



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 28, 2026 – 01:54 PM UTC

PDB ID : 8VTW / pdb_00008vtw
Title : Crystal structure of the wild-type *Thermus thermophilus* 70S ribosome in complex with macrolone MCX-128 and protein Y at 2.35Å resolution
Authors : Aleksandrova, E.V.; Ma, C.-X.; Klepacki, D.; Alizadeh, F.; Vazquez-Laslop, N.; Liang, J.-H.; Polikanov, Y.S.; Mankin, A.S.
Deposited on : 2024-01-27
Resolution : 2.35 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

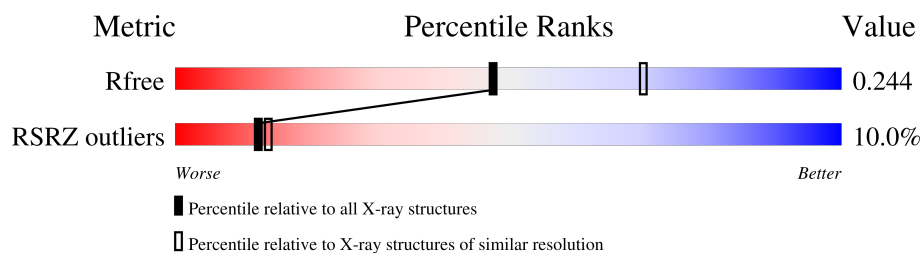
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.35 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	1596 (2.36-2.36)
RSRZ outliers	180081	1598 (2.36-2.36)

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	1675	-	-	-	X
54	MG	2A	3245	-	-	-	X
54	MG	2a	3047	-	-	-	X
54	MG	2a	3058	-	-	-	X
54	MG	2a	3080	-	-	-	X

2 Entry composition

There are 60 unique types of molecules in this entry. The entry contains 296775 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
22	10	83	Total	C	N	O	S	0	0	0
			653	404	139	109	1			
22	20	83	Total	C	N	O	S	0	0	0
			650	401	139	109	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	996	Total	Mg	0	0
			996	996		
54	1B	31	Total	Mg	0	0
			31	31		
54	1D	16	Total	Mg	0	0
			16	16		
54	1E	11	Total	Mg	0	0
			11	11		
54	1F	17	Total	Mg	0	0
			17	17		
54	1G	4	Total	Mg	0	0
			4	4		
54	1H	2	Total	Mg	0	0
			2	2		
54	1N	4	Total	Mg	0	0
			4	4		
54	1O	1	Total	Mg	0	0
			1	1		
54	1P	4	Total	Mg	0	0
			4	4		
54	1Q	4	Total	Mg	0	0
			4	4		
54	1R	5	Total	Mg	0	0
			5	5		
54	1T	6	Total	Mg	0	0
			6	6		
54	1U	5	Total	Mg	0	0
			5	5		
54	1V	6	Total	Mg	0	0
			6	6		
54	1W	5	Total	Mg	0	0
			5	5		
54	1X	1	Total	Mg	0	0
			1	1		
54	1Y	1	Total	Mg	0	0
			1	1		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
54	1Z	1	Total 1	Mg 1	0	0
54	10	9	Total 9	Mg 9	0	0
54	11	5	Total 5	Mg 5	0	0
54	12	1	Total 1	Mg 1	0	0
54	13	3	Total 3	Mg 3	0	0
54	15	9	Total 9	Mg 9	0	0
54	17	5	Total 5	Mg 5	0	0
54	18	2	Total 2	Mg 2	0	0
54	19	2	Total 2	Mg 2	0	0
54	1a	267	Total 267	Mg 267	0	0
54	1b	1	Total 1	Mg 1	0	0
54	1d	5	Total 5	Mg 5	0	0
54	1e	2	Total 2	Mg 2	0	0
54	1f	1	Total 1	Mg 1	0	0
54	1g	2	Total 2	Mg 2	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	2	Total 2	Mg 2	0	0

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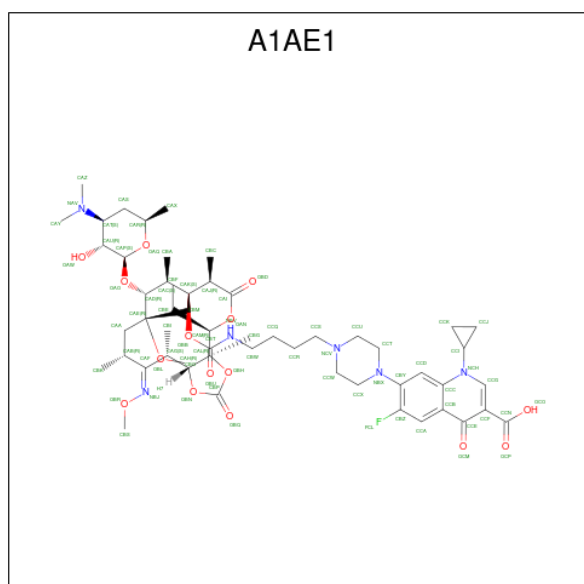
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
54	1r	1	Total 1	Mg 1	0	0
54	1t	2	Total 2	Mg 2	0	0
54	1y	2	Total 2	Mg 2	0	0
54	2A	726	Total 726	Mg 726	0	0
54	2B	18	Total 18	Mg 18	0	0
54	2D	12	Total 12	Mg 12	0	0
54	2E	7	Total 7	Mg 7	0	0
54	2F	4	Total 4	Mg 4	0	0
54	2G	1	Total 1	Mg 1	0	0
54	2I	1	Total 1	Mg 1	0	0
54	2N	1	Total 1	Mg 1	0	0
54	2O	1	Total 1	Mg 1	0	0
54	2P	2	Total 2	Mg 2	0	0
54	2Q	2	Total 2	Mg 2	0	0
54	2R	2	Total 2	Mg 2	0	0
54	2T	4	Total 4	Mg 4	0	0
54	2V	3	Total 3	Mg 3	0	0
54	2W	2	Total 2	Mg 2	0	0
54	20	3	Total 3	Mg 3	0	0
54	23	1	Total 1	Mg 1	0	0
54	25	1	Total 1	Mg 1	0	0

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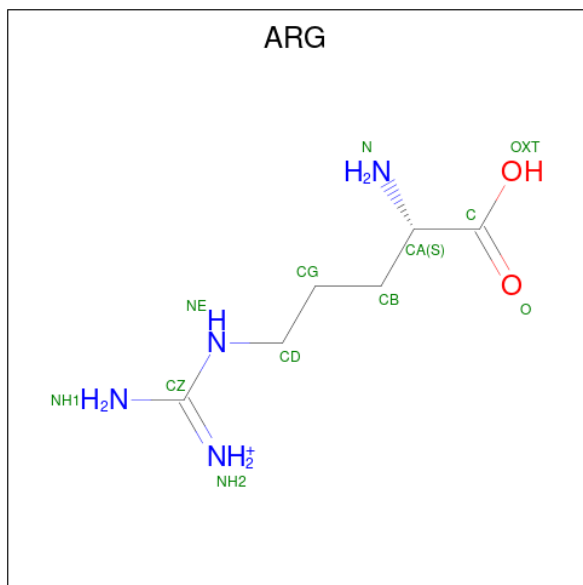
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
54	27	3	Total 3	Mg 3	0	0
54	28	1	Total 1	Mg 1	0	0
54	2a	181	Total 181	Mg 181	0	0
54	2e	1	Total 1	Mg 1	0	0
54	2f	2	Total 2	Mg 2	0	0
54	2h	1	Total 1	Mg 1	0	0
54	2j	1	Total 1	Mg 1	0	0
54	2p	1	Total 1	Mg 1	0	0
54	2r	1	Total 1	Mg 1	0	0
54	2t	1	Total 1	Mg 1	0	0

- Molecule 55 is 1-cyclopropyl-7-(4-{4-[({(3aR,4R,7R,8S,9S,10R,11R,13R,14E,15S,15aR)-10-[(2S,3R,4S,6R)-4-(dimethylamino)-3-hydroxy-6-methyloxan-2-yl]oxy}-4-ethyl-11-methoxy-14-(methoxyimino)-3a,7,9,11,13,15-hexamethyl-2,6-dioxododecahydro-2H,4H-[1,3]dioxolo[4,5-c]oxacyclotetradecin-8-yl]oxy}carbonyl)amino]butyl}piperazin-1-yl)-6-fluoro-4-oxo-1,4-dihydroquinoline-3-carboxylic acid (non-preferred name) (CCD ID: A1AE1) (formula: C₅₄H₈₁FN₆O₁₅) (labeled as "Ligand of Interest" by depositor).



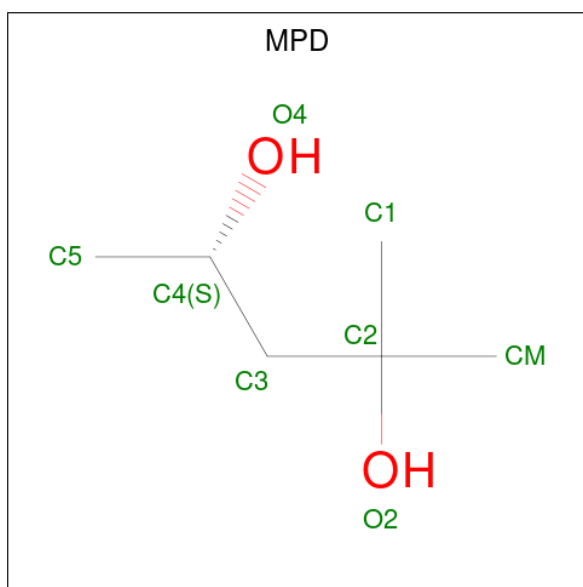
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
55	1A	1	Total	C	F	N	O	0	0
			76	54	1	6	15		
55	2A	1	Total	C	F	N	O	0	0
			76	54	1	6	15		

- Molecule 56 is ARGinine (CCD ID: ARG) (formula: $C_6H_{15}N_4O_2$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
56	1A	1	Total	C	N	O	0	0
			12	6	4	2		
56	1B	1	Total	C	N	O	0	0
			12	6	4	2		

- 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	2B	1	Total	C	O	0	0
			8	6	2		

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

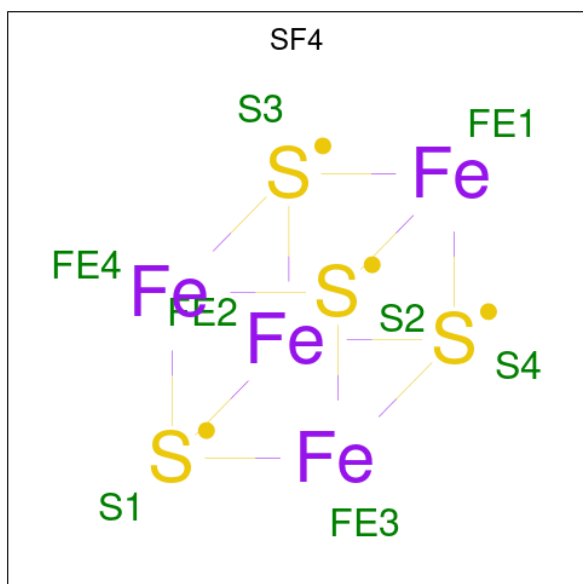
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
58	1Y	1	Total	Zn	0	0
			1	1		
58	14	1	Total	Zn	0	0
			1	1		
58	15	1	Total	Zn	0	0
			1	1		
58	16	1	Total	Zn	0	0
			1	1		
58	19	1	Total	Zn	0	0
			1	1		
58	1n	1	Total	Zn	0	0
			1	1		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
58	2Y	1	Total	Zn	0	0
			1	1		
58	24	1	Total	Zn	0	0
			1	1		
58	25	1	Total	Zn	0	0
			1	1		
58	26	1	Total	Zn	0	0
			1	1		
58	29	1	Total	Zn	0	0
			1	1		
58	2n	1	Total	Zn	0	0
			1	1		

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



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

- Molecule 60 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
60	1A	3773	Total	O	0	0
			3773	3773		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
60	1B	85	Total 85	O 85	0	0
60	1D	105	Total 105	O 105	0	0
60	1E	67	Total 67	O 67	0	0
60	1F	60	Total 60	O 60	0	0
60	1G	13	Total 13	O 13	0	0
60	1H	10	Total 10	O 10	0	0
60	1I	3	Total 3	O 3	0	0
60	1N	46	Total 46	O 46	0	0
60	1O	26	Total 26	O 26	0	0
60	1P	61	Total 61	O 61	0	0
60	1Q	38	Total 38	O 38	0	0
60	1R	33	Total 33	O 33	0	0
60	1S	11	Total 11	O 11	0	0
60	1T	29	Total 29	O 29	0	0
60	1U	45	Total 45	O 45	0	0
60	1V	30	Total 30	O 30	0	0
60	1W	27	Total 27	O 27	0	0
60	1X	23	Total 23	O 23	0	0
60	1Y	14	Total 14	O 14	0	0
60	1Z	8	Total 8	O 8	0	0
60	10	22	Total 22	O 22	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
60	11	26	Total 26	O 26	0	0
60	12	9	Total 9	O 9	0	0
60	13	22	Total 22	O 22	0	0
60	14	1	Total 1	O 1	0	0
60	15	25	Total 25	O 25	0	0
60	16	16	Total 16	O 16	0	0
60	17	19	Total 19	O 19	0	0
60	18	27	Total 27	O 27	0	0
60	19	4	Total 4	O 4	0	0
60	1a	446	Total 446	O 446	0	0
60	1b	1	Total 1	O 1	0	0
60	1c	1	Total 1	O 1	0	0
60	1d	6	Total 6	O 6	0	0
60	1e	5	Total 5	O 5	0	0
60	1f	1	Total 1	O 1	0	0
60	1g	3	Total 3	O 3	0	0
60	1h	4	Total 4	O 4	0	0
60	1j	2	Total 2	O 2	0	0
60	1l	2	Total 2	O 2	0	0
60	1n	1	Total 1	O 1	0	0
60	1o	4	Total 4	O 4	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
60	1p	1	Total 1	O 1	0	0
60	1y	2	Total 2	O 2	0	0
60	2A	1939	Total 1939	O 1939	0	0
60	2B	31	Total 31	O 31	0	0
60	2D	45	Total 45	O 45	0	0
60	2E	23	Total 23	O 23	0	0
60	2F	16	Total 16	O 16	0	0
60	2G	2	Total 2	O 2	0	0
60	2I	1	Total 1	O 1	0	0
60	2N	3	Total 3	O 3	0	0
60	2O	14	Total 14	O 14	0	0
60	2P	24	Total 24	O 24	0	0
60	2Q	7	Total 7	O 7	0	0
60	2R	14	Total 14	O 14	0	0
60	2S	1	Total 1	O 1	0	0
60	2T	7	Total 7	O 7	0	0
60	2U	12	Total 12	O 12	0	0
60	2V	3	Total 3	O 3	0	0
60	2W	15	Total 15	O 15	0	0
60	2X	8	Total 8	O 8	0	0
60	2Z	3	Total 3	O 3	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
60	20	7	Total	O	0	0
			7	7		
60	21	9	Total	O	0	0
			9	9		
60	23	2	Total	O	0	0
			2	2		
60	25	6	Total	O	0	0
			6	6		
60	26	5	Total	O	0	0
			5	5		
60	27	3	Total	O	0	0
			3	3		
60	28	9	Total	O	0	0
			9	9		
60	2a	259	Total	O	0	0
			259	259		
60	2e	2	Total	O	0	0
			2	2		
60	2l	3	Total	O	0	0
			3	3		
60	2n	1	Total	O	0	0
			1	1		
60	2o	2	Total	O	0	0
			2	2		
60	2p	1	Total	O	0	0
			1	1		
60	2r	4	Total	O	0	0
			4	4		
60	2t	3	Total	O	0	0
			3	3		

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

3 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	209.60Å 449.32Å 619.65Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	124.58 – 2.35 124.58 – 2.35	Depositor EDS
% Data completeness (in resolution range)	100.0 (124.58-2.35) 100.0 (124.58-2.35)	Depositor EDS
R_{merge}	0.19	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.19 (at 2.34Å)	Xtriage
Refinement program	PHENIX 1.8.2	Depositor
R, R_{free}	0.207 , 0.243 0.208 , 0.244	Depositor DCC
R_{free} test set	119915 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å ²)	49.6	Xtriage
Anisotropy	0.134	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 47.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.44$, $\langle L^2 \rangle = 0.27$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	296775	wwPDB-VP
Average B, all atoms (Å ²)	60.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.52% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

4 Model quality [i](#)

4.1 Standard geometry [i](#)

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

4.2 Too-close contacts [i](#)

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

4.3 Torsion angles [i](#)

4.3.1 Protein backbone [i](#)

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

4.3.2 Protein sidechains [i](#)

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

4.3.3 RNA [i](#)

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

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
32	4OC	2a	1402	32	20,23,24	0.76	0	25,32,35	0.94	1 (4%)
1	PSU	1A	2605	1	18,21,22	1.36	2 (11%)	21,30,33	1.95	4 (19%)
32	2MG	1a	1207	32	23,26,27	1.23	2 (8%)	33,38,41	2.36	10 (30%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
32	4OC	1a	1402	32	20,23,24	0.74	0	25,32,35	1.01	1 (4%)
1	PSU	2A	2605	1	18,21,22	1.32	3 (16%)	21,30,33	1.92	5 (23%)
1	PSU	1A	1911	1	18,21,22	1.37	2 (11%)	21,30,33	1.98	4 (19%)
32	5MC	2a	1400	32	19,22,23	1.68	3 (15%)	26,32,35	1.19	2 (7%)
32	5MC	2a	1407	32	19,22,23	1.60	3 (15%)	26,32,35	1.15	3 (11%)
1	PSU	2A	1911	1	18,21,22	1.42	3 (16%)	21,30,33	2.00	4 (19%)
32	UR3	2a	1498	32	19,22,23	1.00	1 (5%)	26,32,35	1.71	2 (7%)
32	PSU	2a	516	54,32	18,21,22	1.34	2 (11%)	21,30,33	2.07	5 (23%)
1	OMC	2A	1920	1	19,22,23	0.79	0	25,31,34	0.91	1 (4%)
32	MA6	2a	1518	32	23,26,27	0.40	0	33,38,41	2.01	9 (27%)
1	OMC	1A	1920	1	19,22,23	0.80	0	25,31,34	0.99	1 (4%)
32	5MC	1a	1400	32	19,22,23	1.81	3 (15%)	26,32,35	1.19	2 (7%)
1	5MU	2A	1939	1,54	19,22,23	1.39	6 (31%)	27,32,35	2.23	6 (22%)
1	5MC	2A	1962	1,54	19,22,23	1.61	3 (15%)	26,32,35	1.13	2 (7%)
32	5MC	1a	1407	32	19,22,23	1.80	3 (15%)	26,32,35	1.15	3 (11%)
32	G7M	2a	527	32	23,26,27	1.51	3 (13%)	34,39,42	1.66	5 (14%)
32	UR3	1a	1498	32	19,22,23	1.02	1 (5%)	26,32,35	1.84	4 (15%)
1	2MA	1A	2503	1,54	22,25,26	1.45	6 (27%)	32,37,40	2.36	9 (28%)
1	OMU	1A	2552	1,54	19,22,23	1.21	3 (15%)	25,31,34	1.80	5 (20%)
32	PSU	1a	516	54,32	18,21,22	1.35	2 (11%)	21,30,33	1.87	4 (19%)
32	5MC	2a	1404	32	19,22,23	1.75	3 (15%)	26,32,35	1.17	3 (11%)
1	2MA	2A	2503	1,54	22,25,26	1.41	4 (18%)	32,37,40	2.46	9 (28%)
1	OMU	2A	2552	1,54	19,22,23	1.15	2 (10%)	25,31,34	1.89	6 (24%)
32	G7M	1a	527	54,32	23,26,27	1.51	4 (17%)	34,39,42	1.69	5 (14%)
32	MA6	1a	1518	32	23,26,27	0.39	0	33,38,41	1.98	9 (27%)
1	5MU	1A	1915	1	19,22,23	1.44	5 (26%)	27,32,35	2.37	9 (33%)
32	MA6	1a	1519	32	23,26,27	0.41	0	33,38,41	2.00	9 (27%)
1	5MU	2A	1915	1	19,22,23	1.45	4 (21%)	27,32,35	2.21	9 (33%)
32	M2G	1a	966	32	24,27,28	1.29	3 (12%)	33,40,43	1.78	5 (15%)
32	5MC	1a	1404	32	19,22,23	1.64	3 (15%)	26,32,35	1.08	3 (11%)
43	0TD	2l	92	43	8,9,10	4.43	2 (25%)	6,11,13	3.95	2 (33%)
1	5MC	1A	1962	1	19,22,23	1.58	3 (15%)	26,32,35	1.15	4 (15%)
1	PSU	1A	1917	1	18,21,22	1.34	2 (11%)	21,30,33	1.89	4 (19%)
1	5MU	1A	1939	1,54	19,22,23	1.46	5 (26%)	27,32,35	2.14	6 (22%)
43	0TD	1l	92	43	8,9,10	4.60	2 (25%)	6,11,13	4.25	2 (33%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	OMG	1A	2251	1,54	23,26,27	1.30	3 (13%)	32,38,41	2.03	6 (18%)
32	5MC	1a	967	32	19,22,23	1.63	3 (15%)	26,32,35	1.09	2 (7%)
32	5MC	2a	967	32	19,22,23	1.83	3 (15%)	26,32,35	1.10	2 (7%)
1	5MC	1A	1942	1,54	19,22,23	1.57	3 (15%)	26,32,35	1.10	3 (11%)
1	PSU	2A	1917	1	18,21,22	1.31	2 (11%)	21,30,33	2.02	3 (14%)
1	5MC	2A	1942	1,54	19,22,23	1.66	3 (15%)	26,32,35	1.24	2 (7%)
32	2MG	2a	1207	32	23,26,27	1.22	2 (8%)	33,38,41	2.19	7 (21%)
32	MA6	2a	1519	32	23,26,27	0.40	0	33,38,41	2.11	9 (27%)
32	M2G	2a	966	32	24,27,28	1.28	3 (12%)	33,40,43	1.81	5 (15%)
1	OMG	2A	2251	1,54	23,26,27	1.18	3 (13%)	32,38,41	2.06	7 (21%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
32	4OC	2a	1402	32	-	3/9/29/30	0/2/2/2
1	PSU	1A	2605	1	-	0/7/25/26	0/2/2/2
32	2MG	1a	1207	32	-	2/9/27/28	0/3/3/3
32	4OC	1a	1402	32	-	0/9/29/30	0/2/2/2
1	PSU	2A	2605	1	-	0/7/25/26	0/2/2/2
1	PSU	1A	1911	1	-	0/7/25/26	0/2/2/2
32	5MC	2a	1400	32	-	0/7/25/26	0/2/2/2
32	5MC	2a	1407	32	-	0/7/25/26	0/2/2/2
1	PSU	2A	1911	1	-	0/7/25/26	0/2/2/2
32	UR3	2a	1498	32	-	0/7/25/26	0/2/2/2
32	PSU	2a	516	54,32	-	2/7/25/26	0/2/2/2
1	OMC	2A	1920	1	-	0/9/27/28	0/2/2/2
32	MA6	2a	1518	32	-	1/11/29/30	0/3/3/3
1	OMC	1A	1920	1	-	1/9/27/28	0/2/2/2
32	5MC	1a	1400	32	-	1/7/25/26	0/2/2/2
1	5MU	2A	1939	1,54	-	0/7/25/26	0/2/2/2
1	5MC	2A	1962	1,54	-	0/7/25/26	0/2/2/2
32	5MC	1a	1407	32	-	0/7/25/26	0/2/2/2
32	G7M	2a	527	32	-	0/7/25/26	0/3/3/3
32	UR3	1a	1498	32	-	0/7/25/26	0/2/2/2
1	2MA	1A	2503	1,54	-	1/7/25/26	0/3/3/3
1	OMU	1A	2552	1,54	-	0/9/27/28	0/2/2/2
32	PSU	1a	516	54,32	-	0/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
32	5MC	2a	1404	32	-	0/7/25/26	0/2/2/2
1	2MA	2A	2503	1,54	-	0/7/25/26	0/3/3/3
1	OMU	2A	2552	1,54	-	0/9/27/28	0/2/2/2
32	G7M	1a	527	54,32	-	3/7/25/26	0/3/3/3
32	MA6	1a	1518	32	-	0/11/29/30	0/3/3/3
1	5MU	1A	1915	1	-	2/7/25/26	0/2/2/2
32	MA6	1a	1519	32	-	2/11/29/30	0/3/3/3
1	5MU	2A	1915	1	-	2/7/25/26	0/2/2/2
32	M2G	1a	966	32	-	0/11/29/30	0/3/3/3
32	5MC	1a	1404	32	-	0/7/25/26	0/2/2/2
43	0TD	2l	92	43	-	3/7/12/14	-
1	5MC	1A	1962	1	-	0/7/25/26	0/2/2/2
1	PSU	1A	1917	1	-	0/7/25/26	0/2/2/2
1	5MU	1A	1939	1,54	-	0/7/25/26	0/2/2/2
43	0TD	1l	92	43	-	3/7/12/14	-
1	OMG	1A	2251	1,54	-	0/9/27/28	0/3/3/3
32	5MC	1a	967	32	-	0/7/25/26	0/2/2/2
32	5MC	2a	967	32	-	0/7/25/26	0/2/2/2
1	5MC	1A	1942	1,54	-	0/7/25/26	0/2/2/2
1	PSU	2A	1917	1	-	0/7/25/26	0/2/2/2
1	5MC	2A	1942	1,54	-	0/7/25/26	0/2/2/2
32	2MG	2a	1207	32	-	0/9/27/28	0/3/3/3
32	MA6	2a	1519	32	-	3/11/29/30	0/3/3/3
32	M2G	2a	966	32	-	0/11/29/30	0/3/3/3
1	OMG	2A	2251	1,54	-	0/9/27/28	0/3/3/3

All (118) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
43	1l	92	0TD	CB-SB	-12.44	1.69	1.82
43	2l	92	0TD	CB-SB	-11.89	1.70	1.82
32	2a	967	5MC	C5-C4	6.76	1.49	1.44
32	1a	1407	5MC	C5-C4	6.70	1.49	1.44
32	1a	1400	5MC	C5-C4	6.69	1.49	1.44
32	2a	1404	5MC	C5-C4	6.36	1.48	1.44
32	2a	1400	5MC	C5-C4	6.07	1.48	1.44
32	1a	1404	5MC	C5-C4	5.97	1.48	1.44
1	2A	1942	5MC	C5-C4	5.94	1.48	1.44
32	1a	967	5MC	C5-C4	5.88	1.48	1.44
1	2A	1962	5MC	C5-C4	5.83	1.48	1.44
32	2a	1407	5MC	C5-C4	5.64	1.48	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	1A	1942	5MC	C5-C4	5.54	1.48	1.44
1	1A	1962	5MC	C5-C4	5.53	1.48	1.44
32	1a	527	G7M	C5-N7	-4.81	1.33	1.39
32	2a	527	G7M	C5-N7	-4.71	1.33	1.39
1	2A	2503	2MA	C5-C4	4.11	1.46	1.39
1	1A	2503	2MA	C5-C4	3.98	1.46	1.39
1	2A	1911	PSU	C6-C5	3.67	1.39	1.35
32	1a	516	PSU	C6-C5	3.60	1.39	1.35
1	1A	1917	PSU	C6-C5	3.55	1.39	1.35
1	1A	1911	PSU	C6-C5	3.37	1.39	1.35
1	1A	2251	OMG	C6-N1	-3.34	1.32	1.38
32	2a	516	PSU	C6-C5	3.27	1.38	1.35
32	2a	966	M2G	C5-C4	3.27	1.47	1.38
1	1A	2605	PSU	C6-C5	3.23	1.38	1.35
32	2a	1207	2MG	C5-C4	3.22	1.47	1.38
32	1a	527	G7M	C5-C4	3.19	1.46	1.38
1	2A	1915	5MU	C2-N1	3.18	1.43	1.38
1	2A	1917	PSU	C6-C5	3.16	1.38	1.35
1	1A	1915	5MU	C2-N1	3.13	1.43	1.38
1	2A	1915	5MU	C6-C5	3.13	1.39	1.34
32	1a	966	M2G	C5-C4	3.12	1.47	1.38
32	2a	527	G7M	C5-C4	3.10	1.46	1.38
32	2a	967	5MC	C6-C5	3.04	1.39	1.34
1	1A	2251	OMG	C5-C4	3.03	1.47	1.38
32	1a	1207	2MG	C5-C4	3.02	1.47	1.38
32	2a	1407	5MC	C6-C5	2.98	1.39	1.34
1	2A	2251	OMG	C5-C4	2.97	1.46	1.38
32	2a	1404	5MC	C6-C5	2.96	1.39	1.34
1	2A	2605	PSU	C6-C5	2.96	1.38	1.35
1	1A	2503	2MA	C5-N7	-2.95	1.33	1.39
1	1A	1939	5MU	C6-C5	2.93	1.39	1.34
32	1a	1407	5MC	C6-C5	2.92	1.39	1.34
1	1A	1942	5MC	C6-C5	2.90	1.39	1.34
32	2a	966	M2G	C2-N2	2.89	1.40	1.35
1	1A	2605	PSU	C4-N3	-2.88	1.33	1.38
1	1A	2552	OMU	C4-N3	-2.81	1.33	1.38
32	1a	1400	5MC	C6-C5	2.80	1.39	1.34
1	2A	1939	5MU	C4-N3	-2.80	1.33	1.38
1	2A	1939	5MU	C6-C5	2.79	1.39	1.34
32	1a	967	5MC	C6-C5	2.78	1.39	1.34
1	2A	1962	5MC	C6-C5	2.75	1.39	1.34
1	2A	2605	PSU	C4-N3	-2.74	1.33	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	2a	1400	5MC	C6-C5	2.73	1.39	1.34
32	1a	966	M2G	C6-N1	-2.71	1.33	1.38
1	2A	1942	5MC	C6-C5	2.71	1.39	1.34
32	1a	1404	5MC	C6-C5	2.71	1.39	1.34
1	2A	1911	PSU	C4-N3	-2.69	1.33	1.38
1	1A	1962	5MC	C6-N1	-2.68	1.33	1.38
1	1A	1939	5MU	C6-N1	-2.61	1.33	1.38
1	1A	1939	5MU	C4-N3	-2.60	1.34	1.38
32	1a	966	M2G	C2-N2	2.60	1.39	1.35
43	2l	92	0TD	CB-CA	2.59	1.55	1.54
1	1A	1915	5MU	C4-N3	-2.56	1.34	1.38
1	1A	1915	5MU	C6-C5	2.56	1.38	1.34
32	2a	516	PSU	C4-N3	-2.54	1.34	1.38
1	1A	1939	5MU	C2-N3	-2.51	1.33	1.38
1	1A	1911	PSU	C4-N3	-2.48	1.34	1.38
32	2a	527	G7M	C6-N1	-2.47	1.34	1.38
1	1A	1962	5MC	C6-C5	2.47	1.38	1.34
32	1a	1400	5MC	C6-N1	-2.44	1.33	1.38
1	2A	2251	OMG	C6-N1	-2.44	1.34	1.38
1	1A	1917	PSU	C4-N3	-2.43	1.34	1.38
1	2A	2552	OMU	C4-N3	-2.42	1.34	1.38
1	2A	1915	5MU	C4-N3	-2.42	1.34	1.38
1	2A	1917	PSU	C4-N3	-2.42	1.34	1.38
32	1a	1207	2MG	C6-N1	-2.40	1.34	1.38
1	2A	2503	2MA	C5-C6	2.39	1.47	1.41
1	2A	2605	PSU	C2-N3	-2.38	1.33	1.37
1	2A	1942	5MC	C6-N1	-2.37	1.34	1.38
1	1A	2503	2MA	C4-N9	-2.33	1.32	1.37
1	2A	2251	OMG	C5-N7	-2.32	1.34	1.39
32	1a	516	PSU	C4-N3	-2.32	1.34	1.38
1	2A	1939	5MU	C2-N3	-2.27	1.34	1.38
32	2a	1400	5MC	C6-N1	-2.26	1.34	1.38
1	1A	1939	5MU	C4-C5	2.23	1.48	1.44
32	2a	1498	UR3	C6-C5	2.19	1.40	1.35
1	1A	1915	5MU	C4-C5	2.18	1.48	1.44
1	2A	1939	5MU	C4-C5	2.17	1.48	1.44
32	1a	527	G7M	C6-N1	-2.17	1.34	1.38
32	2a	1404	5MC	C6-N1	-2.16	1.34	1.38
1	2A	2503	2MA	C8-N7	2.16	1.35	1.31
1	2A	1962	5MC	C6-N1	-2.16	1.34	1.38
32	2a	1207	2MG	C6-N1	-2.16	1.34	1.38
32	2a	1407	5MC	C6-N1	-2.15	1.34	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	2A	1915	5MU	C4-C5	2.14	1.48	1.44
1	1A	2251	OMG	C5-N7	-2.14	1.34	1.39
1	1A	1942	5MC	C6-N1	-2.14	1.34	1.38
1	1A	2503	2MA	C8-N7	2.13	1.35	1.31
32	2a	967	5MC	C6-N1	-2.13	1.34	1.38
32	2a	966	M2G	C6-N1	-2.11	1.34	1.38
1	2A	1939	5MU	C2-N1	2.09	1.41	1.38
32	1a	1498	UR3	C2-N1	2.09	1.41	1.38
1	2A	1939	5MU	C6-N1	-2.09	1.34	1.38
1	2A	2503	2MA	C5-N7	-2.09	1.35	1.39
1	1A	2503	2MA	C8-N9	-2.09	1.34	1.37
1	2A	2552	OMU	C2-N3	-2.08	1.34	1.38
32	1a	1404	5MC	C6-N1	-2.08	1.34	1.38
1	2A	1911	PSU	C2-N3	-2.08	1.34	1.37
32	1a	967	5MC	C6-N1	-2.08	1.34	1.38
43	1l	92	0TD	CSB-SB	-2.07	1.75	1.79
1	1A	2552	OMU	C2-N3	-2.05	1.34	1.38
32	1a	1407	5MC	C6-N1	-2.03	1.34	1.38
1	1A	2503	2MA	C5-C6	2.03	1.46	1.41
32	1a	527	G7M	C4-N9	-2.03	1.32	1.38
1	1A	2552	OMU	C6-C5	2.01	1.39	1.35
1	1A	1915	5MU	C2-N3	-2.01	1.34	1.38

All (223) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
43	1l	92	0TD	CSB-SB-CB	-9.98	84.43	102.36
43	2l	92	0TD	CSB-SB-CB	-9.27	85.69	102.36
1	2A	2503	2MA	C5-C4-N3	-7.91	118.85	127.18
1	1A	2503	2MA	C5-C4-N3	-7.74	119.03	127.18
32	1a	1498	UR3	C4-N3-C2	-7.32	118.69	124.58
32	1a	1207	2MG	C2-N3-C4	7.21	121.02	112.00
32	2a	1498	UR3	C4-N3-C2	-7.04	118.92	124.58
1	2A	2503	2MA	N3-C4-N9	6.91	135.76	126.99
32	2a	1207	2MG	C2-N3-C4	6.69	120.36	112.00
1	2A	2251	OMG	C5-C4-N3	-6.47	118.09	128.39
1	1A	2251	OMG	C5-C4-N3	-6.28	118.39	128.39
1	2A	1911	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	2503	2MA	N3-C4-N9	6.24	134.90	126.99
1	1A	1911	PSU	N1-C2-N3	6.19	121.70	115.17
1	2A	1917	PSU	N1-C2-N3	6.09	121.59	115.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1A	2605	PSU	N1-C2-N3	6.01	121.51	115.17
32	1a	1207	2MG	C5-C4-N3	-5.95	118.92	128.39
1	2A	2605	PSU	N1-C2-N3	5.86	121.35	115.17
1	1A	1917	PSU	N1-C2-N3	5.67	121.15	115.17
32	1a	966	M2G	C5-C4-N3	-5.67	119.36	128.39
32	2a	966	M2G	C5-C4-N3	-5.66	119.38	128.39
1	2A	1939	5MU	N3-C2-N1	5.60	122.19	114.89
32	2a	1207	2MG	C5-C4-N3	-5.56	119.55	128.39
1	2A	1939	5MU	C4-N3-C2	-5.52	120.10	127.34
32	1a	516	PSU	N1-C2-N3	5.52	120.99	115.17
1	1A	2251	OMG	C2-N3-C4	5.36	121.53	112.30
1	1A	1939	5MU	C4-N3-C2	-5.34	120.34	127.34
32	1a	527	G7M	N9-C4-N3	5.29	136.52	125.95
1	2A	2251	OMG	C2-N3-C4	5.22	121.28	112.30
1	1A	1939	5MU	N3-C2-N1	5.16	121.61	114.89
32	2a	527	G7M	C5-C4-N3	-5.15	118.41	128.15
1	2A	2552	OMU	C4-N3-C2	-5.15	120.22	126.61
32	2a	527	G7M	N9-C4-N3	5.08	136.12	125.95
1	2A	1915	5MU	N3-C2-N1	5.08	121.50	114.89
32	1a	527	G7M	C5-C4-N3	-5.03	118.64	128.15
32	2a	1519	MA6	N1-C2-N3	-4.92	121.14	128.58
1	1A	1939	5MU	C5-C4-N3	4.86	119.55	115.32
1	1A	1915	5MU	C5-C4-N3	4.86	119.55	115.32
1	2A	2251	OMG	N9-C4-N3	4.81	135.56	125.95
1	1A	1915	5MU	C4-N3-C2	-4.75	121.11	127.34
1	2A	1939	5MU	C5-C4-N3	4.71	119.42	115.32
32	2a	1518	MA6	N1-C2-N3	-4.70	121.47	128.58
1	1A	2503	2MA	N6-C6-N1	4.70	123.36	117.03
1	1A	1915	5MU	C1'-N1-C2	4.68	126.00	117.59
32	2a	527	G7M	C2-N3-C4	4.68	120.36	112.30
1	1A	2552	OMU	N3-C2-N1	4.66	120.96	114.89
1	1A	1915	5MU	N3-C2-N1	4.63	120.92	114.89
1	1A	2552	OMU	C4-N3-C2	-4.63	120.87	126.61
32	1a	1519	MA6	N1-C2-N3	-4.62	121.58	128.58
1	2A	1915	5MU	C4-N3-C2	-4.60	121.31	127.34
32	1a	527	G7M	C2-N3-C4	4.59	120.21	112.30
32	1a	1518	MA6	N1-C2-N3	-4.54	121.71	128.58
32	1a	1519	MA6	C5-C4-N3	-4.53	120.47	126.72
32	2a	1518	MA6	C5-C4-N3	-4.52	120.50	126.72
1	1A	2251	OMG	N9-C4-N3	4.48	134.90	125.95
1	2A	1915	5MU	O4-C4-C5	-4.47	119.81	124.92
32	2a	1519	MA6	C5-C4-N3	-4.41	120.64	126.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	2a	966	M2G	C2-N3-C4	4.36	120.57	112.51
32	1a	1518	MA6	C5-C4-N3	-4.35	120.72	126.72
32	1a	966	M2G	N9-C4-N3	4.30	134.55	125.95
1	1A	1915	5MU	O4-C4-C5	-4.30	120.00	124.92
32	2a	516	PSU	C4-N3-C2	-4.25	120.52	126.37
1	2A	1939	5MU	O4-C4-C5	-4.25	120.06	124.92
1	2A	2552	OMU	N3-C2-N1	4.24	120.42	114.89
1	2A	1917	PSU	O2-C2-N1	-4.23	118.42	122.79
1	1A	1915	5MU	C1'-N1-C6	-4.20	114.23	121.15
32	2a	966	M2G	N9-C4-N3	4.17	134.30	125.95
1	2A	2503	2MA	C4-N9-C8	4.12	110.07	105.74
1	1A	1939	5MU	O4-C4-C5	-4.11	120.21	124.92
32	1a	966	M2G	C2-N3-C4	4.11	120.11	112.51
32	2a	1518	MA6	C2-N1-C6	4.10	121.84	111.83
1	2A	1911	PSU	C4-N3-C2	-4.07	120.76	126.37
1	1A	2605	PSU	C4-N3-C2	-4.07	120.77	126.37
1	2A	1917	PSU	C4-N3-C2	-4.04	120.81	126.37
32	2a	1519	MA6	C4-C5-N7	-4.02	105.99	110.58
32	2a	1519	MA6	C5-N7-C8	4.01	109.75	103.45
32	1a	1207	2MG	C6-C5-N7	4.00	137.56	130.29
1	2A	1915	5MU	C5-C4-N3	3.95	118.76	115.32
1	2A	2605	PSU	C4-N3-C2	-3.95	120.93	126.37
1	2A	1915	5MU	C1'-N1-C2	3.95	124.69	117.59
32	2a	1519	MA6	C2-N1-C6	3.93	121.44	111.83
1	1A	1917	PSU	C4-N3-C2	-3.93	120.95	126.37
32	1a	1518	MA6	C2-N1-C6	3.88	121.32	111.83
1	1A	1911	PSU	C4-N3-C2	-3.88	121.03	126.37
1	2A	2552	OMU	C5-C4-N3	3.84	120.19	114.80
32	1a	1519	MA6	C2-N1-C6	3.83	121.19	111.83
32	1a	516	PSU	C4-N3-C2	-3.79	121.15	126.37
32	1a	1207	2MG	N9-C4-N3	3.79	133.53	125.95
32	1a	1518	MA6	C5-N7-C8	3.76	109.35	103.45
32	2a	1207	2MG	C6-C5-N7	3.71	137.04	130.29
1	2A	1939	5MU	C5-C6-N1	-3.71	119.29	123.31
1	1A	1942	5MC	C5-C6-N1	-3.70	119.29	123.31
32	2a	1518	MA6	C4-C5-N7	-3.70	106.35	110.58
32	1a	1400	5MC	C5-C6-N1	-3.67	119.33	123.31
32	2a	1207	2MG	N1-C2-N2	3.66	120.29	116.56
32	1a	1519	MA6	C4-C5-N7	-3.65	106.40	110.58
32	2a	516	PSU	O2-C2-N1	-3.63	119.05	122.79
32	1a	967	5MC	C5-C6-N1	-3.63	119.37	123.31
1	1A	2251	OMG	C6-C5-N7	3.61	136.87	130.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1A	1911	PSU	O2-C2-N1	-3.61	119.06	122.79
32	1a	1519	MA6	C5-N7-C8	3.60	109.11	103.45
32	2a	1518	MA6	C5-N7-C8	3.60	109.11	103.45
32	2a	1207	2MG	N9-C4-N3	3.59	133.14	125.95
1	2A	1942	5MC	C5-C6-N1	-3.59	119.41	123.31
1	2A	1962	5MC	C5-C6-N1	-3.57	119.43	123.31
32	1a	1518	MA6	C4-C5-N7	-3.54	106.54	110.58
32	2a	1404	5MC	C5-C4-N3	-3.51	118.16	121.75
32	2a	1519	MA6	N9-C8-N7	-3.51	108.96	113.94
32	1a	1207	2MG	N1-C2-N2	3.50	120.13	116.56
32	2a	1519	MA6	C2-N3-C4	3.48	120.32	111.83
32	2a	967	5MC	C5-C6-N1	-3.48	119.54	123.31
1	1A	1939	5MU	C5-C6-N1	-3.46	119.56	123.31
32	2a	1400	5MC	C5-C6-N1	-3.45	119.57	123.31
32	2a	966	M2G	C6-C5-N7	3.41	136.50	130.29
1	1A	2552	OMU	C5-C4-N3	3.41	119.57	114.80
32	1a	1518	MA6	N9-C8-N7	-3.41	109.10	113.94
1	2A	2503	2MA	C4-C5-N7	-3.40	106.69	110.58
32	1a	1519	MA6	C2-N3-C4	3.37	120.07	111.83
1	2A	2552	OMU	O2-C2-N1	-3.32	118.47	122.80
32	2a	1518	MA6	C2-N3-C4	3.27	119.82	111.83
32	1a	1518	MA6	C2-N3-C4	3.25	119.76	111.83
32	2a	1207	2MG	N2-C2-N3	-3.22	116.41	120.51
32	1a	1407	5MC	C5-C6-N1	-3.21	119.82	123.31
32	1a	966	M2G	C6-C5-N7	3.21	136.14	130.29
32	1a	1207	2MG	C4-C5-N7	-3.21	105.59	110.67
1	1A	2503	2MA	C4-C5-N7	-3.20	106.92	110.58
32	1a	516	PSU	O2-C2-N1	-3.19	119.50	122.79
32	1a	1498	UR3	C5-C4-N3	3.19	119.24	115.04
1	2A	2251	OMG	C6-C5-N7	3.12	135.96	130.29
1	2A	1942	5MC	C5-C4-N3	-3.12	118.56	121.75
32	1a	1404	5MC	C5-C6-N1	-3.08	119.97	123.31
32	2a	1498	UR3	C5-C4-N3	3.07	119.09	115.04
32	2a	1207	2MG	C4-C5-N7	-3.07	105.81	110.67
1	2A	2503	2MA	N9-C8-N7	-3.06	109.60	113.94
1	2A	2503	2MA	C5-N7-C8	3.05	108.25	103.45
1	1A	1962	5MC	C5-C6-N1	-3.05	120.00	123.31
32	2a	1518	MA6	N9-C8-N7	-3.04	109.62	113.94
32	1a	1207	2MG	N2-C2-N3	-3.04	116.64	120.51
1	1A	2503	2MA	C4-N9-C8	3.03	108.92	105.74
32	2a	1404	5MC	C5-C6-N1	-3.03	120.02	123.31
32	2a	1407	5MC	C5-C6-N1	-3.03	120.02	123.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1A	2552	OMU	O2-C2-N1	-3.02	118.86	122.80
1	2A	1915	5MU	C1'-N1-C6	-3.01	116.20	121.15
32	1a	1519	MA6	N9-C8-N7	-3.00	109.68	113.94
1	2A	2503	2MA	N6-C6-N1	2.96	121.02	117.03
1	2A	1911	PSU	O2-C2-N1	-2.94	119.76	122.79
32	2a	1407	5MC	C5-C4-N3	-2.94	118.75	121.75
1	2A	2552	OMU	O4-C4-C5	-2.91	120.15	125.16
1	2A	2503	2MA	C2-N1-C6	2.87	122.51	118.10
32	1a	1400	5MC	C5-C4-N3	-2.87	118.82	121.75
32	2a	1518	MA6	C4-C5-C6	2.85	118.86	115.91
32	1a	1518	MA6	N3-C4-N9	2.84	132.00	127.17
1	1A	1917	PSU	O2-C2-N1	-2.80	119.90	122.79
1	2A	1939	5MU	O2-C2-N1	-2.79	119.17	122.80
1	1A	1915	5MU	O2-C2-N3	-2.76	116.40	121.49
32	1a	1402	4OC	C6-C5-C4	2.75	120.31	117.00
1	1A	1939	5MU	O2-C2-N1	-2.73	119.24	122.80
32	1a	1519	MA6	N3-C4-N9	2.71	131.78	127.17
1	1A	2251	OMG	C4-C5-N7	-2.69	106.41	110.67
32	1a	1207	2MG	CM2-N2-C2	-2.67	117.90	123.65
1	1A	2605	PSU	O2-C2-N1	-2.67	120.03	122.79
1	2A	2251	OMG	C4-C5-N7	-2.67	106.44	110.67
32	2a	1518	MA6	N3-C4-N9	2.65	131.67	127.17
32	2a	966	M2G	C4-C5-N7	-2.61	106.53	110.67
32	2a	1519	MA6	N3-C4-N9	2.60	131.59	127.17
32	1a	527	G7M	O6-C6-C5	-2.60	122.20	128.01
32	1a	1404	5MC	C5-C4-N3	-2.59	119.10	121.75
32	1a	1518	MA6	C4-C5-C6	2.58	118.58	115.91
32	2a	1400	5MC	C5-C4-N3	-2.56	119.13	121.75
32	1a	1519	MA6	C4-C5-C6	2.54	118.53	115.91
1	1A	2503	2MA	C5-N7-C8	2.53	107.42	103.45
32	2a	967	5MC	C5-C4-N3	-2.52	119.17	121.75
32	1a	1407	5MC	C5-C4-N3	-2.52	119.17	121.75
32	1a	1407	5MC	O2-C2-N3	-2.46	118.46	122.33
32	2a	1407	5MC	O2-C2-N3	-2.45	118.47	122.33
1	2A	1915	5MU	C5-C6-N1	-2.43	120.68	123.31
32	1a	1498	UR3	C6-N1-C2	-2.42	119.82	121.80
1	2A	1920	OMC	O2-C2-N3	-2.41	118.53	122.33
32	1a	1498	UR3	C3U-N3-C2	2.41	121.52	117.33
1	1A	1962	5MC	C5-C4-N3	-2.40	119.30	121.75
32	2a	516	PSU	C5-C6-N1	-2.38	118.83	122.14
32	1a	967	5MC	C5-C4-N3	-2.38	119.31	121.75
32	2a	516	PSU	O4'-C1'-C2'	2.38	108.44	105.15

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	2A	1915	5MU	O2-C2-N3	-2.38	117.10	121.49
32	1a	966	M2G	C4-C5-N7	-2.37	106.92	110.67
32	2a	1402	4OC	C6-C5-C4	2.33	119.81	117.00
1	1A	1920	OMC	O2-C2-N3	-2.32	118.67	122.33
1	2A	2251	OMG	O6-C6-C5	-2.32	120.41	126.53
1	1A	2503	2MA	N9-C8-N7	-2.30	110.67	113.94
1	1A	1915	5MU	C5-C6-N1	-2.29	120.83	123.31
1	1A	2552	OMU	O4-C4-C5	-2.27	121.24	125.16
1	1A	2503	2MA	C2-N1-C6	2.27	121.59	118.10
1	2A	2605	PSU	O2-C2-N1	-2.25	120.47	122.79
1	2A	1915	5MU	C6-N1-C2	-2.21	119.11	121.30
1	1A	1942	5MC	C5-C4-N3	-2.20	119.50	121.75
1	2A	2503	2MA	C6-C5-N7	2.19	136.31	132.09
1	2A	2552	OMU	C5-C6-N1	-2.18	118.30	121.84
32	2a	527	G7M	O6-C6-C5	-2.18	123.15	128.01
32	1a	516	PSU	C6-C5-C4	-2.17	116.71	118.17
1	1A	1962	5MC	C1'-N1-C6	-2.17	117.58	121.15
32	1a	527	G7M	C5-C6-N1	2.16	116.31	111.84
1	1A	1917	PSU	C6-C5-C4	-2.15	116.72	118.17
1	1A	1915	5MU	C5M-C5-C4	2.15	121.08	118.78
32	1a	1207	2MG	C8-N7-C5	2.14	108.08	104.26
1	1A	2503	2MA	CM2-C2-N1	2.14	120.33	117.13
1	1A	1911	PSU	O4'-C1'-C2'	2.13	108.10	105.15
1	2A	1962	5MC	C5-C4-N3	-2.12	119.58	121.75
32	1a	1404	5MC	O2-C2-N3	-2.12	118.98	122.33
1	2A	2605	PSU	C6-C5-C4	-2.10	116.76	118.17
32	2a	1519	MA6	C4-C5-C6	2.09	118.07	115.91
43	1l	92	0TD	OD2-CG-CB	2.09	117.67	113.15
32	2a	527	G7M	C5-C6-N1	2.08	116.15	111.84
1	1A	1962	5MC	CM5-C5-C6	-2.08	120.03	122.85
1	2A	1911	PSU	C5-C6-N1	-2.08	119.25	122.14
1	1A	1942	5MC	O2-C2-N3	-2.08	119.05	122.33
1	1A	2605	PSU	C5-C6-N1	-2.08	119.25	122.14
1	2A	2605	PSU	O2-C2-N3	-2.07	118.18	121.86
32	1a	1207	2MG	C2-N1-C6	-2.05	122.07	124.55
32	2a	1404	5MC	O2-C2-N3	-2.04	119.11	122.33
1	1A	2251	OMG	C5-C6-N1	2.04	118.45	113.25
43	2l	92	0TD	OD2-CG-CB	2.03	117.54	113.15
1	2A	2251	OMG	C8-N7-C5	2.03	107.88	104.26

There are no chirality outliers.

All (29) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	1A	1915	5MU	O4'-C1'-N1-C2
1	1A	1915	5MU	O4'-C1'-N1-C6
32	1a	1207	2MG	N1-C2-N2-CM2
32	1a	1207	2MG	N3-C2-N2-CM2
43	1l	92	0TD	CA-CB-SB-CSB
43	1l	92	0TD	CG-CB-SB-CSB
1	2A	1915	5MU	O4'-C1'-N1-C2
1	2A	1915	5MU	O4'-C1'-N1-C6
32	1a	1519	MA6	O4'-C4'-C5'-O5'
32	1a	527	G7M	C3'-C4'-C5'-O5'
32	1a	1519	MA6	C3'-C4'-C5'-O5'
32	2a	1519	MA6	O4'-C4'-C5'-O5'
32	2a	1402	4OC	O4'-C4'-C5'-O5'
43	2l	92	0TD	CG-CB-SB-CSB
43	1l	92	0TD	SB-CB-CG-OD1
43	2l	92	0TD	SB-CB-CG-OD1
32	2a	516	PSU	O4'-C1'-C5-C4
1	1A	2503	2MA	C4'-C5'-O5'-P
32	1a	527	G7M	O4'-C4'-C5'-O5'
32	1a	1400	5MC	O4'-C4'-C5'-O5'
32	2a	1518	MA6	O4'-C4'-C5'-O5'
43	2l	92	0TD	CA-CB-SB-CSB
32	1a	527	G7M	C4'-C5'-O5'-P
32	2a	516	PSU	O4'-C1'-C5-C6
32	2a	1519	MA6	C4'-C5'-O5'-P
32	2a	1519	MA6	C3'-C4'-C5'-O5'
32	2a	1402	4OC	C3'-C2'-O2'-CM2
1	1A	1920	OMC	C2'-C1'-N1-C2
32	2a	1402	4OC	C3'-C4'-C5'-O5'

There are no ring outliers.

No monomer is involved in short contacts.

4.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

4.6 Ligand geometry [i](#)

Of 2458 ligands modelled in this entry, 2446 are monoatomic - leaving 12 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
56	ARG	1B	232	-	10,11,11	0.72	0	9,13,13	1.04	1 (11%)
57	MPD	1T	207	-	7,7,7	0.38	0	9,10,10	0.41	0
59	SF4	1d	306	35	0,12,12	-	-	-		
59	SF4	2d	501	35	0,12,12	-	-	-		
55	A1AE1	1A	3996	54	82,82,82	2.31	18 (21%)	116,122,122	2.56	34 (29%)
55	A1AE1	2A	3726	54	82,82,82	2.28	13 (15%)	116,122,122	2.42	31 (26%)
56	ARG	1A	3998	-	10,11,11	0.76	1 (10%)	9,13,13	1.12	1 (11%)
57	MPD	18	103	-	7,7,7	0.29	0	9,10,10	0.26	0
57	MPD	2A	3728	-	7,7,7	0.33	0	9,10,10	0.27	0
57	MPD	1a	1868	32	7,7,7	0.41	0	9,10,10	0.61	0
57	MPD	1A	3999	-	7,7,7	0.44	0	9,10,10	0.32	0
57	MPD	2B	219	-	7,7,7	0.34	0	9,10,10	0.33	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
56	ARG	1B	232	-	-	4/11/11/11	-
57	MPD	1T	207	-	-	3/5/5/5	-
59	SF4	1d	306	35	-	-	0/6/5/5
59	SF4	2d	501	35	-	-	0/6/5/5
55	A1AE1	1A	3996	54	-	16/89/132/132	0/7/7/7
55	A1AE1	2A	3726	54	-	12/89/132/132	0/7/7/7
56	ARG	1A	3998	-	-	4/11/11/11	-
57	MPD	18	103	-	-	2/5/5/5	-
57	MPD	2A	3728	-	-	3/5/5/5	-
57	MPD	1a	1868	32	-	4/5/5/5	-
57	MPD	1A	3999	-	-	2/5/5/5	-
57	MPD	2B	219	-	-	4/5/5/5	-

All (32) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
55	2A	3726	A1AE1	CAG-CAF	-12.58	1.41	1.53
55	1A	3996	A1AE1	CAG-CAF	-12.26	1.41	1.53
55	2A	3726	A1AE1	CAB-CAF	-6.47	1.41	1.52
55	1A	3996	A1AE1	CAB-CAF	-6.32	1.41	1.52
55	1A	3996	A1AE1	OBR-NBJ	5.98	1.54	1.40
55	1A	3996	A1AE1	CCF-CCN	-5.71	1.39	1.48
55	2A	3726	A1AE1	OBR-NBJ	5.61	1.53	1.40
55	2A	3726	A1AE1	CCF-CCN	-5.28	1.40	1.48
55	2A	3726	A1AE1	CAJ-CAI	-5.17	1.40	1.51
55	2A	3726	A1AE1	CCC-NCH	-5.02	1.34	1.40
55	1A	3996	A1AE1	CCB-CCE	-4.81	1.38	1.48
55	1A	3996	A1AE1	CAJ-CAI	-4.75	1.41	1.51
55	1A	3996	A1AE1	OBH-CAL	-4.72	1.40	1.47
55	2A	3726	A1AE1	CCB-CCE	-4.36	1.39	1.48
55	2A	3726	A1AE1	OBH-CAL	-3.98	1.41	1.47
55	1A	3996	A1AE1	CAF-NBJ	3.86	1.34	1.28
55	2A	3726	A1AE1	CAF-NBJ	3.50	1.33	1.28
55	1A	3996	A1AE1	CCG-NCH	3.40	1.40	1.34
55	2A	3726	A1AE1	CCG-NCH	3.13	1.39	1.34
55	2A	3726	A1AE1	CBY-NBX	-2.87	1.35	1.41
55	1A	3996	A1AE1	CCI-NCH	2.69	1.51	1.46
55	1A	3996	A1AE1	CBY-NBX	-2.69	1.35	1.41
55	1A	3996	A1AE1	CCC-NCH	-2.61	1.37	1.40
55	2A	3726	A1AE1	CAG-CAH	2.31	1.57	1.54
55	1A	3996	A1AE1	OBB-CAK	2.29	1.48	1.44
55	2A	3726	A1AE1	FCL-CBZ	-2.25	1.29	1.35
55	1A	3996	A1AE1	OCO-CCN	-2.16	1.24	1.30
56	1A	3998	ARG	OXT-C	-2.11	1.23	1.30
55	1A	3996	A1AE1	OAN-CAM	-2.10	1.42	1.46
55	1A	3996	A1AE1	CAA-CAB	2.09	1.56	1.54
55	1A	3996	A1AE1	CCT-NBX	2.08	1.50	1.46
55	1A	3996	A1AE1	CAA-CAE	2.04	1.55	1.52

All (67) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
55	2A	3726	A1AE1	CAB-CAF-NBJ	-13.01	116.62	126.21
55	1A	3996	A1AE1	CAB-CAF-NBJ	-11.24	117.93	126.21
55	1A	3996	A1AE1	CCC-NCH-CCI	9.94	130.24	119.88
55	1A	3996	A1AE1	OBB-CBT-NBV	7.72	123.59	111.01
55	2A	3726	A1AE1	OBB-CBT-NBV	7.05	122.49	111.01
55	1A	3996	A1AE1	CAK-OBB-CBT	-6.66	107.26	117.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
55	2A	3726	A1AE1	CAK-OBB-CBT	-6.55	107.42	117.04
55	1A	3996	A1AE1	CCD-CCC-NCH	6.46	126.07	120.49
55	1A	3996	A1AE1	CCI-NCH-CCG	-6.37	110.40	119.74
55	2A	3726	A1AE1	CBE-CAM-CAL	-5.38	107.81	115.23
55	2A	3726	A1AE1	CAB-CAF-CAG	5.37	125.07	119.34
55	1A	3996	A1AE1	FCL-CBZ-CBY	5.25	123.37	118.37
55	1A	3996	A1AE1	OBU-CBT-NBV	-5.01	117.39	124.93
55	1A	3996	A1AE1	CCA-CBZ-CBY	-4.53	119.35	123.35
55	2A	3726	A1AE1	OBU-CBT-NBV	-4.50	118.15	124.93
55	2A	3726	A1AE1	CAE-CAA-CAB	-4.46	108.82	116.10
55	2A	3726	A1AE1	CCK-CCI-NCH	-4.26	112.12	118.87
55	2A	3726	A1AE1	CCD-CBY-NBX	-4.24	116.41	122.59
55	2A	3726	A1AE1	CCX-NBX-CCT	4.21	121.03	111.57
55	1A	3996	A1AE1	CAB-CAF-CAG	4.17	123.79	119.34
55	2A	3726	A1AE1	CBZ-CBY-NBX	4.12	125.24	120.42
55	1A	3996	A1AE1	CCX-NBX-CCT	4.11	120.82	111.57
55	2A	3726	A1AE1	CAE-CAD-CAC	-3.86	107.64	113.54
55	2A	3726	A1AE1	FCL-CBZ-CBY	3.78	121.97	118.37
55	1A	3996	A1AE1	OBB-CBT-OBU	-3.77	119.01	124.55
55	2A	3726	A1AE1	CAG-CAF-NBJ	3.76	118.27	114.40
55	1A	3996	A1AE1	CAG-CAF-NBJ	3.76	118.27	114.40
55	2A	3726	A1AE1	OBB-CBT-OBU	-3.53	119.35	124.55
55	2A	3726	A1AE1	CCA-CBZ-CBY	-3.41	120.34	123.35
55	1A	3996	A1AE1	CCG-CCF-CCE	-3.36	117.47	119.94
56	1A	3998	ARG	OXT-C-O	-3.24	116.73	124.08
56	1B	232	ARG	OXT-C-O	-3.01	117.24	124.08
55	1A	3996	A1AE1	CBS-OB-R-NBJ	3.00	111.98	108.32
55	2A	3726	A1AE1	CCF-CCG-NCH	-2.99	120.84	124.42
55	2A	3726	A1AE1	CCJ-CCI-NCH	-2.99	114.14	118.87
55	2A	3726	A1AE1	CCB-CCE-CCF	2.95	119.36	115.64
55	1A	3996	A1AE1	CCD-CCC-CCB	-2.88	116.06	120.18
55	1A	3996	A1AE1	CBW-NBV-CBT	2.80	126.74	121.98
55	1A	3996	A1AE1	CCA-CCB-CCE	-2.77	115.29	119.94
55	1A	3996	A1AE1	CCB-CCE-CCF	2.77	119.14	115.64
55	2A	3726	A1AE1	OAN-CAM-CAL	2.77	111.73	105.48
55	1A	3996	A1AE1	OCM-CCE-CCB	-2.67	117.29	121.57
55	2A	3726	A1AE1	CBI-CAG-CAH	2.65	116.55	112.94
55	1A	3996	A1AE1	CCN-CCF-CCE	2.59	125.47	121.61
55	2A	3726	A1AE1	CCN-CCF-CCE	2.58	125.45	121.61
55	1A	3996	A1AE1	CCA-CCB-CCC	2.57	121.78	118.76
55	1A	3996	A1AE1	CBE-CAM-CAL	-2.54	111.73	115.23
55	2A	3726	A1AE1	OBH-CAL-CBG	2.51	111.22	106.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
55	1A	3996	A1AE1	CAX-CAR-CAS	-2.51	109.48	113.27
55	2A	3726	A1AE1	CAX-CAR-CAS	-2.44	109.58	113.27
55	2A	3726	A1AE1	CBF-CBE-CAM	-2.32	107.51	113.11
55	2A	3726	A1AE1	OCO-CCN-OCP	-2.29	118.44	123.90
55	1A	3996	A1AE1	CCQ-CBW-NBV	-2.27	105.84	112.20
55	1A	3996	A1AE1	OCO-CCN-OCP	-2.26	118.51	123.90
55	1A	3996	A1AE1	OBL-CAE-CAA	2.22	110.38	105.71
55	2A	3726	A1AE1	CCT-NBX-CBY	2.22	121.45	116.19
55	1A	3996	A1AE1	OBH-CAL-CBG	2.17	110.62	106.80
55	2A	3726	A1AE1	CCG-CCF-CCE	-2.16	118.36	119.94
55	1A	3996	A1AE1	CBI-CAG-CAH	2.15	115.88	112.94
55	1A	3996	A1AE1	OBH-CAL-CAM	2.10	110.28	105.63
55	1A	3996	A1AE1	OBR-NBJ-CAF	2.08	117.17	111.25
55	1A	3996	A1AE1	OBB-CAK-CAC	2.07	112.29	107.52
55	2A	3726	A1AE1	CCQ-CBW-NBV	-2.06	106.41	112.20
55	2A	3726	A1AE1	OCM-CCE-CCB	-2.05	118.30	121.57
55	1A	3996	A1AE1	CAH-OBH-CBP	-2.04	106.02	109.45
55	2A	3726	A1AE1	CCB-CCC-NCH	2.03	120.43	118.83
55	1A	3996	A1AE1	OAQ-CAD-CAE	2.01	111.10	106.44

There are no chirality outliers.

All (54) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
55	1A	3996	A1AE1	CCE-CCF-CCN-OCO
55	1A	3996	A1AE1	CCE-CCF-CCN-OCP
55	1A	3996	A1AE1	CCJ-CCI-NCH-CCG
55	1A	3996	A1AE1	CCK-CCI-NCH-CCC
55	1A	3996	A1AE1	CCK-CCI-NCH-CCG
55	2A	3726	A1AE1	CAF-NBJ-OBR-CBS
56	1A	3998	ARG	N-CA-CB-CG
56	1A	3998	ARG	CA-CB-CG-CD
56	1B	232	ARG	C-CA-CB-CG
57	1T	207	MPD	C1-C2-C3-C4
57	18	103	MPD	C2-C3-C4-O4
57	1a	1868	MPD	C2-C3-C4-O4
57	1a	1868	MPD	C2-C3-C4-C5
57	2B	219	MPD	C2-C3-C4-C5
55	1A	3996	A1AE1	CCJ-CCI-NCH-CCC
55	1A	3996	A1AE1	CCG-CCF-CCN-OCO
55	1A	3996	A1AE1	CCG-CCF-CCN-OCP
56	1A	3998	ARG	NE-CD-CG-CB

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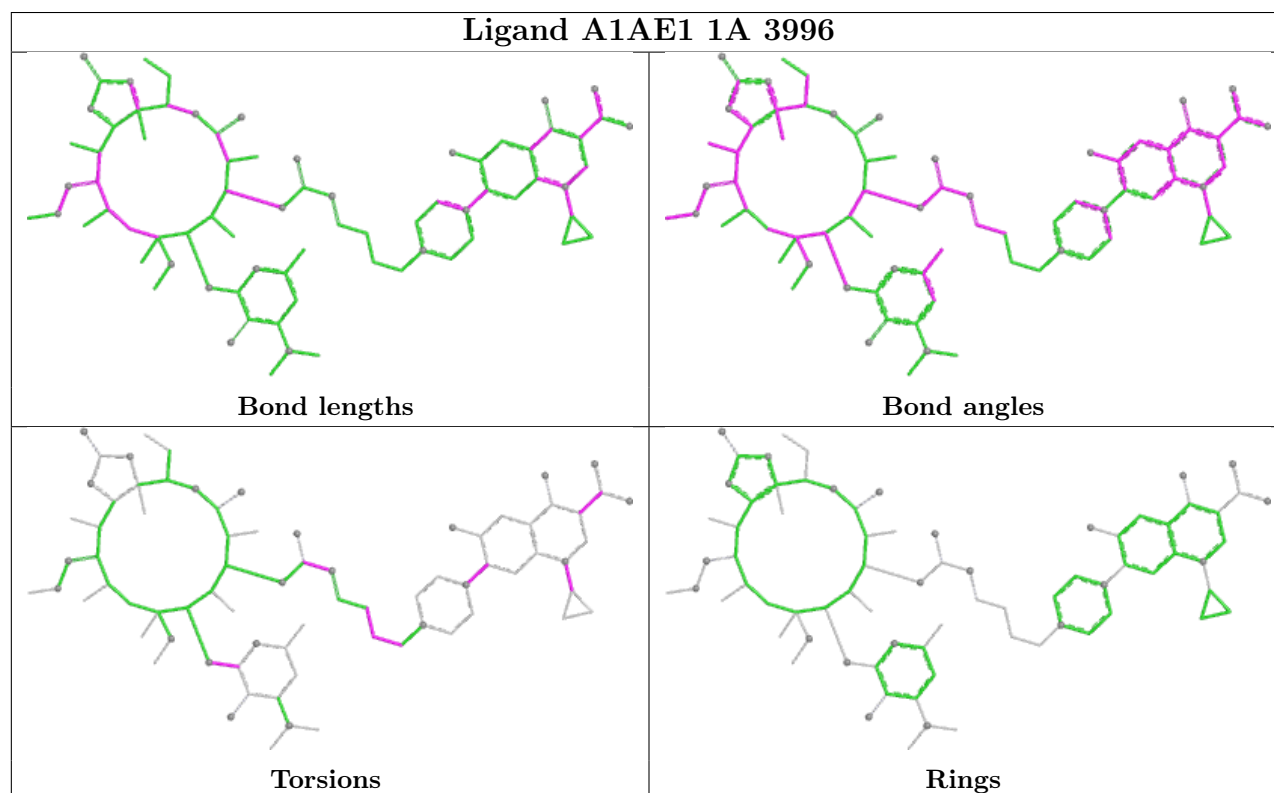
Mol	Chain	Res	Type	Atoms
55	1A	3996	A1AE1	CCQ-CCR-CCS-NCV
55	2A	3726	A1AE1	CCQ-CCR-CCS-NCV
55	1A	3996	A1AE1	CBZ-CBY-NBX-CCX
56	1B	232	ARG	OXT-C-CA-N
55	2A	3726	A1AE1	CCJ-CCI-NCH-CCG
55	2A	3726	A1AE1	CCJ-CCI-NCH-CCC
55	1A	3996	A1AE1	OBB-CBT-NBV-CBW
55	2A	3726	A1AE1	OBB-CBT-NBV-CBW
55	2A	3726	A1AE1	OBU-CBT-NBV-CBW
55	1A	3996	A1AE1	OBU-CBT-NBV-CBW
55	2A	3726	A1AE1	CBE-CAM-OAN-CAI
56	1A	3998	ARG	C-CA-CB-CG
55	1A	3996	A1AE1	CAU-CAP-OAO-CAD
57	1a	1868	MPD	C1-C2-C3-C4
57	2A	3728	MPD	C1-C2-C3-C4
57	2A	3728	MPD	CM-C2-C3-C4
57	1A	3999	MPD	C2-C3-C4-C5
57	1T	207	MPD	C2-C3-C4-C5
57	18	103	MPD	C2-C3-C4-C5
55	1A	3996	A1AE1	OAQ-CAP-OAO-CAD
55	1A	3996	A1AE1	CBW-CCQ-CCR-CCS
55	2A	3726	A1AE1	CBZ-CBY-NBX-CCT
55	2A	3726	A1AE1	CBW-CCQ-CCR-CCS
55	1A	3996	A1AE1	CCD-CBY-NBX-CCX
55	2A	3726	A1AE1	CCD-CBY-NBX-CCT
57	2A	3728	MPD	O2-C2-C3-C4
57	2B	219	MPD	O2-C2-C3-C4
57	1A	3999	MPD	C2-C3-C4-O4
57	2B	219	MPD	C2-C3-C4-O4
55	2A	3726	A1AE1	CAU-CAP-OAO-CAD
55	2A	3726	A1AE1	OAQ-CAP-OAO-CAD
57	1T	207	MPD	CM-C2-C3-C4
57	1a	1868	MPD	CM-C2-C3-C4
57	2B	219	MPD	C1-C2-C3-C4
56	1B	232	ARG	N-CA-CB-CG
56	1B	232	ARG	O-C-CA-N

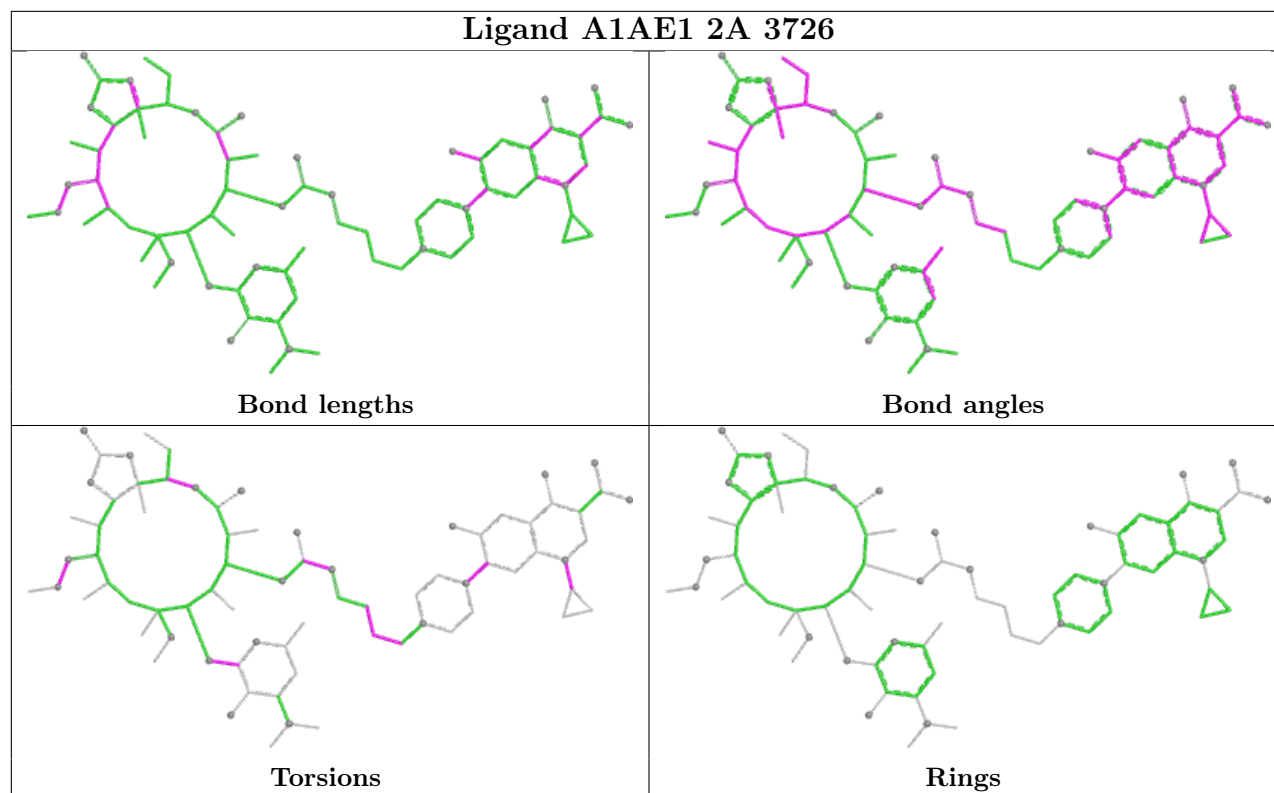
There are no ring outliers.

No monomer is involved in short contacts.

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

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





4.7 Other polymers [i](#)

There are no such residues in this entry.

4.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

5 Fit of model and data ⓘ

5.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	1A	2861/2915 (98%)	-0.49	142 (4%) 34 40	24, 41, 91, 102	0
1	2A	2856/2915 (97%)	-0.06	155 (5%) 31 37	35, 56, 93, 102	0
2	1B	120/121 (99%)	-0.26	3 (2%) 58 64	35, 54, 68, 83	0
2	2B	120/121 (99%)	0.50	1 (0%) 82 86	59, 75, 82, 87	0
3	1D	275/276 (99%)	-0.02	4 (1%) 72 77	25, 40, 54, 78	0
3	2D	275/276 (99%)	0.29	7 (2%) 58 64	35, 50, 61, 77	0
4	1E	204/206 (99%)	0.13	4 (1%) 65 70	24, 44, 64, 76	0
4	2E	204/206 (99%)	0.53	8 (3%) 43 49	36, 58, 72, 82	0
5	1F	203/210 (96%)	0.19	4 (1%) 65 70	24, 46, 71, 82	0
5	2F	203/210 (96%)	0.69	5 (2%) 58 64	35, 65, 78, 84	0
6	1G	181/182 (99%)	0.94	18 (9%) 13 14	52, 66, 79, 87	0
6	2G	181/182 (99%)	1.94	79 (43%) 0 0	70, 80, 86, 91	0
7	1H	174/180 (96%)	0.53	5 (2%) 53 60	44, 57, 69, 76	0
7	2H	173/180 (96%)	1.78	59 (34%) 1 0	67, 78, 85, 86	0
8	1I	147/148 (99%)	1.17	14 (9%) 14 16	44, 71, 80, 82	0
8	2I	146/148 (98%)	1.42	30 (20%) 2 2	57, 74, 82, 84	0
9	1N	140/140 (100%)	0.20	2 (1%) 73 78	31, 44, 64, 77	0
9	2N	140/140 (100%)	0.69	5 (3%) 46 52	49, 63, 75, 81	0
10	1O	122/122 (100%)	0.10	2 (1%) 70 76	32, 43, 61, 67	0
10	2O	122/122 (100%)	0.53	2 (1%) 70 76	46, 56, 68, 74	0
11	1P	149/150 (99%)	0.25	1 (0%) 84 87	24, 49, 68, 79	0
11	2P	149/150 (99%)	0.65	7 (4%) 36 42	37, 66, 79, 85	0
12	1Q	141/141 (100%)	0.21	0 100 100	33, 44, 57, 67	0
12	2Q	141/141 (100%)	0.93	9 (6%) 25 28	45, 63, 71, 79	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
13	1R	118/118 (100%)	0.03	0 100 100	29, 40, 55, 63	0
13	2R	118/118 (100%)	0.46	1 (0%) 82 86	42, 53, 62, 71	0
14	1S	110/112 (98%)	0.62	5 (4%) 38 44	42, 54, 66, 73	0
14	2S	110/112 (98%)	1.47	24 (21%) 2 2	62, 71, 77, 79	0
15	1T	131/146 (89%)	0.39	6 (4%) 37 43	37, 48, 69, 85	0
15	2T	131/146 (89%)	0.72	6 (4%) 37 43	50, 60, 76, 82	0
16	1U	116/118 (98%)	-0.05	1 (0%) 81 84	28, 37, 53, 69	0
16	2U	116/118 (98%)	0.72	3 (2%) 57 63	41, 58, 71, 75	0
17	1V	101/101 (100%)	0.16	2 (1%) 65 70	28, 49, 64, 73	0
17	2V	101/101 (100%)	0.92	6 (5%) 28 32	42, 68, 75, 78	0
18	1W	112/113 (99%)	-0.02	2 (1%) 67 72	31, 38, 57, 84	0
18	2W	112/113 (99%)	0.44	3 (2%) 56 63	39, 51, 67, 87	0
19	1X	95/96 (98%)	0.28	3 (3%) 50 57	31, 41, 65, 73	0
19	2X	95/96 (98%)	0.92	10 (10%) 11 13	47, 59, 75, 82	0
20	1Y	107/110 (97%)	0.59	3 (2%) 55 61	41, 53, 69, 77	0
20	2Y	107/110 (97%)	1.43	21 (19%) 3 3	60, 70, 77, 85	0
21	1Z	203/206 (98%)	0.83	13 (6%) 25 28	46, 61, 76, 84	0
21	2Z	201/206 (97%)	1.51	47 (23%) 2 1	64, 75, 82, 86	0
22	10	83/85 (97%)	0.61	8 (9%) 13 16	34, 42, 76, 84	0
22	20	83/85 (97%)	1.26	11 (13%) 7 8	50, 62, 76, 88	0
23	11	97/98 (98%)	0.29	2 (2%) 63 68	31, 46, 67, 74	0
23	21	97/98 (98%)	0.66	3 (3%) 51 58	41, 57, 74, 79	0
24	12	70/72 (97%)	0.50	2 (2%) 53 60	38, 51, 63, 82	0
24	22	70/72 (97%)	1.02	4 (5%) 29 34	59, 69, 75, 79	0
25	13	59/60 (98%)	0.14	1 (1%) 69 74	31, 43, 67, 75	0
25	23	59/60 (98%)	0.85	4 (6%) 23 26	49, 60, 75, 79	0
26	14	69/71 (97%)	1.60	18 (26%) 1 1	63, 79, 88, 90	0
26	24	69/71 (97%)	2.40	47 (68%) 0 0	78, 85, 91, 92	0
27	15	59/60 (98%)	0.02	1 (1%) 69 74	26, 40, 61, 71	0
27	25	59/60 (98%)	0.32	0 100 100	37, 52, 68, 77	0
28	16	53/54 (98%)	0.16	0 100 100	37, 46, 60, 66	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
28	26	53/54 (98%)	0.71	2 (3%) 44 50	52, 61, 68, 73	0
29	17	48/49 (97%)	0.01	5 (10%) 11 13	24, 31, 54, 65	0
29	27	48/49 (97%)	0.39	6 (12%) 8 9	36, 42, 68, 72	0
30	18	64/65 (98%)	-0.17	0 100 100	31, 38, 44, 57	0
30	28	64/65 (98%)	0.57	2 (3%) 51 58	46, 54, 62, 67	0
31	19	37/37 (100%)	0.20	0 100 100	38, 46, 58, 60	0
31	29	37/37 (100%)	1.30	8 (21%) 2 2	56, 65, 72, 75	0
32	1a	1488/1521 (97%)	0.29	58 (3%) 43 49	40, 68, 90, 102	0
32	2a	1492/1521 (98%)	0.47	66 (4%) 39 45	47, 74, 91, 101	0
33	1b	231/256 (90%)	1.68	64 (27%) 1 1	65, 77, 84, 89	0
33	2b	231/256 (90%)	2.02	106 (45%) 0 0	71, 81, 86, 91	0
34	1c	206/239 (86%)	1.15	27 (13%) 7 8	60, 72, 82, 88	0
34	2c	206/239 (86%)	1.83	79 (38%) 1 0	71, 81, 86, 89	0
35	1d	208/209 (99%)	1.27	35 (16%) 4 4	58, 71, 78, 85	0
35	2d	208/209 (99%)	1.41	38 (18%) 3 3	62, 71, 78, 82	0
36	1e	148/162 (91%)	0.95	8 (5%) 31 37	53, 65, 74, 84	0
36	2e	148/162 (91%)	1.14	17 (11%) 9 11	55, 70, 78, 87	0
37	1f	100/101 (99%)	0.92	3 (3%) 52 59	57, 67, 74, 79	0
37	2f	100/101 (99%)	0.96	5 (5%) 34 40	58, 67, 76, 79	0
38	1g	155/156 (99%)	1.01	12 (7%) 19 22	63, 71, 79, 84	0
38	2g	155/156 (99%)	1.56	39 (25%) 1 1	70, 78, 83, 85	0
39	1h	137/138 (99%)	1.11	10 (7%) 21 24	55, 68, 74, 80	0
39	2h	137/138 (99%)	1.13	12 (8%) 15 18	60, 70, 77, 80	0
40	1i	127/128 (99%)	1.86	49 (38%) 1 0	61, 77, 83, 85	0
40	2i	126/128 (98%)	2.46	77 (61%) 0 0	71, 82, 86, 89	0
41	1j	97/105 (92%)	1.69	32 (32%) 1 0	60, 77, 84, 87	0
41	2j	96/105 (91%)	2.56	65 (67%) 0 0	73, 82, 87, 91	0
42	1k	114/129 (88%)	0.93	8 (7%) 22 25	46, 65, 75, 80	0
42	2k	114/129 (88%)	1.14	14 (12%) 8 10	57, 70, 79, 82	0
43	1l	121/132 (91%)	0.88	13 (10%) 11 13	49, 60, 70, 74	0
43	2l	121/132 (91%)	1.05	13 (10%) 11 13	56, 66, 73, 77	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
44	1m	116/126 (92%)	1.31	16 (13%) 6 7	62, 75, 80, 84	0
44	2m	114/126 (90%)	1.78	34 (29%) 1 1	73, 81, 85, 88	0
45	1n	60/61 (98%)	1.20	8 (13%) 7 8	63, 70, 78, 81	0
45	2n	60/61 (98%)	2.51	37 (61%) 0 0	72, 79, 84, 90	0
46	1o	88/89 (98%)	1.10	7 (7%) 18 21	49, 67, 76, 79	0
46	2o	88/89 (98%)	1.16	9 (10%) 12 13	58, 70, 78, 82	0
47	1p	82/88 (93%)	1.96	40 (48%) 0 0	60, 71, 80, 84	0
47	2p	82/88 (93%)	1.46	17 (20%) 2 2	63, 69, 78, 85	0
48	1q	99/105 (94%)	1.32	14 (14%) 6 7	56, 69, 77, 79	0
48	2q	99/105 (94%)	1.10	8 (8%) 18 20	57, 68, 76, 79	0
49	1r	68/88 (77%)	0.97	6 (8%) 15 18	58, 65, 77, 83	0
49	2r	68/88 (77%)	1.00	4 (5%) 28 32	63, 70, 79, 83	0
50	1s	83/93 (89%)	1.59	22 (26%) 1 1	65, 76, 81, 85	0
50	2s	83/93 (89%)	2.21	48 (57%) 0 0	77, 84, 88, 91	0
51	1t	96/106 (90%)	1.57	23 (23%) 2 1	61, 71, 80, 82	0
51	2t	98/106 (92%)	1.22	14 (14%) 6 7	60, 69, 80, 82	0
52	1u	23/27 (85%)	1.58	8 (34%) 1 0	66, 71, 75, 77	0
52	2u	23/27 (85%)	2.82	17 (73%) 0 0	76, 78, 82, 82	0
53	1y	97/113 (85%)	1.12	12 (12%) 8 9	54, 64, 74, 81	0
53	2y	96/113 (84%)	1.88	34 (35%) 1 0	67, 76, 83, 84	0
All	All	20778/21468 (96%)	0.54	2074 (9%) 12 14	24, 63, 85, 102	0

All (2074) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
45	2n	2	ALA	10.5
22	10	7	LEU	8.6
1	1A	1087	G	8.4
22	20	7	LEU	7.6
45	1n	2	ALA	7.5
53	1y	98	ALA	7.3
51	2t	6	PRO	7.3
53	2y	98	ALA	7.0
26	24	56	VAL	6.5
1	1A	1072	C	6.5

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Mol	Chain	Res	Type	RSRZ
22	10	2	ALA	6.4
40	2i	102	LEU	6.3
51	1t	103	GLY	6.1
15	1T	131	ALA	6.1
7	1H	2	SER	6.1
41	2j	75	ILE	6.1
40	2i	56	LEU	6.1
44	2m	116	THR	6.0
50	2s	2	PRO	6.0
1	1A	1077	A	5.9
41	2j	37	PRO	5.9
51	2t	103	GLY	5.8
1	1A	1080	C	5.8
33	2b	136	VAL	5.8
22	20	4	LYS	5.8
1	1A	1102	C	5.8
33	1b	229	VAL	5.7
22	20	3	HIS	5.7
44	1m	2	ALA	5.7
1	1A	1090	U	5.7
1	2A	2174	C	5.6
7	2H	45	VAL	5.6
41	1j	4	ILE	5.6
22	10	6	GLY	5.6
40	1i	128	ARG	5.5
23	21	2	SER	5.4
26	24	9	LEU	5.4
3	1D	276	LYS	5.4
33	2b	7	VAL	5.3
52	2u	14	TRP	5.3
22	10	3	HIS	5.3
22	20	84	LEU	5.2
1	1A	1089	G	5.2
26	14	56	VAL	5.2
1	1A	1088	A	5.2
1	2A	2124	G	5.2
41	2j	74	ILE	5.1
26	14	49	PHE	5.1
22	20	6	GLY	5.1
46	2o	89	GLY	5.1
22	10	4	LYS	5.1
6	2G	146	TYR	5.1

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Mol	Chain	Res	Type	RSRZ
26	14	63	TYR	5.1
35	1d	2	GLY	5.1
41	2j	34	VAL	5.0
1	1A	1078	U	5.0
15	1T	37	GLY	4.9
1	1A	1081	U	4.9
3	2D	276	LYS	4.9
32	2a	1036	G	4.9
23	11	2	SER	4.9
21	1Z	191	VAL	4.9
1	1A	1075	C	4.8
1	1A	1093	G	4.8
1	1A	1103	A	4.8
21	1Z	192	ALA	4.8
45	2n	3	ARG	4.8
1	2A	2125	G	4.8
1	1A	1086	A	4.7
24	12	70	GLN	4.7
1	1A	1076	C	4.7
6	2G	50	ALA	4.7
38	2g	83	ALA	4.7
1	1A	1091	G	4.7
1	1A	1070	A	4.7
7	2H	71	LEU	4.7
26	24	49	PHE	4.7
40	2i	2	GLU	4.7
45	2n	18	VAL	4.6
6	2G	52	ILE	4.6
15	1T	130	ALA	4.6
26	24	63	TYR	4.6
1	1A	1079	C	4.6
19	1X	95	LEU	4.6
8	1I	147	GLN	4.6
8	2I	146	ALA	4.6
21	2Z	51	ALA	4.6
46	1o	89	GLY	4.5
1	2A	2119	A	4.5
52	2u	6	ARG	4.5
35	2d	5	ILE	4.5
27	15	60	VAL	4.5
1	2A	2135	A	4.5
12	2Q	104	PHE	4.5

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Mol	Chain	Res	Type	RSRZ
7	2H	136	ILE	4.4
52	2u	16	GLY	4.4
26	14	59	PHE	4.4
33	1b	17	PHE	4.4
15	2T	130	ALA	4.4
1	2A	2140	C	4.4
19	2X	95	LEU	4.4
40	2i	14	VAL	4.4
6	2G	76	SER	4.4
33	2b	237	ALA	4.4
53	1y	97	ALA	4.4
1	2A	2152	G	4.4
40	2i	105	ASP	4.4
33	2b	44	LEU	4.4
40	2i	96	LEU	4.4
1	2A	2139	C	4.4
34	2c	207	VAL	4.4
1	2A	2113	U	4.4
1	1A	2602	A	4.4
33	2b	122	PHE	4.4
6	2G	2	PRO	4.3
40	1i	56	LEU	4.3
40	2i	53	VAL	4.3
40	1i	46	ALA	4.3
52	2u	24	ARG	4.3
1	1A	1104	C	4.3
33	2b	236	TYR	4.3
40	2i	62	TYR	4.3
33	1b	237	ALA	4.3
48	1q	63	ARG	4.3
1	2A	2147	G	4.3
32	1a	1036	G	4.3
41	2j	38	ILE	4.3
33	1b	7	VAL	4.3
1	2A	1046	A	4.3
40	1i	66	ARG	4.3
25	23	2	PRO	4.3
1	1A	1071	G	4.3
32	2a	1003	G	4.3
26	24	67	TYR	4.2
33	1b	94	ASN	4.2
41	1j	78	ASN	4.2

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Mol	Chain	Res	Type	RSRZ
15	2T	131	ALA	4.2
51	1t	18	GLN	4.2
1	1A	1064	C	4.2
33	1b	165	VAL	4.2
20	2Y	1	MET	4.2
22	10	84	LEU	4.2
32	2a	1257	U	4.2
1	1A	1092	C	4.2
6	2G	3	LEU	4.2
38	2g	80	VAL	4.2
45	2n	33	VAL	4.2
1	2A	1091	G	4.2
40	2i	125	TYR	4.2
41	2j	91	PRO	4.2
41	2j	32	ALA	4.1
1	2A	2150	U	4.1
26	24	59	PHE	4.1
1	2A	2169	A	4.1
1	2A	2173	A	4.1
6	2G	43	LEU	4.1
51	1t	10	LEU	4.1
40	1i	126	SER	4.1
1	2A	2175	C	4.1
33	2b	232	PRO	4.1
18	2W	112	GLY	4.0
1	2A	2129	C	4.0
53	2y	97	ALA	4.0
52	2u	23	PRO	4.0
1	2A	1536	C	4.0
1	1A	1082	U	4.0
6	2G	53	LEU	4.0
6	2G	139	LEU	4.0
1	1A	1063	G	4.0
40	2i	18	PHE	4.0
34	1c	193	TYR	4.0
33	2b	230	VAL	4.0
39	1h	2	LEU	4.0
49	1r	24	ALA	4.0
40	2i	6	GLY	4.0
41	2j	93	GLY	4.0
40	2i	101	PHE	4.0
1	1A	1062	G	4.0

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Mol	Chain	Res	Type	RSRZ
1	2A	2162	G	4.0
41	2j	78	ASN	4.0
45	2n	21	TYR	4.0
33	1b	19	HIS	3.9
1	1A	1065	U	3.9
1	2A	2138	C	3.9
32	1a	1030	C	3.9
1	1A	1067	A	3.9
1	1A	1085	A	3.9
40	2i	94	ALA	3.9
1	1A	1074	G	3.9
14	2S	35	ILE	3.9
38	1g	85	TYR	3.9
38	2g	154	TYR	3.9
14	1S	3	ARG	3.9
1	1A	1094	U	3.9
33	2b	15	VAL	3.9
47	2p	82	GLN	3.9
33	2b	121	LEU	3.9
1	1A	1069	A	3.9
33	2b	133	LYS	3.9
50	1s	13	ASP	3.9
33	1b	33	TYR	3.9
1	2A	2136	C	3.9
5	1F	208	GLY	3.9
36	1e	21	ALA	3.9
1	2A	1067	A	3.9
32	1a	1286	A	3.9
40	1i	127	LYS	3.9
40	2i	7	THR	3.9
33	2b	21	ARG	3.9
1	2A	2127	G	3.9
47	2p	38	TYR	3.9
33	1b	230	VAL	3.9
33	1b	227	GLY	3.9
1	2A	1509	C	3.9
1	2A	2145	C	3.9
38	2g	117	ALA	3.9
44	1m	116	THR	3.9
1	2A	1085	A	3.9
1	2A	2117	A	3.9
14	2S	53	SER	3.8

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Mol	Chain	Res	Type	RSRZ
1	1A	1068	G	3.8
1	1A	1176	G	3.8
32	2a	1030(A)	G	3.8
1	2A	2146	C	3.8
32	1a	1001	A	3.8
33	1b	37	ASN	3.8
41	2j	47	PHE	3.8
1	1A	1066	U	3.8
41	1j	74	ILE	3.8
41	2j	82	ILE	3.8
32	2a	1001(A)	G	3.8
26	24	54	GLY	3.8
34	2c	94	LEU	3.8
1	2A	2108	C	3.8
1	2A	2137	C	3.8
33	2b	57	PHE	3.8
6	2G	88	ILE	3.8
34	2c	5	ILE	3.8
33	1b	236	TYR	3.8
40	2i	99	LEU	3.8
26	24	66	SER	3.8
34	2c	77	ILE	3.8
38	2g	32	ARG	3.8
33	2b	148	TYR	3.7
34	1c	207	VAL	3.8
41	2j	40	LEU	3.8
32	2a	1031	G	3.7
22	20	2	ALA	3.7
42	2k	89	ALA	3.7
32	2a	1030	C	3.7
1	2A	2602	A	3.7
40	2i	10	ARG	3.7
50	2s	29	ARG	3.7
22	10	8	GLY	3.7
35	1d	170	VAL	3.7
29	27	48	LYS	3.7
32	1a	1024	G	3.7
41	2j	100	THR	3.7
1	2A	2111	C	3.7
1	2A	2109	U	3.7
50	1s	9	VAL	3.7
1	2A	2153	G	3.7

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Mol	Chain	Res	Type	RSRZ
21	1Z	188	ALA	3.7
32	1a	1030(A)	G	3.7
38	2g	7	ALA	3.7
40	1i	94	ALA	3.7
1	1A	1073	A	3.7
1	2A	1084	A	3.7
40	2i	126	SER	3.7
40	2i	127	LYS	3.7
40	1i	102	LEU	3.7
52	2u	4	GLY	3.7
40	2i	9	ARG	3.7
40	2i	13	ALA	3.7
42	2k	25	TYR	3.7
45	2n	30	ALA	3.7
1	1A	1099	G	3.7
41	2j	39	PRO	3.7
1	2A	2126	A	3.7
34	2c	128	PHE	3.6
33	2b	97	TRP	3.6
33	2b	118	LEU	3.6
40	2i	66	ARG	3.6
33	1b	136	VAL	3.6
1	2A	2148	G	3.6
1	2A	2151	G	3.6
32	2a	1033	G	3.6
34	2c	2	GLY	3.6
50	1s	68	GLY	3.6
53	1y	95	ARG	3.6
44	1m	117	VAL	3.6
45	2n	13	THR	3.6
1	2A	2114	A	3.6
32	1a	1026	G	3.6
32	2a	1286	A	3.6
32	1a	1029	C	3.6
23	2l	83	GLU	3.6
44	2m	6	GLY	3.6
44	2m	106	ASN	3.6
33	2b	132	LYS	3.6
40	2i	95	LYS	3.6
33	1b	232	PRO	3.6
52	1u	23	PRO	3.6
38	2g	85	TYR	3.6

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Mol	Chain	Res	Type	RSRZ
11	2P	15	ARG	3.6
8	2I	134	PRO	3.6
44	1m	102	ARG	3.5
1	2A	2143	C	3.5
20	1Y	1	MET	3.5
32	1a	1037	C	3.5
1	1A	2147	G	3.5
33	1b	10	LEU	3.5
33	1b	22	LYS	3.5
51	2t	7	LYS	3.5
7	2H	129	THR	3.5
1	2A	2144	U	3.5
1	1A	2117	A	3.5
32	2a	1035	A	3.5
40	1i	125	TYR	3.5
40	2i	4	TYR	3.5
1	2A	2106	G	3.5
6	2G	77	ILE	3.5
33	2b	11	LEU	3.5
39	2h	2	LEU	3.5
7	2H	3	ARG	3.5
41	2j	46	ARG	3.5
29	17	48	LYS	3.5
1	2A	2142	C	3.5
43	1l	64	TYR	3.5
1	2A	2149	G	3.5
1	2A	2168	G	3.5
50	2s	5	LEU	3.5
52	2u	15	ARG	3.5
21	1Z	1	MET	3.5
1	2A	652(B)	A	3.5
14	2S	22	GLY	3.5
43	1l	63	GLY	3.5
51	1t	100	ILE	3.5
6	2G	152	LEU	3.5
39	1h	133	LEU	3.5
1	2A	2120	G	3.5
1	2A	2130	U	3.5
40	2i	21	PRO	3.4
1	1A	888	C	3.4
1	2A	2107	C	3.4
6	2G	39	ILE	3.4

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Mol	Chain	Res	Type	RSRZ
19	2X	68	ARG	3.4
38	1g	16	LEU	3.4
38	2g	5	ARG	3.4
41	2j	6	ILE	3.4
53	2y	40	ILE	3.4
41	2j	65	LEU	3.4
1	1A	1058	G	3.4
1	2A	2116	G	3.4
1	2A	2118	U	3.4
1	2A	2121	G	3.4
6	2G	87	PRO	3.4
41	2j	35	SER	3.4
45	2n	5	ALA	3.4
50	2s	35	SER	3.4
36	2e	22	GLY	3.4
45	1n	3	ARG	3.4
1	1A	1053	C	3.4
7	2H	92	ILE	3.4
33	1b	39	ILE	3.4
46	2o	3	ILE	3.4
47	1p	48	TRP	3.4
1	2A	2141	G	3.4
40	2i	103	THR	3.4
42	1k	14	VAL	3.4
50	2s	9	VAL	3.4
50	2s	3	ARG	3.4
32	2a	1004	A	3.4
22	10	5	LYS	3.4
43	2l	17	LYS	3.4
1	1A	34	C	3.4
1	2A	1083	U	3.4
32	1a	1030(B)	C	3.4
32	2a	1027	C	3.4
32	2a	1037	C	3.4
7	2H	44	VAL	3.4
40	1i	17	VAL	3.4
1	1A	1098	A	3.4
40	1i	91	ASP	3.4
1	1A	2130	U	3.3
6	1G	52	ILE	3.3
1	2A	2161	C	3.3
44	2m	87	TYR	3.3

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Mol	Chain	Res	Type	RSRZ
1	1A	2116	G	3.3
51	1t	8	ARG	3.3
21	2Z	187	ALA	3.3
43	2l	18	VAL	3.3
50	2s	67	VAL	3.3
1	1A	2173	A	3.3
1	2A	2176	A	3.3
38	2g	16	LEU	3.3
26	24	11	PRO	3.3
40	2i	5	TYR	3.3
40	2i	92	TYR	3.3
45	2n	34	TYR	3.3
50	2s	69	HIS	3.3
52	2u	18	TYR	3.3
40	2i	11	LYS	3.3
51	1t	74	LYS	3.3
33	2b	165	VAL	3.3
40	1i	106	ALA	3.3
47	1p	53	VAL	3.3
7	2H	41	MET	3.3
32	1a	1447	A	3.3
33	1b	187	LEU	3.3
34	2c	42	LEU	3.3
51	1t	99	LEU	3.3
7	2H	21	PRO	3.3
14	2S	17	ARG	3.3
32	2a	1030(B)	C	3.3
40	2i	27	THR	3.3
26	14	67	TYR	3.3
26	14	50	VAL	3.3
34	2c	99	VAL	3.3
40	2i	29	ASN	3.3
40	2i	91	ASP	3.3
32	2a	1025	U	3.3
1	2A	2134	A	3.3
34	1c	87	LEU	3.3
45	2n	39	LEU	3.3
33	2b	200	ILE	3.3
35	2d	70	ILE	3.3
52	1u	24	ARG	3.3
40	2i	90	PRO	3.3
47	1p	46	PRO	3.3

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Mol	Chain	Res	Type	RSRZ
41	1j	87	THR	3.3
41	1j	100	THR	3.3
42	1k	25	TYR	3.3
7	2H	37	VAL	3.3
18	1W	112	GLY	3.2
26	24	65	ASP	3.2
45	2n	12	ARG	3.2
1	1A	2119	A	3.2
32	1a	1005	A	3.2
43	1l	47	LYS	3.2
46	1o	3	ILE	3.2
47	1p	41	PRO	3.2
6	2G	80	PHE	3.2
26	24	10	VAL	3.2
47	2p	2	VAL	3.2
7	2H	42	ARG	3.2
50	2s	84	GLY	3.2
1	1A	2132	U	3.2
32	1a	1032	G	3.2
32	2a	1026	G	3.2
34	1c	90	GLU	3.2
20	2Y	106	LEU	3.2
34	2c	87	LEU	3.2
35	1d	157	LEU	3.2
44	1m	56	LEU	3.2
1	2A	2171	A	3.2
32	2a	1030(D)	A	3.2
50	2s	76	PRO	3.2
33	2b	208	ILE	3.2
41	2j	96	ILE	3.2
53	1y	2	THR	3.2
1	2A	652(T)	C	3.2
32	2a	1029	C	3.2
6	2G	110	ALA	3.2
29	27	45	ALA	3.2
40	1i	15	ALA	3.2
41	2j	26	ALA	3.2
41	2j	36	GLY	3.2
1	1A	1026	U	3.2
1	1A	2113	U	3.2
20	2Y	91	GLU	3.2
1	2A	2159	G	3.2

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Mol	Chain	Res	Type	RSRZ
32	1a	1031	G	3.2
32	2a	1034	G	3.2
40	1i	19	LEU	3.2
45	2n	6	LEU	3.2
7	2H	10	PRO	3.2
26	24	29	PRO	3.2
41	2j	77	PRO	3.2
1	2A	1070	A	3.2
41	1j	98	ILE	3.2
34	2c	95	THR	3.2
1	1A	2174	C	3.2
1	2A	1092	C	3.2
5	1F	6	VAL	3.2
6	2G	46	ALA	3.2
34	1c	2	GLY	3.2
40	2i	119	ALA	3.2
41	2j	44	VAL	3.2
47	1p	79	VAL	3.2
33	1b	40	HIS	3.2
1	2A	1071	G	3.2
1	2A	2110	G	3.2
32	2a	630	G	3.2
33	2b	131	PRO	3.2
36	2e	20	GLN	3.2
44	2m	9	ILE	3.2
21	2Z	170	THR	3.2
36	2e	10	MET	3.2
1	2A	2179	C	3.1
32	1a	1027	C	3.1
33	2b	22	LYS	3.1
1	1A	1061	U	3.1
1	1A	1097	U	3.1
2	1B	1	U	3.1
21	2Z	191	VAL	3.1
41	2j	76	ASN	3.1
50	2s	41	VAL	3.1
6	1G	146	TYR	3.1
14	2S	80	LEU	3.1
41	2j	90	LEU	3.1
50	2s	30	LEU	3.1
1	1A	2159	G	3.1
1	2A	1089	G	3.1

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Mol	Chain	Res	Type	RSRZ
1	2A	2160	G	3.1
1	1A	2158	A	3.1
33	1b	127	ILE	3.1
1	1A	1509	C	3.1
1	2A	2172	U	3.1
33	1b	228	GLY	3.1
35	1d	87	GLY	3.1
35	1d	167	GLY	3.1
33	2b	207	ALA	3.1
49	2r	20	ALA	3.1
21	2Z	42	VAL	3.1
40	2i	42	ARG	3.1
45	1n	12	ARG	3.1
1	1A	1057	A	3.1
1	1A	2125	G	3.1
1	2A	1096	A	3.1
6	1G	182	LYS	3.1
32	1a	1003	G	3.1
32	2a	1030(C)	G	3.1
32	2a	1032	G	3.1
47	1p	22	THR	3.1
1	2A	1076	C	3.1
32	1a	1028	C	3.1
1	1A	1083	U	3.1
22	20	8	GLY	3.1
41	1j	31	GLY	3.1
51	1t	102	GLY	3.1
51	2t	98	PRO	3.1
33	2b	199	TYR	3.1
43	1l	91	LYS	3.1
43	2l	13	LYS	3.1
47	1p	39	TYR	3.1
8	2I	97	ILE	3.1
33	2b	223	ILE	3.1
35	1d	70	ILE	3.1
36	2e	13	ILE	3.1
41	2j	98	ILE	3.1
32	1a	1030(D)	A	3.1
41	2j	64	GLU	3.1
47	2p	48	TRP	3.1
1	2A	2133	G	3.1
1	2A	2154	G	3.1

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Mol	Chain	Res	Type	RSRZ
40	2i	64	THR	3.1
51	1t	73	HIS	3.1
1	1A	1101	U	3.1
32	2a	1038	C	3.1
41	2j	33	GLN	3.1
42	2k	117	ASN	3.1
46	2o	86	GLY	3.1
50	2s	10	PHE	3.1
52	2u	2	GLY	3.1
7	2H	51	ARG	3.1
7	2H	52	VAL	3.1
7	2H	101	ARG	3.1
22	20	5	LYS	3.1
33	1b	234	PRO	3.1
38	2g	76	ARG	3.1
33	2b	8	LYS	3.1
53	2y	45	PRO	3.1
34	2c	101	LEU	3.1
41	2j	85	LEU	3.1
47	1p	6	LEU	3.1
53	2y	27	LEU	3.1
40	2i	88	TYR	3.0
41	2j	67	THR	3.0
1	1A	2127	G	3.0
1	2A	2112	G	3.0
18	1W	111	HIS	3.0
32	1a	1001(A)	G	3.0
38	2g	156	TRP	3.0
47	1p	59	TRP	3.0
41	2j	30	SER	3.0
2	2B	1	U	3.0
1	1A	1100	C	3.0
1	2A	1064	C	3.0
7	2H	66	GLY	3.0
44	2m	100	GLY	3.0
47	1p	80	PHE	3.0
50	2s	68	GLY	3.0
14	2S	3	ARG	3.0
14	2S	33	LYS	3.0
48	1q	100	LYS	3.0
34	2c	61	ALA	3.0
41	1j	27	ALA	3.0

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Mol	Chain	Res	Type	RSRZ
41	2j	27	ALA	3.0
33	1b	125	PRO	3.0
34	1c	99	VAL	3.0
1	2A	229	A	3.0
1	1A	275	G	3.0
32	1a	1023	G	3.0
1	2A	2132	U	3.0
53	2y	42	SER	3.0
14	2S	59	LYS	3.0
29	27	47	ARG	3.0
6	2G	85	GLY	3.0
7	2H	82	GLY	3.0
45	2n	55	GLY	3.0
1	1A	2129	C	3.0
45	2n	14	PRO	3.0
8	2I	3	VAL	3.0
33	1b	231	GLU	3.0
34	2c	152	ILE	3.0
26	24	60	GLN	3.0
12	2Q	59	ARG	3.0
46	1o	68	ARG	3.0
51	1t	68	LYS	3.0
1	1A	2172	U	3.0
32	1a	1000	U	3.0
1	1A	1059	G	3.0
1	2A	2893	G	3.0
32	1a	1030(C)	G	3.0
33	1b	97	TRP	3.0
38	1g	84	ASN	3.0
38	1g	156	TRP	3.0
45	2n	61	TRP	3.0
50	2s	42	PRO	3.0
5	2F	21	ALA	3.0
21	2Z	189	ALA	3.0
40	2i	55	ALA	3.0
41	1j	32	ALA	3.0
50	2s	24	ALA	3.0
34	2c	75	VAL	3.0
40	2i	41	VAL	3.0
41	2j	72	VAL	3.0
45	2n	25	VAL	3.0
20	2Y	44	ILE	3.0

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Mol	Chain	Res	Type	RSRZ
33	2b	127	ILE	3.0
6	2G	75	LYS	3.0
47	1p	82	GLN	3.0
26	24	25	TYR	3.0
35	2d	20	TYR	3.0
42	2k	75	TYR	3.0
1	1A	271(K)	U	3.0
25	23	60	GLU	3.0
47	2p	80	PHE	2.9
7	2H	33	LEU	2.9
21	2Z	90	VAL	2.9
40	2i	17	VAL	2.9
40	2i	65	VAL	2.9
43	1l	18	VAL	2.9
3	2D	275	LYS	2.9
44	2m	110	ARG	2.9
39	1h	134	ILE	2.9
33	2b	47	THR	2.9
41	2j	92	THR	2.9
32	2a	1001	A	2.9
40	1i	5	TYR	2.9
50	2s	12	ASP	2.9
1	2A	2115	G	2.9
1	2A	2123	G	2.9
1	2A	2165	G	2.9
32	2a	1002	G	2.9
6	2G	100	TRP	2.9
21	2Z	136	PHE	2.9
32	2a	1006	C	2.9
35	1d	110	PHE	2.9
33	1b	77	ALA	2.9
39	1h	112	LEU	2.9
40	2i	46	ALA	2.9
51	1t	72	LEU	2.9
51	1t	97	ALA	2.9
53	2y	52	ALA	2.9
6	2G	81	LYS	2.9
43	2l	19	ARG	2.9
44	2m	98	VAL	2.9
47	1p	81	ARG	2.9
53	2y	9	GLN	2.9
53	2y	46	GLN	2.9

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Mol	Chain	Res	Type	RSRZ
53	2y	12	ILE	2.9
53	2y	39	ILE	2.9
26	24	52	THR	2.9
1	1A	2109	U	2.9
1	2A	2158	A	2.9
21	2Z	99	TYR	2.9
26	14	57	GLU	2.9
47	1p	1	MET	2.9
26	14	64	GLY	2.9
41	1j	76	ASN	2.9
50	2s	26	GLY	2.9
53	2y	51	ASP	2.9
40	2i	98	PRO	2.9
1	1A	2115	G	2.9
4	2E	204	ALA	2.9
6	2G	141	PHE	2.9
35	1d	169	LYS	2.9
34	1c	47	LEU	2.9
40	1i	101	PHE	2.9
1	1A	2107	C	2.9
7	2H	60	ARG	2.9
48	2q	98	LEU	2.9
26	24	50	VAL	2.9
34	2c	86	VAL	2.9
1	1A	1105	U	2.9
1	1A	2144	U	2.9
1	2A	2122	U	2.9
26	14	52	THR	2.9
1	1A	6	A	2.9
17	1V	101	GLY	2.9
26	24	43	TYR	2.9
47	1p	37	GLY	2.9
53	2y	43	LYS	2.9
33	2b	140	HIS	2.9
35	2d	47	ARG	2.9
41	2j	62	HIS	2.9
21	1Z	187	ALA	2.9
33	2b	145	LEU	2.9
34	2c	52	LEU	2.9
50	2s	71	LEU	2.9
1	1A	2145	C	2.9
1	2A	2177	C	2.9

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Mol	Chain	Res	Type	RSRZ
8	2I	92	VAL	2.9
6	1G	48	GLU	2.9
6	2G	144	ILE	2.9
34	2c	14	ILE	2.9
50	1s	77	THR	2.9
1	2A	1111	A	2.8
6	1G	76	SER	2.8
15	1T	38	ASN	2.9
32	1a	1493	A	2.8
48	1q	99	SER	2.8
53	2y	4	ASN	2.9
43	1l	20	LYS	2.8
44	2m	31	LYS	2.8
45	2n	50	LYS	2.8
14	2S	7	TYR	2.8
47	1p	5	ARG	2.8
47	1p	66	PRO	2.8
14	2S	58	LEU	2.8
33	2b	61	LEU	2.8
38	2g	99	LEU	2.8
45	2n	53	LEU	2.8
50	2s	15	LEU	2.8
7	2H	20	ALA	2.8
29	17	45	ALA	2.8
40	2i	37	PHE	2.8
1	1A	889	C	2.8
1	1A	2112	G	2.8
1	2A	1087	G	2.8
1	2A	2128	C	2.8
1	2A	2157	G	2.8
8	1I	136	VAL	2.8
40	2i	109	VAL	2.8
41	1j	34	VAL	2.8
41	2j	49	VAL	2.8
44	2m	82	MET	2.8
32	1a	1257	U	2.8
33	1b	214	ILE	2.8
26	24	51	ASP	2.8
34	1c	62	ASP	2.8
51	1t	11	SER	2.8
51	2t	25	ARG	2.8
53	2y	64	SER	2.8

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Mol	Chain	Res	Type	RSRZ
33	2b	40	HIS	2.8
34	1c	107	GLN	2.8
44	1m	87	TYR	2.8
34	2c	175	LEU	2.8
44	2m	90	LEU	2.8
34	1c	71	ALA	2.8
40	2i	52	ALA	2.8
35	1d	179	GLU	2.8
1	2A	2166	G	2.8
6	2G	86	MET	2.8
21	2Z	71	VAL	2.8
29	17	1	MET	2.8
1	2A	271(N)	U	2.8
1	2A	1066	U	2.8
1	2A	2180	U	2.8
3	1D	275	LYS	2.8
26	14	69	LYS	2.8
26	14	68	ARG	2.8
33	2b	73	THR	2.8
33	2b	168	THR	2.8
46	2o	87	ILE	2.8
52	2u	10	ARG	2.8
17	2V	63	GLY	2.8
33	2b	227	GLY	2.8
40	2i	30	GLY	2.8
50	2s	82	GLY	2.8
32	2a	1005	A	2.8
40	2i	49	PRO	2.8
6	2G	12	TYR	2.8
34	2c	48	TYR	2.8
42	1k	75	TYR	2.8
7	2H	7	LEU	2.8
44	2m	75	ALA	2.8
20	2Y	5	MET	2.8
1	1A	2146	C	2.8
40	1i	95	LYS	2.8
1	2A	12	U	2.8
1	2A	614(A)	U	2.8
9	1N	140	VAL	2.8
1	2A	2156	G	2.8
15	1T	129	ARG	2.8
32	1a	1034	G	2.8

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Mol	Chain	Res	Type	RSRZ
38	2g	33	ASP	2.8
40	2i	67	GLY	2.8
1	2A	1088	A	2.8
1	2A	1095	A	2.8
32	1a	1492	A	2.8
51	1t	98	PRO	2.8
34	2c	90	GLU	2.8
6	2G	182	LYS	2.8
45	2n	4	LYS	2.8
14	2S	79	ALA	2.8
33	2b	120	ALA	2.8
34	2c	186	PHE	2.8
35	2d	110	PHE	2.8
45	2n	16	PHE	2.8
7	1H	101	ARG	2.8
13	2R	68	ARG	2.8
1	2A	645	C	2.8
32	2a	1039	C	2.8
35	1d	178	VAL	2.8
1	1A	2148	G	2.7
1	1A	2154	G	2.7
1	2A	2184	G	2.7
8	2I	129	THR	2.7
42	1k	117	ASN	2.7
51	2t	100	ILE	2.7
33	2b	38	GLY	2.7
45	2n	32	SER	2.7
5	2F	14	PRO	2.7
45	2n	54	PRO	2.7
26	24	28	LYS	2.7
53	2y	8	LYS	2.7
6	2G	82	LEU	2.7
14	2S	32	LEU	2.7
35	1d	155	LEU	2.7
41	2j	88	LEU	2.7
53	2y	41	LEU	2.7
35	1d	138	TYR	2.7
40	2i	43	ALA	2.7
43	2l	120	TYR	2.7
49	1r	60	ALA	2.7
50	1s	29	ARG	2.7
1	1A	1175	U	2.7

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Mol	Chain	Res	Type	RSRZ
1	2A	1065	U	2.7
1	2A	1082	U	2.7
32	1a	1040	U	2.7
1	2A	2163	C	2.7
4	1E	75	VAL	2.7
7	2H	43	VAL	2.7
7	2H	50	VAL	2.7
8	1I	107	VAL	2.7
9	2N	140	VAL	2.7
34	2c	138	VAL	2.7
40	2i	26	VAL	2.7
41	2j	69	ASN	2.7
45	1n	13	THR	2.7
45	1n	22	THR	2.7
33	1b	223	ILE	2.7
26	24	45	GLY	2.7
34	1c	80	GLY	2.7
50	2s	4	SER	2.7
32	1a	1004	A	2.7
20	2Y	90	LEU	2.7
26	24	58	ARG	2.7
40	2i	19	LEU	2.7
45	2n	29	ARG	2.7
46	2o	88	ARG	2.7
50	2s	16	LEU	2.7
50	2s	37	ARG	2.7
6	1G	50	ALA	2.7
34	2c	100	ALA	2.7
40	1i	62	TYR	2.7
40	2i	58	HIS	2.7
1	1A	2139	C	2.7
7	2H	15	VAL	2.7
41	1j	72	VAL	2.7
33	2b	37	ASN	2.7
20	2Y	80	GLY	2.7
26	24	5	ILE	2.7
50	1s	40	ILE	2.7
3	2D	38	LYS	2.7
8	2I	137	PRO	2.7
21	2Z	159	PRO	2.7
33	2b	156	LYS	2.7
1	1A	2169	A	2.7

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Mol	Chain	Res	Type	RSRZ
1	1A	2176	A	2.7
33	1b	23	ARG	2.7
39	1h	102	ARG	2.7
41	2j	79	ARG	2.7
42	2k	126	ARG	2.7
46	2o	68	ARG	2.7
52	1u	9	ARG	2.7
33	1b	221	LEU	2.7
34	2c	32	LEU	2.7
33	2b	16	HIS	2.7
34	2c	65	ALA	2.7
19	1X	69	TYR	2.7
6	1G	80	PHE	2.7
6	2G	70	VAL	2.7
7	2H	49	VAL	2.7
33	2b	93	VAL	2.7
34	2c	3	ASN	2.7
38	2g	21	VAL	2.7
40	1i	86	VAL	2.7
51	1t	9	ASN	2.7
26	24	19	GLY	2.7
33	1b	18	GLY	2.7
38	2g	27	ILE	2.7
38	2g	42	ILE	2.7
50	1s	26	GLY	2.7
40	1i	21	PRO	2.7
44	2m	113	PRO	2.7
33	2b	144	ARG	2.7
34	1c	83	ARG	2.7
1	1A	545	G	2.7
1	2A	2207	G	2.7
29	27	1	MET	2.7
32	1a	220	G	2.7
32	2a	1024	G	2.7
41	1j	86	MET	2.7
1	1A	1095	A	2.7
1	2A	2170	A	2.7
32	2a	1357	A	2.7
33	2b	149	LEU	2.7
47	1p	73	LEU	2.7
47	2p	59	TRP	2.7
52	1u	14	TRP	2.7

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Mol	Chain	Res	Type	RSRZ
1	1A	1060	U	2.6
1	1A	1963	U	2.6
21	2Z	188	ALA	2.6
34	1c	60	ALA	2.6
44	2m	5	ALA	2.6
4	2E	151	TYR	2.6
40	1i	33	PHE	2.6
41	2j	54	PHE	2.6
45	2n	36	PHE	2.6
3	2D	99	ASP	2.6
41	1j	44	VAL	2.6
47	2p	20	VAL	2.6
1	1A	2108	C	2.6
6	2G	145	THR	2.6
6	2G	157	ILE	2.6
7	2H	120	GLY	2.6
32	1a	1007	C	2.6
32	2a	1028	C	2.6
41	2j	15	THR	2.6
45	2n	22	THR	2.6
34	2c	8	ILE	2.6
35	1d	23	GLY	2.6
7	2H	39	PRO	2.6
15	2T	111	ARG	2.6
26	14	55	ARG	2.6
33	1b	21	ARG	2.6
34	2c	79	ARG	2.6
35	1d	76	ARG	2.6
35	2d	158	ILE	2.6
45	2n	7	ILE	2.6
46	1o	87	ILE	2.6
47	1p	15	PRO	2.6
47	2p	19	ILE	2.6
1	1A	1055	G	2.6
1	1A	548	A	2.6
1	1A	1045	A	2.6
1	1A	2126	A	2.6
32	2a	1447	A	2.6
34	2c	178	LEU	2.6
6	1G	46	ALA	2.6
40	1i	18	PHE	2.6
40	2i	59	PHE	2.6

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Mol	Chain	Res	Type	RSRZ
49	1r	43	PHE	2.6
52	2u	5	ASP	2.6
7	2H	6	ARG	2.6
12	2Q	60	ARG	2.6
14	2S	20	ARG	2.6
29	17	23	ARG	2.6
35	1d	3	ARG	2.6
5	2F	6	VAL	2.6
24	22	63	VAL	2.6
26	24	27	THR	2.6
34	2c	192	THR	2.6
35	2d	69	GLY	2.6
41	2j	48	THR	2.6
50	1s	84	GLY	2.6
1	2A	2178	C	2.6
1	2A	2183	C	2.6
1	2A	2789	C	2.6
6	2G	112	PRO	2.6
41	1j	77	PRO	2.6
1	2A	1062	G	2.6
1	2A	2155	G	2.6
32	1a	1033	G	2.6
32	2a	994	A	2.6
33	1b	154	LEU	2.6
33	2b	196	LEU	2.6
35	1d	101	LEU	2.6
44	2m	48	LEU	2.6
51	1t	62	LEU	2.6
8	2I	131	LYS	2.6
32	2a	1125	U	2.6
33	2b	139	LYS	2.6
47	1p	50	LYS	2.6
8	2I	55	ALA	2.6
38	2g	2	ALA	2.6
50	2s	34	TRP	2.6
51	1t	66	ALA	2.6
6	2G	83	ARG	2.6
7	2H	8	PRO	2.6
14	2S	92	TYR	2.6
21	2Z	161	VAL	2.6
35	2d	23	GLY	2.6
40	1i	39	GLY	2.6

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Mol	Chain	Res	Type	RSRZ
48	1q	23	VAL	2.6
52	1u	21	TYR	2.6
52	2u	21	TYR	2.6
53	2y	53	THR	2.6
40	2i	123	PRO	2.6
1	1A	2142	C	2.6
33	2b	201	ILE	2.6
50	2s	31	ILE	2.6
43	2l	47	LYS	2.6
50	2s	25	LYS	2.6
1	2A	6	A	2.6
1	2A	1073	A	2.6
40	2i	47	LEU	2.6
1	1A	2206	G	2.6
8	2I	85	GLU	2.6
32	1a	1021	G	2.6
6	1G	83	ARG	2.6
26	24	55	ARG	2.6
45	2n	31	ARG	2.6
34	2c	60	ALA	2.6
6	2G	155	MET	2.6
33	1b	89	GLY	2.6
34	2c	41	GLY	2.6
40	2i	8	GLY	2.6
25	23	59	VAL	2.6
50	2s	59	PRO	2.6
41	1j	6	ILE	2.6
1	1A	2161	C	2.6
1	1A	2175	C	2.6
1	2A	34	C	2.6
23	21	78	LYS	2.6
6	1G	82	LEU	2.5
19	2X	92	LEU	2.5
24	22	3	LEU	2.5
1	2A	1050	A	2.5
1	2A	1086	A	2.5
32	2a	1040	U	2.5
34	1c	42	LEU	2.5
41	2j	8	LEU	2.5
26	14	61	ARG	2.5
6	2G	73	ALA	2.5
33	1b	34	ALA	2.5

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Mol	Chain	Res	Type	RSRZ
34	2c	149	ALA	2.5
34	2c	160	ALA	2.5
34	1c	3	ASN	2.5
37	2f	89	MET	2.5
42	2k	36	ASP	2.5
53	1y	70	MET	2.5
21	2Z	95	PRO	2.5
34	2c	80	GLY	2.5
40	2i	39	GLY	2.5
33	2b	17	PHE	2.5
38	1g	26	PHE	2.5
44	1m	113	PRO	2.5
47	1p	45	THR	2.5
6	2G	109	VAL	2.5
7	2H	169	VAL	2.5
21	2Z	58	VAL	2.5
21	2Z	86	VAL	2.5
6	2G	20	ILE	2.5
26	24	40	HIS	2.5
31	29	20	HIS	2.5
44	2m	27	LYS	2.5
47	1p	51	VAL	2.5
50	1s	19	VAL	2.5
34	2c	157	ILE	2.5
34	2c	182	ILE	2.5
41	1j	75	ILE	2.5
1	1A	1532	C	2.5
1	1A	2136	C	2.5
1	2A	2185	C	2.5
38	1g	13	GLN	2.5
40	1i	4	TYR	2.5
40	2i	36	TYR	2.5
47	1p	17	TYR	2.5
10	1O	108	GLU	2.5
1	1A	2167	U	2.5
49	2r	87	ARG	2.5
6	2G	90	LEU	2.5
33	2b	51	LEU	2.5
1	2A	1045	A	2.5
15	2T	1	MET	2.5
32	2a	1021	G	2.5
33	2b	48	MET	2.5

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Mol	Chain	Res	Type	RSRZ
6	2G	151	ALA	2.5
33	2b	166	ASP	2.5
38	2g	84	ASN	2.5
44	1m	107	ALA	2.5
50	1s	23	ASN	2.5
7	2H	128	PRO	2.5
7	2H	173	PRO	2.5
33	2b	234	PRO	2.5
44	1m	100	GLY	2.5
44	2m	24	GLY	2.5
44	2m	20	THR	2.5
34	2c	18	TRP	2.5
53	2y	38	HIS	2.5
20	2Y	89	PHE	2.5
34	2c	76	VAL	2.5
40	2i	44	VAL	2.5
41	1j	35	SER	2.5
11	2P	75	ILE	2.5
40	2i	63	ILE	2.5
44	2m	39	ILE	2.5
21	1Z	203	GLU	2.5
7	1H	3	ARG	2.5
19	2X	65	ARG	2.5
20	2Y	55	TYR	2.5
32	1a	1038	C	2.5
49	1r	42	ARG	2.5
1	2A	1026	U	2.5
32	2a	1000	U	2.5
7	2H	171	LEU	2.5
33	2b	102	LEU	2.5
34	1c	52	LEU	2.5
38	2g	12	LEU	2.5
40	1i	99	LEU	2.5
1	1A	1046	A	2.5
1	2A	1051	G	2.5
1	2A	1063	G	2.5
1	2A	2131	G	2.5
14	2S	57	LYS	2.5
32	1a	630	G	2.5
34	2c	92	ALA	2.5
47	2p	47	ASP	2.5
50	2s	6	LYS	2.5

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Mol	Chain	Res	Type	RSRZ
6	2G	42	GLY	2.5
33	1b	131	PRO	2.5
36	1e	22	GLY	2.5
44	2m	41	PRO	2.5
37	1f	27	GLN	2.5
41	1j	33	GLN	2.5
41	2j	87	THR	2.5
6	2G	102	PHE	2.5
6	1G	149	VAL	2.5
6	2G	137	GLU	2.5
40	1i	59	PHE	2.5
34	1c	75	VAL	2.5
40	2i	12	GLU	2.5
42	2k	125	PHE	2.5
9	2N	9	VAL	2.5
20	2Y	75	ILE	2.5
41	2j	5	ARG	2.5
1	1A	2138	C	2.5
1	2A	2164	C	2.5
1	2A	1090	U	2.5
44	2m	59	TYR	2.5
5	2F	181	LEU	2.5
33	2b	154	LEU	2.5
34	2c	188	LEU	2.5
35	1d	188	LEU	2.5
37	2f	45	LEU	2.5
40	1i	50	LEU	2.5
48	1q	98	LEU	2.5
1	2A	1077	A	2.5
4	1E	57	LYS	2.5
35	1d	86	LYS	2.5
50	2s	7	LYS	2.5
47	1p	68	ASP	2.5
7	2H	75	ALA	2.5
9	2N	92	ALA	2.5
33	2b	88	ALA	2.5
33	2b	225	ALA	2.5
34	2c	163	ALA	2.5
36	2e	21	ALA	2.5
39	1h	110	ALA	2.5
45	2n	59	ALA	2.5
1	1A	2124	G	2.5

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Mol	Chain	Res	Type	RSRZ
1	1A	2153	G	2.5
1	2A	1068	G	2.5
4	2E	29	GLY	2.5
7	2H	174	GLY	2.5
21	2Z	68	PRO	2.5
32	2a	1124	G	2.5
40	1i	90	PRO	2.5
42	2k	115	PRO	2.5
53	2y	14	PRO	2.5
6	2G	51	ARG	2.4
16	2U	59	ARG	2.4
33	2b	30	ARG	2.4
40	2i	104	ARG	2.4
48	1q	49	GLU	2.4
50	2s	78	ARG	2.4
51	2t	86	ARG	2.4
53	2y	95	ARG	2.4
35	1d	133	VAL	2.4
38	2g	62	PHE	2.4
8	2I	71	ILE	2.4
40	2i	81	ILE	2.4
41	2j	50	ILE	2.4
50	2s	49	ILE	2.4
53	1y	60	VAL	2.4
32	1a	1025	U	2.4
1	1A	2143	C	2.4
1	2A	1079	C	2.4
14	1S	58	LEU	2.4
21	2Z	9	TYR	2.4
33	2b	31	TYR	2.4
33	2b	138	LEU	2.4
33	2b	187	LEU	2.4
40	2i	40	LEU	2.4
8	2I	87	LYS	2.4
12	2Q	103	MET	2.4
20	2Y	81	LYS	2.4
26	24	69	LYS	2.4
34	2c	97	LYS	2.4
41	2j	86	MET	2.4
1	1A	1096	A	2.4
32	1a	1035	A	2.4
33	1b	140	HIS	2.4

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Mol	Chain	Res	Type	RSRZ
48	2q	94	ASN	2.4
7	2H	36	PRO	2.4
20	2Y	50	ARG	2.4
26	14	54	GLY	2.4
26	24	61	ARG	2.4
35	2d	164	ALA	2.4
38	2g	116	ALA	2.4
39	1h	84	ARG	2.4
41	1j	39	PRO	2.4
44	2m	102	ARG	2.4
1	1A	1537	G	2.4
1	1A	2168	G	2.4
47	1p	44	THR	2.4
48	1q	12	SER	2.4
51	1t	70	SER	2.4
14	2S	40	ILE	2.4
26	24	14	ILE	2.4
33	2b	152	PHE	2.4
33	2b	163	PHE	2.4
36	2e	45	PHE	2.4
39	2h	45	ILE	2.4
47	1p	19	ILE	2.4
47	1p	36	ILE	2.4
7	2H	153	LYS	2.4
41	2j	80	LYS	2.4
1	2A	1072	C	2.4
1	2A	1075	C	2.4
11	2P	3	LEU	2.4
21	2Z	125	LEU	2.4
32	2a	1128	C	2.4
33	2b	213	LEU	2.4
50	2s	20	LEU	2.4
44	2m	23	TYR	2.4
1	2A	529	A	2.4
40	2i	75	ASP	2.4
26	24	3	GLU	2.4
26	24	57	GLU	2.4
6	2G	6	ALA	2.4
6	2G	69	ALA	2.4
14	1S	60	GLY	2.4
26	24	64	GLY	2.4
33	1b	62	ALA	2.4

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Mol	Chain	Res	Type	RSRZ
34	1c	109	PRO	2.4
38	2g	128	ALA	2.4
40	1i	100	GLY	2.4
42	2k	15	ALA	2.4
52	1u	2	GLY	2.4
6	2G	71	THR	2.4
6	2G	161	THR	2.4
8	1I	86	THR	2.4
41	1j	42	THR	2.4
52	2u	8	THR	2.4
1	1A	1173	G	2.4
1	1A	2141	G	2.4
43	2l	118	SER	2.4
48	2q	99	SER	2.4
6	2G	117	PHE	2.4
6	2G	159	VAL	2.4
7	2H	89	ILE	2.4
32	1a	841	U	2.4
32	2a	1281	U	2.4
33	2b	71	VAL	2.4
34	2c	10	PHE	2.4
34	2c	55	VAL	2.4
34	2c	84	ILE	2.4
37	1f	88	VAL	2.4
40	1i	41	VAL	2.4
40	2i	86	VAL	2.4
50	2s	45	VAL	2.4
52	2u	13	ILE	2.4
1	2A	2105	C	2.4
32	1a	1008	C	2.4
33	1b	61	LEU	2.4
33	2b	10	LEU	2.4
34	1c	94	LEU	2.4
34	2c	33	LEU	2.4
35	1d	194	LEU	2.4
41	1j	90	LEU	2.4
41	2j	71	LEU	2.4
47	2p	6	LEU	2.4
17	2V	81	TYR	2.4
53	2y	67	HIS	2.4
35	2d	160	GLN	2.4
38	2g	115	ARG	2.4

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Mol	Chain	Res	Type	RSRZ
45	2n	35	ARG	2.4
1	1A	887	A	2.4
6	2G	49	ASP	2.4
16	2U	56	ASP	2.4
6	1G	2	PRO	2.4
34	1c	73	PRO	2.4
4	2E	46	ALA	2.4
34	2c	171	GLY	2.4
35	1d	69	GLY	2.4
35	2d	180	GLY	2.4
50	1s	24	ALA	2.4
20	2Y	34	LYS	2.4
41	2j	42	THR	2.4
1	1A	2123	G	2.4
6	2G	15	VAL	2.4
10	1O	112	MET	2.4
35	2d	8	VAL	2.4
38	1g	144	MET	2.4
41	2j	63	PHE	2.4
21	2Z	67	LEU	2.4
33	2b	69	LEU	2.4
38	1g	12	LEU	2.4
42	2k	103	LEU	2.4
14	1S	20	ARG	2.4
29	27	41	ARG	2.4
43	1l	19	ARG	2.4
50	2s	14	HIS	2.4
1	1A	1584	C	2.4
21	1Z	202	GLU	2.4
33	2b	24	TRP	2.4
35	1d	173	TRP	2.4
20	2Y	107	ASP	2.3
1	1A	2171	A	2.3
35	2d	7	PRO	2.3
7	1H	175	LYS	2.3
8	2I	90	GLY	2.3
21	1Z	189	ALA	2.3
31	29	15	LYS	2.3
33	1b	14	GLY	2.3
39	1h	128	GLY	2.3
44	2m	112	GLY	2.3
45	2n	17	LYS	2.3

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Mol	Chain	Res	Type	RSRZ
53	2y	92	GLY	2.3
8	2I	63	ALA	2.3
50	1s	39	THR	2.3
53	2y	7	SER	2.3
1	1A	1420	U	2.3
1	1A	2118	U	2.3
1	2A	2167	U	2.3
36	1e	10	MET	2.3
1	2A	1044	G	2.3
1	2A	2751	G	2.3
7	2H	72	ILE	2.3
20	2Y	45	VAL	2.3
24	22	25	VAL	2.3
26	24	21	VAL	2.3
26	24	31	ILE	2.3
32	2a	1009	G	2.3
34	2c	68	VAL	2.3
34	2c	124	ILE	2.3
45	2n	27	CYS	2.3
50	2s	74	PHE	2.3
6	2G	118	ARG	2.3
21	2Z	121	HIS	2.3
3	2D	37	LEU	2.3
7	2H	103	LEU	2.3
8	2I	38	LEU	2.3
8	2I	135	GLU	2.3
41	2j	83	GLU	2.3
1	1A	2140	C	2.3
1	2A	1104	C	2.3
32	1a	63	C	2.3
17	1V	26	ASP	2.3
1	1A	229	A	2.3
7	2H	118	PRO	2.3
33	2b	33	TYR	2.3
38	2g	103	TRP	2.3
34	2c	73	PRO	2.3
35	1d	4	TYR	2.3
41	1j	99	LYS	2.3
43	2l	46	LYS	2.3
44	1m	59	TYR	2.3
44	1m	115	LYS	2.3
48	2q	67	LYS	2.3

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Mol	Chain	Res	Type	RSRZ
50	2s	80	TYR	2.3
3	1D	2	ALA	2.3
4	1E	28	ALA	2.3
33	1b	225	ALA	2.3
38	2g	147	ALA	2.3
44	2m	18	ALA	2.3
51	2t	97	ALA	2.3
53	1y	3	MET	2.3
1	1A	12	U	2.3
3	2D	262	ARG	2.3
19	1X	68	ARG	2.3
26	24	13	ARG	2.3
26	24	62	ARG	2.3
35	1d	132	ARG	2.3
39	2h	69	ARG	2.3
41	1j	79	ARG	2.3
26	24	22	ILE	2.3
33	1b	201	ILE	2.3
33	2b	222	ILE	2.3
8	2I	136	VAL	2.3
34	2c	130	VAL	2.3
35	1d	80	GLU	2.3
37	2f	95	GLU	2.3
40	1i	14	VAL	2.3
40	1i	58	HIS	2.3
53	2y	82	GLU	2.3
6	2G	103	LEU	2.3
35	1d	120	LEU	2.3
50	1s	16	LEU	2.3
1	1A	645	C	2.3
6	1G	49	ASP	2.3
21	1Z	198	LYS	2.3
33	2b	79	ASP	2.3
36	2e	5	ASP	2.3
43	2l	126	LYS	2.3
38	2g	14	PRO	2.3
1	2A	2062	A	2.3
7	2H	83	TYR	2.3
20	2Y	35	TYR	2.3
26	24	32	TYR	2.3
28	26	42	TRP	2.3
34	2c	159	GLY	2.3

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Mol	Chain	Res	Type	RSRZ
36	2e	133	TYR	2.3
39	2h	47	GLY	2.3
35	2d	48	ALA	2.3
53	1y	94	ALA	2.3
5	1F	17	ARG	2.3
21	1Z	52	SER	2.3
24	12	69	ARG	2.3
35	2d	3	ARG	2.3
41	2j	43	ARG	2.3
41	2j	68	HIS	2.3
26	24	46	GLN	2.3
43	2l	16	GLU	2.3
6	1G	88	ILE	2.3
36	2e	11	ILE	2.3
6	2G	37	VAL	2.3
7	2H	24	VAL	2.3
7	2H	114	VAL	2.3
26	24	35	VAL	2.3
35	2d	112	VAL	2.3
38	1g	91	VAL	2.3
38	2g	9	VAL	2.3
43	2l	90	VAL	2.3
44	2m	7	VAL	2.3
6	2G	19	LEU	2.3
14	1S	4	LEU	2.3
21	2Z	157	LEU	2.3
1	1A	2160	G	2.3
1	2A	11	G	2.3
1	2A	1171	G	2.3
32	1a	1009	G	2.3
33	1b	133	LYS	2.3
40	1i	79	LEU	2.3
41	1j	88	LEU	2.3
42	1k	63	LEU	2.3
44	2m	81	LEU	2.3
47	2p	49	LEU	2.3
53	1y	41	LEU	2.3
32	2a	470	C	2.3
32	2a	1019	C	2.3
8	2I	34	GLY	2.3
40	2i	68	GLY	2.3
51	2t	102	GLY	2.3

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Mol	Chain	Res	Type	RSRZ
52	1u	16	GLY	2.3
5	2F	7	TYR	2.3
15	1T	108	ARG	2.3
18	2W	92	ARG	2.3
21	2Z	184	ALA	2.3
33	1b	36	ARG	2.3
36	2e	60	TYR	2.3
40	2i	16	ARG	2.3
46	1o	88	ARG	2.3
47	1p	25	ARG	2.3
51	2t	94	ALA	2.3
52	2u	9	ARG	2.3
1	1A	272(A)	U	2.3
32	2a	1020	U	2.3
47	1p	69	THR	2.3
14	2S	34	HIS	2.3
16	2U	117	GLN	2.3
21	2Z	168	GLU	2.3
33	1b	20	GLU	2.3
33	2b	86	GLU	2.3
47	1p	13	HIS	2.3
47	1p	16	HIS	2.3
34	2c	104	GLN	2.3
7	1H	92	ILE	2.3
21	2Z	57	ILE	2.3
43	1l	17	LYS	2.3
43	1l	21	LYS	2.3
44	2m	115	LYS	2.3
51	1t	55	ILE	2.3
6	2G	28	VAL	2.3
6	2G	31	VAL	2.3
8	2I	31	LEU	2.2
12	2Q	65	PHE	2.2
17	2V	5	VAL	2.3
25	23	58	VAL	2.3
29	27	46	VAL	2.3
34	2c	47	LEU	2.2
40	1i	28	VAL	2.3
41	1j	85	LEU	2.2
41	2j	94	VAL	2.3
47	1p	62	VAL	2.3
53	2y	24	LEU	2.2

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Mol	Chain	Res	Type	RSRZ
26	14	51	ASP	2.2
42	2k	110	ASP	2.2
1	2A	885	C	2.2
8	1I	134	PRO	2.2
20	1Y	56	PRO	2.2
32	2a	1149	C	2.2
6	2G	128	ARG	2.2
12	2Q	30	GLY	2.2
31	29	9	ARG	2.2
33	2b	228	GLY	2.2
34	2c	185	GLY	2.2
38	2g	81	GLY	2.2
40	1i	51	ARG	2.2
52	1u	15	ARG	2.2
1	1A	1460	A	2.2
1	1A	2150	U	2.2
1	2A	1060	U	2.2
6	2G	163	ALA	2.2
21	1Z	190	GLU	2.2
26	24	12	ALA	2.2
33	2b	123	ALA	2.2
43	1l	120	TYR	2.2
50	2s	75	ALA	2.2
44	2m	43	THR	2.2
50	2s	79	THR	2.2
53	1y	71	TYR	2.2
21	2Z	166	SER	2.2
45	2n	60	SER	2.2
19	2X	33	LYS	2.2
38	2g	36	LYS	2.2
43	1l	126	LYS	2.2
33	1b	208	ILE	2.2
6	1G	3	LEU	2.2
6	2G	5	VAL	2.2
6	2G	92	VAL	2.2
7	2H	17	VAL	2.2
8	2I	5	LEU	2.2
34	2c	120	VAL	2.2
35	2d	75	PHE	2.2
40	1i	65	VAL	2.2
40	1i	109	VAL	2.2
47	1p	74	LEU	2.2

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Mol	Chain	Res	Type	RSRZ
50	1s	15	LEU	2.2
49	2r	29	PHE	2.2
50	2s	58	VAL	2.2
40	1i	75	ASP	2.2
1	1A	1056	G	2.2
1	1A	2207	G	2.2
1	2A	1047	G	2.2
1	2A	2793	G	2.2
29	17	47	ARG	2.2
34	2c	83	ARG	2.2
36	2e	152	ARG	2.2
1	2A	1052	C	2.2
32	2a	1116	C	2.2
50	1s	46	GLY	2.2
26	24	30	GLU	2.2
32	1a	532	A	2.2
33	1b	35	GLU	2.2
48	1q	48	GLU	2.2
1	2A	958	U	2.2
35	2d	45	GLN	2.2
36	1e	20	GLN	2.2
41	1j	14	LYS	2.2
8	2I	78	THR	2.2
50	2s	33	THR	2.2
52	2u	17	THR	2.2
47	2p	39	TYR	2.2
50	1s	61	TYR	2.2
34	2c	22	TRP	2.2
6	2G	140	ILE	2.2
7	2H	9	ILE	2.2
21	1Z	146	ILE	2.2
21	2Z	133	ILE	2.2
21	2Z	146	ILE	2.2
33	1b	222	ILE	2.2
35	2d	146	ILE	2.2
39	1h	86	ILE	2.2
44	1m	39	ILE	2.2
4	1E	195	LEU	2.2
21	2Z	33	LEU	2.2
36	2e	53	LEU	2.2
33	1b	71	VAL	2.2
37	1f	90	VAL	2.2

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Mol	Chain	Res	Type	RSRZ
40	1i	53	VAL	2.2
50	1s	11	VAL	2.2
50	2s	60	VAL	2.2
21	2Z	88	PHE	2.2
8	1I	14	ASP	2.2
18	2W	60	ASN	2.2
35	2d	168	ARG	2.2
40	1i	20	ARG	2.2
41	2j	58	ASP	2.2
47	1p	42	ARG	2.2
21	2Z	1	MET	2.2
25	13	2	PRO	2.2
33	1b	48	MET	2.2
48	1q	82	MET	2.2
1	2A	2181	G	2.2
14	2S	60	GLY	2.2
21	2Z	160	GLY	2.2
31	29	37	GLY	2.2
34	2c	155	GLY	2.2
1	1A	886	C	2.2
7	2H	34	GLU	2.2
7	2H	53	GLU	2.2
8	2I	10	GLU	2.2
32	1a	1019	C	2.2
32	2a	1007	C	2.2
33	1b	12	GLU	2.2
35	2d	156	GLU	2.2
48	2q	86	GLU	2.2
6	2G	58	GLN	2.2
16	1U	117	GLN	2.2
24	22	70	GLN	2.2
43	2l	23	LYS	2.2
44	1m	27	LYS	2.2
1	1A	1084	A	2.2
1	1A	2135	A	2.2
1	2A	887	A	2.2
32	1a	197	A	2.2
32	1a	1020	U	2.2
32	1a	1212	U	2.2
32	2a	1256	A	2.2
6	2G	158	ALA	2.2
7	2H	165	ALA	2.2

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Mol	Chain	Res	Type	RSRZ
19	2X	91	ALA	2.2
33	2b	29	ALA	2.2
33	2b	34	ALA	2.2
33	2b	161	ALA	2.2
33	2b	177	ALA	2.2
50	2s	77	THR	2.2
39	2h	48	TYR	2.2
6	2G	62	LEU	2.2
33	2b	42	ILE	2.2
34	1c	84	ILE	2.2
34	2c	12	LEU	2.2
34	2c	43	LEU	2.2
38	1g	50	ILE	2.2
38	2g	38	LEU	2.2
40	1i	63	ILE	2.2
6	2G	136	ARG	2.2
9	2N	115	ARG	2.2
41	2j	28	ARG	2.2
47	1p	49	LEU	2.2
48	1q	72	ARG	2.2
6	2G	149	VAL	2.2
7	2H	79	VAL	2.2
4	2E	1	MET	2.2
8	2I	20	ASP	2.2
21	2Z	100	VAL	2.2
35	1d	105	VAL	2.2
35	1d	121	VAL	2.2
39	1h	53	VAL	2.2
39	2h	51	VAL	2.2
33	2b	181	PHE	2.2
34	2c	17	ASP	2.2
50	2s	11	VAL	2.2
50	2s	19	VAL	2.2
36	1e	45	PHE	2.2
53	2y	70	MET	2.2
5	1F	14	PRO	2.2
20	2Y	53	PRO	2.2
38	2g	93	PRO	2.2
46	1o	2	PRO	2.2
46	2o	75	PRO	2.2
6	2G	54	GLU	2.2
20	2Y	88	LYS	2.2

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Mol	Chain	Res	Type	RSRZ
34	2c	4	LYS	2.2
41	2j	14	LYS	2.2
48	1q	37	LYS	2.2
49	2r	46	GLU	2.2
53	2y	26	LYS	2.2
53	2y	66	LYS	2.2
7	2H	166	GLY	2.2
34	2c	6	HIS	2.2
35	2d	16	GLY	2.2
40	2i	117	HIS	2.2
43	1l	95	GLY	2.2
44	1m	6	GLY	2.2
45	2n	51	GLY	2.2
48	2q	93	GLN	2.2
1	1A	2131	G	2.2
1	2A	1074	G	2.2
1	2A	2100	G	2.2
1	2A	2103	C	2.2
32	1a	90	U	2.2
32	2a	80	G	2.2
32	2a	979	C	2.2
8	2I	76	THR	2.2
21	2Z	173	ALA	2.2
21	2Z	192	ALA	2.2
22	20	43	THR	2.2
23	11	54	ALA	2.2
33	2b	124	SER	2.2
34	2c	71	ALA	2.2
34	2c	129	ALA	2.2
35	2d	71	SER	2.2
41	2j	20	ALA	2.2
44	1m	5	ALA	2.2
45	1n	5	ALA	2.2
51	1t	77	ALA	2.2
53	1y	42	SER	2.2
6	2G	11	TYR	2.1
33	1b	148	TYR	2.1
40	1i	36	TYR	2.1
40	2i	114	TYR	2.1
43	2l	89	ARG	2.1
46	2o	17	ARG	2.1
47	1p	32	TYR	2.1

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Mol	Chain	Res	Type	RSRZ
47	1p	38	TYR	2.1
50	2s	52	TYR	2.1
50	2s	61	TYR	2.1
4	2E	77	ILE	2.1
14	2S	54	LEU	2.1
17	2V	96	ILE	2.1
20	2Y	96	ILE	2.1
33	1b	200	ILE	2.1
33	2b	39	ILE	2.1
33	2b	58	ILE	2.1
33	2b	155	LEU	2.1
33	2b	215	LEU	2.1
33	2b	221	LEU	2.1
34	1c	39	ILE	2.1
35	2d	21	LEU	2.1
41	1j	16	LEU	2.1
41	2j	23	ILE	2.1
45	1n	7	ILE	2.1
53	2y	78	ILE	2.1
50	1s	34	TRP	2.1
6	2G	123	ASN	2.1
7	2H	125	VAL	2.1
8	2I	15	VAL	2.1
9	1N	9	VAL	2.1
33	2b	184	VAL	2.1
7	2H	175	LYS	2.1
9	2N	2	LYS	2.1
21	2Z	199	LYS	2.1
19	2X	85	PRO	2.1
26	24	42	PHE	2.1
26	24	53	GLU	2.1
33	1b	122	PHE	2.1
40	1i	37	PHE	2.1
50	1s	74	PHE	2.1
26	14	46	GLN	2.1
42	2k	116	HIS	2.1
50	1s	47	HIS	2.1
53	2y	47	GLY	2.1
1	1A	2149	G	2.1
1	1A	2157	G	2.1
1	1A	2893	G	2.1
1	2A	1093	G	2.1

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Mol	Chain	Res	Type	RSRZ
32	1a	79	G	2.1
32	1a	1533	C	2.1
1	1A	1174	A	2.1
1	1A	2170	A	2.1
1	1A	2790	A	2.1
32	2a	1123	A	2.1
7	2H	150	ALA	2.1
21	2Z	7	ALA	2.1
34	2c	50	ALA	2.1
44	1m	51	ALA	2.1
45	2n	10	ALA	2.1
45	2n	20	ALA	2.1
46	2o	25	THR	2.1
6	2G	72	ARG	2.1
15	2T	115	ARG	2.1
34	2c	11	ARG	2.1
35	2d	50	ARG	2.1
40	2i	83	ARG	2.1
52	2u	22	ARG	2.1
3	1D	37	LEU	2.1
6	2G	47	LYS	2.1
6	2G	60	LEU	2.1
6	2G	135	LEU	2.1
6	2G	148	MET	2.1
12	2Q	137	TYR	2.1
8	1I	38	LEU	2.1
19	2X	1	MET	2.1
38	2g	44	TYR	2.1
53	2y	71	TYR	2.1
33	2b	214	ILE	2.1
42	1k	98	LEU	2.1
44	2m	19	LEU	2.1
48	1q	90	ILE	2.1
3	2D	71	ASP	2.1
21	2Z	87	ASP	2.1
33	2b	129	GLU	2.1
40	1i	105	ASP	2.1
21	1Z	86	VAL	2.1
21	2Z	32	HIS	2.1
33	2b	125	PRO	2.1
34	2c	103	VAL	2.1
34	1c	10	PHE	2.1

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Mol	Chain	Res	Type	RSRZ
36	2e	96	PRO	2.1
37	2f	90	VAL	2.1
38	1g	75	VAL	2.1
39	2h	79	VAL	2.1
42	2k	109	VAL	2.1
44	2m	64	TRP	2.1
38	1g	43	PHE	2.1
38	2g	106	GLN	2.1
53	1y	9	GLN	2.1
33	2b	14	GLY	2.1
36	1e	85	GLY	2.1
41	2j	10	GLY	2.1
41	2j	31	GLY	2.1
48	1q	80	GLY	2.1
50	1s	8	GLY	2.1
32	1a	65	U	2.1
32	2a	1150	U	2.1
2	1B	88	C	2.1
32	1a	217	C	2.1
1	1A	271(M)	G	2.1
1	1A	2134	A	2.1
1	2A	614(B)	G	2.1
8	1I	57	ARG	2.1
7	2H	63	SER	2.1
8	2I	86	THR	2.1
11	2P	102	ARG	2.1
32	1a	196	A	2.1
32	1a	1041	A	2.1
32	2a	963	G	2.1
32	2a	1022	G	2.1
32	2a	1157	A	2.1
40	2i	107	ARG	2.1
41	2j	66	ARG	2.1
44	2m	114	ARG	2.1
47	2p	26	ARG	2.1
8	1I	146	ALA	2.1
8	2I	59	ALA	2.1
12	2Q	117	ALA	2.1
14	2S	37	ALA	2.1
33	1b	13	ALA	2.1
35	1d	32	ALA	2.1
35	2d	149	ALA	2.1

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Mol	Chain	Res	Type	RSRZ
40	2i	45	ALA	2.1
40	2i	82	ALA	2.1
6	1G	81	LYS	2.1
11	2P	76	LYS	2.1
20	2Y	54	LYS	2.1
33	2b	63	MET	2.1
34	2c	93	LYS	2.1
45	1n	4	LYS	2.1
48	2q	14	LYS	2.1
6	2G	133	LEU	2.1
11	2P	99	LEU	2.1
19	2X	8	ILE	2.1
28	26	11	LEU	2.1
33	1b	126	GLU	2.1
8	2I	79	ILE	2.1
33	1b	215	LEU	2.1
35	1d	146	ILE	2.1
35	2d	78	LEU	2.1
35	2d	202	LEU	2.1
39	2h	39	LEU	2.1
41	1j	71	LEU	2.1
51	1t	20	LEU	2.1
51	2t	91	LEU	2.1
21	2Z	34	ASN	2.1
38	2g	37	ASN	2.1
21	2Z	65	GLN	2.1
34	2c	162	GLN	2.1
39	2h	70	GLN	2.1
47	2p	76	GLN	2.1
35	1d	88	VAL	2.1
40	2i	108	VAL	2.1
41	1j	24	VAL	2.1
41	2j	41	PRO	2.1
45	2n	56	VAL	2.1
22	20	45	PHE	2.1
33	1b	57	PHE	2.1
35	2d	167	GLY	2.1
40	2i	69	GLY	2.1
50	2s	8	GLY	2.1
8	2I	52	ARG	2.1
11	1P	15	ARG	2.1
30	28	46	ARG	2.1

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Mol	Chain	Res	Type	RSRZ
42	1k	126	ARG	2.1
44	2m	3	ARG	2.1
48	1q	91	ARG	2.1
49	1r	87	ARG	2.1
2	1B	120	A	2.1
7	2H	56	SER	2.1
26	24	18	CYS	2.1
32	1a	1006	C	2.1
32	2a	1260	C	2.1
1	2A	2186	G	2.1
6	2G	36	LYS	2.1
32	2a	1531	A	2.1
41	1j	15	THR	2.1
32	2a	1023	G	2.1
32	2a	1139	G	2.1
32	2a	1202	G	2.1
34	1c	100	ALA	2.1
34	2c	168	ALA	2.1
40	1i	78	LYS	2.1
33	1b	83	MET	2.1
31	29	28	GLU	2.1
36	2e	81	GLU	2.1
7	2H	111	HIS	2.1
10	2O	90	GLN	2.1
15	2T	114	LEU	2.1
12	2Q	135	ASP	2.1
21	2Z	50	GLN	2.1
35	1d	174	LEU	2.1
35	2d	155	LEU	2.1
35	2d	176	LEU	2.1
38	2g	101	LEU	2.1
33	2b	162	ILE	2.1
33	2b	189	ASP	2.1
35	1d	158	ILE	2.1
36	2e	109	ILE	2.1
40	1i	87	GLN	2.1
41	2j	16	LEU	2.1
47	1p	60	LEU	2.1
47	1p	76	GLN	2.1
51	2t	10	LEU	2.1
33	1b	41	ILE	2.1
47	2p	14	ASN	2.1

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Mol	Chain	Res	Type	RSRZ
26	24	7	PRO	2.1
36	1e	133	TYR	2.1
7	2H	11	VAL	2.1
14	2S	28	VAL	2.1
17	2V	79	VAL	2.1
21	2Z	105	VAL	2.1
31	29	16	VAL	2.1
33	2b	229	VAL	2.1
34	1c	86	VAL	2.1
35	2d	105	VAL	2.1
35	2d	178	VAL	2.1
35	2d	198	VAL	2.1
42	2k	30	VAL	2.1
47	1p	2	VAL	2.1
33	2b	89	GLY	2.1
34	2c	9	GLY	2.1
34	2c	158	GLY	2.1
34	2c	203	PHE	2.1
40	1i	22	GLY	2.1
51	2t	96	GLY	2.1
1	2A	271(K)	U	2.1
1	2A	1081	U	2.1
19	2X	60	ARG	2.1
34	1c	167	TRP	2.1
35	2d	49	ARG	2.1
37	2f	47	ARG	2.1
47	1p	75	ARG	2.1
48	2q	63	ARG	2.1
20	2Y	94	LYS	2.0
1	1A	278	A	2.0
21	2Z	28	MET	2.0
32	1a	1043	C	2.0
32	2a	1008	C	2.0
4	2E	28	ALA	2.0
33	1b	134	GLU	2.0
33	2b	13	ALA	2.0
33	2b	101	MET	2.0
36	2e	48	ALA	2.0
38	2g	46	ALA	2.0
38	2g	65	ALA	2.0
39	2h	22	GLU	2.0
44	2m	76	ALA	2.0

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Mol	Chain	Res	Type	RSRZ
1	1A	274	G	2.0
8	1I	105	HIS	2.0
33	2b	76	GLN	2.0
6	2G	147	ASP	2.0
8	1I	20	ASP	2.0
14	2S	56	LEU	2.0
14	2S	78	LEU	2.0
33	2b	60	ASP	2.0
35	2d	101	LEU	2.0
39	2h	112	LEU	2.0
8	1I	71	ILE	2.0
8	1I	138	ILE	2.0
10	2O	69	ILE	2.0
31	29	17	ILE	2.0
33	2b	108	ILE	2.0
34	1c	77	ILE	2.0
34	2c	57	ILE	2.0
7	2H	168	PRO	2.0
33	2b	26	PRO	2.0
21	2Z	3	TYR	2.0
35	2d	4	TYR	2.0
17	2V	46	VAL	2.0
26	24	68	ARG	2.0
33	2b	164	VAL	2.0
36	2e	55	VAL	2.0
38	2g	155	ARG	2.0
40	1i	44	VAL	2.0
41	1j	46	ARG	2.0
43	1l	90	VAL	2.0
47	2p	79	VAL	2.0
47	2p	81	ARG	2.0
1	2A	157	U	2.0
1	2A	1094	U	2.0
14	2S	81	GLY	2.0
21	2Z	48	PHE	2.0
32	1a	204	U	2.0
33	2b	72	GLY	2.0
35	1d	6	GLY	2.0
35	1d	16	GLY	2.0
38	2g	34	GLY	2.0
39	2h	131	GLY	2.0
33	1b	28	PHE	2.0

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Mol	Chain	Res	Type	RSRZ
33	1b	70	PHE	2.0
33	1b	163	PHE	2.0
22	20	46	LYS	2.0
30	28	21	LYS	2.0
46	1o	5	LYS	2.0
50	1s	18	LYS	2.0
53	2y	3	MET	2.0
51	2t	71	THR	2.0
1	2A	1080	C	2.0
1	2A	2801(A)	A	2.0
8	1I	83	ALA	2.0
11	2P	134	ALA	2.0
32	1a	163	C	2.0
32	2a	848	C	2.0
32	2a	1248	A	2.0
32	2a	1493	A	2.0
40	1i	45	ALA	2.0
49	1r	20	ALA	2.0
51	1t	94	ALA	2.0
1	1A	2133	G	2.0
1	1A	2152	G	2.0
4	2E	195	LEU	2.0
6	1G	126	ASP	2.0
6	2G	173	LEU	2.0
8	2I	12	LEU	2.0
31	29	12	ASP	2.0
32	1a	78	G	2.0
32	1a	102	G	2.0
32	2a	1010	G	2.0
32	2a	1224	G	2.0
36	1e	73	ASN	2.0
45	2n	47	LEU	2.0
51	1t	24	LEU	2.0
53	2y	88	LEU	2.0
6	1G	140	ILE	2.0
6	2G	142	PRO	2.0
21	2Z	197	ILE	2.0
26	14	15	ILE	2.0
26	14	58	ARG	2.0
33	2b	36	ARG	2.0
33	2b	130	ARG	2.0
34	2c	39	ILE	2.0

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Mol	Chain	Res	Type	RSRZ
34	2c	202	ILE	2.0
40	2i	77	ILE	2.0
42	1k	29	ILE	2.0
20	1Y	34	LYS	2.0
33	2b	147	LYS	2.0
35	2d	169	LYS	2.0

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

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
1	5MU	2A	1915	21/22	0.84	0.12	75,83,86,99	0
32	2MG	2a	1207	24/25	0.85	0.12	79,85,90,93	0
1	5MU	1A	1915	21/22	0.86	0.13	72,80,85,91	0
32	M2G	2a	966	25/26	0.88	0.15	60,72,82,86	0
43	0TD	2l	92	10/11	0.89	0.13	62,69,72,79	0
1	PSU	2A	1917	20/21	0.90	0.10	72,76,89,91	0
1	PSU	2A	1911	20/21	0.90	0.10	68,73,78,83	0
32	5MC	2a	967	21/22	0.91	0.14	66,72,81,88	0
1	PSU	1A	1917	20/21	0.92	0.10	66,72,79,82	0
32	PSU	2a	516	20/21	0.92	0.10	71,75,79,82	0
1	PSU	1A	1911	20/21	0.93	0.09	62,67,74,76	0
43	0TD	1l	92	10/11	0.94	0.12	53,61,68,72	0
32	G7M	2a	527	24/25	0.94	0.10	62,68,73,75	0
32	PSU	1a	516	20/21	0.94	0.09	57,67,70,71	0
32	5MC	1a	967	21/22	0.94	0.12	60,67,74,78	0
32	2MG	1a	1207	24/25	0.94	0.09	65,72,75,76	0
1	OMC	2A	1920	21/22	0.94	0.10	62,68,73,74	0
32	5MC	2a	1400	21/22	0.95	0.13	63,69,72,75	0
32	5MC	2a	1404	21/22	0.95	0.09	55,60,65,67	0
32	5MC	2a	1407	21/22	0.95	0.10	55,63,68,70	0
32	UR3	2a	1498	21/22	0.95	0.10	58,63,66,68	0
32	M2G	1a	966	25/26	0.95	0.10	55,63,69,74	0
32	G7M	1a	527	24/25	0.96	0.10	46,57,62,64	0
32	5MC	1a	1400	21/22	0.96	0.10	52,57,62,63	0
32	4OC	1a	1402	22/23	0.96	0.10	50,55,57,68	0
32	5MC	1a	1404	21/22	0.96	0.10	43,49,53,55	0
32	4OC	2a	1402	22/23	0.96	0.09	59,65,71,75	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
32	5MC	1a	1407	21/22	0.96	0.10	47,56,59,64	0
1	5MC	2A	1942	21/22	0.96	0.08	47,53,57,59	0
32	UR3	1a	1498	21/22	0.96	0.10	48,53,56,59	0
32	MA6	2a	1518	24/25	0.96	0.11	54,62,67,70	0
32	MA6	1a	1519	24/25	0.96	0.10	43,51,56,57	0
1	5MC	2A	1962	21/22	0.97	0.09	42,48,54,64	0
1	OMG	2A	2251	24/25	0.97	0.10	40,44,47,49	0
1	2MA	2A	2503	23/24	0.97	0.08	33,39,43,47	0
1	PSU	2A	2605	20/21	0.97	0.07	36,39,46,48	0
1	5MC	1A	1942	21/22	0.97	0.07	36,42,44,50	0
32	MA6	1a	1518	24/25	0.97	0.10	43,51,54,58	0
1	5MU	2A	1939	21/22	0.97	0.07	34,39,42,47	0
32	MA6	2a	1519	24/25	0.97	0.10	55,61,65,66	0
1	OMC	1A	1920	21/22	0.97	0.09	52,60,63,64	0
1	OMU	1A	2552	21/22	0.98	0.07	29,34,37,39	0
1	PSU	1A	2605	20/21	0.98	0.07	26,31,34,42	0
1	5MU	1A	1939	21/22	0.98	0.07	26,33,35,36	0
1	5MC	1A	1962	21/22	0.98	0.07	33,40,44,47	0
1	OMG	1A	2251	24/25	0.98	0.07	25,32,39,40	0
1	2MA	1A	2503	23/24	0.98	0.06	22,28,29,32	0
1	OMU	2A	2552	21/22	0.98	0.07	37,43,46,47	0

5.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	2A	3670	1/1	0.45	0.25	84,84,84,84	0
54	MG	2a	3119	1/1	0.47	0.23	93,93,93,93	0
54	MG	1A	3625	1/1	0.48	0.26	84,84,84,84	0
54	MG	2a	3155	1/1	0.58	0.28	95,95,95,95	0
54	MG	1a	1675	1/1	0.59	0.40	84,84,84,84	0
54	MG	1A	3946	1/1	0.59	0.21	41,41,41,41	0
54	MG	2A	3464	1/1	0.60	0.30	69,69,69,69	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	2A	3658	1/1	0.62	0.28	71,71,71,71	0
54	MG	2A	3452	1/1	0.62	0.19	82,82,82,82	0
54	MG	1A	3411	1/1	0.63	0.17	74,74,74,74	0
54	MG	2A	3577	1/1	0.63	0.15	79,79,79,79	0
54	MG	2A	3454	1/1	0.64	0.24	67,67,67,67	0
54	MG	1A	3763	1/1	0.65	0.36	60,60,60,60	0
54	MG	2A	3717	1/1	0.65	0.15	88,88,88,88	0
54	MG	1A	3680	1/1	0.66	0.28	61,61,61,61	0
54	MG	1A	3854	1/1	0.66	0.27	51,51,51,51	0
54	MG	1a	1830	1/1	0.66	0.36	85,85,85,85	0
54	MG	2A	3656	1/1	0.67	0.29	83,83,83,83	0
54	MG	1A	3925	1/1	0.67	0.23	72,72,72,72	0
54	MG	1a	1740	1/1	0.68	0.19	93,93,93,93	0
54	MG	2A	3421	1/1	0.68	0.23	81,81,81,81	0
54	MG	1a	1774	1/1	0.68	0.21	82,82,82,82	0
54	MG	2A	3704	1/1	0.69	0.14	69,69,69,69	0
54	MG	1A	3508	1/1	0.69	0.16	57,57,57,57	0
54	MG	2B	215	1/1	0.69	0.20	84,84,84,84	0
54	MG	1A	3491	1/1	0.69	0.22	67,67,67,67	0
54	MG	2A	3581	1/1	0.69	0.21	77,77,77,77	0
54	MG	1A	3675	1/1	0.70	0.18	79,79,79,79	0
54	MG	1A	3566	1/1	0.70	0.28	43,43,43,43	0
54	MG	1A	3986	1/1	0.70	0.28	76,76,76,76	0
54	MG	2A	3628	1/1	0.70	0.22	64,64,64,64	0
54	MG	2a	3008	1/1	0.70	0.33	80,80,80,80	0
54	MG	1A	3624	1/1	0.70	0.17	78,78,78,78	0
54	MG	1A	3403	1/1	0.70	0.20	72,72,72,72	0
54	MG	1A	3964	1/1	0.71	0.28	78,78,78,78	0
54	MG	1a	1825	1/1	0.71	0.23	69,69,69,69	0
54	MG	1B	207	1/1	0.71	0.30	73,73,73,73	0
54	MG	2A	3295	1/1	0.71	0.26	72,72,72,72	0
54	MG	1A	3518	1/1	0.72	0.16	51,51,51,51	0
54	MG	1a	1781	1/1	0.72	0.31	77,77,77,77	0
54	MG	1A	3775	1/1	0.72	0.21	55,55,55,55	0
54	MG	1a	1751	1/1	0.72	0.21	82,82,82,82	0
54	MG	2A	3458	1/1	0.72	0.30	76,76,76,76	0
54	MG	2A	3256	1/1	0.72	0.32	76,76,76,76	0
54	MG	2A	3146	1/1	0.73	0.20	73,73,73,73	0
54	MG	1A	3855	1/1	0.73	0.22	62,62,62,62	0
54	MG	1b	301	1/1	0.73	0.23	83,83,83,83	0
54	MG	2A	3681	1/1	0.73	0.33	74,74,74,74	0
54	MG	2A	3416	1/1	0.73	0.37	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	1676	1/1	0.74	0.16	83,83,83,83	0
54	MG	1a	1788	1/1	0.74	0.19	75,75,75,75	0
54	MG	2A	3707	1/1	0.74	0.23	62,62,62,62	0
54	MG	1a	1812	1/1	0.74	0.23	82,82,82,82	0
54	MG	2A	3497	1/1	0.74	0.20	77,77,77,77	0
54	MG	2I	201	1/1	0.74	0.22	75,75,75,75	0
54	MG	2A	3659	1/1	0.74	0.14	55,55,55,55	0
54	MG	2A	3666	1/1	0.74	0.16	77,77,77,77	0
54	MG	1B	228	1/1	0.74	0.24	69,69,69,69	0
54	MG	2A	3348	1/1	0.75	0.20	77,77,77,77	0
54	MG	2A	3380	1/1	0.75	0.26	69,69,69,69	0
54	MG	2A	3661	1/1	0.75	0.20	74,74,74,74	0
54	MG	1a	1623	1/1	0.75	0.23	66,66,66,66	0
54	MG	1A	3958	1/1	0.75	0.23	85,85,85,85	0
54	MG	1A	3607	1/1	0.75	0.20	54,54,54,54	0
54	MG	1A	3306	1/1	0.75	0.40	81,81,81,81	0
54	MG	1a	1854	1/1	0.75	0.19	75,75,75,75	0
54	MG	1A	3370	1/1	0.75	0.22	65,65,65,65	0
54	MG	2A	3024	1/1	0.75	0.20	64,64,64,64	0
54	MG	2A	3076	1/1	0.75	0.32	77,77,77,77	0
54	MG	1A	3660	1/1	0.75	0.24	73,73,73,73	0
54	MG	2a	3022	1/1	0.75	0.20	75,75,75,75	0
54	MG	1T	202	1/1	0.75	0.28	75,75,75,75	0
54	MG	1a	1785	1/1	0.75	0.17	79,79,79,79	0
54	MG	2h	201	1/1	0.75	0.27	84,84,84,84	0
54	MG	1a	1708	1/1	0.76	0.28	74,74,74,74	0
54	MG	1a	1842	1/1	0.76	0.30	77,77,77,77	0
54	MG	1A	3421	1/1	0.76	0.18	38,38,38,38	0
54	MG	1A	3754	1/1	0.76	0.20	47,47,47,47	0
54	MG	1h	201	1/1	0.76	0.20	72,72,72,72	0
54	MG	1A	3283	1/1	0.76	0.24	75,75,75,75	0
54	MG	1A	3937	1/1	0.76	0.33	70,70,70,70	0
54	MG	2A	3079	1/1	0.76	0.30	77,77,77,77	0
54	MG	2A	3499	1/1	0.76	0.24	78,78,78,78	0
54	MG	1A	3533	1/1	0.76	0.26	59,59,59,59	0
54	MG	1a	1640	1/1	0.76	0.22	71,71,71,71	0
54	MG	2A	3279	1/1	0.76	0.21	64,64,64,64	0
54	MG	2a	3080	1/1	0.76	0.53	85,85,85,85	0
54	MG	1A	3815	1/1	0.76	0.17	61,61,61,61	0
54	MG	2A	3657	1/1	0.76	0.28	68,68,68,68	0
54	MG	2a	3169	1/1	0.76	0.35	70,70,70,70	0
54	MG	1A	3833	1/1	0.76	0.14	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	3152	1/1	0.77	0.20	57,57,57,57	0
54	MG	1A	3297	1/1	0.77	0.39	68,68,68,68	0
54	MG	2a	3047	1/1	0.77	0.46	76,76,76,76	0
54	MG	2a	3069	1/1	0.77	0.21	68,68,68,68	0
54	MG	1A	3696	1/1	0.77	0.18	51,51,51,51	0
54	MG	1A	3269	1/1	0.77	0.26	78,78,78,78	0
54	MG	1a	1759	1/1	0.77	0.24	82,82,82,82	0
54	MG	1A	3602	1/1	0.77	0.19	72,72,72,72	0
54	MG	1A	3903	1/1	0.77	0.13	62,62,62,62	0
54	MG	1a	1811	1/1	0.78	0.19	79,79,79,79	0
54	MG	2A	3702	1/1	0.78	0.16	79,79,79,79	0
54	MG	1A	3668	1/1	0.78	0.26	79,79,79,79	0
54	MG	1a	1821	1/1	0.78	0.19	79,79,79,79	0
54	MG	2A	3235	1/1	0.78	0.33	77,77,77,77	0
54	MG	2A	3245	1/1	0.78	0.41	73,73,73,73	0
54	MG	1B	231	1/1	0.78	0.17	79,79,79,79	0
54	MG	1A	3293	1/1	0.78	0.39	65,65,65,65	0
54	MG	2a	3016	1/1	0.78	0.17	73,73,73,73	0
54	MG	1a	1834	1/1	0.78	0.21	68,68,68,68	0
54	MG	2A	3305	1/1	0.78	0.22	68,68,68,68	0
54	MG	1A	3965	1/1	0.78	0.20	60,60,60,60	0
54	MG	1a	1636	1/1	0.78	0.30	72,72,72,72	0
54	MG	1A	3980	1/1	0.78	0.24	80,80,80,80	0
54	MG	2a	3145	1/1	0.78	0.33	80,80,80,80	0
54	MG	1A	3744	1/1	0.78	0.16	70,70,70,70	0
54	MG	1A	3805	1/1	0.78	0.13	62,62,62,62	0
54	MG	2A	3453	1/1	0.78	0.17	70,70,70,70	0
54	MG	1B	225	1/1	0.79	0.15	62,62,62,62	0
54	MG	1a	1798	1/1	0.79	0.21	81,81,81,81	0
54	MG	2B	207	1/1	0.79	0.29	79,79,79,79	0
54	MG	2B	211	1/1	0.79	0.15	63,63,63,63	0
54	MG	1B	227	1/1	0.79	0.23	70,70,70,70	0
54	MG	2A	3349	1/1	0.79	0.17	54,54,54,54	0
54	MG	2A	3366	1/1	0.79	0.34	80,80,80,80	0
54	MG	1A	3311	1/1	0.79	0.31	71,71,71,71	0
54	MG	1A	3826	1/1	0.79	0.16	68,68,68,68	0
54	MG	2a	3034	1/1	0.79	0.14	78,78,78,78	0
54	MG	1A	3584	1/1	0.79	0.15	47,47,47,47	0
54	MG	1A	3981	1/1	0.79	0.13	43,43,43,43	0
54	MG	1A	3450	1/1	0.79	0.11	58,58,58,58	0
54	MG	2a	3090	1/1	0.79	0.31	75,75,75,75	0
54	MG	2a	3098	1/1	0.79	0.31	82,82,82,82	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	1A	3185	1/1	0.79	0.28	61,61,61,61	0
54	MG	2A	3266	1/1	0.79	0.32	77,77,77,77	0
54	MG	1a	1663	1/1	0.79	0.29	72,72,72,72	0
54	MG	2A	3470	1/1	0.79	0.24	71,71,71,71	0
54	MG	2A	3475	1/1	0.79	0.21	76,76,76,76	0
54	MG	2A	3509	1/1	0.80	0.14	64,64,64,64	0
54	MG	2A	3526	1/1	0.80	0.18	71,71,71,71	0
54	MG	2A	3530	1/1	0.80	0.16	49,49,49,49	0
54	MG	2A	3569	1/1	0.80	0.21	57,57,57,57	0
54	MG	2a	3052	1/1	0.80	0.13	83,83,83,83	0
54	MG	2a	3058	1/1	0.80	0.43	83,83,83,83	0
54	MG	2A	3703	1/1	0.80	0.26	73,73,73,73	0
54	MG	1a	1782	1/1	0.80	0.20	86,86,86,86	0
54	MG	1d	305	1/1	0.80	0.11	89,89,89,89	0
54	MG	1A	3536	1/1	0.80	0.18	63,63,63,63	0
54	MG	2A	3412	1/1	0.80	0.23	63,63,63,63	0
54	MG	2A	3302	1/1	0.80	0.19	65,65,65,65	0
54	MG	1A	3320	1/1	0.80	0.15	68,68,68,68	0
54	MG	2A	3431	1/1	0.80	0.17	64,64,64,64	0
54	MG	2a	3176	1/1	0.80	0.19	71,71,71,71	0
54	MG	1A	3757	1/1	0.80	0.21	52,52,52,52	0
54	MG	2A	3123	1/1	0.81	0.18	73,73,73,73	0
54	MG	2B	217	1/1	0.81	0.18	86,86,86,86	0
54	MG	1A	3027	1/1	0.81	0.15	67,67,67,67	0
54	MG	1a	1817	1/1	0.81	0.19	78,78,78,78	0
54	MG	2A	3632	1/1	0.81	0.17	69,69,69,69	0
54	MG	2a	3018	1/1	0.81	0.38	74,74,74,74	0
54	MG	1A	3616	1/1	0.81	0.25	74,74,74,74	0
54	MG	2A	3251	1/1	0.81	0.41	74,74,74,74	0
54	MG	1A	3562	1/1	0.81	0.19	58,58,58,58	0
54	MG	1A	3886	1/1	0.81	0.12	31,31,31,31	0
54	MG	2a	3053	1/1	0.81	0.26	76,76,76,76	0
54	MG	1A	3116	1/1	0.81	0.30	63,63,63,63	0
54	MG	1A	3758	1/1	0.81	0.15	44,44,44,44	0
54	MG	1B	230	1/1	0.81	0.12	70,70,70,70	0
54	MG	2A	3480	1/1	0.81	0.17	68,68,68,68	0
54	MG	2A	3486	1/1	0.81	0.20	74,74,74,74	0
54	MG	1A	3631	1/1	0.81	0.17	60,60,60,60	0
54	MG	1A	3579	1/1	0.81	0.16	69,69,69,69	0
54	MG	1A	3790	1/1	0.81	0.24	83,83,83,83	0
54	MG	1A	3426	1/1	0.81	0.12	68,68,68,68	0
54	MG	1A	3586	1/1	0.81	0.13	55,55,55,55	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	1A	3267	1/1	0.81	0.15	84,84,84,84	0
54	MG	2A	3145	1/1	0.82	0.37	71,71,71,71	0
54	MG	1A	3302	1/1	0.82	0.29	77,77,77,77	0
54	MG	2A	3201	1/1	0.82	0.17	66,66,66,66	0
54	MG	2A	3713	1/1	0.82	0.19	67,67,67,67	0
54	MG	1a	1650	1/1	0.82	0.35	77,77,77,77	0
54	MG	2A	3477	1/1	0.82	0.12	81,81,81,81	0
54	MG	1a	1801	1/1	0.82	0.28	71,71,71,71	0
54	MG	2B	213	1/1	0.82	0.25	73,73,73,73	0
54	MG	1A	3676	1/1	0.82	0.22	66,66,66,66	0
54	MG	1A	3445	1/1	0.82	0.14	55,55,55,55	0
54	MG	2A	3498	1/1	0.82	0.12	64,64,64,64	0
54	MG	1A	3250	1/1	0.82	0.44	75,75,75,75	0
54	MG	1a	1687	1/1	0.82	0.23	72,72,72,72	0
54	MG	1a	1692	1/1	0.82	0.42	75,75,75,75	0
54	MG	2a	3021	1/1	0.82	0.33	79,79,79,79	0
54	MG	1a	1698	1/1	0.82	0.37	69,69,69,69	0
54	MG	2A	3557	1/1	0.82	0.15	53,53,53,53	0
54	MG	1A	3802	1/1	0.82	0.14	62,62,62,62	0
54	MG	2A	3346	1/1	0.82	0.20	77,77,77,77	0
54	MG	1A	3743	1/1	0.82	0.13	45,45,45,45	0
54	MG	2a	3056	1/1	0.82	0.24	68,68,68,68	0
54	MG	1a	1853	1/1	0.82	0.24	77,77,77,77	0
54	MG	1a	1745	1/1	0.82	0.44	64,64,64,64	0
54	MG	1A	3600	1/1	0.82	0.25	65,65,65,65	0
54	MG	2a	3082	1/1	0.82	0.32	68,68,68,68	0
54	MG	2a	3084	1/1	0.82	0.30	61,61,61,61	0
54	MG	1A	3822	1/1	0.82	0.14	72,72,72,72	0
54	MG	1E	305	1/1	0.82	0.14	30,30,30,30	0
54	MG	2a	3100	1/1	0.82	0.25	87,87,87,87	0
54	MG	2A	3417	1/1	0.82	0.18	64,64,64,64	0
54	MG	1a	1780	1/1	0.82	0.24	70,70,70,70	0
54	MG	2A	3046	1/1	0.82	0.20	64,64,64,64	0
54	MG	2a	3166	1/1	0.82	0.14	72,72,72,72	0
54	MG	1A	3198	1/1	0.82	0.16	69,69,69,69	0
54	MG	1A	3201	1/1	0.82	0.20	72,72,72,72	0
54	MG	1A	3850	1/1	0.82	0.11	33,33,33,33	0
56	ARG	1A	3998	12/12	0.82	0.20	56,69,76,77	0
57	MPD	1T	207	8/8	0.82	0.25	67,74,79,79	0
57	MPD	2B	219	8/8	0.82	0.29	59,68,74,77	0
54	MG	1a	1662	1/1	0.83	0.23	70,70,70,70	0
54	MG	2A	3503	1/1	0.83	0.24	76,76,76,76	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	1g	202	1/1	0.83	0.27	80,80,80,80	0
54	MG	2D	308	1/1	0.83	0.14	64,64,64,64	0
54	MG	1A	3569	1/1	0.83	0.11	55,55,55,55	0
54	MG	1A	3608	1/1	0.83	0.17	65,65,65,65	0
54	MG	1A	3955	1/1	0.83	0.38	56,56,56,56	0
54	MG	2A	3381	1/1	0.83	0.13	49,49,49,49	0
54	MG	2A	3407	1/1	0.83	0.30	75,75,75,75	0
54	MG	1a	1790	1/1	0.83	0.13	70,70,70,70	0
54	MG	2a	3029	1/1	0.83	0.31	70,70,70,70	0
54	MG	2A	3616	1/1	0.83	0.23	74,74,74,74	0
54	MG	1A	3191	1/1	0.83	0.27	66,66,66,66	0
54	MG	2A	3088	1/1	0.83	0.25	65,65,65,65	0
54	MG	2A	3639	1/1	0.83	0.19	70,70,70,70	0
54	MG	1A	3285	1/1	0.83	0.23	90,90,90,90	0
54	MG	1A	3683	1/1	0.83	0.27	42,42,42,42	0
54	MG	2a	3062	1/1	0.83	0.34	65,65,65,65	0
54	MG	1a	1702	1/1	0.83	0.45	77,77,77,77	0
54	MG	2A	3184	1/1	0.83	0.40	81,81,81,81	0
54	MG	1a	1707	1/1	0.83	0.23	75,75,75,75	0
54	MG	2A	3662	1/1	0.83	0.20	63,63,63,63	0
54	MG	2A	3455	1/1	0.83	0.16	75,75,75,75	0
54	MG	1A	3457	1/1	0.83	0.12	55,55,55,55	0
54	MG	2A	3462	1/1	0.83	0.16	73,73,73,73	0
54	MG	2a	3108	1/1	0.83	0.19	68,68,68,68	0
54	MG	2A	3683	1/1	0.83	0.20	72,72,72,72	0
54	MG	2a	3138	1/1	0.83	0.14	73,73,73,73	0
54	MG	2A	3696	1/1	0.83	0.09	84,84,84,84	0
54	MG	1a	1728	1/1	0.83	0.18	63,63,63,63	0
54	MG	2a	3160	1/1	0.83	0.27	82,82,82,82	0
54	MG	1T	205	1/1	0.83	0.17	73,73,73,73	0
54	MG	1Z	301	1/1	0.83	0.17	65,65,65,65	0
54	MG	1A	3721	1/1	0.83	0.26	57,57,57,57	0
54	MG	2f	202	1/1	0.83	0.20	81,81,81,81	0
54	MG	1a	1846	1/1	0.83	0.30	75,75,75,75	0
54	MG	1A	3409	1/1	0.83	0.12	74,74,74,74	0
54	MG	1B	203	1/1	0.83	0.28	72,72,72,72	0
57	MPD	1a	1868	8/8	0.83	0.18	53,67,74,76	0
54	MG	1A	3437	1/1	0.83	0.20	65,65,65,65	0
54	MG	1r	101	1/1	0.84	0.27	72,72,72,72	0
54	MG	1A	3475	1/1	0.84	0.10	26,26,26,26	0
54	MG	2A	3437	1/1	0.84	0.24	71,71,71,71	0
54	MG	2A	3438	1/1	0.84	0.23	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	3446	1/1	0.84	0.17	72,72,72,72	0
54	MG	1A	3361	1/1	0.84	0.16	65,65,65,65	0
54	MG	1A	3632	1/1	0.84	0.23	71,71,71,71	0
54	MG	1A	3651	1/1	0.84	0.13	59,59,59,59	0
54	MG	1A	3770	1/1	0.84	0.18	70,70,70,70	0
54	MG	2B	209	1/1	0.84	0.26	72,72,72,72	0
54	MG	2A	3109	1/1	0.84	0.26	67,67,67,67	0
54	MG	2B	212	1/1	0.84	0.30	79,79,79,79	0
54	MG	2A	3115	1/1	0.84	0.30	71,71,71,71	0
54	MG	2B	214	1/1	0.84	0.12	68,68,68,68	0
54	MG	1a	1653	1/1	0.84	0.21	63,63,63,63	0
54	MG	1A	3498	1/1	0.84	0.20	71,71,71,71	0
54	MG	1A	3663	1/1	0.84	0.10	80,80,80,80	0
54	MG	2A	3166	1/1	0.84	0.28	65,65,65,65	0
54	MG	1a	1807	1/1	0.84	0.20	88,88,88,88	0
54	MG	2A	3483	1/1	0.84	0.21	69,69,69,69	0
54	MG	1a	1808	1/1	0.84	0.20	74,74,74,74	0
54	MG	1a	1809	1/1	0.84	0.25	82,82,82,82	0
54	MG	1A	3436	1/1	0.84	0.13	81,81,81,81	0
54	MG	1A	3515	1/1	0.84	0.21	65,65,65,65	0
54	MG	1A	3305	1/1	0.84	0.30	68,68,68,68	0
54	MG	2a	3046	1/1	0.84	0.23	78,78,78,78	0
54	MG	2A	3504	1/1	0.84	0.19	64,64,64,64	0
54	MG	2a	3050	1/1	0.84	0.37	77,77,77,77	0
54	MG	2A	3508	1/1	0.84	0.23	80,80,80,80	0
54	MG	1A	3817	1/1	0.84	0.11	53,53,53,53	0
54	MG	1a	1824	1/1	0.84	0.12	68,68,68,68	0
54	MG	2A	3280	1/1	0.84	0.25	80,80,80,80	0
54	MG	2A	3552	1/1	0.84	0.23	75,75,75,75	0
54	MG	2A	3281	1/1	0.84	0.15	39,39,39,39	0
54	MG	1A	3414	1/1	0.84	0.15	45,45,45,45	0
54	MG	1A	3102	1/1	0.84	0.16	72,72,72,72	0
54	MG	1A	3692	1/1	0.84	0.15	51,51,51,51	0
54	MG	2a	3088	1/1	0.84	0.40	71,71,71,71	0
54	MG	2A	3586	1/1	0.84	0.17	72,72,72,72	0
54	MG	1a	1841	1/1	0.84	0.15	70,70,70,70	0
54	MG	1A	3558	1/1	0.84	0.17	53,53,53,53	0
54	MG	1B	229	1/1	0.84	0.31	70,70,70,70	0
54	MG	2A	3636	1/1	0.84	0.20	84,84,84,84	0
54	MG	2A	3353	1/1	0.84	0.17	51,51,51,51	0
54	MG	2A	3641	1/1	0.84	0.27	53,53,53,53	0
54	MG	2A	3652	1/1	0.84	0.46	83,83,83,83	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	2a	3157	1/1	0.84	0.23	87,87,87,87	0
54	MG	2a	3158	1/1	0.84	0.26	71,71,71,71	0
54	MG	1a	1850	1/1	0.84	0.16	55,55,55,55	0
54	MG	2A	3374	1/1	0.84	0.21	71,71,71,71	0
54	MG	2A	3379	1/1	0.84	0.17	74,74,74,74	0
54	MG	1a	1730	1/1	0.84	0.19	82,82,82,82	0
54	MG	1A	3612	1/1	0.84	0.17	64,64,64,64	0
54	MG	1A	3728	1/1	0.84	0.24	58,58,58,58	0
54	MG	2A	3663	1/1	0.84	0.18	66,66,66,66	0
54	MG	1A	3870	1/1	0.84	0.29	45,45,45,45	0
54	MG	1A	3560	1/1	0.84	0.19	78,78,78,78	0
54	MG	1A	3423	1/1	0.84	0.18	51,51,51,51	0
54	MG	2A	3148	1/1	0.85	0.20	71,71,71,71	0
54	MG	1V	203	1/1	0.85	0.22	62,62,62,62	0
54	MG	2B	205	1/1	0.85	0.17	65,65,65,65	0
54	MG	1W	204	1/1	0.85	0.17	59,59,59,59	0
54	MG	2A	3185	1/1	0.85	0.20	62,62,62,62	0
54	MG	1A	3451	1/1	0.85	0.21	73,73,73,73	0
54	MG	2A	3217	1/1	0.85	0.31	74,74,74,74	0
54	MG	2A	3224	1/1	0.85	0.23	58,58,58,58	0
54	MG	2A	3232	1/1	0.85	0.48	75,75,75,75	0
54	MG	10	107	1/1	0.85	0.19	68,68,68,68	0
54	MG	1a	1749	1/1	0.85	0.20	60,60,60,60	0
54	MG	1A	3665	1/1	0.85	0.15	48,48,48,48	0
54	MG	2G	201	1/1	0.85	0.17	68,68,68,68	0
54	MG	1A	3572	1/1	0.85	0.15	38,38,38,38	0
54	MG	1B	220	1/1	0.85	0.18	69,69,69,69	0
54	MG	2A	3274	1/1	0.85	0.48	71,71,71,71	0
54	MG	1a	1775	1/1	0.85	0.19	80,80,80,80	0
54	MG	2a	3020	1/1	0.85	0.28	70,70,70,70	0
54	MG	1a	1776	1/1	0.85	0.18	71,71,71,71	0
54	MG	1A	3541	1/1	0.85	0.20	55,55,55,55	0
54	MG	1A	3582	1/1	0.85	0.13	70,70,70,70	0
54	MG	2a	3033	1/1	0.85	0.23	68,68,68,68	0
54	MG	1A	3952	1/1	0.85	0.19	47,47,47,47	0
54	MG	2a	3036	1/1	0.85	0.24	74,74,74,74	0
54	MG	1A	3557	1/1	0.85	0.21	54,54,54,54	0
54	MG	1a	1671	1/1	0.85	0.19	69,69,69,69	0
54	MG	1A	3061	1/1	0.85	0.19	57,57,57,57	0
54	MG	2A	3032	1/1	0.85	0.20	64,64,64,64	0
54	MG	1A	3466	1/1	0.85	0.10	27,27,27,27	0
54	MG	2A	3354	1/1	0.85	0.11	80,80,80,80	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	2A	3047	1/1	0.85	0.13	64,64,64,64	0
54	MG	2A	3063	1/1	0.85	0.29	66,66,66,66	0
54	MG	2A	3627	1/1	0.85	0.15	66,66,66,66	0
54	MG	2a	3079	1/1	0.85	0.40	74,74,74,74	0
54	MG	2A	3375	1/1	0.85	0.12	65,65,65,65	0
54	MG	1D	314	1/1	0.85	0.18	76,76,76,76	0
54	MG	2A	3634	1/1	0.85	0.33	51,51,51,51	0
54	MG	1a	1691	1/1	0.85	0.24	68,68,68,68	0
54	MG	1A	3186	1/1	0.85	0.33	68,68,68,68	0
54	MG	2A	3384	1/1	0.85	0.19	59,59,59,59	0
54	MG	2A	3386	1/1	0.85	0.21	58,58,58,58	0
54	MG	2A	3394	1/1	0.85	0.23	67,67,67,67	0
54	MG	2a	3111	1/1	0.85	0.22	78,78,78,78	0
54	MG	2a	3118	1/1	0.85	0.22	72,72,72,72	0
54	MG	2A	3404	1/1	0.85	0.16	61,61,61,61	0
54	MG	2a	3122	1/1	0.85	0.15	74,74,74,74	0
54	MG	2A	3095	1/1	0.85	0.21	64,64,64,64	0
54	MG	2A	3102	1/1	0.85	0.32	71,71,71,71	0
54	MG	2a	3152	1/1	0.85	0.31	74,74,74,74	0
54	MG	2A	3414	1/1	0.85	0.14	86,86,86,86	0
54	MG	1F	313	1/1	0.85	0.36	52,52,52,52	0
54	MG	2A	3113	1/1	0.85	0.20	83,83,83,83	0
54	MG	1a	1699	1/1	0.85	0.40	75,75,75,75	0
54	MG	2a	3162	1/1	0.85	0.16	77,77,77,77	0
54	MG	2A	3118	1/1	0.85	0.18	61,61,61,61	0
54	MG	2a	3167	1/1	0.85	0.30	72,72,72,72	0
54	MG	2A	3120	1/1	0.85	0.23	69,69,69,69	0
54	MG	2A	3682	1/1	0.85	0.18	57,57,57,57	0
54	MG	1P	202	1/1	0.85	0.27	48,48,48,48	0
54	MG	1A	3368	1/1	0.85	0.17	50,50,50,50	0
54	MG	2A	3450	1/1	0.85	0.20	54,54,54,54	0
54	MG	2A	3451	1/1	0.85	0.16	78,78,78,78	0
54	MG	1A	3792	1/1	0.85	0.21	44,44,44,44	0
57	MPD	2A	3728	8/8	0.85	0.22	51,65,69,71	0
54	MG	2A	3147	1/1	0.85	0.31	84,84,84,84	0
54	MG	2A	3276	1/1	0.86	0.17	68,68,68,68	0
54	MG	1A	3501	1/1	0.86	0.12	37,37,37,37	0
54	MG	1A	3936	1/1	0.86	0.18	52,52,52,52	0
54	MG	2A	3489	1/1	0.86	0.14	72,72,72,72	0
54	MG	2A	3493	1/1	0.86	0.14	40,40,40,40	0
54	MG	1T	204	1/1	0.86	0.15	65,65,65,65	0
54	MG	1A	3506	1/1	0.86	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	2V	203	1/1	0.86	0.28	68,68,68,68	0
54	MG	20	102	1/1	0.86	0.16	68,68,68,68	0
54	MG	1A	3943	1/1	0.86	0.24	68,68,68,68	0
54	MG	2A	3501	1/1	0.86	0.14	58,58,58,58	0
54	MG	2A	3303	1/1	0.86	0.20	62,62,62,62	0
54	MG	1A	3574	1/1	0.86	0.12	56,56,56,56	0
54	MG	2A	3331	1/1	0.86	0.12	52,52,52,52	0
54	MG	2A	3041	1/1	0.86	0.17	65,65,65,65	0
54	MG	2a	3023	1/1	0.86	0.37	71,71,71,71	0
54	MG	2A	3043	1/1	0.86	0.35	73,73,73,73	0
54	MG	1A	3442	1/1	0.86	0.17	69,69,69,69	0
54	MG	2A	3539	1/1	0.86	0.21	70,70,70,70	0
54	MG	2a	3035	1/1	0.86	0.23	77,77,77,77	0
54	MG	1A	3444	1/1	0.86	0.15	52,52,52,52	0
54	MG	2a	3037	1/1	0.86	0.29	80,80,80,80	0
54	MG	2a	3043	1/1	0.86	0.23	66,66,66,66	0
54	MG	15	108	1/1	0.86	0.20	56,56,56,56	0
54	MG	2A	3362	1/1	0.86	0.18	73,73,73,73	0
54	MG	1a	1611	1/1	0.86	0.30	80,80,80,80	0
54	MG	2A	3373	1/1	0.86	0.16	61,61,61,61	0
54	MG	1A	3670	1/1	0.86	0.17	72,72,72,72	0
54	MG	2A	3083	1/1	0.86	0.24	61,61,61,61	0
54	MG	2A	3084	1/1	0.86	0.13	56,56,56,56	0
54	MG	1A	3043	1/1	0.86	0.24	62,62,62,62	0
54	MG	1A	3525	1/1	0.86	0.24	71,71,71,71	0
54	MG	1A	3363	1/1	0.86	0.19	59,59,59,59	0
54	MG	1A	3238	1/1	0.86	0.12	76,76,76,76	0
54	MG	2A	3637	1/1	0.86	0.13	78,78,78,78	0
54	MG	2A	3391	1/1	0.86	0.14	66,66,66,66	0
54	MG	1a	1656	1/1	0.86	0.13	72,72,72,72	0
54	MG	1A	3982	1/1	0.86	0.23	59,59,59,59	0
54	MG	1A	3249	1/1	0.86	0.20	65,65,65,65	0
54	MG	1A	3544	1/1	0.86	0.16	64,64,64,64	0
54	MG	1A	3545	1/1	0.86	0.17	63,63,63,63	0
54	MG	1B	213	1/1	0.86	0.24	72,72,72,72	0
54	MG	1a	1677	1/1	0.86	0.14	67,67,67,67	0
54	MG	1A	3837	1/1	0.86	0.21	68,68,68,68	0
54	MG	1A	3464	1/1	0.86	0.10	28,28,28,28	0
54	MG	2a	3135	1/1	0.86	0.14	68,68,68,68	0
54	MG	2A	3435	1/1	0.86	0.15	66,66,66,66	0
54	MG	1A	3738	1/1	0.86	0.18	67,67,67,67	0
54	MG	1a	1697	1/1	0.86	0.29	69,69,69,69	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	2A	3445	1/1	0.86	0.27	76,76,76,76	0
54	MG	1a	1832	1/1	0.86	0.10	68,68,68,68	0
54	MG	2A	3189	1/1	0.86	0.23	66,66,66,66	0
54	MG	2A	3192	1/1	0.86	0.32	72,72,72,72	0
54	MG	1A	3398	1/1	0.86	0.28	70,70,70,70	0
54	MG	1A	3867	1/1	0.86	0.11	69,69,69,69	0
54	MG	1A	3427	1/1	0.86	0.20	67,67,67,67	0
54	MG	1A	3184	1/1	0.86	0.14	59,59,59,59	0
54	MG	1A	3014	1/1	0.86	0.28	66,66,66,66	0
54	MG	2A	3721	1/1	0.86	0.15	81,81,81,81	0
54	MG	2B	204	1/1	0.86	0.16	80,80,80,80	0
54	MG	2r	101	1/1	0.86	0.20	72,72,72,72	0
54	MG	1a	1719	1/1	0.86	0.16	56,56,56,56	0
54	MG	1A	3912	1/1	0.86	0.17	70,70,70,70	0
54	MG	1a	1855	1/1	0.86	0.17	65,65,65,65	0
54	MG	1a	1860	1/1	0.86	0.12	71,71,71,71	0
54	MG	1A	3923	1/1	0.86	0.11	47,47,47,47	0
54	MG	1A	3521	1/1	0.87	0.13	55,55,55,55	0
54	MG	1A	3371	1/1	0.87	0.26	62,62,62,62	0
54	MG	1A	3926	1/1	0.87	0.14	65,65,65,65	0
54	MG	2A	3712	1/1	0.87	0.14	62,62,62,62	0
54	MG	1A	3618	1/1	0.87	0.23	59,59,59,59	0
54	MG	1A	3477	1/1	0.87	0.14	31,31,31,31	0
54	MG	1a	1814	1/1	0.87	0.17	70,70,70,70	0
54	MG	1A	3232	1/1	0.87	0.17	76,76,76,76	0
54	MG	1a	1683	1/1	0.87	0.32	75,75,75,75	0
54	MG	1a	1684	1/1	0.87	0.37	72,72,72,72	0
54	MG	2A	3456	1/1	0.87	0.23	66,66,66,66	0
54	MG	1A	3497	1/1	0.87	0.17	57,57,57,57	0
54	MG	1A	3318	1/1	0.87	0.16	68,68,68,68	0
54	MG	1F	311	1/1	0.87	0.26	65,65,65,65	0
54	MG	2A	3466	1/1	0.87	0.13	64,64,64,64	0
54	MG	1a	1694	1/1	0.87	0.23	70,70,70,70	0
54	MG	1a	1840	1/1	0.87	0.23	78,78,78,78	0
54	MG	2A	3476	1/1	0.87	0.18	59,59,59,59	0
54	MG	2E	306	1/1	0.87	0.27	73,73,73,73	0
54	MG	2A	3246	1/1	0.87	0.28	70,70,70,70	0
54	MG	1A	3739	1/1	0.87	0.17	55,55,55,55	0
54	MG	2A	3252	1/1	0.87	0.27	69,69,69,69	0
54	MG	1A	3366	1/1	0.87	0.13	69,69,69,69	0
54	MG	2a	3003	1/1	0.87	0.32	69,69,69,69	0
54	MG	1A	3550	1/1	0.87	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	1a	1848	1/1	0.87	0.17	72,72,72,72	0
54	MG	1a	1700	1/1	0.87	0.30	68,68,68,68	0
54	MG	1A	3589	1/1	0.87	0.17	41,41,41,41	0
54	MG	1a	1704	1/1	0.87	0.12	72,72,72,72	0
54	MG	1A	3598	1/1	0.87	0.22	42,42,42,42	0
54	MG	2A	3502	1/1	0.87	0.10	61,61,61,61	0
54	MG	1A	3233	1/1	0.87	0.27	72,72,72,72	0
54	MG	1a	1865	1/1	0.87	0.10	70,70,70,70	0
54	MG	1a	1717	1/1	0.87	0.16	62,62,62,62	0
54	MG	1d	302	1/1	0.87	0.11	73,73,73,73	0
54	MG	2A	3522	1/1	0.87	0.11	39,39,39,39	0
54	MG	2A	3308	1/1	0.87	0.20	81,81,81,81	0
54	MG	2A	3314	1/1	0.87	0.20	61,61,61,61	0
54	MG	2A	3535	1/1	0.87	0.23	55,55,55,55	0
54	MG	1V	204	1/1	0.87	0.29	69,69,69,69	0
54	MG	1a	1723	1/1	0.87	0.09	59,59,59,59	0
54	MG	1a	1726	1/1	0.87	0.27	73,73,73,73	0
54	MG	2A	3565	1/1	0.87	0.12	45,45,45,45	0
54	MG	1A	3333	1/1	0.87	0.11	37,37,37,37	0
54	MG	2A	3571	1/1	0.87	0.15	55,55,55,55	0
54	MG	2A	3575	1/1	0.87	0.16	38,38,38,38	0
54	MG	2a	3066	1/1	0.87	0.35	71,71,71,71	0
54	MG	2A	3576	1/1	0.87	0.20	62,62,62,62	0
54	MG	1t	201	1/1	0.87	0.17	63,63,63,63	0
54	MG	1A	3984	1/1	0.87	0.16	68,68,68,68	0
54	MG	1A	3869	1/1	0.87	0.14	67,67,67,67	0
54	MG	11	104	1/1	0.87	0.15	67,67,67,67	0
54	MG	2A	3626	1/1	0.87	0.12	59,59,59,59	0
54	MG	1A	3997	1/1	0.87	0.10	42,42,42,42	0
54	MG	2a	3092	1/1	0.87	0.21	59,59,59,59	0
54	MG	2a	3096	1/1	0.87	0.26	63,63,63,63	0
54	MG	1a	1603	1/1	0.87	0.16	79,79,79,79	0
54	MG	1a	1752	1/1	0.87	0.11	59,59,59,59	0
54	MG	2a	3102	1/1	0.87	0.22	69,69,69,69	0
54	MG	2A	3633	1/1	0.87	0.22	67,67,67,67	0
54	MG	1a	1605	1/1	0.87	0.26	66,66,66,66	0
54	MG	1a	1763	1/1	0.87	0.18	67,67,67,67	0
54	MG	1a	1773	1/1	0.87	0.13	78,78,78,78	0
54	MG	2a	3120	1/1	0.87	0.22	71,71,71,71	0
54	MG	2A	3080	1/1	0.87	0.27	71,71,71,71	0
54	MG	2a	3127	1/1	0.87	0.18	77,77,77,77	0
54	MG	2A	3385	1/1	0.87	0.16	59,59,59,59	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	2A	3081	1/1	0.87	0.34	66,66,66,66	0
54	MG	1B	202	1/1	0.87	0.20	62,62,62,62	0
54	MG	1a	1617	1/1	0.87	0.12	62,62,62,62	0
54	MG	2A	3396	1/1	0.87	0.15	42,42,42,42	0
54	MG	1A	3768	1/1	0.87	0.18	67,67,67,67	0
54	MG	2A	3406	1/1	0.87	0.19	75,75,75,75	0
54	MG	1a	1779	1/1	0.87	0.21	69,69,69,69	0
54	MG	1a	1627	1/1	0.87	0.42	71,71,71,71	0
54	MG	1B	206	1/1	0.87	0.10	51,51,51,51	0
54	MG	2A	3669	1/1	0.87	0.23	67,67,67,67	0
54	MG	1a	1637	1/1	0.87	0.49	80,80,80,80	0
54	MG	2A	3671	1/1	0.87	0.30	70,70,70,70	0
54	MG	1A	3420	1/1	0.87	0.16	64,64,64,64	0
54	MG	1A	3469	1/1	0.87	0.12	33,33,33,33	0
54	MG	1B	218	1/1	0.87	0.12	62,62,62,62	0
54	MG	2A	3692	1/1	0.87	0.25	65,65,65,65	0
54	MG	1A	3781	1/1	0.87	0.20	32,32,32,32	0
54	MG	2A	3697	1/1	0.87	0.13	69,69,69,69	0
54	MG	2A	3701	1/1	0.87	0.11	61,61,61,61	0
54	MG	1a	1659	1/1	0.87	0.22	69,69,69,69	0
54	MG	1A	3795	1/1	0.88	0.16	68,68,68,68	0
54	MG	1A	3424	1/1	0.88	0.16	66,66,66,66	0
54	MG	1a	1862	1/1	0.88	0.11	72,72,72,72	0
54	MG	1a	1645	1/1	0.88	0.31	68,68,68,68	0
54	MG	1a	1762	1/1	0.88	0.13	66,66,66,66	0
54	MG	1A	3621	1/1	0.88	0.23	40,40,40,40	0
54	MG	1a	1766	1/1	0.88	0.29	68,68,68,68	0
54	MG	1a	1768	1/1	0.88	0.24	61,61,61,61	0
54	MG	1A	3812	1/1	0.88	0.17	61,61,61,61	0
54	MG	1l	202	1/1	0.88	0.25	78,78,78,78	0
54	MG	1n	101	1/1	0.88	0.21	80,80,80,80	0
54	MG	1A	3701	1/1	0.88	0.09	75,75,75,75	0
54	MG	1A	3947	1/1	0.88	0.14	51,51,51,51	0
54	MG	1y	201	1/1	0.88	0.15	63,63,63,63	0
54	MG	2A	3001	1/1	0.88	0.15	62,62,62,62	0
54	MG	2A	3317	1/1	0.88	0.23	67,67,67,67	0
54	MG	2A	3520	1/1	0.88	0.24	53,53,53,53	0
54	MG	1A	3483	1/1	0.88	0.13	37,37,37,37	0
54	MG	1E	309	1/1	0.88	0.13	54,54,54,54	0
54	MG	2A	3033	1/1	0.88	0.37	72,72,72,72	0
54	MG	1a	1668	1/1	0.88	0.20	68,68,68,68	0
54	MG	1A	3489	1/1	0.88	0.13	60,60,60,60	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	1A	3446	1/1	0.88	0.13	57,57,57,57	0
54	MG	1F	314	1/1	0.88	0.15	47,47,47,47	0
54	MG	2A	3560	1/1	0.88	0.13	61,61,61,61	0
54	MG	2A	3364	1/1	0.88	0.28	67,67,67,67	0
54	MG	2A	3049	1/1	0.88	0.34	76,76,76,76	0
54	MG	1O	201	1/1	0.88	0.14	58,58,58,58	0
54	MG	1A	3146	1/1	0.88	0.35	46,46,46,46	0
54	MG	1A	3649	1/1	0.88	0.12	69,69,69,69	0
54	MG	2A	3377	1/1	0.88	0.09	39,39,39,39	0
54	MG	2a	3048	1/1	0.88	0.27	73,73,73,73	0
54	MG	2A	3378	1/1	0.88	0.14	61,61,61,61	0
54	MG	2a	3051	1/1	0.88	0.28	77,77,77,77	0
54	MG	1A	3585	1/1	0.88	0.10	48,48,48,48	0
54	MG	2A	3608	1/1	0.88	0.13	78,78,78,78	0
54	MG	1a	1803	1/1	0.88	0.22	76,76,76,76	0
54	MG	1A	3136	1/1	0.88	0.19	69,69,69,69	0
54	MG	2a	3059	1/1	0.88	0.40	65,65,65,65	0
54	MG	1A	3662	1/1	0.88	0.11	78,78,78,78	0
54	MG	2a	3063	1/1	0.88	0.12	77,77,77,77	0
54	MG	1A	3454	1/1	0.88	0.16	64,64,64,64	0
54	MG	1A	3553	1/1	0.88	0.14	66,66,66,66	0
54	MG	2a	3072	1/1	0.88	0.39	70,70,70,70	0
54	MG	2a	3077	1/1	0.88	0.26	74,74,74,74	0
54	MG	2A	3099	1/1	0.88	0.42	78,78,78,78	0
54	MG	2A	3393	1/1	0.88	0.12	37,37,37,37	0
54	MG	1A	3994	1/1	0.88	0.17	62,62,62,62	0
54	MG	1A	3432	1/1	0.88	0.18	57,57,57,57	0
54	MG	2a	3086	1/1	0.88	0.41	68,68,68,68	0
54	MG	2A	3398	1/1	0.88	0.26	63,63,63,63	0
54	MG	10	108	1/1	0.88	0.17	61,61,61,61	0
54	MG	1a	1819	1/1	0.88	0.16	51,51,51,51	0
54	MG	1a	1820	1/1	0.88	0.15	66,66,66,66	0
54	MG	1A	3395	1/1	0.88	0.20	55,55,55,55	0
54	MG	1A	3897	1/1	0.88	0.14	71,71,71,71	0
54	MG	2a	3101	1/1	0.88	0.10	74,74,74,74	0
54	MG	2A	3141	1/1	0.88	0.17	70,70,70,70	0
54	MG	17	105	1/1	0.88	0.14	59,59,59,59	0
54	MG	1B	204	1/1	0.88	0.25	61,61,61,61	0
54	MG	2A	3426	1/1	0.88	0.13	49,49,49,49	0
54	MG	2A	3430	1/1	0.88	0.23	79,79,79,79	0
54	MG	1A	3255	1/1	0.88	0.12	66,66,66,66	0
54	MG	2a	3121	1/1	0.88	0.32	78,78,78,78	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	1A	3911	1/1	0.88	0.11	49,49,49,49	0
54	MG	2A	3159	1/1	0.88	0.16	76,76,76,76	0
54	MG	1a	1836	1/1	0.88	0.18	71,71,71,71	0
54	MG	2a	3136	1/1	0.88	0.12	57,57,57,57	0
54	MG	2A	3444	1/1	0.88	0.23	58,58,58,58	0
54	MG	1A	3401	1/1	0.88	0.27	58,58,58,58	0
54	MG	2A	3684	1/1	0.88	0.24	58,58,58,58	0
54	MG	2A	3686	1/1	0.88	0.12	63,63,63,63	0
54	MG	2A	3688	1/1	0.88	0.15	68,68,68,68	0
54	MG	1A	3922	1/1	0.88	0.13	71,71,71,71	0
54	MG	1A	3175	1/1	0.88	0.37	75,75,75,75	0
54	MG	2a	3161	1/1	0.88	0.29	67,67,67,67	0
54	MG	1a	1845	1/1	0.88	0.31	76,76,76,76	0
54	MG	2a	3163	1/1	0.88	0.23	70,70,70,70	0
54	MG	1a	1629	1/1	0.88	0.28	65,65,65,65	0
54	MG	2A	3209	1/1	0.88	0.28	68,68,68,68	0
54	MG	1a	1847	1/1	0.88	0.24	70,70,70,70	0
54	MG	2A	3218	1/1	0.88	0.20	68,68,68,68	0
54	MG	2a	3178	1/1	0.88	0.15	77,77,77,77	0
54	MG	1a	1735	1/1	0.88	0.13	75,75,75,75	0
54	MG	1a	1849	1/1	0.88	0.28	78,78,78,78	0
54	MG	2j	201	1/1	0.88	0.20	73,73,73,73	0
54	MG	1a	1631	1/1	0.88	0.33	69,69,69,69	0
54	MG	2A	3242	1/1	0.88	0.22	68,68,68,68	0
54	MG	2A	3718	1/1	0.88	0.22	76,76,76,76	0
54	MG	1a	1634	1/1	0.88	0.25	71,71,71,71	0
54	MG	1A	3522	1/1	0.88	0.14	57,57,57,57	0
54	MG	2A	3250	1/1	0.88	0.43	74,74,74,74	0
54	MG	2A	3031	1/1	0.89	0.28	69,69,69,69	0
54	MG	1A	3797	1/1	0.89	0.21	37,37,37,37	0
54	MG	1A	3476	1/1	0.89	0.11	61,61,61,61	0
54	MG	2A	3685	1/1	0.89	0.23	65,65,65,65	0
54	MG	1a	1757	1/1	0.89	0.21	65,65,65,65	0
54	MG	1A	3202	1/1	0.89	0.15	63,63,63,63	0
54	MG	15	103	1/1	0.89	0.25	50,50,50,50	0
54	MG	2A	3387	1/1	0.89	0.17	49,49,49,49	0
54	MG	1A	3807	1/1	0.89	0.10	51,51,51,51	0
54	MG	1A	3376	1/1	0.89	0.10	31,31,31,31	0
54	MG	1a	1602	1/1	0.89	0.19	71,71,71,71	0
54	MG	2A	3070	1/1	0.89	0.26	63,63,63,63	0
54	MG	2A	3075	1/1	0.89	0.14	69,69,69,69	0
54	MG	1A	3688	1/1	0.89	0.12	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	3301	1/1	0.89	0.19	60,60,60,60	0
54	MG	1A	3966	1/1	0.89	0.12	67,67,67,67	0
54	MG	2A	3714	1/1	0.89	0.14	65,65,65,65	0
54	MG	2A	3411	1/1	0.89	0.33	51,51,51,51	0
54	MG	1A	3974	1/1	0.89	0.31	44,44,44,44	0
54	MG	1a	1777	1/1	0.89	0.25	73,73,73,73	0
54	MG	2A	3415	1/1	0.89	0.12	54,54,54,54	0
54	MG	1A	3979	1/1	0.89	0.19	77,77,77,77	0
54	MG	1A	3821	1/1	0.89	0.23	59,59,59,59	0
54	MG	1A	3622	1/1	0.89	0.20	40,40,40,40	0
54	MG	1A	3011	1/1	0.89	0.12	62,62,62,62	0
54	MG	1A	3581	1/1	0.89	0.17	47,47,47,47	0
54	MG	1a	1787	1/1	0.89	0.15	61,61,61,61	0
54	MG	1A	3985	1/1	0.89	0.23	68,68,68,68	0
54	MG	1A	3835	1/1	0.89	0.09	41,41,41,41	0
54	MG	1a	1791	1/1	0.89	0.21	56,56,56,56	0
54	MG	2A	3442	1/1	0.89	0.22	66,66,66,66	0
54	MG	2D	309	1/1	0.89	0.09	34,34,34,34	0
54	MG	1a	1792	1/1	0.89	0.18	67,67,67,67	0
54	MG	2A	3121	1/1	0.89	0.22	74,74,74,74	0
54	MG	1a	1638	1/1	0.89	0.24	78,78,78,78	0
54	MG	2T	203	1/1	0.89	0.15	69,69,69,69	0
54	MG	2A	3126	1/1	0.89	0.20	57,57,57,57	0
54	MG	2A	3132	1/1	0.89	0.29	63,63,63,63	0
54	MG	2A	3140	1/1	0.89	0.23	67,67,67,67	0
54	MG	1A	3626	1/1	0.89	0.16	67,67,67,67	0
54	MG	2a	3014	1/1	0.89	0.09	73,73,73,73	0
54	MG	1a	1644	1/1	0.89	0.29	63,63,63,63	0
54	MG	1a	1805	1/1	0.89	0.09	67,67,67,67	0
54	MG	1A	3845	1/1	0.89	0.14	63,63,63,63	0
54	MG	1A	3848	1/1	0.89	0.13	70,70,70,70	0
54	MG	2A	3158	1/1	0.89	0.23	62,62,62,62	0
54	MG	2A	3463	1/1	0.89	0.16	56,56,56,56	0
54	MG	1A	3148	1/1	0.89	0.21	62,62,62,62	0
54	MG	2a	3031	1/1	0.89	0.34	71,71,71,71	0
54	MG	2A	3160	1/1	0.89	0.11	62,62,62,62	0
54	MG	2A	3163	1/1	0.89	0.21	69,69,69,69	0
54	MG	1a	1654	1/1	0.89	0.28	66,66,66,66	0
54	MG	2A	3168	1/1	0.89	0.11	54,54,54,54	0
54	MG	2A	3175	1/1	0.89	0.12	63,63,63,63	0
54	MG	2a	3040	1/1	0.89	0.35	71,71,71,71	0
54	MG	2A	3177	1/1	0.89	0.25	69,69,69,69	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	2a	3045	1/1	0.89	0.26	72,72,72,72	0
54	MG	1A	3851	1/1	0.89	0.09	42,42,42,42	0
54	MG	1A	3039	1/1	0.89	0.13	47,47,47,47	0
54	MG	2A	3188	1/1	0.89	0.41	76,76,76,76	0
54	MG	1a	1815	1/1	0.89	0.11	76,76,76,76	0
54	MG	2A	3494	1/1	0.89	0.12	65,65,65,65	0
54	MG	2A	3496	1/1	0.89	0.14	62,62,62,62	0
54	MG	1A	3741	1/1	0.89	0.16	65,65,65,65	0
54	MG	1A	3866	1/1	0.89	0.11	78,78,78,78	0
54	MG	2A	3205	1/1	0.89	0.19	71,71,71,71	0
54	MG	1B	215	1/1	0.89	0.08	56,56,56,56	0
54	MG	1A	3742	1/1	0.89	0.15	51,51,51,51	0
54	MG	1a	1823	1/1	0.89	0.09	76,76,76,76	0
54	MG	1A	3633	1/1	0.89	0.13	33,33,33,33	0
54	MG	2A	3228	1/1	0.89	0.19	64,64,64,64	0
54	MG	2A	3230	1/1	0.89	0.12	59,59,59,59	0
54	MG	1B	221	1/1	0.89	0.11	54,54,54,54	0
54	MG	1a	1826	1/1	0.89	0.13	66,66,66,66	0
54	MG	2A	3241	1/1	0.89	0.29	57,57,57,57	0
54	MG	1A	3640	1/1	0.89	0.09	43,43,43,43	0
54	MG	2A	3531	1/1	0.89	0.12	47,47,47,47	0
54	MG	1A	3872	1/1	0.89	0.12	27,27,27,27	0
54	MG	1A	3878	1/1	0.89	0.18	58,58,58,58	0
54	MG	2a	3089	1/1	0.89	0.17	58,58,58,58	0
54	MG	2A	3249	1/1	0.89	0.31	65,65,65,65	0
54	MG	2A	3555	1/1	0.89	0.15	71,71,71,71	0
54	MG	1A	3880	1/1	0.89	0.18	60,60,60,60	0
54	MG	1A	3645	1/1	0.89	0.11	32,32,32,32	0
54	MG	1A	3887	1/1	0.89	0.20	52,52,52,52	0
54	MG	1D	301	1/1	0.89	0.18	73,73,73,73	0
54	MG	1D	309	1/1	0.89	0.28	47,47,47,47	0
54	MG	1A	3890	1/1	0.89	0.20	69,69,69,69	0
54	MG	1A	3546	1/1	0.89	0.12	51,51,51,51	0
54	MG	2a	3113	1/1	0.89	0.17	65,65,65,65	0
54	MG	1A	3548	1/1	0.89	0.11	56,56,56,56	0
54	MG	2A	3580	1/1	0.89	0.17	61,61,61,61	0
54	MG	1A	3760	1/1	0.89	0.14	56,56,56,56	0
54	MG	1a	1703	1/1	0.89	0.33	69,69,69,69	0
54	MG	1A	3658	1/1	0.89	0.16	56,56,56,56	0
54	MG	1A	3125	1/1	0.89	0.19	59,59,59,59	0
54	MG	2A	3625	1/1	0.89	0.15	69,69,69,69	0
54	MG	1F	316	1/1	0.89	0.24	49,49,49,49	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	2A	3304	1/1	0.89	0.16	66,66,66,66	0
54	MG	1a	1709	1/1	0.89	0.14	63,63,63,63	0
54	MG	1a	1714	1/1	0.89	0.15	65,65,65,65	0
54	MG	2A	3311	1/1	0.89	0.19	52,52,52,52	0
54	MG	1A	3461	1/1	0.89	0.14	65,65,65,65	0
54	MG	1A	3369	1/1	0.89	0.14	56,56,56,56	0
54	MG	2A	3322	1/1	0.89	0.11	55,55,55,55	0
54	MG	1T	201	1/1	0.89	0.13	57,57,57,57	0
54	MG	2A	3342	1/1	0.89	0.12	48,48,48,48	0
54	MG	2A	3650	1/1	0.89	0.12	67,67,67,67	0
54	MG	1d	303	1/1	0.89	0.18	73,73,73,73	0
54	MG	1A	3413	1/1	0.89	0.15	39,39,39,39	0
54	MG	1A	3927	1/1	0.89	0.13	59,59,59,59	0
54	MG	2a	3173	1/1	0.89	0.21	58,58,58,58	0
54	MG	2a	3175	1/1	0.89	0.27	69,69,69,69	0
54	MG	1A	3603	1/1	0.89	0.09	52,52,52,52	0
54	MG	1a	1731	1/1	0.89	0.12	74,74,74,74	0
54	MG	1A	3438	1/1	0.89	0.10	44,44,44,44	0
54	MG	1a	1738	1/1	0.89	0.26	61,61,61,61	0
54	MG	1A	3940	1/1	0.89	0.13	63,63,63,63	0
54	MG	2p	101	1/1	0.89	0.18	68,68,68,68	0
54	MG	1t	202	1/1	0.89	0.15	77,77,77,77	0
54	MG	1A	3091	1/1	0.89	0.17	54,54,54,54	0
54	MG	1a	1746	1/1	0.89	0.11	60,60,60,60	0
54	MG	2A	3017	1/1	0.89	0.20	67,67,67,67	0
54	MG	2A	3674	1/1	0.89	0.20	63,63,63,63	0
54	MG	1A	3945	1/1	0.89	0.09	63,63,63,63	0
54	MG	1A	3962	1/1	0.90	0.23	38,38,38,38	0
54	MG	2A	3016	1/1	0.90	0.22	77,77,77,77	0
54	MG	2A	3243	1/1	0.90	0.29	58,58,58,58	0
54	MG	2A	3244	1/1	0.90	0.33	60,60,60,60	0
54	MG	1a	1679	1/1	0.90	0.13	64,64,64,64	0
54	MG	1a	1682	1/1	0.90	0.12	52,52,52,52	0
54	MG	1A	3429	1/1	0.90	0.20	67,67,67,67	0
54	MG	1R	205	1/1	0.90	0.15	49,49,49,49	0
54	MG	1a	1795	1/1	0.90	0.18	73,73,73,73	0
54	MG	2A	3722	1/1	0.90	0.18	70,70,70,70	0
54	MG	2B	201	1/1	0.90	0.27	72,72,72,72	0
54	MG	1a	1796	1/1	0.90	0.13	68,68,68,68	0
54	MG	2A	3253	1/1	0.90	0.14	62,62,62,62	0
54	MG	2A	3467	1/1	0.90	0.10	72,72,72,72	0
54	MG	2A	3469	1/1	0.90	0.12	44,44,44,44	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	1A	3853	1/1	0.90	0.08	53,53,53,53	0
54	MG	2A	3473	1/1	0.90	0.09	60,60,60,60	0
54	MG	2A	3258	1/1	0.90	0.43	70,70,70,70	0
54	MG	1a	1689	1/1	0.90	0.33	74,74,74,74	0
54	MG	2A	3270	1/1	0.90	0.41	74,74,74,74	0
54	MG	1A	3599	1/1	0.90	0.12	63,63,63,63	0
54	MG	1A	3552	1/1	0.90	0.21	63,63,63,63	0
54	MG	2A	3485	1/1	0.90	0.15	62,62,62,62	0
54	MG	2A	3050	1/1	0.90	0.20	51,51,51,51	0
54	MG	2E	307	1/1	0.90	0.09	36,36,36,36	0
54	MG	2A	3058	1/1	0.90	0.21	65,65,65,65	0
54	MG	2A	3490	1/1	0.90	0.28	70,70,70,70	0
54	MG	2N	201	1/1	0.90	0.13	77,77,77,77	0
54	MG	2Q	202	1/1	0.90	0.16	74,74,74,74	0
54	MG	2A	3492	1/1	0.90	0.16	62,62,62,62	0
54	MG	1A	3976	1/1	0.90	0.19	49,49,49,49	0
54	MG	1A	3978	1/1	0.90	0.13	81,81,81,81	0
54	MG	25	101	1/1	0.90	0.18	75,75,75,75	0
54	MG	2A	3298	1/1	0.90	0.08	37,37,37,37	0
54	MG	2a	3004	1/1	0.90	0.12	62,62,62,62	0
54	MG	1A	3856	1/1	0.90	0.12	57,57,57,57	0
54	MG	2a	3011	1/1	0.90	0.23	72,72,72,72	0
54	MG	1A	3761	1/1	0.90	0.18	66,66,66,66	0
54	MG	1A	3036	1/1	0.90	0.14	53,53,53,53	0
54	MG	2A	3500	1/1	0.90	0.12	58,58,58,58	0
54	MG	1A	3270	1/1	0.90	0.14	67,67,67,67	0
54	MG	1A	3276	1/1	0.90	0.15	53,53,53,53	0
54	MG	1A	3771	1/1	0.90	0.10	55,55,55,55	0
54	MG	13	102	1/1	0.90	0.20	73,73,73,73	0
54	MG	2A	3315	1/1	0.90	0.18	58,58,58,58	0
54	MG	1A	3773	1/1	0.90	0.27	59,59,59,59	0
54	MG	2A	3517	1/1	0.90	0.27	68,68,68,68	0
54	MG	2A	3519	1/1	0.90	0.09	62,62,62,62	0
54	MG	2A	3321	1/1	0.90	0.13	56,56,56,56	0
54	MG	2A	3521	1/1	0.90	0.09	59,59,59,59	0
54	MG	1A	3989	1/1	0.90	0.14	56,56,56,56	0
54	MG	2a	3039	1/1	0.90	0.17	73,73,73,73	0
54	MG	2A	3325	1/1	0.90	0.12	53,53,53,53	0
54	MG	2A	3527	1/1	0.90	0.11	63,63,63,63	0
54	MG	2A	3096	1/1	0.90	0.22	69,69,69,69	0
54	MG	2A	3097	1/1	0.90	0.14	67,67,67,67	0
54	MG	2A	3345	1/1	0.90	0.11	45,45,45,45	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	1A	3879	1/1	0.90	0.10	38,38,38,38	0
54	MG	2A	3545	1/1	0.90	0.16	57,57,57,57	0
54	MG	2A	3100	1/1	0.90	0.13	58,58,58,58	0
54	MG	1A	3351	1/1	0.90	0.12	45,45,45,45	0
54	MG	2A	3350	1/1	0.90	0.10	55,55,55,55	0
54	MG	2a	3055	1/1	0.90	0.11	70,70,70,70	0
54	MG	1A	3439	1/1	0.90	0.13	63,63,63,63	0
54	MG	2a	3057	1/1	0.90	0.20	76,76,76,76	0
54	MG	2A	3563	1/1	0.90	0.11	37,37,37,37	0
54	MG	1a	1604	1/1	0.90	0.25	72,72,72,72	0
54	MG	1a	1829	1/1	0.90	0.14	63,63,63,63	0
54	MG	1A	3783	1/1	0.90	0.13	37,37,37,37	0
54	MG	2A	3574	1/1	0.90	0.10	82,82,82,82	0
54	MG	2a	3067	1/1	0.90	0.45	78,78,78,78	0
54	MG	1A	3615	1/1	0.90	0.09	25,25,25,25	0
54	MG	2A	3372	1/1	0.90	0.11	73,73,73,73	0
54	MG	1a	1833	1/1	0.90	0.19	77,77,77,77	0
54	MG	2a	3078	1/1	0.90	0.17	69,69,69,69	0
54	MG	1A	3565	1/1	0.90	0.18	63,63,63,63	0
54	MG	1A	3470	1/1	0.90	0.13	39,39,39,39	0
54	MG	1a	1837	1/1	0.90	0.22	65,65,65,65	0
54	MG	2A	3595	1/1	0.90	0.18	66,66,66,66	0
54	MG	2A	3604	1/1	0.90	0.09	70,70,70,70	0
54	MG	1A	3905	1/1	0.90	0.17	68,68,68,68	0
54	MG	2A	3609	1/1	0.90	0.16	70,70,70,70	0
54	MG	1A	3909	1/1	0.90	0.15	64,64,64,64	0
54	MG	2A	3619	1/1	0.90	0.14	56,56,56,56	0
54	MG	2a	3093	1/1	0.90	0.28	59,59,59,59	0
54	MG	1A	3472	1/1	0.90	0.12	39,39,39,39	0
54	MG	1B	219	1/1	0.90	0.18	58,58,58,58	0
54	MG	2A	3382	1/1	0.90	0.11	50,50,50,50	0
54	MG	1A	3356	1/1	0.90	0.22	72,72,72,72	0
54	MG	1a	1747	1/1	0.90	0.21	67,67,67,67	0
54	MG	2a	3106	1/1	0.90	0.21	71,71,71,71	0
54	MG	1A	3804	1/1	0.90	0.11	46,46,46,46	0
54	MG	2a	3109	1/1	0.90	0.10	60,60,60,60	0
54	MG	1A	3387	1/1	0.90	0.12	57,57,57,57	0
54	MG	2a	3112	1/1	0.90	0.15	83,83,83,83	0
54	MG	2A	3635	1/1	0.90	0.08	76,76,76,76	0
54	MG	1A	3155	1/1	0.90	0.27	59,59,59,59	0
54	MG	2A	3162	1/1	0.90	0.35	74,74,74,74	0
54	MG	2A	3638	1/1	0.90	0.18	66,66,66,66	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	1a	1643	1/1	0.90	0.25	64,64,64,64	0
54	MG	1a	1758	1/1	0.90	0.13	66,66,66,66	0
54	MG	2a	3125	1/1	0.90	0.15	68,68,68,68	0
54	MG	1A	3539	1/1	0.90	0.14	47,47,47,47	0
54	MG	2A	3169	1/1	0.90	0.31	67,67,67,67	0
54	MG	2A	3654	1/1	0.90	0.14	67,67,67,67	0
54	MG	1A	3627	1/1	0.90	0.19	44,44,44,44	0
54	MG	1A	3628	1/1	0.90	0.14	67,67,67,67	0
54	MG	2A	3409	1/1	0.90	0.28	64,64,64,64	0
54	MG	1A	3729	1/1	0.90	0.13	54,54,54,54	0
54	MG	2a	3156	1/1	0.90	0.26	63,63,63,63	0
54	MG	1a	1867	1/1	0.90	0.21	73,73,73,73	0
54	MG	1A	3733	1/1	0.90	0.10	64,64,64,64	0
54	MG	2a	3159	1/1	0.90	0.26	67,67,67,67	0
54	MG	1A	3629	1/1	0.90	0.10	42,42,42,42	0
54	MG	1a	1658	1/1	0.90	0.22	67,67,67,67	0
54	MG	2A	3668	1/1	0.90	0.13	75,75,75,75	0
54	MG	1A	3256	1/1	0.90	0.11	49,49,49,49	0
54	MG	2A	3420	1/1	0.90	0.14	67,67,67,67	0
54	MG	2A	3204	1/1	0.90	0.16	69,69,69,69	0
54	MG	2A	3673	1/1	0.90	0.15	63,63,63,63	0
54	MG	2a	3170	1/1	0.90	0.30	77,77,77,77	0
54	MG	2a	3172	1/1	0.90	0.23	67,67,67,67	0
54	MG	2A	3423	1/1	0.90	0.25	72,72,72,72	0
54	MG	2a	3174	1/1	0.90	0.26	62,62,62,62	0
54	MG	2A	3675	1/1	0.90	0.14	70,70,70,70	0
54	MG	1a	1660	1/1	0.90	0.18	73,73,73,73	0
54	MG	1A	3449	1/1	0.90	0.08	31,31,31,31	0
54	MG	1i	201	1/1	0.90	0.23	75,75,75,75	0
54	MG	1A	3163	1/1	0.90	0.14	61,61,61,61	0
54	MG	2A	3220	1/1	0.90	0.20	68,68,68,68	0
54	MG	1A	3492	1/1	0.90	0.11	43,43,43,43	0
54	MG	1A	3953	1/1	0.90	0.25	48,48,48,48	0
54	MG	1A	3367	1/1	0.90	0.14	62,62,62,62	0
54	MG	1a	1783	1/1	0.90	0.14	76,76,76,76	0
54	MG	2A	3234	1/1	0.90	0.17	60,60,60,60	0
54	MG	2A	3448	1/1	0.90	0.11	63,63,63,63	0
54	MG	1A	3592	1/1	0.90	0.14	65,65,65,65	0
54	MG	1a	1727	1/1	0.91	0.12	78,78,78,78	0
54	MG	1A	3580	1/1	0.91	0.09	46,46,46,46	0
54	MG	1A	3350	1/1	0.91	0.10	46,46,46,46	0
54	MG	12	101	1/1	0.91	0.13	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	1A	3971	1/1	0.91	0.13	62,62,62,62	0
54	MG	1A	3113	1/1	0.91	0.11	45,45,45,45	0
54	MG	1A	3077	1/1	0.91	0.14	58,58,58,58	0
54	MG	2A	3238	1/1	0.91	0.18	64,64,64,64	0
54	MG	2B	202	1/1	0.91	0.19	72,72,72,72	0
54	MG	1a	1743	1/1	0.91	0.13	68,68,68,68	0
54	MG	1A	3296	1/1	0.91	0.14	54,54,54,54	0
54	MG	2A	3472	1/1	0.91	0.14	63,63,63,63	0
54	MG	2B	208	1/1	0.91	0.31	66,66,66,66	0
54	MG	1a	1601	1/1	0.91	0.11	74,74,74,74	0
54	MG	1A	3852	1/1	0.91	0.18	61,61,61,61	0
54	MG	1A	3543	1/1	0.91	0.09	45,45,45,45	0
54	MG	1A	3634	1/1	0.91	0.19	59,59,59,59	0
54	MG	1A	3587	1/1	0.91	0.10	46,46,46,46	0
54	MG	2A	3482	1/1	0.91	0.18	60,60,60,60	0
54	MG	1a	1753	1/1	0.91	0.24	70,70,70,70	0
54	MG	2D	303	1/1	0.91	0.35	49,49,49,49	0
54	MG	2A	3484	1/1	0.91	0.17	60,60,60,60	0
54	MG	1a	1607	1/1	0.91	0.09	71,71,71,71	0
54	MG	2D	312	1/1	0.91	0.14	69,69,69,69	0
54	MG	1a	1608	1/1	0.91	0.11	61,61,61,61	0
54	MG	1A	3746	1/1	0.91	0.10	31,31,31,31	0
54	MG	1a	1760	1/1	0.91	0.22	68,68,68,68	0
54	MG	2A	3003	1/1	0.91	0.09	62,62,62,62	0
54	MG	1A	3749	1/1	0.91	0.06	35,35,35,35	0
54	MG	1A	3643	1/1	0.91	0.07	20,20,20,20	0
54	MG	1a	1764	1/1	0.91	0.14	75,75,75,75	0
54	MG	2V	201	1/1	0.91	0.18	66,66,66,66	0
54	MG	2A	3025	1/1	0.91	0.13	53,53,53,53	0
54	MG	1a	1765	1/1	0.91	0.19	75,75,75,75	0
54	MG	1A	3755	1/1	0.91	0.19	47,47,47,47	0
54	MG	28	101	1/1	0.91	0.20	62,62,62,62	0
54	MG	1A	3991	1/1	0.91	0.08	60,60,60,60	0
54	MG	2A	3282	1/1	0.91	0.30	66,66,66,66	0
54	MG	2a	3005	1/1	0.91	0.26	69,69,69,69	0
54	MG	2a	3007	1/1	0.91	0.52	75,75,75,75	0
54	MG	2A	3034	1/1	0.91	0.30	66,66,66,66	0
54	MG	1A	3756	1/1	0.91	0.13	49,49,49,49	0
54	MG	1A	3117	1/1	0.91	0.15	46,46,46,46	0
54	MG	2A	3505	1/1	0.91	0.25	78,78,78,78	0
54	MG	2A	3507	1/1	0.91	0.21	63,63,63,63	0
54	MG	2a	3019	1/1	0.91	0.10	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	3875	1/1	0.91	0.12	36,36,36,36	0
54	MG	1A	3876	1/1	0.91	0.08	38,38,38,38	0
54	MG	2A	3511	1/1	0.91	0.09	36,36,36,36	0
54	MG	1A	3365	1/1	0.91	0.11	42,42,42,42	0
54	MG	2a	3024	1/1	0.91	0.15	73,73,73,73	0
54	MG	2a	3028	1/1	0.91	0.24	72,72,72,72	0
54	MG	1A	3597	1/1	0.91	0.13	49,49,49,49	0
54	MG	2A	3052	1/1	0.91	0.10	59,59,59,59	0
54	MG	2A	3312	1/1	0.91	0.15	68,68,68,68	0
54	MG	1A	3656	1/1	0.91	0.25	40,40,40,40	0
54	MG	1A	3033	1/1	0.91	0.21	63,63,63,63	0
54	MG	1B	214	1/1	0.91	0.17	67,67,67,67	0
54	MG	2A	3529	1/1	0.91	0.13	43,43,43,43	0
54	MG	1A	3767	1/1	0.91	0.10	59,59,59,59	0
54	MG	1A	3266	1/1	0.91	0.10	71,71,71,71	0
54	MG	2a	3041	1/1	0.91	0.29	68,68,68,68	0
54	MG	2A	3077	1/1	0.91	0.14	51,51,51,51	0
54	MG	1a	1786	1/1	0.91	0.08	78,78,78,78	0
54	MG	2A	3340	1/1	0.91	0.27	67,67,67,67	0
54	MG	2A	3547	1/1	0.91	0.09	52,52,52,52	0
54	MG	2A	3550	1/1	0.91	0.10	65,65,65,65	0
54	MG	1A	3494	1/1	0.91	0.09	55,55,55,55	0
54	MG	1A	3902	1/1	0.91	0.12	50,50,50,50	0
54	MG	2A	3082	1/1	0.91	0.19	63,63,63,63	0
54	MG	1A	3304	1/1	0.91	0.27	65,65,65,65	0
54	MG	1B	224	1/1	0.91	0.13	62,62,62,62	0
54	MG	1A	3904	1/1	0.91	0.11	56,56,56,56	0
54	MG	2A	3089	1/1	0.91	0.34	69,69,69,69	0
54	MG	2A	3570	1/1	0.91	0.11	62,62,62,62	0
54	MG	1A	3096	1/1	0.91	0.14	60,60,60,60	0
54	MG	2A	3355	1/1	0.91	0.18	64,64,64,64	0
54	MG	2A	3358	1/1	0.91	0.23	72,72,72,72	0
54	MG	2a	3064	1/1	0.91	0.14	59,59,59,59	0
54	MG	1A	3212	1/1	0.91	0.12	57,57,57,57	0
54	MG	1A	3778	1/1	0.91	0.11	54,54,54,54	0
54	MG	2A	3098	1/1	0.91	0.20	69,69,69,69	0
54	MG	1a	1670	1/1	0.91	0.40	68,68,68,68	0
54	MG	2a	3074	1/1	0.91	0.25	70,70,70,70	0
54	MG	1A	3502	1/1	0.91	0.08	27,27,27,27	0
54	MG	1a	1672	1/1	0.91	0.19	58,58,58,58	0
54	MG	2A	3597	1/1	0.91	0.12	41,41,41,41	0
54	MG	1a	1806	1/1	0.91	0.14	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	2A	3607	1/1	0.91	0.07	44,44,44,44	0
54	MG	1a	1673	1/1	0.91	0.23	58,58,58,58	0
54	MG	2a	3085	1/1	0.91	0.27	67,67,67,67	0
54	MG	1A	3919	1/1	0.91	0.18	61,61,61,61	0
54	MG	2A	3612	1/1	0.91	0.10	68,68,68,68	0
54	MG	2A	3116	1/1	0.91	0.21	63,63,63,63	0
54	MG	1A	3425	1/1	0.91	0.13	62,62,62,62	0
54	MG	1D	303	1/1	0.91	0.17	70,70,70,70	0
54	MG	1a	1678	1/1	0.91	0.32	74,74,74,74	0
54	MG	1A	3179	1/1	0.91	0.24	73,73,73,73	0
54	MG	1A	3678	1/1	0.91	0.17	35,35,35,35	0
54	MG	2a	3099	1/1	0.91	0.12	53,53,53,53	0
54	MG	1a	1816	1/1	0.91	0.12	75,75,75,75	0
54	MG	2A	3139	1/1	0.91	0.22	61,61,61,61	0
54	MG	1A	3512	1/1	0.91	0.12	60,60,60,60	0
54	MG	1A	3796	1/1	0.91	0.09	17,17,17,17	0
54	MG	1A	3934	1/1	0.91	0.09	39,39,39,39	0
54	MG	1A	3137	1/1	0.91	0.11	63,63,63,63	0
54	MG	1A	3567	1/1	0.91	0.23	62,62,62,62	0
54	MG	1A	3062	1/1	0.91	0.24	54,54,54,54	0
54	MG	1N	203	1/1	0.91	0.14	62,62,62,62	0
54	MG	2A	3646	1/1	0.91	0.15	57,57,57,57	0
54	MG	2A	3648	1/1	0.91	0.22	64,64,64,64	0
54	MG	1a	1696	1/1	0.91	0.26	82,82,82,82	0
54	MG	1a	1827	1/1	0.91	0.26	81,81,81,81	0
54	MG	2A	3410	1/1	0.91	0.12	67,67,67,67	0
54	MG	1A	3941	1/1	0.91	0.14	68,68,68,68	0
54	MG	1A	3942	1/1	0.91	0.11	68,68,68,68	0
54	MG	1P	204	1/1	0.91	0.14	80,80,80,80	0
54	MG	2A	3167	1/1	0.91	0.28	66,66,66,66	0
54	MG	1Q	202	1/1	0.91	0.16	56,56,56,56	0
54	MG	2a	3142	1/1	0.91	0.19	60,60,60,60	0
54	MG	1A	3693	1/1	0.91	0.16	65,65,65,65	0
54	MG	2a	3146	1/1	0.91	0.18	69,69,69,69	0
54	MG	2A	3173	1/1	0.91	0.12	62,62,62,62	0
54	MG	2a	3153	1/1	0.91	0.16	78,78,78,78	0
54	MG	2a	3154	1/1	0.91	0.12	85,85,85,85	0
54	MG	2A	3664	1/1	0.91	0.21	76,76,76,76	0
54	MG	1A	3623	1/1	0.91	0.31	42,42,42,42	0
54	MG	2A	3422	1/1	0.91	0.12	68,68,68,68	0
54	MG	1A	3698	1/1	0.91	0.17	58,58,58,58	0
54	MG	2A	3183	1/1	0.91	0.13	66,66,66,66	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	1A	3468	1/1	0.91	0.07	35,35,35,35	0
54	MG	1A	3705	1/1	0.91	0.15	64,64,64,64	0
54	MG	2A	3432	1/1	0.91	0.12	64,64,64,64	0
54	MG	2A	3433	1/1	0.91	0.10	62,62,62,62	0
54	MG	2a	3165	1/1	0.91	0.27	70,70,70,70	0
54	MG	2A	3677	1/1	0.91	0.27	62,62,62,62	0
54	MG	2A	3679	1/1	0.91	0.16	76,76,76,76	0
54	MG	2a	3168	1/1	0.91	0.29	63,63,63,63	0
54	MG	2A	3680	1/1	0.91	0.17	66,66,66,66	0
54	MG	1A	3391	1/1	0.91	0.11	32,32,32,32	0
54	MG	1a	1712	1/1	0.91	0.18	72,72,72,72	0
54	MG	1A	3722	1/1	0.91	0.24	59,59,59,59	0
54	MG	2A	3439	1/1	0.91	0.32	62,62,62,62	0
54	MG	2A	3441	1/1	0.91	0.14	64,64,64,64	0
54	MG	2A	3200	1/1	0.91	0.34	65,65,65,65	0
54	MG	1A	3723	1/1	0.91	0.27	66,66,66,66	0
54	MG	2A	3203	1/1	0.91	0.16	65,65,65,65	0
54	MG	1Y	201	1/1	0.91	0.09	68,68,68,68	0
54	MG	1a	1722	1/1	0.91	0.13	77,77,77,77	0
54	MG	1A	3724	1/1	0.91	0.17	58,58,58,58	0
54	MG	2A	3212	1/1	0.91	0.17	63,63,63,63	0
54	MG	2A	3213	1/1	0.91	0.27	64,64,64,64	0
56	ARG	1B	232	12/12	0.91	0.12	37,47,60,63	0
54	MG	1a	1725	1/1	0.91	0.20	73,73,73,73	0
54	MG	2A	3706	1/1	0.91	0.11	62,62,62,62	0
54	MG	1A	3284	1/1	0.91	0.18	69,69,69,69	0
54	MG	2A	3709	1/1	0.91	0.18	55,55,55,55	0
54	MG	1a	1646	1/1	0.92	0.31	68,68,68,68	0
54	MG	2A	3048	1/1	0.92	0.28	70,70,70,70	0
54	MG	1A	3377	1/1	0.92	0.07	25,25,25,25	0
54	MG	1A	3900	1/1	0.92	0.13	59,59,59,59	0
54	MG	1A	3381	1/1	0.92	0.09	39,39,39,39	0
54	MG	2A	3053	1/1	0.92	0.08	41,41,41,41	0
54	MG	1a	1655	1/1	0.92	0.15	75,75,75,75	0
54	MG	2D	310	1/1	0.92	0.08	74,74,74,74	0
54	MG	2D	311	1/1	0.92	0.16	69,69,69,69	0
54	MG	2A	3062	1/1	0.92	0.23	54,54,54,54	0
54	MG	1a	1784	1/1	0.92	0.11	65,65,65,65	0
54	MG	1A	3671	1/1	0.92	0.13	47,47,47,47	0
54	MG	2A	3073	1/1	0.92	0.15	50,50,50,50	0
54	MG	1A	3672	1/1	0.92	0.19	64,64,64,64	0
54	MG	1A	3776	1/1	0.92	0.19	39,39,39,39	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	1A	3605	1/1	0.92	0.07	29,29,29,29	0
54	MG	2R	202	1/1	0.92	0.12	71,71,71,71	0
54	MG	2T	202	1/1	0.92	0.12	69,69,69,69	0
54	MG	1A	3910	1/1	0.92	0.09	59,59,59,59	0
54	MG	2T	204	1/1	0.92	0.15	61,61,61,61	0
54	MG	2A	3510	1/1	0.92	0.09	57,57,57,57	0
54	MG	1A	3321	1/1	0.92	0.09	29,29,29,29	0
54	MG	20	101	1/1	0.92	0.12	59,59,59,59	0
54	MG	2A	3514	1/1	0.92	0.12	37,37,37,37	0
54	MG	1a	1665	1/1	0.92	0.15	60,60,60,60	0
54	MG	1a	1666	1/1	0.92	0.13	63,63,63,63	0
54	MG	2a	3002	1/1	0.92	0.09	63,63,63,63	0
54	MG	1a	1667	1/1	0.92	0.41	68,68,68,68	0
54	MG	2A	3323	1/1	0.92	0.09	39,39,39,39	0
54	MG	2A	3324	1/1	0.92	0.11	64,64,64,64	0
54	MG	1A	3322	1/1	0.92	0.11	28,28,28,28	0
54	MG	1a	1799	1/1	0.92	0.15	70,70,70,70	0
54	MG	2A	3336	1/1	0.92	0.20	64,64,64,64	0
54	MG	2a	3012	1/1	0.92	0.30	65,65,65,65	0
54	MG	1A	3610	1/1	0.92	0.09	31,31,31,31	0
54	MG	2A	3094	1/1	0.92	0.17	53,53,53,53	0
54	MG	1A	3921	1/1	0.92	0.08	67,67,67,67	0
54	MG	1A	3611	1/1	0.92	0.13	61,61,61,61	0
54	MG	2A	3347	1/1	0.92	0.10	41,41,41,41	0
54	MG	1A	3685	1/1	0.92	0.14	63,63,63,63	0
54	MG	1D	312	1/1	0.92	0.10	59,59,59,59	0
54	MG	1A	3287	1/1	0.92	0.17	41,41,41,41	0
54	MG	1E	301	1/1	0.92	0.27	52,52,52,52	0
54	MG	1A	3496	1/1	0.92	0.17	70,70,70,70	0
54	MG	1A	3343	1/1	0.92	0.11	69,69,69,69	0
54	MG	1E	310	1/1	0.92	0.14	36,36,36,36	0
54	MG	1F	309	1/1	0.92	0.33	68,68,68,68	0
54	MG	1A	3929	1/1	0.92	0.12	85,85,85,85	0
54	MG	2A	3117	1/1	0.92	0.22	73,73,73,73	0
54	MG	2A	3368	1/1	0.92	0.08	44,44,44,44	0
54	MG	2A	3369	1/1	0.92	0.11	72,72,72,72	0
54	MG	1F	312	1/1	0.92	0.13	30,30,30,30	0
54	MG	1A	3031	1/1	0.92	0.07	38,38,38,38	0
54	MG	1A	3620	1/1	0.92	0.18	52,52,52,52	0
54	MG	1A	3806	1/1	0.92	0.09	35,35,35,35	0
54	MG	2A	3124	1/1	0.92	0.21	58,58,58,58	0
54	MG	2A	3583	1/1	0.92	0.07	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	3041	1/1	0.92	0.13	60,60,60,60	0
54	MG	2A	3588	1/1	0.92	0.12	53,53,53,53	0
54	MG	1a	1695	1/1	0.92	0.27	71,71,71,71	0
54	MG	1A	3811	1/1	0.92	0.17	61,61,61,61	0
54	MG	1A	3405	1/1	0.92	0.10	59,59,59,59	0
54	MG	1A	3814	1/1	0.92	0.17	51,51,51,51	0
54	MG	1A	3716	1/1	0.92	0.11	55,55,55,55	0
54	MG	1A	3503	1/1	0.92	0.06	40,40,40,40	0
54	MG	1A	3407	1/1	0.92	0.12	31,31,31,31	0
54	MG	2A	3613	1/1	0.92	0.07	59,59,59,59	0
54	MG	1A	3353	1/1	0.92	0.10	53,53,53,53	0
54	MG	2a	3061	1/1	0.92	0.14	71,71,71,71	0
54	MG	2A	3388	1/1	0.92	0.14	72,72,72,72	0
54	MG	2A	3155	1/1	0.92	0.11	57,57,57,57	0
54	MG	2A	3156	1/1	0.92	0.23	58,58,58,58	0
54	MG	1A	3121	1/1	0.92	0.14	50,50,50,50	0
54	MG	1A	3829	1/1	0.92	0.09	58,58,58,58	0
54	MG	2a	3068	1/1	0.92	0.09	65,65,65,65	0
54	MG	2A	3630	1/1	0.92	0.13	56,56,56,56	0
54	MG	2a	3070	1/1	0.92	0.23	70,70,70,70	0
54	MG	1A	3300	1/1	0.92	0.21	63,63,63,63	0
54	MG	2A	3401	1/1	0.92	0.13	60,60,60,60	0
54	MG	1A	3578	1/1	0.92	0.13	58,58,58,58	0
54	MG	1V	206	1/1	0.92	0.09	65,65,65,65	0
54	MG	2A	3164	1/1	0.92	0.31	70,70,70,70	0
54	MG	2A	3408	1/1	0.92	0.09	60,60,60,60	0
54	MG	2a	3081	1/1	0.92	0.43	63,63,63,63	0
54	MG	2A	3165	1/1	0.92	0.27	74,74,74,74	0
54	MG	2a	3083	1/1	0.92	0.20	57,57,57,57	0
54	MG	1W	201	1/1	0.92	0.27	60,60,60,60	0
54	MG	1A	3836	1/1	0.92	0.09	47,47,47,47	0
54	MG	2A	3643	1/1	0.92	0.18	62,62,62,62	0
54	MG	2A	3644	1/1	0.92	0.12	46,46,46,46	0
54	MG	1A	3730	1/1	0.92	0.09	55,55,55,55	0
54	MG	1A	3732	1/1	0.92	0.07	55,55,55,55	0
54	MG	10	102	1/1	0.92	0.18	53,53,53,53	0
54	MG	10	106	1/1	0.92	0.14	48,48,48,48	0
54	MG	2a	3095	1/1	0.92	0.37	63,63,63,63	0
54	MG	2A	3653	1/1	0.92	0.20	63,63,63,63	0
54	MG	1A	3970	1/1	0.92	0.10	43,43,43,43	0
54	MG	2A	3419	1/1	0.92	0.10	67,67,67,67	0
54	MG	2A	3179	1/1	0.92	0.35	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	3181	1/1	0.92	0.11	63,63,63,63	0
54	MG	1A	3166	1/1	0.92	0.15	52,52,52,52	0
54	MG	10	109	1/1	0.92	0.10	59,59,59,59	0
54	MG	2a	3107	1/1	0.92	0.15	78,78,78,78	0
54	MG	1A	3735	1/1	0.92	0.09	48,48,48,48	0
54	MG	1A	3520	1/1	0.92	0.16	38,38,38,38	0
54	MG	1A	3463	1/1	0.92	0.17	67,67,67,67	0
54	MG	2A	3190	1/1	0.92	0.12	64,64,64,64	0
54	MG	1a	1864	1/1	0.92	0.10	69,69,69,69	0
54	MG	2a	3114	1/1	0.92	0.17	64,64,64,64	0
54	MG	2a	3115	1/1	0.92	0.11	67,67,67,67	0
54	MG	2A	3195	1/1	0.92	0.14	62,62,62,62	0
54	MG	2A	3436	1/1	0.92	0.18	58,58,58,58	0
54	MG	1a	1736	1/1	0.92	0.12	61,61,61,61	0
54	MG	2A	3672	1/1	0.92	0.21	73,73,73,73	0
54	MG	1a	1866	1/1	0.92	0.13	61,61,61,61	0
54	MG	2a	3124	1/1	0.92	0.13	62,62,62,62	0
54	MG	2A	3202	1/1	0.92	0.34	69,69,69,69	0
54	MG	1A	3210	1/1	0.92	0.19	40,40,40,40	0
54	MG	1A	3583	1/1	0.92	0.13	68,68,68,68	0
54	MG	1A	3638	1/1	0.92	0.25	49,49,49,49	0
54	MG	2A	3207	1/1	0.92	0.11	68,68,68,68	0
54	MG	19	101	1/1	0.92	0.16	59,59,59,59	0
54	MG	1A	3524	1/1	0.92	0.26	58,58,58,58	0
54	MG	1A	3010	1/1	0.92	0.11	49,49,49,49	0
54	MG	1a	1748	1/1	0.92	0.36	78,78,78,78	0
54	MG	1A	3644	1/1	0.92	0.18	75,75,75,75	0
54	MG	1A	3054	1/1	0.92	0.25	65,65,65,65	0
54	MG	1A	3988	1/1	0.92	0.13	54,54,54,54	0
54	MG	1n	102	1/1	0.92	0.21	70,70,70,70	0
54	MG	2A	3695	1/1	0.92	0.10	50,50,50,50	0
54	MG	1o	101	1/1	0.92	0.25	61,61,61,61	0
54	MG	1A	3060	1/1	0.92	0.08	62,62,62,62	0
54	MG	2A	3699	1/1	0.92	0.14	62,62,62,62	0
54	MG	2A	3459	1/1	0.92	0.10	60,60,60,60	0
54	MG	1A	3871	1/1	0.92	0.09	19,19,19,19	0
54	MG	1A	3992	1/1	0.92	0.14	56,56,56,56	0
54	MG	1A	3237	1/1	0.92	0.11	56,56,56,56	0
54	MG	2A	3705	1/1	0.92	0.10	62,62,62,62	0
54	MG	1A	3873	1/1	0.92	0.09	40,40,40,40	0
54	MG	1B	201	1/1	0.92	0.20	71,71,71,71	0
54	MG	2A	3012	1/1	0.92	0.11	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	3655	1/1	0.92	0.15	68,68,68,68	0
54	MG	1A	3317	1/1	0.92	0.09	55,55,55,55	0
54	MG	2A	3022	1/1	0.92	0.18	52,52,52,52	0
54	MG	2A	3716	1/1	0.92	0.09	56,56,56,56	0
54	MG	1A	3596	1/1	0.92	0.25	37,37,37,37	0
54	MG	1A	3542	1/1	0.92	0.12	55,55,55,55	0
54	MG	1A	3002	1/1	0.92	0.11	55,55,55,55	0
54	MG	2e	201	1/1	0.92	0.21	66,66,66,66	0
54	MG	2f	201	1/1	0.92	0.13	60,60,60,60	0
54	MG	1a	1772	1/1	0.92	0.08	64,64,64,64	0
54	MG	1B	208	1/1	0.92	0.34	69,69,69,69	0
54	MG	2A	3255	1/1	0.92	0.26	71,71,71,71	0
54	MG	2B	203	1/1	0.92	0.31	68,68,68,68	0
54	MG	1B	210	1/1	0.92	0.10	56,56,56,56	0
54	MG	2A	3040	1/1	0.92	0.22	68,68,68,68	0
54	MG	2A	3264	1/1	0.92	0.42	72,72,72,72	0
57	MPD	1A	3999	8/8	0.92	0.20	50,53,61,63	0
54	MG	1A	3765	1/1	0.92	0.12	60,60,60,60	0
54	MG	1A	3373	1/1	0.92	0.14	60,60,60,60	0
54	MG	2A	3491	1/1	0.92	0.11	64,64,64,64	0
54	MG	1A	3115	1/1	0.92	0.21	54,54,54,54	0
54	MG	1A	3718	1/1	0.93	0.09	49,49,49,49	0
54	MG	2F	302	1/1	0.93	0.10	51,51,51,51	0
54	MG	1a	1620	1/1	0.93	0.22	61,61,61,61	0
54	MG	1a	1733	1/1	0.93	0.11	68,68,68,68	0
54	MG	1A	3220	1/1	0.93	0.18	65,65,65,65	0
54	MG	2P	201	1/1	0.93	0.12	69,69,69,69	0
54	MG	2P	202	1/1	0.93	0.11	64,64,64,64	0
54	MG	2Q	201	1/1	0.93	0.11	54,54,54,54	0
54	MG	2A	3138	1/1	0.93	0.42	67,67,67,67	0
54	MG	1a	1625	1/1	0.93	0.11	60,60,60,60	0
54	MG	1A	3231	1/1	0.93	0.17	62,62,62,62	0
54	MG	1A	3575	1/1	0.93	0.10	57,57,57,57	0
54	MG	2A	3532	1/1	0.93	0.10	60,60,60,60	0
54	MG	1a	1851	1/1	0.93	0.25	61,61,61,61	0
54	MG	1a	1852	1/1	0.93	0.17	55,55,55,55	0
54	MG	2W	202	1/1	0.93	0.17	63,63,63,63	0
54	MG	2A	3544	1/1	0.93	0.08	58,58,58,58	0
54	MG	2A	3363	1/1	0.93	0.19	61,61,61,61	0
54	MG	1a	1742	1/1	0.93	0.09	52,52,52,52	0
54	MG	1a	1630	1/1	0.93	0.12	48,48,48,48	0
54	MG	2A	3152	1/1	0.93	0.12	55,55,55,55	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	1A	3090	1/1	0.93	0.21	61,61,61,61	0
54	MG	2A	3371	1/1	0.93	0.16	68,68,68,68	0
54	MG	2A	3559	1/1	0.93	0.07	67,67,67,67	0
54	MG	1a	1856	1/1	0.93	0.18	77,77,77,77	0
54	MG	2A	3157	1/1	0.93	0.14	60,60,60,60	0
54	MG	2a	3009	1/1	0.93	0.14	62,62,62,62	0
54	MG	1a	1858	1/1	0.93	0.11	64,64,64,64	0
54	MG	2A	3567	1/1	0.93	0.08	53,53,53,53	0
54	MG	2a	3013	1/1	0.93	0.17	56,56,56,56	0
54	MG	1A	3931	1/1	0.93	0.11	56,56,56,56	0
54	MG	1A	3396	1/1	0.93	0.16	61,61,61,61	0
54	MG	1a	1863	1/1	0.93	0.09	66,66,66,66	0
54	MG	1A	3448	1/1	0.93	0.12	56,56,56,56	0
54	MG	1A	3056	1/1	0.93	0.11	53,53,53,53	0
54	MG	1A	3635	1/1	0.93	0.20	55,55,55,55	0
54	MG	1a	1641	1/1	0.93	0.31	63,63,63,63	0
54	MG	2A	3579	1/1	0.93	0.10	64,64,64,64	0
54	MG	1A	3057	1/1	0.93	0.20	50,50,50,50	0
54	MG	1a	1755	1/1	0.93	0.08	62,62,62,62	0
54	MG	1A	3830	1/1	0.93	0.10	53,53,53,53	0
54	MG	2a	3030	1/1	0.93	0.30	66,66,66,66	0
54	MG	2A	3172	1/1	0.93	0.11	53,53,53,53	0
54	MG	1A	3118	1/1	0.93	0.17	53,53,53,53	0
54	MG	2A	3390	1/1	0.93	0.09	35,35,35,35	0
54	MG	2A	3596	1/1	0.93	0.15	40,40,40,40	0
54	MG	1f	201	1/1	0.93	0.12	53,53,53,53	0
54	MG	1D	313	1/1	0.93	0.09	64,64,64,64	0
54	MG	2a	3038	1/1	0.93	0.17	74,74,74,74	0
54	MG	1a	1649	1/1	0.93	0.37	72,72,72,72	0
54	MG	2A	3180	1/1	0.93	0.30	69,69,69,69	0
54	MG	1A	3944	1/1	0.93	0.11	63,63,63,63	0
54	MG	2A	3611	1/1	0.93	0.13	69,69,69,69	0
54	MG	2A	3400	1/1	0.93	0.22	65,65,65,65	0
54	MG	1A	3737	1/1	0.93	0.13	60,60,60,60	0
54	MG	2A	3402	1/1	0.93	0.07	46,46,46,46	0
54	MG	2A	3403	1/1	0.93	0.12	52,52,52,52	0
54	MG	2A	3620	1/1	0.93	0.20	70,70,70,70	0
54	MG	2A	3622	1/1	0.93	0.09	61,61,61,61	0
54	MG	2A	3624	1/1	0.93	0.15	53,53,53,53	0
54	MG	1A	3642	1/1	0.93	0.11	67,67,67,67	0
54	MG	2a	3054	1/1	0.93	0.22	68,68,68,68	0
54	MG	2A	3405	1/1	0.93	0.12	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	3519	1/1	0.93	0.11	55,55,55,55	0
54	MG	2A	3186	1/1	0.93	0.26	65,65,65,65	0
54	MG	1A	3069	1/1	0.93	0.10	42,42,42,42	0
54	MG	1o	102	1/1	0.93	0.09	67,67,67,67	0
54	MG	1A	3846	1/1	0.93	0.12	40,40,40,40	0
54	MG	2A	3191	1/1	0.93	0.15	63,63,63,63	0
54	MG	1A	3188	1/1	0.93	0.13	51,51,51,51	0
54	MG	2A	3413	1/1	0.93	0.30	58,58,58,58	0
54	MG	2a	3065	1/1	0.93	0.28	70,70,70,70	0
54	MG	2A	3194	1/1	0.93	0.21	65,65,65,65	0
54	MG	1A	3647	1/1	0.93	0.15	53,53,53,53	0
54	MG	1A	3960	1/1	0.93	0.13	65,65,65,65	0
54	MG	1y	202	1/1	0.93	0.17	80,80,80,80	0
54	MG	1A	3460	1/1	0.93	0.06	54,54,54,54	0
54	MG	2A	3002	1/1	0.93	0.17	55,55,55,55	0
54	MG	2a	3073	1/1	0.93	0.17	63,63,63,63	0
54	MG	1A	3359	1/1	0.93	0.09	35,35,35,35	0
54	MG	2A	3647	1/1	0.93	0.16	72,72,72,72	0
54	MG	2A	3010	1/1	0.93	0.13	67,67,67,67	0
54	MG	1A	3748	1/1	0.93	0.06	46,46,46,46	0
54	MG	2A	3651	1/1	0.93	0.08	48,48,48,48	0
54	MG	1a	1778	1/1	0.93	0.14	64,64,64,64	0
54	MG	2A	3211	1/1	0.93	0.26	48,48,48,48	0
54	MG	1A	3299	1/1	0.93	0.23	64,64,64,64	0
54	MG	2A	3655	1/1	0.93	0.12	65,65,65,65	0
54	MG	1A	3967	1/1	0.93	0.15	60,60,60,60	0
54	MG	1A	3968	1/1	0.93	0.11	48,48,48,48	0
54	MG	1A	3595	1/1	0.93	0.26	46,46,46,46	0
54	MG	2A	3219	1/1	0.93	0.17	67,67,67,67	0
54	MG	1Q	204	1/1	0.93	0.18	62,62,62,62	0
54	MG	1R	204	1/1	0.93	0.17	59,59,59,59	0
54	MG	1A	3412	1/1	0.93	0.14	37,37,37,37	0
54	MG	1A	3972	1/1	0.93	0.24	68,68,68,68	0
54	MG	2A	3665	1/1	0.93	0.14	70,70,70,70	0
54	MG	1A	3253	1/1	0.93	0.22	60,60,60,60	0
54	MG	1A	3254	1/1	0.93	0.10	74,74,74,74	0
54	MG	2A	3042	1/1	0.93	0.19	58,58,58,58	0
54	MG	1A	3154	1/1	0.93	0.24	61,61,61,61	0
54	MG	2A	3044	1/1	0.93	0.14	49,49,49,49	0
54	MG	2a	3105	1/1	0.93	0.18	64,64,64,64	0
54	MG	2A	3449	1/1	0.93	0.07	62,62,62,62	0
54	MG	1a	1680	1/1	0.93	0.19	66,66,66,66	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	1A	3303	1/1	0.93	0.19	58,58,58,58	0
54	MG	1a	1794	1/1	0.93	0.13	59,59,59,59	0
54	MG	2a	3110	1/1	0.93	0.11	67,67,67,67	0
54	MG	1A	3122	1/1	0.93	0.13	44,44,44,44	0
54	MG	1V	205	1/1	0.93	0.17	73,73,73,73	0
54	MG	2A	3247	1/1	0.93	0.17	56,56,56,56	0
54	MG	1a	1686	1/1	0.93	0.17	57,57,57,57	0
54	MG	1A	3473	1/1	0.93	0.09	35,35,35,35	0
54	MG	2A	3054	1/1	0.93	0.25	51,51,51,51	0
54	MG	2A	3460	1/1	0.93	0.11	39,39,39,39	0
54	MG	2A	3055	1/1	0.93	0.10	48,48,48,48	0
54	MG	2A	3056	1/1	0.93	0.09	56,56,56,56	0
54	MG	2A	3687	1/1	0.93	0.17	60,60,60,60	0
54	MG	1A	3262	1/1	0.93	0.28	38,38,38,38	0
54	MG	1a	1690	1/1	0.93	0.20	70,70,70,70	0
54	MG	1A	3053	1/1	0.93	0.17	47,47,47,47	0
54	MG	2a	3133	1/1	0.93	0.09	48,48,48,48	0
54	MG	1X	101	1/1	0.93	0.09	68,68,68,68	0
54	MG	1A	3130	1/1	0.93	0.22	45,45,45,45	0
54	MG	1A	3769	1/1	0.93	0.11	58,58,58,58	0
54	MG	2a	3139	1/1	0.93	0.12	68,68,68,68	0
54	MG	2a	3141	1/1	0.93	0.21	71,71,71,71	0
54	MG	1A	3316	1/1	0.93	0.11	41,41,41,41	0
54	MG	1a	1810	1/1	0.93	0.08	64,64,64,64	0
54	MG	1A	3551	1/1	0.93	0.14	66,66,66,66	0
54	MG	2a	3148	1/1	0.93	0.20	65,65,65,65	0
54	MG	2a	3151	1/1	0.93	0.07	73,73,73,73	0
54	MG	1A	3485	1/1	0.93	0.18	64,64,64,64	0
54	MG	2A	3478	1/1	0.93	0.08	69,69,69,69	0
54	MG	1A	3774	1/1	0.93	0.09	56,56,56,56	0
54	MG	1A	3993	1/1	0.93	0.10	66,66,66,66	0
54	MG	2A	3289	1/1	0.93	0.11	51,51,51,51	0
54	MG	2A	3710	1/1	0.93	0.12	61,61,61,61	0
54	MG	2A	3290	1/1	0.93	0.24	58,58,58,58	0
54	MG	2A	3291	1/1	0.93	0.13	71,71,71,71	0
54	MG	2A	3294	1/1	0.93	0.09	58,58,58,58	0
54	MG	1a	1701	1/1	0.93	0.43	73,73,73,73	0
54	MG	1A	3487	1/1	0.93	0.07	62,62,62,62	0
54	MG	1A	3892	1/1	0.93	0.22	60,60,60,60	0
54	MG	2a	3164	1/1	0.93	0.19	62,62,62,62	0
54	MG	1A	3169	1/1	0.93	0.15	64,64,64,64	0
54	MG	2A	3093	1/1	0.93	0.17	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	2A	3725	1/1	0.93	0.15	61,61,61,61	0
54	MG	2A	3727	1/1	0.93	0.14	46,46,46,46	0
54	MG	1a	1705	1/1	0.93	0.12	62,62,62,62	0
54	MG	1a	1822	1/1	0.93	0.20	68,68,68,68	0
54	MG	2A	3310	1/1	0.93	0.23	66,66,66,66	0
54	MG	1A	3172	1/1	0.93	0.15	49,49,49,49	0
54	MG	1A	3689	1/1	0.93	0.13	46,46,46,46	0
54	MG	1A	3434	1/1	0.93	0.12	47,47,47,47	0
54	MG	1A	3561	1/1	0.93	0.12	29,29,29,29	0
54	MG	1A	3493	1/1	0.93	0.07	48,48,48,48	0
54	MG	1a	1715	1/1	0.93	0.26	68,68,68,68	0
54	MG	1A	3379	1/1	0.93	0.08	39,39,39,39	0
54	MG	2A	3112	1/1	0.93	0.44	50,50,50,50	0
54	MG	1A	3273	1/1	0.93	0.25	50,50,50,50	0
54	MG	1A	3702	1/1	0.93	0.08	37,37,37,37	0
54	MG	1A	3704	1/1	0.93	0.13	50,50,50,50	0
54	MG	1A	3385	1/1	0.93	0.11	36,36,36,36	0
54	MG	2A	3337	1/1	0.93	0.11	40,40,40,40	0
54	MG	2A	3513	1/1	0.93	0.10	41,41,41,41	0
54	MG	1A	3715	1/1	0.93	0.10	34,34,34,34	0
54	MG	2A	3515	1/1	0.93	0.07	54,54,54,54	0
54	MG	1a	1610	1/1	0.93	0.25	59,59,59,59	0
54	MG	2E	304	1/1	0.93	0.07	56,56,56,56	0
54	MG	1A	3386	1/1	0.93	0.08	42,42,42,42	0
54	MG	2A	3254	1/1	0.94	0.17	46,46,46,46	0
54	MG	1A	3221	1/1	0.94	0.28	60,60,60,60	0
54	MG	2A	3487	1/1	0.94	0.10	65,65,65,65	0
54	MG	1A	3358	1/1	0.94	0.08	37,37,37,37	0
54	MG	1A	3479	1/1	0.94	0.09	46,46,46,46	0
54	MG	1a	1606	1/1	0.94	0.18	55,55,55,55	0
54	MG	1A	3416	1/1	0.94	0.13	34,34,34,34	0
54	MG	1A	3734	1/1	0.94	0.13	65,65,65,65	0
54	MG	2D	305	1/1	0.94	0.10	55,55,55,55	0
54	MG	2D	307	1/1	0.94	0.21	48,48,48,48	0
54	MG	2A	3272	1/1	0.94	0.08	59,59,59,59	0
54	MG	2A	3495	1/1	0.94	0.10	40,40,40,40	0
54	MG	1a	1609	1/1	0.94	0.10	59,59,59,59	0
54	MG	1A	3226	1/1	0.94	0.09	49,49,49,49	0
54	MG	2A	3277	1/1	0.94	0.14	67,67,67,67	0
54	MG	2E	303	1/1	0.94	0.44	57,57,57,57	0
54	MG	1a	1769	1/1	0.94	0.14	51,51,51,51	0
54	MG	1a	1770	1/1	0.94	0.28	65,65,65,65	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	1a	1771	1/1	0.94	0.09	70,70,70,70	0
54	MG	1A	3289	1/1	0.94	0.12	55,55,55,55	0
54	MG	2A	3283	1/1	0.94	0.06	43,43,43,43	0
54	MG	2A	3287	1/1	0.94	0.10	41,41,41,41	0
54	MG	1a	1616	1/1	0.94	0.12	67,67,67,67	0
54	MG	1A	3362	1/1	0.94	0.12	51,51,51,51	0
54	MG	1A	3490	1/1	0.94	0.09	57,57,57,57	0
54	MG	2A	3293	1/1	0.94	0.14	55,55,55,55	0
54	MG	1A	3173	1/1	0.94	0.21	42,42,42,42	0
54	MG	2R	201	1/1	0.94	0.19	59,59,59,59	0
54	MG	1A	3858	1/1	0.94	0.14	54,54,54,54	0
54	MG	2A	3512	1/1	0.94	0.11	49,49,49,49	0
54	MG	1A	3862	1/1	0.94	0.10	55,55,55,55	0
54	MG	2A	3066	1/1	0.94	0.08	54,54,54,54	0
54	MG	1A	3641	1/1	0.94	0.07	28,28,28,28	0
54	MG	1A	3364	1/1	0.94	0.06	33,33,33,33	0
54	MG	2A	3518	1/1	0.94	0.07	65,65,65,65	0
54	MG	1A	3868	1/1	0.94	0.07	63,63,63,63	0
54	MG	1A	3294	1/1	0.94	0.18	38,38,38,38	0
54	MG	20	103	1/1	0.94	0.13	58,58,58,58	0
54	MG	1A	3745	1/1	0.94	0.13	56,56,56,56	0
54	MG	1A	3139	1/1	0.94	0.11	57,57,57,57	0
54	MG	1A	3176	1/1	0.94	0.11	54,54,54,54	0
54	MG	1a	1639	1/1	0.94	0.12	73,73,73,73	0
54	MG	1A	3431	1/1	0.94	0.09	56,56,56,56	0
54	MG	1A	3751	1/1	0.94	0.06	46,46,46,46	0
54	MG	2a	3006	1/1	0.94	0.13	69,69,69,69	0
54	MG	2A	3320	1/1	0.94	0.09	37,37,37,37	0
54	MG	1B	212	1/1	0.94	0.18	67,67,67,67	0
54	MG	2A	3534	1/1	0.94	0.10	56,56,56,56	0
54	MG	1A	3648	1/1	0.94	0.42	41,41,41,41	0
54	MG	1A	3234	1/1	0.94	0.08	53,53,53,53	0
54	MG	2A	3090	1/1	0.94	0.17	75,75,75,75	0
54	MG	1A	3178	1/1	0.94	0.25	66,66,66,66	0
54	MG	2A	3327	1/1	0.94	0.11	39,39,39,39	0
54	MG	2A	3330	1/1	0.94	0.08	37,37,37,37	0
54	MG	2A	3551	1/1	0.94	0.08	66,66,66,66	0
54	MG	1A	3143	1/1	0.94	0.11	44,44,44,44	0
54	MG	2A	3553	1/1	0.94	0.10	58,58,58,58	0
54	MG	2A	3332	1/1	0.94	0.09	48,48,48,48	0
54	MG	2A	3556	1/1	0.94	0.07	37,37,37,37	0
54	MG	1A	3180	1/1	0.94	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	2a	3027	1/1	0.94	0.10	58,58,58,58	0
54	MG	1a	1797	1/1	0.94	0.11	64,64,64,64	0
54	MG	1a	1651	1/1	0.94	0.33	69,69,69,69	0
54	MG	1A	3372	1/1	0.94	0.20	61,61,61,61	0
54	MG	1a	1800	1/1	0.94	0.17	70,70,70,70	0
54	MG	1A	3888	1/1	0.94	0.07	65,65,65,65	0
54	MG	2A	3101	1/1	0.94	0.19	65,65,65,65	0
54	MG	1A	3659	1/1	0.94	0.34	75,75,75,75	0
54	MG	2A	3106	1/1	0.94	0.15	44,44,44,44	0
54	MG	1A	3008	1/1	0.94	0.08	45,45,45,45	0
54	MG	1A	3896	1/1	0.94	0.06	59,59,59,59	0
54	MG	1A	3509	1/1	0.94	0.08	24,24,24,24	0
54	MG	1A	3898	1/1	0.94	0.10	44,44,44,44	0
54	MG	2A	3578	1/1	0.94	0.11	64,64,64,64	0
54	MG	2a	3042	1/1	0.94	0.13	70,70,70,70	0
54	MG	1a	1661	1/1	0.94	0.15	65,65,65,65	0
54	MG	1A	3092	1/1	0.94	0.11	44,44,44,44	0
54	MG	1A	3443	1/1	0.94	0.10	66,66,66,66	0
54	MG	1a	1664	1/1	0.94	0.29	75,75,75,75	0
54	MG	2A	3365	1/1	0.94	0.13	55,55,55,55	0
54	MG	1A	3591	1/1	0.94	0.11	71,71,71,71	0
54	MG	2A	3591	1/1	0.94	0.07	50,50,50,50	0
54	MG	2A	3592	1/1	0.94	0.09	58,58,58,58	0
54	MG	1A	3669	1/1	0.94	0.14	71,71,71,71	0
54	MG	1A	3516	1/1	0.94	0.09	49,49,49,49	0
54	MG	2A	3370	1/1	0.94	0.09	42,42,42,42	0
54	MG	2A	3601	1/1	0.94	0.11	75,75,75,75	0
54	MG	1A	3906	1/1	0.94	0.07	67,67,67,67	0
54	MG	1A	3772	1/1	0.94	0.10	40,40,40,40	0
54	MG	2A	3134	1/1	0.94	0.14	71,71,71,71	0
54	MG	1A	3012	1/1	0.94	0.11	44,44,44,44	0
54	MG	1D	316	1/1	0.94	0.09	54,54,54,54	0
54	MG	1A	3100	1/1	0.94	0.14	55,55,55,55	0
54	MG	1a	1674	1/1	0.94	0.18	62,62,62,62	0
54	MG	1A	3001	1/1	0.94	0.08	41,41,41,41	0
54	MG	2A	3617	1/1	0.94	0.09	42,42,42,42	0
54	MG	1E	308	1/1	0.94	0.14	31,31,31,31	0
54	MG	1A	3261	1/1	0.94	0.14	37,37,37,37	0
54	MG	2A	3621	1/1	0.94	0.10	55,55,55,55	0
54	MG	1A	3777	1/1	0.94	0.12	54,54,54,54	0
54	MG	2A	3623	1/1	0.94	0.08	42,42,42,42	0
54	MG	2A	3149	1/1	0.94	0.11	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	2A	3150	1/1	0.94	0.12	45,45,45,45	0
54	MG	2A	3151	1/1	0.94	0.08	53,53,53,53	0
54	MG	1F	305	1/1	0.94	0.21	40,40,40,40	0
54	MG	2A	3153	1/1	0.94	0.09	50,50,50,50	0
54	MG	1A	3193	1/1	0.94	0.19	51,51,51,51	0
54	MG	1A	3779	1/1	0.94	0.13	65,65,65,65	0
54	MG	1A	3523	1/1	0.94	0.09	58,58,58,58	0
54	MG	1A	3682	1/1	0.94	0.14	56,56,56,56	0
54	MG	2A	3395	1/1	0.94	0.07	56,56,56,56	0
54	MG	1a	1685	1/1	0.94	0.14	49,49,49,49	0
54	MG	1A	3265	1/1	0.94	0.12	53,53,53,53	0
54	MG	2a	3087	1/1	0.94	0.14	64,64,64,64	0
54	MG	2A	3399	1/1	0.94	0.08	41,41,41,41	0
54	MG	1A	3791	1/1	0.94	0.13	30,30,30,30	0
54	MG	1F	317	1/1	0.94	0.12	55,55,55,55	0
54	MG	2a	3091	1/1	0.94	0.34	62,62,62,62	0
54	MG	1H	201	1/1	0.94	0.11	70,70,70,70	0
54	MG	1N	202	1/1	0.94	0.10	48,48,48,48	0
54	MG	2A	3645	1/1	0.94	0.09	48,48,48,48	0
54	MG	1A	3390	1/1	0.94	0.05	27,27,27,27	0
54	MG	1A	3793	1/1	0.94	0.18	49,49,49,49	0
54	MG	1A	3686	1/1	0.94	0.10	54,54,54,54	0
54	MG	1A	3527	1/1	0.94	0.11	59,59,59,59	0
54	MG	1A	3161	1/1	0.94	0.23	70,70,70,70	0
54	MG	1A	3801	1/1	0.94	0.10	48,48,48,48	0
54	MG	2A	3174	1/1	0.94	0.11	52,52,52,52	0
54	MG	1R	202	1/1	0.94	0.09	43,43,43,43	0
54	MG	1A	3691	1/1	0.94	0.12	35,35,35,35	0
54	MG	1A	3128	1/1	0.94	0.08	52,52,52,52	0
54	MG	1A	3035	1/1	0.94	0.11	59,59,59,59	0
54	MG	1A	3540	1/1	0.94	0.10	55,55,55,55	0
54	MG	1T	203	1/1	0.94	0.09	60,60,60,60	0
54	MG	1a	1859	1/1	0.94	0.07	70,70,70,70	0
54	MG	2A	3418	1/1	0.94	0.12	40,40,40,40	0
54	MG	1A	3397	1/1	0.94	0.10	29,29,29,29	0
54	MG	1a	1706	1/1	0.94	0.25	61,61,61,61	0
54	MG	1A	3323	1/1	0.94	0.18	54,54,54,54	0
54	MG	1T	206	1/1	0.94	0.17	60,60,60,60	0
54	MG	2A	3667	1/1	0.94	0.13	63,63,63,63	0
54	MG	1U	201	1/1	0.94	0.21	59,59,59,59	0
54	MG	1A	3948	1/1	0.94	0.11	52,52,52,52	0
54	MG	2a	3123	1/1	0.94	0.13	56,56,56,56	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	1a	1713	1/1	0.94	0.23	69,69,69,69	0
54	MG	2A	3193	1/1	0.94	0.13	59,59,59,59	0
54	MG	1A	3949	1/1	0.94	0.06	48,48,48,48	0
54	MG	1A	3326	1/1	0.94	0.05	35,35,35,35	0
54	MG	2A	3434	1/1	0.94	0.07	51,51,51,51	0
54	MG	2A	3197	1/1	0.94	0.15	54,54,54,54	0
54	MG	1A	3205	1/1	0.94	0.09	48,48,48,48	0
54	MG	1d	304	1/1	0.94	0.09	65,65,65,65	0
54	MG	1A	3619	1/1	0.94	0.12	59,59,59,59	0
54	MG	1e	201	1/1	0.94	0.11	62,62,62,62	0
54	MG	2A	3440	1/1	0.94	0.14	62,62,62,62	0
54	MG	1A	3708	1/1	0.94	0.07	38,38,38,38	0
54	MG	1g	201	1/1	0.94	0.14	73,73,73,73	0
54	MG	1W	205	1/1	0.94	0.20	52,52,52,52	0
54	MG	1A	3959	1/1	0.94	0.07	64,64,64,64	0
54	MG	2A	3210	1/1	0.94	0.23	65,65,65,65	0
54	MG	1A	3818	1/1	0.94	0.11	38,38,38,38	0
54	MG	2A	3689	1/1	0.94	0.09	54,54,54,54	0
54	MG	1A	3961	1/1	0.94	0.12	46,46,46,46	0
54	MG	2A	3694	1/1	0.94	0.10	56,56,56,56	0
54	MG	10	101	1/1	0.94	0.14	44,44,44,44	0
54	MG	1a	1729	1/1	0.94	0.08	57,57,57,57	0
54	MG	1A	3820	1/1	0.94	0.11	50,50,50,50	0
54	MG	10	103	1/1	0.94	0.08	49,49,49,49	0
54	MG	10	104	1/1	0.94	0.13	56,56,56,56	0
54	MG	1A	3712	1/1	0.94	0.14	40,40,40,40	0
54	MG	1A	3085	1/1	0.94	0.13	52,52,52,52	0
54	MG	1A	3825	1/1	0.94	0.11	32,32,32,32	0
54	MG	2A	3231	1/1	0.94	0.12	56,56,56,56	0
54	MG	1A	3346	1/1	0.94	0.07	36,36,36,36	0
54	MG	2A	3461	1/1	0.94	0.08	68,68,68,68	0
54	MG	2A	3233	1/1	0.94	0.10	45,45,45,45	0
54	MG	1A	3408	1/1	0.94	0.12	29,29,29,29	0
54	MG	2a	3171	1/1	0.94	0.27	75,75,75,75	0
54	MG	1A	3549	1/1	0.94	0.06	65,65,65,65	0
54	MG	2A	3237	1/1	0.94	0.12	48,48,48,48	0
54	MG	1a	1744	1/1	0.94	0.16	72,72,72,72	0
54	MG	2A	3468	1/1	0.94	0.13	34,34,34,34	0
54	MG	2A	3008	1/1	0.94	0.19	44,44,44,44	0
54	MG	2a	3177	1/1	0.94	0.14	77,77,77,77	0
54	MG	1A	3832	1/1	0.94	0.09	44,44,44,44	0
54	MG	1A	3471	1/1	0.94	0.11	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	15	106	1/1	0.94	0.30	74,74,74,74	0
54	MG	2A	3723	1/1	0.94	0.19	62,62,62,62	0
54	MG	2A	3724	1/1	0.94	0.32	68,68,68,68	0
54	MG	2A	3474	1/1	0.94	0.08	45,45,45,45	0
54	MG	1A	3211	1/1	0.94	0.19	42,42,42,42	0
54	MG	15	109	1/1	0.94	0.08	53,53,53,53	0
54	MG	17	104	1/1	0.94	0.13	63,63,63,63	0
54	MG	1A	3975	1/1	0.94	0.07	66,66,66,66	0
54	MG	18	102	1/1	0.94	0.20	39,39,39,39	0
54	MG	1A	3171	1/1	0.94	0.15	69,69,69,69	0
54	MG	2B	206	1/1	0.94	0.14	84,84,84,84	0
54	MG	1A	3050	1/1	0.94	0.23	38,38,38,38	0
54	MG	1A	3843	1/1	0.94	0.14	41,41,41,41	0
54	MG	1A	3467	1/1	0.95	0.08	38,38,38,38	0
54	MG	1A	3063	1/1	0.95	0.16	42,42,42,42	0
54	MG	1A	3347	1/1	0.95	0.07	40,40,40,40	0
54	MG	2A	3333	1/1	0.95	0.08	39,39,39,39	0
54	MG	2A	3335	1/1	0.95	0.14	53,53,53,53	0
54	MG	2F	301	1/1	0.95	0.27	46,46,46,46	0
54	MG	1U	205	1/1	0.95	0.17	40,40,40,40	0
54	MG	2F	303	1/1	0.95	0.17	59,59,59,59	0
54	MG	1A	3037	1/1	0.95	0.08	35,35,35,35	0
54	MG	1A	3236	1/1	0.95	0.08	47,47,47,47	0
54	MG	1A	3410	1/1	0.95	0.08	35,35,35,35	0
54	MG	2A	3542	1/1	0.95	0.13	59,59,59,59	0
54	MG	2A	3343	1/1	0.95	0.16	71,71,71,71	0
54	MG	2A	3344	1/1	0.95	0.13	44,44,44,44	0
54	MG	2A	3125	1/1	0.95	0.09	43,43,43,43	0
54	MG	1A	3141	1/1	0.95	0.08	45,45,45,45	0
54	MG	2A	3129	1/1	0.95	0.17	57,57,57,57	0
54	MG	1a	1831	1/1	0.95	0.07	55,55,55,55	0
54	MG	1A	3727	1/1	0.95	0.10	31,31,31,31	0
54	MG	2A	3135	1/1	0.95	0.17	53,53,53,53	0
54	MG	2A	3351	1/1	0.95	0.07	43,43,43,43	0
54	MG	2A	3137	1/1	0.95	0.16	59,59,59,59	0
54	MG	2W	201	1/1	0.95	0.21	64,64,64,64	0
54	MG	1W	202	1/1	0.95	0.19	56,56,56,56	0
54	MG	1A	3354	1/1	0.95	0.14	28,28,28,28	0
54	MG	2A	3561	1/1	0.95	0.12	52,52,52,52	0
54	MG	1A	3168	1/1	0.95	0.22	42,42,42,42	0
54	MG	23	101	1/1	0.95	0.17	56,56,56,56	0
54	MG	1A	3357	1/1	0.95	0.07	40,40,40,40	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	27	102	1/1	0.95	0.17	47,47,47,47	0
54	MG	2A	3143	1/1	0.95	0.27	52,52,52,52	0
54	MG	2a	3001	1/1	0.95	0.10	49,49,49,49	0
54	MG	1A	3478	1/1	0.95	0.06	26,26,26,26	0
54	MG	1A	3840	1/1	0.95	0.08	61,61,61,61	0
54	MG	1A	3415	1/1	0.95	0.05	24,24,24,24	0
54	MG	2A	3573	1/1	0.95	0.22	66,66,66,66	0
54	MG	2A	3367	1/1	0.95	0.12	70,70,70,70	0
54	MG	1A	3556	1/1	0.95	0.20	58,58,58,58	0
54	MG	1A	3480	1/1	0.95	0.10	69,69,69,69	0
54	MG	1A	3295	1/1	0.95	0.11	52,52,52,52	0
54	MG	10	105	1/1	0.95	0.10	61,61,61,61	0
54	MG	1A	3417	1/1	0.95	0.08	35,35,35,35	0
54	MG	1A	3244	1/1	0.95	0.10	62,62,62,62	0
54	MG	2A	3154	1/1	0.95	0.15	52,52,52,52	0
54	MG	1a	1711	1/1	0.95	0.21	71,71,71,71	0
54	MG	2A	3376	1/1	0.95	0.07	36,36,36,36	0
54	MG	1A	3740	1/1	0.95	0.06	34,34,34,34	0
54	MG	1A	3360	1/1	0.95	0.06	33,33,33,33	0
54	MG	11	101	1/1	0.95	0.10	49,49,49,49	0
54	MG	2A	3594	1/1	0.95	0.10	55,55,55,55	0
54	MG	11	102	1/1	0.95	0.17	55,55,55,55	0
54	MG	1a	1716	1/1	0.95	0.19	58,58,58,58	0
54	MG	2A	3161	1/1	0.95	0.10	45,45,45,45	0
54	MG	2A	3598	1/1	0.95	0.07	40,40,40,40	0
54	MG	2A	3383	1/1	0.95	0.09	50,50,50,50	0
54	MG	2A	3603	1/1	0.95	0.08	60,60,60,60	0
54	MG	11	103	1/1	0.95	0.10	54,54,54,54	0
54	MG	2A	3605	1/1	0.95	0.12	70,70,70,70	0
54	MG	1a	1718	1/1	0.95	0.13	78,78,78,78	0
54	MG	1A	3108	1/1	0.95	0.09	47,47,47,47	0
54	MG	1a	1721	1/1	0.95	0.15	45,45,45,45	0
54	MG	1A	3197	1/1	0.95	0.34	49,49,49,49	0
54	MG	1A	3170	1/1	0.95	0.09	51,51,51,51	0
54	MG	13	103	1/1	0.95	0.08	45,45,45,45	0
54	MG	2A	3614	1/1	0.95	0.08	42,42,42,42	0
54	MG	1A	3568	1/1	0.95	0.11	62,62,62,62	0
54	MG	1A	3123	1/1	0.95	0.25	40,40,40,40	0
54	MG	1A	3052	1/1	0.95	0.13	50,50,50,50	0
54	MG	1d	301	1/1	0.95	0.19	69,69,69,69	0
54	MG	1A	3573	1/1	0.95	0.12	64,64,64,64	0
54	MG	17	102	1/1	0.95	0.17	36,36,36,36	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	1A	3650	1/1	0.95	0.09	58,58,58,58	0
54	MG	2a	3049	1/1	0.95	0.29	71,71,71,71	0
54	MG	1A	3752	1/1	0.95	0.08	28,28,28,28	0
54	MG	1A	3753	1/1	0.95	0.10	37,37,37,37	0
54	MG	2A	3182	1/1	0.95	0.35	51,51,51,51	0
54	MG	1A	3495	1/1	0.95	0.06	28,28,28,28	0
54	MG	19	102	1/1	0.95	0.16	58,58,58,58	0
54	MG	1A	3150	1/1	0.95	0.09	52,52,52,52	0
54	MG	1A	3576	1/1	0.95	0.22	63,63,63,63	0
54	MG	2A	3187	1/1	0.95	0.11	50,50,50,50	0
54	MG	1h	202	1/1	0.95	0.10	68,68,68,68	0
54	MG	1A	3151	1/1	0.95	0.07	39,39,39,39	0
54	MG	1B	205	1/1	0.95	0.07	54,54,54,54	0
54	MG	1m	201	1/1	0.95	0.07	75,75,75,75	0
54	MG	1A	3093	1/1	0.95	0.11	57,57,57,57	0
54	MG	1A	3264	1/1	0.95	0.08	49,49,49,49	0
54	MG	1n	103	1/1	0.95	0.09	57,57,57,57	0
54	MG	2A	3642	1/1	0.95	0.10	40,40,40,40	0
54	MG	1A	3435	1/1	0.95	0.07	53,53,53,53	0
54	MG	1A	3177	1/1	0.95	0.22	55,55,55,55	0
54	MG	1A	3883	1/1	0.95	0.19	45,45,45,45	0
54	MG	1A	3504	1/1	0.95	0.09	60,60,60,60	0
54	MG	1A	3312	1/1	0.95	0.30	54,54,54,54	0
54	MG	1A	3313	1/1	0.95	0.09	33,33,33,33	0
54	MG	2A	3649	1/1	0.95	0.09	45,45,45,45	0
54	MG	2a	3075	1/1	0.95	0.43	68,68,68,68	0
54	MG	1a	1754	1/1	0.95	0.16	68,68,68,68	0
54	MG	1A	3315	1/1	0.95	0.11	42,42,42,42	0
54	MG	1a	1756	1/1	0.95	0.11	71,71,71,71	0
54	MG	1A	3511	1/1	0.95	0.08	24,24,24,24	0
54	MG	1a	1622	1/1	0.95	0.18	56,56,56,56	0
54	MG	1A	3894	1/1	0.95	0.10	54,54,54,54	0
54	MG	1A	3213	1/1	0.95	0.12	47,47,47,47	0
54	MG	2A	3014	1/1	0.95	0.12	58,58,58,58	0
54	MG	2A	3214	1/1	0.95	0.21	53,53,53,53	0
54	MG	1a	1761	1/1	0.95	0.12	62,62,62,62	0
54	MG	1B	222	1/1	0.95	0.09	41,41,41,41	0
54	MG	1a	1628	1/1	0.95	0.21	72,72,72,72	0
54	MG	2A	3023	1/1	0.95	0.16	63,63,63,63	0
54	MG	1A	3673	1/1	0.95	0.07	56,56,56,56	0
54	MG	2A	3225	1/1	0.95	0.12	37,37,37,37	0
54	MG	2A	3226	1/1	0.95	0.10	60,60,60,60	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	1A	3513	1/1	0.95	0.07	54,54,54,54	0
54	MG	2a	3094	1/1	0.95	0.15	63,63,63,63	0
54	MG	2A	3030	1/1	0.95	0.13	61,61,61,61	0
54	MG	1A	3094	1/1	0.95	0.21	46,46,46,46	0
54	MG	1a	1767	1/1	0.95	0.13	71,71,71,71	0
54	MG	1a	1632	1/1	0.95	0.14	44,44,44,44	0
54	MG	1A	3593	1/1	0.95	0.18	38,38,38,38	0
54	MG	2A	3036	1/1	0.95	0.16	53,53,53,53	0
54	MG	2A	3038	1/1	0.95	0.12	59,59,59,59	0
54	MG	2a	3103	1/1	0.95	0.08	56,56,56,56	0
54	MG	2a	3104	1/1	0.95	0.07	69,69,69,69	0
54	MG	2A	3039	1/1	0.95	0.16	53,53,53,53	0
54	MG	2A	3240	1/1	0.95	0.12	63,63,63,63	0
54	MG	2A	3678	1/1	0.95	0.10	50,50,50,50	0
54	MG	1a	1635	1/1	0.95	0.16	51,51,51,51	0
54	MG	1A	3378	1/1	0.95	0.05	29,29,29,29	0
54	MG	1A	3047	1/1	0.95	0.32	51,51,51,51	0
54	MG	1A	3224	1/1	0.95	0.22	53,53,53,53	0
54	MG	1A	3157	1/1	0.95	0.17	46,46,46,46	0
54	MG	1A	3780	1/1	0.95	0.26	44,44,44,44	0
54	MG	1A	3228	1/1	0.95	0.24	52,52,52,52	0
54	MG	1D	311	1/1	0.95	0.21	45,45,45,45	0
54	MG	2a	3116	1/1	0.95	0.20	64,64,64,64	0
54	MG	1A	3687	1/1	0.95	0.08	46,46,46,46	0
54	MG	1A	3784	1/1	0.95	0.09	57,57,57,57	0
54	MG	2A	3051	1/1	0.95	0.20	71,71,71,71	0
54	MG	2A	3690	1/1	0.95	0.07	62,62,62,62	0
54	MG	1A	3918	1/1	0.95	0.10	50,50,50,50	0
54	MG	2A	3693	1/1	0.95	0.07	64,64,64,64	0
54	MG	1A	3785	1/1	0.95	0.07	39,39,39,39	0
54	MG	1A	3920	1/1	0.95	0.09	68,68,68,68	0
54	MG	1A	3788	1/1	0.95	0.11	58,58,58,58	0
54	MG	2a	3128	1/1	0.95	0.07	66,66,66,66	0
54	MG	2a	3130	1/1	0.95	0.07	59,59,59,59	0
54	MG	1A	3278	1/1	0.95	0.07	54,54,54,54	0
54	MG	2A	3698	1/1	0.95	0.08	58,58,58,58	0
54	MG	2A	3259	1/1	0.95	0.09	45,45,45,45	0
54	MG	2A	3260	1/1	0.95	0.33	68,68,68,68	0
54	MG	2A	3261	1/1	0.95	0.16	51,51,51,51	0
54	MG	1A	3282	1/1	0.95	0.13	38,38,38,38	0
54	MG	1A	3329	1/1	0.95	0.11	33,33,33,33	0
54	MG	1A	3331	1/1	0.95	0.07	48,48,48,48	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	1a	1657	1/1	0.95	0.24	57,57,57,57	0
54	MG	2A	3273	1/1	0.95	0.15	56,56,56,56	0
54	MG	2a	3150	1/1	0.95	0.09	73,73,73,73	0
54	MG	2A	3708	1/1	0.95	0.07	68,68,68,68	0
54	MG	2A	3067	1/1	0.95	0.16	52,52,52,52	0
54	MG	2A	3275	1/1	0.95	0.06	65,65,65,65	0
54	MG	2A	3711	1/1	0.95	0.14	56,56,56,56	0
54	MG	2A	3068	1/1	0.95	0.10	57,57,57,57	0
54	MG	1A	3182	1/1	0.95	0.17	62,62,62,62	0
54	MG	1A	3694	1/1	0.95	0.20	38,38,38,38	0
54	MG	2A	3715	1/1	0.95	0.08	63,63,63,63	0
54	MG	1A	3695	1/1	0.95	0.17	47,47,47,47	0
54	MG	1A	3800	1/1	0.95	0.08	62,62,62,62	0
54	MG	1A	3529	1/1	0.95	0.06	40,40,40,40	0
54	MG	2A	3719	1/1	0.95	0.09	59,59,59,59	0
54	MG	1F	315	1/1	0.95	0.13	66,66,66,66	0
54	MG	1A	3335	1/1	0.95	0.09	42,42,42,42	0
54	MG	2A	3288	1/1	0.95	0.09	45,45,45,45	0
54	MG	1A	3938	1/1	0.95	0.07	30,30,30,30	0
54	MG	1G	202	1/1	0.95	0.13	61,61,61,61	0
54	MG	1A	3699	1/1	0.95	0.06	38,38,38,38	0
54	MG	1A	3535	1/1	0.95	0.17	49,49,49,49	0
54	MG	1a	1802	1/1	0.95	0.14	67,67,67,67	0
54	MG	1a	1669	1/1	0.95	0.16	69,69,69,69	0
54	MG	1A	3336	1/1	0.95	0.06	43,43,43,43	0
54	MG	1A	3537	1/1	0.95	0.27	61,61,61,61	0
54	MG	1A	3809	1/1	0.95	0.08	47,47,47,47	0
54	MG	1A	3810	1/1	0.95	0.08	49,49,49,49	0
54	MG	1Q	201	1/1	0.95	0.12	52,52,52,52	0
54	MG	1A	3538	1/1	0.95	0.21	36,36,36,36	0
54	MG	2B	210	1/1	0.95	0.10	70,70,70,70	0
54	MG	2a	3180	1/1	0.95	0.18	65,65,65,65	0
54	MG	1Q	203	1/1	0.95	0.07	46,46,46,46	0
54	MG	1A	3706	1/1	0.95	0.05	28,28,28,28	0
54	MG	1A	3707	1/1	0.95	0.08	57,57,57,57	0
54	MG	1A	3342	1/1	0.95	0.09	46,46,46,46	0
54	MG	1A	3950	1/1	0.95	0.07	24,24,24,24	0
54	MG	1A	3951	1/1	0.95	0.19	59,59,59,59	0
54	MG	2B	218	1/1	0.95	0.09	65,65,65,65	0
54	MG	2t	201	1/1	0.95	0.12	49,49,49,49	0
55	A1AE1	2A	3726	76/76	0.95	0.11	38,48,54,60	0
54	MG	2A	3107	1/1	0.95	0.07	42,42,42,42	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	2A	3108	1/1	0.95	0.08	53,53,53,53	0
54	MG	1a	1818	1/1	0.95	0.12	54,54,54,54	0
54	MG	1A	3710	1/1	0.95	0.07	58,58,58,58	0
57	MPD	18	103	8/8	0.95	0.12	36,45,46,51	0
54	MG	1A	3158	1/1	0.95	0.31	57,57,57,57	0
54	MG	2A	3114	1/1	0.95	0.16	48,48,48,48	0
54	MG	1A	3819	1/1	0.95	0.13	41,41,41,41	0
54	MG	2V	202	1/1	0.96	0.29	49,49,49,49	0
54	MG	1A	3045	1/1	0.96	0.16	55,55,55,55	0
54	MG	1A	3190	1/1	0.96	0.19	51,51,51,51	0
54	MG	1A	3954	1/1	0.96	0.10	57,57,57,57	0
54	MG	2A	3198	1/1	0.96	0.21	43,43,43,43	0
54	MG	2A	3199	1/1	0.96	0.23	48,48,48,48	0
54	MG	1A	3064	1/1	0.96	0.22	43,43,43,43	0
54	MG	1R	203	1/1	0.96	0.13	44,44,44,44	0
54	MG	1A	3956	1/1	0.96	0.05	50,50,50,50	0
54	MG	27	101	1/1	0.96	0.15	46,46,46,46	0
54	MG	1A	3570	1/1	0.96	0.11	56,56,56,56	0
54	MG	2A	3392	1/1	0.96	0.10	54,54,54,54	0
54	MG	2A	3593	1/1	0.96	0.07	59,59,59,59	0
54	MG	1A	3068	1/1	0.96	0.26	50,50,50,50	0
54	MG	1A	3839	1/1	0.96	0.09	49,49,49,49	0
54	MG	2A	3206	1/1	0.96	0.16	43,43,43,43	0
54	MG	1A	3194	1/1	0.96	0.17	40,40,40,40	0
54	MG	2A	3397	1/1	0.96	0.09	50,50,50,50	0
54	MG	1A	3841	1/1	0.96	0.07	28,28,28,28	0
54	MG	1A	3963	1/1	0.96	0.12	19,19,19,19	0
54	MG	1A	3842	1/1	0.96	0.06	55,55,55,55	0
54	MG	1A	3307	1/1	0.96	0.17	62,62,62,62	0
54	MG	2A	3606	1/1	0.96	0.06	46,46,46,46	0
54	MG	1A	3654	1/1	0.96	0.07	52,52,52,52	0
54	MG	1A	3430	1/1	0.96	0.09	45,45,45,45	0
54	MG	2A	3216	1/1	0.96	0.08	46,46,46,46	0
54	MG	2a	3017	1/1	0.96	0.11	53,53,53,53	0
54	MG	1A	3747	1/1	0.96	0.06	47,47,47,47	0
54	MG	1a	1681	1/1	0.96	0.10	55,55,55,55	0
54	MG	1A	3308	1/1	0.96	0.11	52,52,52,52	0
54	MG	1A	3657	1/1	0.96	0.14	61,61,61,61	0
54	MG	1A	3577	1/1	0.96	0.08	25,25,25,25	0
54	MG	1A	3973	1/1	0.96	0.09	43,43,43,43	0
54	MG	1A	3196	1/1	0.96	0.31	44,44,44,44	0
54	MG	2A	3059	1/1	0.96	0.32	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	3059	1/1	0.96	0.14	42,42,42,42	0
54	MG	1A	3259	1/1	0.96	0.08	67,67,67,67	0
54	MG	2A	3064	1/1	0.96	0.28	52,52,52,52	0
54	MG	1A	3070	1/1	0.96	0.24	50,50,50,50	0
54	MG	1A	3507	1/1	0.96	0.06	58,58,58,58	0
54	MG	1A	3098	1/1	0.96	0.13	43,43,43,43	0
54	MG	1a	1693	1/1	0.96	0.17	63,63,63,63	0
54	MG	2A	3071	1/1	0.96	0.14	45,45,45,45	0
54	MG	2A	3629	1/1	0.96	0.05	61,61,61,61	0
54	MG	2A	3239	1/1	0.96	0.13	55,55,55,55	0
54	MG	2A	3631	1/1	0.96	0.06	55,55,55,55	0
54	MG	2A	3072	1/1	0.96	0.36	51,51,51,51	0
54	MG	1A	3133	1/1	0.96	0.10	46,46,46,46	0
54	MG	2A	3424	1/1	0.96	0.06	35,35,35,35	0
54	MG	1A	3134	1/1	0.96	0.10	37,37,37,37	0
54	MG	2a	3044	1/1	0.96	0.13	58,58,58,58	0
54	MG	2A	3428	1/1	0.96	0.05	64,64,64,64	0
54	MG	2A	3429	1/1	0.96	0.06	46,46,46,46	0
54	MG	1A	3207	1/1	0.96	0.09	43,43,43,43	0
54	MG	1A	3075	1/1	0.96	0.09	46,46,46,46	0
54	MG	2A	3640	1/1	0.96	0.12	61,61,61,61	0
54	MG	2A	3078	1/1	0.96	0.10	53,53,53,53	0
54	MG	1A	3764	1/1	0.96	0.09	61,61,61,61	0
54	MG	1A	3987	1/1	0.96	0.17	54,54,54,54	0
54	MG	2A	3248	1/1	0.96	0.05	44,44,44,44	0
54	MG	1A	3588	1/1	0.96	0.07	50,50,50,50	0
54	MG	1A	3766	1/1	0.96	0.14	35,35,35,35	0
54	MG	1A	3076	1/1	0.96	0.14	36,36,36,36	0
54	MG	1A	3106	1/1	0.96	0.17	45,45,45,45	0
54	MG	2A	3087	1/1	0.96	0.12	52,52,52,52	0
54	MG	1A	3677	1/1	0.96	0.23	43,43,43,43	0
54	MG	1A	3877	1/1	0.96	0.09	26,26,26,26	0
54	MG	2A	3443	1/1	0.96	0.06	44,44,44,44	0
54	MG	1A	3995	1/1	0.96	0.08	57,57,57,57	0
54	MG	2A	3257	1/1	0.96	0.12	57,57,57,57	0
54	MG	1A	3382	1/1	0.96	0.08	37,37,37,37	0
54	MG	1A	3679	1/1	0.96	0.07	53,53,53,53	0
54	MG	1A	3383	1/1	0.96	0.08	25,25,25,25	0
54	MG	1A	3174	1/1	0.96	0.11	56,56,56,56	0
54	MG	15	107	1/1	0.96	0.19	32,32,32,32	0
54	MG	2A	3265	1/1	0.96	0.38	67,67,67,67	0
54	MG	2a	3071	1/1	0.96	0.12	60,60,60,60	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	1a	1835	1/1	0.96	0.09	55,55,55,55	0
54	MG	2A	3267	1/1	0.96	0.08	60,60,60,60	0
54	MG	1A	3884	1/1	0.96	0.05	56,56,56,56	0
54	MG	2A	3271	1/1	0.96	0.09	35,35,35,35	0
54	MG	2A	3457	1/1	0.96	0.12	64,64,64,64	0
54	MG	1A	3327	1/1	0.96	0.08	14,14,14,14	0
54	MG	1a	1838	1/1	0.96	0.10	49,49,49,49	0
54	MG	1a	1839	1/1	0.96	0.09	55,55,55,55	0
54	MG	2A	3105	1/1	0.96	0.07	48,48,48,48	0
54	MG	1A	3275	1/1	0.96	0.35	43,43,43,43	0
54	MG	17	103	1/1	0.96	0.19	39,39,39,39	0
54	MG	1A	3452	1/1	0.96	0.10	57,57,57,57	0
54	MG	1A	3453	1/1	0.96	0.08	40,40,40,40	0
54	MG	1B	209	1/1	0.96	0.07	43,43,43,43	0
54	MG	1a	1720	1/1	0.96	0.10	39,39,39,39	0
54	MG	1A	3215	1/1	0.96	0.27	43,43,43,43	0
54	MG	1A	3601	1/1	0.96	0.13	38,38,38,38	0
54	MG	1A	3526	1/1	0.96	0.25	30,30,30,30	0
54	MG	1A	3455	1/1	0.96	0.11	62,62,62,62	0
54	MG	1A	3456	1/1	0.96	0.07	50,50,50,50	0
54	MG	1A	3532	1/1	0.96	0.07	38,38,38,38	0
54	MG	1A	3219	1/1	0.96	0.14	38,38,38,38	0
54	MG	1A	3534	1/1	0.96	0.08	53,53,53,53	0
54	MG	1A	3789	1/1	0.96	0.06	46,46,46,46	0
54	MG	2A	3296	1/1	0.96	0.06	60,60,60,60	0
54	MG	1A	3393	1/1	0.96	0.06	32,32,32,32	0
54	MG	2A	3299	1/1	0.96	0.08	43,43,43,43	0
54	MG	2A	3301	1/1	0.96	0.06	37,37,37,37	0
54	MG	2A	3691	1/1	0.96	0.12	62,62,62,62	0
54	MG	1a	1732	1/1	0.96	0.08	38,38,38,38	0
54	MG	1A	3107	1/1	0.96	0.24	43,43,43,43	0
54	MG	2A	3131	1/1	0.96	0.10	48,48,48,48	0
54	MG	2A	3488	1/1	0.96	0.08	63,63,63,63	0
54	MG	1A	3614	1/1	0.96	0.08	45,45,45,45	0
54	MG	2A	3306	1/1	0.96	0.09	40,40,40,40	0
54	MG	1A	3462	1/1	0.96	0.10	49,49,49,49	0
54	MG	1a	1737	1/1	0.96	0.14	67,67,67,67	0
54	MG	1a	1615	1/1	0.96	0.10	69,69,69,69	0
54	MG	1A	3703	1/1	0.96	0.17	64,64,64,64	0
54	MG	2A	3313	1/1	0.96	0.06	57,57,57,57	0
54	MG	1a	1741	1/1	0.96	0.13	40,40,40,40	0
54	MG	1A	3004	1/1	0.96	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	1a	1618	1/1	0.96	0.15	59,59,59,59	0
54	MG	2A	3319	1/1	0.96	0.07	48,48,48,48	0
54	MG	1a	1619	1/1	0.96	0.07	59,59,59,59	0
54	MG	1A	3913	1/1	0.96	0.06	81,81,81,81	0
54	MG	1A	3915	1/1	0.96	0.06	34,34,34,34	0
54	MG	1A	3337	1/1	0.96	0.10	57,57,57,57	0
54	MG	1A	3799	1/1	0.96	0.06	28,28,28,28	0
54	MG	1e	202	1/1	0.96	0.09	68,68,68,68	0
54	MG	2A	3506	1/1	0.96	0.15	67,67,67,67	0
54	MG	2a	3126	1/1	0.96	0.10	63,63,63,63	0
54	MG	2A	3326	1/1	0.96	0.10	55,55,55,55	0
54	MG	1A	3339	1/1	0.96	0.07	48,48,48,48	0
54	MG	2A	3328	1/1	0.96	0.10	43,43,43,43	0
54	MG	1A	3399	1/1	0.96	0.06	28,28,28,28	0
54	MG	1A	3341	1/1	0.96	0.10	31,31,31,31	0
54	MG	1A	3079	1/1	0.96	0.17	46,46,46,46	0
54	MG	1A	3924	1/1	0.96	0.07	67,67,67,67	0
54	MG	1A	3114	1/1	0.96	0.06	45,45,45,45	0
54	MG	1l	201	1/1	0.96	0.21	66,66,66,66	0
54	MG	1A	3713	1/1	0.96	0.07	55,55,55,55	0
54	MG	2a	3144	1/1	0.96	0.14	59,59,59,59	0
54	MG	2A	3338	1/1	0.96	0.06	37,37,37,37	0
54	MG	1A	3714	1/1	0.96	0.09	51,51,51,51	0
54	MG	1E	306	1/1	0.96	0.07	59,59,59,59	0
54	MG	1A	3406	1/1	0.96	0.08	30,30,30,30	0
54	MG	1A	3930	1/1	0.96	0.15	44,44,44,44	0
54	MG	2A	3523	1/1	0.96	0.07	65,65,65,65	0
54	MG	1A	3344	1/1	0.96	0.07	40,40,40,40	0
54	MG	1A	3932	1/1	0.96	0.11	45,45,45,45	0
54	MG	2A	3528	1/1	0.96	0.09	58,58,58,58	0
54	MG	1A	3286	1/1	0.96	0.18	47,47,47,47	0
54	MG	1a	1642	1/1	0.96	0.16	56,56,56,56	0
54	MG	1A	3227	1/1	0.96	0.13	35,35,35,35	0
54	MG	1A	3080	1/1	0.96	0.25	44,44,44,44	0
54	MG	1A	3081	1/1	0.96	0.13	54,54,54,54	0
54	MG	1A	3048	1/1	0.96	0.21	47,47,47,47	0
54	MG	2A	3537	1/1	0.96	0.09	46,46,46,46	0
54	MG	2B	216	1/1	0.96	0.12	64,64,64,64	0
54	MG	2A	3170	1/1	0.96	0.14	69,69,69,69	0
54	MG	2A	3540	1/1	0.96	0.06	44,44,44,44	0
54	MG	2A	3171	1/1	0.96	0.14	56,56,56,56	0
54	MG	2D	304	1/1	0.96	0.22	44,44,44,44	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	2A	3543	1/1	0.96	0.06	56,56,56,56	0
54	MG	2A	3356	1/1	0.96	0.10	66,66,66,66	0
54	MG	1A	3183	1/1	0.96	0.10	64,64,64,64	0
54	MG	2A	3359	1/1	0.96	0.07	55,55,55,55	0
54	MG	2A	3548	1/1	0.96	0.10	56,56,56,56	0
54	MG	1A	3355	1/1	0.96	0.06	18,18,18,18	0
54	MG	2A	3005	1/1	0.96	0.10	55,55,55,55	0
54	MG	2A	3006	1/1	0.96	0.15	50,50,50,50	0
54	MG	2A	3176	1/1	0.96	0.12	48,48,48,48	0
54	MG	1A	3481	1/1	0.96	0.07	34,34,34,34	0
54	MG	1A	3044	1/1	0.96	0.04	33,33,33,33	0
54	MG	2a	3179	1/1	0.96	0.08	82,82,82,82	0
54	MG	1G	203	1/1	0.96	0.13	50,50,50,50	0
54	MG	2a	3181	1/1	0.96	0.14	57,57,57,57	0
54	MG	2A	3013	1/1	0.96	0.06	22,22,22,22	0
54	MG	1A	3119	1/1	0.96	0.12	58,58,58,58	0
54	MG	1H	202	1/1	0.96	0.10	54,54,54,54	0
54	MG	2A	3562	1/1	0.96	0.08	42,42,42,42	0
54	MG	1N	201	1/1	0.96	0.14	43,43,43,43	0
54	MG	2O	3701	1/1	0.96	0.13	64,64,64,64	0
54	MG	2A	3018	1/1	0.96	0.21	46,46,46,46	0
54	MG	2A	3019	1/1	0.96	0.25	50,50,50,50	0
55	A1AE1	1A	3996	76/76	0.96	0.09	21,36,46,56	0
54	MG	1A	3824	1/1	0.96	0.16	38,38,38,38	0
54	MG	1A	3156	1/1	0.96	0.06	43,43,43,43	0
54	MG	1A	3419	1/1	0.96	0.10	46,46,46,46	0
54	MG	2A	3572	1/1	0.96	0.08	54,54,54,54	0
54	MG	2T	201	1/1	0.96	0.28	65,65,65,65	0
54	MG	1A	3187	1/1	0.96	0.17	41,41,41,41	0
54	MG	2A	3026	1/1	0.96	0.09	56,56,56,56	0
54	MG	1A	3240	1/1	0.96	0.10	52,52,52,52	0
54	MG	1A	3831	1/1	0.96	0.06	57,57,57,57	0
54	MG	2A	3178	1/1	0.97	0.14	54,54,54,54	0
54	MG	1A	3531	1/1	0.97	0.07	41,41,41,41	0
54	MG	1A	3604	1/1	0.97	0.08	23,23,23,23	0
54	MG	1a	1613	1/1	0.97	0.07	66,66,66,66	0
54	MG	1a	1614	1/1	0.97	0.07	62,62,62,62	0
54	MG	1A	3046	1/1	0.97	0.14	42,42,42,42	0
54	MG	2A	3009	1/1	0.97	0.09	46,46,46,46	0
54	MG	1A	3022	1/1	0.97	0.09	46,46,46,46	0
54	MG	2A	3011	1/1	0.97	0.05	35,35,35,35	0
54	MG	1A	3229	1/1	0.97	0.13	43,43,43,43	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	1A	3907	1/1	0.97	0.07	30,30,30,30	0
54	MG	1A	3908	1/1	0.97	0.06	38,38,38,38	0
54	MG	2A	3582	1/1	0.97	0.05	49,49,49,49	0
54	MG	1A	3609	1/1	0.97	0.18	63,63,63,63	0
54	MG	1A	3230	1/1	0.97	0.07	36,36,36,36	0
54	MG	1A	3404	1/1	0.97	0.08	36,36,36,36	0
54	MG	1a	1624	1/1	0.97	0.09	47,47,47,47	0
54	MG	2A	3021	1/1	0.97	0.06	40,40,40,40	0
54	MG	2A	3389	1/1	0.97	0.12	43,43,43,43	0
54	MG	1A	3794	1/1	0.97	0.17	34,34,34,34	0
54	MG	1a	1626	1/1	0.97	0.07	52,52,52,52	0
54	MG	1A	3099	1/1	0.97	0.10	34,34,34,34	0
54	MG	1D	302	1/1	0.97	0.07	43,43,43,43	0
54	MG	2a	3010	1/1	0.97	0.06	55,55,55,55	0
54	MG	1A	3914	1/1	0.97	0.05	31,31,31,31	0
54	MG	1D	305	1/1	0.97	0.13	46,46,46,46	0
54	MG	1D	307	1/1	0.97	0.06	42,42,42,42	0
54	MG	1A	3189	1/1	0.97	0.20	43,43,43,43	0
54	MG	1a	1633	1/1	0.97	0.13	50,50,50,50	0
54	MG	1D	310	1/1	0.97	0.14	33,33,33,33	0
54	MG	2A	3035	1/1	0.97	0.15	50,50,50,50	0
54	MG	1A	3917	1/1	0.97	0.10	52,52,52,52	0
54	MG	2A	3208	1/1	0.97	0.31	46,46,46,46	0
54	MG	1A	3288	1/1	0.97	0.18	37,37,37,37	0
54	MG	1A	3348	1/1	0.97	0.12	38,38,38,38	0
54	MG	1A	3617	1/1	0.97	0.07	40,40,40,40	0
54	MG	1D	315	1/1	0.97	0.07	60,60,60,60	0
54	MG	2a	3025	1/1	0.97	0.12	56,56,56,56	0
54	MG	2a	3026	1/1	0.97	0.17	64,64,64,64	0
54	MG	2A	3615	1/1	0.97	0.07	64,64,64,64	0
54	MG	1A	3349	1/1	0.97	0.07	24,24,24,24	0
54	MG	1A	3127	1/1	0.97	0.19	40,40,40,40	0
54	MG	2A	3215	1/1	0.97	0.09	64,64,64,64	0
54	MG	1E	303	1/1	0.97	0.25	45,45,45,45	0
54	MG	2A	3045	1/1	0.97	0.06	41,41,41,41	0
54	MG	1A	3803	1/1	0.97	0.07	56,56,56,56	0
54	MG	1A	3474	1/1	0.97	0.07	32,32,32,32	0
54	MG	1A	3023	1/1	0.97	0.12	38,38,38,38	0
54	MG	1A	3711	1/1	0.97	0.06	49,49,49,49	0
54	MG	1a	1647	1/1	0.97	0.18	50,50,50,50	0
54	MG	1A	3235	1/1	0.97	0.21	30,30,30,30	0
54	MG	2A	3227	1/1	0.97	0.34	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	1789	1/1	0.97	0.07	73,73,73,73	0
54	MG	1E	311	1/1	0.97	0.13	64,64,64,64	0
54	MG	1F	302	1/1	0.97	0.15	39,39,39,39	0
54	MG	1a	1652	1/1	0.97	0.08	50,50,50,50	0
54	MG	1A	3928	1/1	0.97	0.09	51,51,51,51	0
54	MG	1F	306	1/1	0.97	0.15	43,43,43,43	0
54	MG	2A	3425	1/1	0.97	0.08	65,65,65,65	0
54	MG	1A	3192	1/1	0.97	0.21	45,45,45,45	0
54	MG	2A	3060	1/1	0.97	0.08	54,54,54,54	0
54	MG	2A	3061	1/1	0.97	0.05	31,31,31,31	0
54	MG	1A	3547	1/1	0.97	0.07	39,39,39,39	0
54	MG	1A	3026	1/1	0.97	0.27	39,39,39,39	0
54	MG	1A	3104	1/1	0.97	0.20	33,33,33,33	0
54	MG	2A	3065	1/1	0.97	0.17	45,45,45,45	0
54	MG	1A	3717	1/1	0.97	0.04	23,23,23,23	0
54	MG	1A	3935	1/1	0.97	0.07	54,54,54,54	0
54	MG	1A	3105	1/1	0.97	0.12	43,43,43,43	0
54	MG	2A	3069	1/1	0.97	0.09	53,53,53,53	0
54	MG	1A	3719	1/1	0.97	0.10	57,57,57,57	0
54	MG	2a	3060	1/1	0.97	0.17	62,62,62,62	0
54	MG	1G	201	1/1	0.97	0.07	64,64,64,64	0
54	MG	1A	3243	1/1	0.97	0.11	41,41,41,41	0
54	MG	1A	3016	1/1	0.97	0.27	36,36,36,36	0
54	MG	2A	3074	1/1	0.97	0.04	40,40,40,40	0
54	MG	1G	204	1/1	0.97	0.10	58,58,58,58	0
54	MG	1A	3484	1/1	0.97	0.05	52,52,52,52	0
54	MG	1A	3555	1/1	0.97	0.08	22,22,22,22	0
54	MG	1A	3726	1/1	0.97	0.12	35,35,35,35	0
54	MG	2A	3447	1/1	0.97	0.08	36,36,36,36	0
54	MG	1A	3823	1/1	0.97	0.06	60,60,60,60	0
54	MG	1A	3246	1/1	0.97	0.21	44,44,44,44	0
54	MG	1A	3486	1/1	0.97	0.06	24,24,24,24	0
54	MG	1A	3082	1/1	0.97	0.09	54,54,54,54	0
54	MG	1A	3827	1/1	0.97	0.07	44,44,44,44	0
54	MG	1A	3828	1/1	0.97	0.04	46,46,46,46	0
54	MG	2a	3076	1/1	0.97	0.24	51,51,51,51	0
54	MG	2A	3263	1/1	0.97	0.18	58,58,58,58	0
54	MG	2A	3085	1/1	0.97	0.08	47,47,47,47	0
54	MG	1A	3636	1/1	0.97	0.07	54,54,54,54	0
54	MG	1A	3731	1/1	0.97	0.12	52,52,52,52	0
54	MG	1A	3637	1/1	0.97	0.08	60,60,60,60	0
54	MG	2A	3269	1/1	0.97	0.07	46,46,46,46	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	1A	3422	1/1	0.97	0.05	42,42,42,42	0
54	MG	1A	3200	1/1	0.97	0.18	32,32,32,32	0
54	MG	1A	3138	1/1	0.97	0.12	49,49,49,49	0
54	MG	1A	3563	1/1	0.97	0.07	26,26,26,26	0
54	MG	1A	3957	1/1	0.97	0.14	40,40,40,40	0
54	MG	1A	3030	1/1	0.97	0.09	50,50,50,50	0
54	MG	2A	3676	1/1	0.97	0.14	47,47,47,47	0
54	MG	1a	1828	1/1	0.97	0.07	48,48,48,48	0
54	MG	1A	3838	1/1	0.97	0.09	50,50,50,50	0
54	MG	2A	3278	1/1	0.97	0.07	41,41,41,41	0
54	MG	1A	3112	1/1	0.97	0.13	43,43,43,43	0
54	MG	1A	3206	1/1	0.97	0.17	46,46,46,46	0
54	MG	1A	3142	1/1	0.97	0.15	49,49,49,49	0
54	MG	2A	3103	1/1	0.97	0.07	49,49,49,49	0
54	MG	2A	3104	1/1	0.97	0.27	54,54,54,54	0
54	MG	2A	3284	1/1	0.97	0.04	51,51,51,51	0
54	MG	2A	3285	1/1	0.97	0.09	22,22,22,22	0
54	MG	1A	3260	1/1	0.97	0.10	33,33,33,33	0
54	MG	1U	202	1/1	0.97	0.17	42,42,42,42	0
54	MG	1A	3208	1/1	0.97	0.26	42,42,42,42	0
54	MG	1V	201	1/1	0.97	0.24	36,36,36,36	0
54	MG	1V	202	1/1	0.97	0.24	36,36,36,36	0
54	MG	2A	3110	1/1	0.97	0.32	44,44,44,44	0
54	MG	2A	3111	1/1	0.97	0.15	46,46,46,46	0
54	MG	1A	3571	1/1	0.97	0.08	51,51,51,51	0
54	MG	1A	3086	1/1	0.97	0.21	40,40,40,40	0
54	MG	1A	3847	1/1	0.97	0.09	31,31,31,31	0
54	MG	1A	3652	1/1	0.97	0.17	49,49,49,49	0
54	MG	2A	3300	1/1	0.97	0.08	41,41,41,41	0
54	MG	1A	3653	1/1	0.97	0.10	47,47,47,47	0
54	MG	2A	3700	1/1	0.97	0.17	61,61,61,61	0
54	MG	1a	1844	1/1	0.97	0.17	60,60,60,60	0
54	MG	1A	3263	1/1	0.97	0.23	49,49,49,49	0
54	MG	1A	3087	1/1	0.97	0.27	41,41,41,41	0
54	MG	1A	3088	1/1	0.97	0.07	43,43,43,43	0
54	MG	2A	3122	1/1	0.97	0.07	42,42,42,42	0
54	MG	1A	3374	1/1	0.97	0.07	40,40,40,40	0
54	MG	2A	3309	1/1	0.97	0.17	65,65,65,65	0
54	MG	1A	3505	1/1	0.97	0.08	28,28,28,28	0
54	MG	1A	3375	1/1	0.97	0.06	37,37,37,37	0
54	MG	1A	3977	1/1	0.97	0.21	46,46,46,46	0
54	MG	2A	3128	1/1	0.97	0.15	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	3319	1/1	0.97	0.12	32,32,32,32	0
54	MG	2A	3130	1/1	0.97	0.15	43,43,43,43	0
54	MG	2a	3129	1/1	0.97	0.09	76,76,76,76	0
54	MG	2A	3316	1/1	0.97	0.12	58,58,58,58	0
54	MG	1A	3859	1/1	0.97	0.04	41,41,41,41	0
54	MG	2A	3318	1/1	0.97	0.07	50,50,50,50	0
54	MG	1A	3661	1/1	0.97	0.06	64,64,64,64	0
54	MG	2a	3137	1/1	0.97	0.14	54,54,54,54	0
54	MG	2A	3133	1/1	0.97	0.07	44,44,44,44	0
54	MG	1a	1710	1/1	0.97	0.14	63,63,63,63	0
54	MG	2a	3140	1/1	0.97	0.06	72,72,72,72	0
54	MG	2A	3720	1/1	0.97	0.07	70,70,70,70	0
54	MG	1A	3441	1/1	0.97	0.04	27,27,27,27	0
54	MG	2a	3143	1/1	0.97	0.07	61,61,61,61	0
54	MG	1a	1857	1/1	0.97	0.14	66,66,66,66	0
54	MG	1A	3018	1/1	0.97	0.18	30,30,30,30	0
54	MG	1A	3983	1/1	0.97	0.23	41,41,41,41	0
54	MG	2a	3147	1/1	0.97	0.08	77,77,77,77	0
54	MG	2A	3516	1/1	0.97	0.06	77,77,77,77	0
54	MG	1A	3055	1/1	0.97	0.04	49,49,49,49	0
54	MG	1a	1861	1/1	0.97	0.07	78,78,78,78	0
54	MG	2A	3142	1/1	0.97	0.15	48,48,48,48	0
54	MG	1A	3666	1/1	0.97	0.05	61,61,61,61	0
54	MG	2A	3144	1/1	0.97	0.24	44,44,44,44	0
54	MG	1A	3762	1/1	0.97	0.07	36,36,36,36	0
54	MG	1A	3268	1/1	0.97	0.07	36,36,36,36	0
54	MG	2A	3524	1/1	0.97	0.04	24,24,24,24	0
54	MG	2A	3525	1/1	0.97	0.06	61,61,61,61	0
54	MG	1A	3380	1/1	0.97	0.06	41,41,41,41	0
54	MG	1A	3514	1/1	0.97	0.05	33,33,33,33	0
54	MG	1A	3990	1/1	0.97	0.08	50,50,50,50	0
54	MG	1A	3218	1/1	0.97	0.11	40,40,40,40	0
54	MG	2A	3339	1/1	0.97	0.06	48,48,48,48	0
54	MG	1A	3325	1/1	0.97	0.11	30,30,30,30	0
54	MG	15	102	1/1	0.97	0.07	45,45,45,45	0
54	MG	2A	3533	1/1	0.97	0.10	37,37,37,37	0
54	MG	1A	3181	1/1	0.97	0.18	45,45,45,45	0
54	MG	15	104	1/1	0.97	0.27	39,39,39,39	0
54	MG	15	105	1/1	0.97	0.21	46,46,46,46	0
54	MG	2A	3538	1/1	0.97	0.06	48,48,48,48	0
54	MG	1A	3674	1/1	0.97	0.19	52,52,52,52	0
54	MG	2D	306	1/1	0.97	0.07	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	3384	1/1	0.97	0.10	31,31,31,31	0
54	MG	2A	3541	1/1	0.97	0.05	59,59,59,59	0
54	MG	1A	3590	1/1	0.97	0.23	35,35,35,35	0
54	MG	1A	3881	1/1	0.97	0.04	20,20,20,20	0
54	MG	1A	3020	1/1	0.97	0.27	44,44,44,44	0
54	MG	1A	3153	1/1	0.97	0.21	42,42,42,42	0
54	MG	2E	301	1/1	0.97	0.19	44,44,44,44	0
54	MG	2A	3352	1/1	0.97	0.12	33,33,33,33	0
54	MG	1A	3073	1/1	0.97	0.14	50,50,50,50	0
54	MG	1A	3332	1/1	0.97	0.08	38,38,38,38	0
54	MG	18	101	1/1	0.97	0.10	43,43,43,43	0
54	MG	1A	3034	1/1	0.97	0.13	44,44,44,44	0
54	MG	1a	1739	1/1	0.97	0.06	56,56,56,56	0
54	MG	2A	3554	1/1	0.97	0.06	41,41,41,41	0
54	MG	1A	3279	1/1	0.97	0.17	46,46,46,46	0
54	MG	1A	3891	1/1	0.97	0.07	56,56,56,56	0
54	MG	1A	3280	1/1	0.97	0.07	51,51,51,51	0
54	MG	1A	3281	1/1	0.97	0.17	44,44,44,44	0
54	MG	1B	211	1/1	0.97	0.12	42,42,42,42	0
54	MG	1A	3895	1/1	0.97	0.06	35,35,35,35	0
54	MG	1A	3528	1/1	0.97	0.05	23,23,23,23	0
54	MG	1A	3338	1/1	0.97	0.07	30,30,30,30	0
54	MG	2A	3564	1/1	0.97	0.09	61,61,61,61	0
54	MG	1A	3782	1/1	0.97	0.15	48,48,48,48	0
54	MG	1B	216	1/1	0.97	0.10	54,54,54,54	0
54	MG	2A	3568	1/1	0.97	0.07	33,33,33,33	0
54	MG	1A	3530	1/1	0.97	0.05	39,39,39,39	0
58	ZN	2Y	501	1/1	0.97	0.05	91,91,91,91	0
58	ZN	24	501	1/1	0.97	0.15	122,122,122,122	0
54	MG	1F	310	1/1	0.98	0.08	35,35,35,35	0
54	MG	1A	3559	1/1	0.98	0.09	38,38,38,38	0
54	MG	2A	3307	1/1	0.98	0.04	30,30,30,30	0
54	MG	2A	3007	1/1	0.98	0.04	39,39,39,39	0
54	MG	1A	3067	1/1	0.98	0.04	39,39,39,39	0
54	MG	1A	3006	1/1	0.98	0.05	30,30,30,30	0
54	MG	1A	3124	1/1	0.98	0.23	41,41,41,41	0
54	MG	1A	3214	1/1	0.98	0.19	35,35,35,35	0
54	MG	1A	3340	1/1	0.98	0.06	57,57,57,57	0
54	MG	1A	3736	1/1	0.98	0.09	43,43,43,43	0
54	MG	2a	3032	1/1	0.98	0.13	38,38,38,38	0
54	MG	1A	3834	1/1	0.98	0.08	32,32,32,32	0
54	MG	2A	3479	1/1	0.98	0.05	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	3015	1/1	0.98	0.14	34,34,34,34	0
54	MG	1A	3646	1/1	0.98	0.04	52,52,52,52	0
54	MG	1A	3488	1/1	0.98	0.06	46,46,46,46	0
54	MG	1a	1648	1/1	0.98	0.15	52,52,52,52	0
54	MG	1A	3051	1/1	0.98	0.17	38,38,38,38	0
54	MG	2A	3020	1/1	0.98	0.10	44,44,44,44	0
54	MG	2A	3660	1/1	0.98	0.06	51,51,51,51	0
54	MG	1A	3277	1/1	0.98	0.06	34,34,34,34	0
54	MG	1A	3216	1/1	0.98	0.16	37,37,37,37	0
54	MG	1A	3015	1/1	0.98	0.12	48,48,48,48	0
54	MG	1A	3345	1/1	0.98	0.06	27,27,27,27	0
54	MG	1A	3095	1/1	0.98	0.24	36,36,36,36	0
54	MG	1A	3129	1/1	0.98	0.04	46,46,46,46	0
54	MG	2A	3027	1/1	0.98	0.06	33,33,33,33	0
54	MG	2A	3329	1/1	0.98	0.07	29,29,29,29	0
54	MG	2A	3028	1/1	0.98	0.11	42,42,42,42	0
54	MG	1A	3418	1/1	0.98	0.04	17,17,17,17	0
54	MG	1P	203	1/1	0.98	0.03	35,35,35,35	0
54	MG	1A	3071	1/1	0.98	0.22	37,37,37,37	0
54	MG	2A	3334	1/1	0.98	0.08	35,35,35,35	0
54	MG	1A	3222	1/1	0.98	0.25	38,38,38,38	0
54	MG	1A	3499	1/1	0.98	0.08	27,27,27,27	0
54	MG	1A	3849	1/1	0.98	0.07	44,44,44,44	0
54	MG	1A	3750	1/1	0.98	0.06	47,47,47,47	0
54	MG	2A	3037	1/1	0.98	0.06	40,40,40,40	0
54	MG	1A	3500	1/1	0.98	0.05	28,28,28,28	0
54	MG	1A	3131	1/1	0.98	0.08	35,35,35,35	0
54	MG	1A	3225	1/1	0.98	0.24	36,36,36,36	0
54	MG	1A	3352	1/1	0.98	0.04	19,19,19,19	0
54	MG	1A	3969	1/1	0.98	0.03	57,57,57,57	0
54	MG	1A	3097	1/1	0.98	0.23	40,40,40,40	0
54	MG	1A	3664	1/1	0.98	0.12	29,29,29,29	0
54	MG	1A	3857	1/1	0.98	0.15	37,37,37,37	0
54	MG	1A	3072	1/1	0.98	0.12	38,38,38,38	0
54	MG	1A	3038	1/1	0.98	0.14	44,44,44,44	0
54	MG	1A	3759	1/1	0.98	0.05	47,47,47,47	0
54	MG	1a	1804	1/1	0.98	0.06	72,72,72,72	0
54	MG	1A	3865	1/1	0.98	0.07	46,46,46,46	0
54	MG	1U	203	1/1	0.98	0.24	32,32,32,32	0
54	MG	2A	3196	1/1	0.98	0.28	50,50,50,50	0
54	MG	1U	204	1/1	0.98	0.22	41,41,41,41	0
54	MG	1A	3074	1/1	0.98	0.14	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	3291	1/1	0.98	0.22	43,43,43,43	0
54	MG	1A	3292	1/1	0.98	0.10	49,49,49,49	0
54	MG	1A	3510	1/1	0.98	0.04	41,41,41,41	0
54	MG	2A	3057	1/1	0.98	0.09	43,43,43,43	0
54	MG	1A	3101	1/1	0.98	0.11	35,35,35,35	0
54	MG	1a	1813	1/1	0.98	0.04	67,67,67,67	0
54	MG	1A	3028	1/1	0.98	0.24	36,36,36,36	0
54	MG	1A	3140	1/1	0.98	0.23	33,33,33,33	0
54	MG	1A	3103	1/1	0.98	0.17	38,38,38,38	0
54	MG	1A	3040	1/1	0.98	0.09	38,38,38,38	0
54	MG	1W	203	1/1	0.98	0.13	41,41,41,41	0
54	MG	1A	3594	1/1	0.98	0.22	36,36,36,36	0
54	MG	1a	1688	1/1	0.98	0.13	46,46,46,46	0
54	MG	1A	3298	1/1	0.98	0.06	33,33,33,33	0
54	MG	2A	3536	1/1	0.98	0.04	58,58,58,58	0
54	MG	1A	3029	1/1	0.98	0.19	43,43,43,43	0
54	MG	1A	3145	1/1	0.98	0.23	36,36,36,36	0
54	MG	1A	3681	1/1	0.98	0.22	44,44,44,44	0
54	MG	1A	3078	1/1	0.98	0.25	34,34,34,34	0
54	MG	1A	3882	1/1	0.98	0.04	43,43,43,43	0
54	MG	2a	3097	1/1	0.98	0.05	67,67,67,67	0
54	MG	1A	3147	1/1	0.98	0.11	37,37,37,37	0
54	MG	1A	3239	1/1	0.98	0.15	47,47,47,47	0
54	MG	1A	3885	1/1	0.98	0.06	54,54,54,54	0
54	MG	2A	3221	1/1	0.98	0.15	41,41,41,41	0
54	MG	2A	3546	1/1	0.98	0.14	49,49,49,49	0
54	MG	2A	3222	1/1	0.98	0.09	43,43,43,43	0
54	MG	2A	3223	1/1	0.98	0.11	24,24,24,24	0
54	MG	1A	3021	1/1	0.98	0.11	40,40,40,40	0
54	MG	1A	3242	1/1	0.98	0.23	39,39,39,39	0
54	MG	1A	3149	1/1	0.98	0.07	35,35,35,35	0
54	MG	1A	3889	1/1	0.98	0.05	64,64,64,64	0
54	MG	1A	3058	1/1	0.98	0.07	36,36,36,36	0
54	MG	2A	3229	1/1	0.98	0.17	61,61,61,61	0
54	MG	1A	3690	1/1	0.98	0.04	38,38,38,38	0
54	MG	1A	3110	1/1	0.98	0.23	43,43,43,43	0
54	MG	1A	3309	1/1	0.98	0.10	32,32,32,32	0
54	MG	11	105	1/1	0.98	0.05	37,37,37,37	0
54	MG	1A	3310	1/1	0.98	0.15	44,44,44,44	0
54	MG	2A	3086	1/1	0.98	0.11	47,47,47,47	0
54	MG	2A	3236	1/1	0.98	0.10	52,52,52,52	0
54	MG	13	101	1/1	0.98	0.15	41,41,41,41	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	1A	3013	1/1	0.98	0.08	24,24,24,24	0
54	MG	1A	3786	1/1	0.98	0.07	37,37,37,37	0
54	MG	1A	3787	1/1	0.98	0.10	50,50,50,50	0
54	MG	2A	3091	1/1	0.98	0.06	49,49,49,49	0
54	MG	2A	3092	1/1	0.98	0.06	33,33,33,33	0
54	MG	1A	3899	1/1	0.98	0.08	53,53,53,53	0
54	MG	1A	3195	1/1	0.98	0.16	44,44,44,44	0
54	MG	1A	3901	1/1	0.98	0.06	70,70,70,70	0
54	MG	2D	301	1/1	0.98	0.15	41,41,41,41	0
54	MG	2D	302	1/1	0.98	0.11	55,55,55,55	0
54	MG	1A	3251	1/1	0.98	0.20	49,49,49,49	0
54	MG	2a	3131	1/1	0.98	0.04	77,77,77,77	0
54	MG	1A	3697	1/1	0.98	0.06	30,30,30,30	0
54	MG	1A	3314	1/1	0.98	0.08	32,32,32,32	0
54	MG	1A	3613	1/1	0.98	0.08	33,33,33,33	0
54	MG	17	101	1/1	0.98	0.08	38,38,38,38	0
54	MG	1A	3700	1/1	0.98	0.05	49,49,49,49	0
54	MG	1A	3252	1/1	0.98	0.07	44,44,44,44	0
54	MG	1A	3032	1/1	0.98	0.07	39,39,39,39	0
54	MG	1B	223	1/1	0.98	0.05	43,43,43,43	0
54	MG	1a	1724	1/1	0.98	0.10	49,49,49,49	0
54	MG	2A	3584	1/1	0.98	0.05	43,43,43,43	0
54	MG	2E	302	1/1	0.98	0.07	54,54,54,54	0
54	MG	1A	3083	1/1	0.98	0.05	40,40,40,40	0
54	MG	2A	3587	1/1	0.98	0.05	57,57,57,57	0
54	MG	1A	3017	1/1	0.98	0.30	33,33,33,33	0
54	MG	1A	3798	1/1	0.98	0.07	38,38,38,38	0
54	MG	1A	3024	1/1	0.98	0.06	24,24,24,24	0
54	MG	1A	3257	1/1	0.98	0.18	47,47,47,47	0
54	MG	1A	3258	1/1	0.98	0.05	37,37,37,37	0
54	MG	1A	3388	1/1	0.98	0.08	23,23,23,23	0
54	MG	1A	3916	1/1	0.98	0.05	25,25,25,25	0
54	MG	1A	3709	1/1	0.98	0.06	35,35,35,35	0
54	MG	1A	3389	1/1	0.98	0.09	27,27,27,27	0
54	MG	2A	3599	1/1	0.98	0.05	24,24,24,24	0
54	MG	2A	3600	1/1	0.98	0.06	55,55,55,55	0
54	MG	1D	304	1/1	0.98	0.05	41,41,41,41	0
54	MG	2A	3602	1/1	0.98	0.04	44,44,44,44	0
54	MG	2A	3268	1/1	0.98	0.14	38,38,38,38	0
54	MG	1A	3025	1/1	0.98	0.21	38,38,38,38	0
54	MG	1D	306	1/1	0.98	0.10	20,20,20,20	0
54	MG	2A	3119	1/1	0.98	0.07	36,36,36,36	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	1A	3049	1/1	0.98	0.17	34,34,34,34	0
54	MG	1A	3392	1/1	0.98	0.08	27,27,27,27	0
54	MG	1a	1612	1/1	0.98	0.13	31,31,31,31	0
54	MG	2A	3610	1/1	0.98	0.04	64,64,64,64	0
54	MG	1A	3808	1/1	0.98	0.03	37,37,37,37	0
54	MG	1A	3203	1/1	0.98	0.15	41,41,41,41	0
54	MG	1A	3204	1/1	0.98	0.07	40,40,40,40	0
54	MG	1A	3159	1/1	0.98	0.16	36,36,36,36	0
54	MG	2A	3127	1/1	0.98	0.18	36,36,36,36	0
54	MG	1A	3089	1/1	0.98	0.04	19,19,19,19	0
54	MG	1A	3630	1/1	0.98	0.06	32,32,32,32	0
54	MG	2A	3618	1/1	0.98	0.04	43,43,43,43	0
54	MG	1A	3330	1/1	0.98	0.07	33,33,33,33	0
54	MG	1A	3816	1/1	0.98	0.07	45,45,45,45	0
54	MG	27	103	1/1	0.98	0.11	43,43,43,43	0
54	MG	1a	1750	1/1	0.98	0.06	63,63,63,63	0
54	MG	1E	302	1/1	0.98	0.07	39,39,39,39	0
54	MG	1A	3720	1/1	0.98	0.06	43,43,43,43	0
54	MG	1A	3120	1/1	0.98	0.03	38,38,38,38	0
54	MG	2A	3136	1/1	0.98	0.08	40,40,40,40	0
54	MG	1A	3400	1/1	0.98	0.06	44,44,44,44	0
54	MG	1E	307	1/1	0.98	0.05	46,46,46,46	0
54	MG	2A	3292	1/1	0.98	0.11	45,45,45,45	0
54	MG	1A	3933	1/1	0.98	0.05	31,31,31,31	0
54	MG	1A	3065	1/1	0.98	0.28	38,38,38,38	0
54	MG	1A	3209	1/1	0.98	0.25	36,36,36,36	0
54	MG	1A	3725	1/1	0.98	0.04	29,29,29,29	0
54	MG	2A	3297	1/1	0.98	0.05	43,43,43,43	0
54	MG	1A	3334	1/1	0.98	0.13	45,45,45,45	0
54	MG	1F	303	1/1	0.98	0.17	37,37,37,37	0
54	MG	2a	3015	1/1	0.98	0.10	48,48,48,48	0
54	MG	1A	3167	1/1	0.98	0.10	38,38,38,38	0
54	MG	1A	3482	1/1	0.98	0.09	27,27,27,27	0
54	MG	1F	307	1/1	0.98	0.16	29,29,29,29	0
54	MG	1A	3639	1/1	0.98	0.08	39,39,39,39	0
58	ZN	14	501	1/1	0.98	0.07	110,110,110,110	0
54	MG	2A	3465	1/1	0.98	0.05	39,39,39,39	0
54	MG	2A	3004	1/1	0.98	0.04	39,39,39,39	0
58	ZN	25	102	1/1	0.98	0.03	69,69,69,69	0
58	ZN	29	501	1/1	0.98	0.04	71,71,71,71	0
58	ZN	2n	501	1/1	0.98	0.05	90,90,90,90	0
59	SF4	1d	306	8/8	0.98	0.06	64,69,73,76	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
59	SF4	2d	501	8/8	0.98	0.06	68,78,83,88	0
54	MG	1E	304	1/1	0.99	0.14	36,36,36,36	0
54	MG	1A	3893	1/1	0.99	0.05	58,58,58,58	0
54	MG	1A	3394	1/1	0.99	0.05	24,24,24,24	0
54	MG	2E	305	1/1	0.99	0.10	42,42,42,42	0
54	MG	1A	3844	1/1	0.99	0.08	43,43,43,43	0
54	MG	1A	3667	1/1	0.99	0.03	43,43,43,43	0
54	MG	1A	3465	1/1	0.99	0.10	50,50,50,50	0
54	MG	1A	3135	1/1	0.99	0.06	36,36,36,36	0
54	MG	2a	3132	1/1	0.99	0.06	70,70,70,70	0
54	MG	1A	3428	1/1	0.99	0.05	15,15,15,15	0
54	MG	2a	3134	1/1	0.99	0.10	54,54,54,54	0
54	MG	2F	304	1/1	0.99	0.22	48,48,48,48	0
54	MG	1F	301	1/1	0.99	0.15	33,33,33,33	0
54	MG	1a	1621	1/1	0.99	0.03	53,53,53,53	0
54	MG	1A	3005	1/1	0.99	0.08	25,25,25,25	0
54	MG	1A	3066	1/1	0.99	0.10	34,34,34,34	0
54	MG	1F	304	1/1	0.99	0.13	38,38,38,38	0
54	MG	1A	3042	1/1	0.99	0.04	23,23,23,23	0
54	MG	1A	3126	1/1	0.99	0.25	32,32,32,32	0
54	MG	1A	3433	1/1	0.99	0.03	28,28,28,28	0
54	MG	1F	308	1/1	0.99	0.10	38,38,38,38	0
54	MG	1A	3009	1/1	0.99	0.11	35,35,35,35	0
54	MG	1A	3003	1/1	0.99	0.03	27,27,27,27	0
54	MG	1A	3402	1/1	0.99	0.04	31,31,31,31	0
54	MG	1A	3084	1/1	0.99	0.11	40,40,40,40	0
54	MG	2a	3149	1/1	0.99	0.04	56,56,56,56	0
54	MG	1A	3554	1/1	0.99	0.12	49,49,49,49	0
54	MG	1A	3109	1/1	0.99	0.12	39,39,39,39	0
54	MG	2A	3471	1/1	0.99	0.07	51,51,51,51	0
54	MG	1A	3860	1/1	0.99	0.03	46,46,46,46	0
54	MG	1B	217	1/1	0.99	0.04	47,47,47,47	0
54	MG	1A	3861	1/1	0.99	0.11	49,49,49,49	0
54	MG	2A	3549	1/1	0.99	0.06	37,37,37,37	0
54	MG	2A	3262	1/1	0.99	0.35	45,45,45,45	0
54	MG	1A	3144	1/1	0.99	0.08	37,37,37,37	0
54	MG	1A	3864	1/1	0.99	0.07	32,32,32,32	0
54	MG	1A	3517	1/1	0.99	0.03	25,25,25,25	0
54	MG	1A	3684	1/1	0.99	0.02	42,42,42,42	0
54	MG	1A	3440	1/1	0.99	0.07	33,33,33,33	0
54	MG	2A	3481	1/1	0.99	0.04	39,39,39,39	0
54	MG	1A	3019	1/1	0.99	0.21	31,31,31,31	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	1A	3160	1/1	0.99	0.15	30,30,30,30	0
54	MG	15	101	1/1	0.99	0.14	32,32,32,32	0
54	MG	1B	226	1/1	0.99	0.04	62,62,62,62	0
54	MG	1A	3132	1/1	0.99	0.09	23,23,23,23	0
54	MG	2A	3341	1/1	0.99	0.07	41,41,41,41	0
54	MG	1N	204	1/1	0.99	0.02	53,53,53,53	0
54	MG	1A	3162	1/1	0.99	0.18	33,33,33,33	0
54	MG	1P	201	1/1	0.99	0.25	38,38,38,38	0
54	MG	1A	3290	1/1	0.99	0.09	24,24,24,24	0
54	MG	1A	3564	1/1	0.99	0.08	32,32,32,32	0
54	MG	1A	3874	1/1	0.99	0.04	58,58,58,58	0
54	MG	1a	1843	1/1	0.99	0.07	61,61,61,61	0
54	MG	1A	3606	1/1	0.99	0.08	39,39,39,39	0
54	MG	1A	3199	1/1	0.99	0.08	27,27,27,27	0
54	MG	1A	3447	1/1	0.99	0.05	60,60,60,60	0
54	MG	1A	3111	1/1	0.99	0.07	24,24,24,24	0
54	MG	1R	201	1/1	0.99	0.19	51,51,51,51	0
54	MG	1A	3241	1/1	0.99	0.17	36,36,36,36	0
54	MG	2A	3427	1/1	0.99	0.02	36,36,36,36	0
54	MG	2A	3286	1/1	0.99	0.08	65,65,65,65	0
54	MG	1A	3164	1/1	0.99	0.09	32,32,32,32	0
54	MG	2A	3357	1/1	0.99	0.05	43,43,43,43	0
54	MG	1A	3165	1/1	0.99	0.14	33,33,33,33	0
54	MG	1D	308	1/1	0.99	0.17	37,37,37,37	0
54	MG	2A	3361	1/1	0.99	0.07	42,42,42,42	0
54	MG	2A	3585	1/1	0.99	0.06	44,44,44,44	0
54	MG	1A	3324	1/1	0.99	0.09	24,24,24,24	0
54	MG	1A	3223	1/1	0.99	0.15	31,31,31,31	0
54	MG	1A	3245	1/1	0.99	0.07	47,47,47,47	0
54	MG	2A	3589	1/1	0.99	0.05	48,48,48,48	0
54	MG	2A	3590	1/1	0.99	0.10	63,63,63,63	0
54	MG	1A	3007	1/1	0.99	0.06	35,35,35,35	0
54	MG	1A	3328	1/1	0.99	0.10	41,41,41,41	0
54	MG	2A	3029	1/1	0.99	0.04	24,24,24,24	0
54	MG	1a	1793	1/1	0.99	0.04	77,77,77,77	0
58	ZN	1Y	202	1/1	0.99	0.04	62,62,62,62	0
54	MG	1A	3271	1/1	0.99	0.06	24,24,24,24	0
58	ZN	15	110	1/1	0.99	0.03	59,59,59,59	0
58	ZN	16	501	1/1	0.99	0.06	45,45,45,45	0
58	ZN	19	103	1/1	0.99	0.04	46,46,46,46	0
58	ZN	1n	104	1/1	0.99	0.03	65,65,65,65	0
54	MG	2a	3117	1/1	0.99	0.10	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	3459	1/1	0.99	0.04	34,34,34,34	0
54	MG	1A	3272	1/1	0.99	0.10	19,19,19,19	0
58	ZN	26	501	1/1	0.99	0.03	61,61,61,61	0
54	MG	1A	3247	1/1	0.99	0.22	33,33,33,33	0
54	MG	1a	1734	1/1	0.99	0.08	45,45,45,45	0
54	MG	1A	3274	1/1	0.99	0.10	38,38,38,38	0
54	MG	1A	3248	1/1	0.99	0.20	31,31,31,31	0
54	MG	1A	3458	1/1	1.00	0.02	54,54,54,54	0
54	MG	1A	3813	1/1	1.00	0.04	24,24,24,24	0
54	MG	1A	3217	1/1	1.00	0.01	30,30,30,30	0
54	MG	1A	3939	1/1	1.00	0.06	36,36,36,36	0
54	MG	2A	3558	1/1	1.00	0.03	41,41,41,41	0
54	MG	2A	3566	1/1	1.00	0.04	53,53,53,53	0
54	MG	2A	3360	1/1	1.00	0.05	42,42,42,42	0
54	MG	1A	3863	1/1	1.00	0.06	54,54,54,54	0

5.5 Other polymers [i](#)

There are no such residues in this entry.