14	34,34,34,34	0
54	MG	1A	3274	1/1	0.89	0.16	51,51,51,51	0
54	MG	2Q	202	1/1	0.89	0.26	44,44,44,44	0
54	MG	2A	3215	1/1	0.89	0.25	60,60,60,60	0
54	MG	2A	3505	1/1	0.89	0.08	41,41,41,41	0
54	MG	2A	3220	1/1	0.89	0.24	54,54,54,54	0
54	MG	2A	3226	1/1	0.89	0.29	62,62,62,62	0
54	MG	1A	4027	1/1	0.89	0.12	42,42,42,42	0
54	MG	1a	3034	1/1	0.89	0.12	47,47,47,47	0
54	MG	2A	3230	1/1	0.89	0.16	59,59,59,59	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	1a	3217	1/1	0.89	0.29	72,72,72,72	0
54	MG	2A	3521	1/1	0.89	0.12	53,53,53,53	0
54	MG	2a	3006	1/1	0.89	0.28	67,67,67,67	0
54	MG	1A	3539	1/1	0.89	0.15	55,55,55,55	0
54	MG	1A	3124	1/1	0.89	0.16	50,50,50,50	0
54	MG	1A	3724	1/1	0.89	0.09	32,32,32,32	0
54	MG	1A	3287	1/1	0.89	0.14	62,62,62,62	0
54	MG	1A	3878	1/1	0.89	0.11	41,41,41,41	0
54	MG	2A	3249	1/1	0.89	0.31	46,46,46,46	0
54	MG	1A	3550	1/1	0.89	0.08	24,24,24,24	0
54	MG	2A	3255	1/1	0.89	0.25	57,57,57,57	0
54	MG	1a	3234	1/1	0.89	0.17	64,64,64,64	0
54	MG	1a	3066	1/1	0.89	0.09	66,66,66,66	0
54	MG	1A	3882	1/1	0.89	0.09	34,34,34,34	0
54	MG	2a	3039	1/1	0.89	0.18	77,77,77,77	0
54	MG	1A	3361	1/1	0.89	0.09	45,45,45,45	0
54	MG	1B	205	1/1	0.89	0.07	40,40,40,40	0
54	MG	1a	3267	1/1	0.89	0.15	54,54,54,54	0
54	MG	1B	206	1/1	0.89	0.24	43,43,43,43	0
54	MG	1A	3739	1/1	0.89	0.10	40,40,40,40	0
54	MG	1a	3078	1/1	0.89	0.15	62,62,62,62	0
54	MG	1B	209	1/1	0.89	0.07	55,55,55,55	0
54	MG	2A	3563	1/1	0.89	0.27	61,61,61,61	0
54	MG	2a	3063	1/1	0.89	0.21	77,77,77,77	0
54	MG	1a	3083	1/1	0.89	0.10	69,69,69,69	0
54	MG	1A	3894	1/1	0.89	0.10	31,31,31,31	0
54	MG	2a	3066	1/1	0.89	0.26	59,59,59,59	0
54	MG	2A	3298	1/1	0.89	0.12	48,48,48,48	0
54	MG	2A	3303	1/1	0.89	0.16	49,49,49,49	0
54	MG	2A	3578	1/1	0.89	0.13	32,32,32,32	0
54	MG	1a	3089	1/1	0.89	0.25	66,66,66,66	0
54	MG	1a	3093	1/1	0.89	0.13	43,43,43,43	0
54	MG	1A	3364	1/1	0.89	0.09	45,45,45,45	0
54	MG	1A	3374	1/1	0.89	0.12	21,21,21,21	0
54	MG	2A	3326	1/1	0.89	0.11	51,51,51,51	0
54	MG	2a	3089	1/1	0.89	0.19	71,71,71,71	0
54	MG	2A	3597	1/1	0.89	0.09	66,66,66,66	0
54	MG	2A	3329	1/1	0.89	0.13	35,35,35,35	0
54	MG	1o	102	1/1	0.89	0.14	48,48,48,48	0
54	MG	1A	3917	1/1	0.89	0.11	58,58,58,58	0
54	MG	2A	3344	1/1	0.89	0.13	35,35,35,35	0
54	MG	2A	3611	1/1	0.89	0.12	32,32,32,32	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	2A	3614	1/1	0.89	0.17	47,47,47,47	0
54	MG	1a	3101	1/1	0.89	0.12	48,48,48,48	0
54	MG	1A	3659	1/1	0.89	0.09	49,49,49,49	0
54	MG	1A	3376	1/1	0.89	0.11	42,42,42,42	0
54	MG	2A	3622	1/1	0.89	0.08	66,66,66,66	0
54	MG	2A	3356	1/1	0.89	0.11	59,59,59,59	0
54	MG	1D	316	1/1	0.89	0.15	41,41,41,41	0
54	MG	2a	3121	1/1	0.89	0.21	68,68,68,68	0
54	MG	2A	3362	1/1	0.89	0.09	30,30,30,30	0
54	MG	1E	306	1/1	0.89	0.11	39,39,39,39	0
54	MG	1F	313	1/1	0.89	0.13	58,58,58,58	0
54	MG	2A	3636	1/1	0.89	0.12	57,57,57,57	0
54	MG	1F	315	1/1	0.89	0.14	60,60,60,60	0
54	MG	1A	3289	1/1	0.89	0.19	64,64,64,64	0
54	MG	2a	3148	1/1	0.89	0.11	63,63,63,63	0
54	MG	2a	3151	1/1	0.89	0.18	74,74,74,74	0
54	MG	1A	3673	1/1	0.89	0.09	40,40,40,40	0
54	MG	2a	3168	1/1	0.89	0.11	49,49,49,49	0
54	MG	2a	3169	1/1	0.89	0.11	45,45,45,45	0
54	MG	1A	3214	1/1	0.89	0.07	37,37,37,37	0
54	MG	2a	3174	1/1	0.89	0.09	59,59,59,59	0
54	MG	1a	3124	1/1	0.89	0.14	64,64,64,64	0
54	MG	1A	3940	1/1	0.89	0.10	50,50,50,50	0
54	MG	1P	205	1/1	0.89	0.10	59,59,59,59	0
54	MG	1R	202	1/1	0.89	0.18	29,29,29,29	0
54	MG	1A	3676	1/1	0.89	0.10	14,14,14,14	0
54	MG	2A	3402	1/1	0.89	0.21	62,62,62,62	0
54	MG	2A	3679	1/1	0.89	0.12	30,30,30,30	0
54	MG	2A	3680	1/1	0.89	0.09	29,29,29,29	0
54	MG	1S	201	1/1	0.89	0.10	54,54,54,54	0
54	MG	2A	3687	1/1	0.89	0.10	66,66,66,66	0
54	MG	1A	3381	1/1	0.89	0.15	15,15,15,15	0
54	MG	1T	203	1/1	0.89	0.08	55,55,55,55	0
56	MPD	1a	3280	8/8	0.89	0.16	47,64,65,66	0
54	MG	1A	3597	1/1	0.89	0.22	43,43,43,43	0
54	MG	1U	208	1/1	0.89	0.25	36,36,36,36	0
54	MG	1A	3954	1/1	0.89	0.13	50,50,50,50	0
57	ARG	1B	228	12/12	0.89	0.11	22,42,59,67	0
54	MG	1A	3962	1/1	0.89	0.07	32,32,32,32	0
54	MG	1A	3035	1/1	0.89	0.10	41,41,41,41	0
54	MG	1A	3683	1/1	0.89	0.14	45,45,45,45	0
54	MG	13	103	1/1	0.90	0.12	37,37,37,37	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	1A	3555	1/1	0.90	0.13	58,58,58,58	0
54	MG	2A	3508	1/1	0.90	0.16	61,61,61,61	0
54	MG	1A	3199	1/1	0.90	0.12	33,33,33,33	0
54	MG	2A	3244	1/1	0.90	0.10	45,45,45,45	0
54	MG	1A	3358	1/1	0.90	0.09	26,26,26,26	0
54	MG	1A	3883	1/1	0.90	0.11	48,48,48,48	0
54	MG	1A	3122	1/1	0.90	0.20	33,33,33,33	0
54	MG	1d	301	1/1	0.90	0.14	54,54,54,54	0
54	MG	1A	3212	1/1	0.90	0.18	41,41,41,41	0
54	MG	2E	303	1/1	0.90	0.09	51,51,51,51	0
54	MG	1a	3122	1/1	0.90	0.10	75,75,75,75	0
54	MG	1h	202	1/1	0.90	0.17	61,61,61,61	0
54	MG	1A	3583	1/1	0.90	0.14	36,36,36,36	0
54	MG	1n	101	1/1	0.90	0.16	52,52,52,52	0
54	MG	1a	3002	1/1	0.90	0.14	61,61,61,61	0
54	MG	2A	3530	1/1	0.90	0.20	62,62,62,62	0
54	MG	2A	3278	1/1	0.90	0.12	44,44,44,44	0
54	MG	1A	3756	1/1	0.90	0.10	47,47,47,47	0
54	MG	2R	202	1/1	0.90	0.12	30,30,30,30	0
54	MG	1A	3902	1/1	0.90	0.12	32,32,32,32	0
54	MG	2V	203	1/1	0.90	0.10	54,54,54,54	0
54	MG	1A	3587	1/1	0.90	0.09	63,63,63,63	0
54	MG	2Y	201	1/1	0.90	0.13	54,54,54,54	0
54	MG	2A	3288	1/1	0.90	0.14	48,48,48,48	0
54	MG	1a	3014	1/1	0.90	0.07	55,55,55,55	0
54	MG	1A	3368	1/1	0.90	0.12	51,51,51,51	0
54	MG	2A	3024	1/1	0.90	0.28	51,51,51,51	0
54	MG	1A	3159	1/1	0.90	0.13	33,33,33,33	0
54	MG	2A	3026	1/1	0.90	0.09	43,43,43,43	0
54	MG	2A	3299	1/1	0.90	0.20	53,53,53,53	0
54	MG	1a	3019	1/1	0.90	0.08	52,52,52,52	0
54	MG	2A	3030	1/1	0.90	0.12	44,44,44,44	0
54	MG	1A	3014	1/1	0.90	0.16	46,46,46,46	0
54	MG	2a	3014	1/1	0.90	0.19	71,71,71,71	0
54	MG	1A	3306	1/1	0.90	0.15	65,65,65,65	0
54	MG	1A	3220	1/1	0.90	0.28	34,34,34,34	0
54	MG	2A	3567	1/1	0.90	0.12	41,41,41,41	0
54	MG	2a	3023	1/1	0.90	0.06	51,51,51,51	0
54	MG	2A	3569	1/1	0.90	0.10	26,26,26,26	0
54	MG	2A	3570	1/1	0.90	0.08	51,51,51,51	0
54	MG	1A	3933	1/1	0.90	0.16	26,26,26,26	0
54	MG	2A	3043	1/1	0.90	0.09	42,42,42,42	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	1A	3223	1/1	0.90	0.11	27,27,27,27	0
54	MG	2A	3056	1/1	0.90	0.14	64,64,64,64	0
54	MG	2A	3062	1/1	0.90	0.08	41,41,41,41	0
54	MG	1a	3028	1/1	0.90	0.26	49,49,49,49	0
54	MG	1A	3801	1/1	0.90	0.16	50,50,50,50	0
54	MG	2a	3042	1/1	0.90	0.18	49,49,49,49	0
54	MG	2A	3066	1/1	0.90	0.31	52,52,52,52	0
54	MG	2A	3353	1/1	0.90	0.11	69,69,69,69	0
54	MG	1A	3806	1/1	0.90	0.12	41,41,41,41	0
54	MG	2A	3357	1/1	0.90	0.09	30,30,30,30	0
54	MG	1a	3035	1/1	0.90	0.19	57,57,57,57	0
54	MG	1a	3037	1/1	0.90	0.20	38,38,38,38	0
54	MG	1A	3232	1/1	0.90	0.33	39,39,39,39	0
54	MG	2A	3097	1/1	0.90	0.18	44,44,44,44	0
54	MG	2A	3101	1/1	0.90	0.18	48,48,48,48	0
54	MG	1A	3384	1/1	0.90	0.08	26,26,26,26	0
54	MG	1a	3182	1/1	0.90	0.08	52,52,52,52	0
54	MG	1a	3041	1/1	0.90	0.11	68,68,68,68	0
54	MG	2A	3392	1/1	0.90	0.12	67,67,67,67	0
54	MG	1a	3184	1/1	0.90	0.10	63,63,63,63	0
54	MG	1A	3320	1/1	0.90	0.12	52,52,52,52	0
54	MG	2A	3395	1/1	0.90	0.13	35,35,35,35	0
54	MG	1A	3955	1/1	0.90	0.07	47,47,47,47	0
54	MG	2a	3083	1/1	0.90	0.15	48,48,48,48	0
54	MG	2A	3398	1/1	0.90	0.10	56,56,56,56	0
54	MG	1a	3191	1/1	0.90	0.09	58,58,58,58	0
54	MG	1A	3235	1/1	0.90	0.18	29,29,29,29	0
54	MG	1A	3078	1/1	0.90	0.10	27,27,27,27	0
54	MG	1A	3624	1/1	0.90	0.13	74,74,74,74	0
54	MG	1A	3323	1/1	0.90	0.25	40,40,40,40	0
54	MG	1A	3532	1/1	0.90	0.19	51,51,51,51	0
54	MG	1A	3708	1/1	0.90	0.07	28,28,28,28	0
54	MG	2A	3421	1/1	0.90	0.24	48,48,48,48	0
54	MG	1a	3199	1/1	0.90	0.10	66,66,66,66	0
54	MG	1P	204	1/1	0.90	0.16	47,47,47,47	0
54	MG	2A	3425	1/1	0.90	0.17	45,45,45,45	0
54	MG	1A	3844	1/1	0.90	0.10	43,43,43,43	0
54	MG	1a	3076	1/1	0.90	0.11	56,56,56,56	0
54	MG	1A	3407	1/1	0.90	0.12	22,22,22,22	0
54	MG	1a	3207	1/1	0.90	0.13	56,56,56,56	0
54	MG	1A	3190	1/1	0.90	0.23	56,56,56,56	0
54	MG	1a	3210	1/1	0.90	0.21	58,58,58,58	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	2A	3185	1/1	0.90	0.13	57,57,57,57	0
54	MG	2A	3715	1/1	0.90	0.12	43,43,43,43	0
54	MG	2A	3440	1/1	0.90	0.13	50,50,50,50	0
54	MG	1A	3715	1/1	0.90	0.19	48,48,48,48	0
54	MG	2a	3147	1/1	0.90	0.11	69,69,69,69	0
54	MG	2A	3447	1/1	0.90	0.12	49,49,49,49	0
54	MG	1A	3086	1/1	0.90	0.12	56,56,56,56	0
54	MG	2a	3156	1/1	0.90	0.07	45,45,45,45	0
54	MG	2a	3158	1/1	0.90	0.11	81,81,81,81	0
54	MG	2a	3163	1/1	0.90	0.11	70,70,70,70	0
54	MG	1a	3220	1/1	0.90	0.11	63,63,63,63	0
54	MG	1A	3641	1/1	0.90	0.15	15,15,15,15	0
54	MG	1a	3090	1/1	0.90	0.12	50,50,50,50	0
54	MG	2a	3170	1/1	0.90	0.08	74,74,74,74	0
54	MG	1a	3092	1/1	0.90	0.18	50,50,50,50	0
54	MG	1A	3248	1/1	0.90	0.53	36,36,36,36	0
54	MG	1U	201	1/1	0.90	0.27	26,26,26,26	0
54	MG	1a	3233	1/1	0.90	0.09	65,65,65,65	0
54	MG	2A	3461	1/1	0.90	0.17	44,44,44,44	0
54	MG	2A	3462	1/1	0.90	0.10	37,37,37,37	0
54	MG	2A	3208	1/1	0.90	0.24	70,70,70,70	0
54	MG	1A	3196	1/1	0.90	0.18	28,28,28,28	0
54	MG	1W	201	1/1	0.90	0.11	34,34,34,34	0
54	MG	1a	3100	1/1	0.90	0.23	54,54,54,54	0
54	MG	1A	3432	1/1	0.90	0.08	21,21,21,21	0
54	MG	2A	3221	1/1	0.90	0.13	50,50,50,50	0
54	MG	2e	201	1/1	0.90	0.27	63,63,63,63	0
54	MG	2A	3222	1/1	0.90	0.10	50,50,50,50	0
54	MG	2A	3224	1/1	0.90	0.19	48,48,48,48	0
54	MG	1A	3733	1/1	0.90	0.40	32,32,32,32	0
54	MG	1a	3248	1/1	0.90	0.15	69,69,69,69	0
54	MG	1a	3260	1/1	0.90	0.20	56,56,56,56	0
54	MG	1a	3262	1/1	0.90	0.10	52,52,52,52	0
54	MG	2B	208	1/1	0.90	0.21	57,57,57,57	0
54	MG	2A	3233	1/1	0.90	0.09	49,49,49,49	0
54	MG	1A	3353	1/1	0.90	0.14	27,27,27,27	0
54	MG	2A	3236	1/1	0.90	0.16	35,35,35,35	0
54	MG	1A	3732	1/1	0.91	0.13	38,38,38,38	0
54	MG	1A	3974	1/1	0.91	0.10	60,60,60,60	0
54	MG	1a	3064	1/1	0.91	0.14	71,71,71,71	0
54	MG	1A	3433	1/1	0.91	0.12	19,19,19,19	0
54	MG	2A	3260	1/1	0.91	0.12	50,50,50,50	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	2E	301	1/1	0.91	0.12	35,35,35,35	0
54	MG	2A	3264	1/1	0.91	0.07	57,57,57,57	0
54	MG	1a	3185	1/1	0.91	0.12	44,44,44,44	0
54	MG	2E	306	1/1	0.91	0.14	52,52,52,52	0
54	MG	2A	3270	1/1	0.91	0.25	50,50,50,50	0
54	MG	2A	3527	1/1	0.91	0.10	22,22,22,22	0
54	MG	2A	3037	1/1	0.91	0.18	50,50,50,50	0
54	MG	1A	3436	1/1	0.91	0.08	18,18,18,18	0
54	MG	1a	3187	1/1	0.91	0.07	71,71,71,71	0
54	MG	2O	201	1/1	0.91	0.11	53,53,53,53	0
54	MG	2A	3045	1/1	0.91	0.14	45,45,45,45	0
54	MG	1A	3529	1/1	0.91	0.11	16,16,16,16	0
54	MG	2A	3535	1/1	0.91	0.12	43,43,43,43	0
54	MG	2T	201	1/1	0.91	0.12	63,63,63,63	0
54	MG	2A	3536	1/1	0.91	0.07	46,46,46,46	0
54	MG	2A	3052	1/1	0.91	0.15	53,53,53,53	0
54	MG	1A	3738	1/1	0.91	0.07	23,23,23,23	0
54	MG	2A	3058	1/1	0.91	0.22	60,60,60,60	0
54	MG	2A	3061	1/1	0.91	0.23	43,43,43,43	0
54	MG	1A	3273	1/1	0.91	0.29	61,61,61,61	0
54	MG	1A	3200	1/1	0.91	0.22	47,47,47,47	0
54	MG	1A	3867	1/1	0.91	0.10	38,38,38,38	0
54	MG	1A	3204	1/1	0.91	0.22	30,30,30,30	0
54	MG	2A	3069	1/1	0.91	0.09	55,55,55,55	0
54	MG	2A	3304	1/1	0.91	0.17	52,52,52,52	0
54	MG	1A	3997	1/1	0.91	0.14	45,45,45,45	0
54	MG	2a	3007	1/1	0.91	0.08	62,62,62,62	0
54	MG	2A	3080	1/1	0.91	0.17	57,57,57,57	0
54	MG	2A	3081	1/1	0.91	0.10	47,47,47,47	0
54	MG	2A	3320	1/1	0.91	0.12	38,38,38,38	0
54	MG	2A	3083	1/1	0.91	0.12	39,39,39,39	0
54	MG	1A	3104	1/1	0.91	0.23	27,27,27,27	0
54	MG	2A	3087	1/1	0.91	0.31	55,55,55,55	0
54	MG	1A	3684	1/1	0.91	0.09	48,48,48,48	0
54	MG	1a	3085	1/1	0.91	0.10	52,52,52,52	0
54	MG	2A	3096	1/1	0.91	0.15	77,77,77,77	0
54	MG	1A	3451	1/1	0.91	0.12	51,51,51,51	0
54	MG	2A	3100	1/1	0.91	0.07	53,53,53,53	0
54	MG	1Z	301	1/1	0.91	0.08	62,62,62,62	0
54	MG	1A	3185	1/1	0.91	0.16	52,52,52,52	0
54	MG	2a	3036	1/1	0.91	0.13	50,50,50,50	0
54	MG	2A	3354	1/1	0.91	0.10	40,40,40,40	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	2A	3596	1/1	0.91	0.08	51,51,51,51	0
54	MG	1a	3091	1/1	0.91	0.10	56,56,56,56	0
54	MG	1A	4011	1/1	0.91	0.12	34,34,34,34	0
54	MG	2A	3113	1/1	0.91	0.08	42,42,42,42	0
54	MG	1A	4013	1/1	0.91	0.17	27,27,27,27	0
54	MG	1A	3767	1/1	0.91	0.20	52,52,52,52	0
54	MG	13	105	1/1	0.91	0.11	41,41,41,41	0
54	MG	2a	3053	1/1	0.91	0.19	54,54,54,54	0
54	MG	2A	3128	1/1	0.91	0.34	42,42,42,42	0
54	MG	2a	3056	1/1	0.91	0.18	47,47,47,47	0
54	MG	2A	3130	1/1	0.91	0.17	52,52,52,52	0
54	MG	1A	3392	1/1	0.91	0.09	56,56,56,56	0
54	MG	1A	3472	1/1	0.91	0.07	42,42,42,42	0
54	MG	2A	3391	1/1	0.91	0.11	46,46,46,46	0
54	MG	2A	3140	1/1	0.91	0.17	45,45,45,45	0
54	MG	2a	3067	1/1	0.91	0.20	52,52,52,52	0
54	MG	2A	3142	1/1	0.91	0.11	58,58,58,58	0
54	MG	1A	3695	1/1	0.91	0.12	36,36,36,36	0
54	MG	2A	3633	1/1	0.91	0.08	74,74,74,74	0
54	MG	1A	3890	1/1	0.91	0.18	23,23,23,23	0
54	MG	1A	3402	1/1	0.91	0.10	25,25,25,25	0
54	MG	1a	3229	1/1	0.91	0.09	65,65,65,65	0
54	MG	2a	3076	1/1	0.91	0.12	68,68,68,68	0
54	MG	2a	3079	1/1	0.91	0.20	50,50,50,50	0
54	MG	1A	3477	1/1	0.91	0.09	44,44,44,44	0
54	MG	1A	3900	1/1	0.91	0.08	28,28,28,28	0
54	MG	2A	3166	1/1	0.91	0.12	40,40,40,40	0
54	MG	2A	3663	1/1	0.91	0.12	45,45,45,45	0
54	MG	1A	4045	1/1	0.91	0.21	46,46,46,46	0
54	MG	2A	3168	1/1	0.91	0.18	54,54,54,54	0
54	MG	1A	3794	1/1	0.91	0.11	19,19,19,19	0
54	MG	1A	3556	1/1	0.91	0.22	27,27,27,27	0
54	MG	1A	3371	1/1	0.91	0.07	27,27,27,27	0
54	MG	2a	3101	1/1	0.91	0.16	63,63,63,63	0
54	MG	2A	3422	1/1	0.91	0.08	42,42,42,42	0
54	MG	1a	3243	1/1	0.91	0.23	51,51,51,51	0
54	MG	1A	3921	1/1	0.91	0.09	16,16,16,16	0
54	MG	1A	3803	1/1	0.91	0.11	39,39,39,39	0
54	MG	1a	3258	1/1	0.91	0.11	55,55,55,55	0
54	MG	2A	3685	1/1	0.91	0.08	50,50,50,50	0
54	MG	2a	3118	1/1	0.91	0.07	48,48,48,48	0
54	MG	1A	3804	1/1	0.91	0.14	55,55,55,55	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	2A	3188	1/1	0.91	0.18	56,56,56,56	0
54	MG	2A	3190	1/1	0.91	0.09	47,47,47,47	0
54	MG	2A	3192	1/1	0.91	0.36	73,73,73,73	0
54	MG	2a	3125	1/1	0.91	0.10	66,66,66,66	0
54	MG	2A	3707	1/1	0.91	0.10	52,52,52,52	0
54	MG	1A	3036	1/1	0.91	0.13	44,44,44,44	0
54	MG	2A	3194	1/1	0.91	0.10	57,57,57,57	0
54	MG	2A	3195	1/1	0.91	0.23	66,66,66,66	0
54	MG	2A	3720	1/1	0.91	0.16	54,54,54,54	0
54	MG	2a	3138	1/1	0.91	0.17	59,59,59,59	0
54	MG	1a	3264	1/1	0.91	0.14	50,50,50,50	0
54	MG	1A	3493	1/1	0.91	0.09	14,14,14,14	0
54	MG	1a	3270	1/1	0.91	0.08	56,56,56,56	0
54	MG	1A	3375	1/1	0.91	0.10	42,42,42,42	0
54	MG	1A	3813	1/1	0.91	0.08	69,69,69,69	0
54	MG	2a	3162	1/1	0.91	0.11	58,58,58,58	0
54	MG	1a	3024	1/1	0.91	0.15	55,55,55,55	0
54	MG	1B	216	1/1	0.91	0.10	35,35,35,35	0
54	MG	1A	3579	1/1	0.91	0.09	48,48,48,48	0
54	MG	2A	3209	1/1	0.91	0.09	49,49,49,49	0
54	MG	1a	3139	1/1	0.91	0.07	47,47,47,47	0
54	MG	1A	3816	1/1	0.91	0.17	47,47,47,47	0
54	MG	1d	302	1/1	0.91	0.17	48,48,48,48	0
54	MG	1A	3581	1/1	0.91	0.08	42,42,42,42	0
54	MG	1f	202	1/1	0.91	0.11	36,36,36,36	0
54	MG	1A	3128	1/1	0.91	0.21	27,27,27,27	0
54	MG	1A	3039	1/1	0.91	0.08	34,34,34,34	0
54	MG	1E	305	1/1	0.91	0.09	45,45,45,45	0
54	MG	1a	3158	1/1	0.91	0.14	47,47,47,47	0
54	MG	1A	3722	1/1	0.91	0.13	47,47,47,47	0
54	MG	1A	3588	1/1	0.91	0.08	35,35,35,35	0
54	MG	2A	3231	1/1	0.91	0.09	44,44,44,44	0
54	MG	1A	3343	1/1	0.91	0.11	22,22,22,22	0
54	MG	1a	3163	1/1	0.91	0.15	59,59,59,59	0
54	MG	1a	3164	1/1	0.91	0.13	39,39,39,39	0
54	MG	1A	3177	1/1	0.91	0.23	38,38,38,38	0
54	MG	2A	3009	1/1	0.91	0.12	36,36,36,36	0
54	MG	2A	3497	1/1	0.91	0.07	65,65,65,65	0
54	MG	2A	3012	1/1	0.91	0.10	54,54,54,54	0
54	MG	2A	3021	1/1	0.91	0.14	42,42,42,42	0
54	MG	1a	3044	1/1	0.91	0.12	57,57,57,57	0
54	MG	1a	3049	1/1	0.91	0.12	38,38,38,38	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	2A	3248	1/1	0.91	0.30	40,40,40,40	0
54	MG	1a	3052	1/1	0.91	0.18	57,57,57,57	0
54	MG	2A	3487	1/1	0.92	0.12	52,52,52,52	0
54	MG	1T	205	1/1	0.92	0.10	59,59,59,59	0
54	MG	1a	3121	1/1	0.92	0.12	62,62,62,62	0
54	MG	1A	3952	1/1	0.92	0.07	34,34,34,34	0
54	MG	2A	3494	1/1	0.92	0.19	55,55,55,55	0
54	MG	1A	3046	1/1	0.92	0.10	34,34,34,34	0
54	MG	1A	3431	1/1	0.92	0.09	23,23,23,23	0
54	MG	2A	3001	1/1	0.92	0.26	51,51,51,51	0
54	MG	1A	3345	1/1	0.92	0.09	21,21,21,21	0
54	MG	1A	3270	1/1	0.92	0.13	47,47,47,47	0
54	MG	1A	3798	1/1	0.92	0.12	27,27,27,27	0
54	MG	1a	3134	1/1	0.92	0.15	38,38,38,38	0
54	MG	1A	3071	1/1	0.92	0.08	34,34,34,34	0
54	MG	1A	3802	1/1	0.92	0.08	39,39,39,39	0
54	MG	2A	3517	1/1	0.92	0.09	69,69,69,69	0
54	MG	1A	3675	1/1	0.92	0.14	46,46,46,46	0
54	MG	1A	3356	1/1	0.92	0.08	33,33,33,33	0
54	MG	2N	3801	1/1	0.92	0.06	54,54,54,54	0
54	MG	1A	3805	1/1	0.92	0.06	26,26,26,26	0
54	MG	1a	3145	1/1	0.92	0.20	57,57,57,57	0
54	MG	2A	3253	1/1	0.92	0.15	52,52,52,52	0
54	MG	1A	3439	1/1	0.92	0.09	19,19,19,19	0
54	MG	1A	3571	1/1	0.92	0.09	44,44,44,44	0
54	MG	2T	203	1/1	0.92	0.07	46,46,46,46	0
54	MG	1A	3811	1/1	0.92	0.17	54,54,54,54	0
54	MG	1a	3154	1/1	0.92	0.12	40,40,40,40	0
54	MG	17	103	1/1	0.92	0.31	30,30,30,30	0
54	MG	1A	3180	1/1	0.92	0.43	34,34,34,34	0
54	MG	1A	3574	1/1	0.92	0.08	34,34,34,34	0
54	MG	1A	3575	1/1	0.92	0.10	46,46,46,46	0
54	MG	1A	3686	1/1	0.92	0.10	50,50,50,50	0
54	MG	1A	3999	1/1	0.92	0.09	55,55,55,55	0
54	MG	1a	3005	1/1	0.92	0.12	44,44,44,44	0
54	MG	1A	3445	1/1	0.92	0.09	20,20,20,20	0
54	MG	1a	3010	1/1	0.92	0.21	47,47,47,47	0
54	MG	1a	3011	1/1	0.92	0.27	73,73,73,73	0
54	MG	1A	3578	1/1	0.92	0.08	31,31,31,31	0
54	MG	1A	3359	1/1	0.92	0.08	31,31,31,31	0
54	MG	2A	3291	1/1	0.92	0.18	51,51,51,51	0
54	MG	2A	3070	1/1	0.92	0.11	45,45,45,45	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	2a	3016	1/1	0.92	0.12	65,65,65,65	0
54	MG	1A	4006	1/1	0.92	0.10	33,33,33,33	0
54	MG	2A	3075	1/1	0.92	0.12	24,24,24,24	0
54	MG	2a	3021	1/1	0.92	0.16	60,60,60,60	0
54	MG	2A	3079	1/1	0.92	0.15	54,54,54,54	0
54	MG	1A	3835	1/1	0.92	0.23	36,36,36,36	0
54	MG	1A	4008	1/1	0.92	0.08	55,55,55,55	0
54	MG	1A	3129	1/1	0.92	0.13	27,27,27,27	0
54	MG	2a	3026	1/1	0.92	0.14	43,43,43,43	0
54	MG	1A	3218	1/1	0.92	0.34	20,20,20,20	0
54	MG	1A	3454	1/1	0.92	0.15	48,48,48,48	0
54	MG	2A	3571	1/1	0.92	0.07	38,38,38,38	0
54	MG	2A	3572	1/1	0.92	0.09	62,62,62,62	0
54	MG	1a	3188	1/1	0.92	0.12	60,60,60,60	0
54	MG	1A	3219	1/1	0.92	0.13	43,43,43,43	0
54	MG	2A	3095	1/1	0.92	0.19	60,60,60,60	0
54	MG	2A	3328	1/1	0.92	0.10	33,33,33,33	0
54	MG	1A	4022	1/1	0.92	0.13	51,51,51,51	0
54	MG	1A	3294	1/1	0.92	0.11	44,44,44,44	0
54	MG	2a	3044	1/1	0.92	0.20	55,55,55,55	0
54	MG	2A	3587	1/1	0.92	0.11	70,70,70,70	0
54	MG	2a	3048	1/1	0.92	0.15	70,70,70,70	0
54	MG	2A	3098	1/1	0.92	0.10	47,47,47,47	0
54	MG	1A	4024	1/1	0.92	0.09	48,48,48,48	0
54	MG	1A	3593	1/1	0.92	0.09	22,22,22,22	0
54	MG	1A	4028	1/1	0.92	0.07	29,29,29,29	0
54	MG	1A	3296	1/1	0.92	0.17	27,27,27,27	0
54	MG	2a	3058	1/1	0.92	0.22	52,52,52,52	0
54	MG	1A	3304	1/1	0.92	0.07	39,39,39,39	0
54	MG	1A	3083	1/1	0.92	0.20	25,25,25,25	0
54	MG	2A	3606	1/1	0.92	0.08	62,62,62,62	0
54	MG	1a	3200	1/1	0.92	0.08	55,55,55,55	0
54	MG	1A	3600	1/1	0.92	0.09	41,41,41,41	0
54	MG	2A	3120	1/1	0.92	0.14	46,46,46,46	0
54	MG	1A	3603	1/1	0.92	0.07	28,28,28,28	0
54	MG	2A	3363	1/1	0.92	0.11	37,37,37,37	0
54	MG	2A	3365	1/1	0.92	0.20	48,48,48,48	0
54	MG	1A	3189	1/1	0.92	0.34	44,44,44,44	0
54	MG	2A	3623	1/1	0.92	0.08	39,39,39,39	0
54	MG	1A	3317	1/1	0.92	0.07	47,47,47,47	0
54	MG	1a	3047	1/1	0.92	0.17	59,59,59,59	0
54	MG	2A	3132	1/1	0.92	0.20	47,47,47,47	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	1A	3491	1/1	0.92	0.12	12,12,12,12	0
54	MG	2A	3135	1/1	0.92	0.16	72,72,72,72	0
54	MG	2A	3138	1/1	0.92	0.12	59,59,59,59	0
54	MG	1a	3051	1/1	0.92	0.11	42,42,42,42	0
54	MG	1A	3227	1/1	0.92	0.22	37,37,37,37	0
54	MG	2a	3095	1/1	0.92	0.17	62,62,62,62	0
54	MG	2A	3643	1/1	0.92	0.13	54,54,54,54	0
54	MG	1B	203	1/1	0.92	0.21	58,58,58,58	0
54	MG	1A	3145	1/1	0.92	0.34	28,28,28,28	0
54	MG	1A	3147	1/1	0.92	0.10	28,28,28,28	0
54	MG	1a	3223	1/1	0.92	0.12	55,55,55,55	0
54	MG	2A	3156	1/1	0.92	0.24	48,48,48,48	0
54	MG	2a	3106	1/1	0.92	0.10	46,46,46,46	0
54	MG	1A	3193	1/1	0.92	0.12	68,68,68,68	0
54	MG	2A	3158	1/1	0.92	0.18	47,47,47,47	0
54	MG	1A	3500	1/1	0.92	0.09	28,28,28,28	0
54	MG	1A	3626	1/1	0.92	0.49	30,30,30,30	0
54	MG	2A	3677	1/1	0.92	0.10	53,53,53,53	0
54	MG	1A	3119	1/1	0.92	0.20	43,43,43,43	0
54	MG	1a	3231	1/1	0.92	0.11	43,43,43,43	0
54	MG	2A	3416	1/1	0.92	0.10	38,38,38,38	0
54	MG	1a	3070	1/1	0.92	0.09	60,60,60,60	0
54	MG	1A	3240	1/1	0.92	0.21	56,56,56,56	0
54	MG	1B	217	1/1	0.92	0.08	37,37,37,37	0
54	MG	1A	3892	1/1	0.92	0.12	55,55,55,55	0
54	MG	1A	3244	1/1	0.92	0.22	32,32,32,32	0
54	MG	2A	3427	1/1	0.92	0.24	40,40,40,40	0
54	MG	1A	3896	1/1	0.92	0.11	45,45,45,45	0
54	MG	2A	3181	1/1	0.92	0.09	45,45,45,45	0
54	MG	1A	3328	1/1	0.92	0.08	54,54,54,54	0
54	MG	2a	3139	1/1	0.92	0.08	60,60,60,60	0
54	MG	1A	3523	1/1	0.92	0.10	22,22,22,22	0
54	MG	2A	3718	1/1	0.92	0.12	51,51,51,51	0
54	MG	2A	3187	1/1	0.92	0.14	55,55,55,55	0
54	MG	1E	301	1/1	0.92	0.41	42,42,42,42	0
54	MG	1a	3249	1/1	0.92	0.10	74,74,74,74	0
54	MG	2a	3159	1/1	0.92	0.10	61,61,61,61	0
54	MG	1a	3086	1/1	0.92	0.15	47,47,47,47	0
54	MG	1a	3259	1/1	0.92	0.07	48,48,48,48	0
54	MG	2a	3164	1/1	0.92	0.10	61,61,61,61	0
54	MG	2A	3444	1/1	0.92	0.24	46,46,46,46	0
54	MG	1A	3012	1/1	0.92	0.20	33,33,33,33	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	1A	3753	1/1	0.92	0.06	27,27,27,27	0
54	MG	1F	302	1/1	0.92	0.09	22,22,22,22	0
54	MG	1F	312	1/1	0.92	0.36	39,39,39,39	0
54	MG	1A	3406	1/1	0.92	0.10	39,39,39,39	0
54	MG	1A	3096	1/1	0.92	0.20	42,42,42,42	0
54	MG	2A	3201	1/1	0.92	0.20	53,53,53,53	0
54	MG	2A	3202	1/1	0.92	0.16	40,40,40,40	0
54	MG	1A	3760	1/1	0.92	0.07	62,62,62,62	0
54	MG	1A	3923	1/1	0.92	0.10	32,32,32,32	0
54	MG	1A	3409	1/1	0.92	0.08	18,18,18,18	0
54	MG	2a	3186	1/1	0.92	0.20	58,58,58,58	0
54	MG	2a	3187	1/1	0.92	0.08	62,62,62,62	0
54	MG	2A	3756	1/1	0.92	0.07	53,53,53,53	0
54	MG	2a	3194	1/1	0.92	0.08	72,72,72,72	0
54	MG	1O	201	1/1	0.92	0.12	43,43,43,43	0
54	MG	1A	3766	1/1	0.92	0.08	20,20,20,20	0
54	MG	2a	3198	1/1	0.92	0.14	72,72,72,72	0
54	MG	1A	3929	1/1	0.92	0.09	22,22,22,22	0
54	MG	1A	3331	1/1	0.92	0.11	48,48,48,48	0
54	MG	2f	201	1/1	0.92	0.16	53,53,53,53	0
54	MG	1A	3772	1/1	0.92	0.09	42,42,42,42	0
54	MG	2n	101	1/1	0.92	0.13	65,65,65,65	0
54	MG	2A	3218	1/1	0.92	0.11	63,63,63,63	0
54	MG	1A	3172	1/1	0.92	0.19	25,25,25,25	0
54	MG	1R	206	1/1	0.92	0.11	37,37,37,37	0
54	MG	2A	3477	1/1	0.92	0.13	58,58,58,58	0
54	MG	2A	3478	1/1	0.92	0.08	52,52,52,52	0
54	MG	1A	3656	1/1	0.92	0.24	32,32,32,32	0
54	MG	1A	3339	1/1	0.92	0.07	28,28,28,28	0
54	MG	1A	3785	1/1	0.92	0.11	20,20,20,20	0
54	MG	2A	3486	1/1	0.92	0.07	50,50,50,50	0
54	MG	1a	3032	1/1	0.93	0.10	58,58,58,58	0
54	MG	1a	3033	1/1	0.93	0.11	26,26,26,26	0
54	MG	2A	3725	1/1	0.93	0.08	59,59,59,59	0
54	MG	2A	3123	1/1	0.93	0.07	41,41,41,41	0
54	MG	2A	3396	1/1	0.93	0.08	37,37,37,37	0
54	MG	1A	3082	1/1	0.93	0.06	34,34,34,34	0
54	MG	1A	3777	1/1	0.93	0.12	41,41,41,41	0
54	MG	2A	3399	1/1	0.93	0.16	50,50,50,50	0
54	MG	1A	3279	1/1	0.93	0.20	48,48,48,48	0
54	MG	2A	3739	1/1	0.93	0.11	40,40,40,40	0
54	MG	1A	3903	1/1	0.93	0.14	41,41,41,41	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	1a	3039	1/1	0.93	0.24	54,54,54,54	0
54	MG	1A	3284	1/1	0.93	0.11	53,53,53,53	0
54	MG	1a	3206	1/1	0.93	0.13	64,64,64,64	0
54	MG	1A	3784	1/1	0.93	0.09	45,45,45,45	0
54	MG	1B	208	1/1	0.93	0.10	45,45,45,45	0
54	MG	1A	3682	1/1	0.93	0.06	33,33,33,33	0
54	MG	1a	3045	1/1	0.93	0.18	41,41,41,41	0
54	MG	2A	3148	1/1	0.93	0.33	46,46,46,46	0
54	MG	2A	3755	1/1	0.93	0.20	50,50,50,50	0
54	MG	1a	3218	1/1	0.93	0.11	54,54,54,54	0
54	MG	1A	3787	1/1	0.93	0.09	32,32,32,32	0
54	MG	1A	3285	1/1	0.93	0.12	39,39,39,39	0
54	MG	2A	3426	1/1	0.93	0.12	57,57,57,57	0
54	MG	1B	214	1/1	0.93	0.07	30,30,30,30	0
54	MG	1A	3789	1/1	0.93	0.11	37,37,37,37	0
54	MG	1a	3056	1/1	0.93	0.17	38,38,38,38	0
54	MG	2A	3159	1/1	0.93	0.10	55,55,55,55	0
54	MG	2A	3161	1/1	0.93	0.07	42,42,42,42	0
54	MG	1A	3926	1/1	0.93	0.07	29,29,29,29	0
54	MG	1a	3058	1/1	0.93	0.11	57,57,57,57	0
54	MG	1B	218	1/1	0.93	0.07	31,31,31,31	0
54	MG	2A	3437	1/1	0.93	0.06	45,45,45,45	0
54	MG	2A	3438	1/1	0.93	0.21	48,48,48,48	0
54	MG	1a	3230	1/1	0.93	0.09	48,48,48,48	0
54	MG	1B	223	1/1	0.93	0.11	47,47,47,47	0
54	MG	1A	3109	1/1	0.93	0.14	60,60,60,60	0
54	MG	1A	3928	1/1	0.93	0.11	37,37,37,37	0
54	MG	1A	3531	1/1	0.93	0.08	32,32,32,32	0
54	MG	2D	304	1/1	0.93	0.39	44,44,44,44	0
54	MG	2A	3173	1/1	0.93	0.12	45,45,45,45	0
54	MG	2A	3178	1/1	0.93	0.14	43,43,43,43	0
54	MG	1D	305	1/1	0.93	0.08	31,31,31,31	0
54	MG	2A	3454	1/1	0.93	0.15	42,42,42,42	0
54	MG	1a	3236	1/1	0.93	0.09	52,52,52,52	0
54	MG	1a	3237	1/1	0.93	0.07	62,62,62,62	0
54	MG	1D	306	1/1	0.93	0.16	39,39,39,39	0
54	MG	1A	3288	1/1	0.93	0.12	32,32,32,32	0
54	MG	1A	3335	1/1	0.93	0.09	57,57,57,57	0
54	MG	1a	3074	1/1	0.93	0.16	55,55,55,55	0
54	MG	1A	3337	1/1	0.93	0.08	44,44,44,44	0
54	MG	1A	3693	1/1	0.93	0.08	51,51,51,51	0
54	MG	1a	3255	1/1	0.93	0.07	43,43,43,43	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	1a	3257	1/1	0.93	0.07	64,64,64,64	0
54	MG	1A	3536	1/1	0.93	0.10	43,43,43,43	0
54	MG	1A	3945	1/1	0.93	0.06	41,41,41,41	0
54	MG	2A	3473	1/1	0.93	0.08	42,42,42,42	0
54	MG	1F	308	1/1	0.93	0.13	19,19,19,19	0
54	MG	1A	3615	1/1	0.93	0.08	52,52,52,52	0
54	MG	2A	3476	1/1	0.93	0.10	50,50,50,50	0
54	MG	1A	3950	1/1	0.93	0.08	48,48,48,48	0
54	MG	1A	3616	1/1	0.93	0.11	38,38,38,38	0
54	MG	1a	3269	1/1	0.93	0.13	70,70,70,70	0
54	MG	1A	3179	1/1	0.93	0.12	27,27,27,27	0
54	MG	2A	3484	1/1	0.93	0.19	69,69,69,69	0
54	MG	2I	101	1/1	0.93	0.13	49,49,49,49	0
54	MG	1A	3126	1/1	0.93	0.13	23,23,23,23	0
54	MG	1A	3393	1/1	0.93	0.10	52,52,52,52	0
54	MG	1a	3273	1/1	0.93	0.06	72,72,72,72	0
54	MG	1A	3957	1/1	0.93	0.10	39,39,39,39	0
54	MG	1A	3548	1/1	0.93	0.07	43,43,43,43	0
54	MG	1a	3094	1/1	0.93	0.13	56,56,56,56	0
54	MG	1A	3963	1/1	0.93	0.15	56,56,56,56	0
54	MG	2A	3496	1/1	0.93	0.10	50,50,50,50	0
54	MG	1A	3964	1/1	0.93	0.09	68,68,68,68	0
54	MG	1A	3206	1/1	0.93	0.08	32,32,32,32	0
54	MG	2a	3012	1/1	0.93	0.14	49,49,49,49	0
54	MG	1A	3709	1/1	0.93	0.07	47,47,47,47	0
54	MG	1d	305	1/1	0.93	0.07	82,82,82,82	0
54	MG	2a	3017	1/1	0.93	0.14	51,51,51,51	0
54	MG	1A	3475	1/1	0.93	0.07	28,28,28,28	0
54	MG	1g	201	1/1	0.93	0.25	50,50,50,50	0
54	MG	1A	3629	1/1	0.93	0.25	34,34,34,34	0
54	MG	1A	3975	1/1	0.93	0.07	50,50,50,50	0
54	MG	1a	3106	1/1	0.93	0.10	44,44,44,44	0
54	MG	1A	3064	1/1	0.93	0.07	42,42,42,42	0
54	MG	1T	204	1/1	0.93	0.08	48,48,48,48	0
54	MG	1o	101	1/1	0.93	0.11	49,49,49,49	0
54	MG	1a	3111	1/1	0.93	0.10	29,29,29,29	0
54	MG	2a	3029	1/1	0.93	0.12	63,63,63,63	0
54	MG	2A	3522	1/1	0.93	0.11	59,59,59,59	0
54	MG	1A	3016	1/1	0.93	0.31	33,33,33,33	0
54	MG	2a	3034	1/1	0.93	0.24	52,52,52,52	0
54	MG	1A	3719	1/1	0.93	0.25	34,34,34,34	0
54	MG	1A	3981	1/1	0.93	0.14	66,66,66,66	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	2A	3243	1/1	0.93	0.11	43,43,43,43	0
54	MG	1U	203	1/1	0.93	0.22	28,28,28,28	0
54	MG	2A	3245	1/1	0.93	0.25	42,42,42,42	0
54	MG	1U	207	1/1	0.93	0.13	42,42,42,42	0
54	MG	2A	3003	1/1	0.93	0.07	47,47,47,47	0
54	MG	2A	3005	1/1	0.93	0.17	51,51,51,51	0
54	MG	2a	3045	1/1	0.93	0.17	62,62,62,62	0
54	MG	2A	3534	1/1	0.93	0.14	50,50,50,50	0
54	MG	2A	3006	1/1	0.93	0.23	52,52,52,52	0
54	MG	1A	3839	1/1	0.93	0.09	52,52,52,52	0
54	MG	2A	3251	1/1	0.93	0.29	41,41,41,41	0
54	MG	1V	205	1/1	0.93	0.05	67,67,67,67	0
54	MG	2A	3539	1/1	0.93	0.09	68,68,68,68	0
54	MG	2A	3254	1/1	0.93	0.27	59,59,59,59	0
54	MG	2A	3015	1/1	0.93	0.28	36,36,36,36	0
54	MG	1A	3559	1/1	0.93	0.06	29,29,29,29	0
54	MG	2a	3062	1/1	0.93	0.12	62,62,62,62	0
54	MG	1A	3561	1/1	0.93	0.08	27,27,27,27	0
54	MG	1A	3991	1/1	0.93	0.10	43,43,43,43	0
54	MG	1A	3638	1/1	0.93	0.08	25,25,25,25	0
54	MG	2A	3551	1/1	0.93	0.12	30,30,30,30	0
54	MG	2A	3556	1/1	0.93	0.07	62,62,62,62	0
54	MG	2A	3557	1/1	0.93	0.07	52,52,52,52	0
54	MG	10	107	1/1	0.93	0.08	45,45,45,45	0
54	MG	2A	3267	1/1	0.93	0.11	47,47,47,47	0
54	MG	11	101	1/1	0.93	0.07	36,36,36,36	0
54	MG	2A	3272	1/1	0.93	0.13	26,26,26,26	0
54	MG	11	102	1/1	0.93	0.19	48,48,48,48	0
54	MG	2A	3275	1/1	0.93	0.10	39,39,39,39	0
54	MG	2a	3077	1/1	0.93	0.21	58,58,58,58	0
54	MG	1A	3186	1/1	0.93	0.10	48,48,48,48	0
54	MG	1A	3845	1/1	0.93	0.09	42,42,42,42	0
54	MG	1A	3998	1/1	0.93	0.08	42,42,42,42	0
54	MG	2A	3281	1/1	0.93	0.17	60,60,60,60	0
54	MG	2A	3282	1/1	0.93	0.08	49,49,49,49	0
54	MG	2A	3573	1/1	0.93	0.06	59,59,59,59	0
54	MG	2a	3094	1/1	0.93	0.15	38,38,38,38	0
54	MG	2A	3283	1/1	0.93	0.15	34,34,34,34	0
54	MG	1a	3142	1/1	0.93	0.09	57,57,57,57	0
54	MG	1A	3316	1/1	0.93	0.19	31,31,31,31	0
54	MG	2a	3098	1/1	0.93	0.07	62,62,62,62	0
54	MG	2A	3580	1/1	0.93	0.09	45,45,45,45	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	2A	3044	1/1	0.93	0.08	27,27,27,27	0
54	MG	2A	3582	1/1	0.93	0.06	48,48,48,48	0
54	MG	2a	3103	1/1	0.93	0.10	67,67,67,67	0
54	MG	1A	3849	1/1	0.93	0.09	43,43,43,43	0
54	MG	2A	3046	1/1	0.93	0.12	55,55,55,55	0
54	MG	2A	3047	1/1	0.93	0.11	49,49,49,49	0
54	MG	2A	3590	1/1	0.93	0.07	45,45,45,45	0
54	MG	1a	3147	1/1	0.93	0.18	52,52,52,52	0
54	MG	2a	3113	1/1	0.93	0.10	53,53,53,53	0
54	MG	2A	3051	1/1	0.93	0.16	53,53,53,53	0
54	MG	1A	3726	1/1	0.93	0.10	45,45,45,45	0
54	MG	2a	3117	1/1	0.93	0.10	45,45,45,45	0
54	MG	1A	3728	1/1	0.93	0.08	33,33,33,33	0
54	MG	2A	3302	1/1	0.93	0.11	42,42,42,42	0
54	MG	2A	3057	1/1	0.93	0.09	53,53,53,53	0
54	MG	1A	3643	1/1	0.93	0.07	40,40,40,40	0
54	MG	2A	3306	1/1	0.93	0.07	36,36,36,36	0
54	MG	2a	3124	1/1	0.93	0.12	56,56,56,56	0
54	MG	1A	3570	1/1	0.93	0.09	23,23,23,23	0
54	MG	2a	3127	1/1	0.93	0.15	57,57,57,57	0
54	MG	2A	3608	1/1	0.93	0.12	52,52,52,52	0
54	MG	2a	3131	1/1	0.93	0.08	67,67,67,67	0
54	MG	1A	3489	1/1	0.93	0.09	44,44,44,44	0
54	MG	2A	3612	1/1	0.93	0.07	48,48,48,48	0
54	MG	2a	3134	1/1	0.93	0.12	64,64,64,64	0
54	MG	2A	3315	1/1	0.93	0.09	45,45,45,45	0
54	MG	2A	3318	1/1	0.93	0.13	64,64,64,64	0
54	MG	1A	4010	1/1	0.93	0.34	34,34,34,34	0
54	MG	1A	3647	1/1	0.93	0.11	51,51,51,51	0
54	MG	2a	3140	1/1	0.93	0.08	53,53,53,53	0
54	MG	2a	3141	1/1	0.93	0.16	47,47,47,47	0
54	MG	2a	3145	1/1	0.93	0.06	56,56,56,56	0
54	MG	1a	3003	1/1	0.93	0.25	61,61,61,61	0
54	MG	2A	3323	1/1	0.93	0.12	55,55,55,55	0
54	MG	2A	3625	1/1	0.93	0.08	53,53,53,53	0
54	MG	2a	3152	1/1	0.93	0.09	77,77,77,77	0
54	MG	1A	3158	1/1	0.93	0.34	29,29,29,29	0
54	MG	1A	3131	1/1	0.93	0.12	48,48,48,48	0
54	MG	1A	4020	1/1	0.93	0.13	53,53,53,53	0
54	MG	1A	3262	1/1	0.93	0.17	37,37,37,37	0
54	MG	2A	3335	1/1	0.93	0.09	38,38,38,38	0
54	MG	2A	3337	1/1	0.93	0.11	21,21,21,21	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	1A	3657	1/1	0.93	0.08	68,68,68,68	0
54	MG	2A	3342	1/1	0.93	0.09	35,35,35,35	0
54	MG	2A	3343	1/1	0.93	0.07	27,27,27,27	0
54	MG	1a	3012	1/1	0.93	0.14	24,24,24,24	0
54	MG	1A	3136	1/1	0.93	0.07	40,40,40,40	0
54	MG	2A	3652	1/1	0.93	0.07	58,58,58,58	0
54	MG	1A	3497	1/1	0.93	0.08	24,24,24,24	0
54	MG	2a	3178	1/1	0.93	0.11	47,47,47,47	0
54	MG	1a	3179	1/1	0.93	0.08	64,64,64,64	0
54	MG	1a	3181	1/1	0.93	0.06	60,60,60,60	0
54	MG	2A	3089	1/1	0.93	0.27	43,43,43,43	0
54	MG	2A	3355	1/1	0.93	0.09	28,28,28,28	0
54	MG	2A	3090	1/1	0.93	0.10	33,33,33,33	0
54	MG	1A	3498	1/1	0.93	0.10	37,37,37,37	0
54	MG	1A	3175	1/1	0.93	0.22	31,31,31,31	0
54	MG	2A	3361	1/1	0.93	0.06	35,35,35,35	0
54	MG	2a	3192	1/1	0.93	0.12	56,56,56,56	0
54	MG	1A	3667	1/1	0.93	0.09	47,47,47,47	0
54	MG	1A	3222	1/1	0.93	0.41	33,33,33,33	0
54	MG	1A	3888	1/1	0.93	0.08	22,22,22,22	0
54	MG	1A	4039	1/1	0.93	0.15	34,34,34,34	0
54	MG	2A	3686	1/1	0.93	0.08	64,64,64,64	0
54	MG	1A	3501	1/1	0.93	0.09	29,29,29,29	0
54	MG	1A	3194	1/1	0.93	0.12	49,49,49,49	0
54	MG	1a	3026	1/1	0.93	0.08	50,50,50,50	0
54	MG	2A	3698	1/1	0.93	0.10	58,58,58,58	0
56	MPD	1A	4056	8/8	0.93	0.16	39,46,54,57	0
54	MG	2A	3382	1/1	0.93	0.09	48,48,48,48	0
54	MG	1A	4046	1/1	0.93	0.08	56,56,56,56	0
54	MG	1A	3769	1/1	0.93	0.16	46,46,46,46	0
54	MG	2A	3710	1/1	0.93	0.07	50,50,50,50	0
54	MG	2A	3712	1/1	0.93	0.07	45,45,45,45	0
54	MG	2A	3390	1/1	0.93	0.10	23,23,23,23	0
54	MG	1A	3435	1/1	0.93	0.09	50,50,50,50	0
54	MG	2A	3717	1/1	0.93	0.12	38,38,38,38	0
54	MG	1a	3030	1/1	0.93	0.19	47,47,47,47	0
54	MG	1A	3396	1/1	0.94	0.07	37,37,37,37	0
54	MG	1A	3770	1/1	0.94	0.13	44,44,44,44	0
54	MG	1A	3397	1/1	0.94	0.09	34,34,34,34	0
54	MG	1A	3949	1/1	0.94	0.08	31,31,31,31	0
54	MG	1A	3399	1/1	0.94	0.09	42,42,42,42	0
54	MG	1e	202	1/1	0.94	0.14	55,55,55,55	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	2A	3211	1/1	0.94	0.06	41,41,41,41	0
54	MG	1f	201	1/1	0.94	0.19	61,61,61,61	0
54	MG	1A	3062	1/1	0.94	0.11	33,33,33,33	0
54	MG	2B	209	1/1	0.94	0.10	57,57,57,57	0
54	MG	2A	3214	1/1	0.94	0.21	45,45,45,45	0
54	MG	1a	3104	1/1	0.94	0.15	61,61,61,61	0
54	MG	2B	213	1/1	0.94	0.07	77,77,77,77	0
54	MG	1A	3403	1/1	0.94	0.07	15,15,15,15	0
54	MG	2A	3469	1/1	0.94	0.07	43,43,43,43	0
54	MG	2A	3219	1/1	0.94	0.18	50,50,50,50	0
54	MG	1h	201	1/1	0.94	0.13	29,29,29,29	0
54	MG	1A	3123	1/1	0.94	0.10	21,21,21,21	0
54	MG	1l	201	1/1	0.94	0.15	55,55,55,55	0
54	MG	1A	3649	1/1	0.94	0.16	57,57,57,57	0
54	MG	1A	3026	1/1	0.94	0.30	27,27,27,27	0
54	MG	1A	3960	1/1	0.94	0.17	40,40,40,40	0
54	MG	1A	3654	1/1	0.94	0.20	20,20,20,20	0
54	MG	1A	3541	1/1	0.94	0.09	52,52,52,52	0
54	MG	2A	3483	1/1	0.94	0.07	48,48,48,48	0
54	MG	1A	3038	1/1	0.94	0.10	28,28,28,28	0
54	MG	1A	3967	1/1	0.94	0.06	14,14,14,14	0
54	MG	1U	206	1/1	0.94	0.32	33,33,33,33	0
54	MG	1y	203	1/1	0.94	0.08	59,59,59,59	0
54	MG	1A	3127	1/1	0.94	0.10	42,42,42,42	0
54	MG	2F	302	1/1	0.94	0.10	60,60,60,60	0
54	MG	2F	303	1/1	0.94	0.19	49,49,49,49	0
54	MG	2A	3490	1/1	0.94	0.11	62,62,62,62	0
54	MG	1A	3181	1/1	0.94	0.16	51,51,51,51	0
54	MG	1V	201	1/1	0.94	0.19	29,29,29,29	0
54	MG	2A	3493	1/1	0.94	0.11	35,35,35,35	0
54	MG	1A	3971	1/1	0.94	0.14	37,37,37,37	0
54	MG	1a	3130	1/1	0.94	0.07	53,53,53,53	0
54	MG	2A	3007	1/1	0.94	0.06	37,37,37,37	0
54	MG	2P	201	1/1	0.94	0.09	51,51,51,51	0
54	MG	1A	3972	1/1	0.94	0.09	53,53,53,53	0
54	MG	2Q	203	1/1	0.94	0.07	51,51,51,51	0
54	MG	1A	3231	1/1	0.94	0.21	24,24,24,24	0
54	MG	1A	3182	1/1	0.94	0.17	53,53,53,53	0
54	MG	2A	3020	1/1	0.94	0.19	31,31,31,31	0
54	MG	1A	3324	1/1	0.94	0.10	53,53,53,53	0
54	MG	2A	3510	1/1	0.94	0.16	42,42,42,42	0
54	MG	2W	201	1/1	0.94	0.17	41,41,41,41	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	10	105	1/1	0.94	0.10	54,54,54,54	0
54	MG	2X	102	1/1	0.94	0.12	58,58,58,58	0
54	MG	1A	3668	1/1	0.94	0.15	51,51,51,51	0
54	MG	1A	3430	1/1	0.94	0.07	26,26,26,26	0
54	MG	2A	3515	1/1	0.94	0.08	60,60,60,60	0
54	MG	2A	3516	1/1	0.94	0.08	46,46,46,46	0
54	MG	1A	3233	1/1	0.94	0.14	28,28,28,28	0
54	MG	2A	3028	1/1	0.94	0.11	41,41,41,41	0
54	MG	1A	3092	1/1	0.94	0.30	32,32,32,32	0
54	MG	1A	3184	1/1	0.94	0.06	43,43,43,43	0
54	MG	2A	3262	1/1	0.94	0.18	50,50,50,50	0
54	MG	2a	3005	1/1	0.94	0.09	50,50,50,50	0
54	MG	1A	3094	1/1	0.94	0.12	27,27,27,27	0
54	MG	1A	3678	1/1	0.94	0.11	14,14,14,14	0
54	MG	1A	3986	1/1	0.94	0.08	24,24,24,24	0
54	MG	2A	3038	1/1	0.94	0.14	50,50,50,50	0
54	MG	1a	3152	1/1	0.94	0.13	47,47,47,47	0
54	MG	1A	3988	1/1	0.94	0.11	57,57,57,57	0
54	MG	1A	3010	1/1	0.94	0.15	39,39,39,39	0
54	MG	17	101	1/1	0.94	0.11	37,37,37,37	0
54	MG	17	102	1/1	0.94	0.10	32,32,32,32	0
54	MG	1A	3187	1/1	0.94	0.13	25,25,25,25	0
54	MG	1a	3160	1/1	0.94	0.09	48,48,48,48	0
54	MG	18	101	1/1	0.94	0.15	25,25,25,25	0
54	MG	1A	3334	1/1	0.94	0.16	55,55,55,55	0
54	MG	1A	3440	1/1	0.94	0.10	48,48,48,48	0
54	MG	1A	3100	1/1	0.94	0.18	34,34,34,34	0
54	MG	1A	3821	1/1	0.94	0.10	48,48,48,48	0
54	MG	2a	3027	1/1	0.94	0.23	64,64,64,64	0
54	MG	2A	3541	1/1	0.94	0.10	33,33,33,33	0
54	MG	2A	3542	1/1	0.94	0.06	42,42,42,42	0
54	MG	2A	3059	1/1	0.94	0.22	45,45,45,45	0
54	MG	1A	3138	1/1	0.94	0.08	34,34,34,34	0
54	MG	1a	3170	1/1	0.94	0.06	64,64,64,64	0
54	MG	2A	3293	1/1	0.94	0.08	39,39,39,39	0
54	MG	1A	3824	1/1	0.94	0.11	51,51,51,51	0
54	MG	2a	3038	1/1	0.94	0.05	70,70,70,70	0
54	MG	1a	3173	1/1	0.94	0.13	54,54,54,54	0
54	MG	1a	3174	1/1	0.94	0.12	60,60,60,60	0
54	MG	1A	3251	1/1	0.94	0.11	34,34,34,34	0
54	MG	2A	3300	1/1	0.94	0.09	71,71,71,71	0
54	MG	1a	3177	1/1	0.94	0.07	57,57,57,57	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	2A	3071	1/1	0.94	0.13	34,34,34,34	0
54	MG	1A	4004	1/1	0.94	0.09	36,36,36,36	0
54	MG	2A	3564	1/1	0.94	0.08	55,55,55,55	0
54	MG	1A	3833	1/1	0.94	0.09	46,46,46,46	0
54	MG	2a	3049	1/1	0.94	0.19	44,44,44,44	0
54	MG	2A	3076	1/1	0.94	0.08	44,44,44,44	0
54	MG	2A	3311	1/1	0.94	0.16	49,49,49,49	0
54	MG	2A	3312	1/1	0.94	0.13	42,42,42,42	0
54	MG	1a	3180	1/1	0.94	0.07	63,63,63,63	0
54	MG	2A	3314	1/1	0.94	0.12	47,47,47,47	0
54	MG	1A	3834	1/1	0.94	0.09	21,21,21,21	0
54	MG	2A	3316	1/1	0.94	0.07	19,19,19,19	0
54	MG	1A	3139	1/1	0.94	0.12	21,21,21,21	0
54	MG	1A	3031	1/1	0.94	0.11	17,17,17,17	0
54	MG	1A	3582	1/1	0.94	0.08	48,48,48,48	0
54	MG	1a	3015	1/1	0.94	0.15	63,63,63,63	0
54	MG	1A	3346	1/1	0.94	0.15	12,12,12,12	0
54	MG	1A	3263	1/1	0.94	0.14	34,34,34,34	0
54	MG	1A	4016	1/1	0.94	0.12	25,25,25,25	0
54	MG	1A	4018	1/1	0.94	0.22	53,53,53,53	0
54	MG	1A	3463	1/1	0.94	0.13	55,55,55,55	0
54	MG	2a	3071	1/1	0.94	0.14	61,61,61,61	0
54	MG	2A	3334	1/1	0.94	0.07	34,34,34,34	0
54	MG	1A	3589	1/1	0.94	0.13	45,45,45,45	0
54	MG	1A	3590	1/1	0.94	0.12	33,33,33,33	0
54	MG	1A	3591	1/1	0.94	0.15	50,50,50,50	0
54	MG	2A	3099	1/1	0.94	0.12	59,59,59,59	0
54	MG	2A	3598	1/1	0.94	0.06	57,57,57,57	0
54	MG	1A	3705	1/1	0.94	0.07	52,52,52,52	0
54	MG	1A	3002	1/1	0.94	0.07	38,38,38,38	0
54	MG	1A	3268	1/1	0.94	0.25	24,24,24,24	0
54	MG	2A	3347	1/1	0.94	0.10	31,31,31,31	0
54	MG	2A	3105	1/1	0.94	0.30	45,45,45,45	0
54	MG	2A	3350	1/1	0.94	0.11	50,50,50,50	0
54	MG	1A	3146	1/1	0.94	0.08	39,39,39,39	0
54	MG	2A	3108	1/1	0.94	0.12	46,46,46,46	0
54	MG	1A	3595	1/1	0.94	0.09	18,18,18,18	0
54	MG	1A	4033	1/1	0.94	0.06	29,29,29,29	0
54	MG	1A	3863	1/1	0.94	0.07	39,39,39,39	0
54	MG	1A	3712	1/1	0.94	0.11	39,39,39,39	0
54	MG	2A	3359	1/1	0.94	0.10	26,26,26,26	0
54	MG	2A	3116	1/1	0.94	0.19	61,61,61,61	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	2A	3118	1/1	0.94	0.19	39,39,39,39	0
54	MG	1A	3866	1/1	0.94	0.10	41,41,41,41	0
54	MG	2A	3121	1/1	0.94	0.07	38,38,38,38	0
54	MG	2A	3630	1/1	0.94	0.13	49,49,49,49	0
54	MG	1A	3596	1/1	0.94	0.17	35,35,35,35	0
54	MG	1A	3868	1/1	0.94	0.09	40,40,40,40	0
54	MG	2a	3114	1/1	0.94	0.17	51,51,51,51	0
54	MG	2A	3370	1/1	0.94	0.06	44,44,44,44	0
54	MG	1A	3198	1/1	0.94	0.16	50,50,50,50	0
54	MG	1A	3052	1/1	0.94	0.13	11,11,11,11	0
54	MG	2A	3641	1/1	0.94	0.09	74,74,74,74	0
54	MG	1a	3212	1/1	0.94	0.06	60,60,60,60	0
54	MG	1A	4052	1/1	0.94	0.09	45,45,45,45	0
54	MG	2A	3645	1/1	0.94	0.16	48,48,48,48	0
54	MG	2A	3384	1/1	0.94	0.10	61,61,61,61	0
54	MG	2a	3123	1/1	0.94	0.16	63,63,63,63	0
54	MG	2A	3133	1/1	0.94	0.27	61,61,61,61	0
54	MG	2A	3650	1/1	0.94	0.07	52,52,52,52	0
54	MG	2A	3651	1/1	0.94	0.07	72,72,72,72	0
54	MG	1A	3363	1/1	0.94	0.11	17,17,17,17	0
54	MG	2A	3655	1/1	0.94	0.10	52,52,52,52	0
54	MG	2A	3388	1/1	0.94	0.06	49,49,49,49	0
54	MG	1a	3043	1/1	0.94	0.09	47,47,47,47	0
54	MG	1A	3275	1/1	0.94	0.09	49,49,49,49	0
54	MG	1A	3367	1/1	0.94	0.07	28,28,28,28	0
54	MG	1A	3881	1/1	0.94	0.08	30,30,30,30	0
54	MG	1A	3020	1/1	0.94	0.35	33,33,33,33	0
54	MG	1A	3201	1/1	0.94	0.29	39,39,39,39	0
54	MG	1A	3202	1/1	0.94	0.17	47,47,47,47	0
54	MG	1a	3055	1/1	0.94	0.16	41,41,41,41	0
54	MG	2a	3144	1/1	0.94	0.08	62,62,62,62	0
54	MG	1A	3613	1/1	0.94	0.08	39,39,39,39	0
54	MG	2a	3146	1/1	0.94	0.08	70,70,70,70	0
54	MG	1A	3151	1/1	0.94	0.12	36,36,36,36	0
54	MG	1A	3730	1/1	0.94	0.33	30,30,30,30	0
54	MG	2a	3150	1/1	0.94	0.11	64,64,64,64	0
54	MG	1A	3205	1/1	0.94	0.17	38,38,38,38	0
54	MG	1a	3063	1/1	0.94	0.10	53,53,53,53	0
54	MG	1B	215	1/1	0.94	0.11	50,50,50,50	0
54	MG	2A	3408	1/1	0.94	0.13	41,41,41,41	0
54	MG	1A	3110	1/1	0.94	0.25	27,27,27,27	0
54	MG	2a	3161	1/1	0.94	0.08	66,66,66,66	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	1A	3895	1/1	0.94	0.08	17,17,17,17	0
54	MG	2A	3702	1/1	0.94	0.09	66,66,66,66	0
54	MG	1a	3239	1/1	0.94	0.12	47,47,47,47	0
54	MG	1A	3734	1/1	0.94	0.14	33,33,33,33	0
54	MG	2A	3708	1/1	0.94	0.08	49,49,49,49	0
54	MG	2A	3417	1/1	0.94	0.07	33,33,33,33	0
54	MG	2A	3420	1/1	0.94	0.10	59,59,59,59	0
54	MG	2a	3171	1/1	0.94	0.10	68,68,68,68	0
54	MG	1A	3115	1/1	0.94	0.29	24,24,24,24	0
54	MG	2A	3714	1/1	0.94	0.14	39,39,39,39	0
54	MG	2a	3176	1/1	0.94	0.13	63,63,63,63	0
54	MG	1a	3069	1/1	0.94	0.19	40,40,40,40	0
54	MG	1A	3619	1/1	0.94	0.08	33,33,33,33	0
54	MG	1A	3290	1/1	0.94	0.15	43,43,43,43	0
54	MG	1A	3209	1/1	0.94	0.10	34,34,34,34	0
54	MG	2A	3719	1/1	0.94	0.10	61,61,61,61	0
54	MG	1D	301	1/1	0.94	0.39	28,28,28,28	0
54	MG	1A	3502	1/1	0.94	0.12	15,15,15,15	0
54	MG	1A	3908	1/1	0.94	0.07	37,37,37,37	0
54	MG	1A	3745	1/1	0.94	0.08	48,48,48,48	0
54	MG	2a	3190	1/1	0.94	0.09	60,60,60,60	0
54	MG	2A	3183	1/1	0.94	0.11	51,51,51,51	0
54	MG	2A	3731	1/1	0.94	0.06	70,70,70,70	0
54	MG	1A	3747	1/1	0.94	0.08	32,32,32,32	0
54	MG	1A	3748	1/1	0.94	0.17	61,61,61,61	0
54	MG	1A	3061	1/1	0.94	0.10	40,40,40,40	0
54	MG	1A	3509	1/1	0.94	0.05	26,26,26,26	0
54	MG	2A	3737	1/1	0.94	0.05	67,67,67,67	0
54	MG	1A	3511	1/1	0.94	0.10	26,26,26,26	0
54	MG	2e	202	1/1	0.94	0.07	66,66,66,66	0
54	MG	2A	3740	1/1	0.94	0.13	48,48,48,48	0
54	MG	1A	3300	1/1	0.94	0.08	46,46,46,46	0
54	MG	1A	3755	1/1	0.94	0.06	30,30,30,30	0
54	MG	2A	3745	1/1	0.94	0.16	50,50,50,50	0
54	MG	1A	3633	1/1	0.94	0.07	26,26,26,26	0
54	MG	2A	3442	1/1	0.94	0.07	38,38,38,38	0
54	MG	1A	3168	1/1	0.94	0.07	36,36,36,36	0
54	MG	1A	3216	1/1	0.94	0.15	43,43,43,43	0
54	MG	1A	3079	1/1	0.94	0.14	29,29,29,29	0
54	MG	1a	3277	1/1	0.94	0.10	65,65,65,65	0
54	MG	1a	3278	1/1	0.94	0.20	66,66,66,66	0
54	MG	1A	3310	1/1	0.94	0.08	45,45,45,45	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	2A	3453	1/1	0.94	0.09	54,54,54,54	0
54	MG	1a	3105	1/1	0.95	0.19	46,46,46,46	0
54	MG	1A	3192	1/1	0.95	0.15	44,44,44,44	0
54	MG	1A	3817	1/1	0.95	0.06	38,38,38,38	0
54	MG	1T	202	1/1	0.95	0.08	47,47,47,47	0
54	MG	1A	3149	1/1	0.95	0.16	36,36,36,36	0
54	MG	1A	3121	1/1	0.95	0.21	39,39,39,39	0
54	MG	1A	3699	1/1	0.95	0.08	16,16,16,16	0
54	MG	1A	3243	1/1	0.95	0.12	60,60,60,60	0
54	MG	1A	3495	1/1	0.95	0.07	24,24,24,24	0
54	MG	1A	3979	1/1	0.95	0.09	51,51,51,51	0
54	MG	2A	3216	1/1	0.95	0.09	49,49,49,49	0
54	MG	2A	3466	1/1	0.95	0.08	58,58,58,58	0
54	MG	2A	3217	1/1	0.95	0.12	34,34,34,34	0
54	MG	1A	3826	1/1	0.95	0.12	39,39,39,39	0
54	MG	1n	103	1/1	0.95	0.20	54,54,54,54	0
54	MG	1A	3830	1/1	0.95	0.08	44,44,44,44	0
54	MG	1A	3831	1/1	0.95	0.07	39,39,39,39	0
54	MG	1A	3390	1/1	0.95	0.06	28,28,28,28	0
54	MG	2A	3223	1/1	0.95	0.16	48,48,48,48	0
54	MG	1a	3128	1/1	0.95	0.10	54,54,54,54	0
54	MG	2A	3225	1/1	0.95	0.10	45,45,45,45	0
54	MG	1A	3599	1/1	0.95	0.20	39,39,39,39	0
54	MG	1A	3987	1/1	0.95	0.07	39,39,39,39	0
54	MG	1y	204	1/1	0.95	0.06	63,63,63,63	0
54	MG	1A	3093	1/1	0.95	0.06	29,29,29,29	0
54	MG	1A	3836	1/1	0.95	0.16	28,28,28,28	0
54	MG	2A	3232	1/1	0.95	0.11	50,50,50,50	0
54	MG	1A	3837	1/1	0.95	0.14	26,26,26,26	0
54	MG	1a	3135	1/1	0.95	0.09	41,41,41,41	0
54	MG	1A	3156	1/1	0.95	0.17	23,23,23,23	0
54	MG	2A	3238	1/1	0.95	0.16	35,35,35,35	0
54	MG	1A	3058	1/1	0.95	0.04	39,39,39,39	0
54	MG	1A	3060	1/1	0.95	0.14	27,27,27,27	0
54	MG	2A	3010	1/1	0.95	0.23	58,58,58,58	0
54	MG	1A	3842	1/1	0.95	0.06	24,24,24,24	0
54	MG	2A	3013	1/1	0.95	0.07	24,24,24,24	0
54	MG	1a	3141	1/1	0.95	0.18	64,64,64,64	0
54	MG	2A	3498	1/1	0.95	0.07	38,38,38,38	0
54	MG	1l	104	1/1	0.95	0.06	33,33,33,33	0
54	MG	1A	3607	1/1	0.95	0.15	53,53,53,53	0
54	MG	2P	202	1/1	0.95	0.07	48,48,48,48	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	1A	3252	1/1	0.95	0.18	37,37,37,37	0
54	MG	13	104	1/1	0.95	0.06	46,46,46,46	0
54	MG	1A	3163	1/1	0.95	0.07	45,45,45,45	0
54	MG	1A	3257	1/1	0.95	0.09	37,37,37,37	0
54	MG	2A	3511	1/1	0.95	0.10	66,66,66,66	0
54	MG	1A	4005	1/1	0.95	0.07	61,61,61,61	0
54	MG	1A	3166	1/1	0.95	0.23	40,40,40,40	0
54	MG	15	103	1/1	0.95	0.26	32,32,32,32	0
54	MG	1a	3155	1/1	0.95	0.08	61,61,61,61	0
54	MG	2A	3034	1/1	0.95	0.24	53,53,53,53	0
54	MG	2A	3258	1/1	0.95	0.24	59,59,59,59	0
54	MG	20	101	1/1	0.95	0.15	41,41,41,41	0
54	MG	2A	3259	1/1	0.95	0.06	48,48,48,48	0
54	MG	1A	3099	1/1	0.95	0.17	37,37,37,37	0
54	MG	1A	3514	1/1	0.95	0.10	13,13,13,13	0
54	MG	1A	3265	1/1	0.95	0.14	40,40,40,40	0
54	MG	23	102	1/1	0.95	0.07	35,35,35,35	0
54	MG	25	101	1/1	0.95	0.34	36,36,36,36	0
54	MG	1A	3858	1/1	0.95	0.06	48,48,48,48	0
54	MG	2A	3266	1/1	0.95	0.16	35,35,35,35	0
54	MG	2A	3040	1/1	0.95	0.15	48,48,48,48	0
54	MG	2A	3268	1/1	0.95	0.15	44,44,44,44	0
54	MG	2a	3004	1/1	0.95	0.06	41,41,41,41	0
54	MG	2A	3042	1/1	0.95	0.12	43,43,43,43	0
54	MG	17	104	1/1	0.95	0.10	36,36,36,36	0
54	MG	1A	3169	1/1	0.95	0.07	36,36,36,36	0
54	MG	1A	3620	1/1	0.95	0.07	36,36,36,36	0
54	MG	1A	3408	1/1	0.95	0.08	26,26,26,26	0
54	MG	1A	3267	1/1	0.95	0.26	34,34,34,34	0
54	MG	2A	3048	1/1	0.95	0.12	54,54,54,54	0
54	MG	2A	3280	1/1	0.95	0.07	57,57,57,57	0
54	MG	2A	3049	1/1	0.95	0.12	54,54,54,54	0
54	MG	2a	3018	1/1	0.95	0.07	40,40,40,40	0
54	MG	1a	3167	1/1	0.95	0.12	56,56,56,56	0
54	MG	1A	4019	1/1	0.95	0.10	54,54,54,54	0
54	MG	1A	3410	1/1	0.95	0.07	17,17,17,17	0
54	MG	2A	3055	1/1	0.95	0.11	41,41,41,41	0
54	MG	2A	3287	1/1	0.95	0.09	33,33,33,33	0
54	MG	1a	3171	1/1	0.95	0.06	72,72,72,72	0
54	MG	1A	3008	1/1	0.95	0.09	31,31,31,31	0
54	MG	2A	3545	1/1	0.95	0.07	47,47,47,47	0
54	MG	1A	3018	1/1	0.95	0.13	23,23,23,23	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	1a	3006	1/1	0.95	0.07	57,57,57,57	0
54	MG	1A	3630	1/1	0.95	0.10	45,45,45,45	0
54	MG	2A	3550	1/1	0.95	0.09	25,25,25,25	0
54	MG	1a	3176	1/1	0.95	0.10	45,45,45,45	0
54	MG	2A	3552	1/1	0.95	0.06	47,47,47,47	0
54	MG	2A	3553	1/1	0.95	0.07	47,47,47,47	0
54	MG	2A	3555	1/1	0.95	0.05	47,47,47,47	0
54	MG	2a	3037	1/1	0.95	0.11	55,55,55,55	0
54	MG	2A	3063	1/1	0.95	0.08	46,46,46,46	0
54	MG	1a	3008	1/1	0.95	0.07	46,46,46,46	0
54	MG	1A	3419	1/1	0.95	0.07	19,19,19,19	0
54	MG	1A	3873	1/1	0.95	0.07	24,24,24,24	0
54	MG	2A	3301	1/1	0.95	0.10	27,27,27,27	0
54	MG	1A	3420	1/1	0.95	0.09	19,19,19,19	0
54	MG	1A	3063	1/1	0.95	0.06	24,24,24,24	0
54	MG	1A	4030	1/1	0.95	0.07	36,36,36,36	0
54	MG	1A	3535	1/1	0.95	0.06	40,40,40,40	0
54	MG	2a	3047	1/1	0.95	0.12	53,53,53,53	0
54	MG	2A	3307	1/1	0.95	0.06	28,28,28,28	0
54	MG	1A	3743	1/1	0.95	0.10	55,55,55,55	0
54	MG	1A	3427	1/1	0.95	0.11	50,50,50,50	0
54	MG	2A	3077	1/1	0.95	0.19	51,51,51,51	0
54	MG	1A	3537	1/1	0.95	0.09	23,23,23,23	0
54	MG	1A	4040	1/1	0.95	0.07	55,55,55,55	0
54	MG	1A	4042	1/1	0.95	0.28	40,40,40,40	0
54	MG	1A	4043	1/1	0.95	0.21	43,43,43,43	0
54	MG	1A	3639	1/1	0.95	0.10	45,45,45,45	0
54	MG	2A	3086	1/1	0.95	0.10	43,43,43,43	0
54	MG	1A	3340	1/1	0.95	0.07	29,29,29,29	0
54	MG	1A	3342	1/1	0.95	0.14	54,54,54,54	0
54	MG	2A	3322	1/1	0.95	0.06	38,38,38,38	0
54	MG	1A	3211	1/1	0.95	0.12	27,27,27,27	0
54	MG	2A	3325	1/1	0.95	0.09	35,35,35,35	0
54	MG	1A	3106	1/1	0.95	0.12	18,18,18,18	0
54	MG	1A	3178	1/1	0.95	0.11	25,25,25,25	0
54	MG	1A	3549	1/1	0.95	0.06	57,57,57,57	0
54	MG	2A	3593	1/1	0.95	0.11	45,45,45,45	0
54	MG	2A	3594	1/1	0.95	0.11	49,49,49,49	0
54	MG	1A	3133	1/1	0.95	0.16	21,21,21,21	0
54	MG	2A	3333	1/1	0.95	0.09	50,50,50,50	0
54	MG	2a	3075	1/1	0.95	0.05	51,51,51,51	0
54	MG	1A	3761	1/1	0.95	0.13	38,38,38,38	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	1B	204	1/1	0.95	0.08	40,40,40,40	0
54	MG	1A	3135	1/1	0.95	0.06	42,42,42,42	0
54	MG	2a	3081	1/1	0.95	0.17	60,60,60,60	0
54	MG	1A	3651	1/1	0.95	0.08	32,32,32,32	0
54	MG	1A	3554	1/1	0.95	0.07	44,44,44,44	0
54	MG	1A	3355	1/1	0.95	0.05	28,28,28,28	0
54	MG	1A	3007	1/1	0.95	0.12	41,41,41,41	0
54	MG	2a	3090	1/1	0.95	0.10	63,63,63,63	0
54	MG	2A	3106	1/1	0.95	0.10	37,37,37,37	0
54	MG	1A	3912	1/1	0.95	0.11	35,35,35,35	0
54	MG	1A	3557	1/1	0.95	0.07	48,48,48,48	0
54	MG	1A	3137	1/1	0.95	0.23	36,36,36,36	0
54	MG	1a	3215	1/1	0.95	0.07	73,73,73,73	0
54	MG	1A	3053	1/1	0.95	0.20	24,24,24,24	0
54	MG	1A	3778	1/1	0.95	0.13	28,28,28,28	0
54	MG	1a	3046	1/1	0.95	0.19	41,41,41,41	0
54	MG	1A	3660	1/1	0.95	0.20	28,28,28,28	0
54	MG	1a	3221	1/1	0.95	0.06	35,35,35,35	0
54	MG	2A	3358	1/1	0.95	0.10	49,49,49,49	0
54	MG	1A	3360	1/1	0.95	0.11	34,34,34,34	0
54	MG	1B	220	1/1	0.95	0.11	40,40,40,40	0
54	MG	2A	3126	1/1	0.95	0.13	40,40,40,40	0
54	MG	1B	221	1/1	0.95	0.10	38,38,38,38	0
54	MG	1B	222	1/1	0.95	0.12	45,45,45,45	0
54	MG	1A	3783	1/1	0.95	0.09	51,51,51,51	0
54	MG	1A	3564	1/1	0.95	0.07	20,20,20,20	0
54	MG	1A	3568	1/1	0.95	0.11	42,42,42,42	0
54	MG	1a	3059	1/1	0.95	0.14	48,48,48,48	0
54	MG	2A	3378	1/1	0.95	0.10	73,73,73,73	0
54	MG	1A	3085	1/1	0.95	0.39	37,37,37,37	0
54	MG	1A	3142	1/1	0.95	0.07	26,26,26,26	0
54	MG	1D	304	1/1	0.95	0.08	19,19,19,19	0
54	MG	1A	3450	1/1	0.95	0.07	30,30,30,30	0
54	MG	1A	3790	1/1	0.95	0.07	28,28,28,28	0
54	MG	2A	3653	1/1	0.95	0.08	55,55,55,55	0
54	MG	2A	3144	1/1	0.95	0.04	41,41,41,41	0
54	MG	1D	307	1/1	0.95	0.12	10,10,10,10	0
54	MG	2A	3147	1/1	0.95	0.07	27,27,27,27	0
54	MG	2a	3130	1/1	0.95	0.11	61,61,61,61	0
54	MG	2A	3666	1/1	0.95	0.08	54,54,54,54	0
54	MG	1A	3291	1/1	0.95	0.08	18,18,18,18	0
54	MG	1D	312	1/1	0.95	0.08	32,32,32,32	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	1D	313	1/1	0.95	0.09	43,43,43,43	0
54	MG	2A	3674	1/1	0.95	0.07	42,42,42,42	0
54	MG	1D	314	1/1	0.95	0.08	44,44,44,44	0
54	MG	2A	3155	1/1	0.95	0.06	46,46,46,46	0
54	MG	1a	3244	1/1	0.95	0.07	47,47,47,47	0
54	MG	1a	3245	1/1	0.95	0.06	31,31,31,31	0
54	MG	1a	3246	1/1	0.95	0.09	47,47,47,47	0
54	MG	1A	3365	1/1	0.95	0.09	40,40,40,40	0
54	MG	2A	3681	1/1	0.95	0.09	36,36,36,36	0
54	MG	2A	3160	1/1	0.95	0.15	49,49,49,49	0
54	MG	1a	3073	1/1	0.95	0.21	52,52,52,52	0
54	MG	1D	317	1/1	0.95	0.06	43,43,43,43	0
54	MG	2A	3164	1/1	0.95	0.23	45,45,45,45	0
54	MG	2A	3688	1/1	0.95	0.07	42,42,42,42	0
54	MG	2A	3406	1/1	0.95	0.12	49,49,49,49	0
54	MG	1A	3455	1/1	0.95	0.06	16,16,16,16	0
54	MG	1a	3256	1/1	0.95	0.06	39,39,39,39	0
54	MG	1E	304	1/1	0.95	0.08	15,15,15,15	0
54	MG	2a	3160	1/1	0.95	0.07	57,57,57,57	0
54	MG	2A	3703	1/1	0.95	0.07	55,55,55,55	0
54	MG	2A	3411	1/1	0.95	0.08	54,54,54,54	0
54	MG	2A	3412	1/1	0.95	0.06	27,27,27,27	0
54	MG	1A	3796	1/1	0.95	0.24	39,39,39,39	0
54	MG	1A	3797	1/1	0.95	0.07	45,45,45,45	0
54	MG	1A	3225	1/1	0.95	0.13	28,28,28,28	0
54	MG	2A	3419	1/1	0.95	0.10	37,37,37,37	0
54	MG	1a	3261	1/1	0.95	0.05	55,55,55,55	0
54	MG	1F	303	1/1	0.95	0.19	30,30,30,30	0
54	MG	2A	3174	1/1	0.95	0.23	45,45,45,45	0
54	MG	1a	3263	1/1	0.95	0.10	38,38,38,38	0
54	MG	1A	3799	1/1	0.95	0.09	32,32,32,32	0
54	MG	1a	3087	1/1	0.95	0.18	48,48,48,48	0
54	MG	1A	3113	1/1	0.95	0.27	37,37,37,37	0
54	MG	2A	3182	1/1	0.95	0.15	39,39,39,39	0
54	MG	1A	3114	1/1	0.95	0.15	28,28,28,28	0
54	MG	1A	3466	1/1	0.95	0.10	37,37,37,37	0
54	MG	2A	3727	1/1	0.95	0.09	50,50,50,50	0
54	MG	2A	3728	1/1	0.95	0.07	40,40,40,40	0
54	MG	1A	3958	1/1	0.95	0.08	29,29,29,29	0
54	MG	1A	3301	1/1	0.95	0.08	35,35,35,35	0
54	MG	2a	3188	1/1	0.95	0.08	77,77,77,77	0
54	MG	1G	203	1/1	0.95	0.07	52,52,52,52	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	2A	3433	1/1	0.95	0.09	39,39,39,39	0
54	MG	2A	3434	1/1	0.95	0.10	55,55,55,55	0
54	MG	2A	3735	1/1	0.95	0.14	46,46,46,46	0
54	MG	2A	3189	1/1	0.95	0.12	62,62,62,62	0
54	MG	1A	3054	1/1	0.95	0.07	23,23,23,23	0
54	MG	2A	3738	1/1	0.95	0.10	51,51,51,51	0
54	MG	1H	202	1/1	0.95	0.09	38,38,38,38	0
54	MG	1A	3087	1/1	0.95	0.12	34,34,34,34	0
54	MG	1A	3023	1/1	0.95	0.07	22,22,22,22	0
54	MG	1A	3478	1/1	0.95	0.13	61,61,61,61	0
54	MG	1A	3309	1/1	0.95	0.29	31,31,31,31	0
54	MG	1A	3969	1/1	0.95	0.07	51,51,51,51	0
54	MG	2t	3100	1/1	0.95	0.10	48,48,48,48	0
55	YXM	1A	4055	40/40	0.95	0.10	16,31,46,48	0
54	MG	2A	3747	1/1	0.95	0.09	54,54,54,54	0
54	MG	2A	3445	1/1	0.95	0.09	58,58,58,58	0
54	MG	2A	3446	1/1	0.95	0.07	37,37,37,37	0
54	MG	2A	3198	1/1	0.95	0.18	38,38,38,38	0
54	MG	1d	303	1/1	0.95	0.11	45,45,45,45	0
54	MG	2A	3752	1/1	0.95	0.12	51,51,51,51	0
54	MG	1A	3482	1/1	0.95	0.08	51,51,51,51	0
54	MG	2A	3450	1/1	0.95	0.08	48,48,48,48	0
54	MG	1A	3236	1/1	0.95	0.16	25,25,25,25	0
54	MG	1e	201	1/1	0.95	0.12	44,44,44,44	0
58	ZN	2n	102	1/1	0.95	0.09	93,93,93,93	0
54	MG	1a	3009	1/1	0.96	0.21	44,44,44,44	0
54	MG	1A	3171	1/1	0.96	0.09	47,47,47,47	0
54	MG	2A	3741	1/1	0.96	0.09	40,40,40,40	0
54	MG	1A	3044	1/1	0.96	0.09	22,22,22,22	0
54	MG	1A	3664	1/1	0.96	0.06	28,28,28,28	0
54	MG	1A	3665	1/1	0.96	0.07	48,48,48,48	0
54	MG	1A	4012	1/1	0.96	0.32	35,35,35,35	0
54	MG	1A	3425	1/1	0.96	0.07	21,21,21,21	0
54	MG	2A	3162	1/1	0.96	0.12	48,48,48,48	0
54	MG	1A	3336	1/1	0.96	0.06	47,47,47,47	0
54	MG	1A	3669	1/1	0.96	0.11	45,45,45,45	0
54	MG	2A	3165	1/1	0.96	0.11	54,54,54,54	0
54	MG	1A	4017	1/1	0.96	0.05	60,60,60,60	0
54	MG	1A	3829	1/1	0.96	0.07	40,40,40,40	0
54	MG	1A	3547	1/1	0.96	0.12	22,22,22,22	0
54	MG	1A	3174	1/1	0.96	0.10	35,35,35,35	0
54	MG	1A	3832	1/1	0.96	0.08	54,54,54,54	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	1A	3338	1/1	0.96	0.07	21,21,21,21	0
54	MG	1A	3045	1/1	0.96	0.08	33,33,33,33	0
54	MG	1A	3084	1/1	0.96	0.20	34,34,34,34	0
54	MG	1A	4026	1/1	0.96	0.19	10,10,10,10	0
54	MG	2A	3439	1/1	0.96	0.07	38,38,38,38	0
54	MG	2A	3176	1/1	0.96	0.08	33,33,33,33	0
54	MG	1A	3552	1/1	0.96	0.05	35,35,35,35	0
54	MG	1A	3679	1/1	0.96	0.07	41,41,41,41	0
54	MG	1A	3838	1/1	0.96	0.37	28,28,28,28	0
54	MG	1A	3111	1/1	0.96	0.10	21,21,21,21	0
54	MG	1A	3434	1/1	0.96	0.09	12,12,12,12	0
54	MG	1A	3215	1/1	0.96	0.19	23,23,23,23	0
54	MG	2A	3184	1/1	0.96	0.21	38,38,38,38	0
54	MG	1A	4034	1/1	0.96	0.06	50,50,50,50	0
54	MG	1A	3272	1/1	0.96	0.18	27,27,27,27	0
54	MG	2B	216	1/1	0.96	0.06	53,53,53,53	0
54	MG	1A	3437	1/1	0.96	0.06	48,48,48,48	0
54	MG	1A	3560	1/1	0.96	0.09	35,35,35,35	0
54	MG	1A	4041	1/1	0.96	0.06	41,41,41,41	0
54	MG	1a	3253	1/1	0.96	0.05	61,61,61,61	0
54	MG	2A	3455	1/1	0.96	0.07	51,51,51,51	0
54	MG	2A	3191	1/1	0.96	0.10	61,61,61,61	0
54	MG	2D	307	1/1	0.96	0.10	63,63,63,63	0
54	MG	1A	3687	1/1	0.96	0.06	38,38,38,38	0
54	MG	1A	3022	1/1	0.96	0.06	29,29,29,29	0
54	MG	1A	3347	1/1	0.96	0.15	33,33,33,33	0
54	MG	1A	3690	1/1	0.96	0.08	50,50,50,50	0
54	MG	1A	3349	1/1	0.96	0.08	14,14,14,14	0
54	MG	1A	3565	1/1	0.96	0.04	29,29,29,29	0
54	MG	1A	4049	1/1	0.96	0.09	52,52,52,52	0
54	MG	1A	3856	1/1	0.96	0.07	37,37,37,37	0
54	MG	1A	3566	1/1	0.96	0.14	27,27,27,27	0
54	MG	1a	3053	1/1	0.96	0.19	61,61,61,61	0
54	MG	1A	4053	1/1	0.96	0.14	56,56,56,56	0
54	MG	1A	3567	1/1	0.96	0.04	36,36,36,36	0
54	MG	1A	3441	1/1	0.96	0.08	35,35,35,35	0
54	MG	1A	3351	1/1	0.96	0.13	9,9,9,9	0
54	MG	2A	3207	1/1	0.96	0.09	42,42,42,42	0
54	MG	1A	3443	1/1	0.96	0.06	18,18,18,18	0
54	MG	1a	3060	1/1	0.96	0.21	57,57,57,57	0
54	MG	1a	3061	1/1	0.96	0.16	59,59,59,59	0
54	MG	1A	3444	1/1	0.96	0.10	13,13,13,13	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	1A	3050	1/1	0.96	0.20	30,30,30,30	0
54	MG	2Q	201	1/1	0.96	0.06	60,60,60,60	0
54	MG	2A	3481	1/1	0.96	0.12	19,19,19,19	0
54	MG	1A	3446	1/1	0.96	0.14	32,32,32,32	0
54	MG	2R	201	1/1	0.96	0.15	47,47,47,47	0
54	MG	1A	3051	1/1	0.96	0.17	36,36,36,36	0
54	MG	2R	203	1/1	0.96	0.05	19,19,19,19	0
54	MG	1A	3707	1/1	0.96	0.06	26,26,26,26	0
54	MG	1A	3144	1/1	0.96	0.06	20,20,20,20	0
54	MG	1A	3577	1/1	0.96	0.05	35,35,35,35	0
54	MG	1A	3278	1/1	0.96	0.07	26,26,26,26	0
54	MG	1A	3117	1/1	0.96	0.10	24,24,24,24	0
54	MG	2W	202	1/1	0.96	0.13	53,53,53,53	0
54	MG	1A	3713	1/1	0.96	0.21	24,24,24,24	0
54	MG	1A	3580	1/1	0.96	0.06	46,46,46,46	0
54	MG	1A	3453	1/1	0.96	0.05	39,39,39,39	0
54	MG	1A	3884	1/1	0.96	0.08	56,56,56,56	0
54	MG	1A	3281	1/1	0.96	0.16	22,22,22,22	0
54	MG	1A	3283	1/1	0.96	0.26	40,40,40,40	0
54	MG	1a	3077	1/1	0.96	0.13	39,39,39,39	0
54	MG	1g	203	1/1	0.96	0.14	57,57,57,57	0
54	MG	2A	3499	1/1	0.96	0.08	25,25,25,25	0
54	MG	1A	3221	1/1	0.96	0.10	40,40,40,40	0
54	MG	27	101	1/1	0.96	0.19	38,38,38,38	0
54	MG	1a	3080	1/1	0.96	0.13	37,37,37,37	0
54	MG	28	101	1/1	0.96	0.08	54,54,54,54	0
54	MG	1k	201	1/1	0.96	0.17	36,36,36,36	0
54	MG	2a	3001	1/1	0.96	0.06	31,31,31,31	0
54	MG	2A	3507	1/1	0.96	0.09	53,53,53,53	0
54	MG	1a	3081	1/1	0.96	0.13	53,53,53,53	0
54	MG	2A	3234	1/1	0.96	0.36	45,45,45,45	0
54	MG	1A	3889	1/1	0.96	0.07	45,45,45,45	0
54	MG	1A	3459	1/1	0.96	0.08	45,45,45,45	0
54	MG	2A	3237	1/1	0.96	0.08	43,43,43,43	0
54	MG	2a	3008	1/1	0.96	0.09	36,36,36,36	0
54	MG	2a	3009	1/1	0.96	0.05	67,67,67,67	0
54	MG	1a	3084	1/1	0.96	0.13	70,70,70,70	0
54	MG	2A	3239	1/1	0.96	0.23	40,40,40,40	0
54	MG	1A	3462	1/1	0.96	0.07	45,45,45,45	0
54	MG	1A	3001	1/1	0.96	0.04	26,26,26,26	0
54	MG	1D	302	1/1	0.96	0.18	23,23,23,23	0
54	MG	1D	303	1/1	0.96	0.07	46,46,46,46	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	1A	3068	1/1	0.96	0.15	30,30,30,30	0
54	MG	1A	3465	1/1	0.96	0.08	35,35,35,35	0
54	MG	1A	3224	1/1	0.96	0.26	32,32,32,32	0
54	MG	2A	3523	1/1	0.96	0.08	38,38,38,38	0
54	MG	1A	3729	1/1	0.96	0.11	33,33,33,33	0
54	MG	1D	308	1/1	0.96	0.07	45,45,45,45	0
54	MG	1D	309	1/1	0.96	0.14	25,25,25,25	0
54	MG	1A	3901	1/1	0.96	0.06	24,24,24,24	0
54	MG	1a	3096	1/1	0.96	0.23	43,43,43,43	0
54	MG	1A	3471	1/1	0.96	0.05	35,35,35,35	0
54	MG	1A	3024	1/1	0.96	0.10	12,12,12,12	0
54	MG	1a	3099	1/1	0.96	0.09	54,54,54,54	0
54	MG	2a	3030	1/1	0.96	0.19	53,53,53,53	0
54	MG	2a	3031	1/1	0.96	0.13	56,56,56,56	0
54	MG	1A	3473	1/1	0.96	0.10	44,44,44,44	0
54	MG	1A	3905	1/1	0.96	0.06	41,41,41,41	0
54	MG	1A	3907	1/1	0.96	0.12	18,18,18,18	0
54	MG	2A	3014	1/1	0.96	0.06	44,44,44,44	0
54	MG	1A	3025	1/1	0.96	0.15	40,40,40,40	0
54	MG	2A	3261	1/1	0.96	0.27	58,58,58,58	0
54	MG	2A	3018	1/1	0.96	0.07	36,36,36,36	0
54	MG	2A	3263	1/1	0.96	0.13	44,44,44,44	0
54	MG	1A	3369	1/1	0.96	0.06	19,19,19,19	0
54	MG	1A	3916	1/1	0.96	0.06	56,56,56,56	0
54	MG	2A	3022	1/1	0.96	0.07	31,31,31,31	0
54	MG	2A	3023	1/1	0.96	0.16	40,40,40,40	0
54	MG	1A	3736	1/1	0.96	0.06	15,15,15,15	0
54	MG	1A	3919	1/1	0.96	0.09	44,44,44,44	0
54	MG	1A	3230	1/1	0.96	0.20	32,32,32,32	0
54	MG	2A	3273	1/1	0.96	0.32	48,48,48,48	0
54	MG	1F	304	1/1	0.96	0.17	26,26,26,26	0
54	MG	1F	305	1/1	0.96	0.17	25,25,25,25	0
54	MG	2a	3050	1/1	0.96	0.18	55,55,55,55	0
54	MG	2A	3276	1/1	0.96	0.07	29,29,29,29	0
54	MG	1a	3115	1/1	0.96	0.06	44,44,44,44	0
54	MG	2A	3554	1/1	0.96	0.06	60,60,60,60	0
54	MG	2a	3054	1/1	0.96	0.21	50,50,50,50	0
54	MG	1A	3293	1/1	0.96	0.23	44,44,44,44	0
54	MG	1a	3117	1/1	0.96	0.07	68,68,68,68	0
54	MG	1A	3601	1/1	0.96	0.06	33,33,33,33	0
54	MG	2a	3059	1/1	0.96	0.10	53,53,53,53	0
54	MG	1A	3602	1/1	0.96	0.06	44,44,44,44	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	1A	3479	1/1	0.96	0.06	36,36,36,36	0
54	MG	1A	3150	1/1	0.96	0.33	35,35,35,35	0
54	MG	2A	3284	1/1	0.96	0.06	45,45,45,45	0
54	MG	1A	3481	1/1	0.96	0.08	46,46,46,46	0
54	MG	1A	3097	1/1	0.96	0.10	49,49,49,49	0
54	MG	1a	3126	1/1	0.96	0.08	50,50,50,50	0
54	MG	1G	204	1/1	0.96	0.11	37,37,37,37	0
54	MG	1A	3750	1/1	0.96	0.12	28,28,28,28	0
54	MG	1A	3608	1/1	0.96	0.16	51,51,51,51	0
54	MG	1N	201	1/1	0.96	0.12	40,40,40,40	0
54	MG	1N	202	1/1	0.96	0.14	40,40,40,40	0
54	MG	1a	3132	1/1	0.96	0.06	53,53,53,53	0
54	MG	1N	203	1/1	0.96	0.09	58,58,58,58	0
54	MG	1A	3152	1/1	0.96	0.10	40,40,40,40	0
54	MG	1P	201	1/1	0.96	0.40	34,34,34,34	0
54	MG	1A	3937	1/1	0.96	0.06	39,39,39,39	0
54	MG	2a	3078	1/1	0.96	0.16	33,33,33,33	0
54	MG	2A	3054	1/1	0.96	0.09	37,37,37,37	0
54	MG	2a	3080	1/1	0.96	0.14	49,49,49,49	0
54	MG	1A	3488	1/1	0.96	0.12	47,47,47,47	0
54	MG	1A	3234	1/1	0.96	0.15	33,33,33,33	0
54	MG	1Q	201	1/1	0.96	0.08	26,26,26,26	0
54	MG	2a	3085	1/1	0.96	0.25	53,53,53,53	0
54	MG	2a	3086	1/1	0.96	0.36	45,45,45,45	0
54	MG	1a	3140	1/1	0.96	0.07	49,49,49,49	0
54	MG	1Q	204	1/1	0.96	0.10	37,37,37,37	0
54	MG	2A	3060	1/1	0.96	0.09	27,27,27,27	0
54	MG	1R	201	1/1	0.96	0.14	26,26,26,26	0
54	MG	2a	3093	1/1	0.96	0.11	60,60,60,60	0
54	MG	1A	3614	1/1	0.96	0.06	46,46,46,46	0
54	MG	1R	203	1/1	0.96	0.23	39,39,39,39	0
54	MG	1A	3490	1/1	0.96	0.08	40,40,40,40	0
54	MG	1a	3148	1/1	0.96	0.06	48,48,48,48	0
54	MG	1A	3947	1/1	0.96	0.08	39,39,39,39	0
54	MG	2A	3317	1/1	0.96	0.08	53,53,53,53	0
54	MG	2A	3068	1/1	0.96	0.05	35,35,35,35	0
54	MG	1A	3759	1/1	0.96	0.14	31,31,31,31	0
54	MG	2a	3102	1/1	0.96	0.05	56,56,56,56	0
54	MG	1A	3153	1/1	0.96	0.28	33,33,33,33	0
54	MG	1A	3382	1/1	0.96	0.16	51,51,51,51	0
54	MG	2A	3072	1/1	0.96	0.14	52,52,52,52	0
54	MG	2A	3073	1/1	0.96	0.19	33,33,33,33	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	2A	3324	1/1	0.96	0.12	38,38,38,38	0
54	MG	2a	3110	1/1	0.96	0.08	54,54,54,54	0
54	MG	1A	3098	1/1	0.96	0.05	26,26,26,26	0
54	MG	1A	3019	1/1	0.96	0.19	22,22,22,22	0
54	MG	1A	3157	1/1	0.96	0.16	29,29,29,29	0
54	MG	1a	3157	1/1	0.96	0.06	46,46,46,46	0
54	MG	2A	3331	1/1	0.96	0.09	42,42,42,42	0
54	MG	1A	3621	1/1	0.96	0.09	39,39,39,39	0
54	MG	1A	3388	1/1	0.96	0.06	36,36,36,36	0
54	MG	1A	3959	1/1	0.96	0.07	42,42,42,42	0
54	MG	2A	3628	1/1	0.96	0.05	58,58,58,58	0
54	MG	2A	3082	1/1	0.96	0.25	56,56,56,56	0
54	MG	1A	3057	1/1	0.96	0.12	17,17,17,17	0
54	MG	2A	3339	1/1	0.96	0.07	31,31,31,31	0
54	MG	1A	3961	1/1	0.96	0.06	38,38,38,38	0
54	MG	1A	3625	1/1	0.96	0.28	28,28,28,28	0
54	MG	2a	3126	1/1	0.96	0.11	48,48,48,48	0
54	MG	1A	3311	1/1	0.96	0.12	30,30,30,30	0
54	MG	2A	3088	1/1	0.96	0.09	34,34,34,34	0
54	MG	2A	3637	1/1	0.96	0.04	52,52,52,52	0
54	MG	2A	3639	1/1	0.96	0.07	40,40,40,40	0
54	MG	2A	3345	1/1	0.96	0.12	50,50,50,50	0
54	MG	1V	202	1/1	0.96	0.15	43,43,43,43	0
54	MG	1V	204	1/1	0.96	0.09	40,40,40,40	0
54	MG	2A	3644	1/1	0.96	0.06	57,57,57,57	0
54	MG	2a	3136	1/1	0.96	0.04	47,47,47,47	0
54	MG	2A	3348	1/1	0.96	0.06	24,24,24,24	0
54	MG	1A	3314	1/1	0.96	0.16	31,31,31,31	0
54	MG	1A	3779	1/1	0.96	0.15	38,38,38,38	0
54	MG	2A	3351	1/1	0.96	0.09	21,21,21,21	0
54	MG	1A	3241	1/1	0.96	0.20	36,36,36,36	0
54	MG	2a	3142	1/1	0.96	0.07	62,62,62,62	0
54	MG	10	101	1/1	0.96	0.11	32,32,32,32	0
54	MG	1A	3242	1/1	0.96	0.12	32,32,32,32	0
54	MG	2A	3654	1/1	0.96	0.06	63,63,63,63	0
54	MG	1A	3782	1/1	0.96	0.08	19,19,19,19	0
54	MG	2A	3662	1/1	0.96	0.05	64,64,64,64	0
54	MG	10	104	1/1	0.96	0.08	44,44,44,44	0
54	MG	1A	3077	1/1	0.96	0.10	22,22,22,22	0
54	MG	1A	3504	1/1	0.96	0.07	51,51,51,51	0
54	MG	2a	3154	1/1	0.96	0.06	50,50,50,50	0
54	MG	1A	3505	1/1	0.96	0.08	16,16,16,16	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	2A	3668	1/1	0.96	0.09	49,49,49,49	0
54	MG	1A	3506	1/1	0.96	0.07	15,15,15,15	0
54	MG	1A	3508	1/1	0.96	0.07	59,59,59,59	0
54	MG	1A	3161	1/1	0.96	0.17	40,40,40,40	0
54	MG	1A	3245	1/1	0.96	0.12	32,32,32,32	0
54	MG	2A	3364	1/1	0.96	0.11	70,70,70,70	0
54	MG	1A	3640	1/1	0.96	0.11	46,46,46,46	0
54	MG	2A	3366	1/1	0.96	0.08	42,42,42,42	0
54	MG	2a	3167	1/1	0.96	0.12	65,65,65,65	0
54	MG	1A	3792	1/1	0.96	0.13	38,38,38,38	0
54	MG	2A	3369	1/1	0.96	0.06	44,44,44,44	0
54	MG	1A	3246	1/1	0.96	0.13	26,26,26,26	0
54	MG	2A	3373	1/1	0.96	0.08	53,53,53,53	0
54	MG	1A	3515	1/1	0.96	0.05	53,53,53,53	0
54	MG	2a	3173	1/1	0.96	0.07	47,47,47,47	0
54	MG	1A	3009	1/1	0.96	0.17	25,25,25,25	0
54	MG	1A	3404	1/1	0.96	0.06	20,20,20,20	0
54	MG	15	104	1/1	0.96	0.10	29,29,29,29	0
54	MG	15	105	1/1	0.96	0.25	18,18,18,18	0
54	MG	15	106	1/1	0.96	0.08	41,41,41,41	0
54	MG	2A	3125	1/1	0.96	0.09	34,34,34,34	0
54	MG	2A	3700	1/1	0.96	0.09	56,56,56,56	0
54	MG	1A	3164	1/1	0.96	0.05	23,23,23,23	0
54	MG	16	101	1/1	0.96	0.07	39,39,39,39	0
54	MG	2a	3185	1/1	0.96	0.07	45,45,45,45	0
54	MG	2A	3704	1/1	0.96	0.07	55,55,55,55	0
54	MG	2A	3389	1/1	0.96	0.12	25,25,25,25	0
54	MG	1A	3522	1/1	0.96	0.06	36,36,36,36	0
54	MG	1A	3105	1/1	0.96	0.12	37,37,37,37	0
54	MG	1A	3989	1/1	0.96	0.07	32,32,32,32	0
54	MG	1A	3203	1/1	0.96	0.06	35,35,35,35	0
54	MG	2a	3193	1/1	0.96	0.07	52,52,52,52	0
54	MG	1A	3030	1/1	0.96	0.04	24,24,24,24	0
54	MG	1A	3134	1/1	0.96	0.25	26,26,26,26	0
54	MG	1A	3653	1/1	0.96	0.07	42,42,42,42	0
54	MG	2a	3197	1/1	0.96	0.10	56,56,56,56	0
54	MG	2A	3136	1/1	0.96	0.18	50,50,50,50	0
54	MG	1A	3258	1/1	0.96	0.19	33,33,33,33	0
54	MG	2a	3200	1/1	0.96	0.12	70,70,70,70	0
54	MG	1A	3655	1/1	0.96	0.13	28,28,28,28	0
54	MG	2A	3141	1/1	0.96	0.14	43,43,43,43	0
54	MG	1a	3205	1/1	0.96	0.09	74,74,74,74	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	2A	3722	1/1	0.96	0.11	48,48,48,48	0
54	MG	2A	3143	1/1	0.96	0.13	42,42,42,42	0
54	MG	2A	3403	1/1	0.96	0.07	28,28,28,28	0
54	MG	1A	3808	1/1	0.96	0.09	60,60,60,60	0
55	YXM	2A	3758	40/40	0.96	0.11	28,39,51,52	0
54	MG	2A	3145	1/1	0.96	0.09	28,28,28,28	0
54	MG	1A	3259	1/1	0.96	0.06	65,65,65,65	0
54	MG	1a	3208	1/1	0.96	0.12	53,53,53,53	0
54	MG	1A	3414	1/1	0.96	0.10	15,15,15,15	0
54	MG	2A	3149	1/1	0.96	0.11	48,48,48,48	0
54	MG	1A	3415	1/1	0.96	0.08	19,19,19,19	0
54	MG	2A	3413	1/1	0.96	0.10	56,56,56,56	0
54	MG	2A	3151	1/1	0.96	0.08	50,50,50,50	0
54	MG	1A	3332	1/1	0.96	0.14	46,46,46,46	0
54	MG	1A	3260	1/1	0.96	0.09	39,39,39,39	0
54	MG	2A	3418	1/1	0.96	0.09	28,28,28,28	0
54	MG	1A	3327	1/1	0.97	0.12	42,42,42,42	0
54	MG	1a	3110	1/1	0.97	0.07	20,20,20,20	0
54	MG	1A	3880	1/1	0.97	0.05	47,47,47,47	0
54	MG	2T	202	1/1	0.97	0.11	45,45,45,45	0
54	MG	1W	203	1/1	0.97	0.14	26,26,26,26	0
54	MG	1a	3113	1/1	0.97	0.06	52,52,52,52	0
54	MG	2V	202	1/1	0.97	0.12	42,42,42,42	0
54	MG	1A	3229	1/1	0.97	0.09	40,40,40,40	0
54	MG	1A	3271	1/1	0.97	0.08	36,36,36,36	0
54	MG	1A	3764	1/1	0.97	0.09	24,24,24,24	0
54	MG	1A	3765	1/1	0.97	0.07	30,30,30,30	0
54	MG	1A	3394	1/1	0.97	0.04	24,24,24,24	0
54	MG	2A	3561	1/1	0.97	0.05	43,43,43,43	0
54	MG	2A	3562	1/1	0.97	0.06	60,60,60,60	0
54	MG	1A	3395	1/1	0.97	0.04	34,34,34,34	0
54	MG	10	106	1/1	0.97	0.08	59,59,59,59	0
54	MG	1A	3768	1/1	0.97	0.06	46,46,46,46	0
54	MG	1a	3123	1/1	0.97	0.06	32,32,32,32	0
54	MG	1A	3011	1/1	0.97	0.12	49,49,49,49	0
54	MG	1A	3162	1/1	0.97	0.12	26,26,26,26	0
54	MG	1i	201	1/1	0.97	0.12	56,56,56,56	0
54	MG	1A	4031	1/1	0.97	0.04	33,33,33,33	0
54	MG	1A	3771	1/1	0.97	0.07	32,32,32,32	0
54	MG	13	101	1/1	0.97	0.10	26,26,26,26	0
54	MG	1m	201	1/1	0.97	0.07	66,66,66,66	0
54	MG	2A	3575	1/1	0.97	0.06	45,45,45,45	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	2A	3576	1/1	0.97	0.06	56,56,56,56	0
54	MG	13	102	1/1	0.97	0.07	18,18,18,18	0
54	MG	2A	3175	1/1	0.97	0.07	41,41,41,41	0
54	MG	2A	3579	1/1	0.97	0.06	49,49,49,49	0
54	MG	1A	3037	1/1	0.97	0.15	48,48,48,48	0
54	MG	2A	3177	1/1	0.97	0.05	33,33,33,33	0
54	MG	1A	3400	1/1	0.97	0.14	27,27,27,27	0
54	MG	1A	3776	1/1	0.97	0.06	30,30,30,30	0
54	MG	1A	3897	1/1	0.97	0.06	36,36,36,36	0
54	MG	2A	3372	1/1	0.97	0.04	27,27,27,27	0
54	MG	2A	3589	1/1	0.97	0.15	51,51,51,51	0
54	MG	2a	3015	1/1	0.97	0.15	44,44,44,44	0
54	MG	1A	3066	1/1	0.97	0.06	20,20,20,20	0
54	MG	2A	3374	1/1	0.97	0.09	36,36,36,36	0
54	MG	2A	3376	1/1	0.97	0.05	50,50,50,50	0
54	MG	1A	3197	1/1	0.97	0.07	49,49,49,49	0
54	MG	1A	3277	1/1	0.97	0.19	27,27,27,27	0
54	MG	2A	3379	1/1	0.97	0.09	38,38,38,38	0
54	MG	1A	3672	1/1	0.97	0.10	42,42,42,42	0
54	MG	1A	3165	1/1	0.97	0.14	49,49,49,49	0
54	MG	1A	3088	1/1	0.97	0.05	32,32,32,32	0
54	MG	2A	3601	1/1	0.97	0.07	38,38,38,38	0
54	MG	1A	3237	1/1	0.97	0.17	22,22,22,22	0
54	MG	2A	3603	1/1	0.97	0.06	32,32,32,32	0
54	MG	1A	4047	1/1	0.97	0.10	46,46,46,46	0
54	MG	1A	3167	1/1	0.97	0.10	31,31,31,31	0
54	MG	1A	3089	1/1	0.97	0.08	28,28,28,28	0
54	MG	1A	4050	1/1	0.97	0.10	35,35,35,35	0
54	MG	1A	3091	1/1	0.97	0.18	34,34,34,34	0
54	MG	1A	3286	1/1	0.97	0.09	56,56,56,56	0
54	MG	2A	3613	1/1	0.97	0.07	25,25,25,25	0
54	MG	1a	3150	1/1	0.97	0.09	56,56,56,56	0
54	MG	1A	3413	1/1	0.97	0.05	24,24,24,24	0
54	MG	1A	3344	1/1	0.97	0.10	37,37,37,37	0
54	MG	1A	3141	1/1	0.97	0.05	28,28,28,28	0
54	MG	2A	3016	1/1	0.97	0.17	47,47,47,47	0
54	MG	2A	3017	1/1	0.97	0.14	45,45,45,45	0
54	MG	1A	3416	1/1	0.97	0.09	10,10,10,10	0
54	MG	2A	3626	1/1	0.97	0.07	30,30,30,30	0
54	MG	2A	3019	1/1	0.97	0.10	54,54,54,54	0
54	MG	1A	3793	1/1	0.97	0.09	39,39,39,39	0
54	MG	1A	3116	1/1	0.97	0.12	27,27,27,27	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	2A	3204	1/1	0.97	0.06	41,41,41,41	0
54	MG	1A	3173	1/1	0.97	0.20	29,29,29,29	0
54	MG	2A	3404	1/1	0.97	0.05	29,29,29,29	0
54	MG	1A	3348	1/1	0.97	0.07	14,14,14,14	0
54	MG	1A	3003	1/1	0.97	0.06	24,24,24,24	0
54	MG	2A	3407	1/1	0.97	0.08	23,23,23,23	0
54	MG	1A	3422	1/1	0.97	0.07	31,31,31,31	0
54	MG	1A	3423	1/1	0.97	0.05	21,21,21,21	0
54	MG	2A	3210	1/1	0.97	0.17	33,33,33,33	0
54	MG	1B	212	1/1	0.97	0.05	30,30,30,30	0
54	MG	1A	3932	1/1	0.97	0.06	34,34,34,34	0
54	MG	2a	3057	1/1	0.97	0.10	59,59,59,59	0
54	MG	2A	3029	1/1	0.97	0.08	28,28,28,28	0
54	MG	2A	3414	1/1	0.97	0.05	26,26,26,26	0
54	MG	2a	3060	1/1	0.97	0.08	46,46,46,46	0
54	MG	1A	3424	1/1	0.97	0.11	45,45,45,45	0
54	MG	1A	3935	1/1	0.97	0.10	37,37,37,37	0
54	MG	1a	3166	1/1	0.97	0.07	65,65,65,65	0
54	MG	1A	3118	1/1	0.97	0.06	13,13,13,13	0
54	MG	2A	3035	1/1	0.97	0.15	38,38,38,38	0
54	MG	1A	3004	1/1	0.97	0.08	30,30,30,30	0
54	MG	1A	3512	1/1	0.97	0.07	35,35,35,35	0
54	MG	1A	3941	1/1	0.97	0.05	38,38,38,38	0
54	MG	2A	3656	1/1	0.97	0.06	45,45,45,45	0
54	MG	2A	3658	1/1	0.97	0.05	58,58,58,58	0
54	MG	1a	3018	1/1	0.97	0.06	35,35,35,35	0
54	MG	1A	3040	1/1	0.97	0.09	24,24,24,24	0
54	MG	2A	3664	1/1	0.97	0.06	62,62,62,62	0
54	MG	2A	3041	1/1	0.97	0.13	39,39,39,39	0
54	MG	1A	3944	1/1	0.97	0.08	37,37,37,37	0
54	MG	1a	3021	1/1	0.97	0.09	36,36,36,36	0
54	MG	1A	3055	1/1	0.97	0.09	45,45,45,45	0
54	MG	1A	3605	1/1	0.97	0.07	35,35,35,35	0
54	MG	2A	3229	1/1	0.97	0.07	53,53,53,53	0
54	MG	1A	3516	1/1	0.97	0.07	25,25,25,25	0
54	MG	1A	3948	1/1	0.97	0.06	27,27,27,27	0
54	MG	1A	3809	1/1	0.97	0.07	41,41,41,41	0
54	MG	1A	3297	1/1	0.97	0.05	40,40,40,40	0
54	MG	1A	3357	1/1	0.97	0.07	31,31,31,31	0
54	MG	1A	3249	1/1	0.97	0.20	27,27,27,27	0
54	MG	1A	3521	1/1	0.97	0.08	35,35,35,35	0
54	MG	2a	3088	1/1	0.97	0.28	50,50,50,50	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	2A	3053	1/1	0.97	0.11	42,42,42,42	0
54	MG	1a	3031	1/1	0.97	0.13	45,45,45,45	0
54	MG	1A	3250	1/1	0.97	0.17	32,32,32,32	0
54	MG	2a	3092	1/1	0.97	0.18	53,53,53,53	0
54	MG	1A	3072	1/1	0.97	0.05	24,24,24,24	0
54	MG	1A	3524	1/1	0.97	0.05	49,49,49,49	0
54	MG	2A	3443	1/1	0.97	0.06	47,47,47,47	0
54	MG	2A	3690	1/1	0.97	0.06	59,59,59,59	0
54	MG	1A	3526	1/1	0.97	0.06	34,34,34,34	0
54	MG	2A	3693	1/1	0.97	0.05	38,38,38,38	0
54	MG	1a	3190	1/1	0.97	0.06	50,50,50,50	0
54	MG	2A	3696	1/1	0.97	0.05	45,45,45,45	0
54	MG	2A	3697	1/1	0.97	0.06	48,48,48,48	0
54	MG	1a	3036	1/1	0.97	0.21	50,50,50,50	0
54	MG	2A	3699	1/1	0.97	0.05	44,44,44,44	0
54	MG	2a	3104	1/1	0.97	0.06	61,61,61,61	0
54	MG	1A	3527	1/1	0.97	0.07	13,13,13,13	0
54	MG	2A	3701	1/1	0.97	0.07	30,30,30,30	0
54	MG	1A	3823	1/1	0.97	0.05	37,37,37,37	0
54	MG	2a	3108	1/1	0.97	0.10	48,48,48,48	0
54	MG	1A	3305	1/1	0.97	0.09	40,40,40,40	0
54	MG	1A	3362	1/1	0.97	0.11	45,45,45,45	0
54	MG	1A	3032	1/1	0.97	0.10	36,36,36,36	0
54	MG	2a	3112	1/1	0.97	0.08	47,47,47,47	0
54	MG	1A	3966	1/1	0.97	0.04	17,17,17,17	0
54	MG	2A	3067	1/1	0.97	0.08	37,37,37,37	0
54	MG	1A	3828	1/1	0.97	0.07	40,40,40,40	0
54	MG	1E	302	1/1	0.97	0.06	28,28,28,28	0
54	MG	2A	3711	1/1	0.97	0.06	58,58,58,58	0
54	MG	1A	3717	1/1	0.97	0.13	34,34,34,34	0
54	MG	1A	3307	1/1	0.97	0.08	43,43,43,43	0
54	MG	1A	3720	1/1	0.97	0.05	30,30,30,30	0
54	MG	1a	3048	1/1	0.97	0.13	40,40,40,40	0
54	MG	1F	301	1/1	0.97	0.10	20,20,20,20	0
54	MG	1A	3622	1/1	0.97	0.09	28,28,28,28	0
54	MG	1A	3253	1/1	0.97	0.08	41,41,41,41	0
54	MG	1A	3366	1/1	0.97	0.06	22,22,22,22	0
54	MG	2A	3078	1/1	0.97	0.13	30,30,30,30	0
54	MG	2A	3723	1/1	0.97	0.06	48,48,48,48	0
54	MG	2a	3128	1/1	0.97	0.08	61,61,61,61	0
54	MG	1A	3254	1/1	0.97	0.27	49,49,49,49	0
54	MG	1F	306	1/1	0.97	0.07	24,24,24,24	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	1A	3033	1/1	0.97	0.09	35,35,35,35	0
54	MG	1F	309	1/1	0.97	0.10	29,29,29,29	0
54	MG	1F	311	1/1	0.97	0.12	28,28,28,28	0
54	MG	2A	3729	1/1	0.97	0.09	40,40,40,40	0
54	MG	2A	3269	1/1	0.97	0.16	18,18,18,18	0
54	MG	1A	3627	1/1	0.97	0.28	18,18,18,18	0
54	MG	2A	3271	1/1	0.97	0.07	43,43,43,43	0
54	MG	2A	3085	1/1	0.97	0.22	54,54,54,54	0
54	MG	1A	3125	1/1	0.97	0.04	65,65,65,65	0
54	MG	1F	314	1/1	0.97	0.06	47,47,47,47	0
54	MG	1A	3370	1/1	0.97	0.06	16,16,16,16	0
54	MG	1A	3312	1/1	0.97	0.07	12,12,12,12	0
54	MG	1A	3980	1/1	0.97	0.07	34,34,34,34	0
54	MG	1A	3542	1/1	0.97	0.06	34,34,34,34	0
54	MG	1A	3373	1/1	0.97	0.10	24,24,24,24	0
54	MG	2A	3094	1/1	0.97	0.07	35,35,35,35	0
54	MG	1A	3983	1/1	0.97	0.09	35,35,35,35	0
54	MG	1A	3015	1/1	0.97	0.11	37,37,37,37	0
54	MG	1A	3546	1/1	0.97	0.09	48,48,48,48	0
54	MG	1A	3315	1/1	0.97	0.18	35,35,35,35	0
54	MG	1A	3059	1/1	0.97	0.12	44,44,44,44	0
54	MG	1N	204	1/1	0.97	0.08	47,47,47,47	0
54	MG	1A	3847	1/1	0.97	0.04	31,31,31,31	0
54	MG	2A	3102	1/1	0.97	0.08	27,27,27,27	0
54	MG	2A	3103	1/1	0.97	0.07	49,49,49,49	0
54	MG	1A	3021	1/1	0.97	0.21	32,32,32,32	0
54	MG	1P	202	1/1	0.97	0.26	24,24,24,24	0
54	MG	1A	3990	1/1	0.97	0.15	35,35,35,35	0
54	MG	1a	3238	1/1	0.97	0.07	54,54,54,54	0
54	MG	2A	3501	1/1	0.97	0.09	52,52,52,52	0
54	MG	2a	3166	1/1	0.97	0.06	55,55,55,55	0
54	MG	2A	3502	1/1	0.97	0.10	74,74,74,74	0
54	MG	2A	3295	1/1	0.97	0.07	57,57,57,57	0
54	MG	2A	3504	1/1	0.97	0.07	26,26,26,26	0
54	MG	1A	3850	1/1	0.97	0.05	34,34,34,34	0
54	MG	2A	3297	1/1	0.97	0.06	38,38,38,38	0
54	MG	1a	3079	1/1	0.97	0.15	36,36,36,36	0
54	MG	1A	3155	1/1	0.97	0.11	40,40,40,40	0
54	MG	1A	3047	1/1	0.97	0.07	36,36,36,36	0
54	MG	1Q	203	1/1	0.97	0.04	26,26,26,26	0
54	MG	1A	3853	1/1	0.97	0.10	46,46,46,46	0
54	MG	2B	210	1/1	0.97	0.13	56,56,56,56	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	2a	3179	1/1	0.97	0.10	59,59,59,59	0
54	MG	2A	3117	1/1	0.97	0.19	39,39,39,39	0
54	MG	1A	3854	1/1	0.97	0.06	31,31,31,31	0
54	MG	1A	3456	1/1	0.97	0.10	43,43,43,43	0
54	MG	1A	3744	1/1	0.97	0.08	29,29,29,29	0
54	MG	2A	3308	1/1	0.97	0.05	27,27,27,27	0
54	MG	2A	3309	1/1	0.97	0.06	25,25,25,25	0
54	MG	2A	3122	1/1	0.97	0.15	42,42,42,42	0
54	MG	2A	3520	1/1	0.97	0.12	46,46,46,46	0
54	MG	1A	3264	1/1	0.97	0.16	15,15,15,15	0
54	MG	1a	3250	1/1	0.97	0.04	37,37,37,37	0
54	MG	1R	205	1/1	0.97	0.03	20,20,20,20	0
54	MG	1A	4002	1/1	0.97	0.04	40,40,40,40	0
54	MG	2D	306	1/1	0.97	0.06	44,44,44,44	0
54	MG	1A	3188	1/1	0.97	0.15	32,32,32,32	0
54	MG	2D	308	1/1	0.97	0.10	55,55,55,55	0
54	MG	1A	3048	1/1	0.97	0.19	49,49,49,49	0
54	MG	1A	3749	1/1	0.97	0.07	50,50,50,50	0
54	MG	1A	3385	1/1	0.97	0.13	40,40,40,40	0
54	MG	1A	3865	1/1	0.97	0.13	31,31,31,31	0
54	MG	1A	3558	1/1	0.97	0.04	12,12,12,12	0
54	MG	2A	3531	1/1	0.97	0.07	51,51,51,51	0
54	MG	1A	3132	1/1	0.97	0.05	29,29,29,29	0
54	MG	1A	3049	1/1	0.97	0.12	28,28,28,28	0
54	MG	2A	3137	1/1	0.97	0.06	21,21,21,21	0
54	MG	1U	202	1/1	0.97	0.06	32,32,32,32	0
54	MG	1a	3266	1/1	0.97	0.07	69,69,69,69	0
54	MG	1A	3325	1/1	0.97	0.07	47,47,47,47	0
54	MG	2A	3327	1/1	0.97	0.05	40,40,40,40	0
54	MG	1a	3268	1/1	0.97	0.07	76,76,76,76	0
54	MG	1U	204	1/1	0.97	0.48	33,33,33,33	0
56	MPD	18	102	8/8	0.97	0.09	28,33,38,41	0
54	MG	1U	205	1/1	0.97	0.07	24,24,24,24	0
54	MG	1A	3469	1/1	0.97	0.07	37,37,37,37	0
54	MG	1A	4014	1/1	0.97	0.07	41,41,41,41	0
54	MG	1A	3470	1/1	0.97	0.07	49,49,49,49	0
54	MG	1A	3874	1/1	0.97	0.05	34,34,34,34	0
54	MG	2A	3336	1/1	0.97	0.11	26,26,26,26	0
54	MG	1A	3757	1/1	0.97	0.08	24,24,24,24	0
58	ZN	2Y	202	1/1	0.97	0.07	101,101,101,101	0
54	MG	1A	3269	1/1	0.97	0.06	39,39,39,39	0
54	MG	1a	3108	1/1	0.97	0.16	63,63,63,63	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
59	SF4	2d	501	8/8	0.97	0.05	56,69,75,79	0
54	MG	1A	3931	1/1	0.98	0.03	12,12,12,12	0
54	MG	1A	3553	1/1	0.98	0.04	39,39,39,39	0
54	MG	1A	3042	1/1	0.98	0.07	24,24,24,24	0
54	MG	2A	3252	1/1	0.98	0.14	44,44,44,44	0
54	MG	2A	3721	1/1	0.98	0.06	42,42,42,42	0
54	MG	2A	3119	1/1	0.98	0.19	49,49,49,49	0
54	MG	1a	3169	1/1	0.98	0.07	44,44,44,44	0
54	MG	1a	3054	1/1	0.98	0.10	32,32,32,32	0
54	MG	2A	3546	1/1	0.98	0.10	53,53,53,53	0
54	MG	1A	3934	1/1	0.98	0.04	33,33,33,33	0
54	MG	1A	4036	1/1	0.98	0.04	47,47,47,47	0
54	MG	2A	3124	1/1	0.98	0.08	33,33,33,33	0
54	MG	1A	4037	1/1	0.98	0.07	26,26,26,26	0
54	MG	1A	4038	1/1	0.98	0.05	51,51,51,51	0
54	MG	1A	3610	1/1	0.98	0.08	34,34,34,34	0
54	MG	1A	3418	1/1	0.98	0.04	14,14,14,14	0
54	MG	1A	3612	1/1	0.98	0.04	32,32,32,32	0
54	MG	1A	3938	1/1	0.98	0.04	52,52,52,52	0
54	MG	1A	3939	1/1	0.98	0.06	42,42,42,42	0
54	MG	1A	3457	1/1	0.98	0.07	44,44,44,44	0
54	MG	1A	3195	1/1	0.98	0.23	36,36,36,36	0
54	MG	1A	3507	1/1	0.98	0.05	24,24,24,24	0
54	MG	1A	3043	1/1	0.98	0.13	10,10,10,10	0
54	MG	1A	3261	1/1	0.98	0.05	33,33,33,33	0
54	MG	1A	3510	1/1	0.98	0.07	16,16,16,16	0
54	MG	2A	3742	1/1	0.98	0.07	59,59,59,59	0
54	MG	2A	3139	1/1	0.98	0.12	45,45,45,45	0
54	MG	2A	3004	1/1	0.98	0.05	28,28,28,28	0
54	MG	1A	3758	1/1	0.98	0.04	31,31,31,31	0
54	MG	1A	3076	1/1	0.98	0.15	23,23,23,23	0
54	MG	1A	3685	1/1	0.98	0.08	40,40,40,40	0
54	MG	1V	203	1/1	0.98	0.04	43,43,43,43	0
54	MG	1A	3563	1/1	0.98	0.12	25,25,25,25	0
54	MG	2A	3011	1/1	0.98	0.04	25,25,25,25	0
54	MG	2a	3084	1/1	0.98	0.10	50,50,50,50	0
54	MG	1A	4054	1/1	0.98	0.04	34,34,34,34	0
54	MG	1A	3130	1/1	0.98	0.12	28,28,28,28	0
54	MG	1A	3763	1/1	0.98	0.09	30,30,30,30	0
54	MG	1a	3194	1/1	0.98	0.05	56,56,56,56	0
54	MG	1W	204	1/1	0.98	0.05	25,25,25,25	0
54	MG	1A	3513	1/1	0.98	0.10	40,40,40,40	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	2A	3153	1/1	0.98	0.09	42,42,42,42	0
54	MG	1A	3006	1/1	0.98	0.13	20,20,20,20	0
54	MG	1A	3101	1/1	0.98	0.16	30,30,30,30	0
54	MG	1A	3691	1/1	0.98	0.04	53,53,53,53	0
54	MG	1A	3426	1/1	0.98	0.04	35,35,35,35	0
54	MG	1A	3013	1/1	0.98	0.07	21,21,21,21	0
54	MG	2A	3292	1/1	0.98	0.04	25,25,25,25	0
54	MG	1A	3518	1/1	0.98	0.07	45,45,45,45	0
54	MG	1A	3292	1/1	0.98	0.09	14,14,14,14	0
54	MG	1B	211	1/1	0.98	0.05	27,27,27,27	0
54	MG	1A	3696	1/1	0.98	0.05	49,49,49,49	0
54	MG	1I	103	1/1	0.98	0.05	39,39,39,39	0
54	MG	1A	3857	1/1	0.98	0.27	39,39,39,39	0
54	MG	1A	3965	1/1	0.98	0.07	17,17,17,17	0
54	MG	2A	3595	1/1	0.98	0.05	50,50,50,50	0
54	MG	1A	3090	1/1	0.98	0.06	25,25,25,25	0
54	MG	1A	3859	1/1	0.98	0.06	14,14,14,14	0
54	MG	1A	3774	1/1	0.98	0.06	33,33,33,33	0
54	MG	1a	3213	1/1	0.98	0.05	54,54,54,54	0
54	MG	1a	3214	1/1	0.98	0.03	56,56,56,56	0
54	MG	2A	3305	1/1	0.98	0.07	53,53,53,53	0
54	MG	1A	3573	1/1	0.98	0.06	34,34,34,34	0
54	MG	1a	3216	1/1	0.98	0.04	58,58,58,58	0
54	MG	2D	305	1/1	0.98	0.04	32,32,32,32	0
54	MG	1B	219	1/1	0.98	0.04	33,33,33,33	0
54	MG	1A	3070	1/1	0.98	0.14	25,25,25,25	0
54	MG	1A	3474	1/1	0.98	0.04	37,37,37,37	0
54	MG	2A	3609	1/1	0.98	0.07	52,52,52,52	0
54	MG	1A	3702	1/1	0.98	0.07	44,44,44,44	0
54	MG	1A	3703	1/1	0.98	0.04	43,43,43,43	0
54	MG	1A	3295	1/1	0.98	0.07	46,46,46,46	0
54	MG	2A	3457	1/1	0.98	0.04	51,51,51,51	0
54	MG	2E	302	1/1	0.98	0.04	36,36,36,36	0
54	MG	2A	3616	1/1	0.98	0.09	59,59,59,59	0
54	MG	2A	3617	1/1	0.98	0.06	57,57,57,57	0
54	MG	1A	3081	1/1	0.98	0.18	34,34,34,34	0
54	MG	1A	3870	1/1	0.98	0.07	38,38,38,38	0
54	MG	1B	227	1/1	0.98	0.10	65,65,65,65	0
54	MG	1a	3226	1/1	0.98	0.04	55,55,55,55	0
54	MG	1a	3227	1/1	0.98	0.07	43,43,43,43	0
54	MG	1A	3525	1/1	0.98	0.09	51,51,51,51	0
54	MG	1A	3226	1/1	0.98	0.26	28,28,28,28	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	1A	3298	1/1	0.98	0.03	29,29,29,29	0
54	MG	1A	3398	1/1	0.98	0.06	32,32,32,32	0
54	MG	1A	3710	1/1	0.98	0.05	22,22,22,22	0
54	MG	1A	3877	1/1	0.98	0.07	38,38,38,38	0
54	MG	1A	3170	1/1	0.98	0.06	29,29,29,29	0
54	MG	2A	3632	1/1	0.98	0.11	40,40,40,40	0
54	MG	2A	3470	1/1	0.98	0.06	36,36,36,36	0
54	MG	1A	3228	1/1	0.98	0.15	28,28,28,28	0
54	MG	2A	3472	1/1	0.98	0.09	44,44,44,44	0
54	MG	1A	3584	1/1	0.98	0.07	42,42,42,42	0
54	MG	2a	3143	1/1	0.98	0.04	57,57,57,57	0
54	MG	1A	3644	1/1	0.98	0.09	18,18,18,18	0
54	MG	2A	3638	1/1	0.98	0.05	43,43,43,43	0
54	MG	1A	3585	1/1	0.98	0.11	31,31,31,31	0
54	MG	2A	3640	1/1	0.98	0.07	49,49,49,49	0
54	MG	2A	3330	1/1	0.98	0.06	35,35,35,35	0
54	MG	2a	3149	1/1	0.98	0.04	64,64,64,64	0
54	MG	1A	3586	1/1	0.98	0.05	12,12,12,12	0
54	MG	1A	3302	1/1	0.98	0.10	20,20,20,20	0
54	MG	1a	3241	1/1	0.98	0.06	56,56,56,56	0
54	MG	2a	3153	1/1	0.98	0.04	67,67,67,67	0
54	MG	2A	3480	1/1	0.98	0.12	63,63,63,63	0
54	MG	2a	3155	1/1	0.98	0.05	64,64,64,64	0
54	MG	1D	315	1/1	0.98	0.05	44,44,44,44	0
54	MG	2a	3157	1/1	0.98	0.08	41,41,41,41	0
54	MG	1A	3885	1/1	0.98	0.04	30,30,30,30	0
54	MG	2A	3649	1/1	0.98	0.06	47,47,47,47	0
54	MG	1A	3718	1/1	0.98	0.05	41,41,41,41	0
54	MG	1A	3303	1/1	0.98	0.12	26,26,26,26	0
54	MG	2A	3338	1/1	0.98	0.10	24,24,24,24	0
54	MG	1A	3993	1/1	0.98	0.09	18,18,18,18	0
54	MG	2A	3340	1/1	0.98	0.06	27,27,27,27	0
54	MG	1A	3485	1/1	0.98	0.06	38,38,38,38	0
54	MG	1A	3996	1/1	0.98	0.05	44,44,44,44	0
54	MG	2A	3657	1/1	0.98	0.04	65,65,65,65	0
54	MG	1A	3650	1/1	0.98	0.05	27,27,27,27	0
54	MG	1A	3487	1/1	0.98	0.09	28,28,28,28	0
54	MG	1a	3252	1/1	0.98	0.04	56,56,56,56	0
54	MG	1A	3005	1/1	0.98	0.11	19,19,19,19	0
54	MG	1A	3029	1/1	0.98	0.12	38,38,38,38	0
54	MG	1A	3538	1/1	0.98	0.09	24,24,24,24	0
54	MG	1A	3095	1/1	0.98	0.13	16,16,16,16	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	1A	3727	1/1	0.98	0.12	33,33,33,33	0
54	MG	1F	307	1/1	0.98	0.04	25,25,25,25	0
54	MG	1A	3540	1/1	0.98	0.12	16,16,16,16	0
54	MG	2A	3672	1/1	0.98	0.05	35,35,35,35	0
54	MG	1A	3899	1/1	0.98	0.09	59,59,59,59	0
54	MG	1A	3140	1/1	0.98	0.07	25,25,25,25	0
54	MG	1A	3073	1/1	0.98	0.07	28,28,28,28	0
54	MG	1A	3810	1/1	0.98	0.04	56,56,56,56	0
54	MG	1a	3265	1/1	0.98	0.04	45,45,45,45	0
54	MG	2a	3013	1/1	0.98	0.07	50,50,50,50	0
54	MG	1A	4009	1/1	0.98	0.06	14,14,14,14	0
54	MG	1A	3543	1/1	0.98	0.05	20,20,20,20	0
54	MG	1A	3213	1/1	0.98	0.19	32,32,32,32	0
54	MG	2a	3189	1/1	0.98	0.05	64,64,64,64	0
54	MG	1A	3256	1/1	0.98	0.19	19,19,19,19	0
54	MG	2A	3683	1/1	0.98	0.03	58,58,58,58	0
54	MG	1a	3144	1/1	0.98	0.04	52,52,52,52	0
54	MG	1A	3906	1/1	0.98	0.10	26,26,26,26	0
54	MG	2A	3091	1/1	0.98	0.06	31,31,31,31	0
54	MG	1a	3146	1/1	0.98	0.04	31,31,31,31	0
54	MG	1A	3341	1/1	0.98	0.06	37,37,37,37	0
54	MG	2A	3367	1/1	0.98	0.04	28,28,28,28	0
54	MG	2A	3692	1/1	0.98	0.04	70,70,70,70	0
54	MG	1A	3815	1/1	0.98	0.07	26,26,26,26	0
54	MG	2A	3694	1/1	0.98	0.03	29,29,29,29	0
54	MG	1a	3275	1/1	0.98	0.04	44,44,44,44	0
54	MG	1A	3663	1/1	0.98	0.09	29,29,29,29	0
54	MG	1A	3915	1/1	0.98	0.05	39,39,39,39	0
54	MG	1A	3449	1/1	0.98	0.07	46,46,46,46	0
54	MG	1A	3818	1/1	0.98	0.04	29,29,29,29	0
54	MG	1A	3280	1/1	0.98	0.07	15,15,15,15	0
54	MG	1A	3920	1/1	0.98	0.20	19,19,19,19	0
54	MG	1A	3666	1/1	0.98	0.04	34,34,34,34	0
54	MG	1A	3740	1/1	0.98	0.04	61,61,61,61	0
54	MG	1A	3112	1/1	0.98	0.07	41,41,41,41	0
54	MG	1A	4025	1/1	0.98	0.18	30,30,30,30	0
54	MG	2A	3706	1/1	0.98	0.06	36,36,36,36	0
54	MG	1A	3742	1/1	0.98	0.06	39,39,39,39	0
54	MG	1A	3452	1/1	0.98	0.06	42,42,42,42	0
54	MG	1Q	202	1/1	0.98	0.04	29,29,29,29	0
54	MG	1A	3378	1/1	0.98	0.07	13,13,13,13	0
54	MG	2A	3387	1/1	0.98	0.04	54,54,54,54	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	2A	3112	1/1	0.98	0.07	50,50,50,50	0
54	MG	2A	3713	1/1	0.98	0.05	35,35,35,35	0
54	MG	1A	3827	1/1	0.98	0.18	27,27,27,27	0
58	ZN	29	501	1/1	0.98	0.04	64,64,64,64	0
54	MG	1A	3313	1/1	0.98	0.30	28,28,28,28	0
54	MG	1A	3746	1/1	0.98	0.05	32,32,32,32	0
54	MG	2A	3624	1/1	0.99	0.04	32,32,32,32	0
54	MG	1A	3775	1/1	0.99	0.10	23,23,23,23	0
54	MG	1a	3114	1/1	0.99	0.06	28,28,28,28	0
54	MG	1A	3918	1/1	0.99	0.04	37,37,37,37	0
54	MG	1A	3492	1/1	0.99	0.06	32,32,32,32	0
54	MG	1A	3876	1/1	0.99	0.04	38,38,38,38	0
54	MG	1A	3372	1/1	0.99	0.03	13,13,13,13	0
54	MG	1A	3386	1/1	0.99	0.10	30,30,30,30	0
54	MG	1A	3401	1/1	0.99	0.06	25,25,25,25	0
54	MG	1A	3924	1/1	0.99	0.03	47,47,47,47	0
54	MG	1F	310	1/1	0.99	0.06	45,45,45,45	0
54	MG	1A	3299	1/1	0.99	0.06	28,28,28,28	0
54	MG	1A	3350	1/1	0.99	0.05	19,19,19,19	0
54	MG	1W	202	1/1	0.99	0.13	36,36,36,36	0
54	MG	1A	3160	1/1	0.99	0.12	28,28,28,28	0
54	MG	1A	3282	1/1	0.99	0.09	18,18,18,18	0
54	MG	2A	3109	1/1	0.99	0.07	23,23,23,23	0
54	MG	2A	3495	1/1	0.99	0.05	39,39,39,39	0
54	MG	2A	3110	1/1	0.99	0.04	50,50,50,50	0
54	MG	1A	3848	1/1	0.99	0.05	33,33,33,33	0
54	MG	1A	3670	1/1	0.99	0.12	40,40,40,40	0
54	MG	1A	3671	1/1	0.99	0.13	47,47,47,47	0
54	MG	2A	3568	1/1	0.99	0.05	52,52,52,52	0
54	MG	1A	3210	1/1	0.99	0.11	29,29,29,29	0
54	MG	2A	3648	1/1	0.99	0.03	35,35,35,35	0
54	MG	1A	3819	1/1	0.99	0.14	31,31,31,31	0
54	MG	1A	3700	1/1	0.99	0.08	46,46,46,46	0
54	MG	1A	3080	1/1	0.99	0.12	29,29,29,29	0
54	MG	1A	3891	1/1	0.99	0.07	25,25,25,25	0
54	MG	2A	3371	1/1	0.99	0.03	25,25,25,25	0
54	MG	2A	3506	1/1	0.99	0.04	38,38,38,38	0
54	MG	1A	3379	1/1	0.99	0.07	33,33,33,33	0
54	MG	1A	3893	1/1	0.99	0.04	24,24,24,24	0
54	MG	1A	3731	1/1	0.99	0.04	23,23,23,23	0
54	MG	2A	3375	1/1	0.99	0.04	40,40,40,40	0
54	MG	2A	3659	1/1	0.99	0.05	51,51,51,51	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	2A	3660	1/1	0.99	0.07	24,24,24,24	0
54	MG	2A	3661	1/1	0.99	0.03	28,28,28,28	0
54	MG	1a	3251	1/1	0.99	0.04	39,39,39,39	0
54	MG	2a	3175	1/1	0.99	0.04	68,68,68,68	0
54	MG	1A	3028	1/1	0.99	0.23	20,20,20,20	0
54	MG	1A	3460	1/1	0.99	0.02	15,15,15,15	0
54	MG	2A	3583	1/1	0.99	0.07	26,26,26,26	0
54	MG	1a	3254	1/1	0.99	0.07	49,49,49,49	0
54	MG	1A	3528	1/1	0.99	0.05	17,17,17,17	0
54	MG	2A	3586	1/1	0.99	0.04	41,41,41,41	0
54	MG	1A	3943	1/1	0.99	0.04	41,41,41,41	0
54	MG	2A	3670	1/1	0.99	0.07	57,57,57,57	0
54	MG	1A	3461	1/1	0.99	0.04	32,32,32,32	0
54	MG	2A	3383	1/1	0.99	0.04	38,38,38,38	0
54	MG	2A	3673	1/1	0.99	0.03	38,38,38,38	0
54	MG	2A	3129	1/1	0.99	0.16	31,31,31,31	0
54	MG	1A	3483	1/1	0.99	0.04	35,35,35,35	0
54	MG	2A	3008	1/1	0.99	0.05	35,35,35,35	0
54	MG	1A	3862	1/1	0.99	0.05	36,36,36,36	0
54	MG	1A	3107	1/1	0.99	0.03	26,26,26,26	0
54	MG	1A	3994	1/1	0.99	0.04	15,15,15,15	0
54	MG	1A	3411	1/1	0.99	0.10	15,15,15,15	0
54	MG	1Q	205	1/1	0.99	0.04	27,27,27,27	0
54	MG	2A	3599	1/1	0.99	0.04	45,45,45,45	0
54	MG	1A	3486	1/1	0.99	0.04	20,20,20,20	0
54	MG	2A	3684	1/1	0.99	0.04	42,42,42,42	0
54	MG	1A	3800	1/1	0.99	0.06	25,25,25,25	0
54	MG	1D	311	1/1	0.99	0.16	18,18,18,18	0
54	MG	1A	3951	1/1	0.99	0.04	48,48,48,48	0
54	MG	2A	3604	1/1	0.99	0.04	30,30,30,30	0
54	MG	2A	3689	1/1	0.99	0.03	45,45,45,45	0
54	MG	1A	3428	1/1	0.99	0.03	22,22,22,22	0
54	MG	2B	219	1/1	0.99	0.03	58,58,58,58	0
54	MG	1a	3211	1/1	0.99	0.03	63,63,63,63	0
54	MG	1A	3103	1/1	0.99	0.09	20,20,20,20	0
54	MG	1A	3869	1/1	0.99	0.07	53,53,53,53	0
54	MG	1A	3017	1/1	0.99	0.24	17,17,17,17	0
54	MG	2A	3610	1/1	0.99	0.03	42,42,42,42	0
54	MG	1A	3956	1/1	0.99	0.04	50,50,50,50	0
54	MG	1a	3050	1/1	0.99	0.09	43,43,43,43	0
54	MG	1A	3909	1/1	0.99	0.02	15,15,15,15	0
54	MG	1A	3468	1/1	0.99	0.05	14,14,14,14	0

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

5.5 Other polymers [i](#)

There are no such residues in this entry.