



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 30, 2026 – 09:32 PM UTC

PDB ID : 8FC5 / pdb_00008fc5
Title : Crystal structure of the A2058-N6-dimethylated *Thermus thermophilus* 70S ribosome in complex with protein Y, hygromycin A, and azithromycin at 2.65Å resolution
Authors : Chen, C.-W.; Syroegin, E.A.; Svetlov, M.S.; Polikanov, Y.S.
Deposited on : 2022-12-01
Resolution : 2.65 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	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

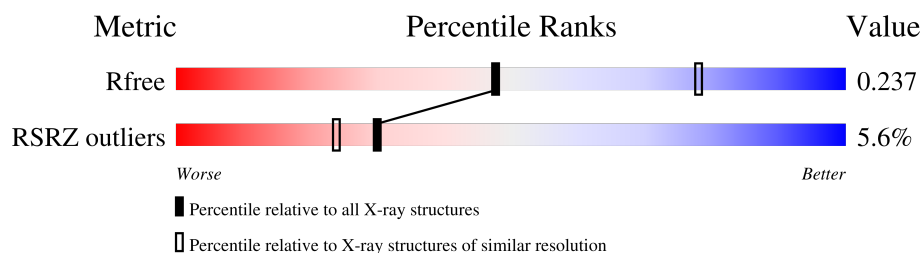
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.65 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1110 (2.66-2.66)
RSRZ outliers	180081	1110 (2.66-2.66)

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	1A	3601	-	-	-	X
54	MG	2A	3090	-	-	-	X
54	MG	2A	3206	-	-	-	X
54	MG	2a	3085	-	-	-	X

2 Entry composition

There are 61 unique types of molecules in this entry. The entry contains 296864 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
			61871	27542	11574	19884	2871			
1	2A	2867	Total	C	N	O	P	0	0	0
			61759	27492	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	1031	Total	Mg	0	0
			1031	1031		
54	1B	29	Total	Mg	0	0
			29	29		
54	1D	18	Total	Mg	0	0
			18	18		
54	1E	10	Total	Mg	0	0
			10	10		
54	1F	18	Total	Mg	0	0
			18	18		
54	1G	4	Total	Mg	0	0
			4	4		
54	1H	2	Total	Mg	0	0
			2	2		
54	1N	4	Total	Mg	0	0
			4	4		
54	1O	1	Total	Mg	0	0
			1	1		
54	1P	7	Total	Mg	0	0
			7	7		
54	1Q	5	Total	Mg	0	0
			5	5		
54	1R	5	Total	Mg	0	0
			5	5		
54	1S	1	Total	Mg	0	0
			1	1		
54	1T	6	Total	Mg	0	0
			6	6		
54	1U	7	Total	Mg	0	0
			7	7		
54	1V	4	Total	Mg	0	0
			4	4		
54	1W	4	Total	Mg	0	0
			4	4		
54	1X	1	Total	Mg	0	0
			1	1		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
54	1Y	1	Total 1	Mg 1	0	0
54	1Z	1	Total 1	Mg 1	0	0
54	10	6	Total 6	Mg 6	0	0
54	11	5	Total 5	Mg 5	0	0
54	13	3	Total 3	Mg 3	0	0
54	15	8	Total 8	Mg 8	0	0
54	17	7	Total 7	Mg 7	0	0
54	18	2	Total 2	Mg 2	0	0
54	19	3	Total 3	Mg 3	0	0
54	1a	281	Total 281	Mg 281	0	0
54	1b	1	Total 1	Mg 1	0	0
54	1d	2	Total 2	Mg 2	0	0
54	1e	3	Total 3	Mg 3	0	0
54	1f	2	Total 2	Mg 2	0	0
54	1g	3	Total 3	Mg 3	0	0
54	1h	2	Total 2	Mg 2	0	0
54	1i	1	Total 1	Mg 1	0	0
54	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
54	1o	1	Total 1	Mg 1	0	0

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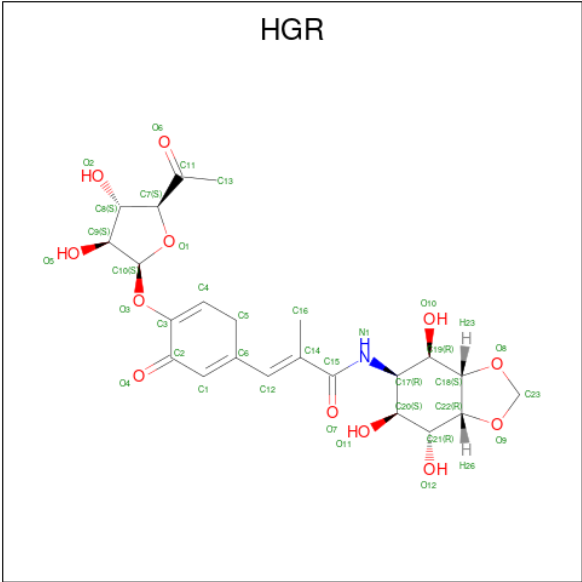
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
54	1t	1	Total 1	Mg 1	0	0
54	1u	1	Total 1	Mg 1	0	0
54	1y	3	Total 3	Mg 3	0	0
54	2A	711	Total 711	Mg 711	0	0
54	2B	18	Total 18	Mg 18	0	0
54	2D	9	Total 9	Mg 9	0	0
54	2E	5	Total 5	Mg 5	0	0
54	2F	4	Total 4	Mg 4	0	0
54	2G	2	Total 2	Mg 2	0	0
54	2I	1	Total 1	Mg 1	0	0
54	2N	1	Total 1	Mg 1	0	0
54	2O	2	Total 2	Mg 2	0	0
54	2P	1	Total 1	Mg 1	0	0
54	2Q	3	Total 3	Mg 3	0	0
54	2R	1	Total 1	Mg 1	0	0
54	2T	3	Total 3	Mg 3	0	0
54	2V	3	Total 3	Mg 3	0	0
54	2W	3	Total 3	Mg 3	0	0
54	2X	1	Total 1	Mg 1	0	0
54	2Y	1	Total 1	Mg 1	0	0
54	20	1	Total 1	Mg 1	0	0

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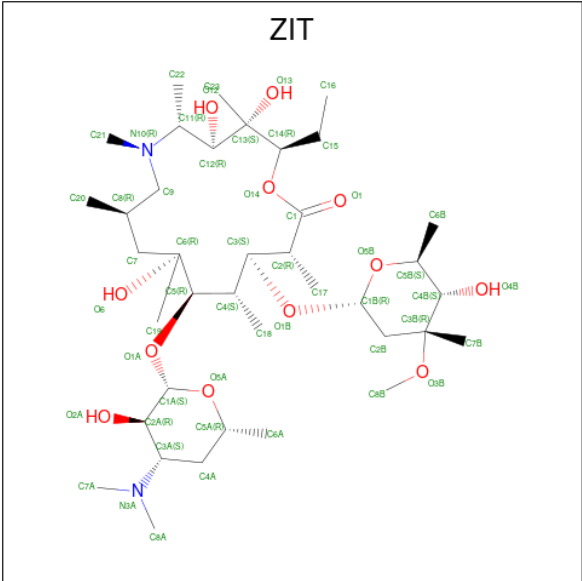
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
54	21	1	Total 1	Mg 1	0	0
54	23	1	Total 1	Mg 1	0	0
54	25	1	Total 1	Mg 1	0	0
54	27	1	Total 1	Mg 1	0	0
54	28	2	Total 2	Mg 2	0	0
54	2a	182	Total 182	Mg 182	0	0
54	2e	2	Total 2	Mg 2	0	0
54	2f	1	Total 1	Mg 1	0	0
54	2j	1	Total 1	Mg 1	0	0
54	2k	1	Total 1	Mg 1	0	0
54	2l	1	Total 1	Mg 1	0	0
54	2n	1	Total 1	Mg 1	0	0
54	2t	1	Total 1	Mg 1	0	0

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



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

- Molecule 56 is AZITHROMYCIN (CCD ID: ZIT) (formula: $C_{38}H_{72}N_2O_{12}$) (labeled as "Ligand of Interest" by depositor).



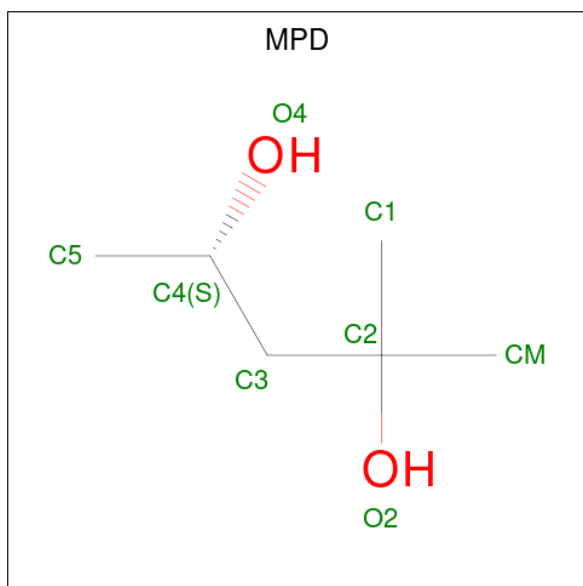
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
56	1A	1	Total	C	N	O	0	0
			52	38	2	12		

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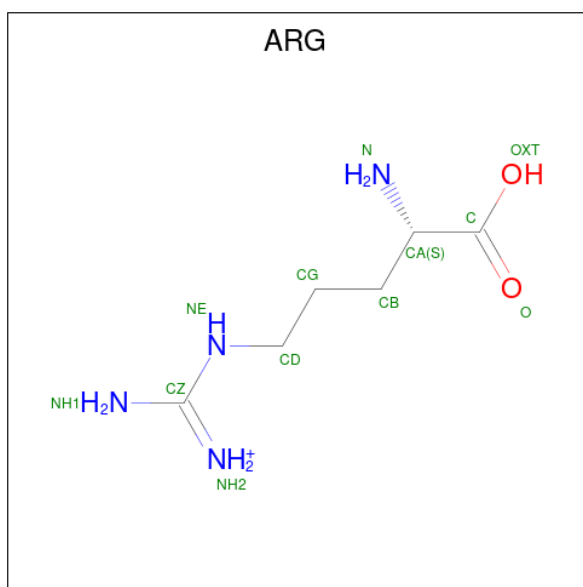
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
56	2A	1	Total	C	N	O	0	0
			52	38	2	12		

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



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

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



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

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

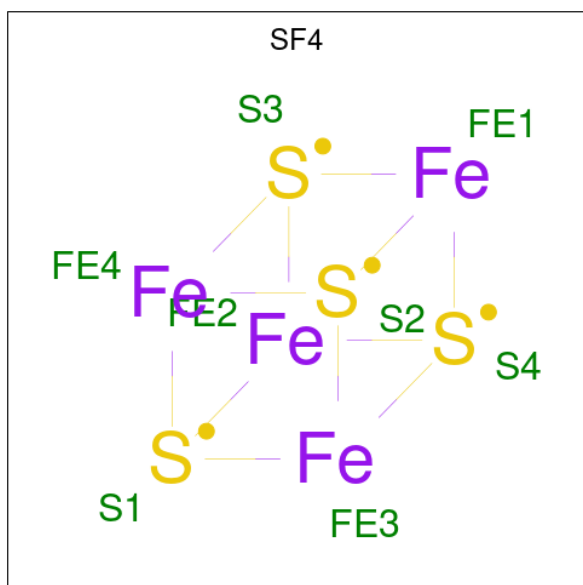
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
59	1Y	1	Total	Zn	0	0
			1	1		
59	14	1	Total	Zn	0	0
			1	1		
59	15	1	Total	Zn	0	0
			1	1		
59	16	1	Total	Zn	0	0
			1	1		
59	19	1	Total	Zn	0	0
			1	1		
59	1n	1	Total	Zn	0	0
			1	1		
59	2Y	1	Total	Zn	0	0
			1	1		
59	24	1	Total	Zn	0	0
			1	1		
59	25	1	Total	Zn	0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

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

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



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

- Molecule 61 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
61	1A	3571	Total	O	0	0
			3571	3571		
61	1B	89	Total	O	0	0
			89	89		
61	1D	109	Total	O	0	0
			109	109		
61	1E	68	Total	O	0	0
			68	68		
61	1F	61	Total	O	0	0
			61	61		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
61	1G	10	Total	O	0	0
			10	10		
61	1H	15	Total	O	0	0
			15	15		
61	1I	4	Total	O	0	0
			4	4		
61	1N	46	Total	O	0	0
			46	46		
61	1O	17	Total	O	0	0
			17	17		
61	1P	53	Total	O	0	0
			53	53		
61	1Q	30	Total	O	0	0
			30	30		
61	1R	29	Total	O	0	0
			29	29		
61	1S	7	Total	O	0	0
			7	7		
61	1T	32	Total	O	0	0
			32	32		
61	1U	38	Total	O	0	0
			38	38		
61	1V	26	Total	O	0	0
			26	26		
61	1W	28	Total	O	0	0
			28	28		
61	1X	23	Total	O	0	0
			23	23		
61	1Y	13	Total	O	0	0
			13	13		
61	1Z	9	Total	O	0	0
			9	9		
61	10	19	Total	O	0	0
			19	19		
61	11	17	Total	O	0	0
			17	17		
61	12	11	Total	O	0	0
			11	11		
61	13	20	Total	O	0	0
			20	20		
61	15	28	Total	O	0	0
			28	28		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
61	16	12	Total 12	O 12	0	0
61	17	12	Total 12	O 12	0	0
61	18	24	Total 24	O 24	0	0
61	19	3	Total 3	O 3	0	0
61	1a	388	Total 388	O 388	0	0
61	1d	9	Total 9	O 9	0	0
61	1f	1	Total 1	O 1	0	0
61	1h	2	Total 2	O 2	0	0
61	1j	1	Total 1	O 1	0	0
61	1l	2	Total 2	O 2	0	0
61	1m	1	Total 1	O 1	0	0
61	1n	2	Total 2	O 2	0	0
61	1o	1	Total 1	O 1	0	0
61	1p	3	Total 3	O 3	0	0
61	1u	1	Total 1	O 1	0	0
61	1y	3	Total 3	O 3	0	0
61	2A	2161	Total 2161	O 2161	0	0
61	2B	48	Total 48	O 48	0	0
61	2D	43	Total 43	O 43	0	0
61	2E	22	Total 22	O 22	0	0
61	2F	25	Total 25	O 25	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
61	2G	1	Total 1	O 1	0	0
61	2H	1	Total 1	O 1	0	0
61	2I	1	Total 1	O 1	0	0
61	2N	5	Total 5	O 5	0	0
61	2O	17	Total 17	O 17	0	0
61	2P	20	Total 20	O 20	0	0
61	2Q	19	Total 19	O 19	0	0
61	2R	15	Total 15	O 15	0	0
61	2S	4	Total 4	O 4	0	0
61	2T	11	Total 11	O 11	0	0
61	2U	15	Total 15	O 15	0	0
61	2V	3	Total 3	O 3	0	0
61	2W	16	Total 16	O 16	0	0
61	2X	6	Total 6	O 6	0	0
61	2Y	2	Total 2	O 2	0	0
61	2Z	6	Total 6	O 6	0	0
61	20	5	Total 5	O 5	0	0
61	21	14	Total 14	O 14	0	0
61	23	3	Total 3	O 3	0	0
61	25	8	Total 8	O 8	0	0
61	26	3	Total 3	O 3	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
61	27	5	Total 5	O 5	0	0
61	28	8	Total 8	O 8	0	0
61	29	1	Total 1	O 1	0	0
61	2a	394	Total 394	O 394	0	0
61	2d	4	Total 4	O 4	0	0
61	2e	2	Total 2	O 2	0	0
61	2f	1	Total 1	O 1	0	0
61	2j	2	Total 2	O 2	0	0
61	2l	4	Total 4	O 4	0	0
61	2n	1	Total 1	O 1	0	0
61	2o	3	Total 3	O 3	0	0
61	2p	3	Total 3	O 3	0	0
61	2q	1	Total 1	O 1	0	0
61	2r	5	Total 5	O 5	0	0
61	2t	2	Total 2	O 2	0	0
61	2y	2	Total 2	O 2	0	0

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	209.55Å 449.77Å 619.46Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	153.31 – 2.65 153.31 – 2.65	Depositor EDS
% Data completeness (in resolution range)	99.8 (153.31-2.65) 99.8 (153.31-2.65)	Depositor EDS
R_{merge}	0.20	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.26 (at 2.65Å)	Xtriage
Refinement program	PHENIX 1.8.2	Depositor
R, R_{free}	0.194 , 0.236 0.197 , 0.237	Depositor DCC
R_{free} test set	83721 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å ²)	59.1	Xtriage
Anisotropy	0.194	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 51.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	296864	wwPDB-VP
Average B, all atoms (Å ²)	62.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.63% 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](#)

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
32	PSU	1a	516	32,54	18,21,22	1.36	2 (11%)	21,30,33	1.98	4 (19%)
1	5MC	1A	1962	1	19,22,23	1.51	3 (15%)	26,32,35	1.06	2 (7%)
1	5MU	1A	1939	1	19,22,23	1.41	5 (26%)	27,32,35	2.19	6 (22%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
32	5MC	2a	967	32	19,22,23	2.01	3 (15%)	26,32,35	1.15	3 (11%)
1	OMU	1A	2552	1,54	19,22,23	1.33	4 (21%)	25,31,34	1.81	6 (24%)
32	5MC	1a	1400	32	19,22,23	1.71	3 (15%)	26,32,35	1.16	2 (7%)
1	OMU	2A	2552	1,54	19,22,23	1.30	2 (10%)	25,31,34	1.89	6 (24%)
32	5MC	2a	1404	32	19,22,23	1.73	3 (15%)	26,32,35	1.24	4 (15%)
1	PSU	1A	2605	1	18,21,22	1.35	3 (16%)	21,30,33	2.08	4 (19%)
32	2MG	2a	1207	32	23,26,27	1.25	4 (17%)	33,38,41	2.15	9 (27%)
32	MA6	1a	1518	32	23,26,27	0.40	0	33,38,41	1.93	8 (24%)
43	0TD	2l	92	43	8,9,10	4.42	1 (12%)	6,11,13	2.32	3 (50%)
1	OMG	2A	2251	1,54	23,26,27	1.22	3 (13%)	32,38,41	1.95	5 (15%)
1	PSU	2A	2605	1	18,21,22	1.36	3 (16%)	21,30,33	2.17	4 (19%)
1	MA6	1A	2058	1,54	23,26,27	0.40	0	33,38,41	2.04	9 (27%)
1	PSU	2A	1917	1	18,21,22	1.35	2 (11%)	21,30,33	2.02	3 (14%)
32	M2G	2a	966	32,54	24,27,28	1.27	3 (12%)	33,40,43	1.82	5 (15%)
32	MA6	1a	1519	32	23,26,27	0.44	0	33,38,41	2.11	9 (27%)
32	5MC	1a	967	32	19,22,23	1.66	3 (15%)	26,32,35	1.07	2 (7%)
1	5MC	2A	1942	1	19,22,23	1.62	3 (15%)	26,32,35	1.28	3 (11%)
32	UR3	1a	1498	32	19,22,23	0.94	1 (5%)	26,32,35	1.83	3 (11%)
32	2MG	1a	1207	32	23,26,27	1.26	2 (8%)	33,38,41	2.44	9 (27%)
1	PSU	1A	1917	1	18,21,22	1.37	2 (11%)	21,30,33	1.86	4 (19%)
32	M2G	1a	966	32	24,27,28	1.31	4 (16%)	33,40,43	1.85	6 (18%)
32	MA6	2a	1518	32	23,26,27	0.41	0	33,38,41	2.02	9 (27%)
1	5MU	2A	1915	1	19,22,23	1.49	4 (21%)	27,32,35	2.27	9 (33%)
1	5MU	2A	1939	1,54	19,22,23	1.47	6 (31%)	27,32,35	2.28	6 (22%)
32	5MC	2a	1407	32	19,22,23	1.53	2 (10%)	26,32,35	1.09	3 (11%)
43	0TD	1l	92	43	8,9,10	4.50	1 (12%)	6,11,13	5.92	3 (50%)
1	OMG	1A	2251	1,54	23,26,27	1.26	3 (13%)	32,38,41	1.99	6 (18%)
1	2MA	1A	2503	1,54	22,25,26	1.50	5 (22%)	32,37,40	2.38	10 (31%)
32	5MC	1a	1404	32	19,22,23	1.60	3 (15%)	26,32,35	1.14	2 (7%)
1	5MC	2A	1962	1,54	19,22,23	1.57	3 (15%)	26,32,35	1.09	2 (7%)
32	MA6	2a	1519	32	23,26,27	0.42	0	33,38,41	2.17	9 (27%)
32	5MC	2a	1400	32	19,22,23	1.60	3 (15%)	26,32,35	1.21	3 (11%)
1	2MA	2A	2503	1,54	22,25,26	1.44	4 (18%)	32,37,40	2.41	9 (28%)
32	4OC	1a	1402	32	20,23,24	0.75	1 (5%)	25,32,35	1.03	1 (4%)
1	OMC	2A	1920	1	19,22,23	0.79	0	25,31,34	0.98	1 (4%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	5MC	1A	1942	1,54	19,22,23	1.54	3 (15%)	26,32,35	1.12	3 (11%)
32	G7M	2a	527	32	23,26,27	2.39	5 (21%)	34,39,42	3.05	10 (29%)
32	UR3	2a	1498	32	19,22,23	0.99	1 (5%)	26,32,35	1.76	3 (11%)
32	PSU	2a	516	32,54	18,21,22	1.34	2 (11%)	21,30,33	2.08	5 (23%)
1	5MU	1A	1915	1,54	19,22,23	1.46	5 (26%)	27,32,35	2.29	8 (29%)
32	G7M	1a	527	32,54	23,26,27	2.33	5 (21%)	34,39,42	3.02	10 (29%)
32	4OC	2a	1402	32	20,23,24	0.76	1 (5%)	25,32,35	0.95	1 (4%)
1	PSU	1A	1911	1	18,21,22	1.36	2 (11%)	21,30,33	2.13	5 (23%)
1	OMC	1A	1920	1,54	19,22,23	0.79	0	25,31,34	0.94	1 (4%)
1	MA6	2A	2058	1	23,26,27	0.38	0	33,38,41	1.95	9 (27%)
32	5MC	1a	1407	32	19,22,23	1.71	3 (15%)	26,32,35	1.19	4 (15%)
1	PSU	2A	1911	1	18,21,22	1.41	3 (16%)	21,30,33	2.06	5 (23%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
32	PSU	1a	516	32,54	-	0/7/25/26	0/2/2/2
1	5MC	1A	1962	1	-	0/7/25/26	0/2/2/2
1	5MU	1A	1939	1	-	0/7/25/26	0/2/2/2
32	5MC	2a	967	32	-	0/7/25/26	0/2/2/2
1	OMU	1A	2552	1,54	-	0/9/27/28	0/2/2/2
32	5MC	1a	1400	32	-	0/7/25/26	0/2/2/2
1	OMU	2A	2552	1,54	-	0/9/27/28	0/2/2/2
32	5MC	2a	1404	32	-	0/7/25/26	0/2/2/2
1	PSU	1A	2605	1	-	0/7/25/26	0/2/2/2
32	2MG	2a	1207	32	-	0/9/27/28	0/3/3/3
32	MA6	1a	1518	32	-	0/11/29/30	0/3/3/3
43	0TD	2l	92	43	-	2/7/12/14	-
1	OMG	2A	2251	1,54	-	0/9/27/28	0/3/3/3
1	PSU	2A	2605	1	-	0/7/25/26	0/2/2/2
1	MA6	1A	2058	1,54	-	0/11/29/30	0/3/3/3
1	PSU	2A	1917	1	-	0/7/25/26	0/2/2/2
32	M2G	2a	966	32,54	-	0/11/29/30	0/3/3/3
32	MA6	1a	1519	32	-	1/11/29/30	0/3/3/3
32	5MC	1a	967	32	-	0/7/25/26	0/2/2/2
1	5MC	2A	1942	1	-	0/7/25/26	0/2/2/2
32	UR3	1a	1498	32	-	0/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
32	2MG	1a	1207	32	-	0/9/27/28	0/3/3/3
1	PSU	1A	1917	1	-	0/7/25/26	0/2/2/2
32	M2G	1a	966	32	-	0/11/29/30	0/3/3/3
32	MA6	2a	1518	32	-	0/11/29/30	0/3/3/3
1	5MU	2A	1915	1	-	2/7/25/26	0/2/2/2
1	5MU	2A	1939	1,54	-	0/7/25/26	0/2/2/2
32	5MC	2a	1407	32	-	0/7/25/26	0/2/2/2
43	0TD	1l	92	43	-	2/7/12/14	-
1	OMG	1A	2251	1,54	-	0/9/27/28	0/3/3/3
1	2MA	1A	2503	1,54	-	1/7/25/26	0/3/3/3
32	5MC	1a	1404	32	-	0/7/25/26	0/2/2/2
1	5MC	2A	1962	1,54	-	0/7/25/26	0/2/2/2
32	MA6	2a	1519	32	-	1/11/29/30	0/3/3/3
32	5MC	2a	1400	32	-	0/7/25/26	0/2/2/2
1	2MA	2A	2503	1,54	-	1/7/25/26	0/3/3/3
32	4OC	1a	1402	32	-	1/9/29/30	0/2/2/2
1	OMC	2A	1920	1	-	2/9/27/28	0/2/2/2
1	5MC	1A	1942	1,54	-	0/7/25/26	0/2/2/2
32	G7M	2a	527	32	-	0/7/25/26	0/3/3/3
32	UR3	2a	1498	32	-	0/7/25/26	0/2/2/2
32	PSU	2a	516	32,54	-	0/7/25/26	0/2/2/2
1	5MU	1A	1915	1,54	-	2/7/25/26	0/2/2/2
32	G7M	1a	527	32,54	-	1/7/25/26	0/3/3/3
32	4OC	2a	1402	32	-	2/9/29/30	0/2/2/2
1	PSU	1A	1911	1	-	0/7/25/26	0/2/2/2
1	OMC	1A	1920	1,54	-	1/9/27/28	0/2/2/2
1	MA6	2A	2058	1	-	0/11/29/30	0/3/3/3
32	5MC	1a	1407	32	-	0/7/25/26	0/2/2/2
1	PSU	2A	1911	1	-	0/7/25/26	0/2/2/2

All (124) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
43	1l	92	0TD	CB-SB	-12.18	1.70	1.82
43	2l	92	0TD	CB-SB	-12.14	1.70	1.82
32	2a	527	G7M	C8-N7	7.77	1.46	1.33
32	2a	967	5MC	C5-C4	7.62	1.49	1.44
32	1a	527	G7M	C8-N7	7.31	1.45	1.33
32	2a	1404	5MC	C5-C4	6.40	1.49	1.44
32	1a	1407	5MC	C5-C4	6.32	1.48	1.44
32	1a	1400	5MC	C5-C4	6.21	1.48	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	1a	967	5MC	C5-C4	6.15	1.48	1.44
1	2A	1942	5MC	C5-C4	5.81	1.48	1.44
32	1a	1404	5MC	C5-C4	5.77	1.48	1.44
32	2a	1400	5MC	C5-C4	5.75	1.48	1.44
1	2A	1962	5MC	C5-C4	5.67	1.48	1.44
32	2a	1407	5MC	C5-C4	5.36	1.48	1.44
1	1A	1942	5MC	C5-C4	5.32	1.48	1.44
1	1A	1962	5MC	C5-C4	4.99	1.47	1.44
32	1a	527	G7M	C5-N7	-4.86	1.33	1.39
32	2a	527	G7M	C5-N7	-4.60	1.33	1.39
1	1A	2503	2MA	C5-C4	4.42	1.47	1.39
32	2a	527	G7M	C8-N9	4.36	1.47	1.35
1	2A	2503	2MA	C5-C4	4.25	1.46	1.39
32	1a	527	G7M	C8-N9	4.09	1.46	1.35
32	1a	527	G7M	C5-C4	3.76	1.47	1.38
32	2a	527	G7M	C5-C4	3.75	1.47	1.38
1	1A	1917	PSU	C6-C5	3.49	1.39	1.35
32	2a	516	PSU	C6-C5	3.48	1.39	1.35
1	1A	1911	PSU	C6-C5	3.46	1.39	1.35
1	2A	1911	PSU	C6-C5	3.42	1.39	1.35
32	1a	516	PSU	C6-C5	3.31	1.39	1.35
32	2a	1207	2MG	C5-C4	3.30	1.47	1.38
1	2A	1915	5MU	C2-N1	3.30	1.43	1.38
1	2A	1917	PSU	C6-C5	3.28	1.38	1.35
32	2a	966	M2G	C5-C4	3.27	1.47	1.38
32	1a	966	M2G	C5-C4	3.19	1.47	1.38
32	2a	967	5MC	C6-C5	3.14	1.39	1.34
1	1A	1915	5MU	C2-N1	3.13	1.43	1.38
1	1A	2251	OMG	C5-C4	3.11	1.47	1.38
1	2A	2251	OMG	C5-C4	3.07	1.47	1.38
1	2A	2605	PSU	C6-C5	3.01	1.38	1.35
32	1a	1207	2MG	C5-C4	3.01	1.47	1.38
1	2A	2552	OMU	C4-N3	-2.97	1.33	1.38
1	1A	1939	5MU	C6-C5	2.94	1.39	1.34
1	1A	1939	5MU	C4-N3	-2.94	1.33	1.38
1	2A	1939	5MU	C4-N3	-2.90	1.33	1.38
32	1a	1400	5MC	C6-C5	2.88	1.39	1.34
1	2A	1915	5MU	C6-C5	2.87	1.39	1.34
1	1A	2552	OMU	C4-N3	-2.85	1.33	1.38
32	1a	966	M2G	C6-N1	-2.84	1.33	1.38
32	1a	1404	5MC	C6-C5	2.82	1.39	1.34
32	2a	1400	5MC	C6-C5	2.81	1.39	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	2a	1407	5MC	C6-C5	2.80	1.39	1.34
1	2A	2251	OMG	C6-N1	-2.79	1.33	1.38
1	2A	1939	5MU	C6-C5	2.77	1.39	1.34
1	2A	2503	2MA	C5-C6	2.76	1.48	1.41
1	1A	1962	5MC	C6-N1	-2.73	1.33	1.38
1	1A	1915	5MU	C4-N3	-2.73	1.33	1.38
1	2A	1942	5MC	C6-C5	2.72	1.39	1.34
1	1A	2605	PSU	C4-N3	-2.71	1.33	1.38
1	1A	1962	5MC	C6-C5	2.69	1.39	1.34
1	1A	2251	OMG	C6-N1	-2.69	1.33	1.38
32	2a	1404	5MC	C6-C5	2.67	1.39	1.34
1	2A	1911	PSU	C4-N3	-2.67	1.33	1.38
32	1a	966	M2G	C2-N2	2.66	1.40	1.35
1	1A	2503	2MA	C5-C6	2.65	1.48	1.41
32	2a	966	M2G	C2-N2	2.65	1.40	1.35
1	2A	1962	5MC	C6-C5	2.64	1.38	1.34
1	1A	1942	5MC	C6-N1	-2.64	1.33	1.38
1	1A	1917	PSU	C4-N3	-2.63	1.33	1.38
1	2A	2605	PSU	C4-N3	-2.58	1.34	1.38
1	1A	1915	5MU	C6-C5	2.58	1.38	1.34
1	2A	1917	PSU	C4-N3	-2.57	1.34	1.38
1	2A	1915	5MU	C4-N3	-2.57	1.34	1.38
32	1a	1407	5MC	C6-C5	2.57	1.38	1.34
1	1A	2251	OMG	C5-N7	-2.55	1.34	1.39
32	1a	967	5MC	C6-C5	2.54	1.38	1.34
1	1A	2503	2MA	C8-N7	2.53	1.36	1.31
1	2A	1939	5MU	C2-N3	-2.53	1.33	1.38
1	2A	1939	5MU	C4-C5	2.52	1.48	1.44
1	1A	2503	2MA	C5-N7	-2.52	1.34	1.39
32	1a	1207	2MG	C6-N1	-2.51	1.34	1.38
1	1A	1911	PSU	C4-N3	-2.51	1.34	1.38
32	2a	516	PSU	C4-N3	-2.48	1.34	1.38
32	1a	516	PSU	C4-N3	-2.47	1.34	1.38
1	1A	1942	5MC	C6-C5	2.46	1.38	1.34
1	1A	2552	OMU	C2-N3	-2.44	1.33	1.38
1	2A	2552	OMU	C2-N3	-2.43	1.33	1.38
1	1A	1939	5MU	C6-N1	-2.42	1.33	1.38
1	2A	1915	5MU	C4-C5	2.41	1.48	1.44
1	1A	2605	PSU	C6-C5	2.39	1.37	1.35
32	2a	527	G7M	C6-N1	-2.36	1.34	1.38
1	2A	1939	5MU	C6-N1	-2.33	1.34	1.38
32	1a	1400	5MC	C6-N1	-2.30	1.34	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	2a	1207	2MG	C6-N1	-2.29	1.34	1.38
1	1A	1939	5MU	C2-N3	-2.29	1.34	1.38
1	1A	2552	OMU	C5-C4	2.28	1.48	1.43
1	1A	1915	5MU	C4-C5	2.28	1.48	1.44
32	2a	966	M2G	C6-N1	-2.27	1.34	1.38
1	2A	2251	OMG	C5-N7	-2.26	1.34	1.39
1	2A	2503	2MA	C8-N7	2.26	1.36	1.31
32	2a	1404	5MC	C6-N1	-2.22	1.34	1.38
32	1a	527	G7M	C6-N1	-2.20	1.34	1.38
32	1a	966	M2G	C5-N7	-2.18	1.34	1.39
32	2a	1207	2MG	C2-N3	2.16	1.36	1.32
1	2A	2605	PSU	C2-N3	-2.16	1.33	1.37
32	1a	1407	5MC	C6-N1	-2.16	1.34	1.38
32	1a	1404	5MC	C6-N1	-2.15	1.34	1.38
1	2A	1942	5MC	C6-N1	-2.15	1.34	1.38
32	2a	1400	5MC	C6-N1	-2.14	1.34	1.38
1	1A	1939	5MU	C4-C5	2.14	1.48	1.44
1	2A	1962	5MC	C6-N1	-2.13	1.34	1.38
32	1a	1498	UR3	C6-C5	2.09	1.39	1.35
32	1a	967	5MC	C6-N1	-2.09	1.34	1.38
1	2A	1939	5MU	C2-N1	2.09	1.41	1.38
1	2A	2503	2MA	C5-N7	-2.09	1.35	1.39
32	2a	1498	UR3	C6-C5	2.08	1.39	1.35
32	1a	1402	4OC	C6-C5	2.08	1.39	1.35
32	2a	1207	2MG	C5-N7	-2.07	1.34	1.39
1	1A	2605	PSU	C2-N1	-2.05	1.34	1.36
1	2A	1911	PSU	C2-N3	-2.05	1.34	1.37
32	2a	967	5MC	C6-N1	-2.05	1.34	1.38
1	1A	1915	5MU	C2-N3	-2.05	1.34	1.38
1	1A	2503	2MA	C4-N9	-2.04	1.33	1.37
1	1A	2552	OMU	C2-N1	2.01	1.41	1.38
32	2a	1402	4OC	C6-C5	2.00	1.39	1.35

All (256) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
43	1l	92	0TD	CSB-SB-CB	13.66	126.92	102.36
1	2A	2503	2MA	C5-C4-N3	-8.38	118.35	127.18
32	2a	527	G7M	CN7-N7-C8	-8.36	112.13	124.79
32	1a	527	G7M	CN7-N7-C8	-8.34	112.16	124.79
1	1A	2503	2MA	C5-C4-N3	-8.31	118.42	127.18
32	1a	1498	UR3	C4-N3-C2	-7.47	118.57	124.58

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	1a	1207	2MG	C2-N3-C4	7.28	121.10	112.00
32	2a	1498	UR3	C4-N3-C2	-7.15	118.83	124.58
32	2a	527	G7M	N9-C8-N7	-6.91	95.70	112.48
32	2a	527	G7M	C8-N7-C5	6.88	116.39	107.78
32	2a	1207	2MG	C2-N3-C4	6.85	120.57	112.00
1	1A	1911	PSU	N1-C2-N3	6.73	122.27	115.17
32	1a	527	G7M	N9-C8-N7	-6.73	96.15	112.48
1	2A	2605	PSU	N1-C2-N3	6.62	122.16	115.17
1	2A	1911	PSU	N1-C2-N3	6.59	122.12	115.17
32	1a	527	G7M	C8-N7-C5	6.42	115.81	107.78
1	2A	2503	2MA	N3-C4-N9	6.39	135.10	126.99
1	2A	1917	PSU	N1-C2-N3	6.28	121.79	115.17
32	2a	516	PSU	N1-C2-N3	6.25	121.76	115.17
1	1A	2605	PSU	N1-C2-N3	6.24	121.75	115.17
1	2A	2251	OMG	C5-C4-N3	-6.24	118.46	128.39
32	1a	966	M2G	C5-C4-N3	-6.23	118.48	128.39
1	1A	2251	OMG	C5-C4-N3	-6.20	118.53	128.39
32	1a	527	G7M	N9-C4-N3	6.15	138.25	125.95
32	2a	527	G7M	N9-C4-N3	6.06	138.07	125.95
32	1a	516	PSU	N1-C2-N3	6.06	121.56	115.17
32	2a	1207	2MG	C5-C4-N3	-6.04	118.78	128.39
32	1a	1207	2MG	C5-C4-N3	-5.92	118.98	128.39
32	2a	966	M2G	C5-C4-N3	-5.86	119.07	128.39
1	2A	1939	5MU	C4-N3-C2	-5.75	119.80	127.34
1	1A	2503	2MA	N3-C4-N9	5.72	134.25	126.99
1	1A	1917	PSU	N1-C2-N3	5.58	121.05	115.17
1	2A	1939	5MU	N3-C2-N1	5.53	122.09	114.89
32	2a	527	G7M	C5-C4-N3	-5.35	118.03	128.15
1	1A	1939	5MU	C4-N3-C2	-5.30	120.40	127.34
1	1A	2058	MA6	N1-C2-N3	-5.27	120.60	128.58
1	1A	1939	5MU	N3-C2-N1	5.25	121.72	114.89
32	1a	527	G7M	C5-C4-N3	-5.22	118.30	128.15
1	1A	2251	OMG	C2-N3-C4	5.00	120.91	112.30
1	2A	1915	5MU	N3-C2-N1	4.99	121.39	114.89
1	1A	2552	OMU	N3-C2-N1	4.99	121.39	114.89
1	2A	2552	OMU	N3-C2-N1	4.93	121.31	114.89
1	1A	1915	5MU	N3-C2-N1	4.91	121.29	114.89
32	1a	1519	MA6	C5-C4-N3	-4.89	119.99	126.72
1	2A	2251	OMG	C2-N3-C4	4.84	120.64	112.30
32	2a	1519	MA6	C5-C4-N3	-4.83	120.06	126.72
1	2A	1939	5MU	C5-C4-N3	4.82	119.52	115.32
32	1a	1518	MA6	N1-C2-N3	-4.78	121.34	128.58

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1A	1915	5MU	C4-N3-C2	-4.76	121.10	127.34
1	2A	2552	OMU	C4-N3-C2	-4.75	120.71	126.61
32	2a	1518	MA6	N1-C2-N3	-4.75	121.39	128.58
32	1a	966	M2G	N9-C4-N3	4.72	135.38	125.95
1	1A	1939	5MU	C5-C4-N3	4.70	119.41	115.32
32	1a	1519	MA6	N1-C2-N3	-4.69	121.49	128.58
32	2a	1519	MA6	N1-C2-N3	-4.67	121.52	128.58
1	2A	1939	5MU	C5-C6-N1	-4.64	118.28	123.31
1	2A	2058	MA6	N1-C2-N3	-4.58	121.65	128.58
1	2A	1915	5MU	C4-N3-C2	-4.56	121.37	127.34
1	2A	2605	PSU	C4-N3-C2	-4.51	120.15	126.37
1	2A	2251	OMG	N9-C4-N3	4.51	134.97	125.95
1	1A	1915	5MU	C5-C4-N3	4.50	119.23	115.32
1	2A	1915	5MU	C1'-N1-C2	4.43	125.55	117.59
1	1A	2605	PSU	C4-N3-C2	-4.43	120.27	126.37
32	2a	527	G7M	C2-N3-C4	4.43	119.93	112.30
32	2a	966	M2G	C2-N3-C4	4.39	120.63	112.51
1	1A	2251	OMG	N9-C4-N3	4.39	134.74	125.95
1	2A	2058	MA6	C5-C4-N3	-4.37	120.70	126.72
32	2a	1207	2MG	N9-C4-N3	4.37	134.69	125.95
32	1a	966	M2G	C2-N3-C4	4.33	120.52	112.51
1	1A	1911	PSU	C4-N3-C2	-4.31	120.44	126.37
1	1A	1915	5MU	C1'-N1-C2	4.31	125.33	117.59
32	1a	527	G7M	C8-N9-C4	4.29	117.72	107.09
32	2a	516	PSU	C4-N3-C2	-4.28	120.48	126.37
32	2a	1519	MA6	C4-C5-N7	-4.25	105.72	110.58
1	1A	1939	5MU	O4-C4-C5	-4.23	120.08	124.92
32	2a	1519	MA6	C5-N7-C8	4.22	110.09	103.45
32	2a	527	G7M	C8-N9-C4	4.22	117.54	107.09
32	1a	527	G7M	C2-N3-C4	4.22	119.56	112.30
43	2l	92	0TD	CSB-SB-CB	4.22	109.94	102.36
1	1A	2058	MA6	C5-C4-N3	-4.20	120.94	126.72
32	1a	527	G7M	CN7-N7-C5	4.19	132.02	126.80
32	2a	966	M2G	N9-C4-N3	4.16	134.27	125.95
1	1A	2503	2MA	C4-C5-N7	-4.14	105.85	110.58
32	2a	1518	MA6	C2-N1-C6	4.13	121.92	111.83
32	1a	516	PSU	C4-N3-C2	-4.09	120.73	126.37
32	2a	1518	MA6	C5-N7-C8	4.02	109.77	103.45
32	1a	1207	2MG	C6-C5-N7	4.02	137.60	130.29
32	1a	1518	MA6	C2-N1-C6	4.01	121.62	111.83
1	2A	2503	2MA	C4-C5-N7	-4.00	106.01	110.58
1	2A	1917	PSU	C4-N3-C2	-4.00	120.87	126.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	2A	1911	PSU	C4-N3-C2	-3.99	120.88	126.37
1	2A	1942	5MC	C5-C6-N1	-3.99	118.98	123.31
32	2a	1518	MA6	C5-C4-N3	-3.96	121.27	126.72
32	2a	1518	MA6	C4-C5-N7	-3.93	106.09	110.58
1	1A	2605	PSU	O2-C2-N1	-3.93	118.74	122.79
1	1A	2552	OMU	C4-N3-C2	-3.90	121.77	126.61
32	2a	1519	MA6	C2-N1-C6	3.89	121.32	111.83
32	1a	1519	MA6	C5-N7-C8	3.87	109.54	103.45
32	1a	1519	MA6	C2-N1-C6	3.86	121.25	111.83
1	2A	1915	5MU	C5-C4-N3	3.84	118.66	115.32
1	2A	2058	MA6	C2-N1-C6	3.83	121.20	111.83
32	1a	1519	MA6	C4-C5-N7	-3.83	106.20	110.58
1	1A	2058	MA6	C2-N1-C6	3.82	121.16	111.83
1	2A	1917	PSU	O2-C2-N1	-3.79	118.88	122.79
1	2A	1915	5MU	O4-C4-C5	-3.78	120.59	124.92
32	2a	527	G7M	CN7-N7-C5	3.76	131.48	126.80
1	1A	1939	5MU	C5-C6-N1	-3.75	119.24	123.31
32	1a	1518	MA6	C5-N7-C8	3.75	109.35	103.45
1	1A	1915	5MU	O4-C4-C5	-3.75	120.62	124.92
1	1A	1911	PSU	O2-C2-N1	-3.75	118.92	122.79
32	1a	1400	5MC	C5-C6-N1	-3.73	119.27	123.31
43	1l	92	0TD	OD2-CG-CB	3.72	121.18	113.15
32	1a	1404	5MC	C5-C6-N1	-3.71	119.28	123.31
32	2a	967	5MC	C5-C6-N1	-3.71	119.28	123.31
1	1A	1917	PSU	C4-N3-C2	-3.70	121.27	126.37
32	2a	1400	5MC	C5-C6-N1	-3.70	119.30	123.31
1	1A	1915	5MU	C1'-N1-C6	-3.68	115.09	121.15
1	1A	2058	MA6	C2-N3-C4	3.66	120.78	111.83
1	1A	2058	MA6	C5-N7-C8	3.66	109.20	103.45
32	2a	1519	MA6	N9-C8-N7	-3.66	108.75	113.94
32	1a	1207	2MG	N9-C4-N3	3.64	133.24	125.95
32	1a	527	G7M	C1'-N9-C8	-3.63	114.48	126.74
1	2A	1915	5MU	C1'-N1-C6	-3.62	115.20	121.15
1	2A	1911	PSU	O2-C2-N1	-3.60	119.07	122.79
32	1a	1518	MA6	C4-C5-N7	-3.60	106.47	110.58
1	2A	2058	MA6	C5-N7-C8	3.58	109.08	103.45
1	2A	2058	MA6	C4-C5-N7	-3.53	106.55	110.58
1	1A	2058	MA6	N9-C8-N7	-3.52	108.94	113.94
32	1a	1518	MA6	C5-C4-N3	-3.52	121.88	126.72
32	2a	1518	MA6	N9-C8-N7	-3.50	108.97	113.94
32	2a	516	PSU	O2-C2-N1	-3.50	119.18	122.79
1	2A	1962	5MC	C5-C6-N1	-3.49	119.53	123.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	1a	1519	MA6	C2-N3-C4	3.48	120.33	111.83
1	2A	1939	5MU	O4-C4-C5	-3.48	120.94	124.92
32	2a	1519	MA6	C2-N3-C4	3.46	120.28	111.83
32	1a	1519	MA6	N9-C8-N7	-3.40	109.11	113.94
1	1A	1962	5MC	C5-C6-N1	-3.40	119.62	123.31
32	1a	1518	MA6	N9-C8-N7	-3.40	109.12	113.94
32	2a	1498	UR3	C5-C4-N3	3.40	119.51	115.04
32	2a	966	M2G	C6-C5-N7	3.36	136.41	130.29
32	1a	1498	UR3	C5-C4-N3	3.36	119.47	115.04
1	1A	1942	5MC	C5-C6-N1	-3.36	119.67	123.31
1	2A	2605	PSU	O2-C2-N1	-3.33	119.36	122.79
32	1a	1207	2MG	N1-C2-N2	3.32	119.95	116.56
1	1A	2503	2MA	N6-C6-N1	3.30	121.47	117.03
1	2A	2058	MA6	C2-N3-C4	3.28	119.84	111.83
1	1A	2552	OMU	C2'-C1'-N1	-3.27	108.04	114.24
32	1a	967	5MC	C5-C6-N1	-3.25	119.78	123.31
1	2A	2552	OMU	C5-C4-N3	3.24	119.34	114.80
1	1A	2058	MA6	C4-C5-N7	-3.24	106.88	110.58
32	1a	516	PSU	O2-C2-N1	-3.22	119.47	122.79
32	2a	527	G7M	C1'-N9-C8	-3.21	115.91	126.74
1	1A	2251	OMG	C6-C5-N7	3.19	136.10	130.29
32	2a	1207	2MG	C6-C5-N7	3.18	136.07	130.29
32	2a	1518	MA6	C2-N3-C4	3.18	119.59	111.83
1	1A	1939	5MU	O2-C2-N1	-3.17	118.67	122.80
1	1A	1917	PSU	O2-C2-N1	-3.16	119.53	122.79
1	2A	2503	2MA	C4-N9-C8	3.12	109.01	105.74
32	1a	1207	2MG	C4-C5-N7	-3.11	105.74	110.67
1	2A	2058	MA6	N9-C8-N7	-3.09	109.55	113.94
32	1a	1518	MA6	C2-N3-C4	3.08	119.36	111.83
1	2A	2251	OMG	C6-C5-N7	3.06	135.85	130.29
32	1a	1519	MA6	N3-C4-N9	3.05	132.36	127.17
32	2a	1404	5MC	C5-C6-N1	-3.03	120.02	123.31
32	2a	1407	5MC	C5-C6-N1	-3.03	120.03	123.31
1	2A	2503	2MA	C5-N7-C8	3.00	108.17	103.45
32	1a	1519	MA6	C4-C5-C6	2.97	118.98	115.91
32	2a	1404	5MC	C5-C4-N3	-2.93	118.76	121.75
1	2A	2552	OMU	C2'-C1'-N1	-2.92	108.70	114.24
32	1a	1407	5MC	C5-C6-N1	-2.92	120.15	123.31
1	1A	2503	2MA	C5-N7-C8	2.90	108.01	103.45
1	1A	2058	MA6	N3-C4-N9	2.89	132.08	127.17
32	2a	1519	MA6	N3-C4-N9	2.87	132.05	127.17
32	1a	966	M2G	C6-C5-N7	2.87	135.52	130.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	2A	2503	2MA	N6-C6-N1	2.87	120.89	117.03
43	2I	92	0TD	OD2-CG-CB	2.87	119.34	113.15
32	2a	1519	MA6	C4-C5-C6	2.86	118.87	115.91
32	1a	1402	4OC	C6-C5-C4	2.86	120.44	117.00
1	1A	1915	5MU	O2-C2-N3	-2.80	116.33	121.49
32	1a	1407	5MC	C5-C4-N3	-2.78	118.90	121.75
1	1A	2503	2MA	CM2-C2-N1	2.78	121.29	117.13
32	1a	527	G7M	O6-C6-C5	-2.73	121.92	128.01
1	1A	2251	OMG	C4-C5-N7	-2.71	106.38	110.67
32	1a	1207	2MG	N2-C2-N3	-2.71	117.06	120.51
32	2a	1400	5MC	C5-C4-N3	-2.69	119.00	121.75
1	2A	2605	PSU	C5-C6-N1	-2.69	118.41	122.14
32	1a	1400	5MC	C5-C4-N3	-2.68	119.00	121.75
1	2A	1939	5MU	O2-C2-N1	-2.66	119.33	122.80
1	2A	1942	5MC	O2-C2-N3	-2.66	118.14	122.33
32	2a	1407	5MC	C5-C4-N3	-2.65	119.03	121.75
1	2A	2058	MA6	N3-C4-N9	2.65	131.67	127.17
32	2a	966	M2G	C4-C5-N7	-2.64	106.49	110.67
32	2a	967	5MC	C5-C4-N3	-2.63	119.05	121.75
1	1A	1942	5MC	C5-C4-N3	-2.61	119.08	121.75
32	2a	1207	2MG	C4-C5-N7	-2.61	106.53	110.67
1	2A	2503	2MA	N9-C8-N7	-2.59	110.26	113.94
1	2A	2552	OMU	O2-C2-N1	-2.59	119.43	122.80
1	1A	1920	OMC	O2-C2-N3	-2.57	118.27	122.33
1	1A	1915	5MU	C5-C6-N1	-2.57	120.52	123.31
1	2A	2251	OMG	C4-C5-N7	-2.54	106.65	110.67
1	2A	1942	5MC	C5-C4-N3	-2.54	119.16	121.75
1	1A	2503	2MA	C6-C5-N7	2.53	136.96	132.09
32	2a	1404	5MC	O2-C2-N3	-2.51	118.37	122.33
1	2A	1915	5MU	O2-C2-N3	-2.51	116.86	121.49
32	1a	1498	UR3	C3U-N3-C2	2.51	121.70	117.33
32	1a	1207	2MG	CM2-N2-C2	-2.50	118.27	123.65
32	2a	516	PSU	O4'-C1'-C2'	2.48	108.58	105.15
32	1a	967	5MC	C5-C4-N3	-2.48	119.21	121.75
1	1A	2552	OMU	C5-C4-N3	2.48	118.27	114.80
43	1I	92	0TD	OD1-CG-CB	-2.47	117.27	122.44
32	2a	1402	4OC	C6-C5-C4	2.45	119.96	117.00
1	2A	2552	OMU	O4-C4-C5	-2.45	120.93	125.16
1	2A	2503	2MA	C6-C5-N7	2.45	136.82	132.09
32	1a	1207	2MG	O3'-C3'-C2'	2.45	119.66	111.82
32	1a	1407	5MC	CM5-C5-C6	-2.44	119.55	122.85
1	2A	2503	2MA	C2-N1-C6	2.42	121.82	118.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	2a	527	G7M	O6-C6-C5	-2.40	122.64	128.01
1	2A	1915	5MU	C5-C6-N1	-2.40	120.70	123.31
1	1A	2605	PSU	C5-C6-N1	-2.39	118.82	122.14
32	1a	1404	5MC	C5-C4-N3	-2.39	119.31	121.75
1	1A	2251	OMG	O6-C6-C5	-2.34	120.35	126.53
32	1a	1407	5MC	O2-C2-N3	-2.34	118.65	122.33
32	2a	1518	MA6	N3-C4-N9	2.32	131.11	127.17
1	2A	1920	OMC	O2-C2-N3	-2.30	118.71	122.33
32	2a	1404	5MC	CM5-C5-C6	-2.30	119.74	122.85
1	2A	2058	MA6	C4-C5-C6	2.29	118.28	115.91
32	1a	966	M2G	C4-C5-N7	-2.28	107.05	110.67
1	1A	2503	2MA	C2-N1-C6	2.28	121.61	118.10
32	2a	1400	5MC	O2-C2-N3	-2.27	118.75	122.33
32	2a	516	PSU	C5-C6-N1	-2.23	119.05	122.14
1	2A	1962	5MC	C5-C4-N3	-2.23	119.47	121.75
1	1A	1962	5MC	C5-C4-N3	-2.23	119.47	121.75
32	2a	1407	5MC	O2-C2-N3	-2.22	118.82	122.33
32	2a	1518	MA6	C4-C5-C6	2.22	118.20	115.91
1	1A	2503	2MA	N9-C8-N7	-2.22	110.79	113.94
1	1A	2503	2MA	C4-N9-C8	2.18	108.02	105.74
1	1A	1911	PSU	C5-C6-N1	-2.17	119.13	122.14
1	1A	2058	MA6	C4-N9-C8	2.14	107.99	105.74
1	1A	2552	OMU	O4-C4-C5	-2.13	121.48	125.16
1	1A	1942	5MC	CM5-C5-C6	-2.12	119.98	122.85
32	1a	966	M2G	O6-C6-C5	-2.10	121.00	126.53
32	2a	1207	2MG	N1-C2-N2	2.09	118.70	116.56
1	2A	1915	5MU	C6-N1-C2	-2.09	119.22	121.30
32	1a	1518	MA6	N3-C4-N9	2.06	130.68	127.17
1	2A	1911	PSU	O4'-C1'-C2'	2.06	108.01	105.15
32	1a	516	PSU	C5-C6-N1	-2.06	119.28	122.14
43	2l	92	0TD	OD1-CG-CB	-2.05	118.14	122.44
1	1A	2552	OMU	O2-C2-N1	-2.04	120.14	122.80
32	2a	1207	2MG	O6-C6-C5	-2.04	121.15	126.53
1	2A	1911	PSU	C5-C6-N1	-2.03	119.32	122.14
32	2a	1498	UR3	C3U-N3-C2	2.03	120.86	117.33
32	2a	1207	2MG	N2-C2-N3	-2.02	117.94	120.51
1	1A	1911	PSU	O4'-C1'-C2'	2.01	107.94	105.15
32	2a	1207	2MG	CM2-N2-C2	-2.00	119.34	123.65
32	2a	967	5MC	CM5-C5-C6	-2.00	120.14	122.85
1	1A	1917	PSU	C6-C5-C4	-2.00	116.82	118.17

There are no chirality outliers.

All (19) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	1A	1915	5MU	O4'-C1'-N1-C2
1	1A	1915	5MU	O4'-C1'-N1-C6
43	1l	92	0TD	CG-CB-SB-CSB
1	2A	1915	5MU	O4'-C1'-N1-C2
1	2A	1915	5MU	O4'-C1'-N1-C6
43	2l	92	0TD	CG-CB-SB-CSB
32	2a	1519	MA6	O4'-C4'-C5'-O5'
1	1A	2503	2MA	C4'-C5'-O5'-P
1	2A	2503	2MA	O4'-C4'-C5'-O5'
32	2a	1402	4OC	C3'-C2'-O2'-CM2
32	1a	1519	MA6	O4'-C4'-C5'-O5'
32	1a	527	G7M	C3'-C4'-C5'-O5'
32	1a	1402	4OC	O4'-C4'-C5'-O5'
43	1l	92	0TD	CA-CB-SB-CSB
43	2l	92	0TD	CA-CB-SB-CSB
32	2a	1402	4OC	C1'-C2'-O2'-CM2
1	1A	1920	OMC	C3'-C2'-O2'-CM2
1	2A	1920	OMC	C3'-C2'-O2'-CM2
1	2A	1920	OMC	C2'-C1'-N1-C2

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 2493 ligands modelled in this entry, 2478 are monoatomic - leaving 15 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
57	MPD	2A	3715	-	7,7,7	0.32	0	9,10,10	0.25	0
57	MPD	2A	3714	-	7,7,7	0.36	0	9,10,10	0.35	0
57	MPD	1A	4034	-	7,7,7	0.36	0	9,10,10	0.38	0
60	SF4	2d	501	35	0,12,12	-	-	-	-	-
56	ZIT	1A	4033	-	54,54,54	0.90	1 (1%)	82,83,83	1.45	11 (13%)
57	MPD	1a	1882	-	7,7,7	0.41	0	9,10,10	0.61	0
58	ARG	1B	230	-	10,11,11	0.76	1 (10%)	9,13,13	1.10	1 (11%)
58	ARG	1F	319	54	10,11,11	0.71	1 (10%)	9,13,13	0.99	1 (11%)
57	MPD	1T	207	-	7,7,7	0.35	0	9,10,10	0.30	0
55	HGR	1A	4032	-	39,39,39	2.42	9 (23%)	48,58,58	1.70	13 (27%)
57	MPD	2B	219	-	7,7,7	0.33	0	9,10,10	0.24	0
57	MPD	18	103	-	7,7,7	0.32	0	9,10,10	0.37	0
55	HGR	2A	3712	-	39,39,39	2.39	8 (20%)	48,58,58	1.66	13 (27%)
60	SF4	1d	303	35	0,12,12	-	-	-	-	-
56	ZIT	2A	3713	-	54,54,54	0.91	1 (1%)	82,83,83	1.66	16 (19%)

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
57	MPD	2A	3715	-	-	5/5/5/5	-
57	MPD	2A	3714	-	-	0/5/5/5	-
57	MPD	1A	4034	-	-	2/5/5/5	-
60	SF4	2d	501	35	-	-	0/6/5/5
56	ZIT	1A	4033	-	-	9/72/107/107	0/3/3/3
57	MPD	1a	1882	-	-	3/5/5/5	-
58	ARG	1B	230	-	-	5/11/11/11	-
58	ARG	1F	319	54	-	5/11/11/11	-
57	MPD	1T	207	-	-	1/5/5/5	-
55	HGR	1A	4032	-	-	5/20/79/79	0/4/4/4
57	MPD	2B	219	-	-	5/5/5/5	-
57	MPD	18	103	-	-	3/5/5/5	-
55	HGR	2A	3712	-	-	5/20/79/79	0/4/4/4
60	SF4	1d	303	35	-	-	0/6/5/5
56	ZIT	2A	3713	-	-	15/72/107/107	0/3/3/3

All (21) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
55	1A	4032	HGR	C12-C14	9.06	1.55	1.33
55	2A	3712	HGR	C12-C14	8.98	1.54	1.33
55	1A	4032	HGR	C5-C4	-5.56	1.39	1.49
55	2A	3712	HGR	C5-C4	-5.54	1.39	1.49
56	2A	3713	ZIT	O14-C1	5.35	1.46	1.34
55	1A	4032	HGR	C5-C6	-5.30	1.39	1.50
55	2A	3712	HGR	C5-C6	-5.28	1.39	1.50
56	1A	4033	ZIT	O14-C1	5.27	1.46	1.34
55	2A	3712	HGR	C3-C2	-4.90	1.39	1.48
55	1A	4032	HGR	C3-C2	-4.67	1.39	1.48
55	1A	4032	HGR	O4-C2	4.44	1.36	1.24
55	2A	3712	HGR	O4-C2	4.28	1.35	1.24
55	1A	4032	HGR	O8-C23	2.79	1.46	1.41
55	1A	4032	HGR	C8-C7	-2.52	1.50	1.53
55	2A	3712	HGR	O8-C23	2.33	1.45	1.41
55	2A	3712	HGR	O1-C10	2.17	1.45	1.41
55	1A	4032	HGR	O1-C10	2.17	1.45	1.41
58	1B	230	ARG	OXT-C	-2.17	1.23	1.30
55	2A	3712	HGR	C1-C2	-2.07	1.39	1.44
55	1A	4032	HGR	C1-C2	-2.07	1.39	1.44
58	1F	319	ARG	OXT-C	-2.04	1.24	1.30

All (55) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
56	1A	4033	ZIT	O1A-C5-C6	4.82	112.14	106.40
56	2A	3713	ZIT	O3B-C3B-C2B	-4.47	106.07	112.95
55	2A	3712	HGR	C4-C5-C6	4.31	121.56	112.35
55	1A	4032	HGR	C4-C5-C6	4.30	121.53	112.35
56	1A	4033	ZIT	O3B-C3B-C4B	4.27	110.05	103.86
55	1A	4032	HGR	C23-O9-C22	-4.00	100.21	106.31
56	2A	3713	ZIT	O3B-C3B-C4B	3.89	109.50	103.86
56	2A	3713	ZIT	C2B-C3B-C4B	3.85	114.23	107.64
56	2A	3713	ZIT	C4A-C3A-N3A	-3.79	104.95	115.59
56	2A	3713	ZIT	O1A-C5-C6	3.52	110.60	106.40
56	1A	4033	ZIT	O14-C1-C2	3.48	118.96	111.53
56	1A	4033	ZIT	C14-O14-C1	-3.29	112.46	118.20
56	1A	4033	ZIT	C8B-O3B-C3B	3.28	124.19	117.51
55	1A	4032	HGR	C4-C3-C2	-3.27	118.99	121.81
56	2A	3713	ZIT	C15-C14-C13	-3.20	109.34	115.20
56	2A	3713	ZIT	O14-C1-C2	3.18	118.33	111.53
58	1B	230	ARG	OXT-C-O	-3.16	116.90	124.08
55	2A	3712	HGR	O9-C22-C18	-3.08	99.51	106.03

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
55	2A	3712	HGR	O1-C10-C9	-2.99	101.17	104.98
55	2A	3712	HGR	O8-C18-C22	-2.99	99.71	106.03
55	2A	3712	HGR	C4-C3-C2	-2.97	119.25	121.81
55	2A	3712	HGR	O4-C2-C3	-2.95	116.85	121.28
56	1A	4033	ZIT	O3B-C3B-C2B	-2.95	108.41	112.95
56	2A	3713	ZIT	C3B-C4B-C5B	2.92	115.36	111.12
55	1A	4032	HGR	O3-C3-C2	2.88	117.74	112.51
56	2A	3713	ZIT	O1B-C3-C4	2.88	111.63	108.23
55	1A	4032	HGR	O3-C10-C9	2.88	111.36	106.69
58	1F	319	ARG	OXT-C-O	-2.85	117.62	124.08
56	2A	3713	ZIT	C6-C5-C4	-2.82	109.80	113.89
55	1A	4032	HGR	O1-C10-C9	-2.81	101.41	104.98
55	2A	3712	HGR	O3-C10-C9	2.72	111.11	106.69
55	1A	4032	HGR	C10-C9-C8	-2.71	98.91	102.29
56	2A	3713	ZIT	C6A-C5A-C4A	-2.71	109.18	113.27
55	2A	3712	HGR	C10-C9-C8	-2.66	98.97	102.29
55	1A	4032	HGR	O9-C22-C18	-2.64	100.45	106.03
55	2A	3712	HGR	C12-C6-C1	-2.60	116.45	119.35
55	1A	4032	HGR	C1-C2-C3	2.59	120.93	116.06
55	2A	3712	HGR	C1-C2-C3	2.57	120.88	116.06
55	1A	4032	HGR	C12-C6-C1	-2.56	116.50	119.35
55	2A	3712	HGR	O3-C3-C2	2.55	117.14	112.51
56	2A	3713	ZIT	O5B-C5B-C6B	2.53	112.36	106.74
56	1A	4033	ZIT	O5B-C5B-C4B	2.52	114.38	110.04
56	1A	4033	ZIT	O1B-C3-C4	2.52	111.21	108.23
56	1A	4033	ZIT	C9-N10-C11	-2.45	107.99	112.06
56	2A	3713	ZIT	C1B-O5B-C5B	2.41	120.43	113.82
55	1A	4032	HGR	O4-C2-C3	-2.39	117.69	121.28
55	2A	3712	HGR	C23-O9-C22	-2.37	102.70	106.31
55	1A	4032	HGR	O8-C18-C22	-2.27	101.23	106.03
55	1A	4032	HGR	C19-C17-N1	2.26	114.78	110.62
55	2A	3712	HGR	C10-O3-C3	-2.14	110.78	115.41
56	2A	3713	ZIT	O14-C1-O1	-2.09	120.18	123.95
56	2A	3713	ZIT	O5A-C5A-C6A	2.04	110.70	106.88
56	1A	4033	ZIT	C6-C5-C4	-2.03	110.94	113.89
56	2A	3713	ZIT	C8B-O3B-C3B	2.00	121.59	117.51
56	1A	4033	ZIT	C4A-C3A-N3A	-2.00	109.97	115.59

There are no chirality outliers.

All (63) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
56	1A	4033	ZIT	C19-C6-C7-C8
56	1A	4033	ZIT	O6-C6-C7-C8
56	1A	4033	ZIT	C12-C11-N10-C21
56	1A	4033	ZIT	C22-C11-N10-C21
56	1A	4033	ZIT	C4B-C3B-O3B-C8B
56	2A	3713	ZIT	C7-C8-C9-N10
56	2A	3713	ZIT	C20-C8-C9-N10
56	2A	3713	ZIT	C2B-C3B-O3B-C8B
56	2A	3713	ZIT	C4B-C3B-O3B-C8B
56	2A	3713	ZIT	C7B-C3B-O3B-C8B
57	1a	1882	MPD	C2-C3-C4-O4
57	1a	1882	MPD	C2-C3-C4-C5
57	2A	3715	MPD	C2-C3-C4-O4
57	2A	3715	MPD	C2-C3-C4-C5
58	1B	230	ARG	NE-CD-CG-CB
58	1F	319	ARG	NE-CD-CG-CB
58	1F	319	ARG	OXT-C-CA-CB
56	1A	4033	ZIT	C2B-C3B-O3B-C8B
58	1F	319	ARG	O-C-CA-CB
58	1F	319	ARG	OXT-C-CA-N
56	1A	4033	ZIT	O1A-C5-C6-C7
56	1A	4033	ZIT	C4-C5-C6-O6
58	1B	230	ARG	CA-CB-CG-CD
58	1B	230	ARG	O-C-CA-N
58	1F	319	ARG	O-C-CA-N
56	2A	3713	ZIT	C22-C11-C12-C13
55	1A	4032	HGR	C12-C14-C15-O7
55	2A	3712	HGR	C12-C14-C15-O7
55	2A	3712	HGR	C12-C14-C15-N1
58	1B	230	ARG	C-CA-CB-CG
57	1A	4034	MPD	O2-C2-C3-C4
57	2A	3715	MPD	O2-C2-C3-C4
55	1A	4032	HGR	C2-C3-O3-C10
55	2A	3712	HGR	C2-C3-O3-C10
57	2B	219	MPD	C2-C3-C4-O4
57	2A	3715	MPD	C1-C2-C3-C4
57	2A	3715	MPD	CM-C2-C3-C4
57	2B	219	MPD	CM-C2-C3-C4
56	2A	3713	ZIT	O12-C12-C13-O13
56	2A	3713	ZIT	N10-C11-C12-O12
56	2A	3713	ZIT	C22-C11-C12-O12
57	2B	219	MPD	C2-C3-C4-C5
55	1A	4032	HGR	C12-C14-C15-N1

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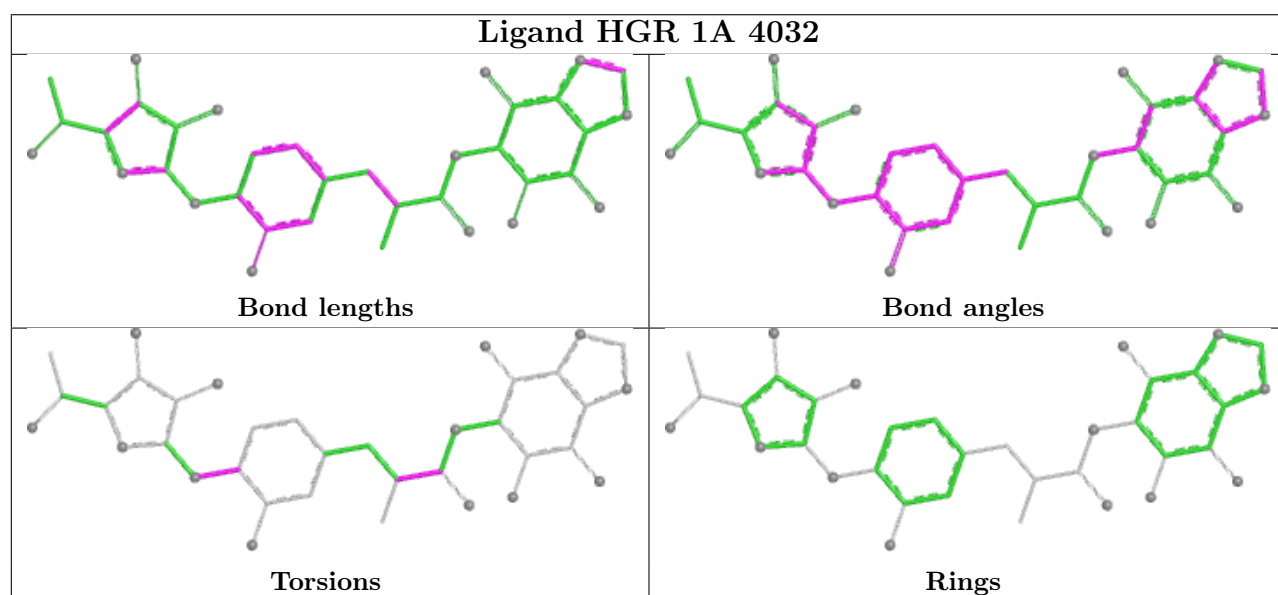
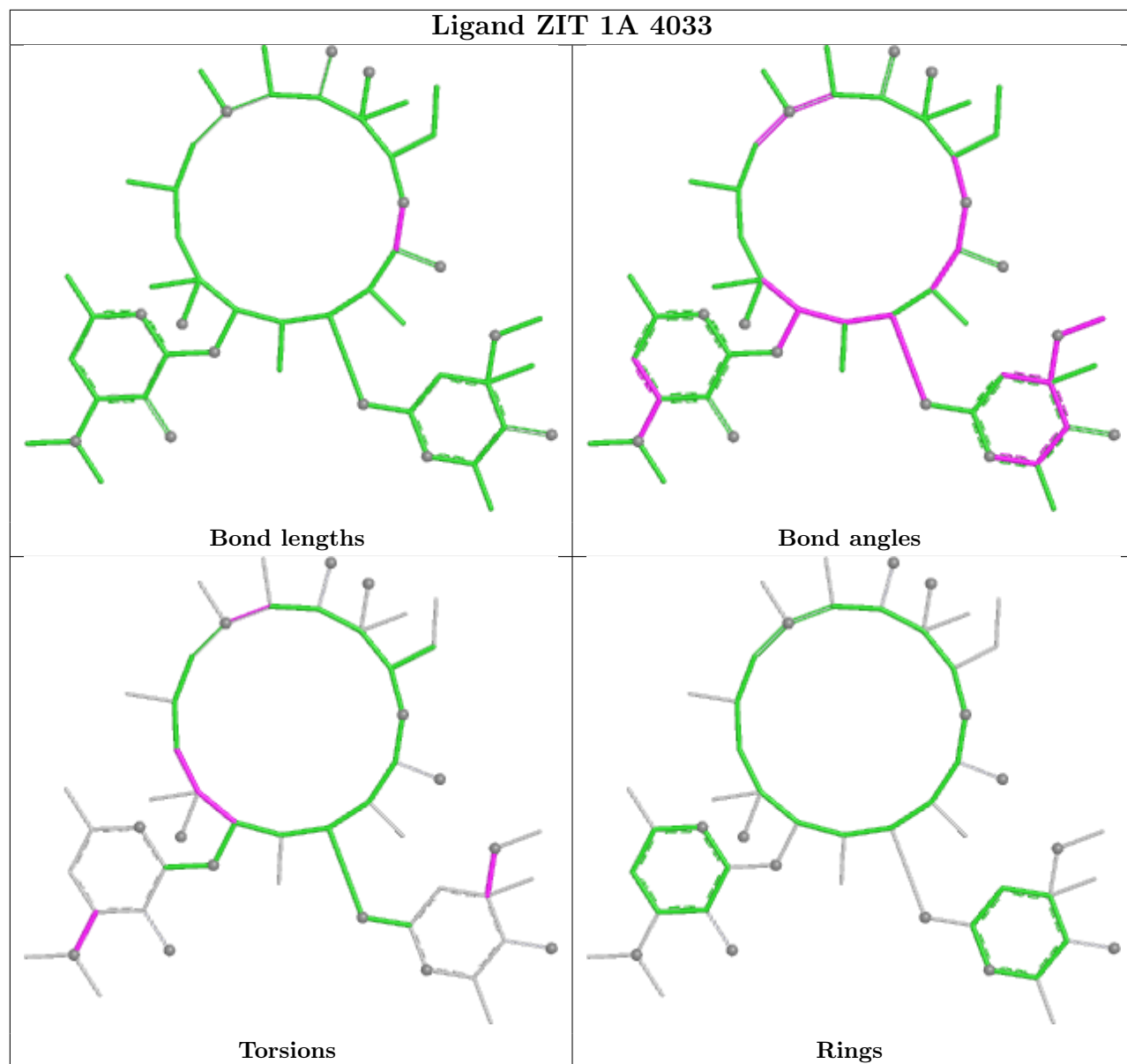
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Mol	Chain	Res	Type	Atoms
56	1A	4033	ZIT	C2A-C3A-N3A-C8A
55	1A	4032	HGR	C16-C14-C15-O7
55	2A	3712	HGR	C16-C14-C15-O7
56	2A	3713	ZIT	C19-C6-C7-C8
56	2A	3713	ZIT	O14-C14-C15-C16
56	2A	3713	ZIT	O12-C12-C13-C14
55	2A	3712	HGR	C16-C14-C15-N1
58	1B	230	ARG	OXT-C-CA-N
57	18	103	MPD	O2-C2-C3-C4
57	2B	219	MPD	O2-C2-C3-C4
57	1A	4034	MPD	C2-C3-C4-O4
57	1T	207	MPD	C2-C3-C4-O4
57	18	103	MPD	C1-C2-C3-C4
57	18	103	MPD	CM-C2-C3-C4
57	1a	1882	MPD	CM-C2-C3-C4
57	2B	219	MPD	C1-C2-C3-C4
56	2A	3713	ZIT	C12-C11-N10-C9
56	2A	3713	ZIT	C11-C12-C13-C23
56	2A	3713	ZIT	C11-C12-C13-O13
55	1A	4032	HGR	C16-C14-C15-N1

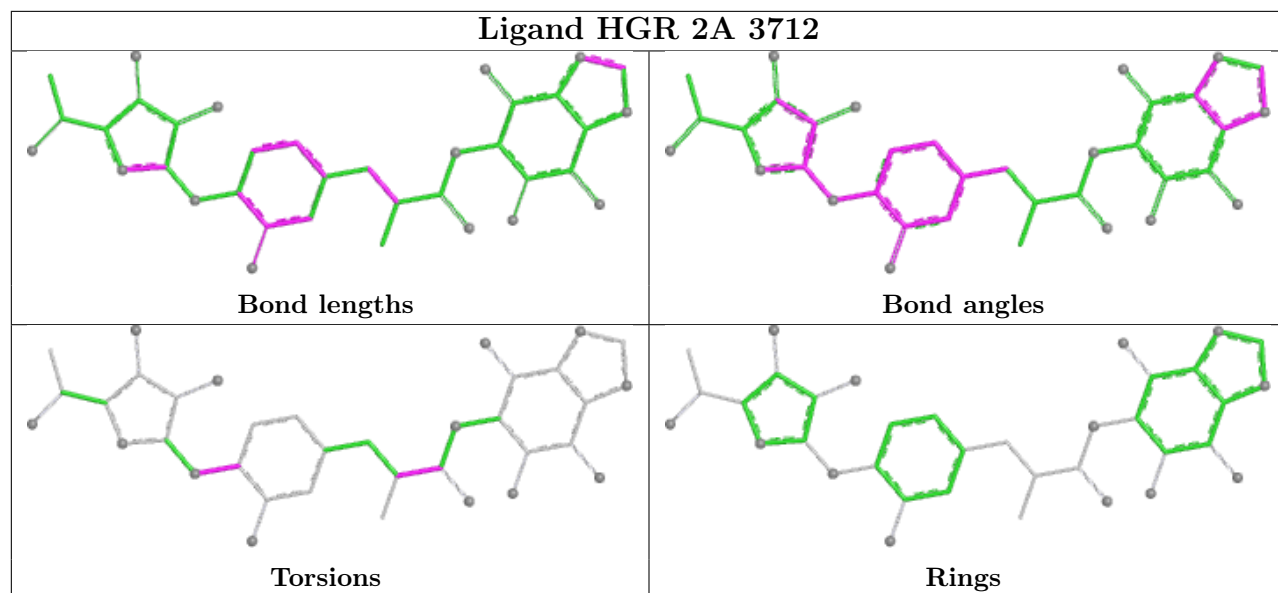
There are no ring outliers.

No monomer is involved in short contacts.

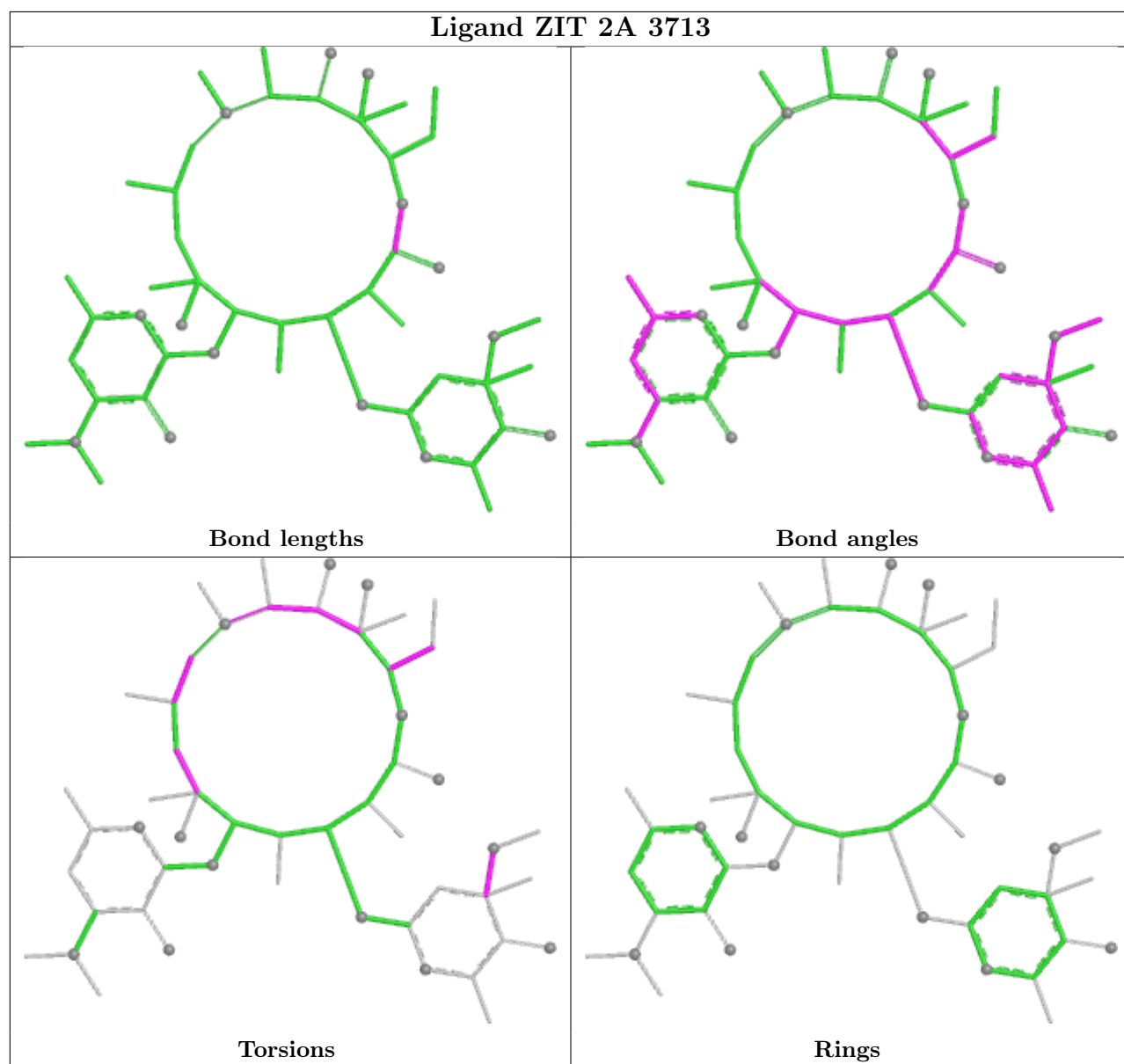
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



Ligand HGR 2A 3712



Ligand ZIT 2A 3713



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	2860/2915 (98%)	-0.58	133 (4%)	36	28	24, 40, 101, 113	0
1	2A	2855/2915 (97%)	-0.17	150 (5%)	32	25	34, 57, 103, 114	0
2	1B	120/121 (99%)	-0.41	1 (0%)	82	79	36, 56, 70, 89	0
2	2B	120/121 (99%)	0.35	1 (0%)	82	79	63, 82, 90, 100	0
3	1D	275/276 (99%)	-0.17	3 (1%)	78	75	24, 40, 55, 81	0
3	2D	275/276 (99%)	0.09	5 (1%)	67	63	32, 51, 64, 87	0
4	1E	204/206 (99%)	-0.19	1 (0%)	87	85	23, 43, 66, 79	0
4	2E	204/206 (99%)	0.16	3 (1%)	72	67	34, 57, 74, 86	0
5	1F	203/210 (96%)	-0.05	3 (1%)	72	67	24, 46, 72, 89	0
5	2F	203/210 (96%)	0.38	3 (1%)	72	67	35, 68, 82, 91	0
6	1G	181/182 (99%)	0.48	8 (4%)	39	31	54, 73, 85, 93	0
6	2G	181/182 (99%)	1.64	58 (32%)	1	0	77, 89, 96, 99	0
7	1H	174/180 (96%)	0.17	2 (1%)	78	75	39, 56, 70, 75	0
7	2H	173/180 (96%)	0.92	13 (7%)	20	15	71, 84, 91, 95	0
8	1I	147/148 (99%)	0.63	6 (4%)	41	33	46, 74, 84, 90	0
8	2I	146/148 (98%)	0.74	6 (4%)	41	33	58, 77, 88, 92	0
9	1N	140/140 (100%)	-0.16	1 (0%)	84	82	30, 43, 65, 81	0
9	2N	140/140 (100%)	0.51	2 (1%)	73	69	47, 65, 78, 87	0
10	1O	122/122 (100%)	-0.28	0	100	100	33, 43, 63, 69	0
10	2O	122/122 (100%)	0.23	0	100	100	45, 57, 70, 77	0
11	1P	149/150 (99%)	0.05	0	100	100	25, 50, 70, 88	0
11	2P	149/150 (99%)	0.34	3 (2%)	65	59	40, 68, 84, 91	0
12	1Q	141/141 (100%)	-0.20	1 (0%)	84	82	30, 44, 56, 71	0
12	2Q	141/141 (100%)	0.60	4 (2%)	55	48	48, 67, 79, 83	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
13	1R	118/118 (100%)	-0.24	0 100 100	30, 40, 57, 65	0
13	2R	118/118 (100%)	0.10	1 (0%) 82 79	39, 53, 66, 71	0
14	1S	110/112 (98%)	0.07	1 (0%) 81 78	45, 57, 71, 75	0
14	2S	110/112 (98%)	1.15	18 (16%) 4 3	66, 77, 84, 87	0
15	1T	131/146 (89%)	0.06	4 (3%) 51 43	36, 48, 71, 86	0
15	2T	131/146 (89%)	0.31	4 (3%) 51 43	50, 60, 78, 86	0
16	1U	116/118 (98%)	-0.38	0 100 100	28, 35, 52, 67	0
16	2U	116/118 (98%)	0.32	1 (0%) 81 78	42, 61, 76, 85	0
17	1V	101/101 (100%)	-0.29	0 100 100	25, 46, 62, 76	0
17	2V	101/101 (100%)	0.44	0 100 100	43, 73, 81, 87	0
18	1W	112/113 (99%)	-0.21	2 (1%) 67 63	28, 36, 56, 86	0
18	2W	112/113 (99%)	-0.01	1 (0%) 81 78	39, 51, 71, 93	0
19	1X	95/96 (98%)	0.01	3 (3%) 50 42	33, 45, 70, 78	0
19	2X	95/96 (98%)	0.41	3 (3%) 50 42	46, 62, 77, 85	0
20	1Y	107/110 (97%)	0.10	2 (1%) 66 61	40, 53, 69, 78	0
20	2Y	107/110 (97%)	0.61	4 (3%) 45 37	59, 71, 82, 87	0
21	1Z	203/206 (98%)	0.37	3 (1%) 72 67	47, 63, 77, 87	0
21	2Z	201/206 (97%)	0.75	3 (1%) 72 67	66, 79, 88, 94	0
22	10	77/85 (90%)	-0.09	1 (1%) 75 71	34, 42, 62, 69	0
22	20	77/85 (90%)	0.64	6 (7%) 19 14	53, 66, 77, 81	0
23	11	97/98 (98%)	0.09	1 (1%) 79 76	31, 50, 74, 84	0
23	21	97/98 (98%)	0.29	2 (2%) 63 57	43, 56, 75, 84	0
24	12	70/72 (97%)	0.11	2 (2%) 53 46	41, 53, 65, 89	0
24	22	70/72 (97%)	0.48	1 (1%) 73 69	61, 72, 79, 80	0
25	13	59/60 (98%)	-0.09	1 (1%) 69 64	32, 41, 68, 76	0
25	23	59/60 (98%)	0.75	4 (6%) 23 17	53, 64, 78, 85	0
26	14	69/71 (97%)	0.77	8 (11%) 9 8	66, 85, 95, 98	0
26	24	69/71 (97%)	1.89	23 (33%) 1 0	86, 95, 100, 103	0
27	15	59/60 (98%)	-0.30	0 100 100	27, 39, 61, 71	0
27	25	59/60 (98%)	-0.15	0 100 100	36, 53, 70, 77	0
28	16	53/54 (98%)	-0.23	0 100 100	37, 47, 61, 65	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
28	26	53/54 (98%)	0.26	1 (1%) 66 61	53, 62, 73, 77	0
29	17	48/49 (97%)	-0.10	4 (8%) 17 12	26, 33, 57, 66	0
29	27	48/49 (97%)	-0.05	4 (8%) 17 12	36, 41, 64, 75	0
30	18	64/65 (98%)	-0.23	0 100 100	33, 40, 46, 60	0
30	28	64/65 (98%)	0.41	0 100 100	48, 57, 64, 71	0
31	19	37/37 (100%)	-0.03	0 100 100	36, 45, 63, 64	0
31	29	37/37 (100%)	1.13	4 (10%) 11 9	59, 70, 78, 80	0
32	1a	1488/1521 (97%)	0.21	49 (3%) 49 40	39, 73, 98, 112	0
32	2a	1492/1521 (98%)	0.41	56 (3%) 44 36	47, 78, 101, 113	0
33	1b	231/256 (90%)	0.94	35 (15%) 5 4	69, 83, 92, 96	0
33	2b	231/256 (90%)	1.22	28 (12%) 8 7	77, 87, 94, 98	0
34	1c	206/239 (86%)	0.81	12 (5%) 29 22	65, 78, 89, 94	0
34	2c	206/239 (86%)	1.28	32 (15%) 5 4	77, 88, 93, 97	0
35	1d	208/209 (99%)	0.75	11 (5%) 32 25	57, 73, 82, 92	0
35	2d	208/209 (99%)	0.77	8 (3%) 44 36	61, 74, 82, 87	0
36	1e	148/162 (91%)	0.37	1 (0%) 84 82	49, 67, 77, 91	0
36	2e	148/162 (91%)	0.77	6 (4%) 41 33	60, 75, 85, 92	0
37	1f	100/101 (99%)	0.43	1 (1%) 79 76	53, 70, 79, 85	0
37	2f	100/101 (99%)	0.44	1 (1%) 79 76	58, 71, 81, 85	0
38	1g	155/156 (99%)	0.66	7 (4%) 38 31	70, 78, 85, 90	0
38	2g	155/156 (99%)	0.92	15 (9%) 13 10	78, 85, 90, 94	0
39	1h	137/138 (99%)	0.59	2 (1%) 72 67	57, 70, 78, 83	0
39	2h	137/138 (99%)	0.65	2 (1%) 72 67	65, 76, 82, 87	0
40	1i	127/128 (99%)	1.38	22 (17%) 4 3	70, 85, 91, 93	0
40	2i	126/128 (98%)	1.91	53 (42%) 0 0	80, 90, 95, 97	0
41	1j	97/105 (92%)	1.11	7 (7%) 21 16	68, 85, 91, 95	0
41	2j	96/105 (91%)	1.81	34 (35%) 1 0	81, 90, 95, 97	0
42	1k	114/129 (88%)	0.40	4 (3%) 47 38	46, 67, 78, 85	0
42	2k	114/129 (88%)	0.97	14 (12%) 8 7	59, 75, 84, 88	0
43	1l	121/132 (91%)	0.44	5 (4%) 41 33	49, 62, 74, 80	0
43	2l	121/132 (91%)	0.58	7 (5%) 29 22	57, 68, 76, 81	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
44	1m	116/126 (92%)	0.74	7 (6%) 27 21	66, 80, 86, 90	0
44	2m	114/126 (90%)	1.62	35 (30%) 1 0	82, 90, 95, 98	0
45	1n	60/61 (98%)	1.06	9 (15%) 5 4	71, 76, 85, 89	0
45	2n	60/61 (98%)	1.99	25 (41%) 0 0	82, 89, 94, 99	0
46	1o	88/89 (98%)	0.74	4 (4%) 38 31	49, 70, 81, 86	0
46	2o	88/89 (98%)	0.92	7 (7%) 18 14	60, 74, 82, 89	0
47	1p	82/88 (93%)	1.13	6 (7%) 21 15	63, 74, 83, 88	0
47	2p	82/88 (93%)	1.06	7 (8%) 16 12	63, 72, 82, 88	0
48	1q	99/105 (94%)	0.95	4 (4%) 42 34	55, 71, 81, 84	0
48	2q	99/105 (94%)	0.75	3 (3%) 52 45	59, 73, 81, 87	0
49	1r	68/88 (77%)	0.40	1 (1%) 72 67	61, 68, 83, 87	0
49	2r	68/88 (77%)	0.70	3 (4%) 39 31	65, 73, 83, 86	0
50	1s	83/93 (89%)	1.08	10 (12%) 9 7	74, 82, 89, 92	0
50	2s	83/93 (89%)	1.99	45 (54%) 0 0	84, 92, 96, 100	0
51	1t	96/106 (90%)	0.96	11 (11%) 9 8	65, 75, 87, 92	0
51	2t	98/106 (92%)	0.63	4 (4%) 41 33	59, 73, 84, 86	0
52	1u	23/27 (85%)	1.11	4 (17%) 4 3	77, 79, 83, 84	0
52	2u	23/27 (85%)	2.54	16 (69%) 0 0	84, 88, 91, 93	0
53	1y	97/113 (85%)	0.59	6 (6%) 26 20	59, 69, 79, 82	0
53	2y	96/113 (84%)	1.59	27 (28%) 1 1	70, 83, 90, 92	0
All	All	20764/21468 (96%)	0.25	1165 (5%) 30 24	23, 66, 93, 114	0

All (1165) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	1A	653	A	9.5
1	2A	653	A	9.1
1	2A	652(U)	G	9.1
45	2n	2	ALA	8.1
1	2A	652(T)	C	8.0
53	1y	98	ALA	8.0
1	1A	654	A	8.0
1	2A	654	A	7.8
1	2A	652(C)	G	7.7
1	2A	652(V)	C	7.6

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Mol	Chain	Res	Type	RSRZ
1	1A	652(V)	C	7.4
1	1A	652(C)	G	7.2
1	1A	1087	G	6.8
53	2y	98	ALA	6.7
1	1A	1076	C	6.7
40	1i	106	ALA	6.3
51	1t	103	GLY	6.3
1	1A	652(D)	C	6.2
26	24	56	VAL	6.2
1	1A	1509	C	6.1
1	1A	652(E)	G	5.8
1	2A	2602	A	5.7
1	1A	1091	G	5.5
1	2A	1509	C	5.5
1	2A	652(E)	G	5.4
1	2A	652(D)	C	5.4
3	1D	276	LYS	5.3
40	2i	127	LYS	5.2
1	1A	652(U)	G	5.1
51	2t	6	PRO	5.1
25	23	2	PRO	5.1
40	1i	126	SER	5.0
1	1A	1090	U	5.0
32	2a	1030(A)	G	4.9
15	1T	131	ALA	4.9
1	1A	2805	G	4.9
32	2a	1202	G	4.9
23	11	2	SER	4.9
40	2i	2	GLU	4.9
1	2A	1536	C	4.9
6	2G	87	PRO	4.9
1	1A	1092	C	4.8
40	2i	125	TYR	4.8
38	1g	84	ASN	4.8
46	2o	86	GLY	4.7
1	1A	2602	A	4.7
1	1A	2804	C	4.7
40	1i	56	LEU	4.7
50	2s	2	PRO	4.7
45	2n	33	VAL	4.7
29	27	48	LYS	4.7
7	1H	2	SER	4.7

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Mol	Chain	Res	Type	RSRZ
53	2y	97	ALA	4.7
40	2i	126	SER	4.7
26	24	49	PHE	4.6
44	2m	98	VAL	4.6
23	2l	2	SER	4.6
1	1A	652(T)	C	4.6
41	2j	75	ILE	4.6
33	2b	237	ALA	4.6
1	1A	1089	G	4.6
1	1A	1077	A	4.5
1	2A	1091	G	4.4
1	1A	1072	C	4.4
1	1A	1088	A	4.4
45	2n	18	VAL	4.4
1	1A	1078	U	4.3
1	1A	1102	C	4.3
40	2i	7	THR	4.3
1	1A	1064	C	4.3
1	1A	1104	C	4.3
1	2A	652(B)	A	4.3
53	1y	97	ALA	4.2
39	2h	2	LEU	4.2
15	1T	104	ASN	4.2
1	1A	2107	C	4.2
6	2G	20	ILE	4.2
1	1A	1176	G	4.2
45	2n	34	TYR	4.1
15	1T	130	ALA	4.1
1	1A	1103	A	4.1
52	2u	24	ARG	4.1
45	2n	13	THR	4.1
32	2a	1030(B)	C	4.1
5	1F	207	GLY	4.1
14	2S	35	ILE	4.1
44	1m	102	ARG	4.1
24	12	70	GLN	4.1
41	2j	34	VAL	4.1
1	1A	652(F)	G	4.0
20	2Y	1	MET	4.0
1	2A	2147	G	4.0
1	2A	2117	A	4.0
45	1n	2	ALA	4.0

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Mol	Chain	Res	Type	RSRZ
40	2i	102	LEU	4.0
1	1A	1075	C	4.0
15	1T	37	GLY	4.0
8	1I	147	GLN	3.9
1	2A	2139	C	3.9
1	1A	1066	U	3.9
35	1d	167	GLY	3.9
43	1l	126	LYS	3.9
12	2Q	104	PHE	3.9
52	2u	14	TRP	3.9
52	2u	16	GLY	3.9
33	1b	7	VAL	3.9
1	2A	34	C	3.9
40	2i	109	VAL	3.9
41	2j	37	PRO	3.8
47	1p	19	ILE	3.8
1	1A	652(S)	C	3.8
33	1b	10	LEU	3.8
8	2I	146	ALA	3.8
1	2A	2133	G	3.8
44	2m	100	GLY	3.8
1	1A	1086	A	3.8
15	2T	130	ALA	3.8
50	2s	76	PRO	3.8
33	1b	236	TYR	3.8
1	2A	1064	C	3.8
1	2A	1076	C	3.8
33	2b	136	VAL	3.8
1	2A	2168	G	3.7
1	1A	2803	C	3.7
51	2t	103	GLY	3.7
1	2A	1046	A	3.7
32	1a	1286	A	3.7
1	1A	1065	U	3.7
11	2P	15	ARG	3.7
1	2A	2116	G	3.7
14	2S	32	LEU	3.7
1	2A	2146	C	3.7
26	14	56	VAL	3.7
34	1c	90	GLU	3.7
40	2i	105	ASP	3.6
43	2l	17	LYS	3.6

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Mol	Chain	Res	Type	RSRZ
1	1A	2145	C	3.6
40	2i	101	PHE	3.6
33	2b	7	VAL	3.6
6	2G	53	LEU	3.6
1	2A	1067	A	3.6
1	2A	2135	A	3.6
3	2D	276	LYS	3.6
26	24	63	TYR	3.6
40	1i	125	TYR	3.6
42	1k	25	TYR	3.6
1	1A	1080	C	3.6
1	2A	2153	G	3.6
1	2A	2155	G	3.6
1	2A	2174	C	3.6
50	2s	67	VAL	3.6
3	1D	275	LYS	3.6
52	2u	6	ARG	3.6
2	2B	1	U	3.6
1	2A	2145	C	3.6
1	1A	1071	G	3.6
51	1t	9	ASN	3.6
18	2W	112	GLY	3.6
32	1a	1257	U	3.6
47	2p	82	GLN	3.6
50	2s	9	VAL	3.6
38	2g	16	LEU	3.6
45	1n	7	ILE	3.5
1	2A	2124	G	3.5
1	2A	2152	G	3.5
21	1Z	192	ALA	3.5
44	2m	76	ALA	3.5
50	2s	82	GLY	3.5
1	1A	888	C	3.5
6	2G	2	PRO	3.5
33	2b	236	TYR	3.5
1	2A	614(A)	U	3.5
40	2i	75	ASP	3.5
45	2n	59	ALA	3.5
1	2A	2803	C	3.5
6	2G	52	ILE	3.5
14	2S	59	LYS	3.5
1	2A	1084	A	3.5

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Mol	Chain	Res	Type	RSRZ
34	2c	160	ALA	3.5
50	2s	59	PRO	3.5
22	20	84	LEU	3.5
43	1l	64	TYR	3.4
2	1B	1	U	3.4
41	2j	76	ASN	3.4
40	1i	19	LEU	3.4
40	2i	117	HIS	3.4
26	14	63	TYR	3.4
6	1G	76	SER	3.4
1	1A	2143	C	3.4
1	1A	2794	C	3.4
25	13	2	PRO	3.4
42	2k	13	GLN	3.4
47	1p	82	GLN	3.4
33	2b	165	VAL	3.4
1	1A	2793	G	3.4
1	2A	2805	G	3.4
32	1a	1036	G	3.4
46	1o	3	ILE	3.4
1	1A	2139	C	3.4
1	2A	2140	C	3.4
5	1F	6	VAL	3.4
26	14	52	THR	3.4
40	2i	10	ARG	3.4
41	1j	4	ILE	3.3
22	20	8	GLY	3.3
1	1A	2117	A	3.3
1	2A	2893	G	3.3
32	2a	1031	G	3.3
26	24	35	VAL	3.3
6	2G	90	LEU	3.3
52	2u	2	GLY	3.3
33	1b	17	PHE	3.3
1	2A	1070	A	3.3
32	2a	1357	A	3.3
34	2c	77	ILE	3.3
34	1c	10	PHE	3.3
38	2g	80	VAL	3.3
40	2i	18	PHE	3.3
32	1a	1001	A	3.3
52	2u	15	ARG	3.3

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Mol	Chain	Res	Type	RSRZ
1	1A	2112	G	3.3
32	1a	1032	G	3.3
6	2G	155	MET	3.3
47	2p	38	TYR	3.3
26	24	54	GLY	3.3
34	2c	159	GLY	3.3
40	2i	46	ALA	3.3
6	2G	147	ASP	3.3
1	1A	2174	C	3.2
1	2A	2136	C	3.2
14	2S	3	ARG	3.2
6	2G	3	LEU	3.2
41	2j	62	HIS	3.2
48	1q	100	LYS	3.2
26	24	67	TYR	3.2
1	2A	1171	G	3.2
32	1a	1030(B)	C	3.2
40	1i	46	ALA	3.2
26	24	65	ASP	3.2
38	2g	5	ARG	3.2
1	2A	2172	U	3.2
32	2a	1257	U	3.2
52	2u	20	LYS	3.2
53	2y	38	HIS	3.2
50	2s	63	THR	3.2
6	1G	44	GLY	3.2
1	2A	2107	C	3.2
15	2T	131	ALA	3.2
6	2G	109	VAL	3.2
41	2j	47	PHE	3.2
40	1i	127	LYS	3.2
4	1E	163	GLU	3.2
6	2G	62	LEU	3.2
1	1A	1093	G	3.2
32	2a	1003	G	3.2
29	17	45	ALA	3.2
40	2i	43	ALA	3.2
40	2i	76	ALA	3.2
1	2A	1075	C	3.1
32	1a	63	C	3.1
45	2n	3	ARG	3.1
26	14	69	LYS	3.1

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Mol	Chain	Res	Type	RSRZ
18	1W	112	GLY	3.1
31	29	21	GLY	3.1
1	2A	1026	U	3.1
6	2G	76	SER	3.1
32	1a	1030(A)	G	3.1
32	1a	1031	G	3.1
42	2k	75	TYR	3.1
52	2u	18	TYR	3.1
1	2A	2142	C	3.1
35	1d	179	GLU	3.1
26	14	54	GLY	3.1
33	2b	230	VAL	3.1
1	2A	2130	U	3.1
41	2j	46	ARG	3.1
41	2j	78	ASN	3.1
6	2G	152	LEU	3.1
52	2u	5	ASP	3.1
1	1A	2147	G	3.1
33	1b	131	PRO	3.1
1	1A	2146	C	3.1
32	2a	1027	C	3.1
3	2D	262	ARG	3.1
51	1t	70	SER	3.1
39	1h	2	LEU	3.1
32	1a	1001(A)	G	3.1
32	2a	1001(A)	G	3.1
46	1o	89	GLY	3.1
14	2S	33	LYS	3.1
26	24	28	LYS	3.1
26	24	58	ARG	3.1
1	1A	34	C	3.1
32	1a	1030	C	3.1
32	2a	1030	C	3.1
33	1b	165	VAL	3.1
1	2A	6	A	3.0
35	1d	155	LEU	3.0
35	1d	166	LYS	3.0
41	2j	48	THR	3.0
26	14	49	PHE	3.0
19	1X	95	LEU	3.0
42	2k	117	ASN	3.0
1	2A	2801(A)	A	3.0

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Mol	Chain	Res	Type	RSRZ
53	2y	9	GLN	3.0
6	1G	52	ILE	3.0
53	2y	7	SER	3.0
6	1G	48	GLU	3.0
1	2A	2112	G	3.0
1	2A	2125	G	3.0
1	2A	2165	G	3.0
1	2A	2119	A	3.0
32	2a	1447	A	3.0
44	2m	6	GLY	3.0
5	2F	21	ALA	3.0
1	2A	2118	U	3.0
32	1a	1000	U	3.0
21	2Z	191	VAL	3.0
34	2c	207	VAL	3.0
50	2s	16	LEU	3.0
26	24	57	GLU	3.0
26	24	66	SER	3.0
12	2Q	59	ARG	3.0
40	1i	7	THR	3.0
1	2A	2793	G	3.0
1	1A	1079	C	3.0
1	2A	2804	C	3.0
45	2n	20	ALA	3.0
1	2A	1085	A	3.0
26	14	59	PHE	3.0
40	2i	56	LEU	2.9
44	2m	66	LEU	2.9
20	1Y	1	MET	2.9
34	2c	79	ARG	2.9
36	2e	13	ILE	2.9
41	2j	36	GLY	2.9
44	2m	24	GLY	2.9
26	24	59	PHE	2.9
50	2s	30	LEU	2.9
1	2A	2802	G	2.9
32	1a	630	G	2.9
32	1a	1033	G	2.9
32	2a	1286	A	2.9
36	2e	10	MET	2.9
6	2G	146	TYR	2.9
46	2o	89	GLY	2.9

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Mol	Chain	Res	Type	RSRZ
50	2s	71	LEU	2.9
1	1A	2108	C	2.9
1	2A	229	A	2.9
1	2A	2111	C	2.9
1	2A	2896	C	2.9
1	2A	2150	U	2.9
1	2A	2897	U	2.9
34	2c	124	ILE	2.9
43	2l	126	LYS	2.9
1	1A	1081	U	2.9
1	1A	1101	U	2.9
1	1A	2142	C	2.9
1	2A	645	C	2.9
1	2A	1073	A	2.9
1	2A	1090	U	2.9
1	2A	2144	U	2.9
32	1a	1030(D)	A	2.9
1	2A	614(B)	G	2.9
1	2A	2151	G	2.9
8	1I	3	VAL	2.9
7	2H	136	ILE	2.8
34	2c	5	ILE	2.8
38	2g	154	TYR	2.8
40	2i	11	LYS	2.8
28	26	11	LEU	2.8
53	2y	73	ALA	2.8
1	1A	2119	A	2.8
1	1A	2167	U	2.8
1	2A	2169	A	2.8
1	2A	2129	C	2.8
1	2A	2138	C	2.8
8	1I	117	GLU	2.8
41	2j	64	GLU	2.8
44	2m	113	PRO	2.8
1	1A	2116	G	2.8
1	2A	2154	G	2.8
1	2A	2162	G	2.8
6	2G	118	ARG	2.8
40	1i	128	ARG	2.8
44	2m	91	ARG	2.8
50	2s	29	ARG	2.8
36	2e	20	GLN	2.8

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Mol	Chain	Res	Type	RSRZ
6	2G	139	LEU	2.8
41	2j	67	THR	2.8
44	2m	72	ALA	2.8
3	2D	113	VAL	2.8
34	1c	207	VAL	2.8
1	1A	1084	A	2.8
32	1a	1041	A	2.8
31	29	17	ILE	2.8
33	1b	22	LYS	2.8
53	2y	54	ILE	2.8
1	1A	1074	G	2.8
1	1A	2115	G	2.8
1	2A	2160	G	2.8
33	1b	11	LEU	2.8
50	2s	15	LEU	2.8
20	2Y	91	GLU	2.8
7	2H	21	PRO	2.8
33	2b	21	ARG	2.8
40	1i	123	PRO	2.8
1	2A	2113	U	2.8
1	1A	887	A	2.8
6	2G	88	ILE	2.8
32	1a	1027	C	2.8
32	1a	1037	C	2.8
32	2a	1116	C	2.8
19	2X	95	LEU	2.8
34	2c	196	LEU	2.8
49	2r	85	LEU	2.8
26	24	51	ASP	2.8
29	17	1	MET	2.8
42	2k	105	VAL	2.8
47	1p	1	MET	2.8
12	2Q	65	PHE	2.8
1	2A	2106	G	2.8
32	1a	79	G	2.8
44	2m	87	TYR	2.8
51	1t	18	GLN	2.7
45	2n	7	ILE	2.7
50	2s	31	ILE	2.7
1	1A	2132	U	2.7
26	24	9	LEU	2.7
41	2j	65	LEU	2.7

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Mol	Chain	Res	Type	RSRZ
43	2l	95	GLY	2.7
6	1G	50	ALA	2.7
50	2s	19	VAL	2.7
50	2s	33	THR	2.7
53	2y	51	ASP	2.7
6	1G	83	ARG	2.7
33	2b	152	PHE	2.7
38	2g	32	ARG	2.7
6	2G	12	TYR	2.7
40	2i	88	TYR	2.7
53	2y	57	PRO	2.7
1	1A	1062	G	2.7
32	2a	1373	G	2.7
33	2b	11	LEU	2.7
35	1d	157	LEU	2.7
8	1I	20	ASP	2.7
40	2i	104	ARG	2.7
1	1A	2158	A	2.7
1	2A	655	A	2.7
1	2A	2126	A	2.7
40	1i	21	PRO	2.7
41	2j	57	LYS	2.7
1	1A	2166	G	2.7
1	1A	2792	G	2.7
1	2A	2148	G	2.7
34	2c	2	GLY	2.7
52	1u	16	GLY	2.7
7	2H	3	ARG	2.7
14	1S	3	ARG	2.7
53	2y	4	ASN	2.7
14	2S	49	VAL	2.7
21	1Z	51	ALA	2.7
26	24	50	VAL	2.7
33	1b	237	ALA	2.7
33	2b	15	VAL	2.7
37	1f	90	VAL	2.7
41	2j	54	PHE	2.7
1	1A	655	A	2.7
1	2A	1096	A	2.7
32	1a	1492	A	2.7
41	1j	74	ILE	2.7
1	2A	2789	C	2.7

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Mol	Chain	Res	Type	RSRZ
32	1a	136	C	2.7
32	1a	1029	C	2.7
5	2F	181	LEU	2.7
6	2G	43	LEU	2.7
36	2e	22	GLY	2.7
52	2u	9	ARG	2.7
50	2s	35	SER	2.7
7	2H	45	VAL	2.7
33	2b	22	LYS	2.7
35	1d	110	PHE	2.7
38	1g	83	ALA	2.7
40	2i	106	ALA	2.7
41	2j	72	VAL	2.7
45	1n	22	THR	2.7
53	1y	2	THR	2.7
32	1a	380	G	2.6
32	2a	1036	G	2.6
1	1A	2144	U	2.6
51	1t	100	ILE	2.6
1	1A	1085	A	2.6
33	1b	187	LEU	2.6
48	2q	98	LEU	2.6
25	23	29	ARG	2.6
43	1l	19	ARG	2.6
1	2A	2179	C	2.6
14	2S	29	PHE	2.6
34	2c	92	ALA	2.6
41	1j	44	VAL	2.6
41	2j	63	PHE	2.6
44	1m	2	ALA	2.6
50	2s	74	PHE	2.6
33	1b	127	ILE	2.6
35	2d	5	ILE	2.6
1	1A	275	G	2.6
1	2A	2159	G	2.6
32	1a	1023	G	2.6
32	2a	1026	G	2.6
32	2a	1030(C)	G	2.6
32	2a	1240	U	2.6
8	1I	38	LEU	2.6
34	1c	87	LEU	2.6
34	2c	94	LEU	2.6

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Mol	Chain	Res	Type	RSRZ
26	24	55	ARG	2.6
29	17	48	LYS	2.6
1	2A	1509(A)	A	2.6
4	2E	204	ALA	2.6
44	2m	106	ASN	2.6
33	2b	97	TRP	2.6
41	2j	30	SER	2.6
45	1n	33	VAL	2.6
1	2A	888	C	2.6
32	2a	1363	C	2.6
48	1q	63	ARG	2.6
45	2n	17	LYS	2.6
1	2A	171	G	2.6
1	2A	1074	G	2.6
32	1a	1026	G	2.6
32	2a	630	G	2.6
32	2a	1022	G	2.6
32	2a	1024	G	2.6
44	2m	75	ALA	2.6
1	2A	887	A	2.6
32	1a	1447	A	2.6
32	2a	532	A	2.6
32	2a	1030(D)	A	2.6
6	2G	7	LEU	2.6
33	1b	36	ARG	2.6
44	1m	115	LYS	2.6
44	2m	31	LYS	2.6
45	1n	4	LYS	2.6
14	2S	60	GLY	2.6
33	1b	38	GLY	2.6
1	2A	1083	U	2.6
6	2G	50	ALA	2.6
34	2c	149	ALA	2.6
40	2i	17	VAL	2.6
40	2i	53	VAL	2.6
40	2i	108	VAL	2.6
40	2i	119	ALA	2.6
49	2r	20	ALA	2.6
50	2s	58	VAL	2.6
24	22	70	GLN	2.6
1	1A	614(B)	G	2.5
1	1A	2125	G	2.5

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Mol	Chain	Res	Type	RSRZ
1	2A	1089	G	2.5
1	2A	2166	G	2.5
32	2a	1033	G	2.5
32	2a	1058	G	2.5
50	2s	66	MET	2.5
40	2i	81	ILE	2.5
44	2m	22	ILE	2.5
53	2y	5	ILE	2.5
1	1A	1057	A	2.5
11	2P	6	LEU	2.5
40	2i	99	LEU	2.5
13	2R	68	ARG	2.5
20	2Y	54	LYS	2.5
33	2b	133	LYS	2.5
40	2i	83	ARG	2.5
33	1b	19	HIS	2.5
40	2i	36	TYR	2.5
6	2G	42	GLY	2.5
33	1b	14	GLY	2.5
6	2G	80	PHE	2.5
6	2G	151	ALA	2.5
33	2b	17	PHE	2.5
44	1m	116	THR	2.5
1	1A	1026	U	2.5
1	2A	2167	U	2.5
53	2y	10	MET	2.5
33	1b	39	ILE	2.5
34	2c	157	ILE	2.5
44	2m	102	ARG	2.5
1	1A	2141	G	2.5
1	1A	2155	G	2.5
32	2a	1002	G	2.5
32	2a	1032	G	2.5
1	2A	1088	A	2.5
33	1b	33	TYR	2.5
42	2k	25	TYR	2.5
52	2u	23	PRO	2.5
49	1r	24	ALA	2.5
1	2A	2143	C	2.5
32	2a	470	C	2.5
51	1t	11	SER	2.5
6	2G	140	ILE	2.5

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Mol	Chain	Res	Type	RSRZ
33	2b	44	LEU	2.5
35	1d	188	LEU	2.5
44	2m	90	LEU	2.5
40	1i	39	GLY	2.5
40	2i	123	PRO	2.5
1	1A	1067	A	2.5
1	1A	1073	A	2.5
1	1A	2159	G	2.5
1	2A	2127	G	2.5
1	2A	2892	A	2.5
32	1a	1030(C)	G	2.5
32	2a	1013	G	2.5
33	1b	230	VAL	2.5
42	2k	15	ALA	2.5
42	2k	125	PHE	2.5
51	1t	97	ALA	2.5
6	2G	145	THR	2.5
41	2j	40	LEU	2.5
45	2n	6	LEU	2.5
45	2n	39	LEU	2.5
1	1A	2138	C	2.5
1	2A	2103	C	2.5
1	2A	2105	C	2.5
32	2a	1038	C	2.5
40	1i	91	ASP	2.5
40	2i	91	ASP	2.5
1	1A	1175	U	2.5
32	2a	1000	U	2.5
34	2c	90	GLU	2.5
35	2d	23	GLY	2.5
40	2i	114	TYR	2.5
41	2j	53	PRO	2.5
53	2y	14	PRO	2.5
6	2G	28	VAL	2.5
6	2G	70	VAL	2.5
34	1c	76	VAL	2.5
4	2E	114	ALA	2.5
33	2b	57	PHE	2.5
40	2i	45	ALA	2.5
45	2n	15	LYS	2.4
46	2o	48	LYS	2.4
26	24	52	THR	2.4

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Mol	Chain	Res	Type	RSRZ
1	1A	529	A	2.4
1	1A	1508	A	2.4
1	1A	1509(A)	A	2.4
1	2A	2170	A	2.4
1	2A	2176	A	2.4
14	2S	61	ASN	2.4
32	2a	994	A	2.4
40	2i	42	ARG	2.4
41	1j	78	ASN	2.4
42	1k	117	ASN	2.4
45	2n	29	ARG	2.4
51	1t	8	ARG	2.4
6	2G	77	ILE	2.4
50	2s	5	LEU	2.4
1	1A	2148	G	2.4
1	2A	2207	G	2.4
32	1a	1003	G	2.4
6	2G	49	ASP	2.4
33	1b	128	GLU	2.4
1	1A	154(A)	C	2.4
1	2A	886	C	2.4
1	1A	1061	U	2.4
1	1A	1963	U	2.4
45	2n	14	PRO	2.4
50	2s	42	PRO	2.4
52	2u	11	GLY	2.4
19	1X	69	TYR	2.4
45	2n	21	TYR	2.4
7	2H	52	VAL	2.4
33	2b	93	VAL	2.4
35	1d	169	LYS	2.4
40	1i	95	LYS	2.4
40	2i	86	VAL	2.4
44	2m	101	GLN	2.4
22	20	69	PHE	2.4
45	1n	5	ALA	2.4
38	2g	79	ARG	2.4
40	1i	107	ARG	2.4
22	10	84	LEU	2.4
50	2s	65	ASN	2.4
1	1A	548	A	2.4
1	2A	1086	A	2.4

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Mol	Chain	Res	Type	RSRZ
1	2A	2158	A	2.4
33	1b	134	GLU	2.4
1	2A	1047	G	2.4
1	2A	1087	G	2.4
1	2A	2894	G	2.4
32	1a	102	G	2.4
32	2a	973	G	2.4
20	2Y	5	MET	2.4
48	2q	100	LYS	2.4
1	2A	1092	C	2.4
1	2A	2108	C	2.4
1	2A	2132	U	2.4
14	2S	7	TYR	2.4
38	1g	85	TYR	2.4
38	2g	85	TYR	2.4
40	2i	4	TYR	2.4
14	2S	12	PHE	2.4
29	27	47	ARG	2.4
33	1b	62	ALA	2.4
33	1b	130	ARG	2.4
40	2i	94	ALA	2.4
52	2u	10	ARG	2.4
40	2i	19	LEU	2.4
40	2i	96	LEU	2.4
38	2g	84	ASN	2.4
1	2A	2114	A	2.4
44	2m	65	LYS	2.4
6	2G	149	VAL	2.4
6	2G	160	VAL	2.4
8	2I	92	VAL	2.4
9	2N	140	VAL	2.4
34	2c	153	VAL	2.4
44	2m	60	VAL	2.4
50	1s	9	VAL	2.4
50	2s	45	VAL	2.4
1	1A	1063	G	2.4
1	2A	2318	G	2.4
6	2G	72	ARG	2.4
34	2c	163	ALA	2.4
38	2g	2	ALA	2.4
50	2s	75	ALA	2.4
51	1t	76	ALA	2.4

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Mol	Chain	Res	Type	RSRZ
1	1A	2150	U	2.4
1	2A	2109	U	2.4
6	2G	157	ILE	2.4
7	2H	89	ILE	2.4
33	2b	10	LEU	2.4
41	1j	75	ILE	2.4
44	2m	84	ILE	2.4
9	1N	68	GLU	2.4
40	2i	110	GLU	2.4
50	2s	64	GLU	2.4
43	2l	23	LYS	2.4
6	2G	134	GLY	2.4
45	2n	38	GLY	2.4
53	2y	92	GLY	2.4
43	2l	89	ARG	2.4
44	1m	117	VAL	2.4
53	1y	95	ARG	2.4
1	1A	2173	A	2.4
19	2X	66	LEU	2.3
35	1d	138	TYR	2.3
42	2k	103	LEU	2.3
6	2G	39	ILE	2.3
41	2j	38	ILE	2.3
52	2u	13	ILE	2.3
53	2y	12	ILE	2.3
1	1A	2130	U	2.3
1	2A	2122	U	2.3
1	2A	2808	U	2.3
21	1Z	203	GLU	2.3
26	24	30	GLU	2.3
33	1b	126	GLU	2.3
34	1c	62	ASP	2.3
38	2g	33	ASP	2.3
53	2y	8	LYS	2.3
53	2y	64	SER	2.3
34	2c	162	GLN	2.3
40	2i	6	GLY	2.3
6	2G	51	ARG	2.3
22	20	74	ARG	2.3
41	2j	45	ARG	2.3
48	1q	91	ARG	2.3
9	2N	9	VAL	2.3

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Mol	Chain	Res	Type	RSRZ
50	2s	41	VAL	2.3
6	2G	102	PHE	2.3
33	1b	13	ALA	2.3
45	2n	37	PHE	2.3
44	2m	96	LEU	2.3
1	1A	2126	A	2.3
50	2s	48	THR	2.3
50	2s	69	HIS	2.3
40	2i	118	LYS	2.3
1	1A	271(K)	U	2.3
1	1A	2113	U	2.3
1	1A	2118	U	2.3
26	14	51	ASP	2.3
44	2m	64	TRP	2.3
1	2A	2115	G	2.3
32	1a	1024	G	2.3
32	1a	1034	G	2.3
32	2a	1190	G	2.3
32	2a	1347	G	2.3
1	2A	2161	C	2.3
32	1a	221	C	2.3
35	1d	2	GLY	2.3
53	2y	46	GLN	2.3
53	2y	83	ARG	2.3
8	2I	5	LEU	2.3
33	2b	122	PHE	2.3
41	2j	90	LEU	2.3
48	2q	71	PHE	2.3
33	1b	214	ILE	2.3
33	2b	208	ILE	2.3
7	2H	129	THR	2.3
14	2S	92	TYR	2.3
6	2G	45	GLU	2.3
6	2G	48	GLU	2.3
33	1b	8	LYS	2.3
40	1i	12	GLU	2.3
1	1A	2629	A	2.3
1	2A	652(A)	A	2.3
1	2A	2173	A	2.3
32	1a	1035	A	2.3
32	2a	1035	A	2.3
41	2j	19	SER	2.3

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Mol	Chain	Res	Type	RSRZ
14	2S	17	ARG	2.3
47	2p	48	TRP	2.3
4	2E	115	GLY	2.3
5	1F	208	GLY	2.3
1	1A	12	U	2.3
1	1A	1082	U	2.3
45	2n	25	VAL	2.3
3	1D	2	ALA	2.3
6	2G	46	ALA	2.3
41	2j	26	ALA	2.3
1	2A	1072	C	2.3
1	2A	2131	G	2.3
1	2A	2149	G	2.3
32	2a	1034	G	2.3
33	1b	200	ILE	2.3
53	2y	39	ILE	2.3
1	2A	2183	C	2.3
22	20	43	THR	2.3
12	1Q	32	TYR	2.3
35	2d	54	TYR	2.3
44	2m	23	TYR	2.3
50	2s	80	TYR	2.3
36	2e	130	ASN	2.3
50	1s	23	ASN	2.3
19	1X	60	ARG	2.3
22	20	9	SER	2.3
33	2b	131	PRO	2.3
38	1g	77	SER	2.3
45	2n	32	SER	2.3
1	1A	229	A	2.3
1	2A	1095	A	2.3
6	2G	100	TRP	2.3
33	1b	97	TRP	2.3
34	1c	2	GLY	2.3
50	2s	8	GLY	2.3
50	2s	34	TRP	2.3
50	2s	20	LEU	2.3
1	1A	2109	U	2.2
1	1A	2172	U	2.2
6	2G	63	ILE	2.2
33	2b	200	ILE	2.2
38	2g	83	ALA	2.2

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Mol	Chain	Res	Type	RSRZ
41	2j	55	LYS	2.2
50	2s	25	LYS	2.2
53	2y	3	MET	2.2
42	2k	87	THR	2.2
45	1n	13	THR	2.2
47	2p	69	THR	2.2
6	2G	137	GLU	2.2
1	2A	2163	C	2.2
1	2A	2175	C	2.2
1	2A	2178	C	2.2
1	1A	2106	G	2.2
1	1A	2133	G	2.2
1	1A	2807	G	2.2
1	2A	2121	G	2.2
38	2g	76	ARG	2.2
33	2b	232	PRO	2.2
38	2g	14	PRO	2.2
40	2i	49	PRO	2.2
50	1s	13	ASP	2.2
35	2d	183	GLY	2.2
7	2H	49	VAL	2.2
34	2c	33	LEU	2.2
41	2j	71	LEU	2.2
1	1A	2176	A	2.2
1	2A	2134	A	2.2
25	23	25	ALA	2.2
26	24	22	ILE	2.2
32	2a	1004	A	2.2
40	2i	37	PHE	2.2
41	2j	32	ALA	2.2
53	2y	66	LYS	2.2
33	1b	12	GLU	2.2
40	1i	64	THR	2.2
41	1j	87	THR	2.2
44	2m	58	GLU	2.2
12	2Q	60	ARG	2.2
45	1n	12	ARG	2.2
45	2n	31	ARG	2.2
47	2p	26	ARG	2.2
6	2G	142	PRO	2.2
33	1b	232	PRO	2.2
46	2o	75	PRO	2.2

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Mol	Chain	Res	Type	RSRZ
1	1A	2111	C	2.2
1	1A	2136	C	2.2
1	2A	2128	C	2.2
1	2A	2137	C	2.2
20	1Y	57	GLN	2.2
32	2a	1028	C	2.2
1	1A	2123	G	2.2
1	1A	2153	G	2.2
1	1A	2894	G	2.2
1	2A	2104	G	2.2
1	2A	2141	G	2.2
7	2H	120	GLY	2.2
14	2S	48	LEU	2.2
14	2S	80	LEU	2.2
32	1a	1042	G	2.2
53	1y	92	GLY	2.2
41	1j	88	LEU	2.2
41	2j	8	LEU	2.2
7	1H	175	LYS	2.2
33	1b	133	LYS	2.2
50	2s	11	VAL	2.2
44	2m	78	ILE	2.2
44	2m	82	MET	2.2
8	2I	7	GLU	2.2
1	1A	652(A)	A	2.2
32	2a	968	A	2.2
44	2m	43	THR	2.2
1	1A	272(A)	U	2.2
32	1a	841	U	2.2
32	2a	1025	U	2.2
32	2a	1358	U	2.2
49	2r	87	ARG	2.2
40	1i	5	TYR	2.2
35	2d	74	GLN	2.2
6	2G	74	LYS	2.2
6	2G	107	LEU	2.2
26	24	45	GLY	2.2
26	24	64	GLY	2.2
40	2i	40	LEU	2.2
40	2i	79	LEU	2.2
41	2j	16	LEU	2.2
43	1l	63	GLY	2.2

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Mol	Chain	Res	Type	RSRZ
45	2n	4	LYS	2.2
52	1u	2	GLY	2.2
52	2u	3	LYS	2.2
6	2G	86	MET	2.2
7	2H	44	VAL	2.2
1	1A	1584	C	2.2
26	24	40	HIS	2.2
32	1a	1007	C	2.2
32	2a	1029	C	2.2
32	2a	1267	C	2.2
33	2b	70	PHE	2.2
35	2d	70	ILE	2.2
21	2Z	192	ALA	2.2
29	27	45	ALA	2.2
45	2n	5	ALA	2.2
34	2c	190	ARG	2.2
50	2s	3	ARG	2.2
50	2s	78	ARG	2.2
1	1A	1046	A	2.2
1	1A	2135	A	2.2
26	24	7	PRO	2.2
32	2a	1001	A	2.2
32	2a	1256	A	2.2
41	2j	91	PRO	2.2
51	2t	98	PRO	2.2
1	1A	1105	U	2.2
1	2A	271(K)	U	2.2
1	2A	1065	U	2.2
1	2A	2180	U	2.2
14	2S	58	LEU	2.2
40	1i	105	ASP	2.2
8	2I	71	ILE	2.2
40	2i	41	VAL	2.2
53	2y	33	HIS	2.2
3	2D	2	ALA	2.1
14	2S	79	ALA	2.1
50	2s	24	ALA	2.1
44	2m	67	GLU	2.1
1	1A	1053	C	2.1
1	1A	2161	C	2.1
1	2A	2185	C	2.1
3	2D	259	THR	2.1

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Mol	Chain	Res	Type	RSRZ
32	1a	219	C	2.1
52	2u	17	THR	2.1
53	1y	53	THR	2.1
1	1A	2149	G	2.1
44	1m	113	PRO	2.1
35	2d	166	LYS	2.1
43	2l	20	LYS	2.1
33	2b	121	LEU	2.1
50	1s	5	LEU	2.1
51	1t	10	LEU	2.1
1	1A	2114	A	2.1
8	1I	13	GLY	2.1
15	2T	69	GLY	2.1
32	2a	975	A	2.1
40	2i	115	GLY	2.1
1	2A	1082	U	2.1
6	2G	92	VAL	2.1
32	1a	992	U	2.1
34	1c	84	ILE	2.1
34	2c	152	ILE	2.1
34	2c	173	VAL	2.1
40	1i	14	VAL	2.1
40	2i	14	VAL	2.1
41	2j	58	ASP	2.1
42	1k	36	ASP	2.1
42	2k	36	ASP	2.1
47	1p	51	VAL	2.1
40	1i	122	ALA	2.1
29	17	47	ARG	2.1
33	1b	23	ARG	2.1
44	1m	114	ARG	2.1
34	2c	95	THR	2.1
42	2k	31	THR	2.1
1	2A	885	C	2.1
16	2U	117	GLN	2.1
6	1G	53	LEU	2.1
35	2d	20	TYR	2.1
51	1t	99	LEU	2.1
50	1s	46	GLY	2.1
1	1A	1537	G	2.1
1	1A	2157	G	2.1
6	2G	101	ILE	2.1

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Mol	Chain	Res	Type	RSRZ
8	2I	20	ASP	2.1
32	1a	376	G	2.1
32	1a	1021	G	2.1
32	2a	971	G	2.1
32	2a	976	G	2.1
38	2g	120	ILE	2.1
42	1k	14	VAL	2.1
45	1n	32	SER	2.1
1	1A	9	U	2.1
1	2A	1098	A	2.1
1	2A	1111	A	2.1
6	2G	69	ALA	2.1
32	1a	1020	U	2.1
33	2b	123	ALA	2.1
6	2G	29	TRP	2.1
24	12	69	ARG	2.1
38	1g	5	ARG	2.1
52	1u	24	ARG	2.1
53	2y	95	ARG	2.1
34	2c	192	THR	2.1
42	2k	28	THR	2.1
45	2n	22	THR	2.1
50	2s	77	THR	2.1
47	1p	15	PRO	2.1
48	1q	82	MET	2.1
7	2H	7	LEU	2.1
34	2c	47	LEU	2.1
39	1h	133	LEU	2.1
50	2s	22	LEU	2.1
33	1b	37	ASN	2.1
6	1G	85	GLY	2.1
14	2S	36	TYR	2.1
40	2i	5	TYR	2.1
42	2k	90	GLY	2.1
50	1s	26	GLY	2.1
50	2s	26	GLY	2.1
1	1A	2140	C	2.1
33	2b	127	ILE	2.1
34	1c	86	VAL	2.1
44	2m	7	VAL	2.1
50	2s	60	VAL	2.1
40	1i	75	ASP	2.1

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Mol	Chain	Res	Type	RSRZ
34	2c	189	ALA	2.1
41	2j	35	SER	2.1
6	2G	91	ARG	2.1
19	2X	68	ARG	2.1
44	2m	28	ALA	2.1
44	2m	69	GLU	2.1
44	2m	88	ARG	2.1
50	1s	29	ARG	2.1
1	1A	2127	G	2.1
1	2A	1533	G	2.1
1	2A	2123	G	2.1
1	2A	2792	G	2.1
6	2G	81	LYS	2.1
23	2l	48	LYS	2.1
32	1a	220	G	2.1
32	1a	378	G	2.1
32	1a	1117	G	2.1
43	1l	47	LYS	2.1
29	27	1	MET	2.1
11	2P	3	LEU	2.1
34	1c	91	LEU	2.1
38	1g	16	LEU	2.1
31	29	20	HIS	2.1
34	2c	80	GLY	2.1
36	1e	85	GLY	2.1
44	2m	68	GLY	2.1
50	1s	47	HIS	2.1
44	2m	9	ILE	2.1
47	2p	33	ILE	2.1
50	2s	61	TYR	2.1
33	1b	15	VAL	2.1
43	2l	18	VAL	2.1
6	2G	116	ASP	2.0
6	2G	141	PHE	2.1
7	2H	116	GLU	2.0
37	2f	47	ARG	2.0
40	2i	9	ARG	2.0
44	2m	80	ARG	2.0
46	2o	68	ARG	2.0
21	2Z	189	ALA	2.0
33	2b	225	ALA	2.0
1	1A	1116	C	2.0

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Mol	Chain	Res	Type	RSRZ
32	1a	132	C	2.0
33	1b	234	PRO	2.0
40	2i	21	PRO	2.0
40	2i	90	PRO	2.0
1	2A	1097	U	2.0
32	2a	1065	U	2.0
32	2a	1205	U	2.0
34	1c	42	LEU	2.0
38	2g	12	LEU	2.0
42	2k	98	LEU	2.0
53	2y	27	LEU	2.0
1	1A	1056	G	2.0
1	1A	1058	G	2.0
1	2A	2110	G	2.0
1	2A	2120	G	2.0
1	2A	2807	G	2.0
32	2a	1224	G	2.0
34	2c	3	ASN	2.0
50	2s	53	ASN	2.0
34	2c	84	ILE	2.0
34	2c	155	GLY	2.0
51	2t	96	GLY	2.0
53	2y	35	ILE	2.0
7	2H	19	VAL	2.0
25	23	6	VAL	2.0
34	1c	99	VAL	2.0
47	1p	17	TYR	2.0
6	2G	136	ARG	2.0
31	29	22	ARG	2.0
45	2n	12	ARG	2.0
50	2s	10	PHE	2.0
52	1u	6	ARG	2.0
6	2G	35	GLU	2.0
34	2c	129	ALA	2.0
36	2e	94	ALA	2.0
41	2j	27	ALA	2.0
53	2y	63	ALA	2.0
15	2T	1	MET	2.0
38	1g	156	TRP	2.0
32	1a	379	C	2.0
32	1a	1354	C	2.0
32	2a	1195	C	2.0

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Mol	Chain	Res	Type	RSRZ
34	2c	188	LEU	2.0
39	2h	70	GLN	2.0
46	2o	71	GLN	2.0
50	1s	22	LEU	2.0
18	1W	111	HIS	2.0
1	1A	1420	U	2.0
32	1a	1040	U	2.0
35	1d	70	ILE	2.0
46	1o	20	GLY	2.0
46	2o	3	ILE	2.0
47	2p	10	GLY	2.0
1	1A	2170	A	2.0
1	2A	1077	A	2.0
32	1a	1493	A	2.0
32	2a	1191	A	2.0
32	2a	1363(A)	A	2.0
34	2c	103	VAL	2.0
46	1o	88	ARG	2.0
50	1s	19	VAL	2.0
50	2s	51	VAL	2.0
5	2F	7	TYR	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(Å ²)	Q<0.9
1	5MU	2A	1915	21/22	0.83	0.11	82,90,98,107	0
1	5MU	1A	1915	21/22	0.85	0.12	75,82,90,97	0
32	2MG	2a	1207	24/25	0.86	0.13	88,95,99,101	0
32	M2G	2a	966	25/26	0.89	0.16	72,77,93,104	0
32	5MC	2a	967	21/22	0.89	0.14	75,79,87,92	0
32	2MG	1a	1207	24/25	0.89	0.11	71,78,82,89	0
1	PSU	2A	1917	20/21	0.90	0.08	77,83,93,95	0
43	0TD	2l	92	10/11	0.90	0.12	66,69,72,88	0
1	PSU	1A	1917	20/21	0.91	0.10	68,76,83,84	0
1	PSU	2A	1911	20/21	0.91	0.08	72,77,88,89	0
32	PSU	2a	516	20/21	0.93	0.08	79,82,86,86	0
32	G7M	2a	527	24/25	0.93	0.10	64,74,76,79	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
32	5MC	1a	967	21/22	0.94	0.11	65,73,82,86	0
1	PSU	1A	1911	20/21	0.94	0.07	65,71,77,77	0
43	0TD	1l	92	10/11	0.94	0.09	53,60,63,71	0
32	5MC	1a	1407	21/22	0.95	0.10	47,54,61,64	0
32	PSU	1a	516	20/21	0.95	0.08	64,68,72,78	0
1	OMC	2A	1920	21/22	0.95	0.08	69,73,78,82	0
1	5MC	2A	1942	21/22	0.95	0.09	51,55,60,64	0
32	4OC	2a	1402	22/23	0.95	0.10	63,70,73,79	0
32	5MC	2a	1404	21/22	0.95	0.09	61,65,69,70	0
32	5MC	2a	1407	21/22	0.95	0.09	61,67,72,78	0
32	UR3	2a	1498	21/22	0.95	0.09	56,62,68,71	0
32	MA6	2a	1518	24/25	0.95	0.11	57,70,75,76	0
32	MA6	2a	1519	24/25	0.95	0.13	58,67,72,75	0
32	M2G	1a	966	25/26	0.95	0.10	61,67,71,75	0
32	G7M	1a	527	24/25	0.96	0.09	48,57,62,71	0
1	OMC	1A	1920	21/22	0.96	0.09	49,61,65,67	0
1	5MU	2A	1939	21/22	0.96	0.09	36,41,45,48	0
32	4OC	1a	1402	22/23	0.96	0.09	52,58,61,71	0
32	5MC	2a	1400	21/22	0.96	0.12	71,78,80,84	0
32	5MC	1a	1404	21/22	0.96	0.08	48,51,55,58	0
1	5MC	2A	1962	21/22	0.97	0.07	44,49,54,68	0
1	MA6	2A	2058	24/25	0.97	0.09	33,40,45,49	0
1	2MA	2A	2503	23/24	0.97	0.08	34,38,40,43	0
32	UR3	1a	1498	21/22	0.97	0.07	47,51,55,64	0
32	MA6	1a	1518	24/25	0.97	0.09	46,49,56,56	0
32	MA6	1a	1519	24/25	0.97	0.08	42,52,56,57	0
32	5MC	1a	1400	21/22	0.97	0.08	47,58,62,67	0
1	5MC	1A	1942	21/22	0.97	0.07	36,42,47,48	0
1	2MA	1A	2503	23/24	0.98	0.06	21,28,31,32	0
1	OMU	1A	2552	21/22	0.98	0.06	30,34,38,43	0
1	PSU	1A	2605	20/21	0.98	0.07	28,32,35,37	0
1	OMG	2A	2251	24/25	0.98	0.09	39,43,46,49	0
1	5MU	1A	1939	21/22	0.98	0.06	28,33,37,38	0
1	OMU	2A	2552	21/22	0.98	0.08	38,43,49,51	0
1	PSU	2A	2605	20/21	0.98	0.07	35,41,46,46	0
1	5MC	1A	1962	21/22	0.98	0.07	28,36,42,49	0
1	MA6	1A	2058	24/25	0.98	0.06	19,27,36,43	0
1	OMG	1A	2251	24/25	0.98	0.06	23,29,31,33	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	2a	3085	1/1	0.21	0.66	97,97,97,97	0
54	MG	2a	3045	1/1	0.22	0.21	91,91,91,91	0
54	MG	2A	3414	1/1	0.39	0.20	82,82,82,82	0
54	MG	1A	3656	1/1	0.46	0.29	85,85,85,85	0
54	MG	2G	201	1/1	0.46	0.25	90,90,90,90	0
54	MG	1A	3854	1/1	0.51	0.27	76,76,76,76	0
54	MG	1A	3657	1/1	0.54	0.30	74,74,74,74	0
54	MG	1A	3983	1/1	0.55	0.16	61,61,61,61	0
54	MG	2G	202	1/1	0.55	0.20	88,88,88,88	0
54	MG	2A	3108	1/1	0.57	0.17	78,78,78,78	0
54	MG	1A	3984	1/1	0.57	0.18	41,41,41,41	0
54	MG	1A	3685	1/1	0.58	0.29	74,74,74,74	0
54	MG	2A	3206	1/1	0.62	0.41	81,81,81,81	0
54	MG	1A	3282	1/1	0.63	0.10	91,91,91,91	0
54	MG	1B	227	1/1	0.64	0.11	79,79,79,79	0
54	MG	2B	206	1/1	0.64	0.40	85,85,85,85	0
54	MG	2A	3355	1/1	0.64	0.17	92,92,92,92	0
54	MG	2n	3101	1/1	0.64	0.30	88,88,88,88	0
54	MG	2B	213	1/1	0.65	0.16	77,77,77,77	0
54	MG	1A	3027	1/1	0.65	0.16	75,75,75,75	0
54	MG	1a	1877	1/1	0.66	0.16	90,90,90,90	0
54	MG	2a	3066	1/1	0.66	0.22	81,81,81,81	0
54	MG	1a	1791	1/1	0.66	0.20	80,80,80,80	0
54	MG	1a	1813	1/1	0.66	0.28	80,80,80,80	0
54	MG	1A	4026	1/1	0.67	0.27	84,84,84,84	0
54	MG	1A	3556	1/1	0.67	0.21	43,43,43,43	0
54	MG	2A	3529	1/1	0.67	0.17	77,77,77,77	0
54	MG	2a	3055	1/1	0.67	0.35	89,89,89,89	0
54	MG	2A	3607	1/1	0.67	0.15	80,80,80,80	0
54	MG	1a	1744	1/1	0.67	0.15	97,97,97,97	0
54	MG	1A	3875	1/1	0.67	0.20	76,76,76,76	0
54	MG	1S	201	1/1	0.68	0.20	68,68,68,68	0
54	MG	2A	3347	1/1	0.68	0.21	82,82,82,82	0
54	MG	1a	1685	1/1	0.68	0.22	76,76,76,76	0
54	MG	1a	1874	1/1	0.68	0.16	79,79,79,79	0
54	MG	1a	1714	1/1	0.68	0.22	81,81,81,81	0
54	MG	2A	3085	1/1	0.68	0.36	79,79,79,79	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	2B	204	1/1	0.68	0.21	85,85,85,85	0
54	MG	1A	3895	1/1	0.68	0.19	64,64,64,64	0
54	MG	2a	3008	1/1	0.69	0.29	81,81,81,81	0
54	MG	2A	3471	1/1	0.69	0.17	84,84,84,84	0
54	MG	2A	3359	1/1	0.69	0.27	71,71,71,71	0
54	MG	2A	3556	1/1	0.69	0.23	68,68,68,68	0
54	MG	2A	3601	1/1	0.69	0.21	88,88,88,88	0
54	MG	2A	3449	1/1	0.69	0.20	75,75,75,75	0
54	MG	1A	3863	1/1	0.70	0.20	76,76,76,76	0
54	MG	1A	3963	1/1	0.70	0.25	72,72,72,72	0
54	MG	2A	3439	1/1	0.70	0.26	65,65,65,65	0
54	MG	1A	3988	1/1	0.70	0.22	82,82,82,82	0
57	MPD	2B	219	8/8	0.70	0.30	70,79,82,82	0
54	MG	1n	103	1/1	0.71	0.19	85,85,85,85	0
54	MG	2a	3056	1/1	0.71	0.30	74,74,74,74	0
54	MG	1A	3910	1/1	0.71	0.15	61,61,61,61	0
54	MG	1A	3887	1/1	0.72	0.15	64,64,64,64	0
54	MG	1A	3998	1/1	0.72	0.30	66,66,66,66	0
54	MG	2a	3113	1/1	0.72	0.23	79,79,79,79	0
54	MG	2a	3164	1/1	0.72	0.15	97,97,97,97	0
54	MG	1A	4000	1/1	0.72	0.32	83,83,83,83	0
54	MG	2A	3430	1/1	0.72	0.15	77,77,77,77	0
54	MG	2A	3089	1/1	0.73	0.20	80,80,80,80	0
54	MG	2a	3061	1/1	0.73	0.13	91,91,91,91	0
54	MG	2A	3090	1/1	0.73	0.43	75,75,75,75	0
54	MG	1A	4020	1/1	0.73	0.19	79,79,79,79	0
54	MG	2A	3572	1/1	0.73	0.13	59,59,59,59	0
54	MG	1a	1850	1/1	0.73	0.22	86,86,86,86	0
54	MG	2A	3267	1/1	0.73	0.34	66,66,66,66	0
54	MG	1A	3300	1/1	0.73	0.14	93,93,93,93	0
54	MG	1A	3165	1/1	0.74	0.23	62,62,62,62	0
54	MG	1A	3542	1/1	0.74	0.15	66,66,66,66	0
54	MG	1a	1693	1/1	0.74	0.29	79,79,79,79	0
54	MG	2A	3470	1/1	0.74	0.18	70,70,70,70	0
54	MG	2A	3185	1/1	0.74	0.21	84,84,84,84	0
54	MG	2A	3371	1/1	0.74	0.17	51,51,51,51	0
54	MG	2A	3409	1/1	0.74	0.13	85,85,85,85	0
54	MG	2I	201	1/1	0.74	0.12	80,80,80,80	0
54	MG	2N	201	1/1	0.74	0.11	75,75,75,75	0
54	MG	1A	3727	1/1	0.74	0.26	57,57,57,57	0
54	MG	1a	1708	1/1	0.75	0.13	98,98,98,98	0
54	MG	2A	3209	1/1	0.75	0.32	80,80,80,80	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	1A	3651	1/1	0.75	0.31	36,36,36,36	0
54	MG	2A	3493	1/1	0.75	0.14	74,74,74,74	0
54	MG	2A	3502	1/1	0.75	0.17	51,51,51,51	0
54	MG	1A	3759	1/1	0.75	0.15	70,70,70,70	0
54	MG	2A	3051	1/1	0.75	0.28	68,68,68,68	0
54	MG	1a	1638	1/1	0.75	0.27	72,72,72,72	0
54	MG	1a	1794	1/1	0.75	0.26	79,79,79,79	0
54	MG	1A	3272	1/1	0.75	0.16	57,57,57,57	0
54	MG	1a	1814	1/1	0.75	0.20	81,81,81,81	0
54	MG	2a	3117	1/1	0.75	0.22	74,74,74,74	0
54	MG	2A	3424	1/1	0.75	0.16	56,56,56,56	0
54	MG	2A	3124	1/1	0.75	0.27	76,76,76,76	0
54	MG	1A	3693	1/1	0.75	0.29	79,79,79,79	0
54	MG	2A	3254	1/1	0.76	0.18	59,59,59,59	0
54	MG	1A	3979	1/1	0.76	0.21	74,74,74,74	0
54	MG	1A	3385	1/1	0.76	0.15	70,70,70,70	0
54	MG	2a	3065	1/1	0.76	0.26	78,78,78,78	0
54	MG	1A	3840	1/1	0.76	0.19	61,61,61,61	0
54	MG	2a	3067	1/1	0.76	0.20	80,80,80,80	0
54	MG	1A	3601	1/1	0.76	0.43	50,50,50,50	0
54	MG	2A	3462	1/1	0.76	0.16	56,56,56,56	0
54	MG	1B	224	1/1	0.76	0.14	64,64,64,64	0
54	MG	2a	3016	1/1	0.76	0.14	94,94,94,94	0
54	MG	2A	3219	1/1	0.76	0.18	70,70,70,70	0
57	MPD	1T	207	8/8	0.76	0.23	73,77,81,82	0
54	MG	2a	3047	1/1	0.76	0.34	72,72,72,72	0
58	ARG	1F	319	12/12	0.76	0.22	60,72,89,89	0
54	MG	1H	201	1/1	0.77	0.17	76,76,76,76	0
54	MG	1A	3237	1/1	0.77	0.29	79,79,79,79	0
54	MG	2A	3153	1/1	0.77	0.18	77,77,77,77	0
54	MG	2A	3376	1/1	0.77	0.21	60,60,60,60	0
54	MG	1a	1879	1/1	0.77	0.15	90,90,90,90	0
54	MG	2a	3103	1/1	0.77	0.12	73,73,73,73	0
54	MG	1n	101	1/1	0.77	0.17	72,72,72,72	0
54	MG	1A	3731	1/1	0.77	0.13	48,48,48,48	0
54	MG	1a	1642	1/1	0.77	0.16	76,76,76,76	0
54	MG	1A	3736	1/1	0.77	0.09	74,74,74,74	0
54	MG	1A	3975	1/1	0.77	0.19	63,63,63,63	0
54	MG	1A	3978	1/1	0.77	0.20	67,67,67,67	0
54	MG	2a	3059	1/1	0.77	0.34	85,85,85,85	0
54	MG	2A	3512	1/1	0.78	0.11	79,79,79,79	0
54	MG	1A	3562	1/1	0.78	0.15	58,58,58,58	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	1A	3797	1/1	0.78	0.24	73,73,73,73	0
54	MG	1a	1647	1/1	0.78	0.30	71,71,71,71	0
54	MG	15	106	1/1	0.78	0.19	58,58,58,58	0
54	MG	2a	3180	1/1	0.78	0.16	86,86,86,86	0
54	MG	2A	3398	1/1	0.78	0.16	70,70,70,70	0
54	MG	2A	3675	1/1	0.78	0.20	55,55,55,55	0
54	MG	2A	3448	1/1	0.78	0.22	67,67,67,67	0
54	MG	2a	3033	1/1	0.78	0.18	84,84,84,84	0
54	MG	1A	3476	1/1	0.79	0.13	58,58,58,58	0
54	MG	2A	3597	1/1	0.79	0.20	48,48,48,48	0
54	MG	2A	3415	1/1	0.79	0.23	71,71,71,71	0
54	MG	1a	1747	1/1	0.79	0.17	78,78,78,78	0
54	MG	1A	3341	1/1	0.79	0.14	49,49,49,49	0
54	MG	1D	318	1/1	0.79	0.19	68,68,68,68	0
54	MG	1a	1652	1/1	0.79	0.25	81,81,81,81	0
54	MG	2a	3080	1/1	0.79	0.20	70,70,70,70	0
54	MG	2A	3282	1/1	0.79	0.17	61,61,61,61	0
54	MG	2A	3292	1/1	0.79	0.14	65,65,65,65	0
54	MG	2A	3465	1/1	0.79	0.18	80,80,80,80	0
54	MG	1A	3733	1/1	0.79	0.22	68,68,68,68	0
54	MG	1a	1821	1/1	0.79	0.17	88,88,88,88	0
54	MG	1A	3814	1/1	0.79	0.24	68,68,68,68	0
54	MG	1T	202	1/1	0.79	0.17	59,59,59,59	0
54	MG	1a	1875	1/1	0.79	0.18	82,82,82,82	0
54	MG	1A	3964	1/1	0.79	0.15	70,70,70,70	0
54	MG	2A	3186	1/1	0.79	0.29	59,59,59,59	0
54	MG	1g	202	1/1	0.80	0.14	69,69,69,69	0
54	MG	1A	3696	1/1	0.80	0.15	71,71,71,71	0
54	MG	2a	3032	1/1	0.80	0.24	74,74,74,74	0
54	MG	1A	3396	1/1	0.80	0.26	71,71,71,71	0
54	MG	1A	3614	1/1	0.80	0.18	75,75,75,75	0
54	MG	2A	3334	1/1	0.80	0.15	83,83,83,83	0
54	MG	2A	3345	1/1	0.80	0.22	81,81,81,81	0
54	MG	1a	1793	1/1	0.80	0.13	71,71,71,71	0
54	MG	2A	3517	1/1	0.80	0.12	61,61,61,61	0
54	MG	1A	3675	1/1	0.80	0.14	34,34,34,34	0
54	MG	1a	1671	1/1	0.80	0.21	81,81,81,81	0
54	MG	1a	1679	1/1	0.80	0.28	71,71,71,71	0
54	MG	1A	3626	1/1	0.80	0.15	85,85,85,85	0
54	MG	1A	3749	1/1	0.80	0.15	59,59,59,59	0
54	MG	2A	3162	1/1	0.80	0.21	68,68,68,68	0
54	MG	2A	3671	1/1	0.80	0.14	67,67,67,67	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	2a	3111	1/1	0.80	0.23	75,75,75,75	0
54	MG	2A	3171	1/1	0.80	0.15	80,80,80,80	0
54	MG	1a	1865	1/1	0.80	0.25	85,85,85,85	0
54	MG	1a	1706	1/1	0.80	0.44	81,81,81,81	0
54	MG	2A	3195	1/1	0.80	0.22	67,67,67,67	0
54	MG	1A	3445	1/1	0.80	0.14	78,78,78,78	0
54	MG	1a	1618	1/1	0.80	0.15	66,66,66,66	0
54	MG	1a	1723	1/1	0.80	0.27	79,79,79,79	0
54	MG	2A	3452	1/1	0.80	0.18	70,70,70,70	0
54	MG	2a	3028	1/1	0.81	0.26	87,87,87,87	0
54	MG	2A	3498	1/1	0.81	0.21	46,46,46,46	0
54	MG	1A	3236	1/1	0.81	0.28	74,74,74,74	0
54	MG	2a	3035	1/1	0.81	0.26	74,74,74,74	0
54	MG	1A	3150	1/1	0.81	0.23	76,76,76,76	0
54	MG	1A	3751	1/1	0.81	0.12	55,55,55,55	0
54	MG	2A	3194	1/1	0.81	0.16	64,64,64,64	0
54	MG	1A	3701	1/1	0.81	0.14	74,74,74,74	0
54	MG	2a	3058	1/1	0.81	0.20	92,92,92,92	0
54	MG	1a	1756	1/1	0.81	0.11	84,84,84,84	0
54	MG	2A	3593	1/1	0.81	0.14	50,50,50,50	0
54	MG	2A	3208	1/1	0.81	0.21	65,65,65,65	0
54	MG	1a	1660	1/1	0.81	0.38	79,79,79,79	0
54	MG	1a	1666	1/1	0.81	0.12	77,77,77,77	0
54	MG	2A	3240	1/1	0.81	0.37	72,72,72,72	0
54	MG	2A	3445	1/1	0.81	0.11	84,84,84,84	0
54	MG	1A	3304	1/1	0.81	0.18	51,51,51,51	0
54	MG	1A	3319	1/1	0.81	0.17	74,74,74,74	0
54	MG	1A	3185	1/1	0.81	0.15	71,71,71,71	0
54	MG	1a	1816	1/1	0.81	0.13	76,76,76,76	0
54	MG	1l	102	1/1	0.81	0.31	63,63,63,63	0
54	MG	1A	3845	1/1	0.81	0.11	53,53,53,53	0
54	MG	2e	202	1/1	0.81	0.34	79,79,79,79	0
54	MG	1A	3972	1/1	0.81	0.13	51,51,51,51	0
54	MG	2A	3477	1/1	0.81	0.27	75,75,75,75	0
54	MG	2a	3011	1/1	0.81	0.33	77,77,77,77	0
54	MG	1a	1871	1/1	0.81	0.15	76,76,76,76	0
54	MG	1A	3856	1/1	0.82	0.16	61,61,61,61	0
54	MG	1A	3318	1/1	0.82	0.19	69,69,69,69	0
54	MG	2A	3043	1/1	0.82	0.32	80,80,80,80	0
54	MG	1a	1798	1/1	0.82	0.31	72,72,72,72	0
54	MG	2A	3264	1/1	0.82	0.19	75,75,75,75	0
54	MG	2A	3052	1/1	0.82	0.28	68,68,68,68	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	2A	3084	1/1	0.82	0.18	80,80,80,80	0
54	MG	13	102	1/1	0.82	0.21	67,67,67,67	0
54	MG	2A	3293	1/1	0.82	0.18	56,56,56,56	0
54	MG	1A	3870	1/1	0.82	0.20	45,45,45,45	0
54	MG	2A	3506	1/1	0.82	0.20	92,92,92,92	0
54	MG	2A	3510	1/1	0.82	0.18	79,79,79,79	0
54	MG	1A	3457	1/1	0.82	0.13	53,53,53,53	0
54	MG	2a	3057	1/1	0.82	0.30	86,86,86,86	0
54	MG	1B	203	1/1	0.82	0.25	67,67,67,67	0
54	MG	1a	1827	1/1	0.82	0.19	88,88,88,88	0
54	MG	1a	1836	1/1	0.82	0.29	74,74,74,74	0
54	MG	2A	3161	1/1	0.82	0.20	83,83,83,83	0
54	MG	1A	3377	1/1	0.82	0.15	61,61,61,61	0
54	MG	2A	3392	1/1	0.82	0.21	78,78,78,78	0
54	MG	1A	3591	1/1	0.82	0.14	76,76,76,76	0
54	MG	2A	3179	1/1	0.82	0.23	82,82,82,82	0
54	MG	1A	3509	1/1	0.82	0.12	29,29,29,29	0
54	MG	2a	3104	1/1	0.82	0.10	85,85,85,85	0
54	MG	1A	3713	1/1	0.82	0.33	54,54,54,54	0
54	MG	2A	3680	1/1	0.82	0.18	64,64,64,64	0
54	MG	2A	3689	1/1	0.82	0.25	70,70,70,70	0
54	MG	1a	1662	1/1	0.82	0.14	70,70,70,70	0
54	MG	2a	3167	1/1	0.82	0.24	89,89,89,89	0
54	MG	1a	1773	1/1	0.82	0.22	64,64,64,64	0
54	MG	2B	208	1/1	0.82	0.29	85,85,85,85	0
54	MG	2B	209	1/1	0.82	0.29	80,80,80,80	0
54	MG	2A	3203	1/1	0.82	0.30	72,72,72,72	0
54	MG	1a	1788	1/1	0.82	0.12	86,86,86,86	0
54	MG	1A	3992	1/1	0.82	0.25	55,55,55,55	0
54	MG	2A	3291	1/1	0.83	0.14	59,59,59,59	0
54	MG	2a	3018	1/1	0.83	0.42	74,74,74,74	0
54	MG	1A	3574	1/1	0.83	0.27	46,46,46,46	0
54	MG	1A	3540	1/1	0.83	0.14	66,66,66,66	0
54	MG	1a	1795	1/1	0.83	0.15	66,66,66,66	0
54	MG	2A	3106	1/1	0.83	0.20	62,62,62,62	0
54	MG	1A	3592	1/1	0.83	0.27	52,52,52,52	0
54	MG	1a	1684	1/1	0.83	0.31	76,76,76,76	0
54	MG	1A	3970	1/1	0.83	0.19	51,51,51,51	0
54	MG	1A	4009	1/1	0.83	0.10	84,84,84,84	0
54	MG	1a	1704	1/1	0.83	0.20	74,74,74,74	0
54	MG	1A	3336	1/1	0.83	0.16	63,63,63,63	0
54	MG	1a	1707	1/1	0.83	0.20	75,75,75,75	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	1a	1615	1/1	0.83	0.10	79,79,79,79	0
54	MG	2A	3612	1/1	0.83	0.20	72,72,72,72	0
54	MG	1A	4024	1/1	0.83	0.17	61,61,61,61	0
54	MG	2A	3187	1/1	0.83	0.25	74,74,74,74	0
54	MG	1a	1717	1/1	0.83	0.33	80,80,80,80	0
54	MG	2A	3686	1/1	0.83	0.18	82,82,82,82	0
54	MG	2a	3099	1/1	0.83	0.13	78,78,78,78	0
54	MG	1a	1720	1/1	0.83	0.41	77,77,77,77	0
54	MG	2A	3691	1/1	0.83	0.20	83,83,83,83	0
54	MG	1a	1626	1/1	0.83	0.09	66,66,66,66	0
54	MG	1a	1727	1/1	0.83	0.16	70,70,70,70	0
54	MG	1A	3551	1/1	0.83	0.30	62,62,62,62	0
54	MG	2a	3145	1/1	0.83	0.16	88,88,88,88	0
54	MG	1A	3621	1/1	0.83	0.14	46,46,46,46	0
54	MG	1B	210	1/1	0.83	0.15	65,65,65,65	0
54	MG	2a	3173	1/1	0.83	0.23	72,72,72,72	0
54	MG	1a	1765	1/1	0.83	0.19	67,67,67,67	0
54	MG	1A	3261	1/1	0.83	0.22	81,81,81,81	0
54	MG	1a	1777	1/1	0.83	0.10	69,69,69,69	0
54	MG	1A	3331	1/1	0.83	0.32	81,81,81,81	0
54	MG	2A	3268	1/1	0.83	0.17	78,78,78,78	0
54	MG	1A	3725	1/1	0.83	0.18	26,26,26,26	0
54	MG	1A	3799	1/1	0.84	0.16	34,34,34,34	0
54	MG	1a	1680	1/1	0.84	0.14	86,86,86,86	0
54	MG	1B	226	1/1	0.84	0.10	78,78,78,78	0
54	MG	1A	3405	1/1	0.84	0.14	51,51,51,51	0
54	MG	1A	3834	1/1	0.84	0.21	47,47,47,47	0
54	MG	1a	1698	1/1	0.84	0.24	78,78,78,78	0
54	MG	1A	3443	1/1	0.84	0.29	82,82,82,82	0
54	MG	1N	203	1/1	0.84	0.14	70,70,70,70	0
54	MG	1A	3707	1/1	0.84	0.15	70,70,70,70	0
54	MG	2A	3227	1/1	0.84	0.27	65,65,65,65	0
54	MG	2A	3234	1/1	0.84	0.26	73,73,73,73	0
54	MG	1A	3981	1/1	0.84	0.25	59,59,59,59	0
54	MG	1A	3145	1/1	0.84	0.17	69,69,69,69	0
54	MG	1A	3454	1/1	0.84	0.23	65,65,65,65	0
54	MG	1d	302	1/1	0.84	0.20	74,74,74,74	0
54	MG	1A	3986	1/1	0.84	0.10	75,75,75,75	0
54	MG	19	103	1/1	0.84	0.21	67,67,67,67	0
54	MG	2A	3548	1/1	0.84	0.14	37,37,37,37	0
54	MG	1a	1603	1/1	0.84	0.22	77,77,77,77	0
54	MG	1a	1612	1/1	0.84	0.20	79,79,79,79	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	1A	3325	1/1	0.84	0.18	66,66,66,66	0
54	MG	2a	3072	1/1	0.84	0.36	67,67,67,67	0
54	MG	1A	3061	1/1	0.84	0.23	64,64,64,64	0
54	MG	2A	3053	1/1	0.84	0.28	69,69,69,69	0
54	MG	1A	3667	1/1	0.84	0.17	65,65,65,65	0
54	MG	2a	3101	1/1	0.84	0.14	71,71,71,71	0
54	MG	1a	1769	1/1	0.84	0.18	63,63,63,63	0
54	MG	1A	3491	1/1	0.84	0.12	60,60,60,60	0
54	MG	1A	4008	1/1	0.84	0.14	61,61,61,61	0
54	MG	1a	1782	1/1	0.84	0.12	76,76,76,76	0
54	MG	1A	3676	1/1	0.84	0.12	49,49,49,49	0
54	MG	2a	3119	1/1	0.84	0.13	65,65,65,65	0
54	MG	1A	3898	1/1	0.84	0.27	40,40,40,40	0
54	MG	2A	3406	1/1	0.84	0.20	92,92,92,92	0
54	MG	2B	202	1/1	0.84	0.16	73,73,73,73	0
54	MG	1A	3107	1/1	0.84	0.15	36,36,36,36	0
54	MG	2a	3178	1/1	0.84	0.19	81,81,81,81	0
54	MG	1A	3931	1/1	0.84	0.17	64,64,64,64	0
54	MG	1a	1665	1/1	0.84	0.17	76,76,76,76	0
54	MG	1A	3530	1/1	0.84	0.12	79,79,79,79	0
54	MG	1a	1809	1/1	0.84	0.28	74,74,74,74	0
54	MG	2A	3438	1/1	0.84	0.37	64,64,64,64	0
54	MG	1A	3694	1/1	0.84	0.23	78,78,78,78	0
54	MG	1a	1869	1/1	0.85	0.13	84,84,84,84	0
54	MG	1a	1729	1/1	0.85	0.19	74,74,74,74	0
54	MG	2A	3228	1/1	0.85	0.16	66,66,66,66	0
54	MG	1a	1872	1/1	0.85	0.11	89,89,89,89	0
54	MG	2A	3632	1/1	0.85	0.12	87,87,87,87	0
54	MG	1A	3699	1/1	0.85	0.16	41,41,41,41	0
54	MG	1A	3926	1/1	0.85	0.15	30,30,30,30	0
54	MG	2A	3259	1/1	0.85	0.20	57,57,57,57	0
54	MG	1a	1749	1/1	0.85	0.13	65,65,65,65	0
54	MG	1a	1750	1/1	0.85	0.20	73,73,73,73	0
54	MG	1d	301	1/1	0.85	0.26	74,74,74,74	0
54	MG	2A	3707	1/1	0.85	0.12	73,73,73,73	0
54	MG	2A	3708	1/1	0.85	0.21	64,64,64,64	0
54	MG	2A	3269	1/1	0.85	0.18	39,39,39,39	0
54	MG	2B	203	1/1	0.85	0.27	74,74,74,74	0
54	MG	1a	1752	1/1	0.85	0.33	71,71,71,71	0
54	MG	1e	201	1/1	0.85	0.21	72,72,72,72	0
54	MG	1A	3479	1/1	0.85	0.12	50,50,50,50	0
54	MG	1h	201	1/1	0.85	0.16	71,71,71,71	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	2A	3297	1/1	0.85	0.21	82,82,82,82	0
54	MG	2E	305	1/1	0.85	0.21	62,62,62,62	0
54	MG	2A	3333	1/1	0.85	0.10	36,36,36,36	0
54	MG	1i	3100	1/1	0.85	0.14	80,80,80,80	0
54	MG	1a	1757	1/1	0.85	0.20	50,50,50,50	0
54	MG	1A	3035	1/1	0.85	0.34	68,68,68,68	0
54	MG	2a	3002	1/1	0.85	0.13	66,66,66,66	0
54	MG	1t	201	1/1	0.85	0.14	70,70,70,70	0
54	MG	1y	203	1/1	0.85	0.11	75,75,75,75	0
54	MG	2A	3012	1/1	0.85	0.14	71,71,71,71	0
54	MG	2A	3024	1/1	0.85	0.24	77,77,77,77	0
54	MG	2a	3020	1/1	0.85	0.28	66,66,66,66	0
54	MG	2a	3021	1/1	0.85	0.20	76,76,76,76	0
54	MG	2a	3022	1/1	0.85	0.22	60,60,60,60	0
54	MG	2A	3036	1/1	0.85	0.20	57,57,57,57	0
54	MG	1A	3189	1/1	0.85	0.13	76,76,76,76	0
54	MG	1A	4019	1/1	0.85	0.12	66,66,66,66	0
54	MG	2A	3408	1/1	0.85	0.18	59,59,59,59	0
54	MG	1a	1774	1/1	0.85	0.14	73,73,73,73	0
54	MG	1A	3583	1/1	0.85	0.12	63,63,63,63	0
54	MG	2a	3049	1/1	0.85	0.34	69,69,69,69	0
54	MG	2A	3073	1/1	0.85	0.28	65,65,65,65	0
54	MG	1a	1682	1/1	0.85	0.12	69,69,69,69	0
54	MG	1a	1601	1/1	0.85	0.15	89,89,89,89	0
54	MG	1A	3659	1/1	0.85	0.23	42,42,42,42	0
54	MG	1A	3079	1/1	0.85	0.18	60,60,60,60	0
54	MG	1A	3538	1/1	0.85	0.10	62,62,62,62	0
54	MG	1A	3866	1/1	0.85	0.12	56,56,56,56	0
54	MG	2A	3120	1/1	0.85	0.23	63,63,63,63	0
54	MG	1a	1796	1/1	0.85	0.18	90,90,90,90	0
54	MG	1A	3600	1/1	0.85	0.18	65,65,65,65	0
54	MG	2A	3160	1/1	0.85	0.14	72,72,72,72	0
54	MG	1a	1630	1/1	0.85	0.16	63,63,63,63	0
54	MG	2a	3086	1/1	0.85	0.28	81,81,81,81	0
54	MG	1A	3455	1/1	0.85	0.14	34,34,34,34	0
54	MG	1a	1710	1/1	0.85	0.25	71,71,71,71	0
54	MG	2A	3486	1/1	0.85	0.15	74,74,74,74	0
54	MG	2A	3491	1/1	0.85	0.09	76,76,76,76	0
54	MG	1a	1641	1/1	0.85	0.17	79,79,79,79	0
54	MG	2A	3180	1/1	0.85	0.19	71,71,71,71	0
54	MG	2a	3116	1/1	0.85	0.22	82,82,82,82	0
54	MG	1A	3610	1/1	0.85	0.30	74,74,74,74	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	1A	3402	1/1	0.85	0.17	72,72,72,72	0
54	MG	2a	3143	1/1	0.85	0.17	70,70,70,70	0
54	MG	1a	1829	1/1	0.85	0.24	74,74,74,74	0
54	MG	2a	3158	1/1	0.85	0.15	88,88,88,88	0
54	MG	1a	1831	1/1	0.85	0.13	62,62,62,62	0
54	MG	2A	3515	1/1	0.85	0.21	82,82,82,82	0
54	MG	1A	3363	1/1	0.85	0.12	71,71,71,71	0
54	MG	2A	3202	1/1	0.85	0.24	63,63,63,63	0
54	MG	2A	3531	1/1	0.85	0.12	87,87,87,87	0
54	MG	1a	1841	1/1	0.85	0.22	79,79,79,79	0
54	MG	2j	201	1/1	0.85	0.08	84,84,84,84	0
54	MG	1a	1849	1/1	0.85	0.15	66,66,66,66	0
57	MPD	1A	4034	8/8	0.85	0.26	54,59,62,65	0
54	MG	1a	1724	1/1	0.85	0.18	64,64,64,64	0
54	MG	2A	3591	1/1	0.85	0.13	55,55,55,55	0
54	MG	1a	1657	1/1	0.85	0.21	84,84,84,84	0
54	MG	2D	308	1/1	0.86	0.10	37,37,37,37	0
54	MG	1A	3036	1/1	0.86	0.10	51,51,51,51	0
54	MG	1a	1867	1/1	0.86	0.12	87,87,87,87	0
54	MG	1a	1659	1/1	0.86	0.24	47,47,47,47	0
54	MG	1a	1870	1/1	0.86	0.17	69,69,69,69	0
54	MG	1A	3152	1/1	0.86	0.19	50,50,50,50	0
54	MG	2O	202	1/1	0.86	0.14	76,76,76,76	0
54	MG	2O	101	1/1	0.86	0.16	78,78,78,78	0
54	MG	1A	3524	1/1	0.86	0.16	56,56,56,56	0
54	MG	1A	3646	1/1	0.86	0.13	30,30,30,30	0
54	MG	2A	3451	1/1	0.86	0.15	67,67,67,67	0
54	MG	1A	3787	1/1	0.86	0.09	24,24,24,24	0
54	MG	1a	1668	1/1	0.86	0.25	82,82,82,82	0
54	MG	1A	3648	1/1	0.86	0.20	55,55,55,55	0
54	MG	1a	1673	1/1	0.86	0.17	61,61,61,61	0
54	MG	1a	1770	1/1	0.86	0.12	68,68,68,68	0
54	MG	1A	3398	1/1	0.86	0.13	53,53,53,53	0
54	MG	2a	3030	1/1	0.86	0.34	72,72,72,72	0
54	MG	2A	3482	1/1	0.86	0.17	65,65,65,65	0
54	MG	2A	3204	1/1	0.86	0.15	67,67,67,67	0
54	MG	2a	3034	1/1	0.86	0.23	92,92,92,92	0
54	MG	2A	3205	1/1	0.86	0.16	74,74,74,74	0
54	MG	1A	3809	1/1	0.86	0.24	59,59,59,59	0
54	MG	1A	3587	1/1	0.86	0.14	57,57,57,57	0
54	MG	2A	3499	1/1	0.86	0.12	67,67,67,67	0
54	MG	2a	3052	1/1	0.86	0.20	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	3941	1/1	0.86	0.18	53,53,53,53	0
54	MG	1A	3947	1/1	0.86	0.13	48,48,48,48	0
54	MG	1a	1690	1/1	0.86	0.39	69,69,69,69	0
54	MG	1A	3956	1/1	0.86	0.12	55,55,55,55	0
54	MG	1y	202	1/1	0.86	0.15	68,68,68,68	0
54	MG	2a	3060	1/1	0.86	0.32	80,80,80,80	0
54	MG	1A	4023	1/1	0.86	0.15	60,60,60,60	0
54	MG	1A	3817	1/1	0.86	0.18	77,77,77,77	0
54	MG	2A	3016	1/1	0.86	0.32	74,74,74,74	0
54	MG	1A	3131	1/1	0.86	0.18	45,45,45,45	0
54	MG	2A	3551	1/1	0.86	0.13	51,51,51,51	0
54	MG	2a	3074	1/1	0.86	0.25	75,75,75,75	0
54	MG	2a	3078	1/1	0.86	0.39	71,71,71,71	0
54	MG	2A	3552	1/1	0.86	0.14	44,44,44,44	0
54	MG	2A	3025	1/1	0.86	0.13	62,62,62,62	0
54	MG	2A	3034	1/1	0.86	0.23	77,77,77,77	0
54	MG	2a	3092	1/1	0.86	0.12	89,89,89,89	0
54	MG	2a	3096	1/1	0.86	0.10	63,63,63,63	0
54	MG	1A	3719	1/1	0.86	0.14	60,60,60,60	0
54	MG	1a	1801	1/1	0.86	0.32	85,85,85,85	0
54	MG	2a	3102	1/1	0.86	0.10	67,67,67,67	0
54	MG	1a	1803	1/1	0.86	0.16	80,80,80,80	0
54	MG	1a	1631	1/1	0.86	0.20	54,54,54,54	0
54	MG	1a	1635	1/1	0.86	0.20	76,76,76,76	0
54	MG	2A	3059	1/1	0.86	0.28	58,58,58,58	0
54	MG	1A	3461	1/1	0.86	0.23	74,74,74,74	0
54	MG	2A	3076	1/1	0.86	0.14	63,63,63,63	0
54	MG	2a	3118	1/1	0.86	0.20	61,61,61,61	0
54	MG	2A	3340	1/1	0.86	0.17	50,50,50,50	0
54	MG	1a	1716	1/1	0.86	0.26	65,65,65,65	0
54	MG	1A	3087	1/1	0.86	0.17	59,59,59,59	0
54	MG	1B	225	1/1	0.86	0.12	72,72,72,72	0
54	MG	1a	1721	1/1	0.86	0.11	75,75,75,75	0
54	MG	2A	3100	1/1	0.86	0.17	71,71,71,71	0
54	MG	2a	3171	1/1	0.86	0.13	83,83,83,83	0
54	MG	2A	3101	1/1	0.86	0.27	61,61,61,61	0
54	MG	2B	201	1/1	0.86	0.14	82,82,82,82	0
54	MG	1a	1644	1/1	0.86	0.27	68,68,68,68	0
54	MG	1A	3543	1/1	0.86	0.08	26,26,26,26	0
54	MG	2A	3112	1/1	0.86	0.35	73,73,73,73	0
54	MG	2A	3113	1/1	0.86	0.19	67,67,67,67	0
54	MG	1A	3148	1/1	0.86	0.11	58,58,58,58	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	1a	1728	1/1	0.86	0.29	65,65,65,65	0
57	MPD	2A	3714	8/8	0.86	0.28	49,56,62,62	0
54	MG	1a	1653	1/1	0.86	0.28	70,70,70,70	0
54	MG	2B	214	1/1	0.86	0.11	76,76,76,76	0
54	MG	2B	212	1/1	0.87	0.09	97,97,97,97	0
54	MG	2A	3375	1/1	0.87	0.12	60,60,60,60	0
54	MG	2A	3082	1/1	0.87	0.16	50,50,50,50	0
54	MG	1a	1805	1/1	0.87	0.17	79,79,79,79	0
54	MG	1a	1806	1/1	0.87	0.18	70,70,70,70	0
54	MG	2A	3404	1/1	0.87	0.15	60,60,60,60	0
54	MG	2A	3088	1/1	0.87	0.21	77,77,77,77	0
54	MG	1A	3822	1/1	0.87	0.11	45,45,45,45	0
54	MG	1a	1810	1/1	0.87	0.21	71,71,71,71	0
54	MG	1a	1811	1/1	0.87	0.16	63,63,63,63	0
54	MG	1a	1812	1/1	0.87	0.19	77,77,77,77	0
54	MG	2A	3423	1/1	0.87	0.15	69,69,69,69	0
54	MG	15	108	1/1	0.87	0.18	76,76,76,76	0
54	MG	1A	3982	1/1	0.87	0.15	68,68,68,68	0
54	MG	1a	1705	1/1	0.87	0.22	75,75,75,75	0
54	MG	1a	1819	1/1	0.87	0.23	68,68,68,68	0
54	MG	2A	3441	1/1	0.87	0.13	68,68,68,68	0
54	MG	1A	3180	1/1	0.87	0.43	67,67,67,67	0
54	MG	2A	3446	1/1	0.87	0.18	69,69,69,69	0
54	MG	2a	3027	1/1	0.87	0.20	77,77,77,77	0
54	MG	2A	3121	1/1	0.87	0.17	70,70,70,70	0
54	MG	1a	1602	1/1	0.87	0.13	81,81,81,81	0
54	MG	2A	3131	1/1	0.87	0.14	71,71,71,71	0
54	MG	2A	3152	1/1	0.87	0.19	66,66,66,66	0
54	MG	1A	3837	1/1	0.87	0.10	54,54,54,54	0
54	MG	2A	3154	1/1	0.87	0.21	62,62,62,62	0
54	MG	2a	3039	1/1	0.87	0.20	80,80,80,80	0
54	MG	1a	1610	1/1	0.87	0.32	60,60,60,60	0
54	MG	1A	3647	1/1	0.87	0.21	69,69,69,69	0
54	MG	1a	1840	1/1	0.87	0.19	51,51,51,51	0
54	MG	1A	3408	1/1	0.87	0.27	68,68,68,68	0
54	MG	1a	1848	1/1	0.87	0.15	65,65,65,65	0
54	MG	2A	3489	1/1	0.87	0.12	83,83,83,83	0
54	MG	1A	3503	1/1	0.87	0.09	33,33,33,33	0
54	MG	1A	3652	1/1	0.87	0.12	59,59,59,59	0
54	MG	1A	3437	1/1	0.87	0.16	76,76,76,76	0
54	MG	1a	1722	1/1	0.87	0.17	64,64,64,64	0
54	MG	1A	4007	1/1	0.87	0.16	53,53,53,53	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	1A	3098	1/1	0.87	0.09	63,63,63,63	0
54	MG	1A	3525	1/1	0.87	0.15	66,66,66,66	0
54	MG	1A	3737	1/1	0.87	0.17	45,45,45,45	0
54	MG	1A	3528	1/1	0.87	0.10	51,51,51,51	0
54	MG	1A	3596	1/1	0.87	0.10	31,31,31,31	0
54	MG	1A	3155	1/1	0.87	0.14	47,47,47,47	0
54	MG	1A	3763	1/1	0.87	0.17	43,43,43,43	0
54	MG	2a	3084	1/1	0.87	0.22	69,69,69,69	0
54	MG	1A	3764	1/1	0.87	0.23	56,56,56,56	0
54	MG	1a	1656	1/1	0.87	0.33	61,61,61,61	0
54	MG	1A	3783	1/1	0.87	0.10	45,45,45,45	0
54	MG	1B	221	1/1	0.87	0.11	59,59,59,59	0
54	MG	2A	3558	1/1	0.87	0.10	78,78,78,78	0
54	MG	1A	3933	1/1	0.87	0.13	61,61,61,61	0
54	MG	1A	3066	1/1	0.87	0.19	57,57,57,57	0
54	MG	1a	1663	1/1	0.87	0.20	75,75,75,75	0
54	MG	1A	3790	1/1	0.87	0.10	30,30,30,30	0
54	MG	2A	3260	1/1	0.87	0.22	68,68,68,68	0
54	MG	1A	3792	1/1	0.87	0.11	45,45,45,45	0
54	MG	1A	3284	1/1	0.87	0.32	74,74,74,74	0
54	MG	2A	3613	1/1	0.87	0.22	81,81,81,81	0
54	MG	2A	3631	1/1	0.87	0.13	53,53,53,53	0
54	MG	1a	1779	1/1	0.87	0.16	72,72,72,72	0
54	MG	2a	3134	1/1	0.87	0.09	80,80,80,80	0
54	MG	2A	3656	1/1	0.87	0.10	78,78,78,78	0
54	MG	2A	3006	1/1	0.87	0.21	71,71,71,71	0
54	MG	1a	1780	1/1	0.87	0.20	78,78,78,78	0
54	MG	1a	1670	1/1	0.87	0.30	61,61,61,61	0
54	MG	1G	203	1/1	0.87	0.12	63,63,63,63	0
54	MG	1a	1789	1/1	0.87	0.17	83,83,83,83	0
54	MG	1A	3297	1/1	0.87	0.13	53,53,53,53	0
54	MG	2a	3175	1/1	0.87	0.09	79,79,79,79	0
54	MG	2A	3330	1/1	0.87	0.13	39,39,39,39	0
54	MG	1A	3803	1/1	0.87	0.23	69,69,69,69	0
54	MG	2e	201	1/1	0.87	0.20	75,75,75,75	0
54	MG	1A	3400	1/1	0.87	0.18	56,56,56,56	0
54	MG	1A	3810	1/1	0.87	0.16	65,65,65,65	0
54	MG	1T	204	1/1	0.87	0.18	67,67,67,67	0
54	MG	1A	3298	1/1	0.87	0.16	74,74,74,74	0
54	MG	2B	205	1/1	0.87	0.20	64,64,64,64	0
54	MG	1a	1799	1/1	0.87	0.11	73,73,73,73	0
54	MG	1a	1689	1/1	0.87	0.27	70,70,70,70	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	1A	3631	1/1	0.87	0.20	53,53,53,53	0
54	MG	2A	3031	1/1	0.88	0.14	68,68,68,68	0
54	MG	1a	1674	1/1	0.88	0.32	66,66,66,66	0
54	MG	2A	3692	1/1	0.88	0.10	89,89,89,89	0
54	MG	2A	3300	1/1	0.88	0.15	63,63,63,63	0
54	MG	2A	3307	1/1	0.88	0.12	54,54,54,54	0
54	MG	2A	3319	1/1	0.88	0.10	48,48,48,48	0
54	MG	2A	3324	1/1	0.88	0.18	65,65,65,65	0
54	MG	1a	1676	1/1	0.88	0.13	75,75,75,75	0
54	MG	2A	3041	1/1	0.88	0.13	50,50,50,50	0
54	MG	1R	205	1/1	0.88	0.19	49,49,49,49	0
54	MG	2A	3046	1/1	0.88	0.11	65,65,65,65	0
54	MG	1A	3974	1/1	0.88	0.19	59,59,59,59	0
54	MG	1a	1681	1/1	0.88	0.15	62,62,62,62	0
54	MG	1A	3430	1/1	0.88	0.15	54,54,54,54	0
54	MG	2A	3357	1/1	0.88	0.09	35,35,35,35	0
54	MG	1A	3198	1/1	0.88	0.14	61,61,61,61	0
54	MG	2A	3361	1/1	0.88	0.20	69,69,69,69	0
54	MG	2D	309	1/1	0.88	0.21	55,55,55,55	0
54	MG	2A	3367	1/1	0.88	0.14	42,42,42,42	0
54	MG	2A	3070	1/1	0.88	0.20	65,65,65,65	0
54	MG	10	103	1/1	0.88	0.13	60,60,60,60	0
54	MG	1A	3616	1/1	0.88	0.12	45,45,45,45	0
54	MG	2A	3388	1/1	0.88	0.09	71,71,71,71	0
54	MG	1A	3536	1/1	0.88	0.11	28,28,28,28	0
54	MG	2P	201	1/1	0.88	0.25	72,72,72,72	0
54	MG	1a	1808	1/1	0.88	0.28	70,70,70,70	0
54	MG	2I	101	1/1	0.88	0.09	88,88,88,88	0
54	MG	1a	1692	1/1	0.88	0.19	62,62,62,62	0
54	MG	1A	3344	1/1	0.88	0.28	51,51,51,51	0
54	MG	1A	3843	1/1	0.88	0.11	54,54,54,54	0
54	MG	1a	1703	1/1	0.88	0.38	78,78,78,78	0
54	MG	1A	3351	1/1	0.88	0.14	70,70,70,70	0
54	MG	1A	3204	1/1	0.88	0.23	64,64,64,64	0
54	MG	1A	3008	1/1	0.88	0.15	50,50,50,50	0
54	MG	1A	3859	1/1	0.88	0.17	54,54,54,54	0
54	MG	2A	3429	1/1	0.88	0.15	62,62,62,62	0
54	MG	1a	1604	1/1	0.88	0.38	78,78,78,78	0
54	MG	2a	3029	1/1	0.88	0.29	64,64,64,64	0
54	MG	2A	3431	1/1	0.88	0.12	66,66,66,66	0
54	MG	1A	3116	1/1	0.88	0.23	47,47,47,47	0
54	MG	2A	3116	1/1	0.88	0.16	76,76,76,76	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	1a	1712	1/1	0.88	0.33	80,80,80,80	0
54	MG	1a	1611	1/1	0.88	0.28	71,71,71,71	0
54	MG	1a	1834	1/1	0.88	0.10	84,84,84,84	0
54	MG	2a	3041	1/1	0.88	0.22	65,65,65,65	0
54	MG	2a	3043	1/1	0.88	0.32	70,70,70,70	0
54	MG	2A	3127	1/1	0.88	0.21	58,58,58,58	0
54	MG	1A	3392	1/1	0.88	0.10	40,40,40,40	0
54	MG	1A	4001	1/1	0.88	0.30	45,45,45,45	0
54	MG	1a	1719	1/1	0.88	0.47	75,75,75,75	0
54	MG	2a	3054	1/1	0.88	0.21	72,72,72,72	0
54	MG	1a	1843	1/1	0.88	0.21	85,85,85,85	0
54	MG	1a	1844	1/1	0.88	0.14	61,61,61,61	0
54	MG	1a	1616	1/1	0.88	0.20	80,80,80,80	0
54	MG	1A	3557	1/1	0.88	0.12	59,59,59,59	0
54	MG	2A	3474	1/1	0.88	0.16	67,67,67,67	0
54	MG	2A	3167	1/1	0.88	0.26	61,61,61,61	0
54	MG	2A	3170	1/1	0.88	0.17	62,62,62,62	0
54	MG	2A	3485	1/1	0.88	0.10	63,63,63,63	0
54	MG	1A	3756	1/1	0.88	0.24	61,61,61,61	0
54	MG	1a	1851	1/1	0.88	0.17	71,71,71,71	0
54	MG	1a	1861	1/1	0.88	0.33	73,73,73,73	0
54	MG	2A	3492	1/1	0.88	0.12	71,71,71,71	0
54	MG	2A	3182	1/1	0.88	0.18	73,73,73,73	0
54	MG	2A	3494	1/1	0.88	0.10	69,69,69,69	0
54	MG	2A	3495	1/1	0.88	0.09	65,65,65,65	0
54	MG	1A	3471	1/1	0.88	0.14	59,59,59,59	0
54	MG	1A	3570	1/1	0.88	0.09	44,44,44,44	0
54	MG	2a	3087	1/1	0.88	0.13	73,73,73,73	0
54	MG	1a	1632	1/1	0.88	0.32	79,79,79,79	0
54	MG	2a	3094	1/1	0.88	0.21	74,74,74,74	0
54	MG	1A	3896	1/1	0.88	0.15	64,64,64,64	0
54	MG	1A	3310	1/1	0.88	0.48	49,49,49,49	0
54	MG	2A	3199	1/1	0.88	0.25	71,71,71,71	0
54	MG	1A	3766	1/1	0.88	0.19	62,62,62,62	0
54	MG	1A	3911	1/1	0.88	0.23	41,41,41,41	0
54	MG	2A	3520	1/1	0.88	0.10	34,34,34,34	0
54	MG	1A	3579	1/1	0.88	0.13	64,64,64,64	0
54	MG	1a	1646	1/1	0.88	0.29	61,61,61,61	0
54	MG	1A	3260	1/1	0.88	0.13	66,66,66,66	0
54	MG	2A	3549	1/1	0.88	0.13	41,41,41,41	0
54	MG	1A	3489	1/1	0.88	0.13	64,64,64,64	0
54	MG	1A	3679	1/1	0.88	0.12	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	3121	1/1	0.88	0.10	76,76,76,76	0
54	MG	2a	3125	1/1	0.88	0.11	81,81,81,81	0
54	MG	2A	3215	1/1	0.88	0.11	58,58,58,58	0
54	MG	2a	3142	1/1	0.88	0.10	83,83,83,83	0
54	MG	1a	1759	1/1	0.88	0.18	68,68,68,68	0
54	MG	1a	1763	1/1	0.88	0.21	64,64,64,64	0
54	MG	2a	3155	1/1	0.88	0.10	72,72,72,72	0
54	MG	2A	3584	1/1	0.88	0.13	53,53,53,53	0
54	MG	2A	3588	1/1	0.88	0.09	70,70,70,70	0
54	MG	1A	3184	1/1	0.88	0.15	52,52,52,52	0
54	MG	1A	3954	1/1	0.88	0.09	30,30,30,30	0
54	MG	1l	202	1/1	0.88	0.23	79,79,79,79	0
54	MG	1A	3401	1/1	0.88	0.08	75,75,75,75	0
54	MG	2a	3177	1/1	0.88	0.24	80,80,80,80	0
54	MG	1D	311	1/1	0.88	0.21	64,64,64,64	0
54	MG	1D	315	1/1	0.88	0.16	74,74,74,74	0
54	MG	1A	3153	1/1	0.88	0.35	72,72,72,72	0
54	MG	1E	306	1/1	0.88	0.18	53,53,53,53	0
54	MG	1F	315	1/1	0.88	0.60	55,55,55,55	0
54	MG	2A	3639	1/1	0.88	0.12	37,37,37,37	0
54	MG	1A	3597	1/1	0.88	0.20	55,55,55,55	0
54	MG	1A	3128	1/1	0.88	0.22	66,66,66,66	0
57	MPD	1a	1882	8/8	0.88	0.11	54,70,76,81	0
54	MG	2A	3286	1/1	0.88	0.10	42,42,42,42	0
54	MG	1A	3191	1/1	0.88	0.33	65,65,65,65	0
54	MG	1O	201	1/1	0.88	0.14	63,63,63,63	0
54	MG	1A	3833	1/1	0.89	0.08	20,20,20,20	0
54	MG	1A	3642	1/1	0.89	0.21	68,68,68,68	0
54	MG	1O	102	1/1	0.89	0.18	47,47,47,47	0
54	MG	2A	3174	1/1	0.89	0.13	63,63,63,63	0
54	MG	2A	3178	1/1	0.89	0.18	75,75,75,75	0
54	MG	1e	202	1/1	0.89	0.28	63,63,63,63	0
54	MG	1f	201	1/1	0.89	0.25	74,74,74,74	0
54	MG	1f	202	1/1	0.89	0.11	49,49,49,49	0
54	MG	2A	3184	1/1	0.89	0.18	66,66,66,66	0
54	MG	1A	3168	1/1	0.89	0.26	63,63,63,63	0
54	MG	1g	203	1/1	0.89	0.18	69,69,69,69	0
54	MG	1a	1783	1/1	0.89	0.24	77,77,77,77	0
54	MG	1A	3838	1/1	0.89	0.16	68,68,68,68	0
54	MG	1A	3839	1/1	0.89	0.12	59,59,59,59	0
54	MG	1A	3586	1/1	0.89	0.18	61,61,61,61	0
54	MG	1A	3332	1/1	0.89	0.14	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	1o	101	1/1	0.89	0.25	58,58,58,58	0
54	MG	17	106	1/1	0.89	0.19	61,61,61,61	0
54	MG	2A	3479	1/1	0.89	0.09	71,71,71,71	0
54	MG	1A	3243	1/1	0.89	0.09	47,47,47,47	0
54	MG	2A	3484	1/1	0.89	0.24	60,60,60,60	0
54	MG	1A	3848	1/1	0.89	0.13	50,50,50,50	0
54	MG	2A	3005	1/1	0.89	0.15	65,65,65,65	0
54	MG	1A	3137	1/1	0.89	0.10	53,53,53,53	0
54	MG	1A	3302	1/1	0.89	0.16	42,42,42,42	0
54	MG	1A	3406	1/1	0.89	0.14	47,47,47,47	0
54	MG	2a	3037	1/1	0.89	0.24	73,73,73,73	0
54	MG	2A	3223	1/1	0.89	0.36	56,56,56,56	0
54	MG	2A	3226	1/1	0.89	0.37	65,65,65,65	0
54	MG	1A	3210	1/1	0.89	0.38	77,77,77,77	0
54	MG	2A	3496	1/1	0.89	0.25	66,66,66,66	0
54	MG	2a	3046	1/1	0.89	0.36	75,75,75,75	0
54	MG	1A	3660	1/1	0.89	0.17	70,70,70,70	0
54	MG	2A	3027	1/1	0.89	0.14	59,59,59,59	0
54	MG	2A	3500	1/1	0.89	0.15	74,74,74,74	0
54	MG	2A	3239	1/1	0.89	0.29	61,61,61,61	0
54	MG	2A	3505	1/1	0.89	0.15	69,69,69,69	0
54	MG	1A	3215	1/1	0.89	0.18	78,78,78,78	0
54	MG	1A	3873	1/1	0.89	0.10	48,48,48,48	0
54	MG	2A	3511	1/1	0.89	0.13	73,73,73,73	0
54	MG	1A	3674	1/1	0.89	0.16	69,69,69,69	0
54	MG	1a	1709	1/1	0.89	0.38	75,75,75,75	0
54	MG	1A	3603	1/1	0.89	0.15	67,67,67,67	0
54	MG	2a	3062	1/1	0.89	0.15	75,75,75,75	0
54	MG	1a	1621	1/1	0.89	0.21	65,65,65,65	0
54	MG	1a	1624	1/1	0.89	0.23	60,60,60,60	0
54	MG	1A	3890	1/1	0.89	0.10	68,68,68,68	0
54	MG	2A	3543	1/1	0.89	0.15	80,80,80,80	0
54	MG	1A	3894	1/1	0.89	0.13	53,53,53,53	0
54	MG	2a	3076	1/1	0.89	0.31	74,74,74,74	0
54	MG	1A	3607	1/1	0.89	0.14	52,52,52,52	0
54	MG	1A	4025	1/1	0.89	0.22	82,82,82,82	0
54	MG	1a	1825	1/1	0.89	0.15	72,72,72,72	0
54	MG	1A	3677	1/1	0.89	0.11	29,29,29,29	0
54	MG	1A	3435	1/1	0.89	0.24	54,54,54,54	0
54	MG	2A	3298	1/1	0.89	0.24	64,64,64,64	0
54	MG	1A	3903	1/1	0.89	0.11	59,59,59,59	0
54	MG	1B	215	1/1	0.89	0.11	50,50,50,50	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	1A	3680	1/1	0.89	0.32	37,37,37,37	0
54	MG	2a	3098	1/1	0.89	0.12	66,66,66,66	0
54	MG	1A	3313	1/1	0.89	0.12	62,62,62,62	0
54	MG	1A	3920	1/1	0.89	0.09	45,45,45,45	0
54	MG	2A	3091	1/1	0.89	0.19	58,58,58,58	0
54	MG	2A	3604	1/1	0.89	0.15	41,41,41,41	0
54	MG	2A	3605	1/1	0.89	0.17	48,48,48,48	0
54	MG	2A	3098	1/1	0.89	0.25	62,62,62,62	0
54	MG	1a	1732	1/1	0.89	0.14	61,61,61,61	0
54	MG	2a	3115	1/1	0.89	0.15	71,71,71,71	0
54	MG	2A	3342	1/1	0.89	0.36	71,71,71,71	0
54	MG	1A	3687	1/1	0.89	0.14	60,60,60,60	0
54	MG	1A	3793	1/1	0.89	0.14	43,43,43,43	0
54	MG	1A	3565	1/1	0.89	0.13	47,47,47,47	0
54	MG	2A	3641	1/1	0.89	0.12	49,49,49,49	0
54	MG	2A	3644	1/1	0.89	0.11	79,79,79,79	0
54	MG	1A	3279	1/1	0.89	0.18	65,65,65,65	0
54	MG	2a	3140	1/1	0.89	0.15	77,77,77,77	0
54	MG	1A	3942	1/1	0.89	0.17	63,63,63,63	0
54	MG	2A	3114	1/1	0.89	0.11	54,54,54,54	0
54	MG	2A	3677	1/1	0.89	0.08	57,57,57,57	0
54	MG	2a	3149	1/1	0.89	0.11	54,54,54,54	0
54	MG	1a	1753	1/1	0.89	0.08	53,53,53,53	0
54	MG	2A	3682	1/1	0.89	0.11	64,64,64,64	0
54	MG	2a	3161	1/1	0.89	0.09	68,68,68,68	0
54	MG	2A	3118	1/1	0.89	0.24	47,47,47,47	0
54	MG	1A	3625	1/1	0.89	0.32	39,39,39,39	0
54	MG	1a	1866	1/1	0.89	0.11	57,57,57,57	0
54	MG	2A	3378	1/1	0.89	0.11	65,65,65,65	0
54	MG	2A	3382	1/1	0.89	0.15	73,73,73,73	0
54	MG	1A	3805	1/1	0.89	0.21	63,63,63,63	0
54	MG	1F	317	1/1	0.89	0.16	52,52,52,52	0
54	MG	1a	1760	1/1	0.89	0.16	81,81,81,81	0
54	MG	2A	3402	1/1	0.89	0.14	71,71,71,71	0
54	MG	2A	3135	1/1	0.89	0.17	68,68,68,68	0
54	MG	2A	3138	1/1	0.89	0.11	49,49,49,49	0
54	MG	1A	3697	1/1	0.89	0.10	78,78,78,78	0
54	MG	2t	201	1/1	0.89	0.20	58,58,58,58	0
54	MG	1A	3961	1/1	0.89	0.11	57,57,57,57	0
54	MG	1A	3217	1/1	0.89	0.18	46,46,46,46	0
54	MG	1A	3039	1/1	0.89	0.35	69,69,69,69	0
54	MG	2A	3419	1/1	0.89	0.14	64,64,64,64	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MPD	2A	3715	8/8	0.89	0.17	68,71,77,78	0
54	MG	1A	3639	1/1	0.89	0.12	66,66,66,66	0
54	MG	1A	3708	1/1	0.89	0.11	53,53,53,53	0
54	MG	2A	3352	1/1	0.90	0.17	57,57,57,57	0
54	MG	1A	3851	1/1	0.90	0.13	53,53,53,53	0
54	MG	1A	3448	1/1	0.90	0.13	44,44,44,44	0
54	MG	1A	3527	1/1	0.90	0.14	58,58,58,58	0
54	MG	1a	1823	1/1	0.90	0.24	74,74,74,74	0
54	MG	2A	3362	1/1	0.90	0.09	69,69,69,69	0
54	MG	1A	3858	1/1	0.90	0.13	42,42,42,42	0
54	MG	2A	3099	1/1	0.90	0.24	55,55,55,55	0
54	MG	2A	3372	1/1	0.90	0.10	57,57,57,57	0
54	MG	18	102	1/1	0.90	0.25	47,47,47,47	0
54	MG	1A	3289	1/1	0.90	0.14	57,57,57,57	0
54	MG	1a	1830	1/1	0.90	0.12	75,75,75,75	0
54	MG	2B	211	1/1	0.90	0.16	74,74,74,74	0
54	MG	1A	3635	1/1	0.90	0.10	24,24,24,24	0
54	MG	2A	3110	1/1	0.90	0.29	67,67,67,67	0
54	MG	1A	3991	1/1	0.90	0.15	46,46,46,46	0
54	MG	2A	3396	1/1	0.90	0.24	73,73,73,73	0
54	MG	2A	3397	1/1	0.90	0.13	51,51,51,51	0
54	MG	1A	3638	1/1	0.90	0.12	42,42,42,42	0
54	MG	2A	3399	1/1	0.90	0.18	67,67,67,67	0
54	MG	2A	3401	1/1	0.90	0.26	69,69,69,69	0
54	MG	1a	1713	1/1	0.90	0.23	72,72,72,72	0
54	MG	1A	3995	1/1	0.90	0.08	89,89,89,89	0
54	MG	1a	1605	1/1	0.90	0.16	63,63,63,63	0
54	MG	1A	3369	1/1	0.90	0.11	47,47,47,47	0
54	MG	1A	3767	1/1	0.90	0.13	44,44,44,44	0
54	MG	2A	3413	1/1	0.90	0.22	86,86,86,86	0
54	MG	25	101	1/1	0.90	0.59	49,49,49,49	0
54	MG	28	102	1/1	0.90	0.25	68,68,68,68	0
54	MG	1A	3773	1/1	0.90	0.17	49,49,49,49	0
54	MG	2a	3003	1/1	0.90	0.42	77,77,77,77	0
54	MG	1A	3881	1/1	0.90	0.18	31,31,31,31	0
54	MG	2A	3128	1/1	0.90	0.18	77,77,77,77	0
54	MG	1A	3190	1/1	0.90	0.12	61,61,61,61	0
54	MG	1A	3889	1/1	0.90	0.08	25,25,25,25	0
54	MG	1A	4014	1/1	0.90	0.13	38,38,38,38	0
54	MG	2A	3144	1/1	0.90	0.23	58,58,58,58	0
54	MG	2A	3148	1/1	0.90	0.28	57,57,57,57	0
54	MG	2A	3433	1/1	0.90	0.16	64,64,64,64	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	1A	3200	1/1	0.90	0.27	53,53,53,53	0
54	MG	1A	3892	1/1	0.90	0.14	53,53,53,53	0
54	MG	1a	1628	1/1	0.90	0.34	70,70,70,70	0
54	MG	2A	3443	1/1	0.90	0.23	60,60,60,60	0
54	MG	1A	3539	1/1	0.90	0.10	26,26,26,26	0
54	MG	1a	1740	1/1	0.90	0.19	58,58,58,58	0
54	MG	1A	3299	1/1	0.90	0.20	50,50,50,50	0
54	MG	2A	3164	1/1	0.90	0.29	56,56,56,56	0
54	MG	1A	3649	1/1	0.90	0.22	59,59,59,59	0
54	MG	2a	3040	1/1	0.90	0.11	84,84,84,84	0
54	MG	1A	3702	1/1	0.90	0.09	71,71,71,71	0
54	MG	2a	3042	1/1	0.90	0.13	66,66,66,66	0
54	MG	2A	3458	1/1	0.90	0.20	75,75,75,75	0
54	MG	2a	3044	1/1	0.90	0.29	80,80,80,80	0
54	MG	2A	3460	1/1	0.90	0.24	74,74,74,74	0
54	MG	2A	3461	1/1	0.90	0.09	71,71,71,71	0
54	MG	1a	1876	1/1	0.90	0.14	76,76,76,76	0
54	MG	1A	4027	1/1	0.90	0.15	69,69,69,69	0
54	MG	1A	3798	1/1	0.90	0.20	63,63,63,63	0
54	MG	1A	3283	1/1	0.90	0.12	41,41,41,41	0
54	MG	1A	3478	1/1	0.90	0.13	44,44,44,44	0
54	MG	1B	220	1/1	0.90	0.25	78,78,78,78	0
54	MG	1A	3912	1/1	0.90	0.09	20,20,20,20	0
54	MG	1a	1651	1/1	0.90	0.29	65,65,65,65	0
54	MG	1a	1761	1/1	0.90	0.27	51,51,51,51	0
54	MG	1A	3916	1/1	0.90	0.10	35,35,35,35	0
54	MG	2A	3189	1/1	0.90	0.32	72,72,72,72	0
54	MG	1a	1764	1/1	0.90	0.28	77,77,77,77	0
54	MG	1A	3709	1/1	0.90	0.29	44,44,44,44	0
54	MG	1A	3711	1/1	0.90	0.11	55,55,55,55	0
54	MG	1A	3928	1/1	0.90	0.08	73,73,73,73	0
54	MG	1a	1772	1/1	0.90	0.17	62,62,62,62	0
54	MG	1n	102	1/1	0.90	0.29	71,71,71,71	0
54	MG	1A	3346	1/1	0.90	0.48	76,76,76,76	0
54	MG	1A	3716	1/1	0.90	0.27	45,45,45,45	0
54	MG	1A	3815	1/1	0.90	0.08	59,59,59,59	0
54	MG	1y	201	1/1	0.90	0.08	72,72,72,72	0
54	MG	2A	3210	1/1	0.90	0.13	59,59,59,59	0
54	MG	2A	3504	1/1	0.90	0.15	59,59,59,59	0
54	MG	1A	3440	1/1	0.90	0.09	28,28,28,28	0
54	MG	2a	3088	1/1	0.90	0.15	76,76,76,76	0
54	MG	1A	3818	1/1	0.90	0.14	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	3221	1/1	0.90	0.25	48,48,48,48	0
54	MG	1A	3441	1/1	0.90	0.11	28,28,28,28	0
54	MG	1F	318	1/1	0.90	0.12	67,67,67,67	0
54	MG	1a	1785	1/1	0.90	0.18	52,52,52,52	0
54	MG	1a	1669	1/1	0.90	0.41	68,68,68,68	0
54	MG	2A	3229	1/1	0.90	0.17	63,63,63,63	0
54	MG	2A	3527	1/1	0.90	0.08	65,65,65,65	0
54	MG	2A	3017	1/1	0.90	0.17	60,60,60,60	0
54	MG	2A	3023	1/1	0.90	0.17	62,62,62,62	0
54	MG	1G	201	1/1	0.90	0.07	79,79,79,79	0
54	MG	2A	3248	1/1	0.90	0.30	48,48,48,48	0
54	MG	1A	3832	1/1	0.90	0.15	66,66,66,66	0
54	MG	1A	3558	1/1	0.90	0.22	58,58,58,58	0
54	MG	2A	3028	1/1	0.90	0.14	44,44,44,44	0
54	MG	1A	3729	1/1	0.90	0.27	41,41,41,41	0
54	MG	1A	3663	1/1	0.90	0.08	49,49,49,49	0
54	MG	2A	3560	1/1	0.90	0.12	54,54,54,54	0
54	MG	1P	203	1/1	0.90	0.24	40,40,40,40	0
54	MG	2A	3037	1/1	0.90	0.25	74,74,74,74	0
54	MG	2A	3279	1/1	0.90	0.12	73,73,73,73	0
54	MG	1P	206	1/1	0.90	0.14	71,71,71,71	0
54	MG	1A	3060	1/1	0.90	0.11	49,49,49,49	0
54	MG	2A	3044	1/1	0.90	0.14	53,53,53,53	0
54	MG	2a	3153	1/1	0.90	0.10	69,69,69,69	0
54	MG	2A	3599	1/1	0.90	0.14	39,39,39,39	0
54	MG	2a	3156	1/1	0.90	0.08	84,84,84,84	0
54	MG	2a	3157	1/1	0.90	0.21	69,69,69,69	0
54	MG	1A	3362	1/1	0.90	0.12	38,38,38,38	0
54	MG	1a	1683	1/1	0.90	0.22	67,67,67,67	0
54	MG	1A	3973	1/1	0.90	0.07	61,61,61,61	0
54	MG	2A	3606	1/1	0.90	0.12	60,60,60,60	0
54	MG	1A	3617	1/1	0.90	0.09	62,62,62,62	0
54	MG	2A	3056	1/1	0.90	0.23	60,60,60,60	0
54	MG	2A	3302	1/1	0.90	0.16	68,68,68,68	0
54	MG	2A	3304	1/1	0.90	0.32	69,69,69,69	0
54	MG	1a	1688	1/1	0.90	0.14	64,64,64,64	0
54	MG	2A	3637	1/1	0.90	0.09	82,82,82,82	0
54	MG	2a	3181	1/1	0.90	0.10	96,96,96,96	0
54	MG	2A	3062	1/1	0.90	0.15	60,60,60,60	0
54	MG	2A	3065	1/1	0.90	0.25	65,65,65,65	0
54	MG	1T	205	1/1	0.90	0.14	73,73,73,73	0
54	MG	1A	3740	1/1	0.90	0.13	70,70,70,70	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	1A	3747	1/1	0.90	0.20	45,45,45,45	0
54	MG	2A	3335	1/1	0.90	0.08	39,39,39,39	0
54	MG	2A	3336	1/1	0.90	0.21	72,72,72,72	0
54	MG	2A	3077	1/1	0.90	0.10	59,59,59,59	0
54	MG	1A	3447	1/1	0.90	0.10	31,31,31,31	0
54	MG	2A	3684	1/1	0.90	0.10	67,67,67,67	0
54	MG	1l	104	1/1	0.90	0.13	55,55,55,55	0
54	MG	1a	1700	1/1	0.90	0.29	78,78,78,78	0
54	MG	1A	3311	1/1	0.91	0.15	59,59,59,59	0
54	MG	1A	3673	1/1	0.91	0.06	29,29,29,29	0
54	MG	1A	3442	1/1	0.91	0.14	27,27,27,27	0
54	MG	2A	3354	1/1	0.91	0.10	71,71,71,71	0
54	MG	1A	3602	1/1	0.91	0.24	58,58,58,58	0
54	MG	2A	3356	1/1	0.91	0.15	64,64,64,64	0
54	MG	1A	3758	1/1	0.91	0.16	63,63,63,63	0
54	MG	1a	1820	1/1	0.91	0.16	71,71,71,71	0
54	MG	2A	3693	1/1	0.91	0.13	80,80,80,80	0
54	MG	2A	3695	1/1	0.91	0.09	74,74,74,74	0
54	MG	2A	3704	1/1	0.91	0.08	49,49,49,49	0
54	MG	1a	1697	1/1	0.91	0.17	67,67,67,67	0
54	MG	1W	203	1/1	0.91	0.09	57,57,57,57	0
54	MG	1A	3053	1/1	0.91	0.24	44,44,44,44	0
54	MG	2A	3368	1/1	0.91	0.13	64,64,64,64	0
54	MG	1a	1701	1/1	0.91	0.22	64,64,64,64	0
54	MG	1A	3860	1/1	0.91	0.10	66,66,66,66	0
54	MG	2A	3374	1/1	0.91	0.14	46,46,46,46	0
54	MG	1A	3125	1/1	0.91	0.23	55,55,55,55	0
54	MG	2A	3111	1/1	0.91	0.15	45,45,45,45	0
54	MG	1A	3987	1/1	0.91	0.11	50,50,50,50	0
54	MG	1a	1833	1/1	0.91	0.20	77,77,77,77	0
54	MG	2A	3386	1/1	0.91	0.09	57,57,57,57	0
54	MG	1A	3678	1/1	0.91	0.12	48,48,48,48	0
54	MG	15	105	1/1	0.91	0.22	36,36,36,36	0
54	MG	2B	216	1/1	0.91	0.07	84,84,84,84	0
54	MG	2B	217	1/1	0.91	0.06	75,75,75,75	0
54	MG	1a	1837	1/1	0.91	0.11	82,82,82,82	0
54	MG	1a	1838	1/1	0.91	0.19	72,72,72,72	0
54	MG	2E	303	1/1	0.91	0.10	32,32,32,32	0
54	MG	1a	1839	1/1	0.91	0.18	52,52,52,52	0
54	MG	1A	3990	1/1	0.91	0.07	22,22,22,22	0
54	MG	1A	3765	1/1	0.91	0.12	60,60,60,60	0
54	MG	1A	3192	1/1	0.91	0.09	67,67,67,67	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	1a	1711	1/1	0.91	0.35	71,71,71,71	0
54	MG	1a	1847	1/1	0.91	0.31	57,57,57,57	0
54	MG	17	107	1/1	0.91	0.12	59,59,59,59	0
54	MG	2T	201	1/1	0.91	0.26	72,72,72,72	0
54	MG	2T	203	1/1	0.91	0.16	61,61,61,61	0
54	MG	1A	3994	1/1	0.91	0.25	43,43,43,43	0
54	MG	19	101	1/1	0.91	0.24	57,57,57,57	0
54	MG	1A	3386	1/1	0.91	0.10	42,42,42,42	0
54	MG	1a	1858	1/1	0.91	0.13	57,57,57,57	0
54	MG	2a	3001	1/1	0.91	0.12	46,46,46,46	0
54	MG	1A	3876	1/1	0.91	0.12	46,46,46,46	0
54	MG	1A	3681	1/1	0.91	0.16	71,71,71,71	0
54	MG	1A	3883	1/1	0.91	0.09	60,60,60,60	0
54	MG	1A	3774	1/1	0.91	0.14	54,54,54,54	0
54	MG	1A	3391	1/1	0.91	0.19	75,75,75,75	0
54	MG	1a	1607	1/1	0.91	0.08	73,73,73,73	0
54	MG	2A	3169	1/1	0.91	0.08	51,51,51,51	0
54	MG	1A	3285	1/1	0.91	0.18	66,66,66,66	0
54	MG	1A	4011	1/1	0.91	0.21	50,50,50,50	0
54	MG	2a	3023	1/1	0.91	0.16	74,74,74,74	0
54	MG	2A	3173	1/1	0.91	0.28	62,62,62,62	0
54	MG	1A	3620	1/1	0.91	0.07	39,39,39,39	0
54	MG	1a	1613	1/1	0.91	0.17	30,30,30,30	0
54	MG	1a	1730	1/1	0.91	0.24	71,71,71,71	0
54	MG	1A	3329	1/1	0.91	0.06	40,40,40,40	0
54	MG	1A	3195	1/1	0.91	0.25	47,47,47,47	0
54	MG	2A	3183	1/1	0.91	0.20	60,60,60,60	0
54	MG	1b	301	1/1	0.91	0.13	84,84,84,84	0
54	MG	2a	3036	1/1	0.91	0.24	67,67,67,67	0
54	MG	2A	3456	1/1	0.91	0.12	74,74,74,74	0
54	MG	2a	3038	1/1	0.91	0.31	67,67,67,67	0
54	MG	1a	1741	1/1	0.91	0.12	77,77,77,77	0
54	MG	1a	1742	1/1	0.91	0.21	65,65,65,65	0
54	MG	1a	1743	1/1	0.91	0.11	63,63,63,63	0
54	MG	1A	4022	1/1	0.91	0.21	66,66,66,66	0
54	MG	1a	1745	1/1	0.91	0.11	68,68,68,68	0
54	MG	2A	3468	1/1	0.91	0.22	65,65,65,65	0
54	MG	1A	3469	1/1	0.91	0.12	64,64,64,64	0
54	MG	1A	3034	1/1	0.91	0.09	52,52,52,52	0
54	MG	1A	3254	1/1	0.91	0.09	72,72,72,72	0
54	MG	1A	3800	1/1	0.91	0.12	63,63,63,63	0
54	MG	1a	1629	1/1	0.91	0.29	72,72,72,72	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	2A	3481	1/1	0.91	0.10	60,60,60,60	0
54	MG	1A	3337	1/1	0.91	0.40	68,68,68,68	0
54	MG	2A	3483	1/1	0.91	0.09	61,61,61,61	0
54	MG	1B	202	1/1	0.91	0.19	77,77,77,77	0
54	MG	2A	3207	1/1	0.91	0.33	65,65,65,65	0
54	MG	1A	3568	1/1	0.91	0.17	48,48,48,48	0
54	MG	1B	205	1/1	0.91	0.10	53,53,53,53	0
54	MG	1B	206	1/1	0.91	0.22	67,67,67,67	0
54	MG	1B	208	1/1	0.91	0.09	55,55,55,55	0
54	MG	2A	3216	1/1	0.91	0.20	71,71,71,71	0
54	MG	1u	101	1/1	0.91	0.13	76,76,76,76	0
54	MG	2A	3220	1/1	0.91	0.19	60,60,60,60	0
54	MG	2a	3068	1/1	0.91	0.33	68,68,68,68	0
54	MG	1B	209	1/1	0.91	0.13	61,61,61,61	0
54	MG	1A	3403	1/1	0.91	0.07	37,37,37,37	0
54	MG	2A	3224	1/1	0.91	0.13	74,74,74,74	0
54	MG	1B	211	1/1	0.91	0.09	64,64,64,64	0
54	MG	2a	3079	1/1	0.91	0.35	59,59,59,59	0
54	MG	1B	214	1/1	0.91	0.09	69,69,69,69	0
54	MG	2a	3082	1/1	0.91	0.17	70,70,70,70	0
54	MG	1A	3645	1/1	0.91	0.09	40,40,40,40	0
54	MG	1A	3340	1/1	0.91	0.08	48,48,48,48	0
54	MG	1A	3577	1/1	0.91	0.10	55,55,55,55	0
54	MG	2A	3236	1/1	0.91	0.09	64,64,64,64	0
54	MG	1A	3257	1/1	0.91	0.31	45,45,45,45	0
54	MG	1A	3718	1/1	0.91	0.20	63,63,63,63	0
54	MG	2A	3241	1/1	0.91	0.17	70,70,70,70	0
54	MG	1A	3110	1/1	0.91	0.10	70,70,70,70	0
54	MG	2A	3518	1/1	0.91	0.14	67,67,67,67	0
54	MG	2A	3253	1/1	0.91	0.24	50,50,50,50	0
54	MG	2a	3100	1/1	0.91	0.13	83,83,83,83	0
54	MG	1A	3827	1/1	0.91	0.13	73,73,73,73	0
54	MG	2A	3255	1/1	0.91	0.29	61,61,61,61	0
54	MG	1B	228	1/1	0.91	0.19	71,71,71,71	0
54	MG	2A	3534	1/1	0.91	0.19	58,58,58,58	0
54	MG	2a	3109	1/1	0.91	0.29	75,75,75,75	0
54	MG	2A	3536	1/1	0.91	0.11	60,60,60,60	0
54	MG	1A	3943	1/1	0.91	0.09	51,51,51,51	0
54	MG	2a	3114	1/1	0.91	0.20	75,75,75,75	0
54	MG	2A	3546	1/1	0.91	0.09	73,73,73,73	0
54	MG	2A	3261	1/1	0.91	0.36	74,74,74,74	0
54	MG	1D	314	1/1	0.91	0.08	63,63,63,63	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	1A	3201	1/1	0.91	0.29	62,62,62,62	0
54	MG	1A	3517	1/1	0.91	0.14	35,35,35,35	0
54	MG	1E	304	1/1	0.91	0.10	27,27,27,27	0
54	MG	2a	3123	1/1	0.91	0.11	79,79,79,79	0
54	MG	2A	3040	1/1	0.91	0.24	61,61,61,61	0
54	MG	1A	3955	1/1	0.91	0.10	62,62,62,62	0
54	MG	2A	3562	1/1	0.91	0.13	74,74,74,74	0
54	MG	2A	3563	1/1	0.91	0.09	52,52,52,52	0
54	MG	1F	314	1/1	0.91	0.38	51,51,51,51	0
54	MG	2A	3577	1/1	0.91	0.17	74,74,74,74	0
54	MG	1A	3523	1/1	0.91	0.11	42,42,42,42	0
54	MG	2A	3045	1/1	0.91	0.14	67,67,67,67	0
54	MG	1a	1797	1/1	0.91	0.26	68,68,68,68	0
54	MG	2A	3296	1/1	0.91	0.15	62,62,62,62	0
54	MG	2A	3047	1/1	0.91	0.12	68,68,68,68	0
54	MG	1A	3960	1/1	0.91	0.09	76,76,76,76	0
54	MG	1A	3133	1/1	0.91	0.24	37,37,37,37	0
54	MG	2A	3602	1/1	0.91	0.23	64,64,64,64	0
54	MG	1a	1800	1/1	0.91	0.23	66,66,66,66	0
54	MG	1a	1678	1/1	0.91	0.26	54,54,54,54	0
54	MG	1A	3962	1/1	0.91	0.13	65,65,65,65	0
54	MG	2A	3317	1/1	0.91	0.12	59,59,59,59	0
54	MG	2A	3318	1/1	0.91	0.14	42,42,42,42	0
54	MG	1a	1804	1/1	0.91	0.11	69,69,69,69	0
54	MG	2A	3618	1/1	0.91	0.12	64,64,64,64	0
54	MG	1A	3595	1/1	0.91	0.15	66,66,66,66	0
54	MG	1A	3353	1/1	0.91	0.11	57,57,57,57	0
54	MG	2A	3331	1/1	0.91	0.16	76,76,76,76	0
54	MG	2A	3072	1/1	0.91	0.16	62,62,62,62	0
54	MG	1a	1807	1/1	0.91	0.08	73,73,73,73	0
54	MG	1A	3113	1/1	0.91	0.13	52,52,52,52	0
56	ZIT	2A	3713	52/52	0.91	0.19	43,67,78,85	0
54	MG	1A	3842	1/1	0.91	0.12	53,53,53,53	0
54	MG	2A	3658	1/1	0.91	0.10	52,52,52,52	0
54	MG	2A	3666	1/1	0.91	0.12	44,44,44,44	0
54	MG	2A	3668	1/1	0.91	0.16	69,69,69,69	0
54	MG	2A	3670	1/1	0.91	0.20	73,73,73,73	0
54	MG	1A	3739	1/1	0.91	0.17	46,46,46,46	0
54	MG	1A	3665	1/1	0.91	0.07	42,42,42,42	0
54	MG	1A	3753	1/1	0.92	0.11	58,58,58,58	0
54	MG	2A	3676	1/1	0.92	0.17	70,70,70,70	0
54	MG	1A	3643	1/1	0.92	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	2A	3107	1/1	0.92	0.12	62,62,62,62	0
54	MG	1A	3266	1/1	0.92	0.36	71,71,71,71	0
54	MG	2A	3365	1/1	0.92	0.08	65,65,65,65	0
54	MG	1A	3270	1/1	0.92	0.16	63,63,63,63	0
54	MG	1A	3161	1/1	0.92	0.27	64,64,64,64	0
54	MG	1A	3277	1/1	0.92	0.26	35,35,35,35	0
54	MG	1A	3927	1/1	0.92	0.09	47,47,47,47	0
54	MG	1A	3545	1/1	0.92	0.13	64,64,64,64	0
54	MG	1F	310	1/1	0.92	0.23	59,59,59,59	0
54	MG	2A	3699	1/1	0.92	0.08	49,49,49,49	0
54	MG	2A	3701	1/1	0.92	0.10	59,59,59,59	0
54	MG	1A	3930	1/1	0.92	0.13	48,48,48,48	0
54	MG	2A	3706	1/1	0.92	0.11	40,40,40,40	0
54	MG	1a	1832	1/1	0.92	0.11	68,68,68,68	0
54	MG	2A	3379	1/1	0.92	0.19	78,78,78,78	0
54	MG	2A	3710	1/1	0.92	0.24	64,64,64,64	0
54	MG	1A	3550	1/1	0.92	0.40	37,37,37,37	0
54	MG	1A	3199	1/1	0.92	0.31	51,51,51,51	0
54	MG	2A	3125	1/1	0.92	0.19	51,51,51,51	0
54	MG	1A	3552	1/1	0.92	0.19	63,63,63,63	0
54	MG	2A	3393	1/1	0.92	0.12	56,56,56,56	0
54	MG	2A	3394	1/1	0.92	0.09	51,51,51,51	0
54	MG	1A	3281	1/1	0.92	0.05	78,78,78,78	0
54	MG	2A	3129	1/1	0.92	0.36	63,63,63,63	0
54	MG	2B	210	1/1	0.92	0.11	71,71,71,71	0
54	MG	1G	202	1/1	0.92	0.07	69,69,69,69	0
54	MG	2A	3133	1/1	0.92	0.20	62,62,62,62	0
54	MG	1A	3780	1/1	0.92	0.19	61,61,61,61	0
54	MG	1A	3134	1/1	0.92	0.06	57,57,57,57	0
54	MG	2A	3140	1/1	0.92	0.33	61,61,61,61	0
54	MG	2A	3405	1/1	0.92	0.24	57,57,57,57	0
54	MG	2D	304	1/1	0.92	0.34	43,43,43,43	0
54	MG	1N	201	1/1	0.92	0.20	49,49,49,49	0
54	MG	2A	3407	1/1	0.92	0.12	50,50,50,50	0
54	MG	2E	301	1/1	0.92	0.22	49,49,49,49	0
54	MG	1A	3046	1/1	0.92	0.17	33,33,33,33	0
54	MG	1A	3173	1/1	0.92	0.14	52,52,52,52	0
54	MG	2A	3411	1/1	0.92	0.10	40,40,40,40	0
54	MG	1A	3791	1/1	0.92	0.15	48,48,48,48	0
54	MG	1A	3959	1/1	0.92	0.10	66,66,66,66	0
54	MG	2A	3158	1/1	0.92	0.14	46,46,46,46	0
54	MG	2A	3416	1/1	0.92	0.28	74,74,74,74	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	1A	3175	1/1	0.92	0.14	63,63,63,63	0
54	MG	2R	201	1/1	0.92	0.12	53,53,53,53	0
54	MG	1A	3666	1/1	0.92	0.13	54,54,54,54	0
54	MG	1A	3178	1/1	0.92	0.17	42,42,42,42	0
54	MG	2Y	201	1/1	0.92	0.20	69,69,69,69	0
54	MG	1A	3670	1/1	0.92	0.40	55,55,55,55	0
54	MG	1A	3569	1/1	0.92	0.08	34,34,34,34	0
54	MG	1A	3965	1/1	0.92	0.14	57,57,57,57	0
54	MG	1Z	301	1/1	0.92	0.12	68,68,68,68	0
54	MG	2A	3437	1/1	0.92	0.10	56,56,56,56	0
54	MG	1A	3967	1/1	0.92	0.11	76,76,76,76	0
54	MG	1a	1868	1/1	0.92	0.24	68,68,68,68	0
54	MG	2a	3006	1/1	0.92	0.08	79,79,79,79	0
54	MG	2a	3007	1/1	0.92	0.47	72,72,72,72	0
54	MG	1A	3290	1/1	0.92	0.13	52,52,52,52	0
54	MG	2A	3442	1/1	0.92	0.10	58,58,58,58	0
54	MG	10	104	1/1	0.92	0.08	58,58,58,58	0
54	MG	1A	3291	1/1	0.92	0.14	43,43,43,43	0
54	MG	1A	3216	1/1	0.92	0.18	62,62,62,62	0
54	MG	1A	3370	1/1	0.92	0.10	51,51,51,51	0
54	MG	15	103	1/1	0.92	0.34	46,46,46,46	0
54	MG	1A	3582	1/1	0.92	0.18	62,62,62,62	0
54	MG	2a	3024	1/1	0.92	0.18	66,66,66,66	0
54	MG	2a	3025	1/1	0.92	0.26	67,67,67,67	0
54	MG	1A	3811	1/1	0.92	0.09	39,39,39,39	0
54	MG	1A	3812	1/1	0.92	0.35	40,40,40,40	0
54	MG	1a	1880	1/1	0.92	0.16	67,67,67,67	0
54	MG	2A	3459	1/1	0.92	0.09	63,63,63,63	0
54	MG	2a	3031	1/1	0.92	0.12	46,46,46,46	0
54	MG	2A	3188	1/1	0.92	0.18	48,48,48,48	0
54	MG	17	102	1/1	0.92	0.17	55,55,55,55	0
54	MG	2A	3190	1/1	0.92	0.20	67,67,67,67	0
54	MG	2A	3192	1/1	0.92	0.08	60,60,60,60	0
54	MG	1A	3813	1/1	0.92	0.11	71,71,71,71	0
54	MG	1a	1731	1/1	0.92	0.19	60,60,60,60	0
54	MG	1A	3470	1/1	0.92	0.20	74,74,74,74	0
54	MG	1a	1733	1/1	0.92	0.14	56,56,56,56	0
54	MG	1a	1737	1/1	0.92	0.09	55,55,55,55	0
54	MG	1A	3139	1/1	0.92	0.27	51,51,51,51	0
54	MG	1A	3472	1/1	0.92	0.11	50,50,50,50	0
54	MG	1A	3985	1/1	0.92	0.11	54,54,54,54	0
54	MG	1A	3683	1/1	0.92	0.17	64,64,64,64	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	1A	3588	1/1	0.92	0.22	51,51,51,51	0
54	MG	1A	3686	1/1	0.92	0.10	50,50,50,50	0
54	MG	1a	1746	1/1	0.92	0.18	43,43,43,43	0
54	MG	1A	3589	1/1	0.92	0.09	23,23,23,23	0
54	MG	2a	3050	1/1	0.92	0.28	64,64,64,64	0
54	MG	2A	3490	1/1	0.92	0.10	59,59,59,59	0
54	MG	1A	3691	1/1	0.92	0.06	55,55,55,55	0
54	MG	2A	3218	1/1	0.92	0.12	65,65,65,65	0
54	MG	1a	1606	1/1	0.92	0.20	58,58,58,58	0
54	MG	1A	3692	1/1	0.92	0.10	59,59,59,59	0
54	MG	1A	3014	1/1	0.92	0.28	68,68,68,68	0
54	MG	1A	3123	1/1	0.92	0.12	38,38,38,38	0
54	MG	1A	3695	1/1	0.92	0.11	65,65,65,65	0
54	MG	2A	3225	1/1	0.92	0.19	66,66,66,66	0
54	MG	1A	3999	1/1	0.92	0.10	58,58,58,58	0
54	MG	2A	3002	1/1	0.92	0.08	58,58,58,58	0
54	MG	2A	3503	1/1	0.92	0.27	49,49,49,49	0
54	MG	2A	3003	1/1	0.92	0.10	65,65,65,65	0
54	MG	1A	3594	1/1	0.92	0.17	70,70,70,70	0
54	MG	1A	3388	1/1	0.92	0.09	47,47,47,47	0
54	MG	2a	3073	1/1	0.92	0.10	68,68,68,68	0
54	MG	2A	3507	1/1	0.92	0.24	68,68,68,68	0
54	MG	2A	3508	1/1	0.92	0.17	66,66,66,66	0
54	MG	1A	4006	1/1	0.92	0.08	58,58,58,58	0
54	MG	1a	1620	1/1	0.92	0.09	65,65,65,65	0
54	MG	1A	3487	1/1	0.92	0.10	49,49,49,49	0
54	MG	2a	3081	1/1	0.92	0.30	63,63,63,63	0
54	MG	2A	3019	1/1	0.92	0.23	52,52,52,52	0
54	MG	1A	3488	1/1	0.92	0.13	57,57,57,57	0
54	MG	1A	3241	1/1	0.92	0.22	63,63,63,63	0
54	MG	1A	3100	1/1	0.92	0.19	57,57,57,57	0
54	MG	2A	3525	1/1	0.92	0.09	53,53,53,53	0
54	MG	1A	4013	1/1	0.92	0.07	36,36,36,36	0
54	MG	2A	3257	1/1	0.92	0.18	55,55,55,55	0
54	MG	1A	3496	1/1	0.92	0.13	55,55,55,55	0
54	MG	2A	3533	1/1	0.92	0.07	88,88,88,88	0
54	MG	1a	1776	1/1	0.92	0.13	73,73,73,73	0
54	MG	1A	4015	1/1	0.92	0.08	28,28,28,28	0
54	MG	2A	3538	1/1	0.92	0.12	44,44,44,44	0
54	MG	1A	4017	1/1	0.92	0.17	71,71,71,71	0
54	MG	1A	4018	1/1	0.92	0.21	63,63,63,63	0
54	MG	1a	1637	1/1	0.92	0.10	48,48,48,48	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	1A	3251	1/1	0.92	0.16	51,51,51,51	0
54	MG	1A	3710	1/1	0.92	0.21	39,39,39,39	0
54	MG	1a	1786	1/1	0.92	0.23	63,63,63,63	0
54	MG	1A	3504	1/1	0.92	0.11	33,33,33,33	0
54	MG	1A	3712	1/1	0.92	0.22	58,58,58,58	0
54	MG	1a	1790	1/1	0.92	0.07	76,76,76,76	0
54	MG	2A	3048	1/1	0.92	0.43	76,76,76,76	0
54	MG	2A	3295	1/1	0.92	0.10	34,34,34,34	0
54	MG	1A	3506	1/1	0.92	0.12	40,40,40,40	0
54	MG	1A	3075	1/1	0.92	0.07	38,38,38,38	0
54	MG	1A	3510	1/1	0.92	0.11	50,50,50,50	0
54	MG	1A	3108	1/1	0.92	0.10	47,47,47,47	0
54	MG	2A	3057	1/1	0.92	0.23	70,70,70,70	0
54	MG	2a	3128	1/1	0.92	0.12	79,79,79,79	0
54	MG	2a	3133	1/1	0.92	0.06	80,80,80,80	0
54	MG	2A	3303	1/1	0.92	0.13	69,69,69,69	0
54	MG	2A	3596	1/1	0.92	0.09	37,37,37,37	0
54	MG	1A	3720	1/1	0.92	0.08	50,50,50,50	0
54	MG	1A	3521	1/1	0.92	0.08	69,69,69,69	0
54	MG	2A	3312	1/1	0.92	0.10	46,46,46,46	0
54	MG	1A	3879	1/1	0.92	0.07	31,31,31,31	0
54	MG	1a	1658	1/1	0.92	0.10	81,81,81,81	0
54	MG	1A	3314	1/1	0.92	0.12	47,47,47,47	0
54	MG	2A	3323	1/1	0.92	0.16	61,61,61,61	0
54	MG	1A	3622	1/1	0.92	0.10	52,52,52,52	0
54	MG	2A	3608	1/1	0.92	0.11	65,65,65,65	0
54	MG	2A	3611	1/1	0.92	0.16	64,64,64,64	0
54	MG	1A	3624	1/1	0.92	0.16	38,38,38,38	0
54	MG	1A	3012	1/1	0.92	0.17	40,40,40,40	0
54	MG	2A	3081	1/1	0.92	0.62	52,52,52,52	0
54	MG	1A	3160	1/1	0.92	0.32	62,62,62,62	0
54	MG	1A	3321	1/1	0.92	0.12	66,66,66,66	0
54	MG	1a	1667	1/1	0.92	0.07	78,78,78,78	0
54	MG	2A	3638	1/1	0.92	0.10	49,49,49,49	0
54	MG	2a	3179	1/1	0.92	0.14	81,81,81,81	0
54	MG	2A	3337	1/1	0.92	0.11	37,37,37,37	0
54	MG	1A	3633	1/1	0.92	0.17	65,65,65,65	0
54	MG	2A	3643	1/1	0.92	0.07	31,31,31,31	0
54	MG	1B	217	1/1	0.92	0.07	47,47,47,47	0
54	MG	2f	201	1/1	0.92	0.17	57,57,57,57	0
54	MG	2A	3646	1/1	0.92	0.09	78,78,78,78	0
54	MG	1A	3324	1/1	0.92	0.10	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	3657	1/1	0.92	0.09	62,62,62,62	0
54	MG	1A	3262	1/1	0.92	0.30	55,55,55,55	0
54	MG	2A	3092	1/1	0.92	0.12	74,74,74,74	0
54	MG	1A	3409	1/1	0.92	0.15	42,42,42,42	0
54	MG	2A	3669	1/1	0.92	0.22	74,74,74,74	0
54	MG	1A	3427	1/1	0.92	0.08	33,33,33,33	0
54	MG	1A	3908	1/1	0.92	0.21	73,73,73,73	0
54	MG	2A	3672	1/1	0.92	0.11	59,59,59,59	0
54	MG	2A	3674	1/1	0.92	0.13	46,46,46,46	0
54	MG	1A	3700	1/1	0.93	0.09	46,46,46,46	0
54	MG	2A	3122	1/1	0.93	0.34	49,49,49,49	0
54	MG	2A	3385	1/1	0.93	0.20	64,64,64,64	0
54	MG	1A	3820	1/1	0.93	0.13	41,41,41,41	0
54	MG	2A	3694	1/1	0.93	0.11	63,63,63,63	0
54	MG	1P	207	1/1	0.93	0.11	64,64,64,64	0
54	MG	2A	3126	1/1	0.93	0.22	67,67,67,67	0
54	MG	1a	1835	1/1	0.93	0.15	63,63,63,63	0
54	MG	1a	1694	1/1	0.93	0.22	75,75,75,75	0
54	MG	1a	1695	1/1	0.93	0.07	82,82,82,82	0
54	MG	1R	203	1/1	0.93	0.21	66,66,66,66	0
54	MG	1A	3238	1/1	0.93	0.27	64,64,64,64	0
54	MG	2A	3134	1/1	0.93	0.09	55,55,55,55	0
54	MG	1A	3091	1/1	0.93	0.09	48,48,48,48	0
54	MG	1T	201	1/1	0.93	0.06	42,42,42,42	0
54	MG	2A	3403	1/1	0.93	0.19	56,56,56,56	0
54	MG	1A	3619	1/1	0.93	0.09	41,41,41,41	0
54	MG	1A	3117	1/1	0.93	0.26	40,40,40,40	0
54	MG	1a	1845	1/1	0.93	0.24	66,66,66,66	0
54	MG	1a	1846	1/1	0.93	0.19	67,67,67,67	0
54	MG	1A	3312	1/1	0.93	0.21	40,40,40,40	0
54	MG	1U	201	1/1	0.93	0.20	44,44,44,44	0
54	MG	2A	3155	1/1	0.93	0.10	73,73,73,73	0
54	MG	2A	3156	1/1	0.93	0.27	48,48,48,48	0
54	MG	1V	203	1/1	0.93	0.12	61,61,61,61	0
54	MG	2A	3159	1/1	0.93	0.16	71,71,71,71	0
54	MG	1A	3247	1/1	0.93	0.12	47,47,47,47	0
54	MG	1W	204	1/1	0.93	0.12	49,49,49,49	0
54	MG	1a	1854	1/1	0.93	0.10	58,58,58,58	0
54	MG	2D	306	1/1	0.93	0.17	55,55,55,55	0
54	MG	1Y	201	1/1	0.93	0.16	68,68,68,68	0
54	MG	2A	3427	1/1	0.93	0.09	66,66,66,66	0
54	MG	2A	3428	1/1	0.93	0.08	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	3249	1/1	0.93	0.08	62,62,62,62	0
54	MG	1A	3097	1/1	0.93	0.09	54,54,54,54	0
54	MG	1A	3253	1/1	0.93	0.07	52,52,52,52	0
54	MG	2A	3432	1/1	0.93	0.07	69,69,69,69	0
54	MG	1A	3841	1/1	0.93	0.08	51,51,51,51	0
54	MG	2A	3435	1/1	0.93	0.21	66,66,66,66	0
54	MG	1A	3412	1/1	0.93	0.07	34,34,34,34	0
54	MG	1A	3632	1/1	0.93	0.12	33,33,33,33	0
54	MG	1A	3844	1/1	0.93	0.13	36,36,36,36	0
54	MG	15	101	1/1	0.93	0.17	41,41,41,41	0
54	MG	15	102	1/1	0.93	0.29	33,33,33,33	0
54	MG	2W	202	1/1	0.93	0.28	55,55,55,55	0
54	MG	1A	3532	1/1	0.93	0.12	55,55,55,55	0
54	MG	1A	3413	1/1	0.93	0.08	37,37,37,37	0
54	MG	1A	3850	1/1	0.93	0.19	54,54,54,54	0
54	MG	2A	3447	1/1	0.93	0.10	57,57,57,57	0
54	MG	15	107	1/1	0.93	0.08	51,51,51,51	0
54	MG	1A	3721	1/1	0.93	0.09	61,61,61,61	0
54	MG	1A	3853	1/1	0.93	0.26	50,50,50,50	0
54	MG	1a	1881	1/1	0.93	0.08	60,60,60,60	0
54	MG	2a	3004	1/1	0.93	0.09	59,59,59,59	0
54	MG	2A	3454	1/1	0.93	0.14	77,77,77,77	0
54	MG	2A	3455	1/1	0.93	0.08	35,35,35,35	0
54	MG	1A	3997	1/1	0.93	0.17	69,69,69,69	0
54	MG	2a	3009	1/1	0.93	0.14	59,59,59,59	0
54	MG	1A	3124	1/1	0.93	0.15	39,39,39,39	0
54	MG	2a	3012	1/1	0.93	0.25	67,67,67,67	0
54	MG	2a	3013	1/1	0.93	0.18	61,61,61,61	0
54	MG	2a	3015	1/1	0.93	0.36	64,64,64,64	0
54	MG	2A	3191	1/1	0.93	0.40	74,74,74,74	0
54	MG	1A	3429	1/1	0.93	0.17	54,54,54,54	0
54	MG	1A	3857	1/1	0.93	0.16	40,40,40,40	0
54	MG	1A	3323	1/1	0.93	0.17	67,67,67,67	0
54	MG	1e	203	1/1	0.93	0.09	66,66,66,66	0
54	MG	2A	3467	1/1	0.93	0.11	43,43,43,43	0
54	MG	2A	3201	1/1	0.93	0.29	74,74,74,74	0
54	MG	1A	4004	1/1	0.93	0.13	67,67,67,67	0
54	MG	1A	3067	1/1	0.93	0.22	41,41,41,41	0
54	MG	2A	3472	1/1	0.93	0.11	65,65,65,65	0
54	MG	1A	3157	1/1	0.93	0.36	37,37,37,37	0
54	MG	1A	3439	1/1	0.93	0.10	49,49,49,49	0
54	MG	1A	3865	1/1	0.93	0.13	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	1h	202	1/1	0.93	0.19	64,64,64,64	0
54	MG	1A	4010	1/1	0.93	0.13	66,66,66,66	0
54	MG	1A	3044	1/1	0.93	0.12	22,22,22,22	0
54	MG	1A	3867	1/1	0.93	0.10	47,47,47,47	0
54	MG	2A	3212	1/1	0.93	0.13	53,53,53,53	0
54	MG	2A	3213	1/1	0.93	0.21	72,72,72,72	0
54	MG	1A	3106	1/1	0.93	0.17	41,41,41,41	0
54	MG	1A	3164	1/1	0.93	0.07	38,38,38,38	0
54	MG	1A	4016	1/1	0.93	0.07	48,48,48,48	0
54	MG	1A	3741	1/1	0.93	0.12	36,36,36,36	0
54	MG	1a	1754	1/1	0.93	0.13	65,65,65,65	0
54	MG	1A	3334	1/1	0.93	0.08	33,33,33,33	0
54	MG	1A	3748	1/1	0.93	0.10	55,55,55,55	0
54	MG	1A	3065	1/1	0.93	0.10	69,69,69,69	0
54	MG	1A	3653	1/1	0.93	0.28	33,33,33,33	0
54	MG	1A	3271	1/1	0.93	0.10	60,60,60,60	0
54	MG	2a	3048	1/1	0.93	0.23	56,56,56,56	0
54	MG	1a	1762	1/1	0.93	0.07	63,63,63,63	0
54	MG	1a	1625	1/1	0.93	0.26	56,56,56,56	0
54	MG	1A	3085	1/1	0.93	0.39	47,47,47,47	0
54	MG	2A	3231	1/1	0.93	0.11	67,67,67,67	0
54	MG	1a	1627	1/1	0.93	0.10	56,56,56,56	0
54	MG	1A	3453	1/1	0.93	0.07	36,36,36,36	0
54	MG	2A	3238	1/1	0.93	0.10	60,60,60,60	0
54	MG	2A	3018	1/1	0.93	0.30	52,52,52,52	0
54	MG	1A	3206	1/1	0.93	0.25	54,54,54,54	0
54	MG	1a	1771	1/1	0.93	0.15	82,82,82,82	0
54	MG	2A	3243	1/1	0.93	0.13	63,63,63,63	0
54	MG	2A	3513	1/1	0.93	0.12	67,67,67,67	0
54	MG	1A	3278	1/1	0.93	0.38	47,47,47,47	0
54	MG	2A	3516	1/1	0.93	0.14	75,75,75,75	0
54	MG	2A	3249	1/1	0.93	0.15	48,48,48,48	0
54	MG	1A	3086	1/1	0.93	0.50	49,49,49,49	0
54	MG	1A	3211	1/1	0.93	0.38	46,46,46,46	0
54	MG	1B	204	1/1	0.93	0.08	51,51,51,51	0
54	MG	2A	3256	1/1	0.93	0.29	66,66,66,66	0
54	MG	1a	1636	1/1	0.93	0.33	67,67,67,67	0
54	MG	2A	3033	1/1	0.93	0.29	57,57,57,57	0
54	MG	1a	1778	1/1	0.93	0.12	72,72,72,72	0
54	MG	1A	3465	1/1	0.93	0.09	52,52,52,52	0
54	MG	1A	3899	1/1	0.93	0.10	58,58,58,58	0
54	MG	2A	3265	1/1	0.93	0.16	60,60,60,60	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	2a	3083	1/1	0.93	0.10	71,71,71,71	0
54	MG	1a	1781	1/1	0.93	0.33	63,63,63,63	0
54	MG	1a	1639	1/1	0.93	0.30	82,82,82,82	0
54	MG	1A	3578	1/1	0.93	0.10	39,39,39,39	0
54	MG	2A	3278	1/1	0.93	0.09	56,56,56,56	0
54	MG	1A	3672	1/1	0.93	0.06	45,45,45,45	0
54	MG	1A	3213	1/1	0.93	0.14	32,32,32,32	0
54	MG	1a	1787	1/1	0.93	0.08	71,71,71,71	0
54	MG	2A	3289	1/1	0.93	0.09	42,42,42,42	0
54	MG	1a	1645	1/1	0.93	0.19	53,53,53,53	0
54	MG	1A	3777	1/1	0.93	0.07	53,53,53,53	0
54	MG	1A	3354	1/1	0.93	0.08	27,27,27,27	0
54	MG	1A	3913	1/1	0.93	0.11	26,26,26,26	0
54	MG	1A	3111	1/1	0.93	0.37	33,33,33,33	0
54	MG	2A	3582	1/1	0.93	0.10	64,64,64,64	0
54	MG	1B	219	1/1	0.93	0.20	43,43,43,43	0
54	MG	2A	3586	1/1	0.93	0.08	79,79,79,79	0
54	MG	1A	3584	1/1	0.93	0.21	62,62,62,62	0
54	MG	1A	3144	1/1	0.93	0.09	40,40,40,40	0
54	MG	1A	3042	1/1	0.93	0.12	60,60,60,60	0
54	MG	2A	3064	1/1	0.93	0.19	62,62,62,62	0
54	MG	1A	3219	1/1	0.93	0.37	44,44,44,44	0
54	MG	2A	3067	1/1	0.93	0.12	51,51,51,51	0
54	MG	2A	3069	1/1	0.93	0.20	52,52,52,52	0
54	MG	1A	3373	1/1	0.93	0.13	54,54,54,54	0
54	MG	2a	3120	1/1	0.93	0.10	77,77,77,77	0
54	MG	2A	3071	1/1	0.93	0.24	53,53,53,53	0
54	MG	1A	3483	1/1	0.93	0.11	27,27,27,27	0
54	MG	1A	3484	1/1	0.93	0.15	58,58,58,58	0
54	MG	1a	1802	1/1	0.93	0.12	58,58,58,58	0
54	MG	2a	3132	1/1	0.93	0.11	75,75,75,75	0
54	MG	1B	229	1/1	0.93	0.16	60,60,60,60	0
54	MG	2A	3079	1/1	0.93	0.41	67,67,67,67	0
54	MG	2a	3137	1/1	0.93	0.07	46,46,46,46	0
54	MG	1A	3934	1/1	0.93	0.11	42,42,42,42	0
54	MG	1A	3936	1/1	0.93	0.13	64,64,64,64	0
54	MG	2A	3616	1/1	0.93	0.08	59,59,59,59	0
54	MG	2a	3144	1/1	0.93	0.10	64,64,64,64	0
54	MG	1A	3374	1/1	0.93	0.09	56,56,56,56	0
54	MG	2A	3627	1/1	0.93	0.10	88,88,88,88	0
54	MG	2a	3152	1/1	0.93	0.09	79,79,79,79	0
54	MG	1A	3221	1/1	0.93	0.27	52,52,52,52	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	1A	3223	1/1	0.93	0.56	44,44,44,44	0
54	MG	2A	3339	1/1	0.93	0.08	36,36,36,36	0
54	MG	1A	3804	1/1	0.93	0.17	60,60,60,60	0
54	MG	2A	3341	1/1	0.93	0.12	77,77,77,77	0
54	MG	1a	1672	1/1	0.93	0.10	62,62,62,62	0
54	MG	1E	308	1/1	0.93	0.12	63,63,63,63	0
54	MG	1A	3950	1/1	0.93	0.06	45,45,45,45	0
54	MG	1A	3688	1/1	0.93	0.25	41,41,41,41	0
54	MG	2A	3648	1/1	0.93	0.07	71,71,71,71	0
54	MG	2A	3651	1/1	0.93	0.08	59,59,59,59	0
54	MG	1a	1677	1/1	0.93	0.17	58,58,58,58	0
54	MG	1A	3806	1/1	0.93	0.06	77,77,77,77	0
54	MG	1A	3293	1/1	0.93	0.22	50,50,50,50	0
54	MG	2A	3659	1/1	0.93	0.13	74,74,74,74	0
54	MG	2A	3105	1/1	0.93	0.12	58,58,58,58	0
54	MG	2a	3182	1/1	0.93	0.08	75,75,75,75	0
54	MG	1A	3227	1/1	0.93	0.17	61,61,61,61	0
54	MG	1A	3500	1/1	0.93	0.08	24,24,24,24	0
54	MG	1A	3501	1/1	0.93	0.08	36,36,36,36	0
54	MG	2A	3109	1/1	0.93	0.22	67,67,67,67	0
54	MG	1a	1824	1/1	0.93	0.20	63,63,63,63	0
54	MG	1A	3232	1/1	0.93	0.42	47,47,47,47	0
56	ZIT	1A	4033	52/52	0.93	0.13	35,56,72,82	0
54	MG	1a	1826	1/1	0.93	0.12	63,63,63,63	0
54	MG	1A	3234	1/1	0.93	0.15	39,39,39,39	0
54	MG	2A	3373	1/1	0.93	0.07	49,49,49,49	0
54	MG	2A	3678	1/1	0.93	0.08	65,65,65,65	0
54	MG	1a	1828	1/1	0.93	0.10	71,71,71,71	0
54	MG	1A	3182	1/1	0.93	0.20	42,42,42,42	0
54	MG	1A	3816	1/1	0.93	0.26	49,49,49,49	0
54	MG	1A	3146	1/1	0.93	0.08	34,34,34,34	0
59	ZN	24	501	1/1	0.93	0.16	146,146,146,146	0
54	MG	1A	3885	1/1	0.94	0.14	43,43,43,43	0
54	MG	1B	207	1/1	0.94	0.34	65,65,65,65	0
54	MG	1a	1648	1/1	0.94	0.26	61,61,61,61	0
54	MG	1a	1649	1/1	0.94	0.19	48,48,48,48	0
54	MG	1A	3529	1/1	0.94	0.08	30,30,30,30	0
54	MG	1A	3421	1/1	0.94	0.16	43,43,43,43	0
54	MG	2A	3363	1/1	0.94	0.12	66,66,66,66	0
54	MG	1A	3228	1/1	0.94	0.21	36,36,36,36	0
54	MG	2A	3366	1/1	0.94	0.10	38,38,38,38	0
54	MG	2A	3683	1/1	0.94	0.15	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	3891	1/1	0.94	0.07	38,38,38,38	0
54	MG	2A	3685	1/1	0.94	0.14	57,57,57,57	0
54	MG	1A	3333	1/1	0.94	0.12	48,48,48,48	0
54	MG	2A	3687	1/1	0.94	0.09	62,62,62,62	0
54	MG	2A	3370	1/1	0.94	0.09	44,44,44,44	0
54	MG	1A	3114	1/1	0.94	0.28	45,45,45,45	0
54	MG	1A	3432	1/1	0.94	0.18	71,71,71,71	0
54	MG	1a	1815	1/1	0.94	0.19	70,70,70,70	0
54	MG	1A	3233	1/1	0.94	0.24	42,42,42,42	0
54	MG	1a	1817	1/1	0.94	0.10	61,61,61,61	0
54	MG	1a	1818	1/1	0.94	0.12	72,72,72,72	0
54	MG	1a	1661	1/1	0.94	0.30	68,68,68,68	0
54	MG	2A	3702	1/1	0.94	0.14	69,69,69,69	0
54	MG	1A	3196	1/1	0.94	0.10	57,57,57,57	0
54	MG	2A	3115	1/1	0.94	0.31	57,57,57,57	0
54	MG	2A	3383	1/1	0.94	0.18	55,55,55,55	0
54	MG	2A	3384	1/1	0.94	0.07	37,37,37,37	0
54	MG	1A	3339	1/1	0.94	0.11	53,53,53,53	0
54	MG	1a	1664	1/1	0.94	0.11	67,67,67,67	0
54	MG	1A	3197	1/1	0.94	0.08	47,47,47,47	0
54	MG	2A	3391	1/1	0.94	0.10	41,41,41,41	0
54	MG	1A	3547	1/1	0.94	0.09	62,62,62,62	0
54	MG	1A	3288	1/1	0.94	0.25	49,49,49,49	0
54	MG	1A	3655	1/1	0.94	0.19	42,42,42,42	0
54	MG	1A	3769	1/1	0.94	0.08	50,50,50,50	0
54	MG	1A	3343	1/1	0.94	0.13	33,33,33,33	0
54	MG	1A	3056	1/1	0.94	0.09	51,51,51,51	0
54	MG	1D	312	1/1	0.94	0.16	30,30,30,30	0
54	MG	1A	3918	1/1	0.94	0.11	25,25,25,25	0
54	MG	1A	3919	1/1	0.94	0.12	26,26,26,26	0
54	MG	1A	3775	1/1	0.94	0.12	50,50,50,50	0
54	MG	1A	3923	1/1	0.94	0.34	46,46,46,46	0
54	MG	1A	3776	1/1	0.94	0.13	65,65,65,65	0
54	MG	2D	303	1/1	0.94	0.42	48,48,48,48	0
54	MG	1A	3658	1/1	0.94	0.12	58,58,58,58	0
54	MG	1E	309	1/1	0.94	0.10	32,32,32,32	0
54	MG	1F	305	1/1	0.94	0.12	43,43,43,43	0
54	MG	2A	3145	1/1	0.94	0.09	48,48,48,48	0
54	MG	1A	3555	1/1	0.94	0.09	61,61,61,61	0
54	MG	1A	3781	1/1	0.94	0.07	32,32,32,32	0
54	MG	1A	3084	1/1	0.94	0.34	44,44,44,44	0
54	MG	2F	301	1/1	0.94	0.26	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	1F	316	1/1	0.94	0.13	63,63,63,63	0
54	MG	1a	1686	1/1	0.94	0.17	65,65,65,65	0
54	MG	1A	3349	1/1	0.94	0.12	40,40,40,40	0
54	MG	1A	3789	1/1	0.94	0.15	44,44,44,44	0
54	MG	1A	3170	1/1	0.94	0.15	39,39,39,39	0
54	MG	1a	1691	1/1	0.94	0.16	45,45,45,45	0
54	MG	2Q	202	1/1	0.94	0.08	65,65,65,65	0
54	MG	1A	3938	1/1	0.94	0.09	47,47,47,47	0
54	MG	1A	3940	1/1	0.94	0.07	63,63,63,63	0
54	MG	1A	3171	1/1	0.94	0.18	51,51,51,51	0
54	MG	2V	203	1/1	0.94	0.10	71,71,71,71	0
54	MG	1A	3244	1/1	0.94	0.16	46,46,46,46	0
54	MG	1A	3669	1/1	0.94	0.14	56,56,56,56	0
54	MG	1a	1863	1/1	0.94	0.09	64,64,64,64	0
54	MG	1A	3795	1/1	0.94	0.12	54,54,54,54	0
54	MG	23	101	1/1	0.94	0.14	57,57,57,57	0
54	MG	1a	1699	1/1	0.94	0.25	70,70,70,70	0
54	MG	1A	3948	1/1	0.94	0.12	56,56,56,56	0
54	MG	1P	205	1/1	0.94	0.13	54,54,54,54	0
54	MG	2A	3440	1/1	0.94	0.10	39,39,39,39	0
54	MG	1A	3355	1/1	0.94	0.14	27,27,27,27	0
54	MG	1A	3952	1/1	0.94	0.07	31,31,31,31	0
54	MG	1Q	205	1/1	0.94	0.08	56,56,56,56	0
54	MG	1A	3356	1/1	0.94	0.13	49,49,49,49	0
54	MG	1A	3246	1/1	0.94	0.13	45,45,45,45	0
54	MG	1A	3571	1/1	0.94	0.13	40,40,40,40	0
54	MG	1A	3573	1/1	0.94	0.25	60,60,60,60	0
54	MG	1A	3120	1/1	0.94	0.31	35,35,35,35	0
54	MG	1a	1878	1/1	0.94	0.25	68,68,68,68	0
54	MG	1A	3468	1/1	0.94	0.14	56,56,56,56	0
54	MG	1A	3103	1/1	0.94	0.08	57,57,57,57	0
54	MG	1T	206	1/1	0.94	0.17	57,57,57,57	0
54	MG	2a	3019	1/1	0.94	0.07	54,54,54,54	0
54	MG	1A	3807	1/1	0.94	0.07	48,48,48,48	0
54	MG	2A	3457	1/1	0.94	0.09	63,63,63,63	0
54	MG	1V	201	1/1	0.94	0.34	34,34,34,34	0
54	MG	1A	3301	1/1	0.94	0.08	47,47,47,47	0
54	MG	2A	3198	1/1	0.94	0.22	52,52,52,52	0
54	MG	1V	204	1/1	0.94	0.15	59,59,59,59	0
54	MG	2A	3200	1/1	0.94	0.34	64,64,64,64	0
54	MG	1W	201	1/1	0.94	0.14	51,51,51,51	0
54	MG	1A	3207	1/1	0.94	0.13	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	3303	1/1	0.94	0.27	38,38,38,38	0
54	MG	1A	3968	1/1	0.94	0.17	58,58,58,58	0
54	MG	1g	201	1/1	0.94	0.32	69,69,69,69	0
54	MG	1A	3473	1/1	0.94	0.10	54,54,54,54	0
54	MG	2A	3473	1/1	0.94	0.07	42,42,42,42	0
54	MG	1A	3971	1/1	0.94	0.06	32,32,32,32	0
54	MG	1A	3376	1/1	0.94	0.09	43,43,43,43	0
54	MG	1A	3209	1/1	0.94	0.38	48,48,48,48	0
54	MG	10	105	1/1	0.94	0.12	55,55,55,55	0
54	MG	2A	3211	1/1	0.94	0.32	70,70,70,70	0
54	MG	11	101	1/1	0.94	0.14	48,48,48,48	0
54	MG	1A	3378	1/1	0.94	0.07	37,37,37,37	0
54	MG	1A	3480	1/1	0.94	0.08	63,63,63,63	0
54	MG	1a	1736	1/1	0.94	0.16	74,74,74,74	0
54	MG	2A	3488	1/1	0.94	0.09	64,64,64,64	0
54	MG	1A	3689	1/1	0.94	0.08	68,68,68,68	0
54	MG	1A	3380	1/1	0.94	0.08	36,36,36,36	0
54	MG	1A	3819	1/1	0.94	0.14	50,50,50,50	0
54	MG	1A	3383	1/1	0.94	0.07	26,26,26,26	0
54	MG	1A	3384	1/1	0.94	0.08	48,48,48,48	0
54	MG	1A	3826	1/1	0.94	0.12	51,51,51,51	0
54	MG	2A	3001	1/1	0.94	0.28	61,61,61,61	0
54	MG	1A	3058	1/1	0.94	0.20	59,59,59,59	0
54	MG	1A	3828	1/1	0.94	0.15	28,28,28,28	0
54	MG	1A	3051	1/1	0.94	0.24	51,51,51,51	0
54	MG	1A	3212	1/1	0.94	0.11	55,55,55,55	0
54	MG	2A	3501	1/1	0.94	0.07	43,43,43,43	0
54	MG	2A	3007	1/1	0.94	0.06	45,45,45,45	0
54	MG	2A	3233	1/1	0.94	0.30	44,44,44,44	0
54	MG	2A	3009	1/1	0.94	0.12	40,40,40,40	0
54	MG	1A	3126	1/1	0.94	0.28	53,53,53,53	0
54	MG	2a	3063	1/1	0.94	0.24	70,70,70,70	0
54	MG	2a	3064	1/1	0.94	0.09	69,69,69,69	0
54	MG	2A	3237	1/1	0.94	0.11	56,56,56,56	0
54	MG	18	101	1/1	0.94	0.19	58,58,58,58	0
54	MG	1A	3835	1/1	0.94	0.08	32,32,32,32	0
54	MG	2A	3509	1/1	0.94	0.06	60,60,60,60	0
54	MG	2a	3070	1/1	0.94	0.22	61,61,61,61	0
54	MG	2a	3071	1/1	0.94	0.14	65,65,65,65	0
54	MG	1A	3836	1/1	0.94	0.07	26,26,26,26	0
54	MG	19	102	1/1	0.94	0.10	65,65,65,65	0
54	MG	2A	3242	1/1	0.94	0.23	71,71,71,71	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	2a	3075	1/1	0.94	0.11	57,57,57,57	0
54	MG	2A	3020	1/1	0.94	0.18	47,47,47,47	0
54	MG	2a	3077	1/1	0.94	0.38	61,61,61,61	0
54	MG	2A	3022	1/1	0.94	0.18	57,57,57,57	0
54	MG	1A	3498	1/1	0.94	0.09	23,23,23,23	0
54	MG	2A	3250	1/1	0.94	0.14	37,37,37,37	0
54	MG	2A	3251	1/1	0.94	0.12	58,58,58,58	0
54	MG	1A	3068	1/1	0.94	0.17	45,45,45,45	0
54	MG	2A	3524	1/1	0.94	0.10	58,58,58,58	0
54	MG	1A	3316	1/1	0.94	0.16	61,61,61,61	0
54	MG	1A	3605	1/1	0.94	0.09	49,49,49,49	0
54	MG	1A	3703	1/1	0.94	0.15	50,50,50,50	0
54	MG	2A	3030	1/1	0.94	0.18	36,36,36,36	0
54	MG	1A	3704	1/1	0.94	0.12	57,57,57,57	0
54	MG	2a	3090	1/1	0.94	0.14	82,82,82,82	0
54	MG	2A	3032	1/1	0.94	0.22	60,60,60,60	0
54	MG	1A	3606	1/1	0.94	0.10	54,54,54,54	0
54	MG	2A	3262	1/1	0.94	0.08	63,63,63,63	0
54	MG	1A	4002	1/1	0.94	0.13	18,18,18,18	0
54	MG	2A	3544	1/1	0.94	0.08	64,64,64,64	0
54	MG	2A	3035	1/1	0.94	0.23	65,65,65,65	0
54	MG	2A	3266	1/1	0.94	0.10	49,49,49,49	0
54	MG	1a	1608	1/1	0.94	0.09	72,72,72,72	0
54	MG	1A	3020	1/1	0.94	0.26	43,43,43,43	0
54	MG	2A	3038	1/1	0.94	0.17	56,56,56,56	0
54	MG	2a	3106	1/1	0.94	0.12	67,67,67,67	0
54	MG	2A	3555	1/1	0.94	0.06	58,58,58,58	0
54	MG	2A	3270	1/1	0.94	0.15	60,60,60,60	0
54	MG	2A	3275	1/1	0.94	0.15	49,49,49,49	0
54	MG	1A	3609	1/1	0.94	0.11	58,58,58,58	0
54	MG	1A	3267	1/1	0.94	0.22	55,55,55,55	0
54	MG	2A	3280	1/1	0.94	0.09	43,43,43,43	0
54	MG	2A	3281	1/1	0.94	0.21	52,52,52,52	0
54	MG	2A	3573	1/1	0.94	0.07	46,46,46,46	0
54	MG	2A	3575	1/1	0.94	0.08	63,63,63,63	0
54	MG	1A	3611	1/1	0.94	0.19	60,60,60,60	0
54	MG	2A	3578	1/1	0.94	0.09	61,61,61,61	0
54	MG	2A	3283	1/1	0.94	0.12	57,57,57,57	0
54	MG	1A	3188	1/1	0.94	0.31	53,53,53,53	0
54	MG	1A	3507	1/1	0.94	0.09	32,32,32,32	0
54	MG	2A	3290	1/1	0.94	0.14	64,64,64,64	0
54	MG	2A	3590	1/1	0.94	0.07	37,37,37,37	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	1a	1617	1/1	0.94	0.09	75,75,75,75	0
54	MG	1A	3322	1/1	0.94	0.20	60,60,60,60	0
54	MG	1a	1619	1/1	0.94	0.09	51,51,51,51	0
54	MG	2A	3294	1/1	0.94	0.13	47,47,47,47	0
54	MG	2A	3598	1/1	0.94	0.11	61,61,61,61	0
54	MG	2A	3050	1/1	0.94	0.10	45,45,45,45	0
54	MG	1A	3618	1/1	0.94	0.09	49,49,49,49	0
54	MG	1A	3132	1/1	0.94	0.15	45,45,45,45	0
54	MG	2a	3151	1/1	0.94	0.07	84,84,84,84	0
54	MG	1a	1623	1/1	0.94	0.07	56,56,56,56	0
54	MG	2A	3054	1/1	0.94	0.26	64,64,64,64	0
54	MG	1A	3511	1/1	0.94	0.10	27,27,27,27	0
54	MG	1a	1784	1/1	0.94	0.10	61,61,61,61	0
54	MG	1A	3513	1/1	0.94	0.08	44,44,44,44	0
54	MG	2A	3609	1/1	0.94	0.07	55,55,55,55	0
54	MG	2A	3610	1/1	0.94	0.06	78,78,78,78	0
54	MG	2a	3163	1/1	0.94	0.08	83,83,83,83	0
54	MG	2A	3061	1/1	0.94	0.07	46,46,46,46	0
54	MG	2a	3165	1/1	0.94	0.08	68,68,68,68	0
54	MG	1A	3404	1/1	0.94	0.11	55,55,55,55	0
54	MG	2A	3063	1/1	0.94	0.11	52,52,52,52	0
54	MG	1A	3519	1/1	0.94	0.12	53,53,53,53	0
54	MG	1A	3728	1/1	0.94	0.09	67,67,67,67	0
54	MG	2A	3626	1/1	0.94	0.07	59,59,59,59	0
54	MG	1A	3158	1/1	0.94	0.22	42,42,42,42	0
54	MG	1A	3093	1/1	0.94	0.32	39,39,39,39	0
54	MG	2A	3327	1/1	0.94	0.07	57,57,57,57	0
54	MG	1A	3627	1/1	0.94	0.20	42,42,42,42	0
54	MG	1a	1792	1/1	0.94	0.13	73,73,73,73	0
54	MG	1A	3630	1/1	0.94	0.19	38,38,38,38	0
54	MG	1A	3327	1/1	0.94	0.13	51,51,51,51	0
54	MG	2A	3075	1/1	0.94	0.13	63,63,63,63	0
54	MG	1A	3328	1/1	0.94	0.23	49,49,49,49	0
54	MG	1A	3878	1/1	0.94	0.11	74,74,74,74	0
54	MG	2A	3338	1/1	0.94	0.06	45,45,45,45	0
54	MG	1A	4030	1/1	0.94	0.13	64,64,64,64	0
54	MG	2A	3652	1/1	0.94	0.08	72,72,72,72	0
54	MG	1B	201	1/1	0.94	0.14	54,54,54,54	0
54	MG	1a	1640	1/1	0.94	0.17	74,74,74,74	0
54	MG	1A	3224	1/1	0.94	0.53	42,42,42,42	0
54	MG	1A	3880	1/1	0.94	0.12	50,50,50,50	0
54	MG	2A	3086	1/1	0.94	0.13	50,50,50,50	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	1A	3076	1/1	0.94	0.23	47,47,47,47	0
58	ARG	1B	230	12/12	0.94	0.10	33,49,59,61	0
54	MG	2A	3353	1/1	0.94	0.12	66,66,66,66	0
54	MG	1A	3745	1/1	0.94	0.12	63,63,63,63	0
54	MG	1A	3010	1/1	0.95	0.14	62,62,62,62	0
54	MG	2A	3010	1/1	0.95	0.11	73,73,73,73	0
54	MG	1A	3537	1/1	0.95	0.06	38,38,38,38	0
54	MG	2A	3015	1/1	0.95	0.21	41,41,41,41	0
54	MG	1A	3229	1/1	0.95	0.21	39,39,39,39	0
54	MG	1A	3154	1/1	0.95	0.20	47,47,47,47	0
54	MG	1A	3348	1/1	0.95	0.07	39,39,39,39	0
54	MG	1a	1768	1/1	0.95	0.12	67,67,67,67	0
54	MG	2B	215	1/1	0.95	0.10	66,66,66,66	0
54	MG	1A	3893	1/1	0.95	0.06	49,49,49,49	0
54	MG	1A	3760	1/1	0.95	0.15	56,56,56,56	0
54	MG	2A	3450	1/1	0.95	0.12	69,69,69,69	0
54	MG	1a	1622	1/1	0.95	0.06	55,55,55,55	0
54	MG	2D	305	1/1	0.95	0.12	49,49,49,49	0
54	MG	1A	3069	1/1	0.95	0.24	41,41,41,41	0
54	MG	1A	3127	1/1	0.95	0.09	52,52,52,52	0
54	MG	1A	3544	1/1	0.95	0.16	43,43,43,43	0
54	MG	1a	1775	1/1	0.95	0.11	68,68,68,68	0
54	MG	1A	3650	1/1	0.95	0.14	50,50,50,50	0
54	MG	1A	3444	1/1	0.95	0.09	28,28,28,28	0
54	MG	1A	3193	1/1	0.95	0.21	55,55,55,55	0
54	MG	2F	303	1/1	0.95	0.16	52,52,52,52	0
54	MG	1A	3072	1/1	0.95	0.06	45,45,45,45	0
54	MG	1A	3654	1/1	0.95	0.21	52,52,52,52	0
54	MG	1A	3296	1/1	0.95	0.14	40,40,40,40	0
54	MG	1A	3449	1/1	0.95	0.11	29,29,29,29	0
54	MG	2A	3466	1/1	0.95	0.12	33,33,33,33	0
54	MG	1B	216	1/1	0.95	0.06	61,61,61,61	0
54	MG	1A	3452	1/1	0.95	0.10	19,19,19,19	0
54	MG	2A	3039	1/1	0.95	0.19	64,64,64,64	0
54	MG	1A	3129	1/1	0.95	0.10	67,67,67,67	0
54	MG	2T	202	1/1	0.95	0.11	70,70,70,70	0
54	MG	1A	3360	1/1	0.95	0.09	15,15,15,15	0
54	MG	2V	201	1/1	0.95	0.12	70,70,70,70	0
54	MG	1A	3782	1/1	0.95	0.07	43,43,43,43	0
54	MG	1A	3922	1/1	0.95	0.06	45,45,45,45	0
54	MG	1A	3054	1/1	0.95	0.17	38,38,38,38	0
54	MG	1A	3661	1/1	0.95	0.15	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	1643	1/1	0.95	0.07	62,62,62,62	0
54	MG	1A	3662	1/1	0.95	0.09	39,39,39,39	0
54	MG	1A	3559	1/1	0.95	0.08	58,58,58,58	0
54	MG	28	101	1/1	0.95	0.10	63,63,63,63	0
54	MG	1A	3561	1/1	0.95	0.14	59,59,59,59	0
54	MG	2A	3252	1/1	0.95	0.29	54,54,54,54	0
54	MG	1D	301	1/1	0.95	0.18	57,57,57,57	0
54	MG	1D	305	1/1	0.95	0.08	44,44,44,44	0
54	MG	1D	310	1/1	0.95	0.16	44,44,44,44	0
54	MG	2a	3005	1/1	0.95	0.31	61,61,61,61	0
54	MG	2A	3055	1/1	0.95	0.09	41,41,41,41	0
54	MG	1A	3163	1/1	0.95	0.11	50,50,50,50	0
54	MG	1A	3459	1/1	0.95	0.11	53,53,53,53	0
54	MG	1D	313	1/1	0.95	0.21	49,49,49,49	0
54	MG	2A	3060	1/1	0.95	0.07	52,52,52,52	0
54	MG	1a	1655	1/1	0.95	0.18	58,58,58,58	0
54	MG	1A	3460	1/1	0.95	0.06	61,61,61,61	0
54	MG	1A	3935	1/1	0.95	0.07	50,50,50,50	0
54	MG	1A	3365	1/1	0.95	0.09	51,51,51,51	0
54	MG	1A	3462	1/1	0.95	0.06	19,19,19,19	0
54	MG	2A	3066	1/1	0.95	0.29	46,46,46,46	0
54	MG	1A	3939	1/1	0.95	0.10	57,57,57,57	0
54	MG	2A	3068	1/1	0.95	0.14	33,33,33,33	0
54	MG	2A	3272	1/1	0.95	0.07	51,51,51,51	0
54	MG	1A	3464	1/1	0.95	0.10	54,54,54,54	0
54	MG	1A	3055	1/1	0.95	0.46	36,36,36,36	0
54	MG	1F	303	1/1	0.95	0.25	38,38,38,38	0
54	MG	1A	3801	1/1	0.95	0.07	40,40,40,40	0
54	MG	1A	3245	1/1	0.95	0.36	49,49,49,49	0
54	MG	2A	3074	1/1	0.95	0.06	47,47,47,47	0
54	MG	1F	312	1/1	0.95	0.14	50,50,50,50	0
54	MG	2A	3284	1/1	0.95	0.07	58,58,58,58	0
54	MG	1F	313	1/1	0.95	0.09	33,33,33,33	0
54	MG	2A	3514	1/1	0.95	0.18	63,63,63,63	0
54	MG	1A	3944	1/1	0.95	0.07	68,68,68,68	0
54	MG	1A	3946	1/1	0.95	0.06	34,34,34,34	0
54	MG	1A	3109	1/1	0.95	0.09	43,43,43,43	0
54	MG	1A	3166	1/1	0.95	0.26	36,36,36,36	0
54	MG	1A	3203	1/1	0.95	0.28	47,47,47,47	0
54	MG	1A	3951	1/1	0.95	0.08	74,74,74,74	0
54	MG	1A	3580	1/1	0.95	0.07	50,50,50,50	0
54	MG	1A	3309	1/1	0.95	0.33	51,51,51,51	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	1A	3250	1/1	0.95	0.30	68,68,68,68	0
54	MG	2A	3530	1/1	0.95	0.06	68,68,68,68	0
54	MG	1A	3167	1/1	0.95	0.10	54,54,54,54	0
54	MG	1A	3957	1/1	0.95	0.11	50,50,50,50	0
54	MG	1N	204	1/1	0.95	0.23	60,60,60,60	0
54	MG	2A	3535	1/1	0.95	0.07	63,63,63,63	0
54	MG	2A	3093	1/1	0.95	0.10	64,64,64,64	0
54	MG	2A	3096	1/1	0.95	0.12	56,56,56,56	0
54	MG	1A	3585	1/1	0.95	0.09	68,68,68,68	0
54	MG	2A	3309	1/1	0.95	0.10	38,38,38,38	0
54	MG	1A	3477	1/1	0.95	0.06	65,65,65,65	0
54	MG	2A	3547	1/1	0.95	0.08	59,59,59,59	0
54	MG	2A	3313	1/1	0.95	0.12	47,47,47,47	0
54	MG	1A	3038	1/1	0.95	0.14	51,51,51,51	0
54	MG	2A	3550	1/1	0.95	0.07	64,64,64,64	0
54	MG	1A	3169	1/1	0.95	0.07	41,41,41,41	0
54	MG	1A	3255	1/1	0.95	0.10	54,54,54,54	0
54	MG	2A	3321	1/1	0.95	0.10	35,35,35,35	0
54	MG	1A	3690	1/1	0.95	0.07	59,59,59,59	0
54	MG	1A	3482	1/1	0.95	0.08	47,47,47,47	0
54	MG	1A	3208	1/1	0.95	0.09	48,48,48,48	0
54	MG	2A	3328	1/1	0.95	0.16	69,69,69,69	0
54	MG	2A	3329	1/1	0.95	0.08	44,44,44,44	0
54	MG	2A	3564	1/1	0.95	0.09	58,58,58,58	0
54	MG	2A	3570	1/1	0.95	0.10	47,47,47,47	0
54	MG	1A	3593	1/1	0.95	0.10	61,61,61,61	0
54	MG	1A	3969	1/1	0.95	0.11	57,57,57,57	0
54	MG	2A	3332	1/1	0.95	0.11	53,53,53,53	0
54	MG	1A	3387	1/1	0.95	0.06	15,15,15,15	0
54	MG	1T	203	1/1	0.95	0.06	57,57,57,57	0
54	MG	1A	3317	1/1	0.95	0.21	47,47,47,47	0
54	MG	1A	3057	1/1	0.95	0.14	56,56,56,56	0
54	MG	1a	1696	1/1	0.95	0.20	55,55,55,55	0
54	MG	1a	1842	1/1	0.95	0.20	78,78,78,78	0
54	MG	2A	3117	1/1	0.95	0.19	57,57,57,57	0
54	MG	1A	3138	1/1	0.95	0.07	53,53,53,53	0
54	MG	1A	3829	1/1	0.95	0.24	43,43,43,43	0
54	MG	1U	202	1/1	0.95	0.13	36,36,36,36	0
54	MG	2A	3343	1/1	0.95	0.09	59,59,59,59	0
54	MG	1U	204	1/1	0.95	0.10	48,48,48,48	0
54	MG	1U	207	1/1	0.95	0.21	45,45,45,45	0
54	MG	2A	3600	1/1	0.95	0.08	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	3351	1/1	0.95	0.21	52,52,52,52	0
54	MG	1a	1702	1/1	0.95	0.35	71,71,71,71	0
54	MG	2A	3603	1/1	0.95	0.07	89,89,89,89	0
54	MG	2a	3091	1/1	0.95	0.07	41,41,41,41	0
54	MG	1A	3598	1/1	0.95	0.09	32,32,32,32	0
54	MG	2a	3093	1/1	0.95	0.12	70,70,70,70	0
54	MG	1A	3599	1/1	0.95	0.16	47,47,47,47	0
54	MG	1A	3393	1/1	0.95	0.08	35,35,35,35	0
54	MG	1A	3495	1/1	0.95	0.12	61,61,61,61	0
54	MG	1a	1855	1/1	0.95	0.20	74,74,74,74	0
54	MG	2A	3132	1/1	0.95	0.12	69,69,69,69	0
54	MG	1A	3320	1/1	0.95	0.09	45,45,45,45	0
54	MG	1a	1859	1/1	0.95	0.12	57,57,57,57	0
54	MG	1A	3002	1/1	0.95	0.09	55,55,55,55	0
54	MG	2A	3136	1/1	0.95	0.13	47,47,47,47	0
54	MG	1A	3265	1/1	0.95	0.19	67,67,67,67	0
54	MG	1A	3028	1/1	0.95	0.29	38,38,38,38	0
54	MG	1A	3176	1/1	0.95	0.24	41,41,41,41	0
54	MG	2A	3369	1/1	0.95	0.16	70,70,70,70	0
54	MG	1A	3608	1/1	0.95	0.09	55,55,55,55	0
54	MG	2A	3147	1/1	0.95	0.26	55,55,55,55	0
54	MG	2A	3635	1/1	0.95	0.06	55,55,55,55	0
54	MG	2A	3636	1/1	0.95	0.10	59,59,59,59	0
54	MG	1A	3269	1/1	0.95	0.09	58,58,58,58	0
54	MG	2A	3151	1/1	0.95	0.16	64,64,64,64	0
54	MG	1A	3029	1/1	0.95	0.17	40,40,40,40	0
54	MG	2A	3640	1/1	0.95	0.09	33,33,33,33	0
54	MG	10	106	1/1	0.95	0.10	65,65,65,65	0
54	MG	1A	3064	1/1	0.95	0.12	34,34,34,34	0
54	MG	2a	3127	1/1	0.95	0.10	74,74,74,74	0
54	MG	1a	1718	1/1	0.95	0.08	72,72,72,72	0
54	MG	1A	3613	1/1	0.95	0.14	51,51,51,51	0
54	MG	2A	3157	1/1	0.95	0.27	57,57,57,57	0
54	MG	1A	3508	1/1	0.95	0.08	33,33,33,33	0
54	MG	2a	3136	1/1	0.95	0.07	73,73,73,73	0
54	MG	1A	3181	1/1	0.95	0.31	50,50,50,50	0
54	MG	2A	3655	1/1	0.95	0.07	37,37,37,37	0
54	MG	1A	3996	1/1	0.95	0.07	55,55,55,55	0
54	MG	1A	3273	1/1	0.95	0.28	39,39,39,39	0
54	MG	1A	3275	1/1	0.95	0.14	59,59,59,59	0
54	MG	2A	3163	1/1	0.95	0.19	62,62,62,62	0
54	MG	2a	3148	1/1	0.95	0.09	68,68,68,68	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	2A	3663	1/1	0.95	0.09	75,75,75,75	0
54	MG	2A	3665	1/1	0.95	0.08	83,83,83,83	0
54	MG	1a	1725	1/1	0.95	0.17	71,71,71,71	0
54	MG	1a	1726	1/1	0.95	0.18	73,73,73,73	0
54	MG	2a	3154	1/1	0.95	0.11	71,71,71,71	0
54	MG	1A	3722	1/1	0.95	0.08	52,52,52,52	0
54	MG	1A	3724	1/1	0.95	0.13	39,39,39,39	0
54	MG	1A	3147	1/1	0.95	0.38	42,42,42,42	0
54	MG	2A	3172	1/1	0.95	0.08	49,49,49,49	0
54	MG	1A	3220	1/1	0.95	0.08	48,48,48,48	0
54	MG	2a	3162	1/1	0.95	0.14	56,56,56,56	0
54	MG	17	101	1/1	0.95	0.07	45,45,45,45	0
54	MG	1A	4003	1/1	0.95	0.06	58,58,58,58	0
54	MG	1A	3518	1/1	0.95	0.07	54,54,54,54	0
54	MG	1a	1734	1/1	0.95	0.08	34,34,34,34	0
54	MG	2a	3168	1/1	0.95	0.13	69,69,69,69	0
54	MG	1a	1735	1/1	0.95	0.15	49,49,49,49	0
54	MG	2a	3172	1/1	0.95	0.10	79,79,79,79	0
54	MG	1A	3417	1/1	0.95	0.08	28,28,28,28	0
54	MG	1A	3045	1/1	0.95	0.18	34,34,34,34	0
54	MG	1a	1739	1/1	0.95	0.09	74,74,74,74	0
54	MG	1A	3732	1/1	0.95	0.07	32,32,32,32	0
54	MG	1A	3425	1/1	0.95	0.12	30,30,30,30	0
54	MG	1A	3734	1/1	0.95	0.07	39,39,39,39	0
54	MG	1A	3426	1/1	0.95	0.06	24,24,24,24	0
54	MG	1A	3871	1/1	0.95	0.07	60,60,60,60	0
54	MG	1A	3280	1/1	0.95	0.18	52,52,52,52	0
54	MG	2A	3418	1/1	0.95	0.08	67,67,67,67	0
54	MG	1A	3874	1/1	0.95	0.10	39,39,39,39	0
54	MG	1A	3526	1/1	0.95	0.13	54,54,54,54	0
54	MG	2l	201	1/1	0.95	0.13	68,68,68,68	0
54	MG	1A	3001	1/1	0.95	0.05	41,41,41,41	0
54	MG	2A	3425	1/1	0.95	0.06	58,58,58,58	0
55	HGR	2A	3712	36/36	0.95	0.12	38,43,49,51	0
54	MG	2A	3197	1/1	0.95	0.10	54,54,54,54	0
54	MG	1A	3186	1/1	0.95	0.27	41,41,41,41	0
54	MG	1A	3016	1/1	0.95	0.34	40,40,40,40	0
54	MG	1A	3433	1/1	0.95	0.07	25,25,25,25	0
54	MG	1A	4021	1/1	0.95	0.09	60,60,60,60	0
54	MG	1a	1755	1/1	0.95	0.12	61,61,61,61	0
54	MG	1A	3636	1/1	0.95	0.07	29,29,29,29	0
54	MG	2A	3434	1/1	0.95	0.09	73,73,73,73	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	1A	3342	1/1	0.95	0.09	56,56,56,56	0
54	MG	1A	3750	1/1	0.95	0.07	39,39,39,39	0
59	ZN	14	501	1/1	0.95	0.16	140,140,140,140	0
54	MG	1a	1614	1/1	0.95	0.07	60,60,60,60	0
54	MG	1A	3494	1/1	0.96	0.05	35,35,35,35	0
54	MG	1A	3415	1/1	0.96	0.06	33,33,33,33	0
54	MG	1A	3258	1/1	0.96	0.26	40,40,40,40	0
54	MG	2A	3008	1/1	0.96	0.08	43,43,43,43	0
54	MG	1A	3671	1/1	0.96	0.12	41,41,41,41	0
54	MG	2V	202	1/1	0.96	0.14	56,56,56,56	0
54	MG	1A	3877	1/1	0.96	0.05	38,38,38,38	0
54	MG	2W	201	1/1	0.96	0.42	51,51,51,51	0
54	MG	2A	3011	1/1	0.96	0.06	40,40,40,40	0
54	MG	1A	3768	1/1	0.96	0.07	55,55,55,55	0
54	MG	2A	3522	1/1	0.96	0.11	37,37,37,37	0
54	MG	2A	3013	1/1	0.96	0.05	26,26,26,26	0
54	MG	1A	3497	1/1	0.96	0.12	59,59,59,59	0
54	MG	2A	3526	1/1	0.96	0.05	83,83,83,83	0
54	MG	2A	3166	1/1	0.96	0.07	61,61,61,61	0
54	MG	1A	3770	1/1	0.96	0.08	58,58,58,58	0
54	MG	1A	3771	1/1	0.96	0.09	46,46,46,46	0
54	MG	1a	1675	1/1	0.96	0.25	53,53,53,53	0
54	MG	2A	3532	1/1	0.96	0.09	67,67,67,67	0
54	MG	1A	3772	1/1	0.96	0.20	43,43,43,43	0
54	MG	1U	205	1/1	0.96	0.30	36,36,36,36	0
54	MG	1U	206	1/1	0.96	0.23	42,42,42,42	0
54	MG	1A	4005	1/1	0.96	0.04	41,41,41,41	0
54	MG	2A	3175	1/1	0.96	0.10	52,52,52,52	0
54	MG	2A	3541	1/1	0.96	0.07	61,61,61,61	0
54	MG	2A	3177	1/1	0.96	0.30	70,70,70,70	0
54	MG	1A	3418	1/1	0.96	0.07	25,25,25,25	0
54	MG	2A	3545	1/1	0.96	0.07	65,65,65,65	0
54	MG	1A	3886	1/1	0.96	0.10	28,28,28,28	0
54	MG	2A	3026	1/1	0.96	0.08	55,55,55,55	0
54	MG	2a	3017	1/1	0.96	0.09	57,57,57,57	0
54	MG	2A	3181	1/1	0.96	0.08	54,54,54,54	0
54	MG	1A	3092	1/1	0.96	0.26	36,36,36,36	0
54	MG	1A	3424	1/1	0.96	0.07	21,21,21,21	0
54	MG	1A	3306	1/1	0.96	0.16	40,40,40,40	0
54	MG	1A	3307	1/1	0.96	0.33	43,43,43,43	0
54	MG	2A	3554	1/1	0.96	0.09	35,35,35,35	0
54	MG	1A	3778	1/1	0.96	0.08	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	1687	1/1	0.96	0.09	55,55,55,55	0
54	MG	2a	3026	1/1	0.96	0.22	60,60,60,60	0
54	MG	1A	3779	1/1	0.96	0.19	64,64,64,64	0
54	MG	1A	3308	1/1	0.96	0.20	49,49,49,49	0
54	MG	1A	3183	1/1	0.96	0.06	62,62,62,62	0
54	MG	1A	3218	1/1	0.96	0.11	51,51,51,51	0
54	MG	1A	3358	1/1	0.96	0.08	24,24,24,24	0
54	MG	2A	3565	1/1	0.96	0.16	49,49,49,49	0
54	MG	2A	3567	1/1	0.96	0.08	48,48,48,48	0
54	MG	1A	3784	1/1	0.96	0.06	35,35,35,35	0
54	MG	1A	3901	1/1	0.96	0.07	55,55,55,55	0
54	MG	1A	3682	1/1	0.96	0.06	50,50,50,50	0
54	MG	2A	3042	1/1	0.96	0.08	29,29,29,29	0
54	MG	2A	3576	1/1	0.96	0.09	73,73,73,73	0
54	MG	1A	3904	1/1	0.96	0.10	48,48,48,48	0
54	MG	11	105	1/1	0.96	0.12	48,48,48,48	0
54	MG	1A	3788	1/1	0.96	0.07	54,54,54,54	0
54	MG	2A	3380	1/1	0.96	0.06	43,43,43,43	0
54	MG	2A	3381	1/1	0.96	0.06	35,35,35,35	0
54	MG	13	103	1/1	0.96	0.07	39,39,39,39	0
54	MG	1A	3018	1/1	0.96	0.23	32,32,32,32	0
54	MG	1A	3040	1/1	0.96	0.10	53,53,53,53	0
54	MG	1A	3512	1/1	0.96	0.07	27,27,27,27	0
54	MG	1a	1822	1/1	0.96	0.10	55,55,55,55	0
54	MG	1A	3071	1/1	0.96	0.20	38,38,38,38	0
54	MG	2A	3389	1/1	0.96	0.09	60,60,60,60	0
54	MG	2a	3051	1/1	0.96	0.09	83,83,83,83	0
54	MG	2A	3390	1/1	0.96	0.13	74,74,74,74	0
54	MG	1A	4029	1/1	0.96	0.09	61,61,61,61	0
54	MG	1A	3156	1/1	0.96	0.24	38,38,38,38	0
54	MG	1A	3367	1/1	0.96	0.09	33,33,33,33	0
54	MG	1A	3315	1/1	0.96	0.17	62,62,62,62	0
54	MG	2A	3395	1/1	0.96	0.05	37,37,37,37	0
54	MG	1A	3099	1/1	0.96	0.14	38,38,38,38	0
54	MG	17	103	1/1	0.96	0.07	41,41,41,41	0
54	MG	17	104	1/1	0.96	0.26	45,45,45,45	0
54	MG	1A	3225	1/1	0.96	0.14	34,34,34,34	0
54	MG	2A	3217	1/1	0.96	0.08	52,52,52,52	0
54	MG	1A	3226	1/1	0.96	0.33	37,37,37,37	0
54	MG	1A	3011	1/1	0.96	0.25	64,64,64,64	0
54	MG	1A	3802	1/1	0.96	0.08	73,73,73,73	0
54	MG	1a	1715	1/1	0.96	0.11	52,52,52,52	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	1A	3101	1/1	0.96	0.21	47,47,47,47	0
54	MG	2a	3069	1/1	0.96	0.31	50,50,50,50	0
54	MG	1A	3130	1/1	0.96	0.06	37,37,37,37	0
54	MG	1A	3162	1/1	0.96	0.09	38,38,38,38	0
54	MG	1A	3698	1/1	0.96	0.08	58,58,58,58	0
54	MG	2A	3629	1/1	0.96	0.06	57,57,57,57	0
54	MG	2A	3410	1/1	0.96	0.09	58,58,58,58	0
54	MG	1A	3451	1/1	0.96	0.08	29,29,29,29	0
54	MG	1A	3808	1/1	0.96	0.08	33,33,33,33	0
54	MG	1A	3381	1/1	0.96	0.05	20,20,20,20	0
54	MG	1A	3033	1/1	0.96	0.20	58,58,58,58	0
54	MG	2A	3232	1/1	0.96	0.50	47,47,47,47	0
54	MG	1A	3535	1/1	0.96	0.08	24,24,24,24	0
54	MG	1A	3022	1/1	0.96	0.05	45,45,45,45	0
54	MG	2A	3421	1/1	0.96	0.06	63,63,63,63	0
54	MG	1A	3077	1/1	0.96	0.29	37,37,37,37	0
54	MG	1B	223	1/1	0.96	0.08	68,68,68,68	0
54	MG	2A	3078	1/1	0.96	0.15	56,56,56,56	0
54	MG	2A	3647	1/1	0.96	0.07	69,69,69,69	0
54	MG	2A	3426	1/1	0.96	0.04	55,55,55,55	0
54	MG	1A	3326	1/1	0.96	0.27	38,38,38,38	0
54	MG	2A	3080	1/1	0.96	0.11	47,47,47,47	0
54	MG	2A	3654	1/1	0.96	0.07	42,42,42,42	0
54	MG	1A	3458	1/1	0.96	0.09	49,49,49,49	0
54	MG	1A	3623	1/1	0.96	0.11	58,58,58,58	0
54	MG	1A	3023	1/1	0.96	0.15	36,36,36,36	0
54	MG	2A	3244	1/1	0.96	0.22	46,46,46,46	0
54	MG	2a	3097	1/1	0.96	0.11	58,58,58,58	0
54	MG	2A	3245	1/1	0.96	0.12	46,46,46,46	0
54	MG	2A	3660	1/1	0.96	0.06	68,68,68,68	0
54	MG	2A	3661	1/1	0.96	0.06	59,59,59,59	0
54	MG	2A	3246	1/1	0.96	0.15	60,60,60,60	0
54	MG	2A	3664	1/1	0.96	0.06	82,82,82,82	0
54	MG	1A	3541	1/1	0.96	0.06	53,53,53,53	0
54	MG	2A	3436	1/1	0.96	0.12	44,44,44,44	0
54	MG	2a	3105	1/1	0.96	0.09	71,71,71,71	0
54	MG	2A	3667	1/1	0.96	0.06	46,46,46,46	0
54	MG	1A	3080	1/1	0.96	0.24	45,45,45,45	0
54	MG	1A	3389	1/1	0.96	0.09	21,21,21,21	0
54	MG	1A	3081	1/1	0.96	0.12	49,49,49,49	0
54	MG	1a	1860	1/1	0.96	0.15	56,56,56,56	0
54	MG	1A	3463	1/1	0.96	0.19	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	1862	1/1	0.96	0.12	44,44,44,44	0
54	MG	1A	3063	1/1	0.96	0.05	40,40,40,40	0
54	MG	1A	3140	1/1	0.96	0.08	36,36,36,36	0
54	MG	2A	3097	1/1	0.96	0.31	63,63,63,63	0
54	MG	2A	3258	1/1	0.96	0.28	51,51,51,51	0
54	MG	1A	3394	1/1	0.96	0.07	35,35,35,35	0
54	MG	1A	3395	1/1	0.96	0.12	40,40,40,40	0
54	MG	1A	3048	1/1	0.96	0.22	56,56,56,56	0
54	MG	2a	3126	1/1	0.96	0.05	71,71,71,71	0
54	MG	1A	3397	1/1	0.96	0.12	53,53,53,53	0
54	MG	2A	3104	1/1	0.96	0.09	56,56,56,56	0
54	MG	2a	3129	1/1	0.96	0.05	61,61,61,61	0
54	MG	2a	3131	1/1	0.96	0.08	83,83,83,83	0
54	MG	2A	3453	1/1	0.96	0.07	65,65,65,65	0
54	MG	1E	301	1/1	0.96	0.17	38,38,38,38	0
54	MG	1A	3172	1/1	0.96	0.22	38,38,38,38	0
54	MG	1E	305	1/1	0.96	0.05	39,39,39,39	0
54	MG	1A	3335	1/1	0.96	0.14	50,50,50,50	0
54	MG	1A	3026	1/1	0.96	0.28	37,37,37,37	0
54	MG	2a	3141	1/1	0.96	0.08	72,72,72,72	0
54	MG	1A	3730	1/1	0.96	0.19	41,41,41,41	0
54	MG	2A	3271	1/1	0.96	0.05	39,39,39,39	0
54	MG	2A	3698	1/1	0.96	0.15	73,73,73,73	0
54	MG	1A	3560	1/1	0.96	0.14	60,60,60,60	0
54	MG	2a	3146	1/1	0.96	0.12	78,78,78,78	0
54	MG	2A	3700	1/1	0.96	0.06	63,63,63,63	0
54	MG	1A	3174	1/1	0.96	0.15	34,34,34,34	0
54	MG	2A	3277	1/1	0.96	0.10	51,51,51,51	0
54	MG	1F	307	1/1	0.96	0.07	43,43,43,43	0
54	MG	2A	3705	1/1	0.96	0.12	46,46,46,46	0
54	MG	1A	3115	1/1	0.96	0.13	36,36,36,36	0
54	MG	1A	3037	1/1	0.96	0.08	40,40,40,40	0
54	MG	1A	3567	1/1	0.96	0.09	38,38,38,38	0
54	MG	1a	1758	1/1	0.96	0.10	55,55,55,55	0
54	MG	1A	3252	1/1	0.96	0.28	33,33,33,33	0
54	MG	2a	3160	1/1	0.96	0.08	78,78,78,78	0
54	MG	2A	3119	1/1	0.96	0.05	42,42,42,42	0
54	MG	1A	3481	1/1	0.96	0.10	50,50,50,50	0
54	MG	2A	3288	1/1	0.96	0.09	37,37,37,37	0
54	MG	1A	3089	1/1	0.96	0.05	41,41,41,41	0
54	MG	1A	3407	1/1	0.96	0.21	57,57,57,57	0
54	MG	2B	207	1/1	0.96	0.09	73,73,73,73	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	1A	3572	1/1	0.96	0.07	56,56,56,56	0
54	MG	1A	3179	1/1	0.96	0.39	42,42,42,42	0
54	MG	1A	3485	1/1	0.96	0.09	63,63,63,63	0
54	MG	1a	1766	1/1	0.96	0.12	57,57,57,57	0
54	MG	1A	3980	1/1	0.96	0.12	53,53,53,53	0
54	MG	1A	3575	1/1	0.96	0.09	36,36,36,36	0
54	MG	1A	3486	1/1	0.96	0.07	58,58,58,58	0
54	MG	1A	3004	1/1	0.96	0.10	44,44,44,44	0
54	MG	1A	3752	1/1	0.96	0.11	26,26,26,26	0
54	MG	1m	201	1/1	0.96	0.04	81,81,81,81	0
54	MG	1A	3411	1/1	0.96	0.08	34,34,34,34	0
54	MG	1A	3754	1/1	0.96	0.10	53,53,53,53	0
54	MG	2A	3137	1/1	0.96	0.10	58,58,58,58	0
54	MG	1A	3345	1/1	0.96	0.17	43,43,43,43	0
54	MG	2D	307	1/1	0.96	0.10	63,63,63,63	0
54	MG	2A	3310	1/1	0.96	0.10	52,52,52,52	0
54	MG	1A	3581	1/1	0.96	0.08	48,48,48,48	0
54	MG	1A	3664	1/1	0.96	0.09	60,60,60,60	0
54	MG	2A	3314	1/1	0.96	0.12	37,37,37,37	0
54	MG	1Q	201	1/1	0.96	0.10	43,43,43,43	0
54	MG	1Q	204	1/1	0.96	0.20	56,56,56,56	0
54	MG	1A	3869	1/1	0.96	0.10	45,45,45,45	0
54	MG	2A	3320	1/1	0.96	0.10	50,50,50,50	0
57	MPD	18	103	8/8	0.96	0.11	32,41,48,49	0
54	MG	2A	3150	1/1	0.96	0.17	61,61,61,61	0
54	MG	2A	3322	1/1	0.96	0.07	39,39,39,39	0
54	MG	1R	202	1/1	0.96	0.11	45,45,45,45	0
54	MG	2O	201	1/1	0.96	0.16	68,68,68,68	0
54	MG	1A	3151	1/1	0.96	0.10	58,58,58,58	0
54	MG	1R	204	1/1	0.96	0.11	49,49,49,49	0
54	MG	1A	3492	1/1	0.96	0.05	56,56,56,56	0
54	MG	2Q	203	1/1	0.96	0.06	75,75,75,75	0
54	MG	1A	3862	1/1	0.97	0.10	26,26,26,26	0
54	MG	2A	3350	1/1	0.97	0.06	62,62,62,62	0
54	MG	1a	1654	1/1	0.97	0.07	47,47,47,47	0
54	MG	2W	203	1/1	0.97	0.12	73,73,73,73	0
54	MG	2A	3537	1/1	0.97	0.07	79,79,79,79	0
54	MG	2A	3021	1/1	0.97	0.05	44,44,44,44	0
54	MG	2A	3540	1/1	0.97	0.05	27,27,27,27	0
54	MG	1G	204	1/1	0.97	0.11	56,56,56,56	0
54	MG	2A	3542	1/1	0.97	0.08	65,65,65,65	0
54	MG	27	101	1/1	0.97	0.19	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	3159	1/1	0.97	0.12	40,40,40,40	0
54	MG	1A	3009	1/1	0.97	0.07	39,39,39,39	0
54	MG	1N	202	1/1	0.97	0.14	49,49,49,49	0
54	MG	1A	3450	1/1	0.97	0.06	30,30,30,30	0
54	MG	2A	3358	1/1	0.97	0.07	65,65,65,65	0
54	MG	1A	3520	1/1	0.97	0.13	30,30,30,30	0
54	MG	1A	3231	1/1	0.97	0.19	35,35,35,35	0
54	MG	2A	3029	1/1	0.97	0.08	47,47,47,47	0
54	MG	1P	202	1/1	0.97	0.28	36,36,36,36	0
54	MG	1A	3522	1/1	0.97	0.08	43,43,43,43	0
54	MG	1P	204	1/1	0.97	0.10	67,67,67,67	0
54	MG	1A	3019	1/1	0.97	0.14	36,36,36,36	0
54	MG	1A	3989	1/1	0.97	0.04	57,57,57,57	0
54	MG	1A	3015	1/1	0.97	0.11	38,38,38,38	0
54	MG	1A	3390	1/1	0.97	0.07	19,19,19,19	0
54	MG	2A	3561	1/1	0.97	0.06	50,50,50,50	0
54	MG	2A	3193	1/1	0.97	0.06	49,49,49,49	0
54	MG	1Q	202	1/1	0.97	0.09	45,45,45,45	0
54	MG	1Q	203	1/1	0.97	0.06	41,41,41,41	0
54	MG	2A	3196	1/1	0.97	0.09	51,51,51,51	0
54	MG	1A	3021	1/1	0.97	0.21	45,45,45,45	0
54	MG	1A	3456	1/1	0.97	0.05	32,32,32,32	0
54	MG	1R	201	1/1	0.97	0.14	46,46,46,46	0
54	MG	1A	3235	1/1	0.97	0.12	31,31,31,31	0
54	MG	1A	3102	1/1	0.97	0.26	38,38,38,38	0
54	MG	1A	3041	1/1	0.97	0.17	47,47,47,47	0
54	MG	1A	3531	1/1	0.97	0.09	50,50,50,50	0
54	MG	1A	3104	1/1	0.97	0.20	26,26,26,26	0
54	MG	2A	3581	1/1	0.97	0.07	41,41,41,41	0
54	MG	1A	3105	1/1	0.97	0.25	35,35,35,35	0
54	MG	2A	3583	1/1	0.97	0.06	38,38,38,38	0
54	MG	1A	3136	1/1	0.97	0.36	33,33,33,33	0
54	MG	1A	3202	1/1	0.97	0.19	39,39,39,39	0
54	MG	2A	3587	1/1	0.97	0.06	71,71,71,71	0
54	MG	1A	3292	1/1	0.97	0.08	49,49,49,49	0
54	MG	1A	3785	1/1	0.97	0.05	47,47,47,47	0
54	MG	1A	3059	1/1	0.97	0.12	21,21,21,21	0
54	MG	1A	3615	1/1	0.97	0.04	37,37,37,37	0
54	MG	2A	3595	1/1	0.97	0.08	57,57,57,57	0
54	MG	1A	3294	1/1	0.97	0.14	47,47,47,47	0
54	MG	1A	3030	1/1	0.97	0.05	39,39,39,39	0
54	MG	1A	3205	1/1	0.97	0.23	41,41,41,41	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	2A	3058	1/1	0.97	0.09	50,50,50,50	0
54	MG	1A	3248	1/1	0.97	0.10	54,54,54,54	0
54	MG	1A	3043	1/1	0.97	0.09	36,36,36,36	0
54	MG	1A	3897	1/1	0.97	0.18	39,39,39,39	0
54	MG	1V	202	1/1	0.97	0.21	38,38,38,38	0
54	MG	1A	3794	1/1	0.97	0.07	49,49,49,49	0
54	MG	2A	3222	1/1	0.97	0.14	53,53,53,53	0
54	MG	1A	3083	1/1	0.97	0.28	38,38,38,38	0
54	MG	1A	3546	1/1	0.97	0.12	26,26,26,26	0
54	MG	1W	202	1/1	0.97	0.15	39,39,39,39	0
54	MG	1A	3902	1/1	0.97	0.13	49,49,49,49	0
54	MG	1A	3143	1/1	0.97	0.07	31,31,31,31	0
54	MG	1A	3062	1/1	0.97	0.18	34,34,34,34	0
54	MG	1A	3907	1/1	0.97	0.08	65,65,65,65	0
54	MG	2A	3230	1/1	0.97	0.11	43,43,43,43	0
54	MG	2A	3614	1/1	0.97	0.09	73,73,73,73	0
54	MG	1A	3031	1/1	0.97	0.05	33,33,33,33	0
54	MG	1A	3706	1/1	0.97	0.22	55,55,55,55	0
54	MG	1A	3112	1/1	0.97	0.32	37,37,37,37	0
54	MG	1A	3553	1/1	0.97	0.08	32,32,32,32	0
54	MG	2A	3235	1/1	0.97	0.21	47,47,47,47	0
54	MG	1A	3628	1/1	0.97	0.22	40,40,40,40	0
54	MG	1A	3914	1/1	0.97	0.05	39,39,39,39	0
54	MG	2A	3634	1/1	0.97	0.06	54,54,54,54	0
54	MG	2A	3420	1/1	0.97	0.11	44,44,44,44	0
54	MG	1A	3629	1/1	0.97	0.07	44,44,44,44	0
54	MG	1A	4028	1/1	0.97	0.20	63,63,63,63	0
54	MG	1A	3917	1/1	0.97	0.04	33,33,33,33	0
54	MG	1A	3554	1/1	0.97	0.09	57,57,57,57	0
54	MG	1A	4031	1/1	0.97	0.05	57,57,57,57	0
54	MG	1A	3177	1/1	0.97	0.12	32,32,32,32	0
54	MG	2A	3083	1/1	0.97	0.09	45,45,45,45	0
54	MG	1A	3414	1/1	0.97	0.08	44,44,44,44	0
54	MG	1A	3714	1/1	0.97	0.20	46,46,46,46	0
54	MG	1A	3715	1/1	0.97	0.08	57,57,57,57	0
54	MG	2A	3087	1/1	0.97	0.17	55,55,55,55	0
54	MG	1A	3925	1/1	0.97	0.09	51,51,51,51	0
54	MG	1A	3032	1/1	0.97	0.05	24,24,24,24	0
54	MG	1A	3634	1/1	0.97	0.05	44,44,44,44	0
54	MG	1A	3416	1/1	0.97	0.05	30,30,30,30	0
54	MG	1A	3214	1/1	0.97	0.24	34,34,34,34	0
54	MG	1a	1856	1/1	0.97	0.06	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	3094	1/1	0.97	0.12	55,55,55,55	0
54	MG	1A	3259	1/1	0.97	0.07	34,34,34,34	0
54	MG	1A	3419	1/1	0.97	0.13	34,34,34,34	0
54	MG	1A	3640	1/1	0.97	0.12	55,55,55,55	0
54	MG	2A	3662	1/1	0.97	0.09	46,46,46,46	0
54	MG	1A	3641	1/1	0.97	0.09	25,25,25,25	0
54	MG	2A	3444	1/1	0.97	0.07	69,69,69,69	0
54	MG	1A	3420	1/1	0.97	0.05	35,35,35,35	0
54	MG	1A	3563	1/1	0.97	0.09	26,26,26,26	0
54	MG	2A	3263	1/1	0.97	0.06	72,72,72,72	0
54	MG	1a	1864	1/1	0.97	0.07	59,59,59,59	0
54	MG	1B	218	1/1	0.97	0.10	35,35,35,35	0
54	MG	1A	3564	1/1	0.97	0.04	33,33,33,33	0
54	MG	1A	3824	1/1	0.97	0.07	51,51,51,51	0
54	MG	1A	3825	1/1	0.97	0.11	53,53,53,53	0
54	MG	1A	3005	1/1	0.97	0.09	22,22,22,22	0
54	MG	1A	3149	1/1	0.97	0.07	49,49,49,49	0
54	MG	1A	3364	1/1	0.97	0.10	29,29,29,29	0
54	MG	1A	3945	1/1	0.97	0.05	75,75,75,75	0
54	MG	2a	3107	1/1	0.97	0.06	74,74,74,74	0
54	MG	2A	3273	1/1	0.97	0.12	20,20,20,20	0
54	MG	2A	3679	1/1	0.97	0.07	69,69,69,69	0
54	MG	2a	3112	1/1	0.97	0.07	71,71,71,71	0
54	MG	1a	1873	1/1	0.97	0.06	54,54,54,54	0
54	MG	2A	3681	1/1	0.97	0.06	60,60,60,60	0
54	MG	1A	3088	1/1	0.97	0.10	52,52,52,52	0
54	MG	1A	3831	1/1	0.97	0.21	42,42,42,42	0
54	MG	1A	3264	1/1	0.97	0.34	37,37,37,37	0
54	MG	1a	1738	1/1	0.97	0.12	47,47,47,47	0
54	MG	1a	1609	1/1	0.97	0.05	64,64,64,64	0
54	MG	1A	3017	1/1	0.97	0.31	39,39,39,39	0
54	MG	1D	302	1/1	0.97	0.09	60,60,60,60	0
54	MG	2a	3122	1/1	0.97	0.14	56,56,56,56	0
54	MG	1D	304	1/1	0.97	0.12	40,40,40,40	0
54	MG	1A	3090	1/1	0.97	0.08	43,43,43,43	0
54	MG	1D	306	1/1	0.97	0.16	44,44,44,44	0
54	MG	1D	308	1/1	0.97	0.06	46,46,46,46	0
54	MG	1A	3738	1/1	0.97	0.08	52,52,52,52	0
54	MG	2A	3696	1/1	0.97	0.06	55,55,55,55	0
54	MG	2a	3130	1/1	0.97	0.05	80,80,80,80	0
54	MG	2A	3697	1/1	0.97	0.09	35,35,35,35	0
54	MG	1A	3953	1/1	0.97	0.06	31,31,31,31	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	2A	3475	1/1	0.97	0.12	57,57,57,57	0
54	MG	2A	3476	1/1	0.97	0.06	74,74,74,74	0
54	MG	2a	3135	1/1	0.97	0.05	72,72,72,72	0
54	MG	1A	3431	1/1	0.97	0.10	31,31,31,31	0
54	MG	2A	3478	1/1	0.97	0.05	30,30,30,30	0
54	MG	2a	3139	1/1	0.97	0.06	78,78,78,78	0
54	MG	2A	3703	1/1	0.97	0.10	52,52,52,52	0
54	MG	1A	3372	1/1	0.97	0.07	31,31,31,31	0
54	MG	2A	3130	1/1	0.97	0.05	36,36,36,36	0
54	MG	1a	1751	1/1	0.97	0.11	59,59,59,59	0
54	MG	1A	3118	1/1	0.97	0.08	46,46,46,46	0
54	MG	1A	3743	1/1	0.97	0.05	35,35,35,35	0
54	MG	2A	3709	1/1	0.97	0.11	64,64,64,64	0
54	MG	2a	3147	1/1	0.97	0.06	76,76,76,76	0
54	MG	1D	316	1/1	0.97	0.09	63,63,63,63	0
54	MG	2A	3711	1/1	0.97	0.05	55,55,55,55	0
54	MG	2A	3299	1/1	0.97	0.14	42,42,42,42	0
54	MG	1D	317	1/1	0.97	0.06	47,47,47,47	0
54	MG	2A	3301	1/1	0.97	0.06	48,48,48,48	0
54	MG	1A	3958	1/1	0.97	0.05	58,58,58,58	0
54	MG	1A	3576	1/1	0.97	0.09	62,62,62,62	0
54	MG	1l	201	1/1	0.97	0.13	62,62,62,62	0
54	MG	2A	3305	1/1	0.97	0.07	46,46,46,46	0
54	MG	2A	3306	1/1	0.97	0.06	48,48,48,48	0
54	MG	1E	302	1/1	0.97	0.20	44,44,44,44	0
54	MG	2A	3142	1/1	0.97	0.17	42,42,42,42	0
54	MG	2A	3143	1/1	0.97	0.10	42,42,42,42	0
54	MG	2A	3311	1/1	0.97	0.08	62,62,62,62	0
54	MG	1A	3268	1/1	0.97	0.13	43,43,43,43	0
54	MG	1A	3375	1/1	0.97	0.06	36,36,36,36	0
54	MG	2A	3146	1/1	0.97	0.18	76,76,76,76	0
54	MG	1A	3050	1/1	0.97	0.18	55,55,55,55	0
54	MG	2a	3169	1/1	0.97	0.08	79,79,79,79	0
54	MG	2a	3170	1/1	0.97	0.06	71,71,71,71	0
54	MG	1E	307	1/1	0.97	0.09	25,25,25,25	0
54	MG	2A	3149	1/1	0.97	0.10	35,35,35,35	0
54	MG	1A	3505	1/1	0.97	0.10	48,48,48,48	0
54	MG	1A	3024	1/1	0.97	0.08	24,24,24,24	0
54	MG	2a	3176	1/1	0.97	0.06	67,67,67,67	0
54	MG	1a	1633	1/1	0.97	0.12	41,41,41,41	0
54	MG	1a	1634	1/1	0.97	0.09	48,48,48,48	0
54	MG	1E	310	1/1	0.97	0.09	60,60,60,60	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	2A	3325	1/1	0.97	0.09	32,32,32,32	0
54	MG	1A	3846	1/1	0.97	0.12	51,51,51,51	0
54	MG	1F	304	1/1	0.97	0.23	40,40,40,40	0
54	MG	1A	3187	1/1	0.97	0.21	42,42,42,42	0
54	MG	1F	306	1/1	0.97	0.12	35,35,35,35	0
54	MG	2F	302	1/1	0.97	0.05	47,47,47,47	0
54	MG	1A	3379	1/1	0.97	0.06	24,24,24,24	0
54	MG	2F	304	1/1	0.97	0.23	50,50,50,50	0
54	MG	1A	3025	1/1	0.97	0.26	48,48,48,48	0
54	MG	1F	311	1/1	0.97	0.06	40,40,40,40	0
55	HGR	1A	4032	36/36	0.97	0.08	25,29,35,40	0
54	MG	2A	3519	1/1	0.97	0.07	59,59,59,59	0
54	MG	1A	3095	1/1	0.97	0.17	43,43,43,43	0
54	MG	1A	3757	1/1	0.97	0.06	64,64,64,64	0
54	MG	1A	3855	1/1	0.97	0.04	51,51,51,51	0
54	MG	1A	3274	1/1	0.97	0.05	44,44,44,44	0
54	MG	2Q	201	1/1	0.97	0.07	63,63,63,63	0
54	MG	1A	3446	1/1	0.97	0.10	31,31,31,31	0
54	MG	2A	3168	1/1	0.97	0.06	55,55,55,55	0
54	MG	2A	3528	1/1	0.97	0.07	66,66,66,66	0
54	MG	1A	3070	1/1	0.97	0.25	37,37,37,37	0
54	MG	1A	3514	1/1	0.97	0.07	72,72,72,72	0
54	MG	1a	1650	1/1	0.97	0.11	55,55,55,55	0
54	MG	1A	3515	1/1	0.97	0.05	33,33,33,33	0
54	MG	1A	3861	1/1	0.97	0.11	45,45,45,45	0
59	ZN	2n	3102	1/1	0.97	0.07	103,103,103,103	0
54	MG	2A	3165	1/1	0.98	0.20	46,46,46,46	0
54	MG	1A	3735	1/1	0.98	0.05	46,46,46,46	0
54	MG	2A	3673	1/1	0.98	0.03	53,53,53,53	0
54	MG	1A	3796	1/1	0.98	0.07	40,40,40,40	0
54	MG	1A	3533	1/1	0.98	0.07	25,25,25,25	0
54	MG	1A	3864	1/1	0.98	0.04	39,39,39,39	0
54	MG	1A	3276	1/1	0.98	0.08	32,32,32,32	0
54	MG	2a	3053	1/1	0.98	0.05	64,64,64,64	0
54	MG	2A	3276	1/1	0.98	0.07	42,42,42,42	0
54	MG	2A	3521	1/1	0.98	0.09	48,48,48,48	0
54	MG	1A	3135	1/1	0.98	0.17	35,35,35,35	0
54	MG	2A	3523	1/1	0.98	0.13	34,34,34,34	0
54	MG	1A	3684	1/1	0.98	0.16	48,48,48,48	0
54	MG	1A	3366	1/1	0.98	0.04	32,32,32,32	0
54	MG	1A	3949	1/1	0.98	0.05	51,51,51,51	0
54	MG	2A	3400	1/1	0.98	0.05	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	3230	1/1	0.98	0.19	44,44,44,44	0
54	MG	2A	3176	1/1	0.98	0.06	71,71,71,71	0
54	MG	1H	202	1/1	0.98	0.06	58,58,58,58	0
54	MG	2A	3690	1/1	0.98	0.04	85,85,85,85	0
54	MG	1A	3742	1/1	0.98	0.04	56,56,56,56	0
54	MG	2A	3285	1/1	0.98	0.04	42,42,42,42	0
54	MG	1A	3872	1/1	0.98	0.08	32,32,32,32	0
54	MG	2A	3287	1/1	0.98	0.07	38,38,38,38	0
54	MG	1A	3368	1/1	0.98	0.10	46,46,46,46	0
54	MG	1A	3744	1/1	0.98	0.05	41,41,41,41	0
54	MG	1A	3119	1/1	0.98	0.13	34,34,34,34	0
54	MG	1P	201	1/1	0.98	0.30	39,39,39,39	0
54	MG	2A	3539	1/1	0.98	0.05	76,76,76,76	0
54	MG	2A	3412	1/1	0.98	0.06	57,57,57,57	0
54	MG	1A	3746	1/1	0.98	0.04	49,49,49,49	0
54	MG	1A	3082	1/1	0.98	0.17	34,34,34,34	0
54	MG	1A	3371	1/1	0.98	0.09	58,58,58,58	0
54	MG	1A	3256	1/1	0.98	0.06	41,41,41,41	0
54	MG	2A	3417	1/1	0.98	0.05	42,42,42,42	0
54	MG	1A	3121	1/1	0.98	0.10	27,27,27,27	0
54	MG	1A	3410	1/1	0.98	0.05	34,34,34,34	0
54	MG	1A	3338	1/1	0.98	0.09	41,41,41,41	0
54	MG	1A	3644	1/1	0.98	0.07	28,28,28,28	0
54	MG	2A	3422	1/1	0.98	0.05	48,48,48,48	0
54	MG	1A	3502	1/1	0.98	0.05	31,31,31,31	0
54	MG	1A	3755	1/1	0.98	0.09	46,46,46,46	0
54	MG	2A	3553	1/1	0.98	0.08	60,60,60,60	0
54	MG	2a	3089	1/1	0.98	0.05	77,77,77,77	0
54	MG	1B	212	1/1	0.98	0.08	47,47,47,47	0
54	MG	1A	3548	1/1	0.98	0.05	45,45,45,45	0
54	MG	1A	3194	1/1	0.98	0.14	39,39,39,39	0
54	MG	1A	3122	1/1	0.98	0.06	29,29,29,29	0
54	MG	2A	3559	1/1	0.98	0.14	58,58,58,58	0
54	MG	2a	3095	1/1	0.98	0.07	53,53,53,53	0
54	MG	2A	3095	1/1	0.98	0.05	45,45,45,45	0
54	MG	1A	3094	1/1	0.98	0.06	40,40,40,40	0
54	MG	1A	3821	1/1	0.98	0.09	55,55,55,55	0
54	MG	1A	3287	1/1	0.98	0.10	17,17,17,17	0
54	MG	1A	3823	1/1	0.98	0.05	42,42,42,42	0
54	MG	2A	3004	1/1	0.98	0.06	43,43,43,43	0
54	MG	2A	3566	1/1	0.98	0.04	57,57,57,57	0
54	MG	1A	3761	1/1	0.98	0.07	26,26,26,26	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	2A	3568	1/1	0.98	0.04	71,71,71,71	0
54	MG	2A	3102	1/1	0.98	0.06	33,33,33,33	0
54	MG	2B	218	1/1	0.98	0.09	66,66,66,66	0
54	MG	2D	301	1/1	0.98	0.19	49,49,49,49	0
54	MG	2a	3108	1/1	0.98	0.16	61,61,61,61	0
54	MG	2D	302	1/1	0.98	0.08	52,52,52,52	0
54	MG	2a	3110	1/1	0.98	0.06	75,75,75,75	0
54	MG	2A	3315	1/1	0.98	0.07	32,32,32,32	0
54	MG	2A	3316	1/1	0.98	0.11	32,32,32,32	0
54	MG	1B	222	1/1	0.98	0.04	55,55,55,55	0
54	MG	1A	3142	1/1	0.98	0.06	43,43,43,43	0
54	MG	1A	3013	1/1	0.98	0.08	29,29,29,29	0
54	MG	1A	3239	1/1	0.98	0.28	39,39,39,39	0
54	MG	2A	3579	1/1	0.98	0.05	70,70,70,70	0
54	MG	1A	3705	1/1	0.98	0.05	58,58,58,58	0
54	MG	2E	302	1/1	0.98	0.14	45,45,45,45	0
54	MG	1A	3604	1/1	0.98	0.08	43,43,43,43	0
54	MG	2E	304	1/1	0.98	0.10	30,30,30,30	0
54	MG	1U	203	1/1	0.98	0.38	43,43,43,43	0
54	MG	1A	3830	1/1	0.98	0.25	44,44,44,44	0
54	MG	2A	3214	1/1	0.98	0.06	67,67,67,67	0
54	MG	2A	3326	1/1	0.98	0.05	33,33,33,33	0
54	MG	2A	3014	1/1	0.98	0.06	51,51,51,51	0
54	MG	1A	3382	1/1	0.98	0.13	33,33,33,33	0
54	MG	1A	3905	1/1	0.98	0.06	29,29,29,29	0
54	MG	2A	3592	1/1	0.98	0.07	65,65,65,65	0
54	MG	1A	3240	1/1	0.98	0.18	36,36,36,36	0
54	MG	2A	3594	1/1	0.98	0.04	48,48,48,48	0
54	MG	1D	303	1/1	0.98	0.09	40,40,40,40	0
54	MG	1A	3096	1/1	0.98	0.09	24,24,24,24	0
54	MG	1A	3909	1/1	0.98	0.03	52,52,52,52	0
54	MG	1A	3423	1/1	0.98	0.07	28,28,28,28	0
54	MG	1A	3466	1/1	0.98	0.11	57,57,57,57	0
54	MG	1D	309	1/1	0.98	0.13	36,36,36,36	0
54	MG	1A	3073	1/1	0.98	0.06	41,41,41,41	0
54	MG	2A	3123	1/1	0.98	0.19	44,44,44,44	0
54	MG	1A	3516	1/1	0.98	0.07	28,28,28,28	0
54	MG	1X	101	1/1	0.98	0.11	43,43,43,43	0
54	MG	2A	3464	1/1	0.98	0.07	66,66,66,66	0
54	MG	1A	3612	1/1	0.98	0.09	27,27,27,27	0
54	MG	1A	3993	1/1	0.98	0.09	63,63,63,63	0
54	MG	10	101	1/1	0.98	0.09	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	3350	1/1	0.98	0.08	54,54,54,54	0
54	MG	2A	3346	1/1	0.98	0.08	57,57,57,57	0
54	MG	2a	3150	1/1	0.98	0.10	54,54,54,54	0
54	MG	1A	3074	1/1	0.98	0.06	36,36,36,36	0
54	MG	2A	3349	1/1	0.98	0.09	44,44,44,44	0
54	MG	1A	3566	1/1	0.98	0.05	36,36,36,36	0
54	MG	1A	3352	1/1	0.98	0.09	25,25,25,25	0
54	MG	2A	3615	1/1	0.98	0.04	82,82,82,82	0
54	MG	1A	3428	1/1	0.98	0.05	27,27,27,27	0
54	MG	2A	3617	1/1	0.98	0.06	64,64,64,64	0
54	MG	1A	3921	1/1	0.98	0.05	21,21,21,21	0
54	MG	2A	3619	1/1	0.98	0.05	53,53,53,53	0
54	MG	2A	3620	1/1	0.98	0.04	71,71,71,71	0
54	MG	1A	3295	1/1	0.98	0.06	48,48,48,48	0
54	MG	1E	303	1/1	0.98	0.09	43,43,43,43	0
54	MG	2A	3628	1/1	0.98	0.05	48,48,48,48	0
54	MG	1A	3052	1/1	0.98	0.26	44,44,44,44	0
54	MG	2a	3166	1/1	0.98	0.11	55,55,55,55	0
54	MG	2A	3480	1/1	0.98	0.05	42,42,42,42	0
54	MG	13	101	1/1	0.98	0.12	33,33,33,33	0
54	MG	2a	3010	1/1	0.98	0.05	54,54,54,54	0
54	MG	2A	3139	1/1	0.98	0.06	42,42,42,42	0
54	MG	1A	3007	1/1	0.98	0.04	44,44,44,44	0
54	MG	2A	3360	1/1	0.98	0.08	48,48,48,48	0
54	MG	2a	3014	1/1	0.98	0.03	61,61,61,61	0
54	MG	2a	3174	1/1	0.98	0.05	64,64,64,64	0
54	MG	2A	3141	1/1	0.98	0.09	59,59,59,59	0
54	MG	1A	3047	1/1	0.98	0.12	16,16,16,16	0
54	MG	2A	3487	1/1	0.98	0.11	43,43,43,43	0
54	MG	1A	3849	1/1	0.98	0.05	41,41,41,41	0
54	MG	2A	3247	1/1	0.98	0.09	23,23,23,23	0
54	MG	2A	3642	1/1	0.98	0.04	42,42,42,42	0
54	MG	1A	3726	1/1	0.98	0.07	49,49,49,49	0
54	MG	1a	1857	1/1	0.98	0.09	72,72,72,72	0
54	MG	1A	3929	1/1	0.98	0.05	59,59,59,59	0
54	MG	15	104	1/1	0.98	0.17	29,29,29,29	0
54	MG	1A	3786	1/1	0.98	0.05	36,36,36,36	0
54	MG	2A	3649	1/1	0.98	0.04	60,60,60,60	0
54	MG	1a	1767	1/1	0.98	0.07	53,53,53,53	0
54	MG	2A	3049	1/1	0.98	0.16	52,52,52,52	0
54	MG	2A	3497	1/1	0.98	0.06	62,62,62,62	0
54	MG	1F	301	1/1	0.98	0.07	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	1F	302	1/1	0.98	0.13	40,40,40,40	0
54	MG	1A	3357	1/1	0.98	0.07	25,25,25,25	0
54	MG	1A	3078	1/1	0.98	0.15	45,45,45,45	0
54	MG	2A	3377	1/1	0.98	0.10	39,39,39,39	0
54	MG	1A	3359	1/1	0.98	0.06	33,33,33,33	0
54	MG	1A	3438	1/1	0.98	0.05	36,36,36,36	0
54	MG	1A	3003	1/1	0.98	0.04	27,27,27,27	0
54	MG	17	105	1/1	0.98	0.17	42,42,42,42	0
54	MG	1F	308	1/1	0.98	0.20	30,30,30,30	0
54	MG	1F	309	1/1	0.98	0.16	35,35,35,35	0
54	MG	1A	3937	1/1	0.98	0.12	47,47,47,47	0
54	MG	1A	3049	1/1	0.98	0.03	27,27,27,27	0
54	MG	1A	3006	1/1	0.98	0.03	29,29,29,29	0
59	ZN	1n	104	1/1	0.98	0.04	74,74,74,74	0
59	ZN	2Y	202	1/1	0.98	0.04	93,93,93,93	0
54	MG	2A	3387	1/1	0.98	0.11	36,36,36,36	0
54	MG	1A	3399	1/1	0.98	0.05	29,29,29,29	0
60	SF4	1d	303	8/8	0.98	0.05	60,65,70,78	0
60	SF4	2d	501	8/8	0.98	0.05	67,82,83,88	0
54	MG	2A	3653	1/1	0.99	0.04	70,70,70,70	0
54	MG	2A	3589	1/1	0.99	0.09	44,44,44,44	0
54	MG	1A	3493	1/1	0.99	0.06	32,32,32,32	0
54	MG	1B	213	1/1	0.99	0.04	42,42,42,42	0
54	MG	2A	3344	1/1	0.99	0.03	36,36,36,36	0
54	MG	1A	3884	1/1	0.99	0.06	43,43,43,43	0
54	MG	1A	3976	1/1	0.99	0.06	26,26,26,26	0
54	MG	1A	3977	1/1	0.99	0.05	35,35,35,35	0
54	MG	2A	3348	1/1	0.99	0.02	38,38,38,38	0
54	MG	1A	4012	1/1	0.99	0.03	63,63,63,63	0
54	MG	1A	3263	1/1	0.99	0.17	34,34,34,34	0
54	MG	1A	3590	1/1	0.99	0.07	50,50,50,50	0
54	MG	1A	3915	1/1	0.99	0.03	55,55,55,55	0
54	MG	1A	3242	1/1	0.99	0.30	34,34,34,34	0
54	MG	2A	3308	1/1	0.99	0.09	50,50,50,50	0
54	MG	1A	3888	1/1	0.99	0.07	43,43,43,43	0
54	MG	1A	3434	1/1	0.99	0.05	42,42,42,42	0
54	MG	2a	3159	1/1	0.99	0.04	64,64,64,64	0
54	MG	1A	3305	1/1	0.99	0.13	25,25,25,25	0
54	MG	1A	3717	1/1	0.99	0.04	44,44,44,44	0
54	MG	11	103	1/1	0.99	0.06	53,53,53,53	0
54	MG	1A	3436	1/1	0.99	0.02	30,30,30,30	0
54	MG	2A	3103	1/1	0.99	0.06	68,68,68,68	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	1A	3330	1/1	0.99	0.09	21,21,21,21	0
54	MG	1A	3222	1/1	0.99	0.03	41,41,41,41	0
54	MG	2A	3364	1/1	0.99	0.03	62,62,62,62	0
54	MG	2A	3557	1/1	0.99	0.04	49,49,49,49	0
54	MG	2A	3274	1/1	0.99	0.06	51,51,51,51	0
54	MG	1A	3924	1/1	0.99	0.03	42,42,42,42	0
54	MG	1A	3868	1/1	0.99	0.06	54,54,54,54	0
54	MG	1A	3286	1/1	0.99	0.10	22,22,22,22	0
54	MG	2A	3463	1/1	0.99	0.06	37,37,37,37	0
54	MG	1A	3762	1/1	0.99	0.11	38,38,38,38	0
54	MG	1a	1852	1/1	0.99	0.03	47,47,47,47	0
54	MG	2A	3622	1/1	0.99	0.03	66,66,66,66	0
54	MG	2A	3623	1/1	0.99	0.06	35,35,35,35	0
54	MG	2A	3688	1/1	0.99	0.04	52,52,52,52	0
54	MG	2A	3624	1/1	0.99	0.05	40,40,40,40	0
54	MG	2A	3625	1/1	0.99	0.04	60,60,60,60	0
54	MG	1a	1853	1/1	0.99	0.05	61,61,61,61	0
54	MG	1A	3847	1/1	0.99	0.04	34,34,34,34	0
54	MG	1A	3549	1/1	0.99	0.06	33,33,33,33	0
54	MG	2A	3469	1/1	0.99	0.03	50,50,50,50	0
54	MG	2A	3630	1/1	0.99	0.11	57,57,57,57	0
54	MG	2A	3569	1/1	0.99	0.03	53,53,53,53	0
54	MG	2k	201	1/1	0.99	0.10	57,57,57,57	0
54	MG	1A	3900	1/1	0.99	0.03	27,27,27,27	0
54	MG	2A	3633	1/1	0.99	0.03	58,58,58,58	0
54	MG	2A	3571	1/1	0.99	0.05	42,42,42,42	0
54	MG	1D	307	1/1	0.99	0.03	19,19,19,19	0
54	MG	1A	3723	1/1	0.99	0.03	36,36,36,36	0
54	MG	2A	3574	1/1	0.99	0.04	41,41,41,41	0
54	MG	2X	101	1/1	0.99	0.07	63,63,63,63	0
54	MG	1A	3932	1/1	0.99	0.06	54,54,54,54	0
54	MG	1A	3668	1/1	0.99	0.04	50,50,50,50	0
54	MG	1A	3474	1/1	0.99	0.04	27,27,27,27	0
54	MG	1A	3966	1/1	0.99	0.03	49,49,49,49	0
54	MG	1A	3852	1/1	0.99	0.06	23,23,23,23	0
54	MG	2A	3580	1/1	0.99	0.06	47,47,47,47	0
54	MG	1A	3475	1/1	0.99	0.06	32,32,32,32	0
54	MG	2A	3645	1/1	0.99	0.03	47,47,47,47	0
54	MG	1A	3906	1/1	0.99	0.05	42,42,42,42	0
59	ZN	1Y	202	1/1	0.99	0.02	62,62,62,62	0
54	MG	1A	3347	1/1	0.99	0.08	30,30,30,30	0
59	ZN	15	109	1/1	0.99	0.02	52,52,52,52	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
59	ZN	16	501	1/1	0.99	0.05	47,47,47,47	0
54	MG	1a	1748	1/1	0.99	0.11	42,42,42,42	0
54	MG	1A	3490	1/1	0.99	0.03	49,49,49,49	0
54	MG	2a	3138	1/1	0.99	0.07	52,52,52,52	0
59	ZN	25	102	1/1	0.99	0.03	68,68,68,68	0
59	ZN	29	501	1/1	0.99	0.03	73,73,73,73	0
54	MG	2A	3650	1/1	0.99	0.04	44,44,44,44	0
54	MG	1A	3141	1/1	0.99	0.13	26,26,26,26	0
54	MG	1A	3422	1/1	0.99	0.08	23,23,23,23	0
54	MG	2A	3621	1/1	1.00	0.02	66,66,66,66	0
59	ZN	19	104	1/1	1.00	0.10	65,65,65,65	0
54	MG	1A	3534	1/1	1.00	0.07	31,31,31,31	0
54	MG	1A	3361	1/1	1.00	0.05	36,36,36,36	0
54	MG	1A	3499	1/1	1.00	0.07	49,49,49,49	0
54	MG	1A	3882	1/1	1.00	0.07	33,33,33,33	0
59	ZN	26	501	1/1	1.00	0.02	65,65,65,65	0
54	MG	1A	3637	1/1	1.00	0.06	32,32,32,32	0
54	MG	1A	3467	1/1	1.00	0.02	27,27,27,27	0
54	MG	2a	3124	1/1	1.00	0.03	60,60,60,60	0
54	MG	2A	3585	1/1	1.00	0.03	43,43,43,43	0

5.5 Other polymers

There are no such residues in this entry.