Full wwPDB X-ray Structure Validation Report ⓘ

Sep 16, 2026 – 07:45 am BST

PDB ID	:	5VP2 / pdb_00005vp2
Title	:	Crystal structure of the Thermus thermophilus 70S ribosome in complex with madumycin II and bound to mRNA and A-, P- and E-site tRNAs at 2.8A resolution
Authors	:	Osterman, I.A.; Khabibullina, N.F.; Komarova, E.S.; Kasatsky, P.; Kartsev, V.G.; Bogdanov, A.A.; Dontsova, O.A.; Konevega, A.L.; Sergiev, P.V.; Polikanov, Y.S.
Deposited on	:	2017-05-04
Resolution	:	2.80 Å(reported)

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

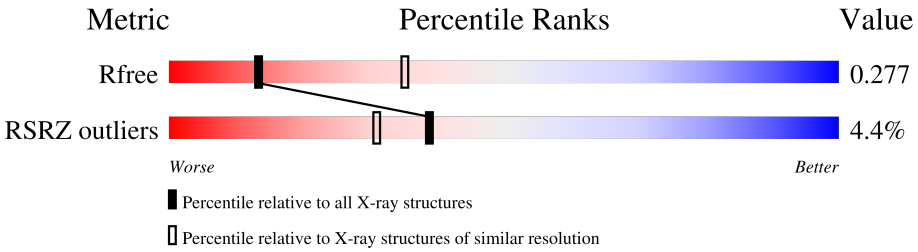
MolProbity	:	FAILED
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.015 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	3866 (2.80-2.80)
RSRZ outliers	180081	3869 (2.80-2.80)

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

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
56	MG	2A	3084	-	-	-	X
56	MG	2A	3204	-	-	-	X

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

2 Entry composition (i)

There are 61 unique types of molecules in this entry. The entry contains 300935 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	2871	Total	C	N	O	P	0	0	0
			61852	27531	11572	19878	2871			
1	2A	2800	Total	C	N	O	P	0	0	0
			60322	26848	11284	19390	2800			

- 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
			2577	1146	476	835	120			
2	2B	120	Total	C	N	O	P	0	0	0
			2575	1146	476	833	120			

- 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
			2136	1349	423	361	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
			1423	913	253	253	4			
6	2G	181	Total	C	N	O	S	0	0	0
			1428	913	258	253	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	174	Total	C	N	O	S	0	0	0
			1330	845	248	236	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	1I	146	Total	C	N	O	S	0	0	0
			1097	701	191	204	1			
8	2I	146	Total	C	N	O	S	0	0	0
			1064	681	186	196	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
			1117	719	207	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 933	C 588	N 171	O 170	S 4	0	0	0

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
14	1S	110	Total 873	C 550	N 174	O 149	0	0	0
14	2S	110	Total 870	C 549	N 173	O 148	0	0	0

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

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

- 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
			771	495	140	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
			806	517	152	131	6			
20	2Y	107	Total	C	N	O	S	0	0	0
			806	517	152	131	6			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
21	1Z	154	Total	C	N	O	S	0	0	0
			1240	795	222	220	3			
21	2Z	160	Total	C	N	O	S	0	0	0
			1271	814	228	227	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
			653	404	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
			755	475	148	131	1			
23	21	97	Total	C	N	O	S	0	0	0
			755	475	148	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
			588	365	118	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
			552	349	99	99	5			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
26	24	69	Total	C	N	O	S	0	0	0
			532	339	97	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
			455	285	89	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	1503	Total	C	N	O	P	0	0	0
			32327	14396	5990	10438	1503			

- 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
			1846	1179	331	331	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
			1548	973	301	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
			1655	1038	326	284	7			
35	2d	208	Total	C	N	O	S	0	0	0
			1674	1050	333	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
			1129	714	213	198	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
			810	514	144	149	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
			1231	766	243	216	6			
38	2g	155	Total	C	N	O	S	0	0	0
			1235	769	244	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
			1088	689	206	191	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
			983	623	193	167			
40	2i	127	Total	C	N	O	0	0	0
			978	619	190	169			

- 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
			709	440	138	131			
41	2j	96	Total	C	N	O	0	0	0
			714	445	138	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
			829	516	155	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	123	Total	C	N	O	S	0	0	0
			958	592	198	166	2			
44	2m	122	Total	C	N	O	S	0	0	0
			950	586	197	165	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
			652	417	120	113	2			
50	2s	83	Total	C	N	O	S	0	0	0
			646	412	119	113	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
			728	446	156	124	2			
51	2t	96	Total	C	N	O	S	0	0	0
			727	446	155	124	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 RNA chain called mRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
53	1v	13	Total	C	N	O	P	0	0	0
			277	125	51	88	13			
53	2v	13	Total	C	N	O	P	0	0	0
			277	125	51	88	13			

- Molecule 54 is a RNA chain called A-site and E-site tRNAs.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
54	1w	72	Total	C	N	O	P	S	0	0	0
			1550	694	277	505	72	2			
54	1y	74	Total	C	N	O	P	S	0	0	0
			1585	707	285	518	74	1			
54	2w	69	Total	C	N	O	P	S	0	0	0
			1482	662	267	482	69	2			
54	2y	73	Total	C	N	O	P	S	0	0	0
			1565	698	283	510	73	1			

- Molecule 55 is a RNA chain called P-site tRNA.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
55	1x	76	Total	C	N	O	P	S	0	0	0
			1625	725	294	529	76	1			
55	2x	76	Total	C	N	O	P	S	0	0	0
			1625	725	294	529	76	1			

- Molecule 56 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
56	1A	1143	Total	Mg	0	0
			1143	1143		
56	1B	36	Total	Mg	0	0
			36	36		
56	1D	14	Total	Mg	0	0
			14	14		
56	1E	12	Total	Mg	0	0
			12	12		
56	1F	8	Total	Mg	0	0
			8	8		
56	1G	5	Total	Mg	0	0
			5	5		
56	1I	1	Total	Mg	0	0
			1	1		
56	1N	6	Total	Mg	0	0
			6	6		

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
56	1O	5	Total Mg 5 5	0	0
56	1P	3	Total Mg 3 3	0	0
56	1Q	5	Total Mg 5 5	0	0
56	1R	4	Total Mg 4 4	0	0
56	1S	3	Total Mg 3 3	0	0
56	1T	3	Total Mg 3 3	0	0
56	1U	7	Total Mg 7 7	0	0
56	1V	2	Total Mg 2 2	0	0
56	1W	7	Total Mg 7 7	0	0
56	1X	5	Total Mg 5 5	0	0
56	1Y	3	Total Mg 3 3	0	0
56	1Z	4	Total Mg 4 4	0	0
56	10	8	Total Mg 8 8	0	0
56	11	4	Total Mg 4 4	0	0
56	12	2	Total Mg 2 2	0	0
56	13	1	Total Mg 1 1	0	0
56	15	3	Total Mg 3 3	0	0
56	16	2	Total Mg 2 2	0	0
56	17	3	Total Mg 3 3	0	0
56	18	4	Total Mg 4 4	0	0
56	19	2	Total Mg 2 2	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
56	1a	235	Total Mg 235 235	0	0
56	1b	2	Total Mg 2 2	0	0
56	1d	1	Total Mg 1 1	0	0
56	1e	1	Total Mg 1 1	0	0
56	1f	2	Total Mg 2 2	0	0
56	1l	3	Total Mg 3 3	0	0
56	1m	1	Total Mg 1 1	0	0
56	1n	2	Total Mg 2 2	0	0
56	1p	1	Total Mg 1 1	0	0
56	1s	1	Total Mg 1 1	0	0
56	1t	1	Total Mg 1 1	0	0
56	1v	1	Total Mg 1 1	0	0
56	1w	11	Total Mg 11 11	0	0
56	1x	15	Total Mg 15 15	0	0
56	1y	5	Total Mg 5 5	0	0
56	2A	876	Total Mg 876 876	0	0
56	2B	21	Total Mg 21 21	0	0
56	2D	7	Total Mg 7 7	0	0
56	2E	7	Total Mg 7 7	0	0
56	2F	4	Total Mg 4 4	0	0
56	2G	1	Total Mg 1 1	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
56	2O	1	Total Mg 1 1	0	0
56	2Q	4	Total Mg 4 4	0	0
56	2R	2	Total Mg 2 2	0	0
56	2T	3	Total Mg 3 3	0	0
56	2U	6	Total Mg 6 6	0	0
56	2V	1	Total Mg 1 1	0	0
56	2W	2	Total Mg 2 2	0	0
56	2X	2	Total Mg 2 2	0	0
56	2Z	1	Total Mg 1 1	0	0
56	20	2	Total Mg 2 2	0	0
56	23	1	Total Mg 1 1	0	0
56	25	4	Total Mg 4 4	0	0
56	26	1	Total Mg 1 1	0	0
56	27	1	Total Mg 1 1	0	0
56	28	1	Total Mg 1 1	0	0
56	2a	230	Total Mg 230 230	0	0
56	2d	2	Total Mg 2 2	0	0
56	2e	1	Total Mg 1 1	0	0
56	2f	1	Total Mg 1 1	0	0
56	2g	1	Total Mg 1 1	0	0
56	2j	2	Total Mg 2 2	0	0

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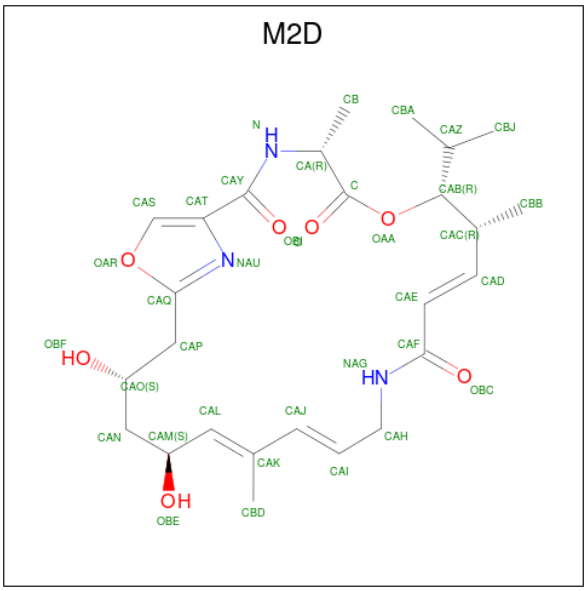
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
56	2l	2	Total Mg 2 2	0	0
56	2p	1	Total Mg 1 1	0	0
56	2q	3	Total Mg 3 3	0	0
56	2r	2	Total Mg 2 2	0	0
56	2t	1	Total Mg 1 1	0	0
56	2v	3	Total Mg 3 3	0	0
56	2w	7	Total Mg 7 7	0	0
56	2x	6	Total Mg 6 6	0	0
56	2y	6	Total Mg 6 6	0	0

- Molecule 57 is POTASSIUM ION (CCD ID: K) (formula: K).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
57	1A	1	Total K 1 1	0	0
57	2A	1	Total K 1 1	0	0

- Molecule 58 is Madumycin II (CCD ID: M2D) (formula: $C_{26}H_{37}N_3O_7$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
58	1A	1	Total C N O 36 26 3 7	0	0
58	2A	1	Total C N O 36 26 3 7	0	0

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

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

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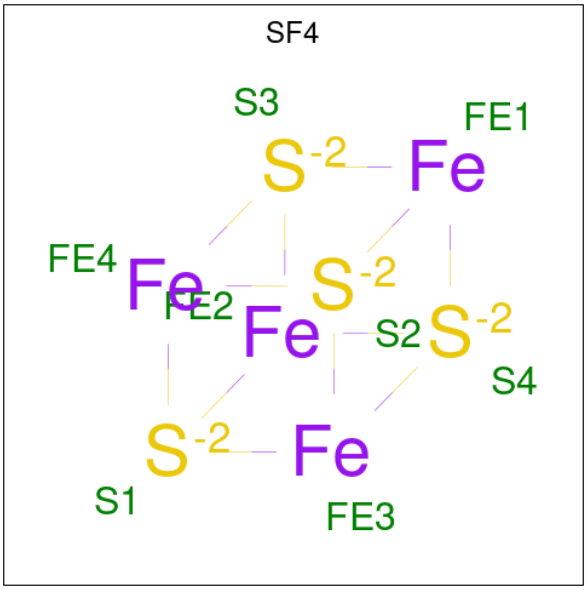
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
59	29	1	Total Zn 1 1	0	0
59	2n	1	Total Zn 1 1	0	0

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



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

- Molecule 61 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
61	1A	2255	Total O 2255 2255	0	0
61	1B	68	Total O 68 68	0	0
61	1D	30	Total O 30 30	0	0
61	1E	28	Total O 28 28	0	0
61	1F	21	Total O 21 21	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
61	1G	5	Total O 5 5	0	0
61	1H	1	Total O 1 1	0	0
61	1I	2	Total O 2 2	0	0
61	1N	8	Total O 8 8	0	0
61	1O	11	Total O 11 11	0	0
61	1P	25	Total O 25 25	0	0
61	1Q	13	Total O 13 13	0	0
61	1R	15	Total O 15 15	0	0
61	1S	4	Total O 4 4	0	0
61	1T	5	Total O 5 5	0	0
61	1U	13	Total O 13 13	0	0
61	1V	10	Total O 10 10	0	0
61	1W	9	Total O 9 9	0	0
61	1X	6	Total O 6 6	0	0
61	1Y	5	Total O 5 5	0	0
61	1Z	1	Total O 1 1	0	0
61	10	8	Total O 8 8	0	0
61	11	14	Total O 14 14	0	0
61	12	4	Total O 4 4	0	0
61	13	4	Total O 4 4	0	0
61	14	1	Total O 1 1	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
61	15	7	Total O 7 7	0	0
61	16	4	Total O 4 4	0	0
61	17	7	Total O 7 7	0	0
61	18	13	Total O 13 13	0	0
61	19	3	Total O 3 3	0	0
61	1a	454	Total O 454 454	0	0
61	1b	1	Total O 1 1	0	0
61	1f	1	Total O 1 1	0	0
61	1l	7	Total O 7 7	0	0
61	1m	2	Total O 2 2	0	0
61	1o	1	Total O 1 1	0	0
61	1q	3	Total O 3 3	0	0
61	1r	1	Total O 1 1	0	0
61	1u	1	Total O 1 1	0	0
61	1v	6	Total O 6 6	0	0
61	1w	18	Total O 18 18	0	0
61	1x	16	Total O 16 16	0	0
61	1y	3	Total O 3 3	0	0
61	2A	1418	Total O 1418 1418	0	0
61	2B	26	Total O 26 26	0	0
61	2D	29	Total O 29 29	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
61	2E	14	Total O 14 14	0	0
61	2F	15	Total O 15 15	0	0
61	2I	4	Total O 4 4	0	0
61	2N	2	Total O 2 2	0	0
61	2O	1	Total O 1 1	0	0
61	2P	13	Total O 13 13	0	0
61	2Q	2	Total O 2 2	0	0
61	2R	2	Total O 2 2	0	0
61	2T	4	Total O 4 4	0	0
61	2U	2	Total O 2 2	0	0
61	2V	1	Total O 1 1	0	0
61	2W	3	Total O 3 3	0	0
61	2X	5	Total O 5 5	0	0
61	2Y	1	Total O 1 1	0	0
61	2Z	2	Total O 2 2	0	0
61	20	5	Total O 5 5	0	0
61	21	14	Total O 14 14	0	0
61	22	1	Total O 1 1	0	0
61	23	2	Total O 2 2	0	0
61	25	5	Total O 5 5	0	0
61	26	1	Total O 1 1	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
61	27	3	Total O 3 3	0	0
61	28	5	Total O 5 5	0	0
61	29	1	Total O 1 1	0	0
61	2a	392	Total O 392 392	0	0
61	2c	2	Total O 2 2	0	0
61	2d	4	Total O 4 4	0	0
61	2e	2	Total O 2 2	0	0
61	2g	1	Total O 1 1	0	0
61	2j	4	Total O 4 4	0	0
61	2k	1	Total O 1 1	0	0
61	2l	6	Total O 6 6	0	0
61	2o	4	Total O 4 4	0	0
61	2p	2	Total O 2 2	0	0
61	2q	1	Total O 1 1	0	0
61	2r	1	Total O 1 1	0	0
61	2t	3	Total O 3 3	0	0
61	2u	1	Total O 1 1	0	0
61	2v	4	Total O 4 4	0	0
61	2w	1	Total O 1 1	0	0
61	2x	6	Total O 6 6	0	0
61	2y	19	Total O 19 19	0	0

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

3 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	209.94Å 451.23Å 622.44Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	155.61 – 2.80 155.61 – 2.80	Depositor EDS
% Data completeness (in resolution range)	96.6 (155.61-2.80) 96.6 (155.61-2.80)	Depositor EDS
R_{merge}	0.15	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.32 (at 2.82Å)	Xtriage
Refinement program	PHENIX 1.8.2	Depositor
R, R_{free}	0.229 , 0.278 0.230 , 0.277	Depositor DCC
R_{free} test set	69403 reflections (4.85%)	wwPDB-VP
Wilson B-factor (Å^2)	53.5	Xtriage
Anisotropy	0.220	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 69.8	EDS
L-test for twinning[2]	$< \|L\| > = 0.39$, $< L^2 > = 0.21$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.89	EDS
Total number of atoms	300935	wwPDB-VP
Average B, all atoms (Å^2)	51.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.66% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

4 Model quality

4.1 Standard geometry

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

4.2 Too-close contacts

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

4.3 Torsion angles

4.3.1 Protein backbone

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

4.3.2 Protein sidechains

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

4.3.3 RNA

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

4.4 Non-standard residues in protein, DNA, RNA chains

84 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	$\#\|Z\| > 2$
55	PSU	1x	55	55	18,21,22	1.35	2 (11%)	22,30,33	1.89	3 (13%)
32	5MC	1a	1407	32	18,22,23	0.91	2 (11%)	26,32,35	1.14	2 (7%)
1	5MU	1A	1937	1	19,22,23	1.43	5 (26%)	28,32,35	2.02	6 (21%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
54	5MU	2w	54	54	19,22,23	1.36	5 (26%)	28,32,35	1.97	7 (25%)
55	4SU	1x	8	55	18,21,22	2.00	5 (27%)	26,30,33	1.63	5 (19%)
54	PSU	1y	32	54	18,21,22	1.35	2 (11%)	22,30,33	1.83	3 (13%)
54	PSU	1y	39	54	18,21,22	1.32	2 (11%)	22,30,33	1.95	3 (13%)
54	MIA	2w	37	54	24,27,32	1.99	5 (20%)	34,39,47	2.25	11 (32%)
1	PSU	1A	1939	1	18,21,22	1.34	2 (11%)	22,30,33	1.89	3 (13%)
54	PSU	2w	39	54	18,21,22	1.34	2 (11%)	22,30,33	1.75	3 (13%)
32	4OC	1a	1402	32	20,23,24	0.74	0	26,32,35	0.91	1 (3%)
54	7MG	1y	46	54	22,26,27	1.35	3 (13%)	29,39,42	2.60	6 (20%)
54	PSU	2w	55	54	18,21,22	1.36	2 (11%)	22,30,33	1.88	3 (13%)
54	PSU	1w	32	54	18,21,22	1.35	2 (11%)	22,30,33	1.78	3 (13%)
32	MA6	2a	1519	32	23,26,27	1.52	4 (17%)	34,38,41	2.29	13 (38%)
1	PSU	1A	1933	1	18,21,22	1.35	2 (11%)	22,30,33	1.86	3 (13%)
1	5MC	1A	1984	1,56	18,22,23	0.97	2 (11%)	26,32,35	1.11	2 (7%)
54	4SU	1w	8	54	18,21,22	1.78	5 (27%)	26,30,33	1.95	5 (19%)
32	UR3	2a	1498	32	19,22,23	1.03	1 (5%)	26,32,35	1.50	1 (3%)
43	0TD	1l	92	43	7,9,10	4.71	1 (14%)	6,11,13	4.76	2 (33%)
54	PSU	1y	55	54	18,21,22	1.37	2 (11%)	22,30,33	1.91	3 (13%)
32	5MC	2a	1404	32	18,22,23	0.97	2 (11%)	26,32,35	1.20	3 (11%)
1	2MU	1A	2564	1,56	19,22,24	1.29	3 (15%)	26,31,36	1.75	6 (23%)
55	5MU	1x	54	56,55	19,22,23	1.39	5 (26%)	28,32,35	1.94	7 (25%)
55	PSU	2x	55	56,55	18,21,22	1.34	2 (11%)	22,30,33	1.88	3 (13%)
32	5MC	1a	1404	32	18,22,23	0.97	2 (11%)	26,32,35	1.13	2 (7%)
55	5MU	2x	54	55	19,22,23	1.41	5 (26%)	28,32,35	2.16	6 (21%)
54	7MG	1w	46	54	22,26,27	1.43	4 (18%)	29,39,42	2.48	7 (24%)
1	4OC	1A	1942	1	19,22,24	0.81	0	26,31,35	0.95	1 (3%)
1	PSU	2A	2605	1	18,21,22	1.34	2 (11%)	22,30,33	1.87	4 (18%)
1	4OC	2A	1920	1	19,22,24	0.81	0	26,31,35	0.86	0
32	PSU	2a	516	32	18,21,22	1.33	2 (11%)	22,30,33	1.84	4 (18%)
54	4SU	2y	8	56,54	18,21,22	1.76	5 (27%)	26,30,33	2.10	4 (15%)
1	PSU	2A	1911	1	18,21,22	1.32	2 (11%)	22,30,33	1.84	3 (13%)
54	MIA	1y	37	54	21,24,32	1.56	4 (19%)	31,35,47	2.02	8 (25%)
54	PSU	2y	55	54	18,21,22	1.33	2 (11%)	22,30,33	1.91	3 (13%)
1	OMG	2A	2251	1,56,55	23,26,27	1.22	3 (13%)	33,38,41	1.94	5 (15%)
54	PSU	2w	32	54	18,21,22	1.32	2 (11%)	22,30,33	1.85	3 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
54	5MU	2y	54	54	19,22,23	1.46	5 (26%)	28,32,35	1.73	7 (25%)
54	PSU	1w	55	54	18,21,22	1.36	2 (11%)	22,30,33	1.90	3 (13%)
1	PSU	1A	2617	1,56	18,21,22	1.35	2 (11%)	22,30,33	1.81	3 (13%)
32	PSU	1a	516	32,56	18,21,22	1.35	2 (11%)	22,30,33	1.90	4 (18%)
54	5MU	1y	54	54	19,22,23	1.44	6 (31%)	28,32,35	2.04	6 (21%)
1	5MU	2A	1939	1,56	19,22,23	1.41	6 (31%)	28,32,35	2.13	6 (21%)
32	M2G	2a	966	32	24,27,28	1.29	4 (16%)	35,40,43	1.82	6 (17%)
32	7MG	1a	527	32,56	22,26,27	1.34	4 (18%)	29,39,42	2.48	7 (24%)
54	MIA	2y	37	54	21,24,32	1.55	3 (14%)	31,35,47	2.06	9 (29%)
54	PSU	2y	39	54	18,21,22	1.26	2 (11%)	22,30,33	2.03	4 (18%)
32	MA6	2a	1518	32	23,26,27	1.53	3 (13%)	34,38,41	2.28	13 (38%)
1	2MA	2A	2503	1,56	22,25,26	1.46	4 (18%)	33,37,40	2.13	9 (27%)
32	5MC	2a	1407	32	18,22,23	0.95	2 (11%)	26,32,35	1.15	3 (11%)
32	5MC	2a	967	32	18,22,23	0.97	2 (11%)	26,32,35	1.12	2 (7%)
54	MIA	1w	37	54	28,31,32	2.33	6 (21%)	40,44,47	2.64	14 (35%)
1	PSU	2A	1917	1	18,21,22	1.33	2 (11%)	22,30,33	1.87	3 (13%)
32	7MG	2a	527	32,56	22,26,27	1.34	4 (18%)	29,39,42	2.51	7 (24%)
1	5MC	1A	1964	1,56	18,22,23	0.93	2 (11%)	26,32,35	1.12	2 (7%)
32	5MC	1a	1400	32	18,22,23	0.97	2 (11%)	26,32,35	1.16	3 (11%)
55	4SU	2x	8	55	18,21,22	1.93	6 (33%)	26,30,33	1.70	6 (23%)
32	2MG	2a	1207	32	23,26,27	1.25	4 (17%)	32,38,41	2.19	6 (18%)
55	5MC	2x	32	55	18,22,23	1.01	2 (11%)	26,32,35	1.21	3 (11%)
54	PSU	1w	39	54	18,21,22	1.31	2 (11%)	22,30,33	1.92	3 (13%)
1	OMG	1A	2263	1,56,55	23,26,27	1.22	3 (13%)	33,38,41	2.00	6 (18%)
54	7MG	2y	46	54	22,26,27	1.35	3 (13%)	29,39,42	2.67	8 (27%)
32	4OC	2a	1402	32	20,23,24	0.80	0	26,32,35	1.05	2 (7%)
32	M2G	1a	966	32	24,27,28	1.31	4 (16%)	35,40,43	1.83	6 (17%)
1	5MC	2A	1942	1	18,22,23	0.96	2 (11%)	26,32,35	1.14	2 (7%)
1	2MA	1A	2515	1,56	22,25,26	1.40	5 (22%)	33,37,40	2.17	9 (27%)
54	PSU	2y	32	54	18,21,22	1.35	2 (11%)	22,30,33	1.82	3 (13%)
32	UR3	1a	1498	32	19,22,23	0.98	1 (5%)	26,32,35	1.39	1 (3%)
54	5MU	1w	54	54	19,22,23	1.40	5 (26%)	28,32,35	1.99	6 (21%)
54	7MG	2w	46	54	22,26,27	1.35	4 (18%)	29,39,42	2.52	7 (24%)
32	MA6	1a	1519	32	23,26,27	1.53	4 (17%)	34,38,41	2.33	11 (32%)
54	4SU	2w	8	54	18,21,22	1.70	4 (22%)	26,30,33	2.32	5 (19%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
1	5MC	2A	1962	1,56	18,22,23	0.97	2 (11%)	26,32,35	1.10	2 (7%)
1	2MU	2A	2552	1,56	19,22,24	1.28	2 (10%)	26,31,36	1.69	5 (19%)
43	0TD	2l	92	43	7,9,10	4.85	1 (14%)	6,11,13	5.20	3 (50%)
32	MA6	1a	1518	32	23,26,27	1.48	3 (13%)	34,38,41	2.31	14 (41%)
32	2MG	1a	1207	32	23,26,27	1.27	4 (17%)	32,38,41	2.11	5 (15%)
1	5MU	1A	1961	1,56	19,22,23	1.42	6 (31%)	28,32,35	2.19	6 (21%)
32	5MC	2a	1400	32	18,22,23	0.95	2 (11%)	26,32,35	1.16	2 (7%)
55	5MC	1x	32	55	18,22,23	0.98	2 (11%)	26,32,35	1.15	2 (7%)
32	5MC	1a	967	32	18,22,23	0.97	2 (11%)	26,32,35	1.19	3 (11%)
54	4SU	1y	8	54	18,21,22	1.68	4 (22%)	26,30,33	2.15	4 (15%)
1	5MU	2A	1915	1	19,22,23	1.47	6 (31%)	28,32,35	2.07	6 (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
55	PSU	1x	55	55	-	0/7/25/26	0/2/2/2
32	5MC	1a	1407	32	-	0/7/25/26	0/2/2/2
1	5MU	1A	1937	1	-	0/7/25/26	0/2/2/2
54	5MU	2w	54	54	-	0/7/25/26	0/2/2/2
55	4SU	1x	8	55	-	0/7/25/26	0/2/2/2
54	PSU	1y	32	54	-	0/7/25/26	0/2/2/2
54	PSU	1y	39	54	-	0/7/25/26	0/2/2/2
54	MIA	2w	37	54	-	2/11/29/34	0/3/3/3
1	PSU	1A	1939	1	-	0/7/25/26	0/2/2/2
54	PSU	2w	39	54	-	0/7/25/26	0/2/2/2
32	4OC	1a	1402	32	-	2/9/29/30	0/2/2/2
54	7MG	1y	46	54	-	2/7/37/38	0/3/3/3
54	PSU	2w	55	54	-	0/7/25/26	0/2/2/2
54	PSU	1w	32	54	-	0/7/25/26	0/2/2/2
32	MA6	2a	1519	32	-	5/11/29/30	0/3/3/3
1	PSU	1A	1933	1	-	0/7/25/26	0/2/2/2
1	5MC	1A	1984	1,56	-	0/7/25/26	0/2/2/2
54	4SU	1w	8	54	-	0/7/25/26	0/2/2/2
32	UR3	2a	1498	32	-	0/7/25/26	0/2/2/2
43	0TD	1l	92	43	-	3/7/12/14	-
54	PSU	1y	55	54	-	2/7/25/26	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	2MU	1A	2564	1,56	-	0/9/27/28	0/2/2/2
55	5MU	1x	54	56,55	-	0/7/25/26	0/2/2/2
55	PSU	2x	55	56,55	-	0/7/25/26	0/2/2/2
32	5MC	1a	1404	32	-	0/7/25/26	0/2/2/2
55	5MU	2x	54	55	-	0/7/25/26	0/2/2/2
54	7MG	1w	46	54	-	3/7/37/38	0/3/3/3
1	4OC	1A	1942	1	-	1/9/27/30	0/2/2/2
1	PSU	2A	2605	1	-	0/7/25/26	0/2/2/2
1	4OC	2A	1920	1	-	2/9/27/30	0/2/2/2
32	PSU	2a	516	32	-	0/7/25/26	0/2/2/2
54	4SU	2y	8	56,54	-	2/7/25/26	0/2/2/2
1	PSU	2A	1911	1	-	0/7/25/26	0/2/2/2
54	MIA	1y	37	54	-	2/7/25/34	0/3/3/3
54	PSU	2y	55	54	-	2/7/25/26	0/2/2/2
1	OMG	2A	2251	1,56,55	-	1/9/27/28	0/3/3/3
54	PSU	2w	32	54	-	0/7/25/26	0/2/2/2
54	5MU	2y	54	54	-	0/7/25/26	0/2/2/2
54	PSU	1w	55	54	-	0/7/25/26	0/2/2/2
1	PSU	1A	2617	1,56	-	0/7/25/26	0/2/2/2
32	PSU	1a	516	32,56	-	0/7/25/26	0/2/2/2
54	5MU	1y	54	54	-	0/7/25/26	0/2/2/2
1	5MU	2A	1939	1,56	-	0/7/25/26	0/2/2/2
32	M2G	2a	966	32	-	0/11/29/30	0/3/3/3
32	7MG	1a	527	32,56	-	2/7/37/38	0/3/3/3
54	MIA	2y	37	54	-	2/7/25/34	0/3/3/3
54	PSU	2y	39	54	-	0/7/25/26	0/2/2/2
32	MA6	2a	1518	32	-	3/11/29/30	0/3/3/3
1	2MA	2A	2503	1,56	-	2/7/25/26	0/3/3/3
32	5MC	2a	1407	32	-	0/7/25/26	0/2/2/2
32	5MC	2a	967	32	-	1/7/25/26	0/2/2/2
54	MIA	1w	37	54	-	1/15/33/34	0/3/3/3
1	PSU	2A	1917	1	-	0/7/25/26	0/2/2/2
32	7MG	2a	527	32,56	-	2/7/37/38	0/3/3/3
1	5MC	1A	1964	1,56	-	0/7/25/26	0/2/2/2
32	5MC	1a	1400	32	-	0/7/25/26	0/2/2/2
55	4SU	2x	8	55	-	1/7/25/26	0/2/2/2
32	2MG	2a	1207	32	-	2/9/27/28	0/3/3/3
55	5MC	2x	32	55	-	0/7/25/26	0/2/2/2
54	PSU	1w	39	54	-	0/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	OMG	1A	2263	1,56,55	-	0/9/27/28	0/3/3/3
54	7MG	2y	46	54	-	3/7/37/38	0/3/3/3
32	4OC	2a	1402	32	-	2/9/29/30	0/2/2/2
32	M2G	1a	966	32	-	0/11/29/30	0/3/3/3
1	5MC	2A	1942	1	-	0/7/25/26	0/2/2/2
1	2MA	1A	2515	1,56	-	2/7/25/26	0/3/3/3
54	PSU	2y	32	54	-	0/7/25/26	0/2/2/2
32	UR3	1a	1498	32	-	0/7/25/26	0/2/2/2
54	5MU	1w	54	54	-	0/7/25/26	0/2/2/2
54	7MG	2w	46	54	-	4/7/37/38	0/3/3/3
32	MA6	1a	1519	32	-	3/11/29/30	0/3/3/3
54	4SU	2w	8	54	-	1/7/25/26	0/2/2/2
1	5MC	2A	1962	1,56	-	1/7/25/26	0/2/2/2
1	2MU	2A	2552	1,56	-	0/9/27/28	0/2/2/2
43	0TD	2l	92	43	-	2/7/12/14	-
32	MA6	1a	1518	32	-	2/11/29/30	0/3/3/3
32	2MG	1a	1207	32	-	1/9/27/28	0/3/3/3
1	5MU	1A	1961	1,56	-	0/7/25/26	0/2/2/2
32	5MC	2a	1400	32	-	0/7/25/26	0/2/2/2
55	5MC	1x	32	55	-	0/7/25/26	0/2/2/2
32	5MC	1a	967	32	-	2/7/25/26	0/2/2/2
54	4SU	1y	8	54	-	3/7/25/26	0/2/2/2
1	5MU	2A	1915	1	-	0/7/25/26	0/2/2/2

All (249) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
43	2l	92	0TD	CB-SB	-12.55	1.69	1.82
43	1l	92	0TD	CB-SB	-12.15	1.69	1.82
54	1w	37	MIA	C13-C14	7.14	1.52	1.32
54	1w	37	MIA	C2-S10	-6.84	1.69	1.75
54	2w	37	MIA	C2-S10	-6.53	1.70	1.75
32	2a	1518	MA6	C5-C4	4.84	1.48	1.39
32	2a	1519	MA6	C5-C4	4.76	1.47	1.39
54	2y	37	MIA	C5-C4	4.74	1.47	1.39
32	1a	1519	MA6	C5-C4	4.72	1.47	1.39
54	1y	37	MIA	C5-C4	4.71	1.47	1.39
54	1w	37	MIA	C5-C4	4.70	1.47	1.39
54	2w	37	MIA	C5-C4	4.59	1.47	1.39
54	2y	8	4SU	C4-S4	-4.57	1.59	1.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	1a	1518	MA6	C5-C4	4.47	1.47	1.39
54	1w	8	4SU	C4-S4	-4.47	1.59	1.68
54	2w	8	4SU	C4-S4	-4.43	1.60	1.68
55	1x	8	4SU	C4-S4	-4.42	1.60	1.68
55	2x	8	4SU	C4-S4	-4.42	1.60	1.68
1	2A	2503	2MA	C5-C4	4.32	1.47	1.39
54	1y	8	4SU	C4-S4	-4.30	1.60	1.68
55	1x	8	4SU	C4-N3	-4.29	1.33	1.37
1	1A	2515	2MA	C5-C4	4.07	1.46	1.39
55	2x	8	4SU	C4-N3	-3.98	1.33	1.37
54	2w	55	PSU	C6-C5	3.63	1.39	1.35
54	1w	55	PSU	C6-C5	3.62	1.39	1.35
54	1y	32	PSU	C6-C5	3.54	1.39	1.35
54	2y	32	PSU	C6-C5	3.47	1.39	1.35
54	2y	55	PSU	C6-C5	3.45	1.39	1.35
54	1y	55	PSU	C6-C5	3.43	1.39	1.35
55	1x	55	PSU	C6-C5	3.39	1.39	1.35
54	2w	39	PSU	C6-C5	3.38	1.39	1.35
54	1w	46	7MG	C4-N9	-3.36	1.33	1.37
54	1y	39	PSU	C6-C5	3.34	1.39	1.35
55	2x	55	PSU	C6-C5	3.34	1.39	1.35
1	1A	1939	PSU	C6-C5	3.33	1.39	1.35
32	2a	516	PSU	C6-C5	3.29	1.39	1.35
54	1w	8	4SU	C4-N3	-3.28	1.34	1.37
54	2w	32	PSU	C6-C5	3.27	1.39	1.35
1	1A	2263	OMG	C5-C4	3.26	1.47	1.38
54	2y	46	7MG	C5-C4	3.26	1.48	1.38
1	1A	1933	PSU	C6-C5	3.25	1.39	1.35
1	2A	1911	PSU	C6-C5	3.24	1.39	1.35
1	2A	1917	PSU	C6-C5	3.23	1.39	1.35
55	1x	8	4SU	C2-N3	-3.22	1.32	1.38
54	1w	39	PSU	C6-C5	3.22	1.39	1.35
54	1y	46	7MG	C5-C4	3.22	1.48	1.38
54	1w	32	PSU	C6-C5	3.21	1.39	1.35
32	1a	516	PSU	C6-C5	3.20	1.39	1.35
1	2A	2251	OMG	C5-C4	3.20	1.47	1.38
32	2a	966	M2G	C5-C4	3.16	1.47	1.38
55	1x	8	4SU	C5-C4	-3.15	1.38	1.42
32	2a	1207	2MG	C5-C4	3.15	1.47	1.38
54	2y	8	4SU	C4-N3	-3.13	1.34	1.37
1	2A	2605	PSU	C6-C5	3.11	1.38	1.35
54	1y	8	4SU	C4-N3	-3.11	1.34	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
54	2y	39	PSU	C6-C5	3.10	1.38	1.35
54	1w	46	7MG	C5-C4	3.09	1.48	1.38
32	1a	1207	2MG	C5-C4	3.08	1.47	1.38
32	1a	527	7MG	C5-C4	3.08	1.48	1.38
1	2A	1915	5MU	C6-C5	3.08	1.39	1.34
55	2x	8	4SU	C5-C4	-3.06	1.38	1.42
32	1a	966	M2G	C5-C4	3.06	1.47	1.38
32	2a	1518	MA6	C5-C6	3.01	1.49	1.41
32	2a	527	7MG	C4-N9	-3.00	1.34	1.37
54	2w	46	7MG	C4-N9	-2.99	1.34	1.37
54	2w	46	7MG	C5-C4	2.99	1.47	1.38
1	1A	2617	PSU	C6-C5	2.98	1.38	1.35
32	2a	527	7MG	C5-C4	2.94	1.47	1.38
32	2a	1519	MA6	C5-C6	2.92	1.49	1.41
32	2a	1404	5MC	C6-C5	2.91	1.39	1.34
54	2y	37	MIA	C5-C6	2.91	1.49	1.41
55	2x	32	5MC	C6-C5	2.90	1.39	1.34
55	1x	32	5MC	C6-C5	2.89	1.39	1.34
54	1y	54	5MU	C6-C5	2.89	1.39	1.34
1	1A	2564	2MU	C4-N3	-2.87	1.33	1.38
54	1y	37	MIA	C5-C6	2.87	1.49	1.41
1	1A	1961	5MU	C4-N3	-2.87	1.33	1.38
32	1a	1519	MA6	C5-C6	2.86	1.49	1.41
32	1a	966	M2G	C2-N2	2.85	1.40	1.35
1	1A	1937	5MU	C6-C5	2.85	1.39	1.34
32	1a	1518	MA6	C5-C6	2.85	1.49	1.41
55	2x	54	5MU	C6-C5	2.82	1.39	1.34
32	1a	1404	5MC	C6-C5	2.82	1.39	1.34
1	1A	1961	5MU	C6-C5	2.81	1.39	1.34
32	1a	1400	5MC	C6-C5	2.80	1.39	1.34
54	2w	8	4SU	C4-N3	-2.79	1.34	1.37
54	1w	54	5MU	C6-C5	2.79	1.39	1.34
32	2a	967	5MC	C6-C5	2.79	1.39	1.34
1	2A	2605	PSU	C4-N3	-2.77	1.33	1.38
1	1A	1984	5MC	C6-C5	2.76	1.39	1.34
54	2y	54	5MU	C6-C5	2.76	1.39	1.34
32	1a	527	7MG	C4-N9	-2.75	1.34	1.37
1	2A	1962	5MC	C6-C5	2.75	1.39	1.34
1	2A	1942	5MC	C6-C5	2.74	1.39	1.34
1	1A	2617	PSU	C4-N3	-2.73	1.33	1.38
54	2w	54	5MU	C6-C5	2.73	1.39	1.34
1	2A	1939	5MU	C6-C5	2.73	1.39	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	1a	967	5MC	C6-C5	2.71	1.39	1.34
54	2y	8	4SU	C5-C4	-2.70	1.39	1.42
1	2A	1939	5MU	C4-N3	-2.70	1.33	1.38
32	2a	1400	5MC	C6-C5	2.69	1.39	1.34
1	2A	1915	5MU	C4-N3	-2.68	1.33	1.38
54	2y	54	5MU	C4-N3	-2.67	1.33	1.38
54	1y	54	5MU	C4-N3	-2.66	1.33	1.38
54	2y	54	5MU	C2-N1	2.66	1.42	1.38
54	1w	8	4SU	C5-C4	-2.65	1.39	1.42
1	1A	1964	5MC	C6-C5	2.64	1.38	1.34
1	2A	2503	2MA	C5-C6	2.64	1.48	1.41
54	2w	8	4SU	C5-C4	-2.63	1.39	1.42
1	2A	2552	2MU	C4-N3	-2.62	1.33	1.38
32	2a	966	M2G	C2-N2	2.61	1.40	1.35
32	1a	516	PSU	C4-N3	-2.61	1.34	1.38
55	1x	54	5MU	C6-C5	2.61	1.38	1.34
1	1A	1937	5MU	C4-N3	-2.61	1.34	1.38
1	2A	1915	5MU	C4-C5	2.60	1.49	1.44
54	1w	37	MIA	C5-C6	2.60	1.48	1.41
1	2A	2503	2MA	C8-N7	2.60	1.36	1.31
54	1w	54	5MU	C4-N3	-2.60	1.34	1.38
1	1A	1933	PSU	C4-N3	-2.59	1.34	1.38
32	2a	1407	5MC	C6-C5	2.59	1.38	1.34
1	1A	1939	PSU	C4-N3	-2.58	1.34	1.38
32	1a	966	M2G	C6-N1	-2.58	1.34	1.38
55	1x	54	5MU	C4-N3	-2.58	1.34	1.38
54	1w	46	7MG	C6-N1	-2.57	1.34	1.38
32	1a	1207	2MG	C6-N1	-2.57	1.34	1.38
54	1w	32	PSU	C4-N3	-2.56	1.34	1.38
54	2y	55	PSU	C4-N3	-2.55	1.34	1.38
54	2w	39	PSU	C4-N3	-2.55	1.34	1.38
54	2w	37	MIA	C5-C6	2.54	1.48	1.41
54	1y	55	PSU	C4-N3	-2.54	1.34	1.38
1	2A	1917	PSU	C4-N3	-2.54	1.34	1.38
54	2y	37	MIA	C8-N7	2.54	1.36	1.31
55	2x	54	5MU	C4-N3	-2.52	1.34	1.38
54	2w	8	4SU	C2-N1	2.52	1.42	1.38
54	1y	39	PSU	C4-N3	-2.51	1.34	1.38
1	2A	2251	OMG	C6-N1	-2.50	1.34	1.38
32	1a	1407	5MC	C6-C5	2.50	1.38	1.34
54	1y	37	MIA	C8-N7	2.50	1.36	1.31
1	2A	1911	PSU	C4-N3	-2.50	1.34	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
54	1y	54	5MU	C4-C5	2.49	1.48	1.44
55	2x	55	PSU	C4-N3	-2.49	1.34	1.38
54	2w	55	PSU	C4-N3	-2.48	1.34	1.38
54	2w	37	MIA	C8-N7	2.47	1.36	1.31
55	2x	8	4SU	C2-N3	-2.47	1.33	1.38
54	2w	32	PSU	C4-N3	-2.46	1.34	1.38
1	1A	2515	2MA	C5-C6	2.45	1.47	1.41
1	1A	1937	5MU	C2-N1	2.45	1.42	1.38
32	2a	966	M2G	C6-N1	-2.45	1.34	1.38
54	1y	32	PSU	C4-N3	-2.43	1.34	1.38
54	1w	39	PSU	C4-N3	-2.43	1.34	1.38
32	2a	516	PSU	C4-N3	-2.42	1.34	1.38
55	2x	54	5MU	C4-C5	2.42	1.48	1.44
54	2w	54	5MU	C4-N3	-2.42	1.34	1.38
54	1y	46	7MG	C6-N1	-2.41	1.34	1.38
55	1x	55	PSU	C4-N3	-2.41	1.34	1.38
54	2y	32	PSU	C4-N3	-2.40	1.34	1.38
54	2y	46	7MG	C6-N1	-2.40	1.34	1.38
54	1w	54	5MU	C4-C5	2.39	1.48	1.44
54	2w	54	5MU	C4-C5	2.38	1.48	1.44
1	1A	1937	5MU	C4-C5	2.37	1.48	1.44
1	2A	2552	2MU	C5-C4	2.37	1.48	1.43
32	2a	1518	MA6	C8-N7	2.37	1.36	1.31
54	2w	46	7MG	C8-N9	2.36	1.47	1.46
1	1A	2263	OMG	C6-N1	-2.35	1.34	1.38
32	1a	1519	MA6	C8-N7	2.35	1.36	1.31
1	1A	1961	5MU	C2-N3	-2.34	1.33	1.38
55	2x	8	4SU	C2-N1	2.34	1.42	1.38
54	1w	55	PSU	C4-N3	-2.34	1.34	1.38
1	2A	1915	5MU	C2-N1	2.33	1.42	1.38
1	1A	2564	2MU	C2-N3	-2.32	1.33	1.38
54	1y	8	4SU	C5-C4	-2.32	1.39	1.42
1	1A	1984	5MC	C6-N1	-2.32	1.34	1.38
54	1y	46	7MG	C8-N9	2.32	1.47	1.46
1	2A	1939	5MU	C6-N1	-2.32	1.34	1.38
54	1w	37	MIA	C8-N7	2.32	1.36	1.31
32	2a	1207	2MG	C6-N1	-2.31	1.34	1.38
32	2a	1519	MA6	C8-N7	2.31	1.36	1.31
1	2A	1939	5MU	C4-C5	2.31	1.48	1.44
32	2a	527	7MG	C6-N1	-2.30	1.34	1.38
32	1a	1518	MA6	C8-N7	2.29	1.35	1.31
32	2a	1400	5MC	C6-N1	-2.29	1.34	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	1A	2564	2MU	C5-C4	2.29	1.48	1.43
55	2x	54	5MU	C2-N1	2.28	1.42	1.38
54	2y	54	5MU	C4-C5	2.28	1.48	1.44
54	2y	46	7MG	C8-N9	2.27	1.47	1.46
55	1x	54	5MU	C4-C5	2.26	1.48	1.44
55	1x	54	5MU	C2-N1	2.25	1.42	1.38
32	1a	527	7MG	C6-N1	-2.25	1.34	1.38
32	1a	967	5MC	C6-N1	-2.24	1.34	1.38
1	2A	2503	2MA	C5-N7	-2.24	1.34	1.39
32	1a	1407	5MC	C6-N1	-2.23	1.34	1.38
1	1A	2263	OMG	C5-N7	-2.23	1.34	1.39
1	2A	1962	5MC	C6-N1	-2.22	1.34	1.38
32	2a	1407	5MC	C6-N1	-2.22	1.34	1.38
54	2y	39	PSU	C4-N3	-2.22	1.34	1.38
32	2a	1207	2MG	C2-N3	2.22	1.36	1.31
1	1A	1961	5MU	C6-N1	-2.21	1.34	1.38
32	1a	966	M2G	C5-N7	-2.21	1.34	1.39
54	1w	8	4SU	C2-N1	2.21	1.42	1.38
54	2y	8	4SU	C2-N1	2.21	1.42	1.38
1	1A	1964	5MC	C6-N1	-2.21	1.34	1.38
54	1y	54	5MU	C2-N1	2.21	1.42	1.38
55	1x	32	5MC	C6-N1	-2.20	1.34	1.38
1	2A	2251	OMG	C5-N7	-2.20	1.34	1.39
54	1y	8	4SU	C2-N1	2.20	1.42	1.38
1	2A	1942	5MC	C6-N1	-2.19	1.34	1.38
1	1A	1961	5MU	C4-C5	2.18	1.48	1.44
55	2x	54	5MU	C6-N1	-2.17	1.34	1.38
32	1a	1519	MA6	C5-N7	-2.17	1.34	1.39
32	1a	1404	5MC	C6-N1	-2.17	1.34	1.38
32	2a	1404	5MC	C6-N1	-2.16	1.34	1.38
54	1y	54	5MU	C6-N1	-2.16	1.34	1.38
32	1a	1400	5MC	C6-N1	-2.15	1.34	1.38
54	2w	37	MIA	C5-N7	-2.14	1.35	1.39
32	2a	1498	UR3	C2-N1	2.13	1.41	1.38
55	1x	54	5MU	C6-N1	-2.13	1.34	1.38
54	1w	8	4SU	C2-N3	-2.13	1.34	1.38
54	1w	37	MIA	C5-N7	-2.12	1.35	1.39
1	1A	2515	2MA	C5-N7	-2.12	1.35	1.39
1	2A	1915	5MU	C6-N1	-2.12	1.34	1.38
1	2A	1939	5MU	C2-N1	2.12	1.41	1.38
54	1w	54	5MU	C2-N1	2.11	1.41	1.38
54	2w	54	5MU	C6-N1	-2.10	1.34	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	2a	966	M2G	C5-N7	-2.10	1.35	1.39
1	1A	2515	2MA	C8-N7	2.10	1.35	1.31
54	1y	37	MIA	C5-N7	-2.09	1.35	1.39
54	1w	46	7MG	C8-N9	2.08	1.47	1.46
32	1a	1207	2MG	C5-N7	-2.08	1.35	1.39
32	1a	1207	2MG	C2-N3	2.08	1.35	1.31
54	1w	54	5MU	C6-N1	-2.08	1.34	1.38
1	2A	1939	5MU	C2-N3	-2.07	1.34	1.38
32	2a	1207	2MG	C5-N7	-2.07	1.35	1.39
32	2a	967	5MC	C6-N1	-2.07	1.34	1.38
1	1A	1937	5MU	C6-N1	-2.07	1.34	1.38
32	1a	1498	UR3	C6-C5	2.06	1.39	1.35
55	2x	8	4SU	O2-C2	2.06	1.26	1.23
54	1y	54	5MU	C2-N3	-2.05	1.34	1.38
1	2A	1915	5MU	C2-N3	-2.05	1.34	1.38
32	2a	527	7MG	C8-N9	2.05	1.47	1.46
55	1x	8	4SU	C2-N1	2.05	1.41	1.38
1	1A	1961	5MU	C2-N1	2.05	1.41	1.38
54	2w	46	7MG	C6-N1	-2.04	1.35	1.38
1	1A	2515	2MA	C4-N9	-2.03	1.33	1.37
55	2x	32	5MC	C6-N1	-2.03	1.34	1.38
32	1a	527	7MG	C8-N9	2.03	1.47	1.46
54	2y	54	5MU	C2-N3	-2.03	1.34	1.38
32	2a	1519	MA6	C5-N7	-2.02	1.35	1.39
54	2y	8	4SU	C2-N3	-2.01	1.34	1.38
54	2w	54	5MU	C2-N1	2.00	1.41	1.38

All (404) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
43	2l	92	0TD	CSB-SB-CB	-11.92	80.88	102.44
43	1l	92	0TD	CSB-SB-CB	-10.99	82.56	102.44
54	2y	46	7MG	N9-C4-N3	9.91	140.30	125.47
54	1y	46	7MG	N9-C4-N3	9.56	139.78	125.47
54	1w	46	7MG	N9-C4-N3	8.91	138.79	125.47
32	1a	527	7MG	N9-C4-N3	8.72	138.51	125.47
32	2a	527	7MG	N9-C4-N3	8.68	138.45	125.47
54	2w	46	7MG	N9-C4-N3	8.65	138.41	125.47
54	1w	37	MIA	C12-C13-C14	-8.10	111.38	127.14
54	1w	37	MIA	C5-C4-N3	-7.75	118.47	127.19
54	2w	37	MIA	C5-C4-N3	-7.47	118.78	127.19
1	2A	2503	2MA	C5-C4-N3	-7.45	118.81	127.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
32	2a	1207	2MG	C2-N3-C4	7.12	120.86	112.04
54	2w	8	4SU	C4-N3-C2	-7.02	120.52	127.34
1	1A	2515	2MA	C5-C4-N3	-6.97	119.35	127.19
32	1a	1207	2MG	C2-N3-C4	6.92	120.61	112.04
54	1y	8	4SU	C4-N3-C2	-6.72	120.81	127.34
1	1A	2263	OMG	C5-C4-N3	-6.37	118.12	128.46
32	2a	1498	UR3	C4-N3-C2	-6.34	118.59	124.56
1	2A	2251	OMG	C5-C4-N3	-6.32	118.21	128.46
32	1a	1519	MA6	C5-C4-N3	-6.25	118.59	126.75
54	2y	39	PSU	N1-C2-N3	6.22	122.17	115.13
54	2y	8	4SU	C4-N3-C2	-6.17	121.34	127.34
32	1a	966	M2G	C5-C4-N3	-6.17	118.45	128.46
54	1y	37	MIA	C5-C4-N3	-6.14	118.74	126.75
54	2y	37	MIA	C5-C4-N3	-6.11	118.78	126.75
54	1y	55	PSU	N1-C2-N3	6.11	122.05	115.13
54	1w	37	MIA	N3-C4-N9	6.06	135.40	126.99
54	1y	39	PSU	N1-C2-N3	6.05	121.99	115.13
54	2y	55	PSU	N1-C2-N3	6.04	121.98	115.13
55	1x	55	PSU	N1-C2-N3	6.03	121.96	115.13
32	1a	516	PSU	N1-C2-N3	6.03	121.96	115.13
32	2a	966	M2G	C5-C4-N3	-6.02	118.69	128.46
55	2x	55	PSU	N1-C2-N3	5.97	121.89	115.13
32	2a	1207	2MG	C5-C4-N3	-5.95	118.80	128.46
54	1w	39	PSU	N1-C2-N3	5.95	121.87	115.13
32	2a	1519	MA6	C5-C4-N3	-5.93	119.02	126.75
54	2y	46	7MG	C5-C4-N3	-5.90	116.88	128.13
1	2A	1917	PSU	N1-C2-N3	5.90	121.81	115.13
54	2y	8	4SU	C5-C4-N3	5.89	120.15	114.69
54	1w	55	PSU	N1-C2-N3	5.87	121.78	115.13
54	2w	8	4SU	C5-C4-N3	5.86	120.12	114.69
1	1A	1939	PSU	N1-C2-N3	5.85	121.76	115.13
54	2w	55	PSU	N1-C2-N3	5.84	121.75	115.13
54	1y	46	7MG	C5-C4-N3	-5.84	117.00	128.13
54	2w	32	PSU	N1-C2-N3	5.83	121.73	115.13
32	2a	516	PSU	N1-C2-N3	5.82	121.72	115.13
54	1y	32	PSU	N1-C2-N3	5.80	121.70	115.13
54	2y	32	PSU	N1-C2-N3	5.80	121.70	115.13
1	1A	1933	PSU	N1-C2-N3	5.78	121.68	115.13
1	1A	2515	2MA	N3-C4-N9	5.78	135.00	126.99
1	2A	1911	PSU	N1-C2-N3	5.75	121.65	115.13
32	1a	1207	2MG	C5-C4-N3	-5.75	119.13	128.46
54	1w	32	PSU	N1-C2-N3	5.73	121.62	115.13

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	2A	2605	PSU	N1-C2-N3	5.72	121.61	115.13
54	1w	8	4SU	C5-C4-N3	5.66	119.94	114.69
54	2w	37	MIA	N3-C4-N9	5.65	134.83	126.99
32	1a	1498	UR3	C4-N3-C2	-5.63	119.26	124.56
32	1a	1518	MA6	C5-C4-N3	-5.63	119.41	126.75
32	2a	1518	MA6	C5-C4-N3	-5.62	119.42	126.75
1	1A	2617	PSU	N1-C2-N3	5.60	121.47	115.13
54	1w	8	4SU	C4-N3-C2	-5.57	121.93	127.34
1	1A	1961	5MU	C4-N3-C2	-5.57	120.15	127.35
54	1y	8	4SU	C5-C4-N3	5.52	119.81	114.69
55	2x	54	5MU	C4-N3-C2	-5.49	120.25	127.35
1	2A	2503	2MA	N3-C4-N9	5.44	134.53	126.99
54	2w	39	PSU	N1-C2-N3	5.42	121.27	115.13
32	1a	527	7MG	C5-C4-N3	-5.41	117.83	128.13
32	2a	527	7MG	N9-C8-N7	-5.38	95.68	103.38
1	2A	1939	5MU	C4-N3-C2	-5.36	120.42	127.35
54	2w	46	7MG	C5-C4-N3	-5.30	118.03	128.13
1	2A	1915	5MU	C4-N3-C2	-5.29	120.50	127.35
1	2A	1915	5MU	N3-C2-N1	5.24	121.85	114.89
54	2w	46	7MG	N9-C8-N7	-5.23	95.89	103.38
32	2a	527	7MG	C5-C4-N3	-5.23	118.16	128.13
54	1w	46	7MG	N9-C8-N7	-5.23	95.90	103.38
1	1A	1961	5MU	N3-C2-N1	5.18	121.77	114.89
55	2x	54	5MU	N3-C2-N1	5.17	121.76	114.89
54	1y	54	5MU	C4-N3-C2	-5.09	120.77	127.35
1	1A	2564	2MU	N3-C2-N1	5.08	121.63	114.89
1	1A	1937	5MU	C4-N3-C2	-5.05	120.82	127.35
1	1A	1961	5MU	C5-C4-N3	5.01	119.58	115.31
1	1A	2263	OMG	C2-N3-C4	5.00	121.20	112.30
54	1y	54	5MU	N3-C2-N1	4.98	121.50	114.89
32	1a	527	7MG	N9-C8-N7	-4.97	96.26	103.38
54	1w	54	5MU	C4-N3-C2	-4.94	120.95	127.35
1	1A	1937	5MU	N3-C2-N1	4.91	121.41	114.89
1	2A	2552	2MU	N3-C2-N1	4.90	121.40	114.89
1	2A	2251	OMG	C2-N3-C4	4.88	120.99	112.30
1	2A	1939	5MU	N3-C2-N1	4.87	121.35	114.89
54	1w	54	5MU	N3-C2-N1	4.85	121.33	114.89
54	2w	54	5MU	C4-N3-C2	-4.82	121.11	127.35
1	2A	1939	5MU	C5-C4-N3	4.80	119.41	115.31
1	1A	2263	OMG	N9-C4-N3	4.74	135.45	125.94
54	1w	46	7MG	C5-C4-N3	-4.74	119.10	128.13
1	2A	2251	OMG	N9-C4-N3	4.73	135.43	125.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
55	2x	8	4SU	C5-C4-N3	4.69	119.04	114.69
54	2y	37	MIA	N3-C4-N9	4.69	134.81	127.08
32	2a	1518	MA6	C2-N1-C6	4.69	122.82	111.75
55	1x	54	5MU	C4-N3-C2	-4.68	121.29	127.35
54	1y	46	7MG	N9-C8-N7	-4.68	96.68	103.38
54	2y	46	7MG	N9-C8-N7	-4.65	96.72	103.38
32	2a	1518	MA6	C9-N6-C6	-4.64	108.36	120.40
54	1y	37	MIA	N3-C4-N9	4.64	134.73	127.08
54	2w	54	5MU	N3-C2-N1	4.64	121.05	114.89
55	1x	54	5MU	N3-C2-N1	4.63	121.03	114.89
32	1a	1519	MA6	N3-C4-N9	4.61	134.68	127.08
32	1a	966	M2G	N9-C4-N3	4.61	135.20	125.94
55	2x	54	5MU	C5-C4-N3	4.61	119.24	115.31
32	2a	966	M2G	N9-C4-N3	4.60	135.19	125.94
32	1a	1518	MA6	C2-N1-C6	4.60	122.61	111.75
32	1a	966	M2G	C2-N3-C4	4.59	120.99	112.51
54	2y	46	7MG	C2-N3-C4	4.53	120.37	112.30
1	1A	1937	5MU	C5-C4-N3	4.51	119.16	115.31
32	2a	1519	MA6	C2-N1-C6	4.51	122.39	111.75
55	1x	8	4SU	C5-C4-N3	4.50	118.86	114.69
54	1y	46	7MG	C2-N3-C4	4.49	120.30	112.30
32	2a	1519	MA6	N3-C4-N9	4.47	134.45	127.08
32	2a	966	M2G	C2-N3-C4	4.45	120.73	112.51
54	2y	39	PSU	C4-N3-C2	-4.44	119.94	126.34
1	1A	1961	5MU	C5-C6-N1	-4.41	118.80	123.34
32	1a	1519	MA6	C2-N1-C6	4.40	122.14	111.75
54	2w	46	7MG	C2-N3-C4	4.40	120.14	112.30
1	2A	1915	5MU	C5-C4-N3	4.39	119.05	115.31
54	1y	54	5MU	C5-C4-N3	4.34	119.02	115.31
32	2a	1519	MA6	C9-N6-C6	-4.32	109.19	120.40
32	2a	527	7MG	C2-N3-C4	4.30	119.97	112.30
54	1w	54	5MU	C5-C4-N3	4.29	118.97	115.31
32	1a	527	7MG	C2-N3-C4	4.28	119.93	112.30
1	1A	2564	2MU	C4-N3-C2	-4.28	120.94	126.58
54	2w	54	5MU	C5-C4-N3	4.27	118.96	115.31
1	2A	2552	2MU	C4-N3-C2	-4.25	120.97	126.58
54	1y	8	4SU	N3-C2-N1	4.24	120.52	114.89
32	1a	1518	MA6	N3-C4-N9	4.23	134.05	127.08
32	2a	1207	2MG	N9-C4-N3	4.22	134.42	125.94
54	1w	37	MIA	C15-C14-C13	-4.20	110.51	122.65
32	1a	1518	MA6	C9-N6-C6	-4.20	109.52	120.40
32	2a	1518	MA6	C4-C5-N7	-4.17	105.54	110.62

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	1A	1961	5MU	O4-C4-C5	-4.15	120.09	124.90
54	2w	8	4SU	N3-C2-N1	4.15	120.40	114.89
32	1a	1207	2MG	N9-C4-N3	4.15	134.27	125.94
54	1y	39	PSU	C4-N3-C2	-4.12	120.40	126.34
55	2x	8	4SU	C1'-N1-C2	4.10	124.99	117.57
55	2x	54	5MU	O4-C4-C5	-4.09	120.16	124.90
1	2A	1915	5MU	C5-C6-N1	-4.09	119.14	123.34
1	2A	2605	PSU	C4-N3-C2	-4.08	120.46	126.34
55	1x	54	5MU	C5-C4-N3	4.06	118.77	115.31
1	2A	1939	5MU	C5-C6-N1	-4.04	119.18	123.34
1	2A	1939	5MU	O4-C4-C5	-4.02	120.24	124.90
32	1a	1519	MA6	C9-N6-C6	-4.02	109.98	120.40
54	2w	54	5MU	O4-C4-C5	-4.02	120.25	124.90
54	1w	39	PSU	C4-N3-C2	-4.01	120.57	126.34
1	1A	1939	PSU	C4-N3-C2	-4.00	120.58	126.34
54	2w	8	4SU	C5-C4-S4	-4.00	119.32	124.47
32	2a	1518	MA6	N3-C4-N9	3.99	133.65	127.08
54	2y	39	PSU	O2-C2-N1	-3.97	118.42	122.79
54	2y	54	5MU	C5-C4-N3	3.95	118.68	115.31
54	2y	55	PSU	C4-N3-C2	-3.94	120.67	126.34
54	1w	37	MIA	C16-C14-C13	-3.91	111.35	122.65
32	1a	516	PSU	C4-N3-C2	-3.89	120.73	126.34
54	2y	37	MIA	C2-N3-C4	3.88	120.93	111.75
54	2w	32	PSU	C4-N3-C2	-3.86	120.77	126.34
32	1a	1518	MA6	C4-C5-N7	-3.86	105.92	110.62
54	1y	37	MIA	C2-N3-C4	3.85	120.85	111.75
1	2A	1917	PSU	C4-N3-C2	-3.83	120.82	126.34
32	2a	1519	MA6	C4-C5-N7	-3.83	105.96	110.62
32	2a	1400	5MC	C5-C6-N1	-3.83	119.40	123.34
32	2a	1519	MA6	C2-N3-C4	3.82	120.76	111.75
32	1a	1519	MA6	C2-N3-C4	3.81	120.75	111.75
54	1y	54	5MU	C5-C6-N1	-3.81	119.42	123.34
54	1w	55	PSU	O2-C2-N1	-3.81	118.60	122.79
54	1y	55	PSU	O2-C2-N1	-3.80	118.60	122.79
1	1A	1933	PSU	C4-N3-C2	-3.80	120.87	126.34
55	2x	55	PSU	C4-N3-C2	-3.79	120.87	126.34
55	2x	54	5MU	C5-C6-N1	-3.79	119.44	123.34
54	1w	46	7MG	C2-N3-C4	3.79	119.05	112.30
32	1a	1519	MA6	C4-C5-N7	-3.79	106.01	110.62
54	2y	8	4SU	C5-C4-S4	-3.78	119.59	124.47
1	2A	1911	PSU	C4-N3-C2	-3.78	120.89	126.34
32	2a	516	PSU	C4-N3-C2	-3.77	120.91	126.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
54	1w	54	5MU	O4-C4-C5	-3.77	120.54	124.90
32	1a	1518	MA6	C2-N3-C4	3.75	120.62	111.75
1	1A	1937	5MU	O4-C4-C5	-3.75	120.56	124.90
54	1y	55	PSU	C4-N3-C2	-3.74	120.95	126.34
55	1x	55	PSU	C4-N3-C2	-3.74	120.95	126.34
54	1w	39	PSU	O2-C2-N1	-3.72	118.70	122.79
54	2w	55	PSU	C4-N3-C2	-3.71	120.99	126.34
1	1A	2617	PSU	C4-N3-C2	-3.69	121.02	126.34
32	2a	1518	MA6	C2-N3-C4	3.68	120.44	111.75
32	1a	1404	5MC	C5-C6-N1	-3.67	119.56	123.34
54	2y	32	PSU	C4-N3-C2	-3.66	121.06	126.34
55	1x	32	5MC	C5-C6-N1	-3.66	119.57	123.34
54	1w	55	PSU	C4-N3-C2	-3.66	121.07	126.34
55	1x	55	PSU	O2-C2-N1	-3.65	118.77	122.79
55	1x	54	5MU	O4-C4-C5	-3.65	120.67	124.90
54	2y	54	5MU	C4-N3-C2	-3.65	122.63	127.35
54	1y	39	PSU	O2-C2-N1	-3.64	118.78	122.79
32	1a	1400	5MC	C5-C6-N1	-3.62	119.61	123.34
54	1y	32	PSU	C4-N3-C2	-3.62	121.12	126.34
54	2y	8	4SU	N3-C2-N1	3.61	119.68	114.89
54	2y	54	5MU	N3-C2-N1	3.56	119.61	114.89
1	1A	1984	5MC	C5-C6-N1	-3.55	119.69	123.34
54	1w	32	PSU	C4-N3-C2	-3.54	121.24	126.34
54	2w	39	PSU	C4-N3-C2	-3.52	121.26	126.34
1	2A	1911	PSU	O2-C2-N1	-3.51	118.92	122.79
32	2a	1404	5MC	C5-C6-N1	-3.51	119.73	123.34
54	1y	54	5MU	O4-C4-C5	-3.50	120.84	124.90
54	2w	55	PSU	O2-C2-N1	-3.50	118.93	122.79
55	2x	55	PSU	O2-C2-N1	-3.50	118.93	122.79
1	1A	1933	PSU	O2-C2-N1	-3.50	118.94	122.79
32	2a	967	5MC	C5-C6-N1	-3.50	119.74	123.34
1	2A	1962	5MC	C5-C6-N1	-3.50	119.74	123.34
1	1A	2515	2MA	N6-C6-N1	3.49	121.97	117.03
54	2y	37	MIA	C4-C5-N7	-3.48	106.38	110.62
54	1y	8	4SU	C5-C4-S4	-3.45	120.02	124.47
1	2A	2503	2MA	C4-C5-N7	-3.44	106.42	110.62
1	1A	1937	5MU	C5-C6-N1	-3.43	119.81	123.34
1	2A	1917	PSU	O2-C2-N1	-3.43	119.01	122.79
43	2l	92	0TD	OD2-CG-CB	3.43	120.56	113.15
54	1w	54	5MU	C5-C6-N1	-3.43	119.81	123.34
54	2w	37	MIA	C2-N3-C4	3.43	121.37	112.35
54	1y	37	MIA	C4-C5-N7	-3.43	106.45	110.62

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
54	2y	37	MIA	N3-C2-N1	-3.42	123.25	128.60
54	2y	54	5MU	O4-C4-C5	-3.42	120.94	124.90
54	1y	32	PSU	O2-C2-N1	-3.42	119.03	122.79
32	1a	1207	2MG	C6-C5-N7	3.41	136.59	130.25
1	1A	2515	2MA	C4-N9-C8	3.41	109.42	105.73
32	2a	1207	2MG	C6-C5-N7	3.40	136.57	130.25
1	1A	2617	PSU	O2-C2-N1	-3.38	119.06	122.79
54	1y	37	MIA	N3-C2-N1	-3.37	123.33	128.60
1	2A	1915	5MU	O4-C4-C5	-3.37	121.00	124.90
1	1A	1939	PSU	O2-C2-N1	-3.37	119.08	122.79
54	2y	55	PSU	O2-C2-N1	-3.36	119.09	122.79
55	1x	8	4SU	C1'-N1-C2	3.36	123.65	117.57
54	2w	32	PSU	O2-C2-N1	-3.35	119.10	122.79
54	1w	37	MIA	C2-N3-C4	3.34	121.15	112.35
1	2A	1942	5MC	C5-C6-N1	-3.32	119.92	123.34
32	1a	1518	MA6	N1-C2-N3	-3.32	123.41	128.60
54	2y	32	PSU	O2-C2-N1	-3.30	119.16	122.79
1	1A	1964	5MC	C5-C6-N1	-3.30	119.95	123.34
32	1a	1407	5MC	C5-C6-N1	-3.29	119.95	123.34
54	2w	37	MIA	C12-N6-C6	-3.29	120.03	122.87
54	2w	8	4SU	C1'-N1-C2	3.28	123.51	117.57
54	1w	46	7MG	C5-C4-N9	-3.28	102.09	106.35
54	1w	8	4SU	C5-C4-S4	-3.27	120.25	124.47
32	2a	1518	MA6	C5-N7-C8	3.27	108.16	103.51
54	1w	8	4SU	N3-C2-N1	3.26	119.22	114.89
32	2a	516	PSU	O2-C2-N1	-3.21	119.26	122.79
32	1a	1518	MA6	C5-N7-C8	3.20	108.05	103.51
32	1a	516	PSU	O2-C2-N1	-3.19	119.27	122.79
32	2a	1518	MA6	N1-C2-N3	-3.19	123.61	128.60
54	2w	37	MIA	C6-C5-N7	3.19	135.85	132.39
54	2w	37	MIA	C4-C5-N7	-3.19	106.73	110.62
32	2a	1519	MA6	N1-C2-N3	-3.18	123.62	128.60
54	1w	37	MIA	C12-N6-C6	-3.16	117.86	122.55
54	1w	37	MIA	C4-C5-N7	-3.15	106.78	110.62
55	2x	32	5MC	C5-C6-N1	-3.15	120.10	123.34
54	1w	32	PSU	O2-C2-N1	-3.14	119.33	122.79
55	1x	54	5MU	C5-C6-N1	-3.14	120.11	123.34
32	1a	966	M2G	C6-C5-N7	3.13	136.07	130.25
32	2a	966	M2G	C6-C5-N7	3.12	136.06	130.25
54	2w	54	5MU	C5-C6-N1	-3.11	120.14	123.34
32	2a	1519	MA6	C5-N7-C8	3.09	107.90	103.51
1	1A	2564	2MU	O2-C2-N1	-3.09	118.68	122.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
32	2a	1407	5MC	C5-C6-N1	-3.09	120.16	123.34
1	1A	2263	OMG	C6-C5-N7	3.08	135.98	130.25
32	1a	1519	MA6	N1-C2-N3	-3.06	123.82	128.60
54	1w	37	MIA	C6-C5-N7	3.05	135.69	132.39
32	1a	967	5MC	C5-C6-N1	-3.04	120.21	123.34
32	1a	1519	MA6	C5-N7-C8	3.04	107.83	103.51
1	2A	2251	OMG	C6-C5-N7	3.00	135.83	130.25
1	2A	2605	PSU	O2-C2-N1	-2.96	119.53	122.79
54	2y	37	MIA	C5-N7-C8	2.92	107.66	103.51
55	1x	8	4SU	C6-C5-C4	-2.92	117.43	119.95
32	1a	1518	MA6	C4-N9-C8	2.91	108.89	105.73
1	1A	2515	2MA	C4-C5-N7	-2.88	107.11	110.62
43	1l	92	0TD	OD2-CG-CB	2.85	119.32	113.15
32	2a	527	7MG	C5-C6-N1	2.85	116.01	110.99
54	2y	54	5MU	C5-C6-N1	-2.83	120.42	123.34
1	1A	2515	2MA	C2-N1-C6	2.83	122.49	118.08
1	2A	2552	2MU	C5-C4-N3	2.82	119.06	114.84
32	2a	1207	2MG	C4-C5-N7	-2.82	106.26	110.72
1	2A	2503	2MA	C5-N7-C8	2.82	107.51	103.51
54	2w	39	PSU	O2-C2-N1	-2.82	119.69	122.79
55	1x	32	5MC	C5-C4-N3	-2.81	118.64	121.67
54	1y	37	MIA	C5-N7-C8	2.80	107.49	103.51
32	1a	1207	2MG	C4-C5-N7	-2.78	106.32	110.72
1	1A	2564	2MU	C5-C4-N3	2.77	118.98	114.84
54	2w	46	7MG	C5-C6-N1	2.77	115.86	110.99
32	1a	1519	MA6	N1-C6-N6	2.75	120.09	117.08
1	1A	2263	OMG	C4-C5-N7	-2.74	106.38	110.72
32	1a	1518	MA6	C10-N6-C6	-2.72	113.33	120.40
54	2y	46	7MG	C5-C4-N9	-2.72	102.81	106.35
1	1A	2515	2MA	C5-N7-C8	2.72	107.37	103.51
32	2a	1404	5MC	C5-C4-N3	-2.70	118.76	121.67
55	2x	54	5MU	O2-C2-N1	-2.69	119.21	122.79
55	1x	8	4SU	O2-C2-N1	2.68	126.34	122.79
55	2x	32	5MC	O2-C2-N3	-2.67	117.98	122.33
32	1a	527	7MG	C5-C6-N1	2.67	115.70	110.99
1	2A	2503	2MA	N6-C6-N1	2.66	120.80	117.03
32	2a	1407	5MC	C5-C4-N3	-2.66	118.81	121.67
54	2w	37	MIA	C5-N7-C8	2.65	107.28	103.51
32	1a	1407	5MC	C5-C4-N3	-2.65	118.81	121.67
1	2A	2552	2MU	O2-C2-N1	-2.64	119.28	122.79
54	1w	37	MIA	C5-N7-C8	2.63	107.25	103.51
32	1a	966	M2G	C4-C5-N7	-2.63	106.55	110.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	2A	2251	OMG	C4-C5-N7	-2.63	106.56	110.72
1	2A	2503	2MA	C2-N1-C6	2.63	122.17	118.08
1	1A	1964	5MC	C5-C4-N3	-2.60	118.87	121.67
1	2A	1942	5MC	C5-C4-N3	-2.59	118.88	121.67
32	1a	967	5MC	C5-C4-N3	-2.57	118.90	121.67
1	1A	1984	5MC	C5-C4-N3	-2.57	118.90	121.67
54	2y	46	7MG	C5-C6-N1	2.57	115.51	110.99
55	2x	32	5MC	C5-C4-N3	-2.57	118.91	121.67
54	1w	54	5MU	O2-C2-N1	-2.56	119.38	122.79
54	1w	37	MIA	C11-S10-C2	-2.56	100.36	102.27
32	2a	1519	MA6	C4-N9-C8	2.55	108.50	105.73
32	2a	966	M2G	C4-C5-N7	-2.54	106.70	110.72
32	2a	1519	MA6	C10-N6-C6	-2.54	113.82	120.40
54	1w	37	MIA	C2-N1-C6	2.54	122.13	117.28
1	2A	2503	2MA	C4-N9-C8	2.53	108.47	105.73
32	1a	1404	5MC	C5-C4-N3	-2.53	118.95	121.67
1	1A	2515	2MA	N9-C8-N7	-2.53	110.46	113.91
54	2w	54	5MU	O2-C2-N1	-2.53	119.43	122.79
55	2x	8	4SU	C5-C4-S4	-2.52	121.22	124.47
54	1y	54	5MU	O2-C2-N1	-2.52	119.44	122.79
32	2a	967	5MC	C5-C4-N3	-2.51	118.97	121.67
54	1y	46	7MG	C5-C6-N1	2.51	115.41	110.99
32	2a	1518	MA6	C6-C5-N7	2.49	137.47	133.28
32	1a	1519	MA6	C10-N6-C6	-2.49	113.94	120.40
32	2a	1518	MA6	C10-N6-C9	-2.48	108.12	116.12
32	1a	1400	5MC	C5-C4-N3	-2.48	119.00	121.67
1	2A	1915	5MU	O2-C2-N1	-2.48	119.49	122.79
1	2A	2552	2MU	O4-C4-C5	-2.47	120.81	125.16
32	2a	1518	MA6	C4-N9-C8	2.47	108.40	105.73
43	2l	92	0TD	OD1-CG-CB	-2.47	117.27	122.44
54	2y	37	MIA	C4-N9-C8	2.46	108.39	105.73
55	2x	8	4SU	C4-N3-C2	-2.45	124.97	127.34
54	2w	37	MIA	C2-N1-C6	2.44	121.95	117.28
32	2a	1404	5MC	O2-C2-N3	-2.44	118.36	122.33
54	2w	37	MIA	N6-C6-N1	2.44	121.55	118.50
32	1a	1402	4OC	C6-C5-C4	2.44	119.94	116.96
1	1A	2564	2MU	C2'-C1'-N1	-2.44	109.49	114.22
1	2A	2503	2MA	C6-C5-N7	2.43	136.55	132.02
54	2w	37	MIA	N3-C2-N1	-2.43	122.49	126.95
32	1a	1518	MA6	N9-C8-N7	-2.43	110.60	113.91
1	2A	1939	5MU	O2-C2-N1	-2.42	119.57	122.79
1	2A	1962	5MC	C5-C4-N3	-2.42	119.07	121.67

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
55	1x	8	4SU	O2-C2-N3	-2.41	117.00	121.50
54	1y	46	7MG	C5-C4-N9	-2.41	103.22	106.35
55	2x	8	4SU	C6-C5-C4	-2.38	117.89	119.95
54	2y	54	5MU	C1'-N1-C2	2.38	121.88	117.57
1	1A	1961	5MU	O2-C2-N1	-2.37	119.64	122.79
54	1w	37	MIA	C4-N9-C8	2.34	108.26	105.73
1	1A	1937	5MU	O2-C2-N1	-2.32	119.70	122.79
32	2a	1402	4OC	C6-C5-C4	2.31	119.79	116.96
54	2w	37	MIA	C4-N9-C8	2.30	108.23	105.73
32	2a	527	7MG	C5-C4-N9	-2.29	103.38	106.35
55	1x	54	5MU	O2-C2-N1	-2.29	119.75	122.79
32	2a	1400	5MC	C5-C4-N3	-2.28	119.21	121.67
54	1w	37	MIA	N3-C2-N1	-2.28	122.77	126.95
55	2x	8	4SU	C1'-N1-C6	-2.28	115.88	120.84
32	1a	1518	MA6	C6-C5-N7	2.28	137.10	133.28
32	1a	1400	5MC	O2-C2-N3	-2.27	118.64	122.33
54	2y	54	5MU	C1'-N1-C6	-2.27	117.35	121.12
54	1y	37	MIA	C4-N9-C8	2.26	108.18	105.73
54	2w	46	7MG	O6-C6-C5	-2.26	122.00	127.54
32	1a	1519	MA6	C4-N9-C8	2.25	108.17	105.73
1	1A	1942	4OC	O2-C2-N3	-2.22	118.72	122.33
55	1x	54	5MU	C5M-C5-C4	2.21	121.19	118.77
54	2y	37	MIA	C6-C5-N7	2.20	136.13	132.02
1	1A	2564	2MU	O4-C4-C5	-2.20	121.30	125.16
32	1a	1518	MA6	C10-N6-C9	-2.20	109.04	116.12
32	1a	967	5MC	C1'-N1-C6	-2.20	117.47	121.12
1	1A	2515	2MA	C6-C5-N7	2.19	136.10	132.02
32	2a	1519	MA6	C6-C5-N7	2.19	136.96	133.28
1	1A	2263	OMG	O6-C6-C5	-2.18	120.81	126.60
1	2A	2503	2MA	N9-C8-N7	-2.18	110.94	113.91
32	1a	516	PSU	O4'-C1'-C2'	2.17	108.21	105.14
32	2a	1407	5MC	O2-C2-N3	-2.17	118.81	122.33
32	2a	1518	MA6	N9-C8-N7	-2.15	110.97	113.91
32	2a	1402	4OC	O2-C2-N3	-2.15	118.83	122.33
54	2w	46	7MG	C5-C4-N9	-2.15	103.56	106.35
32	2a	527	7MG	O6-C6-C5	-2.14	122.29	127.54
54	1y	37	MIA	C6-C5-N7	2.13	136.00	132.02
32	2a	966	M2G	O6-C6-C5	-2.12	120.98	126.60
32	1a	527	7MG	CM7-N7-C5	2.11	131.84	126.40
54	1w	46	7MG	C5-C6-N1	2.09	114.67	110.99
1	2A	2605	PSU	C5-C6-N1	-2.09	118.98	122.11
54	2y	46	7MG	O6-C6-C5	-2.08	122.43	127.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
32	2a	1518	MA6	C10-N6-C6	-2.08	115.02	120.40
32	1a	1518	MA6	N1-C6-N6	2.07	119.35	117.08
32	1a	527	7MG	C5-C4-N9	-2.07	103.66	106.35
32	1a	966	M2G	O6-C6-C5	-2.06	121.14	126.60
54	1w	46	7MG	CM7-N7-C5	2.06	131.72	126.40
54	2y	39	PSU	C5-C6-N1	-2.05	119.03	122.11
32	2a	1519	MA6	N9-C8-N7	-2.05	111.11	113.91
32	2a	1207	2MG	O6-C6-C5	-2.03	121.20	126.60
54	2y	46	7MG	CM7-N7-C5	2.03	131.64	126.40
54	2w	54	5MU	C5M-C5-C4	2.02	120.99	118.77
32	2a	516	PSU	O4'-C1'-C2'	2.02	107.99	105.14
54	2y	37	MIA	N9-C8-N7	-2.01	111.16	113.91
32	2a	1519	MA6	N1-C6-N6	2.01	119.28	117.08
54	1w	8	4SU	C1'-N1-C2	2.01	121.21	117.57

There are no chirality outliers.

All (71) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
32	1a	527	7MG	C3'-C4'-C5'-O5'
32	1a	967	5MC	O4'-C4'-C5'-O5'
32	1a	967	5MC	C3'-C4'-C5'-O5'
32	1a	1207	2MG	N3-C2-N2-CM2
32	1a	1518	MA6	C5-C6-N6-C10
43	1l	92	0TD	O-C-CA-CB
32	2a	1402	4OC	O4'-C4'-C5'-O5'
32	2a	1518	MA6	C5-C6-N6-C9
32	2a	1519	MA6	O4'-C4'-C5'-O5'
32	2a	1519	MA6	C3'-C4'-C5'-O5'
32	2a	1519	MA6	C5-C6-N6-C10
43	2l	92	0TD	O-C-CA-CB
54	1y	8	4SU	O4'-C4'-C5'-O5'
54	1w	37	MIA	C12-C13-C14-C16
54	2w	37	MIA	N1-C6-N6-C12
32	1a	1519	MA6	O4'-C4'-C5'-O5'
32	1a	1519	MA6	C3'-C4'-C5'-O5'
32	2a	1402	4OC	C3'-C4'-C5'-O5'
54	1y	8	4SU	C3'-C4'-C5'-O5'
54	2y	8	4SU	O4'-C4'-C5'-O5'
54	1w	46	7MG	C4'-C5'-O5'-P
54	2y	8	4SU	C3'-C4'-C5'-O5'
32	2a	1518	MA6	N1-C6-N6-C9

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Mol	Chain	Res	Type	Atoms
54	1y	37	MIA	C3'-C4'-C5'-O5'
54	2y	37	MIA	C3'-C4'-C5'-O5'
32	1a	527	7MG	O4'-C4'-C5'-O5'
32	2a	1207	2MG	O4'-C4'-C5'-O5'
32	1a	1518	MA6	C5-C6-N6-C9
32	1a	1519	MA6	C5-C6-N6-C10
32	2a	1519	MA6	C5-C6-N6-C9
54	2w	46	7MG	C2'-C1'-N9-C8
54	2y	37	MIA	O4'-C4'-C5'-O5'
54	1w	46	7MG	C3'-C4'-C5'-O5'
32	1a	1402	4OC	O4'-C4'-C5'-O5'
54	1y	37	MIA	O4'-C4'-C5'-O5'
54	1w	46	7MG	O4'-C4'-C5'-O5'
1	2A	1920	4OC	C1'-C2'-O2'-CM2
43	2l	92	0TD	CG-CB-SB-CSB
32	2a	1519	MA6	C4'-C5'-O5'-P
54	2y	46	7MG	C4'-C5'-O5'-P
54	2w	46	7MG	O4'-C4'-C5'-O5'
54	2y	46	7MG	C2'-C1'-N9-C8
54	1y	46	7MG	C4'-C5'-O5'-P
32	2a	1518	MA6	C5-C6-N6-C10
32	2a	527	7MG	C4'-C5'-O5'-P
32	2a	527	7MG	C3'-C4'-C5'-O5'
54	1y	55	PSU	O4'-C1'-C5-C4
54	2y	55	PSU	O4'-C1'-C5-C4
1	2A	2503	2MA	O4'-C4'-C5'-O5'
54	2w	46	7MG	O4'-C1'-N9-C8
1	2A	2251	OMG	C4'-C5'-O5'-P
1	2A	2503	2MA	C4'-C5'-O5'-P
32	2a	967	5MC	O4'-C4'-C5'-O5'
32	2a	1207	2MG	C3'-C4'-C5'-O5'
54	2w	37	MIA	C5-C6-N6-C12
43	1l	92	0TD	SB-CB-CG-OD2
54	2w	46	7MG	C3'-C4'-C5'-O5'
1	2A	1920	4OC	C3'-C2'-O2'-CM2
1	1A	1942	4OC	C2'-C1'-N1-C2
43	1l	92	0TD	CG-CB-SB-CSB
54	1y	55	PSU	O4'-C1'-C5-C6
54	2y	55	PSU	O4'-C1'-C5-C6
54	2w	8	4SU	C2'-C1'-N1-C2
54	2y	46	7MG	O4'-C1'-N9-C8
1	1A	2515	2MA	O4'-C4'-C5'-O5'

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Mol	Chain	Res	Type	Atoms
32	1a	1402	4OC	C3'-C4'-C5'-O5'
54	1y	46	7MG	C2'-C1'-N9-C8
55	2x	8	4SU	C2'-C1'-N1-C2
1	1A	2515	2MA	C4'-C5'-O5'-P
1	2A	1962	5MC	C2'-C1'-N1-C6
54	1y	8	4SU	C4'-C5'-O5'-P

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 2821 ligands modelled in this entry, 2817 are monoatomic - leaving 4 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	$\#\|Z\| > 2$
60	SF4	2d	302	35	0,12,12	-	-	-		
58	M2D	1A	4118	-	37,37,37	2.90	16 (43%)	46,50,50	3.01	10 (21%)
58	M2D	2A	3864	-	37,37,37	2.97	15 (40%)	46,50,50	2.93	12 (26%)
60	SF4	1d	501	35	0,12,12	-	-	-		

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
60	SF4	2d	302	35	-	-	0/6/5/5

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
58	M2D	1A	4118	-	-	5/48/48/48	0/1/2/2
58	M2D	2A	3864	-	-	6/48/48/48	0/1/2/2
60	SF4	1d	501	35	-	-	0/6/5/5

All (31) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
58	2A	3864	M2D	CAM-CAL	-8.05	1.40	1.50
58	2A	3864	M2D	CAT-CAY	-7.89	1.33	1.48
58	1A	4118	M2D	CAT-CAY	-7.76	1.33	1.48
58	1A	4118	M2D	CAM-CAL	-7.27	1.41	1.50
58	2A	3864	M2D	CAP-CAQ	-5.76	1.39	1.49
58	1A	4118	M2D	CBD-CAK	-5.43	1.39	1.50
58	1A	4118	M2D	CAP-CAQ	-5.37	1.39	1.49
58	2A	3864	M2D	CBD-CAK	-5.27	1.40	1.50
58	1A	4118	M2D	CAC-CAD	-4.34	1.40	1.51
58	2A	3864	M2D	CAE-CAF	-4.23	1.39	1.48
58	2A	3864	M2D	CAC-CAD	-4.17	1.40	1.51
58	1A	4118	M2D	CAE-CAF	-4.12	1.39	1.48
58	1A	4118	M2D	CAQ-NAU	3.85	1.33	1.29
58	2A	3864	M2D	CAQ-NAU	3.83	1.33	1.29
58	1A	4118	M2D	CAF-NAG	3.75	1.42	1.34
58	2A	3864	M2D	CAF-NAG	3.61	1.42	1.34
58	1A	4118	M2D	CAJ-CAI	3.56	1.41	1.32
58	1A	4118	M2D	CA-C	-3.53	1.39	1.51
58	2A	3864	M2D	CAJ-CAI	3.50	1.41	1.32
58	2A	3864	M2D	CA-C	-3.46	1.39	1.51
58	2A	3864	M2D	CAE-CAD	3.13	1.39	1.32
58	1A	4118	M2D	CAE-CAD	3.12	1.39	1.32
58	2A	3864	M2D	CAY-N	2.91	1.40	1.34
58	1A	4118	M2D	CAY-N	2.54	1.39	1.34
58	2A	3864	M2D	CAH-CAI	-2.54	1.40	1.50
58	1A	4118	M2D	CAH-CAI	-2.49	1.40	1.50
58	2A	3864	M2D	CAJ-CAK	-2.43	1.40	1.45
58	1A	4118	M2D	CAT-NAU	-2.43	1.33	1.38
58	2A	3864	M2D	CAT-NAU	-2.40	1.33	1.38
58	1A	4118	M2D	CAJ-CAK	-2.38	1.40	1.45
58	1A	4118	M2D	CAL-CAK	2.12	1.41	1.34

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
58	1A	4118	M2D	OAR-CAQ-CAP	11.10	133.68	117.96
58	2A	3864	M2D	OAR-CAQ-CAP	10.84	133.30	117.96
58	1A	4118	M2D	OAR-CAQ-NAU	-8.20	107.15	113.75
58	1A	4118	M2D	CAI-CAJ-CAK	7.81	137.69	125.89
58	2A	3864	M2D	CAT-NAU-CAQ	7.61	109.04	104.55
58	1A	4118	M2D	CAT-NAU-CAQ	7.46	108.95	104.55
58	2A	3864	M2D	OAR-CAQ-NAU	-7.39	107.80	113.75
58	2A	3864	M2D	CAI-CAJ-CAK	6.59	135.85	125.89
58	2A	3864	M2D	CAP-CAQ-NAU	-6.43	118.87	128.75
58	1A	4118	M2D	CAP-CAQ-NAU	-6.25	119.14	128.75
58	2A	3864	M2D	CBD-CAK-CAJ	3.48	123.56	118.08
58	1A	4118	M2D	CBD-CAK-CAJ	3.24	123.19	118.08
58	1A	4118	M2D	CAH-NAG-CAF	2.80	126.56	122.03
58	2A	3864	M2D	CAH-NAG-CAF	2.63	126.28	122.03
58	2A	3864	M2D	CAB-OAA-C	-2.54	113.42	117.78
58	2A	3864	M2D	CAN-CAM-CAL	2.47	116.91	111.94
58	2A	3864	M2D	CAC-CAB-CAZ	-2.44	109.97	115.98
58	1A	4118	M2D	CAE-CAF-NAG	2.32	119.35	114.97
58	1A	4118	M2D	CAN-CAO-CAP	-2.28	108.66	113.19
58	1A	4118	M2D	CAT-CAY-N	2.12	118.34	115.22
58	2A	3864	M2D	CAC-CAD-CAE	-2.08	120.75	126.44
58	2A	3864	M2D	CAT-CAY-N	2.08	118.28	115.22

There are no chirality outliers.

All (11) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
58	1A	4118	M2D	CAM-CAN-CAO-CAP
58	1A	4118	M2D	CAM-CAN-CAO-OBF
58	2A	3864	M2D	CAM-CAN-CAO-OBF
58	2A	3864	M2D	CAI-CAH-NAG-CAF
58	2A	3864	M2D	CBB-CAC-CAD-CAE
58	1A	4118	M2D	CAI-CAH-NAG-CAF
58	1A	4118	M2D	CBB-CAC-CAD-CAE
58	1A	4118	M2D	CAB-CAC-CAD-CAE
58	2A	3864	M2D	CAB-CAC-CAD-CAE
58	2A	3864	M2D	O-C-CA-CB
58	2A	3864	M2D	OAA-C-CA-CB

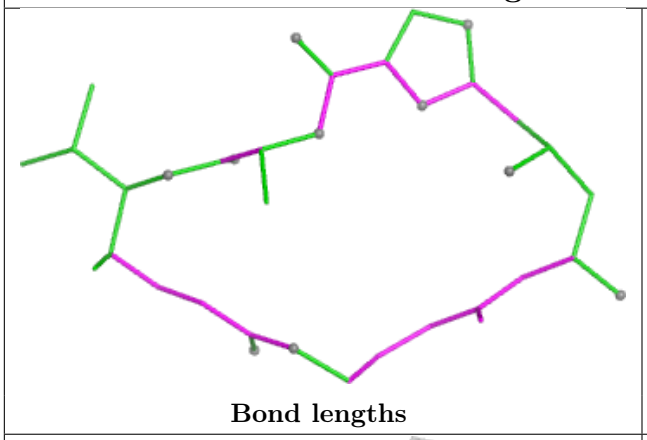
There are no ring outliers.

No monomer is involved in short contacts.

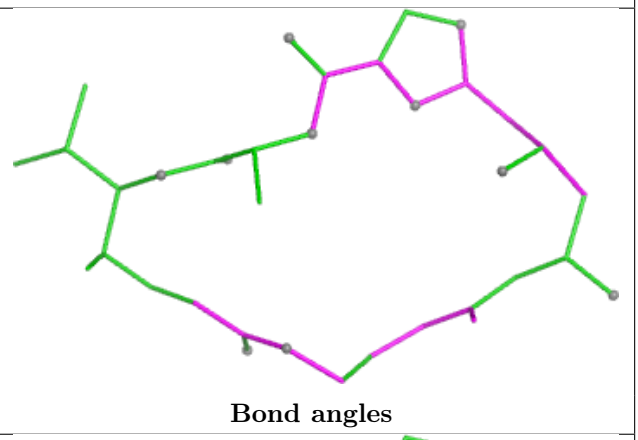
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths,

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

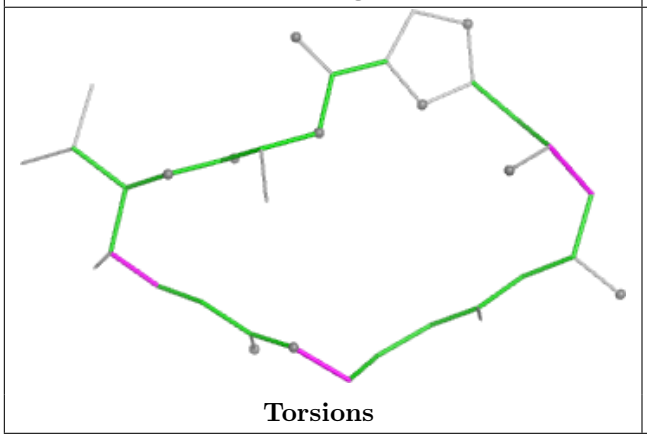
Ligand M2D 1A 4118



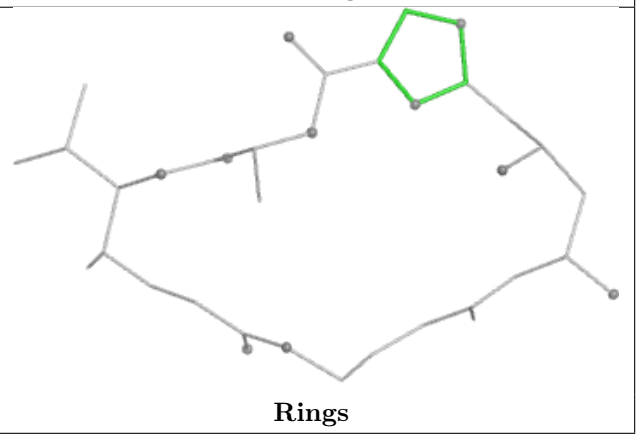
Bond lengths



Bond angles

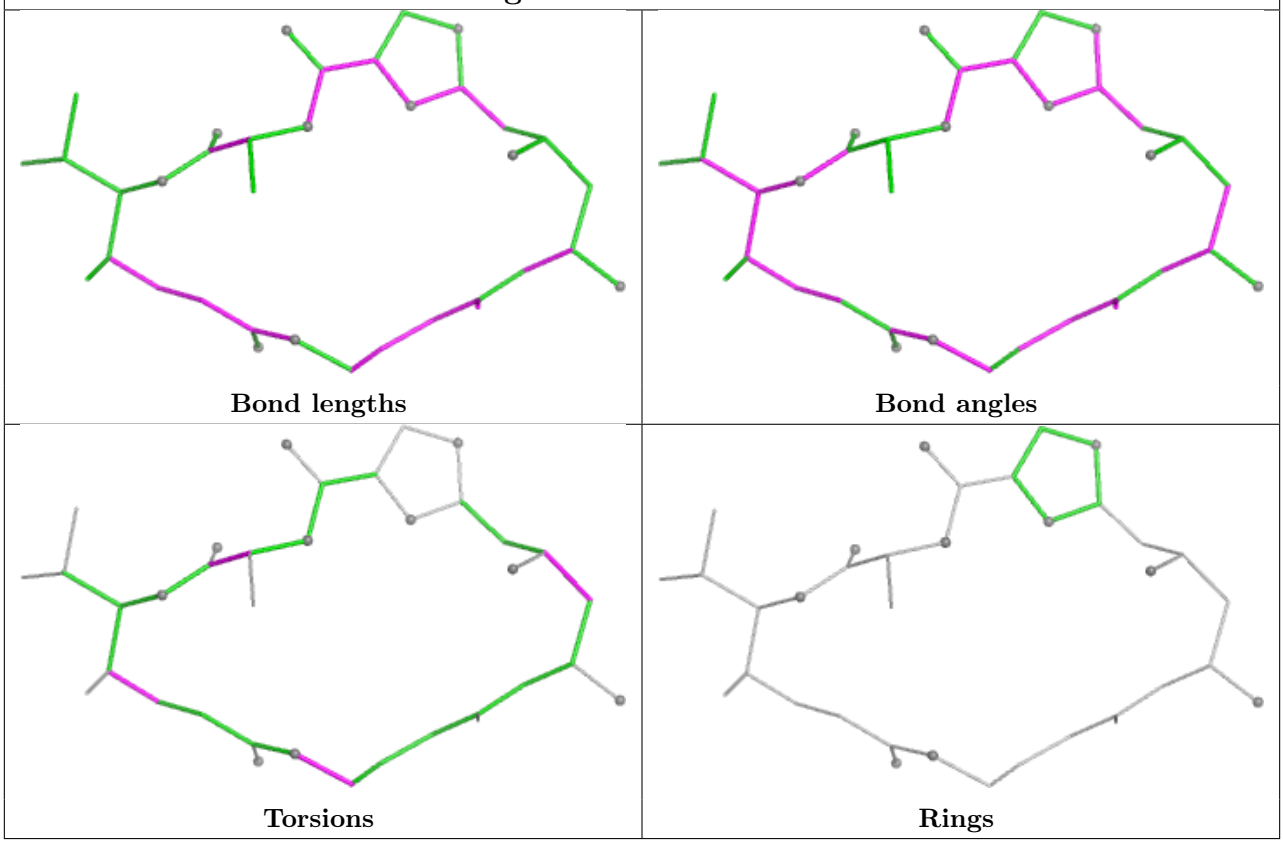


Torsions



Rings

Ligand M2D 2A 3864



4.7 Other polymers

There are no such residues in this entry.

4.8 Polymer linkage issues

There are no chain breaks in this entry.

5 Fit of model and data

5.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	1A	2860/2915 (98%)	-0.45	50 (1%) 69 60	10, 26, 82, 97	0
1	2A	2789/2915 (95%)	0.09	73 (2%) 57 47	25, 51, 82, 96	0
2	1B	120/121 (99%)	-0.42	0 100 100	19, 38, 50, 74	0
2	2B	120/121 (99%)	0.75	2 (1%) 69 60	55, 70, 76, 82	0
3	1D	275/276 (99%)	-0.19	1 (0%) 88 84	12, 29, 43, 62	0
3	2D	275/276 (99%)	0.29	1 (0%) 88 84	25, 43, 56, 69	0
4	1E	204/206 (99%)	-0.25	1 (0%) 87 82	11, 29, 48, 68	0
4	2E	204/206 (99%)	0.17	1 (0%) 87 82	29, 51, 62, 71	0
5	1F	203/210 (96%)	-0.16	0 100 100	12, 32, 62, 75	0
5	2F	203/210 (96%)	0.52	2 (0%) 79 72	28, 58, 70, 80	0
6	1G	181/182 (99%)	0.26	3 (1%) 69 60	28, 46, 61, 72	0
6	2G	181/182 (99%)	1.05	17 (9%) 14 10	59, 69, 78, 88	0
7	1H	174/180 (96%)	0.09	1 (0%) 85 80	24, 42, 54, 60	0
7	2H	174/180 (96%)	1.06	16 (9%) 14 10	55, 72, 81, 84	0
8	1I	146/148 (98%)	0.56	3 (2%) 63 54	35, 63, 72, 78	0
8	2I	146/148 (98%)	0.69	3 (2%) 63 54	44, 62, 72, 76	0
9	1N	140/140 (100%)	-0.23	0 100 100	15, 27, 46, 57	0
9	2N	140/140 (100%)	0.68	7 (5%) 34 26	40, 57, 67, 74	0
10	1O	122/122 (100%)	-0.22	0 100 100	20, 30, 45, 55	0
10	2O	122/122 (100%)	0.44	2 (1%) 70 61	38, 53, 63, 68	0
11	1P	149/150 (99%)	-0.07	0 100 100	12, 36, 59, 70	0
11	2P	149/150 (99%)	0.48	2 (1%) 75 66	31, 59, 71, 79	0
12	1Q	141/141 (100%)	-0.19	0 100 100	19, 32, 44, 66	0
12	2Q	141/141 (100%)	0.74	11 (7%) 19 14	44, 60, 73, 77	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
13	1R	118/118 (100%)	-0.37	0 100 100	14, 24, 36, 43	0
13	2R	118/118 (100%)	0.12	0 100 100	33, 44, 55, 64	0
14	1S	110/112 (98%)	-0.05	0 100 100	27, 38, 50, 59	0
14	2S	110/112 (98%)	1.00	8 (7%) 21 15	55, 65, 71, 75	0
15	1T	131/146 (89%)	-0.01	2 (1%) 72 63	23, 33, 55, 64	0
15	2T	131/146 (89%)	0.51	4 (3%) 51 41	41, 55, 68, 81	0
16	1U	116/118 (98%)	-0.42	1 (0%) 81 74	12, 19, 37, 59	0
16	2U	116/118 (98%)	0.55	4 (3%) 48 39	38, 53, 68, 76	0
17	1V	101/101 (100%)	-0.45	0 100 100	12, 27, 43, 51	0
17	2V	101/101 (100%)	0.64	4 (3%) 42 33	39, 60, 69, 78	0
18	1W	112/113 (99%)	-0.41	1 (0%) 81 74	15, 21, 44, 69	0
18	2W	112/113 (99%)	0.30	2 (1%) 67 58	30, 41, 55, 81	0
19	1X	95/96 (98%)	-0.15	2 (2%) 63 54	17, 29, 46, 63	0
19	2X	95/96 (98%)	0.53	1 (1%) 78 70	37, 53, 62, 68	0
20	1Y	107/110 (97%)	0.20	2 (1%) 66 57	26, 40, 55, 72	0
20	2Y	107/110 (97%)	1.01	13 (12%) 8 6	51, 61, 69, 75	0
21	1Z	154/206 (74%)	0.39	4 (2%) 57 47	30, 50, 75, 82	0
21	2Z	160/206 (77%)	1.35	25 (15%) 5 4	61, 73, 81, 84	0
22	10	83/85 (97%)	0.28	7 (8%) 17 12	19, 28, 59, 80	0
22	20	83/85 (97%)	0.76	8 (9%) 13 10	46, 57, 69, 78	0
23	11	97/98 (98%)	0.20	1 (1%) 79 72	15, 35, 58, 63	0
23	21	97/98 (98%)	0.48	4 (4%) 41 33	32, 49, 67, 71	0
24	12	70/72 (97%)	0.10	1 (1%) 73 64	25, 39, 50, 69	0
24	22	70/72 (97%)	0.46	1 (1%) 73 64	49, 60, 69, 73	0
25	13	59/60 (98%)	-0.25	0 100 100	15, 26, 46, 64	0
25	23	59/60 (98%)	0.48	0 100 100	46, 56, 70, 78	0
26	14	69/71 (97%)	0.50	4 (5%) 29 22	40, 59, 76, 82	0
26	24	69/71 (97%)	1.33	11 (15%) 5 4	64, 75, 83, 84	0
27	15	59/60 (98%)	-0.39	1 (1%) 69 60	11, 22, 41, 58	0
27	25	59/60 (98%)	0.12	0 100 100	31, 44, 54, 65	0
28	16	53/54 (98%)	-0.38	0 100 100	22, 32, 46, 48	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
28	26	53/54 (98%)	0.67	1 (1%) 66 57	43, 53, 61, 66	0
29	17	48/49 (97%)	-0.24	0 100 100	13, 19, 51, 54	0
29	27	48/49 (97%)	0.11	2 (4%) 40 32	26, 33, 54, 65	0
30	18	64/65 (98%)	-0.14	0 100 100	17, 24, 32, 43	0
30	28	64/65 (98%)	0.36	0 100 100	39, 47, 55, 57	0
31	19	37/37 (100%)	-0.25	0 100 100	18, 30, 46, 50	0
31	29	37/37 (100%)	1.06	2 (5%) 31 24	51, 63, 68, 70	0
32	1a	1488/1521 (97%)	0.28	33 (2%) 62 52	28, 57, 81, 96	0
32	2a	1491/1521 (98%)	0.70	82 (5%) 30 23	48, 69, 85, 95	0
33	1b	231/256 (90%)	0.99	33 (14%) 6 5	55, 68, 79, 83	0
33	2b	231/256 (90%)	1.37	39 (16%) 4 3	65, 77, 83, 86	0
34	1c	206/239 (86%)	0.63	10 (4%) 35 27	50, 63, 74, 80	0
34	2c	206/239 (86%)	1.38	47 (22%) 2 1	65, 75, 82, 88	0
35	1d	208/209 (99%)	0.90	15 (7%) 21 16	47, 62, 71, 82	0
35	2d	208/209 (99%)	0.88	12 (5%) 29 22	52, 63, 72, 73	0
36	1e	148/162 (91%)	0.45	1 (0%) 84 77	44, 56, 62, 69	0
36	2e	148/162 (91%)	1.18	23 (15%) 5 4	58, 69, 77, 80	0
37	1f	100/101 (99%)	0.60	0 100 100	46, 59, 68, 71	0
37	2f	100/101 (99%)	0.50	1 (1%) 79 72	52, 63, 70, 72	0
38	1g	155/156 (99%)	0.65	7 (4%) 38 30	48, 59, 70, 81	0
38	2g	155/156 (99%)	1.16	22 (14%) 6 5	60, 69, 78, 90	0
39	1h	137/138 (99%)	0.60	1 (0%) 84 77	47, 58, 66, 72	0
39	2h	137/138 (99%)	1.17	15 (10%) 10 8	59, 69, 75, 78	0
40	1i	127/128 (99%)	1.08	7 (5%) 30 23	42, 66, 74, 76	0
40	2i	127/128 (99%)	1.41	31 (24%) 2 1	65, 75, 82, 85	0
41	1j	97/105 (92%)	1.06	11 (11%) 10 7	50, 68, 77, 80	0
41	2j	96/105 (91%)	1.73	37 (38%) 1 0	67, 76, 84, 94	0
42	1k	114/129 (88%)	0.61	1 (0%) 81 74	36, 54, 65, 69	0
42	2k	114/129 (88%)	1.04	9 (7%) 18 13	44, 65, 72, 75	0
43	1l	121/132 (91%)	0.32	2 (1%) 69 60	38, 46, 58, 65	0
43	2l	121/132 (91%)	0.65	2 (1%) 69 60	49, 61, 69, 74	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
44	1m	123/126 (97%)	0.50	5 (4%) 41 33	44, 57, 67, 72	0
44	2m	122/126 (96%)	1.41	21 (17%) 4 3	60, 72, 77, 82	0
45	1n	60/61 (98%)	0.82	3 (5%) 34 26	52, 58, 65, 71	0
45	2n	60/61 (98%)	1.97	29 (48%) 0 0	69, 75, 81, 84	0
46	1o	88/89 (98%)	0.43	2 (2%) 61 51	41, 55, 65, 69	0
46	2o	88/89 (98%)	0.86	8 (9%) 15 11	50, 64, 71, 77	0
47	1p	82/88 (93%)	0.90	5 (6%) 27 20	49, 60, 68, 73	0
47	2p	82/88 (93%)	0.94	2 (2%) 59 49	48, 60, 68, 70	0
48	1q	99/105 (94%)	0.65	1 (1%) 79 72	44, 56, 66, 70	0
48	2q	99/105 (94%)	0.84	3 (3%) 52 42	56, 64, 71, 74	0
49	1r	68/88 (77%)	0.52	1 (1%) 72 63	45, 56, 68, 74	0
49	2r	68/88 (77%)	0.59	0 100 100	55, 63, 70, 77	0
50	1s	83/93 (89%)	0.57	2 (2%) 59 49	48, 60, 68, 73	0
50	2s	83/93 (89%)	1.56	19 (22%) 2 1	67, 76, 81, 84	0
51	1t	96/106 (90%)	0.76	4 (4%) 40 32	47, 59, 70, 75	0
51	2t	96/106 (90%)	0.70	5 (5%) 33 25	50, 61, 71, 75	0
52	1u	23/27 (85%)	0.94	3 (13%) 7 6	50, 55, 61, 62	0
52	2u	23/27 (85%)	1.70	8 (34%) 1 0	64, 69, 74, 76	0
53	1v	13/24 (54%)	0.36	0 100 100	39, 52, 75, 87	0
53	2v	13/24 (54%)	1.92	6 (46%) 0 0	60, 75, 88, 90	0
54	1w	65/76 (85%)	0.72	6 (9%) 14 10	48, 76, 89, 95	0
54	1y	67/76 (88%)	0.93	5 (7%) 20 15	25, 79, 88, 91	0
54	2w	62/76 (81%)	1.26	10 (16%) 4 4	71, 83, 91, 97	0
54	2y	66/76 (86%)	1.35	11 (16%) 4 3	45, 86, 91, 92	0
55	1x	72/77 (93%)	0.13	0 100 100	35, 52, 70, 80	0
55	2x	72/77 (93%)	0.61	0 100 100	55, 70, 80, 83	0
All	All	20870/21748 (95%)	0.34	912 (4%) 39 31	10, 55, 80, 97	0

All (912) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
22	10	6	GLY	8.8
45	1n	2	ALA	7.3

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Mol	Chain	Res	Type	RSRZ
38	2g	80	VAL	7.0
38	1g	80	VAL	5.5
32	1a	1002	G	5.4
44	2m	102	ARG	5.4
1	2A	883	G	5.3
22	10	4	LYS	5.1
1	1A	942	A	5.0
38	2g	84	ASN	5.0
22	10	3	HIS	4.9
33	1b	237	ALA	4.8
38	2g	82	GLY	4.8
44	2m	6	GLY	4.8
7	1H	2	SER	4.7
22	10	5	LYS	4.7
40	2i	109	VAL	4.7
45	2n	7	ILE	4.7
44	2m	60	VAL	4.7
53	2v	14	A	4.6
44	2m	124	PRO	4.5
34	2c	2	GLY	4.5
45	2n	39	LEU	4.5
32	1a	1001(A)	G	4.4
21	2Z	21	ALA	4.3
1	1A	1555	C	4.3
44	1m	124	PRO	4.3
1	2A	2133	G	4.3
38	2g	81	GLY	4.2
32	2a	1033	G	4.2
34	2c	129	ALA	4.2
41	2j	59	SER	4.1
32	2a	1030(B)	C	4.1
34	2c	198	VAL	4.0
32	2a	1532	U	4.0
40	2i	14	VAL	4.0
7	2H	2	SER	4.0
44	2m	5	ALA	4.0
22	10	7	LEU	3.9
21	2Z	172	ALA	3.9
45	2n	37	PHE	3.9
41	2j	50	ILE	3.9
22	10	2	ALA	3.9
41	2j	65	LEU	3.8

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Mol	Chain	Res	Type	RSRZ
4	2E	10	GLY	3.8
52	2u	16	GLY	3.8
22	20	6	GLY	3.8
32	1a	1003	G	3.7
44	2m	123	ALA	3.7
45	2n	38	GLY	3.7
1	1A	932	C	3.6
6	2G	50	ALA	3.6
26	24	59	PHE	3.6
7	2H	136	ILE	3.6
32	2a	1030(A)	G	3.6
33	2b	165	VAL	3.6
33	2b	152	PHE	3.6
1	2A	1536	C	3.6
42	2k	14	VAL	3.6
1	2A	2896	C	3.5
41	2j	42	THR	3.5
21	2Z	173	ALA	3.5
32	1a	204	U	3.5
41	1j	72	VAL	3.5
50	2s	9	VAL	3.5
33	1b	12	GLU	3.5
21	1Z	146	ILE	3.4
6	2G	28	VAL	3.4
1	1A	1103	A	3.4
45	2n	2	ALA	3.4
36	2e	22	GLY	3.4
40	1i	2	GLU	3.4
54	2w	3	C	3.4
41	2j	47	PHE	3.4
45	2n	34	TYR	3.4
54	1w	1	G	3.3
40	2i	10	ARG	3.3
46	2o	64	ARG	3.3
1	1A	1126	C	3.3
41	2j	74	ILE	3.3
47	1p	68	ASP	3.3
1	2A	2175	C	3.3
34	2c	182	ILE	3.3
32	2a	1356	G	3.3
41	1j	76	ASN	3.3
1	2A	2176	A	3.3

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Mol	Chain	Res	Type	RSRZ
36	2e	31	LEU	3.3
33	1b	136	VAL	3.3
32	1a	1034	G	3.3
52	2u	14	TRP	3.3
6	2G	20	ILE	3.2
41	2j	54	PHE	3.2
53	2v	12	A	3.2
33	2b	112	VAL	3.2
1	1A	943	C	3.2
48	2q	99	SER	3.2
33	2b	161	ALA	3.2
33	1b	15	VAL	3.2
43	1l	16	GLU	3.2
23	11	2	SER	3.2
32	2a	1030	C	3.2
32	1a	1033	G	3.2
26	24	56	VAL	3.2
44	1m	122	LYS	3.2
51	1t	69	GLY	3.2
53	2v	13	A	3.2
33	2b	237	ALA	3.2
32	1a	1447	A	3.1
54	2w	73	A	3.1
29	27	47	ARG	3.1
34	2c	188	LEU	3.1
22	20	3	HIS	3.1
33	2b	184	VAL	3.1
34	2c	68	VAL	3.1
41	1j	77	PRO	3.1
38	2g	4	ARG	3.1
32	2a	1183	A	3.1
1	2A	886	C	3.1
44	2m	4	ILE	3.1
50	2s	77	THR	3.1
21	1Z	141	VAL	3.1
45	2n	44	LEU	3.1
38	2g	152	ALA	3.1
34	2c	48	TYR	3.1
1	1A	1133	G	3.1
32	1a	1001	A	3.1
32	2a	1061	G	3.1
21	2Z	122	ARG	3.1

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Mol	Chain	Res	Type	RSRZ
21	2Z	170	THR	3.1
32	2a	1060	C	3.1
45	1n	59	ALA	3.0
16	2U	87	GLY	3.0
20	2Y	44	ILE	3.0
41	2j	91	PRO	3.0
1	2A	2802	G	3.0
54	1w	70	G	3.0
1	1A	2136	A	3.0
34	2c	195	VAL	3.0
45	2n	18	VAL	3.0
1	2A	2149	G	3.0
6	2G	146	TYR	3.0
9	2N	83	LYS	3.0
36	2e	20	GLN	3.0
1	2A	2117	A	3.0
32	2a	1092	A	3.0
14	2S	58	LEU	3.0
1	2A	2155	G	3.0
32	2a	89	C	3.0
31	29	25	VAL	3.0
6	2G	139	LEU	2.9
43	2l	29	GLY	2.9
45	2n	47	LEU	2.9
23	21	2	SER	2.9
1	2A	884	C	2.9
33	1b	163	PHE	2.9
45	2n	25	VAL	2.9
29	27	48	LYS	2.9
17	2V	50	PRO	2.9
45	1n	8	GLU	2.9
26	24	65	ASP	2.9
32	2a	962	C	2.9
41	2j	60	ARG	2.9
22	20	7	LEU	2.9
38	2g	16	LEU	2.9
41	2j	52	GLY	2.9
35	2d	179	GLU	2.9
32	1a	1531	A	2.9
54	1w	73	A	2.9
54	2y	36	A	2.9
33	2b	200	ILE	2.9

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Mol	Chain	Res	Type	RSRZ
34	2c	157	ILE	2.9
50	2s	5	LEU	2.9
1	2A	279	C	2.9
22	10	8	GLY	2.9
32	2a	1182	G	2.9
54	1w	71	G	2.9
15	1T	131	ALA	2.9
20	2Y	48	ALA	2.9
33	2b	229	VAL	2.9
50	2s	24	ALA	2.9
21	2Z	149	SER	2.9
34	2c	128	PHE	2.9
53	2v	24	A	2.9
26	14	54	GLY	2.8
50	2s	68	GLY	2.8
1	1A	1110	C	2.8
1	1A	1140	U	2.8
32	2a	1027	C	2.8
33	1b	236	TYR	2.8
7	2H	24	VAL	2.8
12	2Q	121	ALA	2.8
33	1b	186	ALA	2.8
35	1d	111	ALA	2.8
40	2i	15	ALA	2.8
40	2i	17	VAL	2.8
44	1m	123	ALA	2.8
45	2n	3	ARG	2.8
1	2A	901	A	2.8
50	2s	84	GLY	2.8
3	2D	38	LYS	2.8
1	2A	2132	U	2.8
32	1a	1257	U	2.8
1	2A	885	C	2.8
1	2A	2146	C	2.8
26	14	56	VAL	2.8
34	2c	137	ALA	2.8
35	1d	122	ARG	2.8
40	2i	84	ALA	2.8
34	2c	39	ILE	2.8
1	2A	2159	G	2.8
32	1a	1023	G	2.8
32	2a	1031	G	2.8

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Mol	Chain	Res	Type	RSRZ
32	2a	1224	G	2.8
1	1A	945	A	2.8
26	24	17	GLY	2.8
36	2e	99	GLY	2.8
41	1j	10	GLY	2.8
41	2j	55	LYS	2.8
38	1g	13	GLN	2.8
51	2t	8	ARG	2.8
41	2j	56	HIS	2.8
34	2c	17	ASP	2.8
50	2s	26	GLY	2.8
1	1A	930	G	2.8
1	2A	2160	G	2.8
20	2Y	57	GLN	2.8
32	2a	1503	A	2.8
33	1b	126	GLU	2.8
52	2u	24	ARG	2.8
50	2s	11	VAL	2.8
33	2b	92	TYR	2.8
43	2l	32	PHE	2.8
1	1A	2135	U	2.8
21	1Z	166	SER	2.8
32	2a	1223	C	2.8
32	2a	1260	C	2.8
54	2w	72	C	2.8
36	2e	114	GLY	2.8
50	2s	2	PRO	2.8
1	1A	1141	A	2.7
1	2A	881	G	2.7
33	2b	196	LEU	2.7
40	1i	50	LEU	2.7
44	2m	78	ILE	2.7
32	2a	1257	U	2.7
16	2U	84	LYS	2.7
21	2Z	154	ASP	2.7
34	2c	41	GLY	2.7
34	2c	174	PRO	2.7
32	1a	1027	C	2.7
21	2Z	139	VAL	2.7
33	2b	71	VAL	2.7
33	1b	201	ILE	2.7
1	2A	906	G	2.7

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Mol	Chain	Res	Type	RSRZ
1	2A	2156	G	2.7
32	2a	1034	G	2.7
32	2a	1184	G	2.7
35	2d	154	ASN	2.7
7	2H	55	PRO	2.7
33	2b	167	PRO	2.7
1	1A	2807	C	2.7
19	2X	92	LEU	2.7
33	1b	207	ALA	2.7
1	2A	896	A	2.7
1	2A	2169	A	2.7
32	2a	1286	A	2.7
1	1A	1124	U	2.7
18	2W	112	GLY	2.7
36	2e	29	GLY	2.7
41	2j	100	THR	2.7
44	2m	100	GLY	2.7
54	1y	20	U	2.7
1	2A	882	G	2.7
1	2A	2112	G	2.7
54	2w	71	G	2.7
54	2y	44	G	2.7
21	2Z	52	SER	2.7
50	2s	64	GLU	2.7
34	2c	91	LEU	2.7
41	2j	8	LEU	2.7
1	1A	2814	C	2.7
40	2i	114	TYR	2.7
35	1d	180	GLY	2.7
39	2h	3	THR	2.7
1	1A	1127	U	2.7
32	2a	88	A	2.7
6	2G	48	GLU	2.7
33	2b	213	LEU	2.7
21	2Z	164	ALA	2.6
45	2n	5	ALA	2.6
1	2A	2319	G	2.6
38	2g	85	TYR	2.6
54	1w	74	C	2.6
12	2Q	30	GLY	2.6
31	29	37	GLY	2.6
34	1c	13	GLY	2.6

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Mol	Chain	Res	Type	RSRZ
34	2c	161	GLU	2.6
41	1j	40	LEU	2.6
44	2m	90	LEU	2.6
32	2a	1531	A	2.6
34	2c	160	ALA	2.6
45	2n	20	ALA	2.6
1	1A	1221	G	2.6
1	1A	2181	G	2.6
1	2A	2805	G	2.6
39	2h	90	GLY	2.6
52	1u	2	GLY	2.6
44	2m	103	THR	2.6
1	2A	2145	C	2.6
35	1d	135	LEU	2.6
35	2d	161	ASN	2.6
51	2t	24	LEU	2.6
9	2N	69	GLN	2.6
24	22	66	GLU	2.6
27	15	60	VAL	2.6
33	2b	185	ILE	2.6
44	2m	22	ILE	2.6
32	2a	994	A	2.6
33	2b	40	HIS	2.6
1	1A	2816	G	2.6
1	2A	2168	G	2.6
7	2H	33	LEU	2.6
32	2a	630	G	2.6
32	2a	1036	G	2.6
32	2a	1222	G	2.6
54	2w	6	G	2.6
16	1U	117	GLN	2.6
47	1p	1	MET	2.6
40	1i	106	ALA	2.6
41	2j	32	ALA	2.6
42	2k	89	ALA	2.6
1	1A	935	C	2.6
1	2A	2128	C	2.6
1	2A	2174	C	2.6
1	1A	1128	U	2.6
5	2F	57	VAL	2.6
33	2b	15	VAL	2.6
33	2b	197	VAL	2.6

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Mol	Chain	Res	Type	RSRZ
12	2Q	28	ALA	2.6
20	2Y	60	PHE	2.6
40	2i	122	ALA	2.6
1	2A	2147	G	2.5
32	2a	973	G	2.5
32	2a	1117	G	2.5
54	2w	70	G	2.5
45	2n	31	ARG	2.5
32	2a	1116	C	2.5
1	2A	2119	A	2.5
1	2A	2170	A	2.5
32	2a	1287	A	2.5
12	2Q	24	GLY	2.5
21	2Z	150	LEU	2.5
33	1b	44	LEU	2.5
34	1c	39	ILE	2.5
24	12	70	GLN	2.5
28	26	4	GLU	2.5
20	2Y	89	PHE	2.5
38	2g	3	ARG	2.5
45	2n	45	ARG	2.5
1	1A	1220	U	2.5
35	1d	83	SER	2.5
1	1A	1104	G	2.5
1	2A	2115	G	2.5
1	2A	2154	G	2.5
32	2a	1283	G	2.5
54	1y	15	G	2.5
1	2A	897	C	2.5
32	2a	1114	C	2.5
39	2h	72	PRO	2.5
33	1b	14	GLY	2.5
45	2n	28	GLY	2.5
34	2c	5	ILE	2.5
32	2a	996	A	2.5
32	2a	1030(D)	A	2.5
33	1b	17	PHE	2.5
45	2n	59	ALA	2.5
20	2Y	73	ARG	2.5
1	2A	1026	U	2.5
21	1Z	149	SER	2.5
16	2U	98	LEU	2.5

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Mol	Chain	Res	Type	RSRZ
33	1b	11	LEU	2.5
34	2c	178	LEU	2.5
8	1I	106	GLY	2.5
23	21	28	GLY	2.5
33	2b	162	ILE	2.5
34	2c	124	ILE	2.5
5	2F	89	VAL	2.5
41	2j	94	VAL	2.5
32	2a	1028	C	2.5
32	2a	1038	C	2.5
32	2a	1354	C	2.5
40	2i	101	PHE	2.5
33	2b	207	ALA	2.5
51	1t	59	ALA	2.5
36	2e	25	ARG	2.5
34	2c	94	LEU	2.5
39	2h	39	LEU	2.5
41	2j	90	LEU	2.5
8	2I	137	PRO	2.5
33	1b	233	SER	2.5
33	2b	216	SER	2.5
39	2h	101	PRO	2.5
1	2A	2109	U	2.5
50	2s	82	GLY	2.5
51	1t	103	GLY	2.5
54	2y	45	U	2.5
7	2H	79	VAL	2.5
17	2V	5	VAL	2.5
33	2b	188	ALA	2.5
34	2c	88	ARG	2.5
44	1m	2	ALA	2.5
45	2n	41	ARG	2.5
49	1r	24	ALA	2.5
51	2t	83	ARG	2.5
1	1A	2815	C	2.5
36	2e	98	THR	2.5
32	2a	1131	G	2.5
32	1a	1035	A	2.5
42	2k	36	ASP	2.4
50	2s	15	LEU	2.4
41	2j	82	ILE	2.4
52	2u	23	PRO	2.4

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Mol	Chain	Res	Type	RSRZ
21	2Z	71	VAL	2.4
26	24	66	SER	2.4
34	2c	55	VAL	2.4
39	2h	137	VAL	2.4
7	2H	3	ARG	2.4
35	2d	73	ARG	2.4
33	1b	225	ALA	2.4
34	2c	168	ALA	2.4
41	1j	32	ALA	2.4
38	2g	24	THR	2.4
50	2s	79	THR	2.4
50	2s	14	HIS	2.4
1	2A	1509	C	2.4
8	1I	140	LEU	2.4
22	20	84	LEU	2.4
1	2A	2131	G	2.4
1	2A	2157	G	2.4
33	1b	234	PRO	2.4
36	2e	109	ILE	2.4
41	2j	6	ILE	2.4
45	2n	14	PRO	2.4
7	2H	45	VAL	2.4
11	2P	109	GLY	2.4
36	2e	33	VAL	2.4
46	2o	60	VAL	2.4
46	2o	89	GLY	2.4
47	1p	25	ARG	2.4
32	1a	1532	U	2.4
41	2j	83	GLU	2.4
34	1c	187	ALA	2.4
33	2b	31	TYR	2.4
42	2k	50	TYR	2.4
44	2m	59	TYR	2.4
40	2i	64	THR	2.4
14	2S	32	LEU	2.4
33	2b	61	LEU	2.4
34	1c	12	LEU	2.4
39	2h	63	LEU	2.4
40	2i	56	LEU	2.4
21	2Z	53	ILE	2.4
41	2j	96	ILE	2.4
1	2A	2138	C	2.4

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Mol	Chain	Res	Type	RSRZ
7	2H	17	VAL	2.4
8	2I	15	VAL	2.4
33	2b	7	VAL	2.4
34	2c	145	GLY	2.4
40	2i	65	VAL	2.4
1	1A	1132	A	2.4
1	1A	2141	A	2.4
32	1a	1286	A	2.4
34	2c	79	ARG	2.4
38	1g	79	ARG	2.4
12	2Q	104	PHE	2.4
32	1a	1036	G	2.4
40	1i	15	ALA	2.4
32	2a	1219	U	2.4
34	2c	201	TYR	2.4
52	2u	17	THR	2.4
50	2s	49	ILE	2.4
33	2b	37	ASN	2.4
9	2N	9	VAL	2.4
21	2Z	165	VAL	2.4
47	2p	2	VAL	2.4
26	24	51	ASP	2.4
36	2e	107	ARG	2.4
40	2i	127	LYS	2.4
1	1A	2160	C	2.4
1	2A	888	C	2.4
1	2A	2137	C	2.4
32	2a	1149	C	2.4
54	2y	56	C	2.4
35	2d	164	ALA	2.4
36	2e	86	ALA	2.4
44	2m	72	ALA	2.4
7	2H	63	SER	2.4
38	2g	86	GLN	2.4
45	2n	32	SER	2.4
32	2a	1253	G	2.4
21	2Z	137	ILE	2.4
40	2i	90	PRO	2.4
33	1b	71	VAL	2.3
36	2e	32	VAL	2.3
40	1i	86	VAL	2.3
19	1X	94	GLY	2.3

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Mol	Chain	Res	Type	RSRZ
40	1i	91	ASP	2.3
41	2j	89	ASP	2.3
15	1T	130	ALA	2.3
33	1b	34	ALA	2.3
1	1A	931	C	2.3
1	2A	894	C	2.3
32	2a	1363	C	2.3
20	1Y	1	MET	2.3
32	1a	1030(D)	A	2.3
32	2a	965	A	2.3
35	1d	152	SER	2.3
34	2c	67	THR	2.3
45	2n	6	LEU	2.3
34	2c	45	LYS	2.3
41	2j	37	PRO	2.3
1	2A	2151	G	2.3
32	1a	1031	G	2.3
32	2a	1190	G	2.3
34	2c	151	VAL	2.3
39	2h	129	VAL	2.3
52	1u	24	ARG	2.3
54	1y	18	G	2.3
20	2Y	10	GLY	2.3
38	1g	81	GLY	2.3
14	2S	12	PHE	2.3
35	1d	110	PHE	2.3
40	2i	2	GLU	2.3
21	2Z	153	SER	2.3
21	2Z	157	LEU	2.3
33	2b	109	SER	2.3
41	2j	40	LEU	2.3
32	1a	91	C	2.3
1	1A	1142	A	2.3
34	1c	14	ILE	2.3
40	2i	4	TYR	2.3
40	2i	49	PRO	2.3
46	2o	68	ARG	2.3
21	2Z	96	VAL	2.3
26	24	50	VAL	2.3
38	2g	66	VAL	2.3
45	2n	56	VAL	2.3
45	2n	51	GLY	2.3

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Mol	Chain	Res	Type	RSRZ
1	1A	2137	G	2.3
1	2A	1533	G	2.3
1	2A	2153	G	2.3
6	1G	48	GLU	2.3
44	2m	58	GLU	2.3
19	1X	95	LEU	2.3
33	2b	221	LEU	2.3
6	1G	182	LYS	2.3
47	1p	69	THR	2.3
6	2G	136	ARG	2.3
38	1g	32	ARG	2.3
40	2i	128	ARG	2.3
41	2j	41	PRO	2.3
1	2A	2111	C	2.3
32	2a	999	C	2.3
32	2a	1059	C	2.3
41	2j	44	VAL	2.3
54	2y	33	U	2.3
39	2h	128	GLY	2.3
34	2c	3	ASN	2.3
36	2e	130	ASN	2.3
7	2H	20	ALA	2.3
20	2Y	1	MET	2.3
22	20	2	ALA	2.3
33	1b	129	GLU	2.3
33	2b	101	MET	2.3
36	2e	54	ALA	2.3
39	1h	2	LEU	2.3
40	2i	99	LEU	2.3
14	2S	33	LYS	2.3
41	2j	99	LYS	2.3
9	2N	38	HIS	2.3
32	1a	1032	G	2.3
32	2a	987	G	2.3
32	2a	1042	G	2.3
32	2a	1058	G	2.3
41	2j	62	HIS	2.3
43	1l	6	THR	2.3
21	2Z	27	VAL	2.3
33	1b	164	VAL	2.3
36	2e	55	VAL	2.3
12	2Q	15	GLY	2.3

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Mol	Chain	Res	Type	RSRZ
21	2Z	143	GLY	2.3
40	2i	39	GLY	2.3
51	2t	103	GLY	2.3
52	2u	11	GLY	2.3
1	1A	944	C	2.2
32	1a	1030	C	2.2
54	2w	7	A	2.2
54	2y	67	C	2.2
8	1I	43	ASN	2.2
8	2I	46	ALA	2.2
18	2W	89	ALA	2.2
34	2c	187	ALA	2.2
36	2e	30	ALA	2.2
40	2i	102	LEU	2.2
41	2j	85	LEU	2.2
23	21	78	LYS	2.2
50	2s	56	GLN	2.2
34	1c	62	ASP	2.2
38	2g	27	ILE	2.2
39	2h	35	ILE	2.2
20	2Y	6	HIS	2.2
35	1d	153	ARG	2.2
38	2g	76	ARG	2.2
36	2e	120	THR	2.2
21	2Z	174	VAL	2.2
33	1b	7	VAL	2.2
33	1b	202	PRO	2.2
34	2c	193	TYR	2.2
42	2k	25	TYR	2.2
1	1A	926	G	2.2
1	1A	2187	G	2.2
32	1a	1026	G	2.2
32	2a	1024	G	2.2
32	2a	1032	G	2.2
54	2y	53	G	2.2
34	2c	13	GLY	2.2
21	2Z	88	PHE	2.2
1	1A	2906	U	2.2
33	2b	170	GLU	2.2
34	2c	200	ALA	2.2
45	2n	30	ALA	2.2
39	2h	133	LEU	2.2

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Mol	Chain	Res	Type	RSRZ
1	2A	2139	C	2.2
32	2a	977	A	2.2
32	2a	1004	A	2.2
32	2a	1285	A	2.2
33	1b	187	LEU	2.2
6	2G	52	ILE	2.2
26	14	58	ARG	2.2
34	2c	6	HIS	2.2
34	2c	62	ASP	2.2
6	2G	160	VAL	2.2
34	2c	95	THR	2.2
47	1p	67	THR	2.2
7	2H	38	SER	2.2
20	2Y	55	TYR	2.2
34	2c	158	GLY	2.2
35	1d	167	GLY	2.2
40	2i	67	GLY	2.2
34	2c	10	PHE	2.2
1	2A	2308	G	2.2
10	2O	76	ALA	2.2
14	2S	57	LYS	2.2
1	1A	2173	G	2.2
32	2a	1215	G	2.2
32	2a	1276	G	2.2
34	2c	53	ALA	2.2
38	2g	2	ALA	2.2
44	1m	27	LYS	2.2
44	2m	122	LYS	2.2
48	2q	98	LEU	2.2
50	2s	70	LYS	2.2
54	2y	65	G	2.2
9	2N	115	ARG	2.2
33	1b	208	ILE	2.2
35	1d	35	ARG	2.2
36	2e	24	ARG	2.2
41	2j	98	ILE	2.2
46	2o	65	ARG	2.2
32	2a	1035	A	2.2
32	2a	1029	C	2.2
32	2a	1210	C	2.2
45	2n	49	HIS	2.2
54	1w	72	C	2.2

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Mol	Chain	Res	Type	RSRZ
6	2G	97	ASP	2.2
6	2G	87	PRO	2.2
38	2g	88	PRO	2.2
42	2k	114	VAL	2.2
41	2j	87	THR	2.2
9	2N	1	MET	2.2
20	2Y	80	GLY	2.2
21	2Z	3	TYR	2.2
40	2i	68	GLY	2.2
40	2i	71	SER	2.2
40	2i	126	SER	2.2
33	2b	17	PHE	2.2
40	2i	18	PHE	2.2
50	2s	22	LEU	2.2
38	2g	83	ALA	2.2
42	2k	15	ALA	2.2
34	2c	8	ILE	2.2
1	1A	1143	U	2.2
1	2A	2113	U	2.2
41	2j	5	ARG	2.2
50	2s	78	ARG	2.2
6	2G	41	GLN	2.2
1	1A	694	G	2.2
1	2A	2110	G	2.2
32	2a	1274	G	2.2
33	1b	19	HIS	2.2
1	2A	866	A	2.2
1	2A	2134	A	2.2
7	2H	11	VAL	2.2
17	2V	52	VAL	2.2
21	2Z	87	ASP	2.2
32	1a	1503	A	2.2
34	2c	106	VAL	2.2
37	2f	6	VAL	2.2
39	2h	4	ASP	2.2
42	2k	113	PRO	2.2
46	2o	27	VAL	2.2
15	2T	1	MET	2.2
32	2a	1244	C	2.2
36	2e	10	MET	2.2
54	2w	4	C	2.2
17	2V	101	GLY	2.2

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Mol	Chain	Res	Type	RSRZ
39	2h	88	LYS	2.2
41	2j	10	GLY	2.2
44	2m	26	GLY	2.2
52	2u	19	GLY	2.2
45	2n	21	TYR	2.2
38	2g	5	ARG	2.1
38	2g	110	GLN	2.1
48	1q	93	GLN	2.1
1	1A	271	U	2.1
33	2b	125	PRO	2.1
41	2j	72	VAL	2.1
40	2i	105	ASP	2.1
1	1A	2146	G	2.1
1	2A	2127	G	2.1
1	2A	2162	G	2.1
32	1a	78	G	2.1
32	2a	1030(C)	G	2.1
32	2a	1047	G	2.1
32	2a	1160	G	2.1
33	2b	47	THR	2.1
38	1g	132	GLY	2.1
53	2v	15	A	2.1
54	1y	69	G	2.1
54	2w	65	G	2.1
1	1A	2167	C	2.1
6	1G	80	PHE	2.1
6	2G	133	LEU	2.1
32	2a	1043	C	2.1
33	2b	121	LEU	2.1
46	1o	69	TYR	2.1
21	2Z	152	ALA	2.1
33	2b	225	ALA	2.1
39	2h	29	SER	2.1
40	2i	119	ALA	2.1
42	2k	24	SER	2.1
33	2b	175	ARG	2.1
34	1c	79	ARG	2.1
33	1b	41	ILE	2.1
39	2h	86	ILE	2.1
45	2n	42	ILE	2.1
18	1W	111	HIS	2.1
20	2Y	45	VAL	2.1

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Mol	Chain	Res	Type	RSRZ
32	1a	203	U	2.1
32	2a	90	U	2.1
50	1s	9	VAL	2.1
35	2d	165	MET	2.1
6	2G	74	LYS	2.1
12	2Q	22	LYS	2.1
11	2P	26	GLY	2.1
40	2i	8	GLY	2.1
52	2u	8	THR	2.1
35	2d	188	LEU	2.1
40	1i	59	PHE	2.1
44	2m	81	LEU	2.1
46	2o	18	PHE	2.1
1	2A	2171	A	2.1
2	2B	120	A	2.1
32	2a	975	A	2.1
33	2b	21	ARG	2.1
35	1d	118	ARG	2.1
38	2g	79	ARG	2.1
40	2i	13	ALA	2.1
41	2j	26	ALA	2.1
45	2n	29	ARG	2.1
53	2v	23	A	2.1
1	2A	2893	G	2.1
14	2S	40	ILE	2.1
32	2a	1017	G	2.1
32	2a	1255	G	2.1
32	2a	1355	G	2.1
1	2A	2804	C	2.1
32	1a	1038	C	2.1
54	2w	13	C	2.1
35	2d	160	GLN	2.1
36	1e	72	GLN	2.1
3	1D	275	LYS	2.1
22	20	4	LYS	2.1
41	1j	78	ASN	2.1
32	2a	997	U	2.1
6	2G	43	LEU	2.1
7	2H	174	GLY	2.1
35	1d	124	GLY	2.1
33	1b	24	TRP	2.1
35	1d	132	ARG	2.1

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Mol	Chain	Res	Type	RSRZ
41	1j	43	ARG	2.1
14	2S	7	TYR	2.1
34	1c	84	ILE	2.1
41	1j	97	GLU	2.1
1	2A	2135	A	2.1
32	1a	149	A	2.1
32	2a	1447	A	2.1
51	2t	73	HIS	2.1
1	1A	1105	G	2.1
1	1A	1117	G	2.1
1	1A	2228	G	2.1
1	2A	2100	G	2.1
1	2A	2304	G	2.1
54	1y	62	C	2.1
20	2Y	42	VAL	2.1
22	20	5	LYS	2.1
32	1a	346	G	2.1
32	1a	1024	G	2.1
32	1a	1030(A)	G	2.1
32	2a	1202	G	2.1
36	2e	51	VAL	2.1
26	24	29	PRO	2.1
41	2j	71	LEU	2.1
47	2p	74	LEU	2.1
48	2q	31	LEU	2.1
6	2G	24	GLY	2.1
26	24	54	GLY	2.1
34	2c	9	GLY	2.1
36	2e	28	PHE	2.1
6	2G	115	ARG	2.1
33	1b	13	ALA	2.1
35	1d	5	ILE	2.1
35	2d	204	ILE	2.1
34	2c	29	TYR	2.1
38	2g	154	TYR	2.1
7	2H	41	MET	2.0
33	1b	40	HIS	2.0
1	1A	946	A	2.0
32	1a	160	A	2.0
32	2a	1179	A	2.0
34	1c	207	VAL	2.0
1	1A	2168	C	2.0

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Mol	Chain	Res	Type	RSRZ
1	2A	2108	C	2.0
32	2a	1214	C	2.0
41	1j	8	LEU	2.0
1	1A	2163	G	2.0
1	2A	2116	G	2.0
2	2B	19	G	2.0
12	2Q	6	ARG	2.0
16	2U	73	GLY	2.0
23	21	76	ARG	2.0
32	1a	630	G	2.0
32	2a	1001(A)	G	2.0
35	2d	23	GLY	2.0
35	2d	209	ARG	2.0
36	2e	84	PHE	2.0
44	2m	29	ARG	2.0
46	2o	88	ARG	2.0
52	1u	19	GLY	2.0
54	2y	1	G	2.0
54	2y	18	G	2.0
14	2S	35	ILE	2.0
51	1t	94	ALA	2.0
12	2Q	139	GLU	2.0
34	1c	18	TRP	2.0
12	2Q	18	LYS	2.0
33	1b	33	TYR	2.0
15	2T	66	VAL	2.0
33	1b	229	VAL	2.0
33	1b	125	PRO	2.0
45	2n	40	CYS	2.0
1	2A	229	A	2.0
1	2A	278	A	2.0
33	2b	142	LEU	2.0
33	2b	180	LEU	2.0
35	1d	157	LEU	2.0
44	2m	66	LEU	2.0
54	2y	35	A	2.0
20	1Y	50	ARG	2.0
22	20	11	ARG	2.0
26	24	49	PHE	2.0
41	1j	36	GLY	2.0
46	1o	89	GLY	2.0
32	1a	1030(B)	C	2.0

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Mol	Chain	Res	Type	RSRZ
12	2Q	49	ALA	2.0
15	2T	130	ALA	2.0
15	2T	131	ALA	2.0
35	2d	48	ALA	2.0
38	1g	83	ALA	2.0
38	2g	150	ALA	2.0
41	2j	67	THR	2.0
1	1A	1112	U	2.0
1	2A	2118	U	2.0
1	2A	2150	U	2.0
9	2N	136	GLU	2.0
10	2O	81	ASP	2.0
32	2a	1062	U	2.0
33	2b	189	ASP	2.0
40	2i	91	ASP	2.0
42	1k	36	ASP	2.0
50	1s	13	ASP	2.0
1	1A	1584	G	2.0
1	2A	2106	G	2.0
1	2A	2318	G	2.0
4	1E	73	GLU	2.0
32	2a	1021	G	2.0
32	2a	1220	G	2.0
34	2c	167	TRP	2.0
26	14	63	TYR	2.0
26	24	63	TYR	2.0
7	2H	26	VAL	2.0
44	2m	74	VAL	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(Å^2)	Q<0.9
54	PSU	2y	55	20/21	0.57	0.20	79,93,100,105	0
54	7MG	2y	46	24/25	0.59	0.20	84,90,96,114	0
54	7MG	1w	46	24/25	0.59	0.15	67,77,94,110	0
54	7MG	1y	46	24/25	0.63	0.17	73,85,99,104	0
54	7MG	2w	46	24/25	0.64	0.16	71,87,94,109	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
54	5MU	2y	54	21/22	0.65	0.17	76,85,92,102	0
54	PSU	1y	55	20/21	0.66	0.15	78,86,93,105	0
54	MIA	2y	37	22/30	0.66	0.17	64,78,97,111	0
54	4SU	2w	8	20/21	0.70	0.15	78,86,91,102	0
54	MIA	1y	37	22/30	0.75	0.15	62,72,77,85	0
54	5MU	1y	54	21/22	0.76	0.14	78,82,88,97	0
43	0TD	2l	92	10/11	0.78	0.16	52,60,64,75	0
54	4SU	2y	8	20/21	0.79	0.13	79,88,94,100	0
54	PSU	2y	32	20/21	0.80	0.19	65,77,84,86	0
32	2MG	2a	1207	24/25	0.82	0.14	68,74,82,88	0
54	PSU	1y	32	20/21	0.83	0.17	64,71,75,82	0
54	PSU	2w	55	20/21	0.83	0.12	64,79,86,88	0
54	4SU	1y	8	20/21	0.83	0.12	77,82,89,92	0
54	PSU	2y	39	20/21	0.84	0.15	72,77,89,97	0
54	5MU	2w	54	21/22	0.84	0.10	66,71,77,82	0
54	PSU	2w	32	20/21	0.85	0.12	70,78,89,93	0
1	5MU	2A	1915	21/22	0.86	0.13	63,70,76,88	0
43	0TD	1l	92	10/11	0.86	0.16	38,44,52,72	0
55	5MU	2x	54	21/22	0.86	0.11	65,73,79,82	0
55	PSU	2x	55	20/21	0.86	0.11	66,75,77,78	0
55	5MC	2x	32	21/22	0.87	0.15	57,66,73,74	0
32	M2G	2a	966	25/26	0.88	0.14	48,59,69,78	0
1	PSU	2A	1911	20/21	0.88	0.12	54,62,67,68	0
55	4SU	2x	8	20/21	0.88	0.12	64,75,77,77	0
54	PSU	1w	55	20/21	0.89	0.11	54,67,73,75	0
54	PSU	1y	39	20/21	0.89	0.12	61,69,75,82	0
32	5MC	2a	1400	21/22	0.89	0.18	63,66,71,75	0
1	4OC	2A	1920	21/23	0.89	0.13	53,60,63,65	0
32	PSU	2a	516	20/21	0.90	0.10	61,68,74,74	0
54	MIA	2w	37	25/30	0.90	0.12	63,70,76,85	0
32	7MG	2a	527	24/25	0.90	0.13	51,57,66,74	0
1	PSU	2A	1917	20/21	0.90	0.10	52,61,72,74	0
54	4SU	1w	8	20/21	0.91	0.09	65,70,76,79	0
32	4OC	2a	1402	22/23	0.91	0.12	52,62,65,65	0
54	5MU	1w	54	21/22	0.91	0.10	46,56,65,71	0
54	PSU	2w	39	20/21	0.91	0.10	63,71,75,79	0
32	5MC	2a	1407	21/22	0.91	0.12	45,53,58,61	0
32	5MC	2a	967	21/22	0.91	0.12	56,62,70,74	0
54	PSU	1w	32	20/21	0.91	0.12	54,60,77,78	0
32	UR3	2a	1498	21/22	0.92	0.13	44,57,63,66	0
55	5MU	1x	54	21/22	0.92	0.09	50,57,63,68	0
55	5MC	1x	32	21/22	0.93	0.12	43,50,54,58	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
32	5MC	2a	1404	21/22	0.93	0.12	50,56,61,66	0
32	MA6	2a	1518	24/25	0.93	0.11	46,64,67,69	0
55	4SU	1x	8	20/21	0.93	0.11	46,54,68,74	0
55	PSU	1x	55	20/21	0.93	0.09	41,51,60,65	0
1	5MU	1A	1937	21/22	0.93	0.10	38,48,53,61	0
1	5MU	2A	1939	21/22	0.94	0.10	30,38,42,42	0
1	PSU	1A	1939	20/21	0.94	0.10	38,45,50,52	0
32	PSU	1a	516	20/21	0.94	0.09	39,50,55,56	0
32	7MG	1a	527	24/25	0.94	0.10	39,45,48,52	0
32	M2G	1a	966	25/26	0.94	0.11	33,45,55,56	0
32	2MG	1a	1207	24/25	0.94	0.10	50,59,63,65	0
32	MA6	2a	1519	24/25	0.94	0.12	46,57,63,65	0
54	PSU	1w	39	20/21	0.95	0.10	44,55,60,63	0
32	5MC	1a	967	21/22	0.95	0.10	38,49,53,55	0
32	5MC	1a	1404	21/22	0.95	0.10	30,36,40,44	0
1	5MC	2A	1962	21/22	0.95	0.09	39,48,55,58	0
1	5MC	1A	1964	21/22	0.96	0.09	24,30,36,39	0
32	5MC	1a	1407	21/22	0.96	0.08	29,34,39,42	0
54	MIA	1w	37	29/30	0.96	0.10	35,48,55,63	0
1	5MU	1A	1961	21/22	0.96	0.09	15,21,26,34	0
1	5MC	2A	1942	21/22	0.96	0.10	44,52,59,61	0
32	5MC	1a	1400	21/22	0.96	0.09	33,44,49,57	0
1	OMG	2A	2251	24/25	0.96	0.09	34,40,45,47	0
1	2MA	2A	2503	23/24	0.96	0.09	26,29,33,34	0
1	PSU	2A	2605	20/21	0.96	0.08	26,37,41,42	0
32	4OC	1a	1402	22/23	0.96	0.09	37,41,51,56	0
32	UR3	1a	1498	21/22	0.97	0.07	28,35,39,40	0
32	MA6	1a	1518	24/25	0.97	0.10	25,33,39,39	0
32	MA6	1a	1519	24/25	0.97	0.08	29,35,39,41	0
1	2MU	2A	2552	21/23	0.97	0.09	32,38,45,57	0
1	2MU	1A	2564	21/23	0.97	0.07	14,20,26,28	0
1	4OC	1A	1942	21/23	0.97	0.09	27,36,42,43	0
1	PSU	1A	1933	20/21	0.98	0.07	33,40,47,48	0
1	PSU	1A	2617	20/21	0.98	0.06	15,18,23,23	0
1	5MC	1A	1984	21/22	0.98	0.07	20,27,30,40	0
1	OMG	1A	2263	24/25	0.98	0.07	13,19,21,24	0
1	2MA	1A	2515	23/24	0.98	0.07	7,11,15,21	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(Å^2)	Q<0.9
56	MG	2a	3208	1/1	0.42	0.26	69,69,69,69	0
56	MG	2A	3675	1/1	0.54	0.29	63,63,63,63	0
56	MG	1A	3975	1/1	0.55	0.23	21,21,21,21	0
56	MG	1w	110	1/1	0.55	0.17	79,79,79,79	0
56	MG	2y	104	1/1	0.55	0.19	85,85,85,85	0
56	MG	2j	8001	1/1	0.57	0.16	77,77,77,77	0
56	MG	1a	3109	1/1	0.57	0.24	70,70,70,70	0
56	MG	2a	3194	1/1	0.58	0.22	71,71,71,71	0
56	MG	2a	3113	1/1	0.58	0.19	72,72,72,72	0
56	MG	2A	3723	1/1	0.60	0.18	65,65,65,65	0
56	MG	1A	3891	1/1	0.60	0.23	74,74,74,74	0
56	MG	2A	3850	1/1	0.62	0.22	67,67,67,67	0
56	MG	2A	3290	1/1	0.65	0.21	77,77,77,77	0
56	MG	2A	3575	1/1	0.65	0.19	38,38,38,38	0
56	MG	2U	202	1/1	0.65	0.15	63,63,63,63	0
56	MG	1a	3145	1/1	0.65	0.25	78,78,78,78	0
56	MG	2A	3542	1/1	0.66	0.17	52,52,52,52	0
56	MG	2A	3741	1/1	0.67	0.25	76,76,76,76	0
56	MG	1A	4023	1/1	0.67	0.15	31,31,31,31	0
56	MG	1A	3916	1/1	0.67	0.15	26,26,26,26	0
56	MG	1A	3770	1/1	0.67	0.16	43,43,43,43	0
56	MG	2a	3198	1/1	0.68	0.20	59,59,59,59	0
56	MG	2A	3650	1/1	0.68	0.24	53,53,53,53	0
56	MG	2A	3671	1/1	0.68	0.14	47,47,47,47	0
56	MG	1a	3194	1/1	0.68	0.19	55,55,55,55	0
56	MG	2B	3009	1/1	0.69	0.16	60,60,60,60	0
56	MG	2R	202	1/1	0.69	0.17	51,51,51,51	0
56	MG	2A	3669	1/1	0.69	0.15	64,64,64,64	0
56	MG	1A	3244	1/1	0.70	0.14	65,65,65,65	0
56	MG	1a	3187	1/1	0.70	0.17	77,77,77,77	0
56	MG	2v	102	1/1	0.70	0.18	62,62,62,62	0
56	MG	2y	101	1/1	0.70	0.20	59,59,59,59	0
56	MG	2A	3651	1/1	0.70	0.13	56,56,56,56	0
56	MG	2A	3627	1/1	0.71	0.14	60,60,60,60	0
56	MG	2A	3338	1/1	0.71	0.20	66,66,66,66	0
56	MG	2A	3224	1/1	0.71	0.23	58,58,58,58	0
56	MG	2A	3204	1/1	0.71	0.43	68,68,68,68	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	2A	3743	1/1	0.71	0.18	47,47,47,47	0
56	MG	2A	3766	1/1	0.71	0.17	85,85,85,85	0
56	MG	2A	3022	1/1	0.72	0.10	51,51,51,51	0
56	MG	2A	3247	1/1	0.72	0.30	64,64,64,64	0
56	MG	2A	3584	1/1	0.72	0.14	52,52,52,52	0
56	MG	2A	3089	1/1	0.72	0.24	56,56,56,56	0
56	MG	1A	4078	1/1	0.72	0.13	37,37,37,37	0
56	MG	1A	4019	1/1	0.73	0.14	29,29,29,29	0
56	MG	2A	3863	1/1	0.73	0.15	70,70,70,70	0
56	MG	1a	3169	1/1	0.73	0.22	57,57,57,57	0
56	MG	2B	3017	1/1	0.73	0.12	58,58,58,58	0
56	MG	2j	8002	1/1	0.73	0.16	77,77,77,77	0
56	MG	2A	3207	1/1	0.73	0.09	48,48,48,48	0
56	MG	2A	3757	1/1	0.73	0.15	50,50,50,50	0
56	MG	1A	3968	1/1	0.73	0.14	53,53,53,53	0
56	MG	2a	3195	1/1	0.74	0.13	69,69,69,69	0
56	MG	2A	3115	1/1	0.74	0.20	64,64,64,64	0
56	MG	2A	3170	1/1	0.74	0.23	66,66,66,66	0
56	MG	28	101	1/1	0.74	0.19	60,60,60,60	0
56	MG	2A	3686	1/1	0.74	0.20	52,52,52,52	0
56	MG	2a	3178	1/1	0.74	0.30	70,70,70,70	0
56	MG	2a	3180	1/1	0.74	0.18	65,65,65,65	0
56	MG	1A	4009	1/1	0.74	0.14	56,56,56,56	0
56	MG	2A	3006	1/1	0.75	0.13	51,51,51,51	0
56	MG	2F	301	1/1	0.75	0.16	58,58,58,58	0
56	MG	2G	3001	1/1	0.75	0.20	62,62,62,62	0
56	MG	2A	3659	1/1	0.75	0.12	64,64,64,64	0
56	MG	2A	3244	1/1	0.75	0.17	65,65,65,65	0
56	MG	20	3001	1/1	0.75	0.14	57,57,57,57	0
56	MG	1A	3458	1/1	0.75	0.12	49,49,49,49	0
56	MG	2A	3285	1/1	0.75	0.14	68,68,68,68	0
56	MG	2A	3084	1/1	0.75	0.43	71,71,71,71	0
56	MG	2A	3690	1/1	0.75	0.19	68,68,68,68	0
56	MG	1A	4033	1/1	0.75	0.20	55,55,55,55	0
56	MG	2A	3473	1/1	0.75	0.12	71,71,71,71	0
56	MG	1A	3591	1/1	0.75	0.27	38,38,38,38	0
56	MG	2A	3165	1/1	0.75	0.14	53,53,53,53	0
56	MG	15	104	1/1	0.75	0.16	40,40,40,40	0
56	MG	2A	3810	1/1	0.75	0.12	44,44,44,44	0
56	MG	2A	3587	1/1	0.75	0.23	68,68,68,68	0
56	MG	1A	3187	1/1	0.75	0.14	51,51,51,51	0
56	MG	1y	105	1/1	0.75	0.10	81,81,81,81	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	1a	3221	1/1	0.76	0.22	61,61,61,61	0
56	MG	2A	3695	1/1	0.76	0.12	55,55,55,55	0
56	MG	1v	3001	1/1	0.76	0.16	67,67,67,67	0
56	MG	1w	104	1/1	0.76	0.22	54,54,54,54	0
56	MG	2A	3154	1/1	0.76	0.14	56,56,56,56	0
56	MG	1B	3027	1/1	0.76	0.12	59,59,59,59	0
56	MG	1A	3837	1/1	0.76	0.14	22,22,22,22	0
56	MG	19	101	1/1	0.76	0.25	33,33,33,33	0
56	MG	1B	3007	1/1	0.76	0.20	56,56,56,56	0
56	MG	2A	3075	1/1	0.76	0.17	62,62,62,62	0
56	MG	2Q	204	1/1	0.77	0.14	49,49,49,49	0
56	MG	2A	3682	1/1	0.77	0.18	37,37,37,37	0
56	MG	2A	3425	1/1	0.77	0.15	56,56,56,56	0
56	MG	2A	3168	1/1	0.77	0.16	71,71,71,71	0
56	MG	2A	3481	1/1	0.77	0.15	47,47,47,47	0
56	MG	2a	3033	1/1	0.77	0.23	61,61,61,61	0
56	MG	1B	3023	1/1	0.77	0.12	65,65,65,65	0
56	MG	2A	3021	1/1	0.77	0.21	64,64,64,64	0
56	MG	1A	3777	1/1	0.77	0.14	37,37,37,37	0
56	MG	1A	3924	1/1	0.77	0.15	40,40,40,40	0
56	MG	2A	3607	1/1	0.77	0.14	56,56,56,56	0
56	MG	2A	3225	1/1	0.77	0.17	69,69,69,69	0
56	MG	2a	3200	1/1	0.77	0.22	64,64,64,64	0
56	MG	1A	3676	1/1	0.77	0.19	32,32,32,32	0
56	MG	1a	3028	1/1	0.77	0.17	53,53,53,53	0
56	MG	1a	3097	1/1	0.77	0.17	59,59,59,59	0
56	MG	1A	3845	1/1	0.77	0.18	41,41,41,41	0
56	MG	2w	3002	1/1	0.77	0.11	46,46,46,46	0
56	MG	2A	3323	1/1	0.77	0.22	54,54,54,54	0
56	MG	1A	3611	1/1	0.77	0.09	63,63,63,63	0
56	MG	2A	3443	1/1	0.78	0.11	50,50,50,50	0
56	MG	2A	3143	1/1	0.78	0.15	51,51,51,51	0
56	MG	2a	3149	1/1	0.78	0.18	62,62,62,62	0
56	MG	2a	3172	1/1	0.78	0.24	67,67,67,67	0
56	MG	2A	3837	1/1	0.78	0.14	62,62,62,62	0
56	MG	1A	4058	1/1	0.78	0.13	71,71,71,71	0
56	MG	1a	3001	1/1	0.78	0.29	65,65,65,65	0
56	MG	1a	3235	1/1	0.78	0.12	68,68,68,68	0
56	MG	2B	3015	1/1	0.78	0.14	54,54,54,54	0
56	MG	2a	3199	1/1	0.78	0.22	57,57,57,57	0
56	MG	1a	3016	1/1	0.78	0.12	51,51,51,51	0
56	MG	1a	3149	1/1	0.78	0.24	67,67,67,67	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	2A	3603	1/1	0.78	0.12	44,44,44,44	0
56	MG	1A	3939	1/1	0.78	0.11	32,32,32,32	0
56	MG	2A	3343	1/1	0.78	0.16	65,65,65,65	0
56	MG	2v	103	1/1	0.78	0.20	60,60,60,60	0
56	MG	1a	3055	1/1	0.78	0.20	68,68,68,68	0
56	MG	2A	3745	1/1	0.78	0.12	56,56,56,56	0
56	MG	2A	3432	1/1	0.78	0.13	65,65,65,65	0
56	MG	1V	202	1/1	0.79	0.11	52,52,52,52	0
56	MG	2A	3830	1/1	0.79	0.19	51,51,51,51	0
56	MG	1A	4034	1/1	0.79	0.14	53,53,53,53	0
56	MG	2A	3838	1/1	0.79	0.12	61,61,61,61	0
56	MG	2A	3510	1/1	0.79	0.13	37,37,37,37	0
56	MG	1A	3282	1/1	0.79	0.14	48,48,48,48	0
56	MG	2A	3563	1/1	0.79	0.11	46,46,46,46	0
56	MG	1A	3253	1/1	0.79	0.12	43,43,43,43	0
56	MG	1a	3167	1/1	0.79	0.13	51,51,51,51	0
56	MG	2A	3346	1/1	0.79	0.11	70,70,70,70	0
56	MG	2A	3588	1/1	0.79	0.27	70,70,70,70	0
56	MG	2a	3224	1/1	0.79	0.10	51,51,51,51	0
56	MG	2A	3377	1/1	0.79	0.16	56,56,56,56	0
56	MG	2A	3396	1/1	0.79	0.10	58,58,58,58	0
56	MG	1A	3803	1/1	0.79	0.11	24,24,24,24	0
56	MG	1A	3495	1/1	0.79	0.10	61,61,61,61	0
56	MG	1A	3681	1/1	0.79	0.24	49,49,49,49	0
56	MG	2w	3005	1/1	0.79	0.10	66,66,66,66	0
56	MG	2x	3002	1/1	0.79	0.17	69,69,69,69	0
56	MG	2A	3767	1/1	0.79	0.12	39,39,39,39	0
56	MG	2a	3105	1/1	0.79	0.24	55,55,55,55	0
56	MG	2a	3170	1/1	0.80	0.21	55,55,55,55	0
56	MG	2a	3171	1/1	0.80	0.10	53,53,53,53	0
56	MG	2A	3742	1/1	0.80	0.16	69,69,69,69	0
56	MG	1A	3502	1/1	0.80	0.11	62,62,62,62	0
56	MG	1A	3884	1/1	0.80	0.20	35,35,35,35	0
56	MG	2A	3261	1/1	0.80	0.16	57,57,57,57	0
56	MG	2A	3192	1/1	0.80	0.22	67,67,67,67	0
56	MG	1A	3940	1/1	0.80	0.18	36,36,36,36	0
56	MG	1A	3825	1/1	0.80	0.10	28,28,28,28	0
56	MG	1A	3713	1/1	0.80	0.11	66,66,66,66	0
56	MG	2a	3201	1/1	0.80	0.18	70,70,70,70	0
56	MG	2A	3339	1/1	0.80	0.10	68,68,68,68	0
56	MG	2a	3211	1/1	0.80	0.17	62,62,62,62	0
56	MG	2A	3608	1/1	0.80	0.23	63,63,63,63	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	2a	3008	1/1	0.80	0.17	54,54,54,54	0
56	MG	2a	3025	1/1	0.80	0.16	58,58,58,58	0
56	MG	2A	3841	1/1	0.80	0.14	62,62,62,62	0
56	MG	2a	3050	1/1	0.80	0.12	57,57,57,57	0
56	MG	2a	3076	1/1	0.80	0.31	64,64,64,64	0
56	MG	2A	3493	1/1	0.80	0.19	46,46,46,46	0
56	MG	2x	3001	1/1	0.80	0.19	60,60,60,60	0
56	MG	2A	3856	1/1	0.80	0.18	35,35,35,35	0
56	MG	2a	3141	1/1	0.80	0.10	71,71,71,71	0
56	MG	1A	4039	1/1	0.80	0.12	54,54,54,54	0
56	MG	2A	3549	1/1	0.81	0.12	34,34,34,34	0
56	MG	1A	3161	1/1	0.81	0.18	49,49,49,49	0
56	MG	1a	3183	1/1	0.81	0.18	64,64,64,64	0
56	MG	2a	3024	1/1	0.81	0.10	58,58,58,58	0
56	MG	1A	3810	1/1	0.81	0.12	27,27,27,27	0
56	MG	2A	3036	1/1	0.81	0.17	66,66,66,66	0
56	MG	1A	4036	1/1	0.81	0.11	37,37,37,37	0
56	MG	2a	3055	1/1	0.81	0.19	70,70,70,70	0
56	MG	1a	3069	1/1	0.81	0.12	53,53,53,53	0
56	MG	2A	3873	1/1	0.81	0.26	41,41,41,41	0
56	MG	1A	3932	1/1	0.81	0.11	25,25,25,25	0
56	MG	1A	3821	1/1	0.81	0.16	49,49,49,49	0
56	MG	2A	3625	1/1	0.81	0.14	53,53,53,53	0
56	MG	2A	3139	1/1	0.81	0.20	69,69,69,69	0
56	MG	1A	3765	1/1	0.81	0.14	18,18,18,18	0
56	MG	1A	4080	1/1	0.81	0.11	39,39,39,39	0
56	MG	1x	102	1/1	0.81	0.20	50,50,50,50	0
56	MG	2x	3004	1/1	0.81	0.17	59,59,59,59	0
56	MG	1a	3013	1/1	0.81	0.21	48,48,48,48	0
56	MG	2a	3189	1/1	0.81	0.14	73,73,73,73	0
56	MG	1B	3034	1/1	0.82	0.15	59,59,59,59	0
56	MG	2a	3125	1/1	0.82	0.10	78,78,78,78	0
56	MG	1O	3001	1/1	0.82	0.12	60,60,60,60	0
56	MG	1A	3997	1/1	0.82	0.14	52,52,52,52	0
56	MG	2A	3455	1/1	0.82	0.17	61,61,61,61	0
56	MG	1Z	303	1/1	0.82	0.07	56,56,56,56	0
56	MG	2A	3478	1/1	0.82	0.15	40,40,40,40	0
56	MG	1A	3392	1/1	0.82	0.12	33,33,33,33	0
56	MG	2A	3672	1/1	0.82	0.12	67,67,67,67	0
56	MG	2B	3014	1/1	0.82	0.12	58,58,58,58	0
56	MG	1A	3258	1/1	0.82	0.14	47,47,47,47	0
56	MG	2A	3291	1/1	0.82	0.16	67,67,67,67	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	2B	3021	1/1	0.82	0.22	69,69,69,69	0
56	MG	2A	3292	1/1	0.82	0.19	51,51,51,51	0
56	MG	2A	3299	1/1	0.82	0.09	46,46,46,46	0
56	MG	1x	110	1/1	0.82	0.17	63,63,63,63	0
56	MG	2A	3703	1/1	0.82	0.16	41,41,41,41	0
56	MG	1A	3793	1/1	0.82	0.12	25,25,25,25	0
56	MG	2A	3736	1/1	0.82	0.21	72,72,72,72	0
56	MG	2A	3579	1/1	0.82	0.17	65,65,65,65	0
56	MG	1a	3002	1/1	0.82	0.18	50,50,50,50	0
56	MG	2a	3011	1/1	0.82	0.21	62,62,62,62	0
56	MG	1a	3173	1/1	0.82	0.10	55,55,55,55	0
56	MG	1A	3610	1/1	0.82	0.15	51,51,51,51	0
56	MG	2A	3596	1/1	0.82	0.18	63,63,63,63	0
56	MG	2a	3034	1/1	0.82	0.25	51,51,51,51	0
56	MG	1A	3155	1/1	0.82	0.18	56,56,56,56	0
56	MG	2A	3378	1/1	0.82	0.19	57,57,57,57	0
56	MG	1A	3768	1/1	0.82	0.11	47,47,47,47	0
56	MG	2A	3622	1/1	0.82	0.11	56,56,56,56	0
56	MG	2A	3382	1/1	0.83	0.13	62,62,62,62	0
56	MG	2A	3388	1/1	0.83	0.20	45,45,45,45	0
56	MG	1y	104	1/1	0.83	0.33	63,63,63,63	0
56	MG	2A	3404	1/1	0.83	0.28	65,65,65,65	0
56	MG	2A	3411	1/1	0.83	0.16	71,71,71,71	0
56	MG	2a	3014	1/1	0.83	0.23	60,60,60,60	0
56	MG	1A	3281	1/1	0.83	0.16	40,40,40,40	0
56	MG	2A	3678	1/1	0.83	0.11	60,60,60,60	0
56	MG	2A	3680	1/1	0.83	0.10	52,52,52,52	0
56	MG	1A	3461	1/1	0.83	0.15	40,40,40,40	0
56	MG	1A	3635	1/1	0.83	0.09	18,18,18,18	0
56	MG	2A	3444	1/1	0.83	0.12	35,35,35,35	0
56	MG	1A	3055	1/1	0.83	0.18	63,63,63,63	0
56	MG	2A	3226	1/1	0.83	0.10	47,47,47,47	0
56	MG	2a	3110	1/1	0.83	0.26	60,60,60,60	0
56	MG	2A	3234	1/1	0.83	0.26	53,53,53,53	0
56	MG	2A	3734	1/1	0.83	0.13	65,65,65,65	0
56	MG	1A	4018	1/1	0.83	0.12	52,52,52,52	0
56	MG	2A	3056	1/1	0.83	0.14	56,56,56,56	0
56	MG	2a	3163	1/1	0.83	0.24	65,65,65,65	0
56	MG	2A	3497	1/1	0.83	0.14	46,46,46,46	0
56	MG	2A	3248	1/1	0.83	0.27	51,51,51,51	0
56	MG	2A	3255	1/1	0.83	0.15	63,63,63,63	0
56	MG	1A	3089	1/1	0.83	0.18	51,51,51,51	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	2A	3554	1/1	0.83	0.18	51,51,51,51	0
56	MG	2A	3262	1/1	0.83	0.25	59,59,59,59	0
56	MG	2A	3806	1/1	0.83	0.20	55,55,55,55	0
56	MG	1A	3712	1/1	0.83	0.10	10,10,10,10	0
56	MG	1A	3446	1/1	0.83	0.20	54,54,54,54	0
56	MG	2A	3583	1/1	0.83	0.12	27,27,27,27	0
56	MG	1N	3006	1/1	0.83	0.28	46,46,46,46	0
56	MG	2A	3839	1/1	0.83	0.18	55,55,55,55	0
56	MG	1a	3060	1/1	0.83	0.34	59,59,59,59	0
56	MG	1a	3068	1/1	0.83	0.09	54,54,54,54	0
56	MG	2a	3218	1/1	0.83	0.18	60,60,60,60	0
56	MG	2a	3220	1/1	0.83	0.17	57,57,57,57	0
56	MG	1A	3738	1/1	0.83	0.15	23,23,23,23	0
56	MG	2A	3597	1/1	0.83	0.21	50,50,50,50	0
56	MG	2A	3160	1/1	0.83	0.11	33,33,33,33	0
56	MG	1a	3092	1/1	0.83	0.32	62,62,62,62	0
56	MG	1R	203	1/1	0.83	0.14	30,30,30,30	0
56	MG	2A	3169	1/1	0.83	0.17	61,61,61,61	0
56	MG	2A	3624	1/1	0.83	0.11	50,50,50,50	0
56	MG	2A	3352	1/1	0.83	0.14	57,57,57,57	0
56	MG	1A	3756	1/1	0.83	0.12	37,37,37,37	0
56	MG	2A	3636	1/1	0.83	0.11	62,62,62,62	0
56	MG	2A	3643	1/1	0.83	0.12	57,57,57,57	0
56	MG	2A	3176	1/1	0.83	0.25	62,62,62,62	0
56	MG	1A	3883	1/1	0.84	0.09	13,13,13,13	0
56	MG	1A	3096	1/1	0.84	0.27	54,54,54,54	0
56	MG	1A	4105	1/1	0.84	0.18	44,44,44,44	0
56	MG	1A	3160	1/1	0.84	0.17	66,66,66,66	0
56	MG	2A	3712	1/1	0.84	0.08	59,59,59,59	0
56	MG	2A	3286	1/1	0.84	0.23	46,46,46,46	0
56	MG	2A	3726	1/1	0.84	0.10	61,61,61,61	0
56	MG	1a	3175	1/1	0.84	0.10	70,70,70,70	0
56	MG	2A	3545	1/1	0.84	0.10	56,56,56,56	0
56	MG	1A	3393	1/1	0.84	0.16	44,44,44,44	0
56	MG	2a	3080	1/1	0.84	0.30	56,56,56,56	0
56	MG	2a	3084	1/1	0.84	0.19	60,60,60,60	0
56	MG	1a	3026	1/1	0.84	0.19	48,48,48,48	0
56	MG	1A	4020	1/1	0.84	0.18	44,44,44,44	0
56	MG	2A	3320	1/1	0.84	0.20	62,62,62,62	0
56	MG	1a	3052	1/1	0.84	0.19	45,45,45,45	0
56	MG	2A	3324	1/1	0.84	0.17	58,58,58,58	0
56	MG	1A	3606	1/1	0.84	0.15	37,37,37,37	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	2A	3794	1/1	0.84	0.15	67,67,67,67	0
56	MG	2A	3797	1/1	0.84	0.10	57,57,57,57	0
56	MG	2A	3798	1/1	0.84	0.16	51,51,51,51	0
56	MG	1b	3002	1/1	0.84	0.19	54,54,54,54	0
56	MG	2A	3342	1/1	0.84	0.20	57,57,57,57	0
56	MG	1E	307	1/1	0.84	0.10	55,55,55,55	0
56	MG	1w	102	1/1	0.84	0.12	54,54,54,54	0
56	MG	1w	103	1/1	0.84	0.11	55,55,55,55	0
56	MG	2A	3356	1/1	0.84	0.18	51,51,51,51	0
56	MG	1a	3062	1/1	0.84	0.19	65,65,65,65	0
56	MG	1A	3608	1/1	0.84	0.10	15,15,15,15	0
56	MG	2A	3205	1/1	0.84	0.08	44,44,44,44	0
56	MG	1A	3776	1/1	0.84	0.17	46,46,46,46	0
56	MG	1A	3475	1/1	0.84	0.24	67,67,67,67	0
56	MG	2a	3210	1/1	0.84	0.15	56,56,56,56	0
56	MG	1A	3874	1/1	0.84	0.08	35,35,35,35	0
56	MG	2a	3212	1/1	0.84	0.18	54,54,54,54	0
56	MG	1a	3107	1/1	0.84	0.13	55,55,55,55	0
56	MG	2A	3415	1/1	0.84	0.16	56,56,56,56	0
56	MG	2B	3016	1/1	0.84	0.17	63,63,63,63	0
56	MG	2A	3418	1/1	0.84	0.31	65,65,65,65	0
56	MG	2B	3018	1/1	0.84	0.14	74,74,74,74	0
56	MG	1A	3876	1/1	0.84	0.12	30,30,30,30	0
56	MG	2A	3429	1/1	0.84	0.16	60,60,60,60	0
56	MG	2A	3235	1/1	0.84	0.12	47,47,47,47	0
56	MG	2w	3004	1/1	0.84	0.17	60,60,60,60	0
56	MG	1a	3111	1/1	0.84	0.15	54,54,54,54	0
56	MG	2w	3006	1/1	0.84	0.14	78,78,78,78	0
56	MG	1a	3137	1/1	0.84	0.12	46,46,46,46	0
56	MG	2T	3001	1/1	0.84	0.13	57,57,57,57	0
56	MG	1A	4065	1/1	0.84	0.11	41,41,41,41	0
56	MG	2A	3472	1/1	0.84	0.14	50,50,50,50	0
56	MG	2A	3251	1/1	0.84	0.12	52,52,52,52	0
56	MG	2a	3039	1/1	0.85	0.21	61,61,61,61	0
56	MG	2a	3048	1/1	0.85	0.11	61,61,61,61	0
56	MG	2A	3762	1/1	0.85	0.11	51,51,51,51	0
56	MG	1w	108	1/1	0.85	0.18	80,80,80,80	0
56	MG	2a	3068	1/1	0.85	0.23	70,70,70,70	0
56	MG	1A	3617	1/1	0.85	0.09	36,36,36,36	0
56	MG	1A	3842	1/1	0.85	0.19	28,28,28,28	0
56	MG	1A	4092	1/1	0.85	0.14	10,10,10,10	0
56	MG	1A	3457	1/1	0.85	0.18	56,56,56,56	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	1A	3858	1/1	0.85	0.12	21,21,21,21	0
56	MG	1a	3077	1/1	0.85	0.10	58,58,58,58	0
56	MG	2A	3821	1/1	0.85	0.12	47,47,47,47	0
56	MG	2A	3198	1/1	0.85	0.19	58,58,58,58	0
56	MG	2A	3454	1/1	0.85	0.17	52,52,52,52	0
56	MG	2a	3155	1/1	0.85	0.11	75,75,75,75	0
56	MG	2A	3203	1/1	0.85	0.25	53,53,53,53	0
56	MG	2A	3647	1/1	0.85	0.12	39,39,39,39	0
56	MG	2A	3465	1/1	0.85	0.09	54,54,54,54	0
56	MG	1A	3034	1/1	0.85	0.12	56,56,56,56	0
56	MG	1a	3188	1/1	0.85	0.13	55,55,55,55	0
56	MG	2A	3663	1/1	0.85	0.18	55,55,55,55	0
56	MG	2A	3666	1/1	0.85	0.18	58,58,58,58	0
56	MG	2A	3326	1/1	0.85	0.18	50,50,50,50	0
56	MG	1A	3947	1/1	0.85	0.09	23,23,23,23	0
56	MG	2A	3483	1/1	0.85	0.12	35,35,35,35	0
56	MG	2A	3211	1/1	0.85	0.17	58,58,58,58	0
56	MG	1a	3106	1/1	0.85	0.20	55,55,55,55	0
56	MG	2A	3508	1/1	0.85	0.10	30,30,30,30	0
56	MG	2B	3019	1/1	0.85	0.10	75,75,75,75	0
56	MG	2A	3509	1/1	0.85	0.12	51,51,51,51	0
56	MG	2E	301	1/1	0.85	0.12	53,53,53,53	0
56	MG	1a	3228	1/1	0.85	0.18	58,58,58,58	0
56	MG	1A	3806	1/1	0.85	0.20	41,41,41,41	0
56	MG	2A	3229	1/1	0.85	0.07	44,44,44,44	0
56	MG	2a	3223	1/1	0.85	0.09	54,54,54,54	0
56	MG	1A	3498	1/1	0.85	0.14	43,43,43,43	0
56	MG	2A	3358	1/1	0.85	0.14	35,35,35,35	0
56	MG	2A	3560	1/1	0.85	0.11	40,40,40,40	0
56	MG	2r	101	1/1	0.85	0.10	75,75,75,75	0
56	MG	2A	3375	1/1	0.85	0.30	47,47,47,47	0
56	MG	1F	308	1/1	0.85	0.21	44,44,44,44	0
56	MG	2a	3002	1/1	0.85	0.18	50,50,50,50	0
56	MG	2A	3138	1/1	0.85	0.14	40,40,40,40	0
56	MG	2A	3737	1/1	0.85	0.21	47,47,47,47	0
56	MG	2a	3012	1/1	0.85	0.14	59,59,59,59	0
56	MG	1a	3121	1/1	0.85	0.20	59,59,59,59	0
56	MG	2A	3142	1/1	0.85	0.12	41,41,41,41	0
56	MG	1A	3143	1/1	0.85	0.18	30,30,30,30	0
56	MG	2A	3403	1/1	0.85	0.17	52,52,52,52	0
56	MG	2y	103	1/1	0.85	0.12	51,51,51,51	0
56	MG	1A	3543	1/1	0.85	0.21	47,47,47,47	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	2A	3688	1/1	0.86	0.12	50,50,50,50	0
56	MG	2A	3103	1/1	0.86	0.15	59,59,59,59	0
56	MG	2a	3019	1/1	0.86	0.10	50,50,50,50	0
56	MG	2A	3482	1/1	0.86	0.13	54,54,54,54	0
56	MG	2A	3109	1/1	0.86	0.11	52,52,52,52	0
56	MG	1a	3180	1/1	0.86	0.09	55,55,55,55	0
56	MG	1a	3037	1/1	0.86	0.21	44,44,44,44	0
56	MG	2A	3503	1/1	0.86	0.11	25,25,25,25	0
56	MG	2A	3732	1/1	0.86	0.12	43,43,43,43	0
56	MG	2A	3295	1/1	0.86	0.23	62,62,62,62	0
56	MG	2a	3054	1/1	0.86	0.22	65,65,65,65	0
56	MG	1a	3046	1/1	0.86	0.18	55,55,55,55	0
56	MG	1A	3994	1/1	0.86	0.16	48,48,48,48	0
56	MG	2A	3539	1/1	0.86	0.27	46,46,46,46	0
56	MG	1A	3426	1/1	0.86	0.15	48,48,48,48	0
56	MG	1a	3197	1/1	0.86	0.12	46,46,46,46	0
56	MG	2a	3098	1/1	0.86	0.15	58,58,58,58	0
56	MG	1A	3861	1/1	0.86	0.11	15,15,15,15	0
56	MG	1a	3224	1/1	0.86	0.19	49,49,49,49	0
56	MG	1A	3328	1/1	0.86	0.18	44,44,44,44	0
56	MG	1A	3204	1/1	0.86	0.11	41,41,41,41	0
56	MG	1A	3536	1/1	0.86	0.14	33,33,33,33	0
56	MG	1m	3001	1/1	0.86	0.22	48,48,48,48	0
56	MG	2A	3188	1/1	0.86	0.48	41,41,41,41	0
56	MG	1a	3074	1/1	0.86	0.17	49,49,49,49	0
56	MG	2a	3165	1/1	0.86	0.19	52,52,52,52	0
56	MG	1A	3200	1/1	0.86	0.18	47,47,47,47	0
56	MG	2A	3372	1/1	0.86	0.28	51,51,51,51	0
56	MG	2A	3595	1/1	0.86	0.12	73,73,73,73	0
56	MG	1a	3087	1/1	0.86	0.26	63,63,63,63	0
56	MG	1A	3709	1/1	0.86	0.10	12,12,12,12	0
56	MG	2A	3599	1/1	0.86	0.14	52,52,52,52	0
56	MG	1A	3900	1/1	0.86	0.12	42,42,42,42	0
56	MG	1A	3915	1/1	0.86	0.13	8,8,8,8	0
56	MG	12	3001	1/1	0.86	0.10	45,45,45,45	0
56	MG	2A	3621	1/1	0.86	0.18	62,62,62,62	0
56	MG	2A	3389	1/1	0.86	0.26	49,49,49,49	0
56	MG	2A	3220	1/1	0.86	0.23	60,60,60,60	0
56	MG	2a	3207	1/1	0.86	0.14	57,57,57,57	0
56	MG	2B	3007	1/1	0.86	0.11	53,53,53,53	0
56	MG	2A	3401	1/1	0.86	0.30	52,52,52,52	0
56	MG	2A	3626	1/1	0.86	0.12	31,31,31,31	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	1A	3564	1/1	0.86	0.10	51,51,51,51	0
56	MG	2a	3216	1/1	0.86	0.19	51,51,51,51	0
56	MG	1x	115	1/1	0.86	0.15	62,62,62,62	0
56	MG	1A	3420	1/1	0.86	0.15	62,62,62,62	0
56	MG	1A	3421	1/1	0.86	0.15	46,46,46,46	0
56	MG	2A	3416	1/1	0.86	0.23	52,52,52,52	0
56	MG	2a	3229	1/1	0.86	0.13	72,72,72,72	0
56	MG	1A	3752	1/1	0.86	0.08	58,58,58,58	0
56	MG	1a	3006	1/1	0.86	0.10	49,49,49,49	0
56	MG	1A	3829	1/1	0.86	0.15	52,52,52,52	0
56	MG	2A	3665	1/1	0.86	0.10	47,47,47,47	0
56	MG	1a	3155	1/1	0.86	0.18	50,50,50,50	0
56	MG	2A	3047	1/1	0.86	0.10	46,46,46,46	0
56	MG	1A	3479	1/1	0.86	0.12	38,38,38,38	0
56	MG	2A	3072	1/1	0.86	0.25	61,61,61,61	0
56	MG	1a	3022	1/1	0.86	0.13	52,52,52,52	0
56	MG	25	105	1/1	0.86	0.10	55,55,55,55	0
56	MG	1A	3485	1/1	0.86	0.20	33,33,33,33	0
56	MG	2x	3003	1/1	0.86	0.24	66,66,66,66	0
56	MG	2A	3268	1/1	0.86	0.17	59,59,59,59	0
56	MG	2A	3276	1/1	0.86	0.07	46,46,46,46	0
56	MG	2a	3010	1/1	0.86	0.21	56,56,56,56	0
56	MG	1A	3766	1/1	0.86	0.12	44,44,44,44	0
56	MG	2V	201	1/1	0.87	0.13	58,58,58,58	0
56	MG	2A	3649	1/1	0.87	0.11	54,54,54,54	0
56	MG	25	102	1/1	0.87	0.20	60,60,60,60	0
56	MG	1A	3248	1/1	0.87	0.10	35,35,35,35	0
56	MG	2A	3408	1/1	0.87	0.12	48,48,48,48	0
56	MG	2A	3655	1/1	0.87	0.09	55,55,55,55	0
56	MG	2a	3004	1/1	0.87	0.18	58,58,58,58	0
56	MG	1A	3332	1/1	0.87	0.08	46,46,46,46	0
56	MG	2A	3661	1/1	0.87	0.11	53,53,53,53	0
56	MG	1A	3380	1/1	0.87	0.10	37,37,37,37	0
56	MG	1a	3066	1/1	0.87	0.19	49,49,49,49	0
56	MG	1A	4113	1/1	0.87	0.09	44,44,44,44	0
56	MG	2a	3017	1/1	0.87	0.14	65,65,65,65	0
56	MG	2A	3668	1/1	0.87	0.13	57,57,57,57	0
56	MG	2A	3423	1/1	0.87	0.12	48,48,48,48	0
56	MG	1A	4127	1/1	0.87	0.14	23,23,23,23	0
56	MG	1a	3070	1/1	0.87	0.19	44,44,44,44	0
56	MG	1A	3481	1/1	0.87	0.20	66,66,66,66	0
56	MG	1x	112	1/1	0.87	0.20	67,67,67,67	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	2A	3679	1/1	0.87	0.14	54,54,54,54	0
56	MG	2A	3243	1/1	0.87	0.17	62,62,62,62	0
56	MG	1A	3800	1/1	0.87	0.10	35,35,35,35	0
56	MG	2A	3685	1/1	0.87	0.11	47,47,47,47	0
56	MG	1A	3631	1/1	0.87	0.11	45,45,45,45	0
56	MG	2a	3069	1/1	0.87	0.13	55,55,55,55	0
56	MG	2a	3073	1/1	0.87	0.13	73,73,73,73	0
56	MG	1B	3028	1/1	0.87	0.09	38,38,38,38	0
56	MG	2a	3077	1/1	0.87	0.14	44,44,44,44	0
56	MG	2A	3466	1/1	0.87	0.17	48,48,48,48	0
56	MG	2A	3468	1/1	0.87	0.09	53,53,53,53	0
56	MG	2a	3086	1/1	0.87	0.25	57,57,57,57	0
56	MG	2A	3250	1/1	0.87	0.08	46,46,46,46	0
56	MG	1A	3388	1/1	0.87	0.10	39,39,39,39	0
56	MG	2a	3106	1/1	0.87	0.15	43,43,43,43	0
56	MG	2A	3722	1/1	0.87	0.11	57,57,57,57	0
56	MG	1D	313	1/1	0.87	0.27	35,35,35,35	0
56	MG	1A	3955	1/1	0.87	0.10	48,48,48,48	0
56	MG	2a	3126	1/1	0.87	0.12	70,70,70,70	0
56	MG	1A	3654	1/1	0.87	0.17	51,51,51,51	0
56	MG	1A	3673	1/1	0.87	0.13	24,24,24,24	0
56	MG	2A	3490	1/1	0.87	0.18	65,65,65,65	0
56	MG	1A	3492	1/1	0.87	0.19	71,71,71,71	0
56	MG	1A	3252	1/1	0.87	0.27	53,53,53,53	0
56	MG	2a	3166	1/1	0.87	0.10	66,66,66,66	0
56	MG	1a	3140	1/1	0.87	0.10	37,37,37,37	0
56	MG	2A	3079	1/1	0.87	0.07	50,50,50,50	0
56	MG	1A	3708	1/1	0.87	0.16	27,27,27,27	0
56	MG	2a	3173	1/1	0.87	0.11	62,62,62,62	0
56	MG	1A	3123	1/1	0.87	0.17	62,62,62,62	0
56	MG	2A	3516	1/1	0.87	0.17	74,74,74,74	0
56	MG	2A	3523	1/1	0.87	0.15	58,58,58,58	0
56	MG	2A	3293	1/1	0.87	0.21	67,67,67,67	0
56	MG	1A	3125	1/1	0.87	0.05	17,17,17,17	0
56	MG	2A	3296	1/1	0.87	0.07	63,63,63,63	0
56	MG	1A	3847	1/1	0.87	0.14	26,26,26,26	0
56	MG	17	102	1/1	0.87	0.09	36,36,36,36	0
56	MG	2A	3120	1/1	0.87	0.20	56,56,56,56	0
56	MG	2A	3123	1/1	0.87	0.12	50,50,50,50	0
56	MG	18	101	1/1	0.87	0.16	59,59,59,59	0
56	MG	1A	3277	1/1	0.87	0.13	49,49,49,49	0
56	MG	1A	4026	1/1	0.87	0.36	42,42,42,42	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	1A	3715	1/1	0.87	0.09	48,48,48,48	0
56	MG	2A	3146	1/1	0.87	0.16	51,51,51,51	0
56	MG	1A	3280	1/1	0.87	0.06	25,25,25,25	0
56	MG	1A	3545	1/1	0.87	0.21	60,60,60,60	0
56	MG	1a	3189	1/1	0.87	0.12	56,56,56,56	0
56	MG	1A	3061	1/1	0.87	0.08	22,22,22,22	0
56	MG	2A	3369	1/1	0.87	0.35	58,58,58,58	0
56	MG	2A	3600	1/1	0.87	0.10	53,53,53,53	0
56	MG	2A	3371	1/1	0.87	0.21	49,49,49,49	0
56	MG	2q	203	1/1	0.87	0.18	55,55,55,55	0
56	MG	1A	4041	1/1	0.87	0.16	45,45,45,45	0
56	MG	2r	102	1/1	0.87	0.07	75,75,75,75	0
56	MG	1A	4053	1/1	0.87	0.10	45,45,45,45	0
56	MG	2A	3612	1/1	0.87	0.22	60,60,60,60	0
56	MG	2A	3614	1/1	0.87	0.15	68,68,68,68	0
56	MG	2w	3003	1/1	0.87	0.10	51,51,51,51	0
56	MG	1a	3222	1/1	0.87	0.16	60,60,60,60	0
56	MG	1A	3180	1/1	0.87	0.09	38,38,38,38	0
56	MG	2A	3191	1/1	0.87	0.15	43,43,43,43	0
56	MG	2E	307	1/1	0.87	0.13	49,49,49,49	0
56	MG	1A	4061	1/1	0.87	0.13	27,27,27,27	0
56	MG	1a	3230	1/1	0.87	0.12	49,49,49,49	0
56	MG	2A	3390	1/1	0.87	0.23	57,57,57,57	0
56	MG	1a	3038	1/1	0.87	0.17	50,50,50,50	0
56	MG	1A	3593	1/1	0.87	0.14	41,41,41,41	0
56	MG	1A	3308	1/1	0.87	0.12	29,29,29,29	0
56	MG	1A	3494	1/1	0.88	0.08	41,41,41,41	0
56	MG	1A	3929	1/1	0.88	0.11	28,28,28,28	0
56	MG	16	103	1/1	0.88	0.17	33,33,33,33	0
56	MG	2A	3181	1/1	0.88	0.17	49,49,49,49	0
56	MG	2a	3031	1/1	0.88	0.33	62,62,62,62	0
56	MG	2A	3331	1/1	0.88	0.22	51,51,51,51	0
56	MG	2A	3710	1/1	0.88	0.10	71,71,71,71	0
56	MG	2a	3036	1/1	0.88	0.13	50,50,50,50	0
56	MG	2A	3337	1/1	0.88	0.22	44,44,44,44	0
56	MG	2A	3183	1/1	0.88	0.13	54,54,54,54	0
56	MG	1A	3251	1/1	0.88	0.18	49,49,49,49	0
56	MG	1A	3835	1/1	0.88	0.12	26,26,26,26	0
56	MG	1A	3760	1/1	0.88	0.12	40,40,40,40	0
56	MG	2a	3064	1/1	0.88	0.23	51,51,51,51	0
56	MG	2A	3345	1/1	0.88	0.07	54,54,54,54	0
56	MG	2A	3735	1/1	0.88	0.13	46,46,46,46	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	1A	3838	1/1	0.88	0.09	35,35,35,35	0
56	MG	2A	3348	1/1	0.88	0.13	50,50,50,50	0
56	MG	2A	3200	1/1	0.88	0.19	51,51,51,51	0
56	MG	1A	3159	1/1	0.88	0.13	26,26,26,26	0
56	MG	2A	3576	1/1	0.88	0.13	35,35,35,35	0
56	MG	2A	3577	1/1	0.88	0.11	49,49,49,49	0
56	MG	2a	3087	1/1	0.88	0.22	53,53,53,53	0
56	MG	2A	3750	1/1	0.88	0.11	48,48,48,48	0
56	MG	2a	3102	1/1	0.88	0.16	60,60,60,60	0
56	MG	2a	3104	1/1	0.88	0.13	34,34,34,34	0
56	MG	1a	3146	1/1	0.88	0.14	44,44,44,44	0
56	MG	1A	3391	1/1	0.88	0.21	47,47,47,47	0
56	MG	1A	3692	1/1	0.88	0.10	56,56,56,56	0
56	MG	2a	3112	1/1	0.88	0.09	61,61,61,61	0
56	MG	1A	3700	1/1	0.88	0.12	49,49,49,49	0
56	MG	2a	3120	1/1	0.88	0.10	75,75,75,75	0
56	MG	2A	3769	1/1	0.88	0.08	46,46,46,46	0
56	MG	2A	3779	1/1	0.88	0.11	27,27,27,27	0
56	MG	2a	3137	1/1	0.88	0.10	48,48,48,48	0
56	MG	2A	3789	1/1	0.88	0.16	62,62,62,62	0
56	MG	2a	3142	1/1	0.88	0.12	56,56,56,56	0
56	MG	2A	3213	1/1	0.88	0.09	61,61,61,61	0
56	MG	2a	3153	1/1	0.88	0.10	68,68,68,68	0
56	MG	2A	3594	1/1	0.88	0.09	38,38,38,38	0
56	MG	2a	3161	1/1	0.88	0.14	70,70,70,70	0
56	MG	1A	3297	1/1	0.88	0.12	42,42,42,42	0
56	MG	2A	3802	1/1	0.88	0.16	60,60,60,60	0
56	MG	1B	3020	1/1	0.88	0.09	28,28,28,28	0
56	MG	1B	3022	1/1	0.88	0.16	48,48,48,48	0
56	MG	2A	3062	1/1	0.88	0.08	56,56,56,56	0
56	MG	2A	3826	1/1	0.88	0.11	62,62,62,62	0
56	MG	1a	3176	1/1	0.88	0.17	63,63,63,63	0
56	MG	2A	3074	1/1	0.88	0.09	47,47,47,47	0
56	MG	1A	3862	1/1	0.88	0.12	15,15,15,15	0
56	MG	2a	3182	1/1	0.88	0.21	56,56,56,56	0
56	MG	2a	3185	1/1	0.88	0.15	47,47,47,47	0
56	MG	2a	3187	1/1	0.88	0.08	54,54,54,54	0
56	MG	1A	4016	1/1	0.88	0.12	32,32,32,32	0
56	MG	2a	3192	1/1	0.88	0.14	64,64,64,64	0
56	MG	2A	3609	1/1	0.88	0.19	35,35,35,35	0
56	MG	1a	3041	1/1	0.88	0.10	59,59,59,59	0
56	MG	1A	3484	1/1	0.88	0.20	33,33,33,33	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	1B	3033	1/1	0.88	0.10	53,53,53,53	0
56	MG	2A	3108	1/1	0.88	0.07	43,43,43,43	0
56	MG	2B	3002	1/1	0.88	0.09	50,50,50,50	0
56	MG	2A	3623	1/1	0.88	0.16	57,57,57,57	0
56	MG	1A	3789	1/1	0.88	0.11	26,26,26,26	0
56	MG	2A	3253	1/1	0.88	0.07	58,58,58,58	0
56	MG	1A	3877	1/1	0.88	0.14	31,31,31,31	0
56	MG	1A	3356	1/1	0.88	0.16	47,47,47,47	0
56	MG	1A	3401	1/1	0.88	0.09	29,29,29,29	0
56	MG	2a	3217	1/1	0.88	0.20	62,62,62,62	0
56	MG	2A	3640	1/1	0.88	0.09	34,34,34,34	0
56	MG	2A	3266	1/1	0.88	0.10	53,53,53,53	0
56	MG	2a	3221	1/1	0.88	0.17	57,57,57,57	0
56	MG	2A	3125	1/1	0.88	0.14	51,51,51,51	0
56	MG	2D	304	1/1	0.88	0.15	59,59,59,59	0
56	MG	2a	3227	1/1	0.88	0.27	49,49,49,49	0
56	MG	2A	3440	1/1	0.88	0.09	40,40,40,40	0
56	MG	2A	3274	1/1	0.88	0.13	47,47,47,47	0
56	MG	1A	3588	1/1	0.88	0.12	24,24,24,24	0
56	MG	2A	3445	1/1	0.88	0.16	50,50,50,50	0
56	MG	2A	3450	1/1	0.88	0.19	46,46,46,46	0
56	MG	2A	3453	1/1	0.88	0.20	52,52,52,52	0
56	MG	1A	3898	1/1	0.88	0.11	23,23,23,23	0
56	MG	1A	3733	1/1	0.88	0.12	15,15,15,15	0
56	MG	2A	3287	1/1	0.88	0.10	45,45,45,45	0
56	MG	1T	3003	1/1	0.88	0.10	34,34,34,34	0
56	MG	1A	3647	1/1	0.88	0.13	27,27,27,27	0
56	MG	1X	104	1/1	0.88	0.21	30,30,30,30	0
56	MG	1Y	503	1/1	0.88	0.10	58,58,58,58	0
56	MG	2A	3163	1/1	0.88	0.11	53,53,53,53	0
56	MG	1A	3748	1/1	0.88	0.11	29,29,29,29	0
56	MG	1a	3098	1/1	0.88	0.23	60,60,60,60	0
56	MG	2A	3311	1/1	0.88	0.10	38,38,38,38	0
56	MG	2A	3312	1/1	0.88	0.18	51,51,51,51	0
56	MG	2A	3683	1/1	0.88	0.22	51,51,51,51	0
56	MG	2A	3318	1/1	0.88	0.11	52,52,52,52	0
56	MG	1a	3031	1/1	0.89	0.16	48,48,48,48	0
56	MG	2a	3001	1/1	0.89	0.10	56,56,56,56	0
56	MG	1A	3584	1/1	0.89	0.12	7,7,7,7	0
56	MG	1A	3088	1/1	0.89	0.22	43,43,43,43	0
56	MG	1A	3802	1/1	0.89	0.11	20,20,20,20	0
56	MG	1B	3003	1/1	0.89	0.18	49,49,49,49	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	1n	502	1/1	0.89	0.25	57,57,57,57	0
56	MG	1t	3001	1/1	0.89	0.18	53,53,53,53	0
56	MG	1a	3048	1/1	0.89	0.24	52,52,52,52	0
56	MG	2a	3015	1/1	0.89	0.16	46,46,46,46	0
56	MG	2a	3016	1/1	0.89	0.08	47,47,47,47	0
56	MG	1A	3346	1/1	0.89	0.12	45,45,45,45	0
56	MG	1B	3008	1/1	0.89	0.20	53,53,53,53	0
56	MG	2a	3022	1/1	0.89	0.22	53,53,53,53	0
56	MG	1a	3058	1/1	0.89	0.08	53,53,53,53	0
56	MG	1w	107	1/1	0.89	0.07	48,48,48,48	0
56	MG	2a	3030	1/1	0.89	0.25	51,51,51,51	0
56	MG	1A	3235	1/1	0.89	0.23	46,46,46,46	0
56	MG	2A	3673	1/1	0.89	0.12	38,38,38,38	0
56	MG	1A	3376	1/1	0.89	0.16	39,39,39,39	0
56	MG	2A	3434	1/1	0.89	0.11	38,38,38,38	0
56	MG	1A	3813	1/1	0.89	0.13	51,51,51,51	0
56	MG	2a	3044	1/1	0.89	0.13	68,68,68,68	0
56	MG	2a	3046	1/1	0.89	0.16	52,52,52,52	0
56	MG	1x	108	1/1	0.89	0.15	47,47,47,47	0
56	MG	1A	3241	1/1	0.89	0.12	46,46,46,46	0
56	MG	1A	3961	1/1	0.89	0.09	19,19,19,19	0
56	MG	1A	3718	1/1	0.89	0.10	42,42,42,42	0
56	MG	2a	3056	1/1	0.89	0.21	46,46,46,46	0
56	MG	2a	3059	1/1	0.89	0.08	52,52,52,52	0
56	MG	1A	3973	1/1	0.89	0.11	23,23,23,23	0
56	MG	1A	3729	1/1	0.89	0.15	10,10,10,10	0
56	MG	2A	3239	1/1	0.89	0.12	46,46,46,46	0
56	MG	1a	3086	1/1	0.89	0.17	46,46,46,46	0
56	MG	2a	3075	1/1	0.89	0.25	54,54,54,54	0
56	MG	2A	3699	1/1	0.89	0.12	60,60,60,60	0
56	MG	2A	3013	1/1	0.89	0.18	52,52,52,52	0
56	MG	2a	3078	1/1	0.89	0.21	60,60,60,60	0
56	MG	2A	3706	1/1	0.89	0.08	58,58,58,58	0
56	MG	2A	3467	1/1	0.89	0.11	32,32,32,32	0
56	MG	2A	3246	1/1	0.89	0.18	55,55,55,55	0
56	MG	2A	3017	1/1	0.89	0.20	37,37,37,37	0
56	MG	2a	3091	1/1	0.89	0.10	60,60,60,60	0
56	MG	1A	3983	1/1	0.89	0.09	14,14,14,14	0
56	MG	2a	3101	1/1	0.89	0.13	66,66,66,66	0
56	MG	1E	309	1/1	0.89	0.09	45,45,45,45	0
56	MG	2a	3103	1/1	0.89	0.25	68,68,68,68	0
56	MG	2A	3480	1/1	0.89	0.10	33,33,33,33	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	2A	3030	1/1	0.89	0.15	56,56,56,56	0
56	MG	1F	305	1/1	0.89	0.08	36,36,36,36	0
56	MG	2A	3038	1/1	0.89	0.14	46,46,46,46	0
56	MG	2A	3043	1/1	0.89	0.13	53,53,53,53	0
56	MG	2A	3740	1/1	0.89	0.11	55,55,55,55	0
56	MG	1A	3991	1/1	0.89	0.20	41,41,41,41	0
56	MG	2A	3049	1/1	0.89	0.09	30,30,30,30	0
56	MG	1A	3834	1/1	0.89	0.14	57,57,57,57	0
56	MG	2a	3128	1/1	0.89	0.12	57,57,57,57	0
56	MG	2a	3131	1/1	0.89	0.07	87,87,87,87	0
56	MG	2A	3272	1/1	0.89	0.13	43,43,43,43	0
56	MG	1A	3456	1/1	0.89	0.10	41,41,41,41	0
56	MG	2A	3064	1/1	0.89	0.15	59,59,59,59	0
56	MG	2A	3068	1/1	0.89	0.22	54,54,54,54	0
56	MG	1a	3108	1/1	0.89	0.16	60,60,60,60	0
56	MG	2A	3536	1/1	0.89	0.08	32,32,32,32	0
56	MG	2a	3156	1/1	0.89	0.09	56,56,56,56	0
56	MG	1A	4006	1/1	0.89	0.07	53,53,53,53	0
56	MG	2A	3541	1/1	0.89	0.12	50,50,50,50	0
56	MG	1A	3735	1/1	0.89	0.08	25,25,25,25	0
56	MG	2A	3076	1/1	0.89	0.13	53,53,53,53	0
56	MG	1A	3387	1/1	0.89	0.06	42,42,42,42	0
56	MG	1A	3021	1/1	0.89	0.14	20,20,20,20	0
56	MG	2A	3799	1/1	0.89	0.15	59,59,59,59	0
56	MG	2A	3294	1/1	0.89	0.22	61,61,61,61	0
56	MG	2A	3805	1/1	0.89	0.14	42,42,42,42	0
56	MG	2a	3179	1/1	0.89	0.12	53,53,53,53	0
56	MG	2A	3562	1/1	0.89	0.10	32,32,32,32	0
56	MG	2A	3085	1/1	0.89	0.19	49,49,49,49	0
56	MG	2A	3570	1/1	0.89	0.13	33,33,33,33	0
56	MG	1A	3618	1/1	0.89	0.11	34,34,34,34	0
56	MG	2A	3827	1/1	0.89	0.17	64,64,64,64	0
56	MG	2A	3090	1/1	0.89	0.16	38,38,38,38	0
56	MG	2A	3308	1/1	0.89	0.14	50,50,50,50	0
56	MG	2A	3098	1/1	0.89	0.07	32,32,32,32	0
56	MG	2a	3196	1/1	0.89	0.22	53,53,53,53	0
56	MG	1Z	301	1/1	0.89	0.16	35,35,35,35	0
56	MG	1A	3509	1/1	0.89	0.25	47,47,47,47	0
56	MG	2A	3845	1/1	0.89	0.15	44,44,44,44	0
56	MG	2A	3846	1/1	0.89	0.13	41,41,41,41	0
56	MG	10	108	1/1	0.89	0.07	45,45,45,45	0
56	MG	1A	3263	1/1	0.89	0.16	31,31,31,31	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	2a	3209	1/1	0.89	0.14	55,55,55,55	0
56	MG	2A	3117	1/1	0.89	0.17	36,36,36,36	0
56	MG	2A	3869	1/1	0.89	0.13	55,55,55,55	0
56	MG	2A	3118	1/1	0.89	0.13	35,35,35,35	0
56	MG	1A	3473	1/1	0.89	0.08	23,23,23,23	0
56	MG	2B	3004	1/1	0.89	0.17	53,53,53,53	0
56	MG	1A	3324	1/1	0.89	0.09	42,42,42,42	0
56	MG	2A	3124	1/1	0.89	0.24	52,52,52,52	0
56	MG	2B	3012	1/1	0.89	0.11	63,63,63,63	0
56	MG	1A	3865	1/1	0.89	0.17	14,14,14,14	0
56	MG	2A	3127	1/1	0.89	0.31	61,61,61,61	0
56	MG	2A	3131	1/1	0.89	0.13	51,51,51,51	0
56	MG	1A	3662	1/1	0.89	0.10	26,26,26,26	0
56	MG	1A	3546	1/1	0.89	0.21	57,57,57,57	0
56	MG	1A	3172	1/1	0.89	0.16	22,22,22,22	0
56	MG	1A	3572	1/1	0.89	0.12	34,34,34,34	0
56	MG	2D	301	1/1	0.89	0.10	36,36,36,36	0
56	MG	2A	3617	1/1	0.89	0.10	48,48,48,48	0
56	MG	2t	3001	1/1	0.89	0.16	48,48,48,48	0
56	MG	2A	3620	1/1	0.89	0.25	50,50,50,50	0
56	MG	2E	304	1/1	0.89	0.15	58,58,58,58	0
56	MG	1a	3003	1/1	0.89	0.18	49,49,49,49	0
56	MG	2A	3149	1/1	0.89	0.30	56,56,56,56	0
56	MG	1A	3784	1/1	0.89	0.11	42,42,42,42	0
56	MG	2A	3158	1/1	0.89	0.11	47,47,47,47	0
56	MG	1A	3787	1/1	0.89	0.13	40,40,40,40	0
56	MG	2w	3007	1/1	0.89	0.12	60,60,60,60	0
56	MG	1A	3788	1/1	0.89	0.07	15,15,15,15	0
56	MG	2A	3164	1/1	0.89	0.06	18,18,18,18	0
56	MG	2U	205	1/1	0.89	0.09	46,46,46,46	0
56	MG	1A	3573	1/1	0.89	0.12	22,22,22,22	0
56	MG	1A	3905	1/1	0.89	0.12	43,43,43,43	0
56	MG	1A	3791	1/1	0.89	0.16	32,32,32,32	0
56	MG	1a	3029	1/1	0.89	0.21	63,63,63,63	0
56	MG	1A	3104	1/1	0.90	0.08	29,29,29,29	0
56	MG	2A	3231	1/1	0.90	0.29	52,52,52,52	0
56	MG	1A	3447	1/1	0.90	0.12	32,32,32,32	0
56	MG	2a	3032	1/1	0.90	0.23	59,59,59,59	0
56	MG	2A	3448	1/1	0.90	0.14	23,23,23,23	0
56	MG	1a	3110	1/1	0.90	0.18	50,50,50,50	0
56	MG	2A	3236	1/1	0.90	0.08	50,50,50,50	0
56	MG	2A	3691	1/1	0.90	0.18	51,51,51,51	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	1A	3868	1/1	0.90	0.10	43,43,43,43	0
56	MG	2A	3048	1/1	0.90	0.08	43,43,43,43	0
56	MG	2A	3457	1/1	0.90	0.11	51,51,51,51	0
56	MG	1a	3112	1/1	0.90	0.16	48,48,48,48	0
56	MG	2A	3245	1/1	0.90	0.09	58,58,58,58	0
56	MG	1A	3453	1/1	0.90	0.11	44,44,44,44	0
56	MG	1A	3515	1/1	0.90	0.09	49,49,49,49	0
56	MG	2a	3058	1/1	0.90	0.09	50,50,50,50	0
56	MG	2A	3469	1/1	0.90	0.16	50,50,50,50	0
56	MG	1A	3524	1/1	0.90	0.20	30,30,30,30	0
56	MG	1a	3144	1/1	0.90	0.15	43,43,43,43	0
56	MG	1A	3242	1/1	0.90	0.21	33,33,33,33	0
56	MG	1A	4040	1/1	0.90	0.10	52,52,52,52	0
56	MG	1A	3663	1/1	0.90	0.07	32,32,32,32	0
56	MG	2A	3257	1/1	0.90	0.17	43,43,43,43	0
56	MG	2A	3738	1/1	0.90	0.11	46,46,46,46	0
56	MG	2A	3260	1/1	0.90	0.09	48,48,48,48	0
56	MG	2a	3079	1/1	0.90	0.18	53,53,53,53	0
56	MG	1A	4044	1/1	0.90	0.06	17,17,17,17	0
56	MG	2A	3077	1/1	0.90	0.09	44,44,44,44	0
56	MG	2A	3494	1/1	0.90	0.10	46,46,46,46	0
56	MG	2A	3744	1/1	0.90	0.08	76,76,76,76	0
56	MG	2A	3263	1/1	0.90	0.29	68,68,68,68	0
56	MG	2a	3092	1/1	0.90	0.32	59,59,59,59	0
56	MG	2a	3093	1/1	0.90	0.16	60,60,60,60	0
56	MG	2a	3096	1/1	0.90	0.11	62,62,62,62	0
56	MG	2a	3097	1/1	0.90	0.12	54,54,54,54	0
56	MG	1a	3157	1/1	0.90	0.10	46,46,46,46	0
56	MG	1a	3160	1/1	0.90	0.12	62,62,62,62	0
56	MG	2A	3269	1/1	0.90	0.10	54,54,54,54	0
56	MG	1A	3261	1/1	0.90	0.16	23,23,23,23	0
56	MG	1A	4055	1/1	0.90	0.13	56,56,56,56	0
56	MG	1A	3674	1/1	0.90	0.14	38,38,38,38	0
56	MG	1A	3899	1/1	0.90	0.07	28,28,28,28	0
56	MG	2a	3108	1/1	0.90	0.15	48,48,48,48	0
56	MG	1a	3005	1/1	0.90	0.12	52,52,52,52	0
56	MG	2A	3105	1/1	0.90	0.21	51,51,51,51	0
56	MG	1A	3094	1/1	0.90	0.15	43,43,43,43	0
56	MG	1a	3007	1/1	0.90	0.26	56,56,56,56	0
56	MG	2a	3123	1/1	0.90	0.10	75,75,75,75	0
56	MG	2A	3548	1/1	0.90	0.11	25,25,25,25	0
56	MG	1A	3678	1/1	0.90	0.17	43,43,43,43	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	2A	3550	1/1	0.90	0.12	43,43,43,43	0
56	MG	2A	3552	1/1	0.90	0.12	40,40,40,40	0
56	MG	2a	3134	1/1	0.90	0.12	60,60,60,60	0
56	MG	2a	3135	1/1	0.90	0.14	55,55,55,55	0
56	MG	1A	3910	1/1	0.90	0.10	45,45,45,45	0
56	MG	2A	3813	1/1	0.90	0.22	51,51,51,51	0
56	MG	2A	3815	1/1	0.90	0.25	59,59,59,59	0
56	MG	1A	3264	1/1	0.90	0.09	48,48,48,48	0
56	MG	1a	3023	1/1	0.90	0.07	47,47,47,47	0
56	MG	1a	3196	1/1	0.90	0.10	51,51,51,51	0
56	MG	2A	3564	1/1	0.90	0.14	34,34,34,34	0
56	MG	2a	3160	1/1	0.90	0.09	66,66,66,66	0
56	MG	2A	3298	1/1	0.90	0.10	47,47,47,47	0
56	MG	1A	4096	1/1	0.90	0.15	39,39,39,39	0
56	MG	1a	3211	1/1	0.90	0.09	65,65,65,65	0
56	MG	2A	3840	1/1	0.90	0.08	68,68,68,68	0
56	MG	1A	3682	1/1	0.90	0.09	12,12,12,12	0
56	MG	1A	3922	1/1	0.90	0.10	63,63,63,63	0
56	MG	2A	3136	1/1	0.90	0.10	54,54,54,54	0
56	MG	1A	3796	1/1	0.90	0.18	41,41,41,41	0
56	MG	2a	3177	1/1	0.90	0.10	58,58,58,58	0
56	MG	1a	3226	1/1	0.90	0.11	55,55,55,55	0
56	MG	2A	3140	1/1	0.90	0.15	44,44,44,44	0
56	MG	2A	3141	1/1	0.90	0.13	53,53,53,53	0
56	MG	1A	3548	1/1	0.90	0.17	45,45,45,45	0
56	MG	1A	3562	1/1	0.90	0.35	26,26,26,26	0
56	MG	1A	3934	1/1	0.90	0.07	14,14,14,14	0
56	MG	1A	3464	1/1	0.90	0.14	29,29,29,29	0
56	MG	2A	3150	1/1	0.90	0.22	53,53,53,53	0
56	MG	1f	3002	1/1	0.90	0.22	60,60,60,60	0
56	MG	1B	3021	1/1	0.90	0.11	50,50,50,50	0
56	MG	1A	3176	1/1	0.90	0.10	52,52,52,52	0
56	MG	1A	3334	1/1	0.90	0.10	46,46,46,46	0
56	MG	2A	3349	1/1	0.90	0.19	45,45,45,45	0
56	MG	1a	3056	1/1	0.90	0.19	56,56,56,56	0
56	MG	1A	3579	1/1	0.90	0.11	27,27,27,27	0
56	MG	2a	3205	1/1	0.90	0.16	66,66,66,66	0
56	MG	2A	3619	1/1	0.90	0.11	50,50,50,50	0
56	MG	1A	3476	1/1	0.90	0.12	44,44,44,44	0
56	MG	1B	3031	1/1	0.90	0.17	59,59,59,59	0
56	MG	1a	3063	1/1	0.90	0.12	41,41,41,41	0
56	MG	2A	3171	1/1	0.90	0.13	48,48,48,48	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	2E	306	1/1	0.90	0.11	45,45,45,45	0
56	MG	2a	3214	1/1	0.90	0.07	51,51,51,51	0
56	MG	1A	3717	1/1	0.90	0.09	23,23,23,23	0
56	MG	2A	3376	1/1	0.90	0.16	47,47,47,47	0
56	MG	2A	3178	1/1	0.90	0.10	41,41,41,41	0
56	MG	2a	3219	1/1	0.90	0.24	53,53,53,53	0
56	MG	1a	3067	1/1	0.90	0.15	44,44,44,44	0
56	MG	1A	3399	1/1	0.90	0.12	42,42,42,42	0
56	MG	2A	3185	1/1	0.90	0.09	46,46,46,46	0
56	MG	2A	3186	1/1	0.90	0.11	43,43,43,43	0
56	MG	1A	3726	1/1	0.90	0.10	12,12,12,12	0
56	MG	1A	3223	1/1	0.90	0.16	47,47,47,47	0
56	MG	2a	3230	1/1	0.90	0.18	61,61,61,61	0
56	MG	2A	3397	1/1	0.90	0.08	59,59,59,59	0
56	MG	1A	3347	1/1	0.90	0.14	34,34,34,34	0
56	MG	2l	202	1/1	0.90	0.16	62,62,62,62	0
56	MG	1A	3348	1/1	0.90	0.13	46,46,46,46	0
56	MG	1y	103	1/1	0.90	0.17	80,80,80,80	0
56	MG	2A	3660	1/1	0.90	0.12	31,31,31,31	0
56	MG	1A	3144	1/1	0.90	0.22	39,39,39,39	0
56	MG	1A	3430	1/1	0.90	0.11	32,32,32,32	0
56	MG	2a	3006	1/1	0.90	0.16	53,53,53,53	0
56	MG	1a	3090	1/1	0.90	0.18	27,27,27,27	0
56	MG	2a	3009	1/1	0.90	0.17	58,58,58,58	0
56	MG	1A	3440	1/1	0.90	0.10	54,54,54,54	0
56	MG	2A	3016	1/1	0.90	0.24	58,58,58,58	0
56	MG	1O	3004	1/1	0.90	0.15	41,41,41,41	0
56	MG	1A	3754	1/1	0.90	0.08	21,21,21,21	0
56	MG	2A	3222	1/1	0.90	0.18	53,53,53,53	0
56	MG	1A	3859	1/1	0.90	0.09	27,27,27,27	0
56	MG	1A	3497	1/1	0.90	0.12	34,34,34,34	0
56	MG	2A	3438	1/1	0.90	0.21	47,47,47,47	0
56	MG	2x	3006	1/1	0.90	0.20	58,58,58,58	0
56	MG	2a	3021	1/1	0.90	0.24	64,64,64,64	0
56	MG	2A	3439	1/1	0.90	0.11	51,51,51,51	0
56	MG	2A	3031	1/1	0.90	0.13	55,55,55,55	0
56	MG	2Q	202	1/1	0.91	0.12	31,31,31,31	0
56	MG	2A	3572	1/1	0.91	0.09	25,25,25,25	0
56	MG	1A	3414	1/1	0.91	0.10	27,27,27,27	0
56	MG	1A	3153	1/1	0.91	0.30	23,23,23,23	0
56	MG	2T	3003	1/1	0.91	0.07	59,59,59,59	0
56	MG	1D	301	1/1	0.91	0.18	29,29,29,29	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	2A	3578	1/1	0.91	0.10	31,31,31,31	0
56	MG	2A	3271	1/1	0.91	0.08	50,50,50,50	0
56	MG	2Z	8001	1/1	0.91	0.15	47,47,47,47	0
56	MG	2A	3582	1/1	0.91	0.12	57,57,57,57	0
56	MG	1a	3096	1/1	0.91	0.26	45,45,45,45	0
56	MG	2A	3273	1/1	0.91	0.15	51,51,51,51	0
56	MG	1A	3751	1/1	0.91	0.09	14,14,14,14	0
56	MG	2A	3275	1/1	0.91	0.09	47,47,47,47	0
56	MG	1E	306	1/1	0.91	0.11	32,32,32,32	0
56	MG	1a	3101	1/1	0.91	0.17	48,48,48,48	0
56	MG	1a	3102	1/1	0.91	0.27	59,59,59,59	0
56	MG	2A	3071	1/1	0.91	0.21	53,53,53,53	0
56	MG	1A	3988	1/1	0.91	0.08	28,28,28,28	0
56	MG	1A	3989	1/1	0.91	0.08	21,21,21,21	0
56	MG	1E	310	1/1	0.91	0.16	28,28,28,28	0
56	MG	1A	3057	1/1	0.91	0.08	36,36,36,36	0
56	MG	1A	3852	1/1	0.91	0.10	17,17,17,17	0
56	MG	1A	3855	1/1	0.91	0.12	32,32,32,32	0
56	MG	2A	3080	1/1	0.91	0.17	59,59,59,59	0
56	MG	2A	3297	1/1	0.91	0.08	52,52,52,52	0
56	MG	2A	3615	1/1	0.91	0.12	54,54,54,54	0
56	MG	2A	3082	1/1	0.91	0.08	52,52,52,52	0
56	MG	2A	3618	1/1	0.91	0.07	35,35,35,35	0
56	MG	2A	3083	1/1	0.91	0.13	51,51,51,51	0
56	MG	2A	3303	1/1	0.91	0.07	35,35,35,35	0
56	MG	1A	3998	1/1	0.91	0.09	51,51,51,51	0
56	MG	1a	3115	1/1	0.91	0.20	38,38,38,38	0
56	MG	2A	3087	1/1	0.91	0.10	61,61,61,61	0
56	MG	1O	3002	1/1	0.91	0.24	40,40,40,40	0
56	MG	1a	3128	1/1	0.91	0.08	36,36,36,36	0
56	MG	2A	3091	1/1	0.91	0.18	50,50,50,50	0
56	MG	2a	3037	1/1	0.91	0.10	53,53,53,53	0
56	MG	1a	3130	1/1	0.91	0.10	53,53,53,53	0
56	MG	2A	3632	1/1	0.91	0.10	42,42,42,42	0
56	MG	2a	3045	1/1	0.91	0.15	55,55,55,55	0
56	MG	1A	3628	1/1	0.91	0.08	17,17,17,17	0
56	MG	2a	3047	1/1	0.91	0.14	56,56,56,56	0
56	MG	2A	3637	1/1	0.91	0.10	53,53,53,53	0
56	MG	2a	3049	1/1	0.91	0.16	79,79,79,79	0
56	MG	2A	3328	1/1	0.91	0.08	45,45,45,45	0
56	MG	2a	3053	1/1	0.91	0.09	57,57,57,57	0
56	MG	1A	3227	1/1	0.91	0.14	28,28,28,28	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	2A	3106	1/1	0.91	0.23	37,37,37,37	0
56	MG	1a	3142	1/1	0.91	0.13	63,63,63,63	0
56	MG	1A	3342	1/1	0.91	0.24	31,31,31,31	0
56	MG	2A	3341	1/1	0.91	0.20	43,43,43,43	0
56	MG	2A	3110	1/1	0.91	0.13	49,49,49,49	0
56	MG	2A	3658	1/1	0.91	0.10	31,31,31,31	0
56	MG	2A	3112	1/1	0.91	0.13	34,34,34,34	0
56	MG	2a	3071	1/1	0.91	0.07	55,55,55,55	0
56	MG	1U	203	1/1	0.91	0.13	22,22,22,22	0
56	MG	1V	201	1/1	0.91	0.07	25,25,25,25	0
56	MG	1A	3005	1/1	0.91	0.08	32,32,32,32	0
56	MG	1a	3153	1/1	0.91	0.12	43,43,43,43	0
56	MG	1A	3864	1/1	0.91	0.11	23,23,23,23	0
56	MG	1A	3441	1/1	0.91	0.09	40,40,40,40	0
56	MG	1A	3523	1/1	0.91	0.34	31,31,31,31	0
56	MG	2a	3082	1/1	0.91	0.20	50,50,50,50	0
56	MG	2A	3363	1/1	0.91	0.14	52,52,52,52	0
56	MG	2A	3367	1/1	0.91	0.16	35,35,35,35	0
56	MG	2A	3368	1/1	0.91	0.27	49,49,49,49	0
56	MG	1a	3165	1/1	0.91	0.22	45,45,45,45	0
56	MG	2A	3676	1/1	0.91	0.09	48,48,48,48	0
56	MG	2A	3128	1/1	0.91	0.16	50,50,50,50	0
56	MG	1A	3077	1/1	0.91	0.22	21,21,21,21	0
56	MG	10	105	1/1	0.91	0.18	30,30,30,30	0
56	MG	1A	3671	1/1	0.91	0.07	40,40,40,40	0
56	MG	11	104	1/1	0.91	0.10	53,53,53,53	0
56	MG	1A	3113	1/1	0.91	0.15	40,40,40,40	0
56	MG	1A	4035	1/1	0.91	0.07	13,13,13,13	0
56	MG	2A	3384	1/1	0.91	0.11	42,42,42,42	0
56	MG	1A	3448	1/1	0.91	0.10	28,28,28,28	0
56	MG	1A	3355	1/1	0.91	0.14	43,43,43,43	0
56	MG	2A	3692	1/1	0.91	0.09	43,43,43,43	0
56	MG	2A	3693	1/1	0.91	0.07	54,54,54,54	0
56	MG	1A	3885	1/1	0.91	0.08	18,18,18,18	0
56	MG	2A	3698	1/1	0.91	0.15	51,51,51,51	0
56	MG	1A	3887	1/1	0.91	0.20	50,50,50,50	0
56	MG	1A	4042	1/1	0.91	0.12	64,64,64,64	0
56	MG	2A	3704	1/1	0.91	0.20	58,58,58,58	0
56	MG	1A	3085	1/1	0.91	0.29	37,37,37,37	0
56	MG	2A	3156	1/1	0.91	0.23	52,52,52,52	0
56	MG	1A	4049	1/1	0.91	0.14	36,36,36,36	0
56	MG	1a	3198	1/1	0.91	0.07	48,48,48,48	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	1A	3359	1/1	0.91	0.06	33,33,33,33	0
56	MG	1a	3219	1/1	0.91	0.08	53,53,53,53	0
56	MG	1A	3367	1/1	0.91	0.24	14,14,14,14	0
56	MG	1A	3036	1/1	0.91	0.30	25,25,25,25	0
56	MG	1a	3012	1/1	0.91	0.11	50,50,50,50	0
56	MG	1a	3225	1/1	0.91	0.24	62,62,62,62	0
56	MG	2A	3428	1/1	0.91	0.07	41,41,41,41	0
56	MG	1A	3571	1/1	0.91	0.11	28,28,28,28	0
56	MG	2A	3174	1/1	0.91	0.08	43,43,43,43	0
56	MG	1A	3126	1/1	0.91	0.12	35,35,35,35	0
56	MG	1A	4076	1/1	0.91	0.10	34,34,34,34	0
56	MG	1A	3801	1/1	0.91	0.14	56,56,56,56	0
56	MG	1A	3472	1/1	0.91	0.08	52,52,52,52	0
56	MG	2a	3169	1/1	0.91	0.15	59,59,59,59	0
56	MG	1a	3027	1/1	0.91	0.23	42,42,42,42	0
56	MG	1l	203	1/1	0.91	0.13	55,55,55,55	0
56	MG	1A	3306	1/1	0.91	0.11	43,43,43,43	0
56	MG	1A	3923	1/1	0.91	0.09	56,56,56,56	0
56	MG	2a	3176	1/1	0.91	0.14	55,55,55,55	0
56	MG	2A	3765	1/1	0.91	0.10	39,39,39,39	0
56	MG	1p	101	1/1	0.91	0.15	46,46,46,46	0
56	MG	1A	4102	1/1	0.91	0.09	11,11,11,11	0
56	MG	1A	3004	1/1	0.91	0.06	23,23,23,23	0
56	MG	2A	3770	1/1	0.91	0.09	40,40,40,40	0
56	MG	2A	3778	1/1	0.91	0.10	57,57,57,57	0
56	MG	2A	3202	1/1	0.91	0.34	51,51,51,51	0
56	MG	1A	4108	1/1	0.91	0.12	28,28,28,28	0
56	MG	2a	3191	1/1	0.91	0.17	61,61,61,61	0
56	MG	2A	3464	1/1	0.91	0.08	29,29,29,29	0
56	MG	1a	3039	1/1	0.91	0.23	59,59,59,59	0
56	MG	1A	3926	1/1	0.91	0.09	31,31,31,31	0
56	MG	1w	105	1/1	0.91	0.15	48,48,48,48	0
56	MG	2a	3197	1/1	0.91	0.18	54,54,54,54	0
56	MG	1A	4121	1/1	0.91	0.27	23,23,23,23	0
56	MG	2A	3804	1/1	0.91	0.21	40,40,40,40	0
56	MG	1A	4125	1/1	0.91	0.12	27,27,27,27	0
56	MG	2A	3215	1/1	0.91	0.14	49,49,49,49	0
56	MG	2a	3202	1/1	0.91	0.18	57,57,57,57	0
56	MG	2A	3217	1/1	0.91	0.12	40,40,40,40	0
56	MG	2A	3475	1/1	0.91	0.08	28,28,28,28	0
56	MG	2A	3218	1/1	0.91	0.12	49,49,49,49	0
56	MG	1a	3051	1/1	0.91	0.13	65,65,65,65	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	1A	3714	1/1	0.91	0.09	59,59,59,59	0
56	MG	1A	4132	1/1	0.91	0.11	29,29,29,29	0
56	MG	2A	3828	1/1	0.91	0.10	40,40,40,40	0
56	MG	1x	109	1/1	0.91	0.12	68,68,68,68	0
56	MG	1A	4133	1/1	0.91	0.18	29,29,29,29	0
56	MG	1A	3314	1/1	0.91	0.07	44,44,44,44	0
56	MG	1A	3316	1/1	0.91	0.26	49,49,49,49	0
56	MG	2A	3232	1/1	0.91	0.06	42,42,42,42	0
56	MG	1A	3323	1/1	0.91	0.12	41,41,41,41	0
56	MG	1A	3827	1/1	0.91	0.20	22,22,22,22	0
56	MG	1a	3064	1/1	0.91	0.10	57,57,57,57	0
56	MG	1A	3605	1/1	0.91	0.07	32,32,32,32	0
56	MG	2a	3225	1/1	0.91	0.12	72,72,72,72	0
56	MG	1A	3091	1/1	0.91	0.09	35,35,35,35	0
56	MG	2A	3517	1/1	0.91	0.08	32,32,32,32	0
56	MG	2A	3520	1/1	0.91	0.17	62,62,62,62	0
56	MG	2d	303	1/1	0.91	0.11	65,65,65,65	0
56	MG	1A	3956	1/1	0.91	0.12	58,58,58,58	0
56	MG	2A	3533	1/1	0.91	0.07	54,54,54,54	0
56	MG	1A	3325	1/1	0.91	0.18	44,44,44,44	0
56	MG	2q	201	1/1	0.91	0.15	46,46,46,46	0
56	MG	2B	3006	1/1	0.91	0.16	60,60,60,60	0
56	MG	2A	3018	1/1	0.91	0.15	36,36,36,36	0
56	MG	2A	3540	1/1	0.91	0.12	32,32,32,32	0
56	MG	2B	3010	1/1	0.91	0.13	64,64,64,64	0
56	MG	1A	3402	1/1	0.91	0.14	27,27,27,27	0
56	MG	1B	3030	1/1	0.91	0.08	44,44,44,44	0
56	MG	2A	3026	1/1	0.91	0.11	47,47,47,47	0
56	MG	2A	3547	1/1	0.91	0.09	48,48,48,48	0
56	MG	2A	3028	1/1	0.91	0.13	30,30,30,30	0
56	MG	2A	3252	1/1	0.91	0.06	35,35,35,35	0
56	MG	2A	3029	1/1	0.91	0.17	52,52,52,52	0
56	MG	1a	3075	1/1	0.91	0.28	58,58,58,58	0
56	MG	1A	3970	1/1	0.91	0.10	25,25,25,25	0
56	MG	2A	3556	1/1	0.91	0.11	52,52,52,52	0
56	MG	1a	3084	1/1	0.91	0.11	42,42,42,42	0
56	MG	2A	3037	1/1	0.91	0.23	44,44,44,44	0
56	MG	1B	3032	1/1	0.91	0.07	35,35,35,35	0
56	MG	2A	3042	1/1	0.91	0.21	52,52,52,52	0
56	MG	2A	3565	1/1	0.91	0.08	51,51,51,51	0
56	MG	2A	3264	1/1	0.91	0.11	47,47,47,47	0
56	MG	1a	3134	1/1	0.92	0.10	38,38,38,38	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	2A	3039	1/1	0.92	0.12	54,54,54,54	0
56	MG	16	102	1/1	0.92	0.09	46,46,46,46	0
56	MG	1a	3138	1/1	0.92	0.07	30,30,30,30	0
56	MG	2A	3045	1/1	0.92	0.19	52,52,52,52	0
56	MG	2a	3026	1/1	0.92	0.08	43,43,43,43	0
56	MG	2A	3046	1/1	0.92	0.09	56,56,56,56	0
56	MG	1A	4081	1/1	0.92	0.07	40,40,40,40	0
56	MG	1A	4083	1/1	0.92	0.15	41,41,41,41	0
56	MG	2A	3233	1/1	0.92	0.06	41,41,41,41	0
56	MG	1A	3173	1/1	0.92	0.09	30,30,30,30	0
56	MG	1A	3839	1/1	0.92	0.17	30,30,30,30	0
56	MG	2A	3061	1/1	0.92	0.08	38,38,38,38	0
56	MG	1A	3948	1/1	0.92	0.06	42,42,42,42	0
56	MG	2a	3041	1/1	0.92	0.09	43,43,43,43	0
56	MG	2a	3043	1/1	0.92	0.08	51,51,51,51	0
56	MG	1A	3840	1/1	0.92	0.10	29,29,29,29	0
56	MG	2A	3689	1/1	0.92	0.12	56,56,56,56	0
56	MG	1A	3525	1/1	0.92	0.24	51,51,51,51	0
56	MG	1A	4109	1/1	0.92	0.39	32,32,32,32	0
56	MG	1A	3059	1/1	0.92	0.14	42,42,42,42	0
56	MG	2A	3459	1/1	0.92	0.16	64,64,64,64	0
56	MG	1A	3962	1/1	0.92	0.09	15,15,15,15	0
56	MG	2a	3052	1/1	0.92	0.21	55,55,55,55	0
56	MG	2A	3696	1/1	0.92	0.10	42,42,42,42	0
56	MG	1a	3161	1/1	0.92	0.10	45,45,45,45	0
56	MG	1a	3164	1/1	0.92	0.12	41,41,41,41	0
56	MG	1A	3650	1/1	0.92	0.25	43,43,43,43	0
56	MG	1A	3537	1/1	0.92	0.19	38,38,38,38	0
56	MG	1A	4131	1/1	0.92	0.13	16,16,16,16	0
56	MG	1a	3171	1/1	0.92	0.09	55,55,55,55	0
56	MG	2a	3067	1/1	0.92	0.16	45,45,45,45	0
56	MG	1A	3658	1/1	0.92	0.13	15,15,15,15	0
56	MG	2A	3474	1/1	0.92	0.12	40,40,40,40	0
56	MG	1A	3660	1/1	0.92	0.10	8,8,8,8	0
56	MG	2a	3072	1/1	0.92	0.12	44,44,44,44	0
56	MG	1A	3540	1/1	0.92	0.13	29,29,29,29	0
56	MG	2a	3074	1/1	0.92	0.24	43,43,43,43	0
56	MG	2A	3729	1/1	0.92	0.10	66,66,66,66	0
56	MG	1A	3769	1/1	0.92	0.08	37,37,37,37	0
56	MG	2A	3733	1/1	0.92	0.10	70,70,70,70	0
56	MG	1A	3459	1/1	0.92	0.13	41,41,41,41	0
56	MG	1A	3052	1/1	0.92	0.12	29,29,29,29	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	1a	3030	1/1	0.92	0.22	46,46,46,46	0
56	MG	2A	3092	1/1	0.92	0.12	41,41,41,41	0
56	MG	1A	3184	1/1	0.92	0.10	37,37,37,37	0
56	MG	2A	3739	1/1	0.92	0.11	69,69,69,69	0
56	MG	1a	3192	1/1	0.92	0.07	53,53,53,53	0
56	MG	2a	3088	1/1	0.92	0.17	67,67,67,67	0
56	MG	2a	3089	1/1	0.92	0.16	56,56,56,56	0
56	MG	1a	3033	1/1	0.92	0.33	56,56,56,56	0
56	MG	1a	3036	1/1	0.92	0.22	40,40,40,40	0
56	MG	1A	3781	1/1	0.92	0.14	42,42,42,42	0
56	MG	1A	3062	1/1	0.92	0.16	36,36,36,36	0
56	MG	1A	4004	1/1	0.92	0.08	62,62,62,62	0
56	MG	1a	3212	1/1	0.92	0.14	54,54,54,54	0
56	MG	2a	3099	1/1	0.92	0.22	51,51,51,51	0
56	MG	2a	3100	1/1	0.92	0.11	51,51,51,51	0
56	MG	2A	3114	1/1	0.92	0.24	52,52,52,52	0
56	MG	2A	3518	1/1	0.92	0.19	49,49,49,49	0
56	MG	1a	3218	1/1	0.92	0.07	55,55,55,55	0
56	MG	2A	3289	1/1	0.92	0.07	58,58,58,58	0
56	MG	2A	3526	1/1	0.92	0.07	57,57,57,57	0
56	MG	1A	3247	1/1	0.92	0.13	31,31,31,31	0
56	MG	2A	3534	1/1	0.92	0.15	52,52,52,52	0
56	MG	2A	3535	1/1	0.92	0.16	48,48,48,48	0
56	MG	2a	3111	1/1	0.92	0.20	46,46,46,46	0
56	MG	1A	3017	1/1	0.92	0.09	17,17,17,17	0
56	MG	2A	3783	1/1	0.92	0.09	40,40,40,40	0
56	MG	2A	3788	1/1	0.92	0.08	57,57,57,57	0
56	MG	1A	3084	1/1	0.92	0.20	50,50,50,50	0
56	MG	1a	3223	1/1	0.92	0.19	48,48,48,48	0
56	MG	1a	3050	1/1	0.92	0.11	51,51,51,51	0
56	MG	1A	4017	1/1	0.92	0.15	57,57,57,57	0
56	MG	2A	3126	1/1	0.92	0.13	39,39,39,39	0
56	MG	1A	3209	1/1	0.92	0.08	45,45,45,45	0
56	MG	1a	3227	1/1	0.92	0.20	46,46,46,46	0
56	MG	1A	3212	1/1	0.92	0.13	36,36,36,36	0
56	MG	2A	3132	1/1	0.92	0.27	57,57,57,57	0
56	MG	2A	3135	1/1	0.92	0.10	53,53,53,53	0
56	MG	2a	3144	1/1	0.92	0.09	76,76,76,76	0
56	MG	2A	3309	1/1	0.92	0.08	55,55,55,55	0
56	MG	2a	3152	1/1	0.92	0.10	67,67,67,67	0
56	MG	2A	3555	1/1	0.92	0.22	55,55,55,55	0
56	MG	2A	3817	1/1	0.92	0.12	47,47,47,47	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	2A	3820	1/1	0.92	0.14	41,41,41,41	0
56	MG	2A	3310	1/1	0.92	0.21	59,59,59,59	0
56	MG	1A	3794	1/1	0.92	0.14	37,37,37,37	0
56	MG	1D	302	1/1	0.92	0.31	29,29,29,29	0
56	MG	2A	3315	1/1	0.92	0.08	40,40,40,40	0
56	MG	2A	3316	1/1	0.92	0.16	52,52,52,52	0
56	MG	2A	3831	1/1	0.92	0.14	56,56,56,56	0
56	MG	1A	3890	1/1	0.92	0.08	51,51,51,51	0
56	MG	1D	314	1/1	0.92	0.25	34,34,34,34	0
56	MG	2A	3571	1/1	0.92	0.17	38,38,38,38	0
56	MG	1E	304	1/1	0.92	0.14	44,44,44,44	0
56	MG	1A	4025	1/1	0.92	0.11	18,18,18,18	0
56	MG	1A	3213	1/1	0.92	0.27	27,27,27,27	0
56	MG	1A	4030	1/1	0.92	0.08	32,32,32,32	0
56	MG	1A	3317	1/1	0.92	0.08	36,36,36,36	0
56	MG	2A	3336	1/1	0.92	0.11	45,45,45,45	0
56	MG	1A	3429	1/1	0.92	0.07	39,39,39,39	0
56	MG	2a	3184	1/1	0.92	0.09	46,46,46,46	0
56	MG	2A	3866	1/1	0.92	0.08	31,31,31,31	0
56	MG	1A	3493	1/1	0.92	0.11	63,63,63,63	0
56	MG	1A	3319	1/1	0.92	0.14	38,38,38,38	0
56	MG	2A	3157	1/1	0.92	0.25	58,58,58,58	0
56	MG	1A	3601	1/1	0.92	0.16	55,55,55,55	0
56	MG	2A	3593	1/1	0.92	0.24	58,58,58,58	0
56	MG	1A	3911	1/1	0.92	0.06	34,34,34,34	0
56	MG	2B	3008	1/1	0.92	0.12	49,49,49,49	0
56	MG	2A	3344	1/1	0.92	0.06	48,48,48,48	0
56	MG	2A	3162	1/1	0.92	0.06	42,42,42,42	0
56	MG	1a	3083	1/1	0.92	0.13	53,53,53,53	0
56	MG	1A	3912	1/1	0.92	0.07	43,43,43,43	0
56	MG	1P	201	1/1	0.92	0.12	20,20,20,20	0
56	MG	1Q	3003	1/1	0.92	0.07	40,40,40,40	0
56	MG	2A	3606	1/1	0.92	0.09	35,35,35,35	0
56	MG	2A	3353	1/1	0.92	0.18	44,44,44,44	0
56	MG	1x	106	1/1	0.92	0.20	52,52,52,52	0
56	MG	1A	3368	1/1	0.92	0.07	42,42,42,42	0
56	MG	2A	3611	1/1	0.92	0.07	61,61,61,61	0
56	MG	2A	3359	1/1	0.92	0.21	43,43,43,43	0
56	MG	1A	3370	1/1	0.92	0.07	29,29,29,29	0
56	MG	1a	3093	1/1	0.92	0.23	35,35,35,35	0
56	MG	1x	111	1/1	0.92	0.12	52,52,52,52	0
56	MG	1U	201	1/1	0.92	0.17	22,22,22,22	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	1A	3320	1/1	0.92	0.14	28,28,28,28	0
56	MG	1U	205	1/1	0.92	0.12	35,35,35,35	0
56	MG	2O	8001	1/1	0.92	0.08	54,54,54,54	0
56	MG	2A	3373	1/1	0.92	0.24	47,47,47,47	0
56	MG	2Q	203	1/1	0.92	0.07	47,47,47,47	0
56	MG	1A	3822	1/1	0.92	0.07	47,47,47,47	0
56	MG	1A	3377	1/1	0.92	0.09	25,25,25,25	0
56	MG	1a	3103	1/1	0.92	0.09	57,57,57,57	0
56	MG	2A	3011	1/1	0.92	0.14	42,42,42,42	0
56	MG	1a	3104	1/1	0.92	0.11	49,49,49,49	0
56	MG	2U	204	1/1	0.92	0.09	57,57,57,57	0
56	MG	1A	3379	1/1	0.92	0.07	39,39,39,39	0
56	MG	1A	4059	1/1	0.92	0.12	34,34,34,34	0
56	MG	2W	202	1/1	0.92	0.08	38,38,38,38	0
56	MG	2p	3001	1/1	0.92	0.11	45,45,45,45	0
56	MG	1A	3615	1/1	0.92	0.07	22,22,22,22	0
56	MG	2q	202	1/1	0.92	0.10	64,64,64,64	0
56	MG	1A	3931	1/1	0.92	0.06	36,36,36,36	0
56	MG	10	102	1/1	0.92	0.10	49,49,49,49	0
56	MG	1A	4068	1/1	0.92	0.07	42,42,42,42	0
56	MG	26	502	1/1	0.92	0.24	62,62,62,62	0
56	MG	2A	3399	1/1	0.92	0.24	53,53,53,53	0
56	MG	2A	3648	1/1	0.92	0.10	33,33,33,33	0
56	MG	2A	3400	1/1	0.92	0.19	51,51,51,51	0
56	MG	2a	3003	1/1	0.92	0.10	53,53,53,53	0
56	MG	2A	3206	1/1	0.92	0.07	57,57,57,57	0
56	MG	10	107	1/1	0.92	0.12	53,53,53,53	0
56	MG	2A	3208	1/1	0.92	0.05	29,29,29,29	0
56	MG	2A	3406	1/1	0.92	0.29	59,59,59,59	0
56	MG	1A	4069	1/1	0.92	0.11	26,26,26,26	0
56	MG	1a	3117	1/1	0.92	0.15	31,31,31,31	0
56	MG	1A	3513	1/1	0.92	0.06	34,34,34,34	0
56	MG	2A	3216	1/1	0.92	0.34	53,53,53,53	0
56	MG	1A	3045	1/1	0.92	0.08	22,22,22,22	0
56	MG	2A	3421	1/1	0.92	0.33	54,54,54,54	0
56	MG	1A	3382	1/1	0.92	0.11	41,41,41,41	0
56	MG	2a	3018	1/1	0.92	0.15	50,50,50,50	0
56	MG	1A	3050	1/1	0.93	0.21	39,39,39,39	0
56	MG	10	104	1/1	0.93	0.06	30,30,30,30	0
56	MG	1A	3592	1/1	0.93	0.10	46,46,46,46	0
56	MG	2A	3305	1/1	0.93	0.12	53,53,53,53	0
56	MG	2A	3585	1/1	0.93	0.17	45,45,45,45	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	2A	3586	1/1	0.93	0.23	41,41,41,41	0
56	MG	2A	3306	1/1	0.93	0.06	45,45,45,45	0
56	MG	1A	3878	1/1	0.93	0.10	30,30,30,30	0
56	MG	2A	3592	1/1	0.93	0.09	48,48,48,48	0
56	MG	1A	3002	1/1	0.93	0.13	40,40,40,40	0
56	MG	1A	4052	1/1	0.93	0.10	49,49,49,49	0
56	MG	1A	3285	1/1	0.93	0.23	32,32,32,32	0
56	MG	1A	4054	1/1	0.93	0.10	37,37,37,37	0
56	MG	1A	3468	1/1	0.93	0.12	26,26,26,26	0
56	MG	2A	3113	1/1	0.93	0.13	47,47,47,47	0
56	MG	1A	3761	1/1	0.93	0.10	47,47,47,47	0
56	MG	2A	3319	1/1	0.93	0.10	51,51,51,51	0
56	MG	2A	3605	1/1	0.93	0.08	46,46,46,46	0
56	MG	1a	3172	1/1	0.93	0.11	65,65,65,65	0
56	MG	1A	3764	1/1	0.93	0.14	16,16,16,16	0
56	MG	1A	3375	1/1	0.93	0.06	25,25,25,25	0
56	MG	2A	3325	1/1	0.93	0.06	33,33,33,33	0
56	MG	1A	3894	1/1	0.93	0.07	36,36,36,36	0
56	MG	1A	3292	1/1	0.93	0.07	22,22,22,22	0
56	MG	1a	3182	1/1	0.93	0.10	56,56,56,56	0
56	MG	2A	3332	1/1	0.93	0.09	43,43,43,43	0
56	MG	2A	3334	1/1	0.93	0.13	63,63,63,63	0
56	MG	2A	3335	1/1	0.93	0.09	48,48,48,48	0
56	MG	2a	3013	1/1	0.93	0.17	44,44,44,44	0
56	MG	1A	3224	1/1	0.93	0.07	41,41,41,41	0
56	MG	1A	4070	1/1	0.93	0.10	49,49,49,49	0
56	MG	1A	3299	1/1	0.93	0.08	27,27,27,27	0
56	MG	1A	3612	1/1	0.93	0.15	16,16,16,16	0
56	MG	1A	3772	1/1	0.93	0.09	14,14,14,14	0
56	MG	1a	3010	1/1	0.93	0.10	53,53,53,53	0
56	MG	2A	3133	1/1	0.93	0.09	44,44,44,44	0
56	MG	1A	3301	1/1	0.93	0.19	54,54,54,54	0
56	MG	1A	4082	1/1	0.93	0.08	29,29,29,29	0
56	MG	2A	3137	1/1	0.93	0.12	35,35,35,35	0
56	MG	2A	3633	1/1	0.93	0.07	59,59,59,59	0
56	MG	2a	3028	1/1	0.93	0.32	58,58,58,58	0
56	MG	2a	3029	1/1	0.93	0.26	43,43,43,43	0
56	MG	2A	3347	1/1	0.93	0.08	58,58,58,58	0
56	MG	1a	3015	1/1	0.93	0.11	60,60,60,60	0
56	MG	1A	3225	1/1	0.93	0.14	42,42,42,42	0
56	MG	1A	4089	1/1	0.93	0.11	34,34,34,34	0
56	MG	2A	3644	1/1	0.93	0.08	55,55,55,55	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	2a	3035	1/1	0.93	0.23	53,53,53,53	0
56	MG	1A	3011	1/1	0.93	0.07	26,26,26,26	0
56	MG	1A	4093	1/1	0.93	0.17	25,25,25,25	0
56	MG	1A	3231	1/1	0.93	0.08	25,25,25,25	0
56	MG	1A	4097	1/1	0.93	0.17	40,40,40,40	0
56	MG	2a	3042	1/1	0.93	0.05	63,63,63,63	0
56	MG	1A	3390	1/1	0.93	0.09	32,32,32,32	0
56	MG	1A	3634	1/1	0.93	0.11	12,12,12,12	0
56	MG	2A	3151	1/1	0.93	0.10	46,46,46,46	0
56	MG	2A	3153	1/1	0.93	0.12	47,47,47,47	0
56	MG	1A	3233	1/1	0.93	0.23	24,24,24,24	0
56	MG	1A	3041	1/1	0.93	0.06	16,16,16,16	0
56	MG	2A	3662	1/1	0.93	0.07	34,34,34,34	0
56	MG	1a	3035	1/1	0.93	0.13	43,43,43,43	0
56	MG	2a	3051	1/1	0.93	0.09	52,52,52,52	0
56	MG	1A	3928	1/1	0.93	0.07	42,42,42,42	0
56	MG	1A	4115	1/1	0.93	0.08	32,32,32,32	0
56	MG	1A	3792	1/1	0.93	0.08	22,22,22,22	0
56	MG	1A	3163	1/1	0.93	0.09	32,32,32,32	0
56	MG	2A	3670	1/1	0.93	0.12	50,50,50,50	0
56	MG	1e	201	1/1	0.93	0.06	63,63,63,63	0
56	MG	1A	3044	1/1	0.93	0.10	14,14,14,14	0
56	MG	2A	3386	1/1	0.93	0.22	51,51,51,51	0
56	MG	2A	3674	1/1	0.93	0.07	62,62,62,62	0
56	MG	1A	3322	1/1	0.93	0.12	31,31,31,31	0
56	MG	1a	3047	1/1	0.93	0.19	52,52,52,52	0
56	MG	2a	3070	1/1	0.93	0.21	46,46,46,46	0
56	MG	1A	3128	1/1	0.93	0.10	38,38,38,38	0
56	MG	2A	3393	1/1	0.93	0.09	30,30,30,30	0
56	MG	1A	3403	1/1	0.93	0.05	29,29,29,29	0
56	MG	1A	3405	1/1	0.93	0.10	30,30,30,30	0
56	MG	2A	3175	1/1	0.93	0.17	45,45,45,45	0
56	MG	1A	3665	1/1	0.93	0.07	14,14,14,14	0
56	MG	1A	3950	1/1	0.93	0.16	46,46,46,46	0
56	MG	2A	3402	1/1	0.93	0.09	39,39,39,39	0
56	MG	2A	3179	1/1	0.93	0.10	56,56,56,56	0
56	MG	1B	3010	1/1	0.93	0.16	32,32,32,32	0
56	MG	1A	3174	1/1	0.93	0.12	48,48,48,48	0
56	MG	2a	3083	1/1	0.93	0.16	42,42,42,42	0
56	MG	1A	3807	1/1	0.93	0.08	42,42,42,42	0
56	MG	1a	3061	1/1	0.93	0.09	50,50,50,50	0
56	MG	2A	3414	1/1	0.93	0.21	55,55,55,55	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	1A	3958	1/1	0.93	0.09	8,8,8,8	0
56	MG	2A	3697	1/1	0.93	0.12	51,51,51,51	0
56	MG	1A	3129	1/1	0.93	0.25	20,20,20,20	0
56	MG	1A	3177	1/1	0.93	0.09	26,26,26,26	0
56	MG	2A	3702	1/1	0.93	0.07	37,37,37,37	0
56	MG	2A	3420	1/1	0.93	0.06	40,40,40,40	0
56	MG	2A	3194	1/1	0.93	0.14	30,30,30,30	0
56	MG	2A	3195	1/1	0.93	0.07	41,41,41,41	0
56	MG	2A	3707	1/1	0.93	0.15	65,65,65,65	0
56	MG	1x	105	1/1	0.93	0.23	66,66,66,66	0
56	MG	2A	3427	1/1	0.93	0.12	58,58,58,58	0
56	MG	2A	3714	1/1	0.93	0.10	44,44,44,44	0
56	MG	2A	3718	1/1	0.93	0.22	56,56,56,56	0
56	MG	2A	3720	1/1	0.93	0.10	54,54,54,54	0
56	MG	1A	3815	1/1	0.93	0.06	48,48,48,48	0
56	MG	2A	3201	1/1	0.93	0.19	52,52,52,52	0
56	MG	1x	107	1/1	0.93	0.12	53,53,53,53	0
56	MG	2A	3433	1/1	0.93	0.23	51,51,51,51	0
56	MG	1A	3424	1/1	0.93	0.07	31,31,31,31	0
56	MG	1A	3531	1/1	0.93	0.09	35,35,35,35	0
56	MG	1A	3823	1/1	0.93	0.11	17,17,17,17	0
56	MG	2a	3114	1/1	0.93	0.19	47,47,47,47	0
56	MG	1A	3976	1/1	0.93	0.08	17,17,17,17	0
56	MG	1a	3071	1/1	0.93	0.08	41,41,41,41	0
56	MG	1A	3978	1/1	0.93	0.12	57,57,57,57	0
56	MG	1y	102	1/1	0.93	0.06	40,40,40,40	0
56	MG	1A	3679	1/1	0.93	0.11	43,43,43,43	0
56	MG	2a	3129	1/1	0.93	0.07	64,64,64,64	0
56	MG	1A	3826	1/1	0.93	0.10	41,41,41,41	0
56	MG	1a	3082	1/1	0.93	0.17	45,45,45,45	0
56	MG	2A	3002	1/1	0.93	0.16	49,49,49,49	0
56	MG	1D	312	1/1	0.93	0.20	20,20,20,20	0
56	MG	1A	3131	1/1	0.93	0.08	29,29,29,29	0
56	MG	2A	3012	1/1	0.93	0.07	24,24,24,24	0
56	MG	2A	3461	1/1	0.93	0.07	30,30,30,30	0
56	MG	2a	3146	1/1	0.93	0.07	76,76,76,76	0
56	MG	1a	3085	1/1	0.93	0.21	53,53,53,53	0
56	MG	2a	3150	1/1	0.93	0.09	68,68,68,68	0
56	MG	2A	3015	1/1	0.93	0.15	35,35,35,35	0
56	MG	1A	3132	1/1	0.93	0.24	32,32,32,32	0
56	MG	2a	3154	1/1	0.93	0.10	66,66,66,66	0
56	MG	2A	3228	1/1	0.93	0.07	41,41,41,41	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	1A	3339	1/1	0.93	0.07	44,44,44,44	0
56	MG	2a	3158	1/1	0.93	0.11	66,66,66,66	0
56	MG	1a	3088	1/1	0.93	0.06	52,52,52,52	0
56	MG	2A	3019	1/1	0.93	0.21	45,45,45,45	0
56	MG	2a	3162	1/1	0.93	0.15	57,57,57,57	0
56	MG	2A	3776	1/1	0.93	0.08	48,48,48,48	0
56	MG	2a	3164	1/1	0.93	0.08	49,49,49,49	0
56	MG	1A	3431	1/1	0.93	0.10	40,40,40,40	0
56	MG	1A	3435	1/1	0.93	0.10	51,51,51,51	0
56	MG	2A	3023	1/1	0.93	0.07	34,34,34,34	0
56	MG	2A	3476	1/1	0.93	0.09	52,52,52,52	0
56	MG	1A	4000	1/1	0.93	0.12	34,34,34,34	0
56	MG	1a	3094	1/1	0.93	0.17	39,39,39,39	0
56	MG	2A	3240	1/1	0.93	0.09	43,43,43,43	0
56	MG	2A	3242	1/1	0.93	0.07	47,47,47,47	0
56	MG	1A	3029	1/1	0.93	0.16	28,28,28,28	0
56	MG	2A	3487	1/1	0.93	0.07	27,27,27,27	0
56	MG	2A	3803	1/1	0.93	0.09	52,52,52,52	0
56	MG	1F	302	1/1	0.93	0.06	31,31,31,31	0
56	MG	2A	3491	1/1	0.93	0.10	35,35,35,35	0
56	MG	1A	3711	1/1	0.93	0.06	28,28,28,28	0
56	MG	1a	3099	1/1	0.93	0.12	51,51,51,51	0
56	MG	1A	3344	1/1	0.93	0.06	29,29,29,29	0
56	MG	2a	3188	1/1	0.93	0.12	72,72,72,72	0
56	MG	1G	3001	1/1	0.93	0.13	28,28,28,28	0
56	MG	2A	3507	1/1	0.93	0.09	52,52,52,52	0
56	MG	1G	3002	1/1	0.93	0.07	38,38,38,38	0
56	MG	1G	3004	1/1	0.93	0.07	39,39,39,39	0
56	MG	1I	3001	1/1	0.93	0.06	50,50,50,50	0
56	MG	2A	3511	1/1	0.93	0.10	38,38,38,38	0
56	MG	1A	4010	1/1	0.93	0.13	54,54,54,54	0
56	MG	2A	3829	1/1	0.93	0.08	40,40,40,40	0
56	MG	2A	3254	1/1	0.93	0.09	53,53,53,53	0
56	MG	1A	3443	1/1	0.93	0.07	46,46,46,46	0
56	MG	2A	3833	1/1	0.93	0.06	42,42,42,42	0
56	MG	2A	3834	1/1	0.93	0.07	47,47,47,47	0
56	MG	2a	3203	1/1	0.93	0.15	64,64,64,64	0
56	MG	1A	3843	1/1	0.93	0.20	23,23,23,23	0
56	MG	2A	3258	1/1	0.93	0.15	40,40,40,40	0
56	MG	2A	3525	1/1	0.93	0.06	38,38,38,38	0
56	MG	2A	3259	1/1	0.93	0.07	46,46,46,46	0
56	MG	1A	3260	1/1	0.93	0.11	44,44,44,44	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	1O	3005	1/1	0.93	0.07	62,62,62,62	0
56	MG	2A	3050	1/1	0.93	0.12	38,38,38,38	0
56	MG	2a	3213	1/1	0.93	0.14	56,56,56,56	0
56	MG	1A	3568	1/1	0.93	0.12	51,51,51,51	0
56	MG	2A	3851	1/1	0.93	0.08	43,43,43,43	0
56	MG	2A	3852	1/1	0.93	0.06	43,43,43,43	0
56	MG	2A	3538	1/1	0.93	0.16	47,47,47,47	0
56	MG	1P	203	1/1	0.93	0.14	34,34,34,34	0
56	MG	2A	3865	1/1	0.93	0.23	39,39,39,39	0
56	MG	1A	3849	1/1	0.93	0.10	28,28,28,28	0
56	MG	2a	3222	1/1	0.93	0.10	51,51,51,51	0
56	MG	2A	3867	1/1	0.93	0.09	36,36,36,36	0
56	MG	2A	3267	1/1	0.93	0.11	49,49,49,49	0
56	MG	2A	3871	1/1	0.93	0.15	36,36,36,36	0
56	MG	2a	3226	1/1	0.93	0.16	55,55,55,55	0
56	MG	1a	3119	1/1	0.93	0.06	28,28,28,28	0
56	MG	2A	3875	1/1	0.93	0.17	32,32,32,32	0
56	MG	2A	3876	1/1	0.93	0.11	43,43,43,43	0
56	MG	2d	301	1/1	0.93	0.26	58,58,58,58	0
56	MG	1a	3120	1/1	0.93	0.17	46,46,46,46	0
56	MG	2A	3270	1/1	0.93	0.06	41,41,41,41	0
56	MG	2B	3005	1/1	0.93	0.10	55,55,55,55	0
56	MG	1A	4021	1/1	0.93	0.07	45,45,45,45	0
56	MG	1a	3124	1/1	0.93	0.13	40,40,40,40	0
56	MG	1a	3127	1/1	0.93	0.14	33,33,33,33	0
56	MG	1A	3197	1/1	0.93	0.09	44,44,44,44	0
56	MG	2A	3553	1/1	0.93	0.08	39,39,39,39	0
56	MG	1A	3047	1/1	0.93	0.26	47,47,47,47	0
56	MG	1A	3147	1/1	0.93	0.14	36,36,36,36	0
56	MG	2A	3279	1/1	0.93	0.13	51,51,51,51	0
56	MG	2A	3557	1/1	0.93	0.21	41,41,41,41	0
56	MG	2A	3078	1/1	0.93	0.17	31,31,31,31	0
56	MG	1A	3577	1/1	0.93	0.07	16,16,16,16	0
56	MG	1U	207	1/1	0.93	0.17	22,22,22,22	0
56	MG	1A	3150	1/1	0.93	0.09	39,39,39,39	0
56	MG	1a	3141	1/1	0.93	0.18	53,53,53,53	0
56	MG	1A	3734	1/1	0.93	0.09	14,14,14,14	0
56	MG	1a	3143	1/1	0.93	0.15	52,52,52,52	0
56	MG	2E	302	1/1	0.93	0.07	28,28,28,28	0
56	MG	1A	3583	1/1	0.93	0.10	31,31,31,31	0
56	MG	2E	305	1/1	0.93	0.15	39,39,39,39	0
56	MG	2A	3088	1/1	0.93	0.19	35,35,35,35	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	1A	3736	1/1	0.93	0.12	16,16,16,16	0
56	MG	1A	3063	1/1	0.93	0.13	14,14,14,14	0
56	MG	2F	303	1/1	0.93	0.09	38,38,38,38	0
56	MG	1A	3362	1/1	0.93	0.26	41,41,41,41	0
58	M2D	2A	3864	36/36	0.93	0.12	32,41,50,52	0
56	MG	1A	3723	1/1	0.94	0.13	46,46,46,46	0
56	MG	1A	4038	1/1	0.94	0.08	39,39,39,39	0
56	MG	1A	3575	1/1	0.94	0.10	21,21,21,21	0
56	MG	1A	3162	1/1	0.94	0.27	32,32,32,32	0
56	MG	1A	3731	1/1	0.94	0.07	20,20,20,20	0
56	MG	1a	3168	1/1	0.94	0.06	44,44,44,44	0
56	MG	1A	3578	1/1	0.94	0.10	47,47,47,47	0
56	MG	1A	4043	1/1	0.94	0.05	30,30,30,30	0
56	MG	1A	3249	1/1	0.94	0.09	49,49,49,49	0
56	MG	1A	3081	1/1	0.94	0.14	23,23,23,23	0
56	MG	1a	3174	1/1	0.94	0.09	76,76,76,76	0
56	MG	1A	4050	1/1	0.94	0.08	34,34,34,34	0
56	MG	1A	3009	1/1	0.94	0.08	16,16,16,16	0
56	MG	2A	3130	1/1	0.94	0.13	49,49,49,49	0
56	MG	2A	3610	1/1	0.94	0.06	42,42,42,42	0
56	MG	2X	3001	1/1	0.94	0.09	52,52,52,52	0
56	MG	1A	3109	1/1	0.94	0.09	28,28,28,28	0
56	MG	1A	3740	1/1	0.94	0.07	44,44,44,44	0
56	MG	20	3002	1/1	0.94	0.07	40,40,40,40	0
56	MG	1A	3880	1/1	0.94	0.19	16,16,16,16	0
56	MG	2A	3134	1/1	0.94	0.15	42,42,42,42	0
56	MG	1A	3881	1/1	0.94	0.07	18,18,18,18	0
56	MG	1A	3742	1/1	0.94	0.08	15,15,15,15	0
56	MG	1A	4060	1/1	0.94	0.07	25,25,25,25	0
56	MG	1A	3467	1/1	0.94	0.19	31,31,31,31	0
56	MG	1a	3193	1/1	0.94	0.08	37,37,37,37	0
56	MG	1A	3255	1/1	0.94	0.09	38,38,38,38	0
56	MG	2A	3351	1/1	0.94	0.11	59,59,59,59	0
56	MG	2a	3007	1/1	0.94	0.10	38,38,38,38	0
56	MG	1A	3886	1/1	0.94	0.11	34,34,34,34	0
56	MG	1A	3470	1/1	0.94	0.12	33,33,33,33	0
56	MG	2A	3355	1/1	0.94	0.15	29,29,29,29	0
56	MG	1A	3471	1/1	0.94	0.12	41,41,41,41	0
56	MG	2A	3628	1/1	0.94	0.07	34,34,34,34	0
56	MG	2A	3629	1/1	0.94	0.10	56,56,56,56	0
56	MG	2A	3357	1/1	0.94	0.18	37,37,37,37	0
56	MG	1A	4072	1/1	0.94	0.07	44,44,44,44	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	2A	3148	1/1	0.94	0.10	35,35,35,35	0
56	MG	2A	3362	1/1	0.94	0.20	26,26,26,26	0
56	MG	2A	3639	1/1	0.94	0.10	62,62,62,62	0
56	MG	1A	4073	1/1	0.94	0.07	39,39,39,39	0
56	MG	2A	3641	1/1	0.94	0.08	56,56,56,56	0
56	MG	1a	3217	1/1	0.94	0.09	35,35,35,35	0
56	MG	2a	3023	1/1	0.94	0.17	49,49,49,49	0
56	MG	1A	3602	1/1	0.94	0.10	24,24,24,24	0
56	MG	1A	3757	1/1	0.94	0.12	8,8,8,8	0
56	MG	1A	3897	1/1	0.94	0.10	40,40,40,40	0
56	MG	1a	3024	1/1	0.94	0.19	37,37,37,37	0
56	MG	1A	3758	1/1	0.94	0.10	59,59,59,59	0
56	MG	2A	3374	1/1	0.94	0.19	39,39,39,39	0
56	MG	2A	3653	1/1	0.94	0.14	51,51,51,51	0
56	MG	1A	3214	1/1	0.94	0.10	46,46,46,46	0
56	MG	2A	3656	1/1	0.94	0.08	44,44,44,44	0
56	MG	1A	3389	1/1	0.94	0.17	36,36,36,36	0
56	MG	2A	3161	1/1	0.94	0.07	36,36,36,36	0
56	MG	1A	4088	1/1	0.94	0.07	49,49,49,49	0
56	MG	2A	3381	1/1	0.94	0.15	43,43,43,43	0
56	MG	1A	3901	1/1	0.94	0.13	37,37,37,37	0
56	MG	1A	3902	1/1	0.94	0.08	34,34,34,34	0
56	MG	2A	3664	1/1	0.94	0.09	50,50,50,50	0
56	MG	2A	3385	1/1	0.94	0.10	36,36,36,36	0
56	MG	1a	3032	1/1	0.94	0.17	20,20,20,20	0
56	MG	2A	3387	1/1	0.94	0.13	39,39,39,39	0
56	MG	1a	3232	1/1	0.94	0.13	54,54,54,54	0
56	MG	1A	3762	1/1	0.94	0.07	13,13,13,13	0
56	MG	1a	3034	1/1	0.94	0.18	49,49,49,49	0
56	MG	1A	3218	1/1	0.94	0.19	33,33,33,33	0
56	MG	2A	3394	1/1	0.94	0.08	48,48,48,48	0
56	MG	2A	3395	1/1	0.94	0.20	45,45,45,45	0
56	MG	1A	3609	1/1	0.94	0.19	6,6,6,6	0
56	MG	1A	3221	1/1	0.94	0.06	34,34,34,34	0
56	MG	1A	3018	1/1	0.94	0.08	28,28,28,28	0
56	MG	1A	3115	1/1	0.94	0.12	19,19,19,19	0
56	MG	1A	3394	1/1	0.94	0.09	39,39,39,39	0
56	MG	1a	3042	1/1	0.94	0.08	55,55,55,55	0
56	MG	2A	3182	1/1	0.94	0.18	51,51,51,51	0
56	MG	2a	3060	1/1	0.94	0.09	49,49,49,49	0
56	MG	2a	3061	1/1	0.94	0.17	40,40,40,40	0
56	MG	2a	3062	1/1	0.94	0.21	48,48,48,48	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	2a	3063	1/1	0.94	0.09	46,46,46,46	0
56	MG	1A	3398	1/1	0.94	0.12	48,48,48,48	0
56	MG	1A	3487	1/1	0.94	0.10	25,25,25,25	0
56	MG	2A	3687	1/1	0.94	0.21	37,37,37,37	0
56	MG	2A	3407	1/1	0.94	0.25	45,45,45,45	0
56	MG	1A	3622	1/1	0.94	0.09	37,37,37,37	0
56	MG	2A	3409	1/1	0.94	0.30	65,65,65,65	0
56	MG	1A	3624	1/1	0.94	0.07	39,39,39,39	0
56	MG	1A	3782	1/1	0.94	0.14	35,35,35,35	0
56	MG	1A	3783	1/1	0.94	0.07	24,24,24,24	0
56	MG	2A	3694	1/1	0.94	0.07	44,44,44,44	0
56	MG	2A	3193	1/1	0.94	0.18	40,40,40,40	0
56	MG	1A	3268	1/1	0.94	0.15	15,15,15,15	0
56	MG	1w	109	1/1	0.94	0.11	51,51,51,51	0
56	MG	2A	3197	1/1	0.94	0.06	46,46,46,46	0
56	MG	2A	3422	1/1	0.94	0.17	31,31,31,31	0
56	MG	2A	3700	1/1	0.94	0.08	36,36,36,36	0
56	MG	2A	3701	1/1	0.94	0.07	32,32,32,32	0
56	MG	1A	3400	1/1	0.94	0.14	50,50,50,50	0
56	MG	1x	101	1/1	0.94	0.10	43,43,43,43	0
56	MG	1A	4144	1/1	0.94	0.13	27,27,27,27	0
56	MG	2A	3705	1/1	0.94	0.16	51,51,51,51	0
56	MG	1a	3059	1/1	0.94	0.16	40,40,40,40	0
56	MG	1B	3001	1/1	0.94	0.17	27,27,27,27	0
56	MG	1A	3335	1/1	0.94	0.06	28,28,28,28	0
56	MG	2A	3711	1/1	0.94	0.14	61,61,61,61	0
56	MG	2a	3095	1/1	0.94	0.11	59,59,59,59	0
56	MG	1A	3119	1/1	0.94	0.32	24,24,24,24	0
56	MG	1A	3944	1/1	0.94	0.11	53,53,53,53	0
56	MG	2A	3717	1/1	0.94	0.06	39,39,39,39	0
56	MG	1A	3790	1/1	0.94	0.07	19,19,19,19	0
56	MG	1B	3011	1/1	0.94	0.14	29,29,29,29	0
56	MG	2A	3210	1/1	0.94	0.09	42,42,42,42	0
56	MG	1B	3015	1/1	0.94	0.06	29,29,29,29	0
56	MG	2A	3724	1/1	0.94	0.08	55,55,55,55	0
56	MG	2A	3725	1/1	0.94	0.10	67,67,67,67	0
56	MG	2A	3212	1/1	0.94	0.12	54,54,54,54	0
56	MG	2A	3727	1/1	0.94	0.07	45,45,45,45	0
56	MG	1x	114	1/1	0.94	0.05	54,54,54,54	0
56	MG	2A	3214	1/1	0.94	0.06	38,38,38,38	0
56	MG	1A	3638	1/1	0.94	0.07	27,27,27,27	0
56	MG	1A	3646	1/1	0.94	0.08	15,15,15,15	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	1A	3951	1/1	0.94	0.12	56,56,56,56	0
56	MG	1A	3087	1/1	0.94	0.13	8,8,8,8	0
56	MG	2a	3116	1/1	0.94	0.09	73,73,73,73	0
56	MG	2A	3219	1/1	0.94	0.16	42,42,42,42	0
56	MG	1A	3343	1/1	0.94	0.12	32,32,32,32	0
56	MG	2A	3460	1/1	0.94	0.10	35,35,35,35	0
56	MG	2A	3221	1/1	0.94	0.17	46,46,46,46	0
56	MG	2a	3127	1/1	0.94	0.10	66,66,66,66	0
56	MG	1A	3006	1/1	0.94	0.10	44,44,44,44	0
56	MG	2A	3003	1/1	0.94	0.07	44,44,44,44	0
56	MG	2a	3130	1/1	0.94	0.10	67,67,67,67	0
56	MG	1B	3029	1/1	0.94	0.13	59,59,59,59	0
56	MG	2A	3009	1/1	0.94	0.12	36,36,36,36	0
56	MG	1A	3345	1/1	0.94	0.08	34,34,34,34	0
56	MG	2A	3746	1/1	0.94	0.08	58,58,58,58	0
56	MG	2a	3138	1/1	0.94	0.20	48,48,48,48	0
56	MG	2A	3749	1/1	0.94	0.11	66,66,66,66	0
56	MG	1A	3186	1/1	0.94	0.37	31,31,31,31	0
56	MG	2A	3755	1/1	0.94	0.06	53,53,53,53	0
56	MG	1A	3423	1/1	0.94	0.12	53,53,53,53	0
56	MG	1A	3518	1/1	0.94	0.08	48,48,48,48	0
56	MG	1A	3664	1/1	0.94	0.06	13,13,13,13	0
56	MG	1A	3028	1/1	0.94	0.31	22,22,22,22	0
56	MG	1A	3667	1/1	0.94	0.05	35,35,35,35	0
56	MG	2A	3768	1/1	0.94	0.09	24,24,24,24	0
56	MG	2A	3477	1/1	0.94	0.08	44,44,44,44	0
56	MG	1D	304	1/1	0.94	0.18	48,48,48,48	0
56	MG	2A	3773	1/1	0.94	0.06	57,57,57,57	0
56	MG	1a	3091	1/1	0.94	0.29	38,38,38,38	0
56	MG	1D	311	1/1	0.94	0.07	29,29,29,29	0
56	MG	1A	3811	1/1	0.94	0.08	41,41,41,41	0
56	MG	2A	3782	1/1	0.94	0.08	44,44,44,44	0
56	MG	2A	3025	1/1	0.94	0.09	28,28,28,28	0
56	MG	2A	3785	1/1	0.94	0.07	63,63,63,63	0
56	MG	2A	3485	1/1	0.94	0.07	33,33,33,33	0
56	MG	1A	3979	1/1	0.94	0.07	63,63,63,63	0
56	MG	2A	3488	1/1	0.94	0.12	30,30,30,30	0
56	MG	1A	3980	1/1	0.94	0.07	61,61,61,61	0
56	MG	1A	3668	1/1	0.94	0.11	21,21,21,21	0
56	MG	2A	3492	1/1	0.94	0.06	27,27,27,27	0
56	MG	2a	3175	1/1	0.94	0.07	51,51,51,51	0
56	MG	1A	3984	1/1	0.94	0.07	21,21,21,21	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	1A	3985	1/1	0.94	0.07	20,20,20,20	0
56	MG	1A	3237	1/1	0.94	0.10	28,28,28,28	0
56	MG	2A	3499	1/1	0.94	0.09	33,33,33,33	0
56	MG	1A	3819	1/1	0.94	0.08	10,10,10,10	0
56	MG	2A	3809	1/1	0.94	0.06	27,27,27,27	0
56	MG	2a	3183	1/1	0.94	0.08	59,59,59,59	0
56	MG	1F	301	1/1	0.94	0.23	26,26,26,26	0
56	MG	2A	3812	1/1	0.94	0.14	52,52,52,52	0
56	MG	1A	3428	1/1	0.94	0.10	26,26,26,26	0
56	MG	2A	3041	1/1	0.94	0.16	46,46,46,46	0
56	MG	1A	3526	1/1	0.94	0.12	18,18,18,18	0
56	MG	2a	3190	1/1	0.94	0.08	61,61,61,61	0
56	MG	2A	3818	1/1	0.94	0.08	38,38,38,38	0
56	MG	2A	3256	1/1	0.94	0.09	35,35,35,35	0
56	MG	2a	3193	1/1	0.94	0.13	54,54,54,54	0
56	MG	2A	3513	1/1	0.94	0.12	36,36,36,36	0
56	MG	2A	3822	1/1	0.94	0.20	48,48,48,48	0
56	MG	1A	3995	1/1	0.94	0.07	52,52,52,52	0
56	MG	1A	3529	1/1	0.94	0.13	32,32,32,32	0
56	MG	1A	3677	1/1	0.94	0.10	44,44,44,44	0
56	MG	1A	3351	1/1	0.94	0.09	27,27,27,27	0
56	MG	1A	3535	1/1	0.94	0.23	38,38,38,38	0
56	MG	1A	4005	1/1	0.94	0.06	34,34,34,34	0
56	MG	2A	3832	1/1	0.94	0.10	41,41,41,41	0
56	MG	1A	3296	1/1	0.94	0.08	34,34,34,34	0
56	MG	2A	3051	1/1	0.94	0.05	40,40,40,40	0
56	MG	2a	3206	1/1	0.94	0.11	58,58,58,58	0
56	MG	2A	3054	1/1	0.94	0.08	39,39,39,39	0
56	MG	1a	3116	1/1	0.94	0.14	35,35,35,35	0
56	MG	1A	3188	1/1	0.94	0.07	24,24,24,24	0
56	MG	1a	3118	1/1	0.94	0.15	37,37,37,37	0
56	MG	2A	3063	1/1	0.94	0.06	33,33,33,33	0
56	MG	1A	3298	1/1	0.94	0.09	45,45,45,45	0
56	MG	2A	3066	1/1	0.94	0.12	43,43,43,43	0
56	MG	2A	3067	1/1	0.94	0.10	35,35,35,35	0
56	MG	2a	3215	1/1	0.94	0.08	68,68,68,68	0
56	MG	1A	4011	1/1	0.94	0.08	35,35,35,35	0
56	MG	1A	3693	1/1	0.94	0.09	45,45,45,45	0
56	MG	1A	3439	1/1	0.94	0.07	35,35,35,35	0
56	MG	2A	3858	1/1	0.94	0.18	57,57,57,57	0
56	MG	1a	3126	1/1	0.94	0.15	45,45,45,45	0
56	MG	2A	3283	1/1	0.94	0.07	38,38,38,38	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	1A	3706	1/1	0.94	0.06	48,48,48,48	0
56	MG	1Q	3004	1/1	0.94	0.05	36,36,36,36	0
56	MG	1R	201	1/1	0.94	0.16	23,23,23,23	0
56	MG	2A	3870	1/1	0.94	0.11	40,40,40,40	0
56	MG	1a	3131	1/1	0.94	0.12	46,46,46,46	0
56	MG	1a	3132	1/1	0.94	0.12	51,51,51,51	0
56	MG	1a	3133	1/1	0.94	0.18	48,48,48,48	0
56	MG	1A	3042	1/1	0.94	0.11	15,15,15,15	0
56	MG	2B	3001	1/1	0.94	0.15	54,54,54,54	0
56	MG	2A	3561	1/1	0.94	0.10	46,46,46,46	0
56	MG	2e	3001	1/1	0.94	0.12	58,58,58,58	0
56	MG	1R	204	1/1	0.94	0.16	34,34,34,34	0
56	MG	1A	3043	1/1	0.94	0.11	28,28,28,28	0
56	MG	1A	3304	1/1	0.94	0.07	49,49,49,49	0
56	MG	1A	3245	1/1	0.94	0.11	19,19,19,19	0
56	MG	1A	3372	1/1	0.94	0.20	25,25,25,25	0
56	MG	1A	3848	1/1	0.94	0.14	48,48,48,48	0
56	MG	1A	3373	1/1	0.94	0.08	30,30,30,30	0
56	MG	2B	3011	1/1	0.94	0.21	48,48,48,48	0
56	MG	2A	3574	1/1	0.94	0.09	49,49,49,49	0
56	MG	2B	3013	1/1	0.94	0.12	57,57,57,57	0
56	MG	1A	4032	1/1	0.94	0.07	19,19,19,19	0
56	MG	2A	3304	1/1	0.94	0.06	44,44,44,44	0
56	MG	1W	201	1/1	0.94	0.13	28,28,28,28	0
56	MG	2A	3093	1/1	0.94	0.06	55,55,55,55	0
56	MG	1W	203	1/1	0.94	0.12	35,35,35,35	0
56	MG	2A	3580	1/1	0.94	0.08	45,45,45,45	0
56	MG	2A	3100	1/1	0.94	0.16	43,43,43,43	0
56	MG	1a	3150	1/1	0.94	0.12	56,56,56,56	0
56	MG	1a	3151	1/1	0.94	0.12	45,45,45,45	0
56	MG	2D	306	1/1	0.94	0.23	34,34,34,34	0
56	MG	1A	3449	1/1	0.94	0.14	49,49,49,49	0
56	MG	1A	3374	1/1	0.94	0.08	27,27,27,27	0
56	MG	2x	3005	1/1	0.94	0.07	59,59,59,59	0
56	MG	2E	303	1/1	0.94	0.17	55,55,55,55	0
56	MG	1A	3203	1/1	0.94	0.19	25,25,25,25	0
56	MG	1a	3159	1/1	0.94	0.09	52,52,52,52	0
56	MG	2A	3589	1/1	0.94	0.10	38,38,38,38	0
56	MG	2y	106	1/1	0.94	0.15	64,64,64,64	0
57	K	2A	3398	1/1	0.94	0.15	70,70,70,70	0
56	MG	2A	3591	1/1	0.94	0.11	54,54,54,54	0
56	MG	1A	3844	1/1	0.95	0.18	21,21,21,21	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	1y	101	1/1	0.95	0.06	22,22,22,22	0
56	MG	1A	3071	1/1	0.95	0.25	26,26,26,26	0
56	MG	1A	3504	1/1	0.95	0.12	39,39,39,39	0
56	MG	1A	3507	1/1	0.95	0.13	36,36,36,36	0
56	MG	1A	3675	1/1	0.95	0.17	32,32,32,32	0
56	MG	1A	3118	1/1	0.95	0.12	29,29,29,29	0
56	MG	1A	3511	1/1	0.95	0.09	15,15,15,15	0
56	MG	1A	3046	1/1	0.95	0.07	40,40,40,40	0
56	MG	1A	4066	1/1	0.95	0.12	32,32,32,32	0
56	MG	1A	4067	1/1	0.95	0.12	40,40,40,40	0
56	MG	1A	3078	1/1	0.95	0.06	20,20,20,20	0
56	MG	2B	3020	1/1	0.95	0.19	66,66,66,66	0
56	MG	1A	3680	1/1	0.95	0.09	46,46,46,46	0
56	MG	2A	3566	1/1	0.95	0.08	35,35,35,35	0
56	MG	2D	303	1/1	0.95	0.22	40,40,40,40	0
56	MG	1A	3001	1/1	0.95	0.13	22,22,22,22	0
56	MG	2A	3265	1/1	0.95	0.25	39,39,39,39	0
56	MG	2D	307	1/1	0.95	0.31	43,43,43,43	0
56	MG	1a	3043	1/1	0.95	0.12	49,49,49,49	0
56	MG	2A	3573	1/1	0.95	0.09	44,44,44,44	0
56	MG	1A	3521	1/1	0.95	0.10	17,17,17,17	0
56	MG	1A	3683	1/1	0.95	0.11	39,39,39,39	0
56	MG	1A	3866	1/1	0.95	0.07	35,35,35,35	0
56	MG	1a	3049	1/1	0.95	0.08	35,35,35,35	0
56	MG	1A	4077	1/1	0.95	0.08	53,53,53,53	0
56	MG	1A	3685	1/1	0.95	0.07	37,37,37,37	0
56	MG	2A	3024	1/1	0.95	0.09	45,45,45,45	0
56	MG	1A	3871	1/1	0.95	0.10	18,18,18,18	0
56	MG	1a	3053	1/1	0.95	0.15	46,46,46,46	0
56	MG	1a	3054	1/1	0.95	0.16	57,57,57,57	0
56	MG	1A	3873	1/1	0.95	0.10	40,40,40,40	0
56	MG	2A	3280	1/1	0.95	0.14	43,43,43,43	0
56	MG	2R	201	1/1	0.95	0.09	39,39,39,39	0
56	MG	2A	3281	1/1	0.95	0.08	60,60,60,60	0
56	MG	2A	3282	1/1	0.95	0.07	41,41,41,41	0
56	MG	1A	3690	1/1	0.95	0.07	40,40,40,40	0
56	MG	2A	3284	1/1	0.95	0.07	41,41,41,41	0
56	MG	1A	3048	1/1	0.95	0.10	26,26,26,26	0
56	MG	1A	4086	1/1	0.95	0.16	31,31,31,31	0
56	MG	1A	3037	1/1	0.95	0.26	28,28,28,28	0
56	MG	2W	201	1/1	0.95	0.14	42,42,42,42	0
56	MG	1A	3326	1/1	0.95	0.17	32,32,32,32	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	1A	4091	1/1	0.95	0.08	28,28,28,28	0
56	MG	1A	3702	1/1	0.95	0.05	31,31,31,31	0
56	MG	1A	3705	1/1	0.95	0.10	39,39,39,39	0
56	MG	1A	3250	1/1	0.95	0.11	56,56,56,56	0
56	MG	23	3001	1/1	0.95	0.05	46,46,46,46	0
56	MG	2A	3601	1/1	0.95	0.07	45,45,45,45	0
56	MG	25	103	1/1	0.95	0.14	47,47,47,47	0
56	MG	2A	3044	1/1	0.95	0.12	36,36,36,36	0
56	MG	1A	3528	1/1	0.95	0.23	45,45,45,45	0
56	MG	1A	4099	1/1	0.95	0.07	43,43,43,43	0
56	MG	1A	4101	1/1	0.95	0.09	23,23,23,23	0
56	MG	1A	3412	1/1	0.95	0.08	41,41,41,41	0
56	MG	1A	3530	1/1	0.95	0.21	42,42,42,42	0
56	MG	2A	3302	1/1	0.95	0.07	50,50,50,50	0
56	MG	2a	3005	1/1	0.95	0.14	42,42,42,42	0
56	MG	1A	4106	1/1	0.95	0.09	17,17,17,17	0
56	MG	1A	3330	1/1	0.95	0.13	20,20,20,20	0
56	MG	2A	3613	1/1	0.95	0.06	38,38,38,38	0
56	MG	1A	3533	1/1	0.95	0.29	39,39,39,39	0
56	MG	1a	3080	1/1	0.95	0.13	40,40,40,40	0
56	MG	2A	3058	1/1	0.95	0.21	47,47,47,47	0
56	MG	1A	4112	1/1	0.95	0.25	31,31,31,31	0
56	MG	1A	3417	1/1	0.95	0.10	19,19,19,19	0
56	MG	1A	3892	1/1	0.95	0.07	30,30,30,30	0
56	MG	1A	3086	1/1	0.95	0.16	40,40,40,40	0
56	MG	2A	3313	1/1	0.95	0.09	46,46,46,46	0
56	MG	1A	3039	1/1	0.95	0.05	23,23,23,23	0
56	MG	1A	3422	1/1	0.95	0.06	24,24,24,24	0
56	MG	1A	3194	1/1	0.95	0.07	35,35,35,35	0
56	MG	2A	3069	1/1	0.95	0.06	43,43,43,43	0
56	MG	2A	3070	1/1	0.95	0.09	34,34,34,34	0
56	MG	2A	3321	1/1	0.95	0.14	50,50,50,50	0
56	MG	1A	3724	1/1	0.95	0.11	34,34,34,34	0
56	MG	2A	3631	1/1	0.95	0.06	44,44,44,44	0
56	MG	1A	3336	1/1	0.95	0.06	27,27,27,27	0
56	MG	1A	4137	1/1	0.95	0.12	20,20,20,20	0
56	MG	2A	3635	1/1	0.95	0.08	50,50,50,50	0
56	MG	1A	4143	1/1	0.95	0.18	26,26,26,26	0
56	MG	1A	3338	1/1	0.95	0.13	37,37,37,37	0
56	MG	2A	3329	1/1	0.95	0.15	29,29,29,29	0
56	MG	2A	3330	1/1	0.95	0.25	47,47,47,47	0
56	MG	1A	3730	1/1	0.95	0.07	21,21,21,21	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	1A	3547	1/1	0.95	0.08	39,39,39,39	0
56	MG	1B	3006	1/1	0.95	0.07	29,29,29,29	0
56	MG	2A	3645	1/1	0.95	0.10	42,42,42,42	0
56	MG	1A	3427	1/1	0.95	0.05	35,35,35,35	0
56	MG	1a	3100	1/1	0.95	0.18	41,41,41,41	0
56	MG	1A	3550	1/1	0.95	0.06	26,26,26,26	0
56	MG	1A	3552	1/1	0.95	0.30	44,44,44,44	0
56	MG	1A	3558	1/1	0.95	0.12	42,42,42,42	0
56	MG	1B	3012	1/1	0.95	0.05	39,39,39,39	0
56	MG	1A	3918	1/1	0.95	0.08	51,51,51,51	0
56	MG	1B	3016	1/1	0.95	0.07	22,22,22,22	0
56	MG	1B	3018	1/1	0.95	0.09	51,51,51,51	0
56	MG	1A	3559	1/1	0.95	0.26	30,30,30,30	0
56	MG	1A	3739	1/1	0.95	0.08	21,21,21,21	0
56	MG	1A	3040	1/1	0.95	0.12	35,35,35,35	0
56	MG	2A	3094	1/1	0.95	0.07	43,43,43,43	0
56	MG	1A	3925	1/1	0.95	0.08	39,39,39,39	0
56	MG	2A	3350	1/1	0.95	0.17	60,60,60,60	0
56	MG	2A	3099	1/1	0.95	0.06	43,43,43,43	0
56	MG	1a	3113	1/1	0.95	0.12	37,37,37,37	0
56	MG	2a	3057	1/1	0.95	0.05	53,53,53,53	0
56	MG	1A	3340	1/1	0.95	0.12	44,44,44,44	0
56	MG	1A	3744	1/1	0.95	0.07	55,55,55,55	0
56	MG	1A	3746	1/1	0.95	0.06	15,15,15,15	0
56	MG	1A	3198	1/1	0.95	0.11	26,26,26,26	0
56	MG	1A	3569	1/1	0.95	0.09	23,23,23,23	0
56	MG	1A	3199	1/1	0.95	0.11	37,37,37,37	0
56	MG	2A	3111	1/1	0.95	0.19	29,29,29,29	0
56	MG	2a	3066	1/1	0.95	0.09	49,49,49,49	0
56	MG	1A	3935	1/1	0.95	0.14	41,41,41,41	0
56	MG	2A	3364	1/1	0.95	0.24	34,34,34,34	0
56	MG	2A	3677	1/1	0.95	0.28	43,43,43,43	0
56	MG	1A	3936	1/1	0.95	0.06	40,40,40,40	0
56	MG	1B	3036	1/1	0.95	0.07	27,27,27,27	0
56	MG	1A	3136	1/1	0.95	0.11	48,48,48,48	0
56	MG	2A	3116	1/1	0.95	0.07	41,41,41,41	0
56	MG	1A	3139	1/1	0.95	0.05	28,28,28,28	0
56	MG	2A	3684	1/1	0.95	0.05	46,46,46,46	0
56	MG	1a	3129	1/1	0.95	0.06	46,46,46,46	0
56	MG	1A	3941	1/1	0.95	0.10	40,40,40,40	0
56	MG	2A	3121	1/1	0.95	0.10	49,49,49,49	0
56	MG	1D	310	1/1	0.95	0.06	34,34,34,34	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	1A	3942	1/1	0.95	0.06	31,31,31,31	0
56	MG	1A	3142	1/1	0.95	0.15	16,16,16,16	0
56	MG	2A	3379	1/1	0.95	0.19	36,36,36,36	0
56	MG	1A	3945	1/1	0.95	0.08	39,39,39,39	0
56	MG	1A	3022	1/1	0.95	0.16	38,38,38,38	0
56	MG	1A	3269	1/1	0.95	0.14	20,20,20,20	0
56	MG	1A	3949	1/1	0.95	0.07	58,58,58,58	0
56	MG	1A	3444	1/1	0.95	0.07	37,37,37,37	0
56	MG	1A	3270	1/1	0.95	0.22	18,18,18,18	0
56	MG	1A	3353	1/1	0.95	0.16	23,23,23,23	0
56	MG	1A	3587	1/1	0.95	0.06	39,39,39,39	0
56	MG	1A	3354	1/1	0.95	0.07	36,36,36,36	0
56	MG	2A	3392	1/1	0.95	0.18	35,35,35,35	0
56	MG	1F	303	1/1	0.95	0.11	14,14,14,14	0
56	MG	1A	3767	1/1	0.95	0.08	25,25,25,25	0
56	MG	1F	307	1/1	0.95	0.09	34,34,34,34	0
56	MG	1A	3271	1/1	0.95	0.20	25,25,25,25	0
56	MG	1A	3964	1/1	0.95	0.06	73,73,73,73	0
56	MG	1A	3965	1/1	0.95	0.08	65,65,65,65	0
56	MG	2A	3708	1/1	0.95	0.06	48,48,48,48	0
56	MG	2A	3709	1/1	0.95	0.08	43,43,43,43	0
56	MG	1G	3003	1/1	0.95	0.06	47,47,47,47	0
56	MG	1A	3450	1/1	0.95	0.06	22,22,22,22	0
56	MG	2A	3145	1/1	0.95	0.07	33,33,33,33	0
56	MG	1G	3005	1/1	0.95	0.08	50,50,50,50	0
56	MG	2A	3716	1/1	0.95	0.12	63,63,63,63	0
56	MG	1A	3452	1/1	0.95	0.06	40,40,40,40	0
56	MG	1a	3163	1/1	0.95	0.07	47,47,47,47	0
56	MG	2A	3719	1/1	0.95	0.10	64,64,64,64	0
56	MG	2a	3115	1/1	0.95	0.06	56,56,56,56	0
56	MG	1N	3005	1/1	0.95	0.05	18,18,18,18	0
56	MG	2A	3721	1/1	0.95	0.06	49,49,49,49	0
56	MG	1A	3594	1/1	0.95	0.07	18,18,18,18	0
56	MG	2a	3124	1/1	0.95	0.07	56,56,56,56	0
56	MG	2A	3152	1/1	0.95	0.06	37,37,37,37	0
56	MG	1A	3773	1/1	0.95	0.07	26,26,26,26	0
56	MG	2A	3412	1/1	0.95	0.08	37,37,37,37	0
56	MG	1A	3596	1/1	0.95	0.06	20,20,20,20	0
56	MG	1O	3003	1/1	0.95	0.05	42,42,42,42	0
56	MG	2A	3728	1/1	0.95	0.07	55,55,55,55	0
56	MG	1A	3597	1/1	0.95	0.06	25,25,25,25	0
56	MG	2A	3730	1/1	0.95	0.05	63,63,63,63	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	1A	3030	1/1	0.95	0.05	27,27,27,27	0
56	MG	2A	3159	1/1	0.95	0.08	28,28,28,28	0
56	MG	1A	3455	1/1	0.95	0.12	23,23,23,23	0
56	MG	1A	3981	1/1	0.95	0.05	49,49,49,49	0
56	MG	1A	3604	1/1	0.95	0.08	29,29,29,29	0
56	MG	1A	3357	1/1	0.95	0.09	12,12,12,12	0
56	MG	1a	3177	1/1	0.95	0.08	46,46,46,46	0
56	MG	1A	3146	1/1	0.95	0.14	38,38,38,38	0
56	MG	1A	3986	1/1	0.95	0.06	13,13,13,13	0
56	MG	2a	3151	1/1	0.95	0.07	53,53,53,53	0
56	MG	2A	3431	1/1	0.95	0.22	47,47,47,47	0
56	MG	1A	3360	1/1	0.95	0.10	27,27,27,27	0
56	MG	1S	3003	1/1	0.95	0.08	69,69,69,69	0
56	MG	1T	3001	1/1	0.95	0.20	50,50,50,50	0
56	MG	1T	3002	1/1	0.95	0.05	33,33,33,33	0
56	MG	1a	3191	1/1	0.95	0.10	64,64,64,64	0
56	MG	2A	3748	1/1	0.95	0.15	48,48,48,48	0
56	MG	1A	3093	1/1	0.95	0.11	41,41,41,41	0
56	MG	1A	3363	1/1	0.95	0.18	29,29,29,29	0
56	MG	2A	3751	1/1	0.95	0.07	68,68,68,68	0
56	MG	2A	3752	1/1	0.95	0.06	47,47,47,47	0
56	MG	1A	3217	1/1	0.95	0.08	33,33,33,33	0
56	MG	2A	3756	1/1	0.95	0.08	45,45,45,45	0
56	MG	2A	3180	1/1	0.95	0.17	45,45,45,45	0
56	MG	2A	3759	1/1	0.95	0.07	74,74,74,74	0
56	MG	2A	3760	1/1	0.95	0.10	34,34,34,34	0
56	MG	2A	3447	1/1	0.95	0.08	44,44,44,44	0
56	MG	2A	3763	1/1	0.95	0.07	29,29,29,29	0
56	MG	1A	3031	1/1	0.95	0.07	21,21,21,21	0
56	MG	1A	3290	1/1	0.95	0.12	37,37,37,37	0
56	MG	1A	3095	1/1	0.95	0.06	29,29,29,29	0
56	MG	2A	3184	1/1	0.95	0.13	36,36,36,36	0
56	MG	1a	3202	1/1	0.95	0.09	53,53,53,53	0
56	MG	1A	3795	1/1	0.95	0.07	32,32,32,32	0
56	MG	2a	3181	1/1	0.95	0.17	52,52,52,52	0
56	MG	2A	3771	1/1	0.95	0.06	30,30,30,30	0
56	MG	2A	3187	1/1	0.95	0.33	43,43,43,43	0
56	MG	1A	4001	1/1	0.95	0.07	59,59,59,59	0
56	MG	2A	3190	1/1	0.95	0.06	30,30,30,30	0
56	MG	2A	3463	1/1	0.95	0.06	40,40,40,40	0
56	MG	2A	3780	1/1	0.95	0.09	37,37,37,37	0
56	MG	1A	4002	1/1	0.95	0.08	53,53,53,53	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	1A	3222	1/1	0.95	0.23	28,28,28,28	0
56	MG	1A	3025	1/1	0.95	0.19	12,12,12,12	0
56	MG	2A	3786	1/1	0.95	0.08	57,57,57,57	0
56	MG	1A	3156	1/1	0.95	0.14	28,28,28,28	0
56	MG	1A	3097	1/1	0.95	0.08	15,15,15,15	0
56	MG	1Z	304	1/1	0.95	0.11	40,40,40,40	0
56	MG	2A	3796	1/1	0.95	0.08	25,25,25,25	0
56	MG	2A	3470	1/1	0.95	0.05	32,32,32,32	0
56	MG	10	101	1/1	0.95	0.08	43,43,43,43	0
56	MG	1A	3300	1/1	0.95	0.07	40,40,40,40	0
56	MG	1A	3804	1/1	0.95	0.07	30,30,30,30	0
56	MG	1A	4014	1/1	0.95	0.17	35,35,35,35	0
56	MG	1A	3632	1/1	0.95	0.06	27,27,27,27	0
56	MG	1A	3098	1/1	0.95	0.17	25,25,25,25	0
56	MG	2a	3204	1/1	0.95	0.05	66,66,66,66	0
56	MG	1a	3231	1/1	0.95	0.16	41,41,41,41	0
56	MG	2A	3808	1/1	0.95	0.08	46,46,46,46	0
56	MG	11	101	1/1	0.95	0.10	39,39,39,39	0
56	MG	1a	3234	1/1	0.95	0.05	38,38,38,38	0
56	MG	11	102	1/1	0.95	0.09	47,47,47,47	0
56	MG	1b	3001	1/1	0.95	0.06	69,69,69,69	0
56	MG	1A	3303	1/1	0.95	0.32	25,25,25,25	0
56	MG	1d	502	1/1	0.95	0.20	41,41,41,41	0
56	MG	1A	3637	1/1	0.95	0.08	14,14,14,14	0
56	MG	15	102	1/1	0.95	0.24	28,28,28,28	0
56	MG	1A	3100	1/1	0.95	0.10	15,15,15,15	0
56	MG	1A	3642	1/1	0.95	0.06	15,15,15,15	0
56	MG	1A	4022	1/1	0.95	0.06	29,29,29,29	0
56	MG	1A	3383	1/1	0.95	0.09	28,28,28,28	0
56	MG	2A	3496	1/1	0.95	0.12	42,42,42,42	0
56	MG	1s	3001	1/1	0.95	0.12	42,42,42,42	0
56	MG	1A	4024	1/1	0.95	0.08	14,14,14,14	0
56	MG	1A	3486	1/1	0.95	0.23	26,26,26,26	0
56	MG	2A	3506	1/1	0.95	0.10	50,50,50,50	0
56	MG	1A	3386	1/1	0.95	0.05	34,34,34,34	0
56	MG	2A	3223	1/1	0.95	0.12	55,55,55,55	0
56	MG	2A	3835	1/1	0.95	0.13	53,53,53,53	0
56	MG	1A	3652	1/1	0.95	0.05	41,41,41,41	0
56	MG	2a	3228	1/1	0.95	0.15	53,53,53,53	0
56	MG	1A	3489	1/1	0.95	0.09	47,47,47,47	0
56	MG	1A	3656	1/1	0.95	0.08	12,12,12,12	0
56	MG	2A	3227	1/1	0.95	0.19	69,69,69,69	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	2A	3514	1/1	0.95	0.10	42,42,42,42	0
56	MG	2A	3844	1/1	0.95	0.08	34,34,34,34	0
56	MG	2f	3001	1/1	0.95	0.12	42,42,42,42	0
56	MG	1w	106	1/1	0.95	0.14	50,50,50,50	0
56	MG	1A	3035	1/1	0.95	0.07	27,27,27,27	0
56	MG	2l	201	1/1	0.95	0.06	53,53,53,53	0
56	MG	2A	3847	1/1	0.95	0.10	54,54,54,54	0
56	MG	2A	3849	1/1	0.95	0.11	24,24,24,24	0
56	MG	2A	3230	1/1	0.95	0.06	40,40,40,40	0
56	MG	1A	3659	1/1	0.95	0.09	6,6,6,6	0
56	MG	1A	3831	1/1	0.95	0.06	40,40,40,40	0
56	MG	2A	3854	1/1	0.95	0.09	50,50,50,50	0
56	MG	2A	3855	1/1	0.95	0.10	48,48,48,48	0
56	MG	1A	3832	1/1	0.95	0.08	34,34,34,34	0
56	MG	2v	101	1/1	0.95	0.29	48,48,48,48	0
56	MG	1w	111	1/1	0.95	0.05	37,37,37,37	0
56	MG	2A	3530	1/1	0.95	0.06	45,45,45,45	0
56	MG	2A	3532	1/1	0.95	0.11	42,42,42,42	0
56	MG	1A	3833	1/1	0.95	0.08	46,46,46,46	0
56	MG	1A	3068	1/1	0.95	0.28	50,50,50,50	0
56	MG	2A	3238	1/1	0.95	0.07	30,30,30,30	0
56	MG	1x	103	1/1	0.95	0.07	38,38,38,38	0
56	MG	1A	3311	1/1	0.95	0.21	40,40,40,40	0
56	MG	2A	3872	1/1	0.95	0.24	37,37,37,37	0
56	MG	1a	3017	1/1	0.95	0.08	37,37,37,37	0
56	MG	2A	3874	1/1	0.95	0.09	37,37,37,37	0
56	MG	1A	3312	1/1	0.95	0.20	41,41,41,41	0
56	MG	1A	3496	1/1	0.95	0.40	40,40,40,40	0
56	MG	2A	3877	1/1	0.95	0.10	57,57,57,57	0
56	MG	1A	3069	1/1	0.95	0.03	16,16,16,16	0
56	MG	2y	102	1/1	0.95	0.07	59,59,59,59	0
56	MG	1a	3025	1/1	0.95	0.14	42,42,42,42	0
56	MG	2A	3546	1/1	0.95	0.09	57,57,57,57	0
56	MG	1A	3666	1/1	0.95	0.06	33,33,33,33	0
56	MG	1A	3240	1/1	0.95	0.05	31,31,31,31	0
56	MG	1A	3501	1/1	0.95	0.13	22,22,22,22	0
56	MG	2A	3322	1/1	0.96	0.04	32,32,32,32	0
56	MG	1E	311	1/1	0.96	0.08	41,41,41,41	0
56	MG	1A	3818	1/1	0.96	0.14	28,28,28,28	0
56	MG	1A	3278	1/1	0.96	0.09	37,37,37,37	0
56	MG	1A	3992	1/1	0.96	0.07	28,28,28,28	0
56	MG	2A	3616	1/1	0.96	0.09	31,31,31,31	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	1a	3125	1/1	0.96	0.17	37,37,37,37	0
56	MG	1A	3108	1/1	0.96	0.05	23,23,23,23	0
56	MG	1F	306	1/1	0.96	0.10	34,34,34,34	0
56	MG	1A	3138	1/1	0.96	0.20	16,16,16,16	0
56	MG	2A	3095	1/1	0.96	0.12	39,39,39,39	0
56	MG	2A	3097	1/1	0.96	0.14	38,38,38,38	0
56	MG	1A	3038	1/1	0.96	0.12	26,26,26,26	0
56	MG	2U	203	1/1	0.96	0.12	47,47,47,47	0
56	MG	1A	3349	1/1	0.96	0.10	47,47,47,47	0
56	MG	1A	3534	1/1	0.96	0.24	40,40,40,40	0
56	MG	1A	3283	1/1	0.96	0.14	46,46,46,46	0
56	MG	1A	3828	1/1	0.96	0.10	21,21,21,21	0
56	MG	1A	3175	1/1	0.96	0.08	35,35,35,35	0
56	MG	2A	3107	1/1	0.96	0.18	30,30,30,30	0
56	MG	2X	3002	1/1	0.96	0.09	40,40,40,40	0
56	MG	1a	3136	1/1	0.96	0.06	52,52,52,52	0
56	MG	1A	3830	1/1	0.96	0.13	40,40,40,40	0
56	MG	1N	3001	1/1	0.96	0.30	34,34,34,34	0
56	MG	1A	3438	1/1	0.96	0.06	30,30,30,30	0
56	MG	1A	4007	1/1	0.96	0.13	45,45,45,45	0
56	MG	1A	3538	1/1	0.96	0.13	45,45,45,45	0
56	MG	25	104	1/1	0.96	0.09	45,45,45,45	0
56	MG	1A	3287	1/1	0.96	0.07	25,25,25,25	0
56	MG	1A	3542	1/1	0.96	0.11	29,29,29,29	0
56	MG	1A	3140	1/1	0.96	0.10	32,32,32,32	0
56	MG	1A	4015	1/1	0.96	0.06	40,40,40,40	0
56	MG	1a	3147	1/1	0.96	0.05	32,32,32,32	0
56	MG	2A	3119	1/1	0.96	0.08	30,30,30,30	0
56	MG	1A	3226	1/1	0.96	0.12	42,42,42,42	0
56	MG	1A	3686	1/1	0.96	0.08	34,34,34,34	0
56	MG	2A	3122	1/1	0.96	0.10	41,41,41,41	0
56	MG	1A	3442	1/1	0.96	0.13	40,40,40,40	0
56	MG	2A	3360	1/1	0.96	0.19	30,30,30,30	0
56	MG	2A	3361	1/1	0.96	0.20	36,36,36,36	0
56	MG	2A	3654	1/1	0.96	0.05	46,46,46,46	0
56	MG	1A	3293	1/1	0.96	0.13	41,41,41,41	0
56	MG	1a	3154	1/1	0.96	0.09	38,38,38,38	0
56	MG	1A	3841	1/1	0.96	0.13	12,12,12,12	0
56	MG	2A	3366	1/1	0.96	0.12	31,31,31,31	0
56	MG	1a	3156	1/1	0.96	0.18	30,30,30,30	0
56	MG	1A	3294	1/1	0.96	0.11	30,30,30,30	0
56	MG	1a	3158	1/1	0.96	0.08	43,43,43,43	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	1A	3694	1/1	0.96	0.10	49,49,49,49	0
56	MG	1S	3002	1/1	0.96	0.09	37,37,37,37	0
56	MG	2a	3020	1/1	0.96	0.09	32,32,32,32	0
56	MG	1A	3699	1/1	0.96	0.07	55,55,55,55	0
56	MG	1A	3141	1/1	0.96	0.21	21,21,21,21	0
56	MG	2A	3667	1/1	0.96	0.06	33,33,33,33	0
56	MG	1A	3846	1/1	0.96	0.12	18,18,18,18	0
56	MG	1A	3701	1/1	0.96	0.06	42,42,42,42	0
56	MG	1a	3166	1/1	0.96	0.10	55,55,55,55	0
56	MG	2a	3027	1/1	0.96	0.20	45,45,45,45	0
56	MG	1A	4029	1/1	0.96	0.07	35,35,35,35	0
56	MG	1A	3178	1/1	0.96	0.09	42,42,42,42	0
56	MG	1U	204	1/1	0.96	0.19	22,22,22,22	0
56	MG	1a	3170	1/1	0.96	0.12	49,49,49,49	0
56	MG	2A	3383	1/1	0.96	0.15	43,43,43,43	0
56	MG	1A	4031	1/1	0.96	0.12	37,37,37,37	0
56	MG	1A	3703	1/1	0.96	0.12	24,24,24,24	0
56	MG	1A	3851	1/1	0.96	0.07	28,28,28,28	0
56	MG	1A	3556	1/1	0.96	0.08	9,9,9,9	0
56	MG	2A	3147	1/1	0.96	0.12	37,37,37,37	0
56	MG	2A	3681	1/1	0.96	0.10	52,52,52,52	0
56	MG	2a	3040	1/1	0.96	0.12	47,47,47,47	0
56	MG	1A	3853	1/1	0.96	0.07	7,7,7,7	0
56	MG	1A	3016	1/1	0.96	0.14	33,33,33,33	0
56	MG	1A	3856	1/1	0.96	0.11	40,40,40,40	0
56	MG	1a	3178	1/1	0.96	0.05	41,41,41,41	0
56	MG	1a	3179	1/1	0.96	0.09	64,64,64,64	0
56	MG	1X	105	1/1	0.96	0.08	36,36,36,36	0
56	MG	1Y	502	1/1	0.96	0.13	37,37,37,37	0
56	MG	2A	3155	1/1	0.96	0.13	37,37,37,37	0
56	MG	1A	3181	1/1	0.96	0.16	24,24,24,24	0
56	MG	1a	3184	1/1	0.96	0.08	63,63,63,63	0
56	MG	1a	3185	1/1	0.96	0.08	60,60,60,60	0
56	MG	1A	3182	1/1	0.96	0.14	25,25,25,25	0
56	MG	1Z	302	1/1	0.96	0.05	26,26,26,26	0
56	MG	1A	3860	1/1	0.96	0.07	14,14,14,14	0
56	MG	1A	3710	1/1	0.96	0.13	22,22,22,22	0
56	MG	1A	3239	1/1	0.96	0.10	49,49,49,49	0
56	MG	1A	3863	1/1	0.96	0.10	46,46,46,46	0
56	MG	10	103	1/1	0.96	0.17	24,24,24,24	0
56	MG	2A	3166	1/1	0.96	0.10	36,36,36,36	0
56	MG	1A	4047	1/1	0.96	0.07	32,32,32,32	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	1A	3566	1/1	0.96	0.06	25,25,25,25	0
56	MG	10	106	1/1	0.96	0.08	48,48,48,48	0
56	MG	1a	3201	1/1	0.96	0.06	51,51,51,51	0
56	MG	1A	3302	1/1	0.96	0.10	23,23,23,23	0
56	MG	2a	3065	1/1	0.96	0.10	36,36,36,36	0
56	MG	1A	3114	1/1	0.96	0.05	18,18,18,18	0
56	MG	1A	3080	1/1	0.96	0.27	28,28,28,28	0
56	MG	1A	3869	1/1	0.96	0.06	39,39,39,39	0
56	MG	11	103	1/1	0.96	0.05	27,27,27,27	0
56	MG	1A	3116	1/1	0.96	0.05	28,28,28,28	0
56	MG	1A	3872	1/1	0.96	0.16	12,12,12,12	0
56	MG	12	3002	1/1	0.96	0.14	41,41,41,41	0
56	MG	13	101	1/1	0.96	0.07	31,31,31,31	0
56	MG	2A	3430	1/1	0.96	0.16	61,61,61,61	0
56	MG	1A	3010	1/1	0.96	0.08	22,22,22,22	0
56	MG	1A	3722	1/1	0.96	0.05	28,28,28,28	0
56	MG	1A	3193	1/1	0.96	0.06	24,24,24,24	0
56	MG	1A	3576	1/1	0.96	0.07	39,39,39,39	0
56	MG	2A	3436	1/1	0.96	0.06	40,40,40,40	0
56	MG	1A	3148	1/1	0.96	0.09	23,23,23,23	0
56	MG	2a	3081	1/1	0.96	0.09	70,70,70,70	0
56	MG	1A	3879	1/1	0.96	0.16	20,20,20,20	0
56	MG	18	103	1/1	0.96	0.09	29,29,29,29	0
56	MG	1A	3727	1/1	0.96	0.16	32,32,32,32	0
56	MG	2a	3085	1/1	0.96	0.20	41,41,41,41	0
56	MG	1A	3462	1/1	0.96	0.06	38,38,38,38	0
56	MG	1A	3463	1/1	0.96	0.12	49,49,49,49	0
56	MG	1A	3313	1/1	0.96	0.10	23,23,23,23	0
56	MG	1a	3004	1/1	0.96	0.17	43,43,43,43	0
56	MG	2a	3090	1/1	0.96	0.21	64,64,64,64	0
56	MG	1A	3466	1/1	0.96	0.13	19,19,19,19	0
56	MG	2A	3452	1/1	0.96	0.15	42,42,42,42	0
56	MG	1A	4074	1/1	0.96	0.09	36,36,36,36	0
56	MG	2a	3094	1/1	0.96	0.07	64,64,64,64	0
56	MG	1A	3195	1/1	0.96	0.06	8,8,8,8	0
56	MG	1A	3083	1/1	0.96	0.05	41,41,41,41	0
56	MG	2A	3456	1/1	0.96	0.10	31,31,31,31	0
56	MG	1A	3385	1/1	0.96	0.09	35,35,35,35	0
56	MG	2A	3458	1/1	0.96	0.10	40,40,40,40	0
56	MG	1A	3737	1/1	0.96	0.07	17,17,17,17	0
56	MG	1A	3121	1/1	0.96	0.16	32,32,32,32	0
56	MG	1A	3154	1/1	0.96	0.21	34,34,34,34	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	1A	3896	1/1	0.96	0.09	60,60,60,60	0
56	MG	1a	3018	1/1	0.96	0.16	44,44,44,44	0
56	MG	2A	3209	1/1	0.96	0.15	55,55,55,55	0
56	MG	1a	3019	1/1	0.96	0.07	49,49,49,49	0
56	MG	1A	4084	1/1	0.96	0.10	24,24,24,24	0
56	MG	1A	4085	1/1	0.96	0.08	25,25,25,25	0
56	MG	1A	3054	1/1	0.96	0.07	37,37,37,37	0
56	MG	1A	3741	1/1	0.96	0.05	11,11,11,11	0
56	MG	2A	3471	1/1	0.96	0.09	34,34,34,34	0
56	MG	1A	3201	1/1	0.96	0.09	26,26,26,26	0
56	MG	2A	3753	1/1	0.96	0.09	36,36,36,36	0
56	MG	1A	4090	1/1	0.96	0.07	32,32,32,32	0
56	MG	2a	3118	1/1	0.96	0.06	68,68,68,68	0
56	MG	1A	3202	1/1	0.96	0.09	22,22,22,22	0
56	MG	1A	3600	1/1	0.96	0.09	14,14,14,14	0
56	MG	1A	3477	1/1	0.96	0.19	30,30,30,30	0
56	MG	1A	3065	1/1	0.96	0.13	20,20,20,20	0
56	MG	2A	3761	1/1	0.96	0.09	42,42,42,42	0
56	MG	1A	3480	1/1	0.96	0.05	34,34,34,34	0
56	MG	1A	3259	1/1	0.96	0.15	37,37,37,37	0
56	MG	1A	4100	1/1	0.96	0.27	18,18,18,18	0
56	MG	1A	3755	1/1	0.96	0.04	34,34,34,34	0
56	MG	1A	3913	1/1	0.96	0.08	34,34,34,34	0
56	MG	2A	3484	1/1	0.96	0.06	32,32,32,32	0
56	MG	1A	4104	1/1	0.96	0.09	47,47,47,47	0
56	MG	2A	3486	1/1	0.96	0.10	46,46,46,46	0
56	MG	1A	3482	1/1	0.96	0.08	18,18,18,18	0
56	MG	2a	3140	1/1	0.96	0.06	52,52,52,52	0
56	MG	1A	3607	1/1	0.96	0.11	40,40,40,40	0
56	MG	2A	3489	1/1	0.96	0.11	38,38,38,38	0
56	MG	2a	3143	1/1	0.96	0.06	51,51,51,51	0
56	MG	1a	3040	1/1	0.96	0.21	39,39,39,39	0
56	MG	1A	3483	1/1	0.96	0.13	23,23,23,23	0
56	MG	1A	3013	1/1	0.96	0.15	9,9,9,9	0
56	MG	1A	4110	1/1	0.96	0.17	31,31,31,31	0
56	MG	1a	3044	1/1	0.96	0.09	50,50,50,50	0
56	MG	2A	3495	1/1	0.96	0.09	22,22,22,22	0
56	MG	1a	3045	1/1	0.96	0.10	38,38,38,38	0
56	MG	1A	3327	1/1	0.96	0.13	40,40,40,40	0
56	MG	1A	3205	1/1	0.96	0.17	47,47,47,47	0
56	MG	2A	3792	1/1	0.96	0.06	37,37,37,37	0
56	MG	2A	3501	1/1	0.96	0.06	24,24,24,24	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	1A	3099	1/1	0.96	0.07	24,24,24,24	0
56	MG	2A	3505	1/1	0.96	0.07	34,34,34,34	0
56	MG	2A	3001	1/1	0.96	0.24	41,41,41,41	0
56	MG	1A	4116	1/1	0.96	0.15	38,38,38,38	0
56	MG	2A	3801	1/1	0.96	0.10	47,47,47,47	0
56	MG	2A	3241	1/1	0.96	0.10	66,66,66,66	0
56	MG	1A	4117	1/1	0.96	0.11	52,52,52,52	0
56	MG	2a	3167	1/1	0.96	0.12	37,37,37,37	0
56	MG	2A	3005	1/1	0.96	0.12	38,38,38,38	0
56	MG	1A	4120	1/1	0.96	0.09	23,23,23,23	0
56	MG	2A	3512	1/1	0.96	0.05	29,29,29,29	0
56	MG	2A	3807	1/1	0.96	0.06	42,42,42,42	0
56	MG	2A	3007	1/1	0.96	0.06	29,29,29,29	0
56	MG	1A	3613	1/1	0.96	0.06	18,18,18,18	0
56	MG	2A	3515	1/1	0.96	0.08	42,42,42,42	0
56	MG	2A	3811	1/1	0.96	0.04	54,54,54,54	0
56	MG	1A	4122	1/1	0.96	0.09	35,35,35,35	0
56	MG	1A	4123	1/1	0.96	0.17	18,18,18,18	0
56	MG	1A	3927	1/1	0.96	0.07	33,33,33,33	0
56	MG	2A	3519	1/1	0.96	0.07	39,39,39,39	0
56	MG	2A	3014	1/1	0.96	0.07	28,28,28,28	0
56	MG	2A	3819	1/1	0.96	0.07	48,48,48,48	0
56	MG	2A	3522	1/1	0.96	0.08	30,30,30,30	0
56	MG	1A	4126	1/1	0.96	0.13	34,34,34,34	0
56	MG	1A	3331	1/1	0.96	0.29	14,14,14,14	0
56	MG	2A	3823	1/1	0.96	0.07	48,48,48,48	0
56	MG	2A	3825	1/1	0.96	0.11	58,58,58,58	0
56	MG	1A	3616	1/1	0.96	0.04	23,23,23,23	0
56	MG	1A	3490	1/1	0.96	0.19	31,31,31,31	0
56	MG	1A	3491	1/1	0.96	0.05	40,40,40,40	0
56	MG	1A	3619	1/1	0.96	0.05	18,18,18,18	0
56	MG	1A	3056	1/1	0.96	0.07	33,33,33,33	0
56	MG	1A	3333	1/1	0.96	0.12	37,37,37,37	0
56	MG	1A	4145	1/1	0.96	0.19	28,28,28,28	0
56	MG	2A	3537	1/1	0.96	0.14	54,54,54,54	0
56	MG	1A	3266	1/1	0.96	0.08	32,32,32,32	0
56	MG	1A	3630	1/1	0.96	0.07	12,12,12,12	0
56	MG	2A	3836	1/1	0.96	0.08	44,44,44,44	0
56	MG	1B	3004	1/1	0.96	0.11	43,43,43,43	0
56	MG	1A	3404	1/1	0.96	0.13	21,21,21,21	0
56	MG	1A	3027	1/1	0.96	0.14	16,16,16,16	0
56	MG	1A	3407	1/1	0.96	0.11	29,29,29,29	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	2A	3032	1/1	0.96	0.08	56,56,56,56	0
56	MG	2A	3842	1/1	0.96	0.15	41,41,41,41	0
56	MG	2A	3843	1/1	0.96	0.06	32,32,32,32	0
56	MG	2A	3035	1/1	0.96	0.14	19,19,19,19	0
56	MG	1B	3009	1/1	0.96	0.14	34,34,34,34	0
56	MG	1a	3076	1/1	0.96	0.07	46,46,46,46	0
56	MG	1A	3408	1/1	0.96	0.09	39,39,39,39	0
56	MG	1a	3078	1/1	0.96	0.16	47,47,47,47	0
56	MG	1A	3946	1/1	0.96	0.13	30,30,30,30	0
56	MG	1A	3409	1/1	0.96	0.16	52,52,52,52	0
56	MG	1A	3411	1/1	0.96	0.16	22,22,22,22	0
56	MG	2A	3853	1/1	0.96	0.07	37,37,37,37	0
56	MG	1A	3106	1/1	0.96	0.10	28,28,28,28	0
56	MG	2A	3277	1/1	0.96	0.10	46,46,46,46	0
56	MG	2A	3559	1/1	0.96	0.07	23,23,23,23	0
56	MG	2A	3278	1/1	0.96	0.05	35,35,35,35	0
56	MG	2A	3862	1/1	0.96	0.06	35,35,35,35	0
56	MG	1A	3505	1/1	0.96	0.14	25,25,25,25	0
56	MG	1A	3413	1/1	0.96	0.12	32,32,32,32	0
56	MG	1A	3337	1/1	0.96	0.10	38,38,38,38	0
56	MG	1A	3651	1/1	0.96	0.09	12,12,12,12	0
56	MG	1a	3089	1/1	0.96	0.23	37,37,37,37	0
56	MG	1A	3510	1/1	0.96	0.17	29,29,29,29	0
56	MG	1A	3959	1/1	0.96	0.05	26,26,26,26	0
56	MG	1A	3415	1/1	0.96	0.21	23,23,23,23	0
56	MG	1A	3655	1/1	0.96	0.06	17,17,17,17	0
56	MG	2A	3288	1/1	0.96	0.14	48,48,48,48	0
56	MG	2A	3057	1/1	0.96	0.06	42,42,42,42	0
56	MG	1A	3963	1/1	0.96	0.06	16,16,16,16	0
56	MG	2A	3060	1/1	0.96	0.09	47,47,47,47	0
56	MG	2g	8001	1/1	0.96	0.10	70,70,70,70	0
56	MG	1a	3095	1/1	0.96	0.23	42,42,42,42	0
56	MG	1A	3797	1/1	0.96	0.13	25,25,25,25	0
56	MG	2B	3003	1/1	0.96	0.15	44,44,44,44	0
56	MG	1A	3416	1/1	0.96	0.25	27,27,27,27	0
56	MG	1A	3966	1/1	0.96	0.12	41,41,41,41	0
56	MG	2A	3581	1/1	0.96	0.08	42,42,42,42	0
56	MG	1A	3967	1/1	0.96	0.15	56,56,56,56	0
56	MG	1A	3514	1/1	0.96	0.12	33,33,33,33	0
56	MG	1A	3165	1/1	0.96	0.13	29,29,29,29	0
56	MG	1A	3418	1/1	0.96	0.06	36,36,36,36	0
56	MG	2A	3300	1/1	0.96	0.11	37,37,37,37	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	2A	3301	1/1	0.96	0.06	39,39,39,39	0
56	MG	1A	3661	1/1	0.96	0.07	48,48,48,48	0
56	MG	1D	305	1/1	0.96	0.20	24,24,24,24	0
56	MG	2A	3590	1/1	0.96	0.12	41,41,41,41	0
56	MG	1A	3805	1/1	0.96	0.09	40,40,40,40	0
56	MG	2A	3073	1/1	0.96	0.08	25,25,25,25	0
56	MG	1A	3519	1/1	0.96	0.05	43,43,43,43	0
56	MG	2A	3307	1/1	0.96	0.05	41,41,41,41	0
56	MG	1A	3168	1/1	0.96	0.11	20,20,20,20	0
56	MG	1A	3809	1/1	0.96	0.08	32,32,32,32	0
56	MG	1A	3272	1/1	0.96	0.07	30,30,30,30	0
56	MG	1E	301	1/1	0.96	0.17	18,18,18,18	0
56	MG	1A	3274	1/1	0.96	0.09	28,28,28,28	0
56	MG	2D	305	1/1	0.96	0.10	27,27,27,27	0
56	MG	1A	3276	1/1	0.96	0.14	33,33,33,33	0
56	MG	2A	3314	1/1	0.96	0.07	40,40,40,40	0
56	MG	2A	3081	1/1	0.96	0.13	38,38,38,38	0
56	MG	1A	3220	1/1	0.96	0.10	17,17,17,17	0
56	MG	1E	308	1/1	0.96	0.13	14,14,14,14	0
56	MG	1A	3816	1/1	0.96	0.11	36,36,36,36	0
57	K	1A	3527	1/1	0.96	0.18	57,57,57,57	0
56	MG	1A	3817	1/1	0.96	0.06	28,28,28,28	0
58	M2D	1A	4118	36/36	0.96	0.10	13,19,23,24	0
56	MG	2A	3086	1/1	0.96	0.14	39,39,39,39	0
59	ZN	24	501	1/1	0.96	0.05	86,86,86,86	0
59	ZN	29	501	1/1	0.96	0.06	77,77,77,77	0
59	ZN	2n	501	1/1	0.96	0.07	93,93,93,93	0
56	MG	1B	3024	1/1	0.97	0.07	49,49,49,49	0
56	MG	1B	3026	1/1	0.97	0.06	27,27,27,27	0
56	MG	2A	3435	1/1	0.97	0.06	62,62,62,62	0
56	MG	1a	3057	1/1	0.97	0.09	47,47,47,47	0
56	MG	1A	3238	1/1	0.97	0.13	25,25,25,25	0
56	MG	1A	3544	1/1	0.97	0.14	32,32,32,32	0
56	MG	1A	3451	1/1	0.97	0.07	35,35,35,35	0
56	MG	1A	3092	1/1	0.97	0.12	11,11,11,11	0
56	MG	1A	3117	1/1	0.97	0.06	24,24,24,24	0
56	MG	1x	113	1/1	0.97	0.09	46,46,46,46	0
56	MG	1A	3454	1/1	0.97	0.07	29,29,29,29	0
56	MG	1A	3549	1/1	0.97	0.14	45,45,45,45	0
56	MG	1a	3065	1/1	0.97	0.12	54,54,54,54	0
56	MG	1A	3060	1/1	0.97	0.15	32,32,32,32	0
56	MG	1A	3551	1/1	0.97	0.10	26,26,26,26	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	1A	3149	1/1	0.97	0.07	18,18,18,18	0
56	MG	1A	3554	1/1	0.97	0.05	36,36,36,36	0
56	MG	1A	3555	1/1	0.97	0.09	11,11,11,11	0
56	MG	1A	3691	1/1	0.97	0.10	34,34,34,34	0
56	MG	1a	3073	1/1	0.97	0.10	34,34,34,34	0
56	MG	2A	3004	1/1	0.97	0.11	40,40,40,40	0
56	MG	1D	307	1/1	0.97	0.10	41,41,41,41	0
56	MG	1D	308	1/1	0.97	0.20	26,26,26,26	0
56	MG	1D	309	1/1	0.97	0.13	23,23,23,23	0
56	MG	2A	3008	1/1	0.97	0.11	39,39,39,39	0
56	MG	1A	3189	1/1	0.97	0.19	29,29,29,29	0
56	MG	2A	3715	1/1	0.97	0.07	56,56,56,56	0
56	MG	2A	3010	1/1	0.97	0.05	31,31,31,31	0
56	MG	1A	3836	1/1	0.97	0.07	39,39,39,39	0
56	MG	1a	3079	1/1	0.97	0.13	30,30,30,30	0
56	MG	1A	3305	1/1	0.97	0.14	23,23,23,23	0
56	MG	1a	3081	1/1	0.97	0.15	47,47,47,47	0
56	MG	1A	3190	1/1	0.97	0.04	31,31,31,31	0
56	MG	2a	3038	1/1	0.97	0.04	37,37,37,37	0
56	MG	1A	3696	1/1	0.97	0.05	31,31,31,31	0
56	MG	1A	3246	1/1	0.97	0.08	28,28,28,28	0
56	MG	1A	3563	1/1	0.97	0.16	19,19,19,19	0
56	MG	1E	305	1/1	0.97	0.08	26,26,26,26	0
56	MG	1A	3381	1/1	0.97	0.07	25,25,25,25	0
56	MG	1A	3565	1/1	0.97	0.05	25,25,25,25	0
56	MG	1A	3020	1/1	0.97	0.04	18,18,18,18	0
56	MG	1A	3704	1/1	0.97	0.04	37,37,37,37	0
56	MG	1A	3567	1/1	0.97	0.05	41,41,41,41	0
56	MG	2A	3731	1/1	0.97	0.05	64,64,64,64	0
56	MG	1A	3151	1/1	0.97	0.10	14,14,14,14	0
56	MG	1A	3152	1/1	0.97	0.14	20,20,20,20	0
56	MG	1A	3120	1/1	0.97	0.14	16,16,16,16	0
56	MG	1A	3315	1/1	0.97	0.16	31,31,31,31	0
56	MG	2A	3249	1/1	0.97	0.12	48,48,48,48	0
56	MG	1A	3469	1/1	0.97	0.05	36,36,36,36	0
56	MG	1A	3574	1/1	0.97	0.08	27,27,27,27	0
56	MG	2A	3033	1/1	0.97	0.16	44,44,44,44	0
56	MG	2A	3034	1/1	0.97	0.12	43,43,43,43	0
56	MG	1A	3079	1/1	0.97	0.16	25,25,25,25	0
56	MG	1A	3026	1/1	0.97	0.18	14,14,14,14	0
56	MG	1A	3857	1/1	0.97	0.04	22,22,22,22	0
56	MG	1A	3318	1/1	0.97	0.04	25,25,25,25	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	1A	3023	1/1	0.97	0.16	18,18,18,18	0
56	MG	1A	3474	1/1	0.97	0.18	21,21,21,21	0
56	MG	2A	3747	1/1	0.97	0.05	59,59,59,59	0
56	MG	1A	3719	1/1	0.97	0.04	37,37,37,37	0
56	MG	1a	3105	1/1	0.97	0.05	35,35,35,35	0
56	MG	2A	3500	1/1	0.97	0.12	60,60,60,60	0
56	MG	1A	3580	1/1	0.97	0.10	33,33,33,33	0
56	MG	1A	3581	1/1	0.97	0.04	30,30,30,30	0
56	MG	1N	3003	1/1	0.97	0.08	32,32,32,32	0
56	MG	2A	3754	1/1	0.97	0.05	42,42,42,42	0
56	MG	1A	3254	1/1	0.97	0.05	32,32,32,32	0
56	MG	1A	3725	1/1	0.97	0.06	29,29,29,29	0
56	MG	1A	3157	1/1	0.97	0.16	17,17,17,17	0
56	MG	2A	3758	1/1	0.97	0.06	42,42,42,42	0
56	MG	1A	3586	1/1	0.97	0.10	16,16,16,16	0
56	MG	1A	3256	1/1	0.97	0.06	20,20,20,20	0
56	MG	2A	3053	1/1	0.97	0.12	30,30,30,30	0
56	MG	1a	3114	1/1	0.97	0.09	26,26,26,26	0
56	MG	1A	3478	1/1	0.97	0.07	38,38,38,38	0
56	MG	1A	3590	1/1	0.97	0.05	21,21,21,21	0
56	MG	1A	3158	1/1	0.97	0.05	12,12,12,12	0
56	MG	2A	3059	1/1	0.97	0.10	29,29,29,29	0
56	MG	1P	202	1/1	0.97	0.25	16,16,16,16	0
56	MG	1A	3082	1/1	0.97	0.23	34,34,34,34	0
56	MG	1Q	3001	1/1	0.97	0.04	26,26,26,26	0
56	MG	1A	3127	1/1	0.97	0.08	19,19,19,19	0
56	MG	2A	3521	1/1	0.97	0.13	50,50,50,50	0
56	MG	2A	3775	1/1	0.97	0.06	51,51,51,51	0
56	MG	1a	3122	1/1	0.97	0.25	46,46,46,46	0
56	MG	2A	3777	1/1	0.97	0.07	55,55,55,55	0
56	MG	2A	3065	1/1	0.97	0.14	37,37,37,37	0
56	MG	1a	3123	1/1	0.97	0.17	40,40,40,40	0
56	MG	1A	4046	1/1	0.97	0.05	38,38,38,38	0
56	MG	1A	3032	1/1	0.97	0.11	8,8,8,8	0
56	MG	1R	202	1/1	0.97	0.29	25,25,25,25	0
56	MG	1A	3262	1/1	0.97	0.23	36,36,36,36	0
56	MG	1A	3206	1/1	0.97	0.10	34,34,34,34	0
56	MG	1S	3001	1/1	0.97	0.07	30,30,30,30	0
56	MG	1A	4051	1/1	0.97	0.06	44,44,44,44	0
56	MG	2A	3790	1/1	0.97	0.05	32,32,32,32	0
56	MG	2A	3791	1/1	0.97	0.05	45,45,45,45	0
56	MG	1A	3598	1/1	0.97	0.05	7,7,7,7	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	1A	3066	1/1	0.97	0.09	21,21,21,21	0
56	MG	1A	3211	1/1	0.97	0.09	33,33,33,33	0
56	MG	1A	3067	1/1	0.97	0.05	8,8,8,8	0
56	MG	2a	3107	1/1	0.97	0.21	38,38,38,38	0
56	MG	1a	3135	1/1	0.97	0.05	46,46,46,46	0
56	MG	1A	4056	1/1	0.97	0.07	45,45,45,45	0
56	MG	2A	3800	1/1	0.97	0.06	26,26,26,26	0
56	MG	1A	3603	1/1	0.97	0.07	15,15,15,15	0
56	MG	1A	3488	1/1	0.97	0.06	42,42,42,42	0
56	MG	1A	3164	1/1	0.97	0.05	31,31,31,31	0
56	MG	1A	3888	1/1	0.97	0.06	23,23,23,23	0
56	MG	1A	4063	1/1	0.97	0.10	17,17,17,17	0
56	MG	2a	3117	1/1	0.97	0.07	51,51,51,51	0
56	MG	1A	4064	1/1	0.97	0.07	48,48,48,48	0
56	MG	1A	3749	1/1	0.97	0.08	38,38,38,38	0
56	MG	2a	3121	1/1	0.97	0.07	62,62,62,62	0
56	MG	1W	202	1/1	0.97	0.17	31,31,31,31	0
56	MG	1A	3105	1/1	0.97	0.19	25,25,25,25	0
56	MG	1W	207	1/1	0.97	0.10	9,9,9,9	0
56	MG	1X	103	1/1	0.97	0.05	22,22,22,22	0
56	MG	1A	3410	1/1	0.97	0.08	20,20,20,20	0
56	MG	2A	3558	1/1	0.97	0.05	29,29,29,29	0
56	MG	2A	3814	1/1	0.97	0.07	45,45,45,45	0
56	MG	1A	3753	1/1	0.97	0.04	31,31,31,31	0
56	MG	2A	3816	1/1	0.97	0.07	55,55,55,55	0
56	MG	2a	3132	1/1	0.97	0.12	67,67,67,67	0
56	MG	1a	3152	1/1	0.97	0.05	55,55,55,55	0
56	MG	1A	3215	1/1	0.97	0.06	29,29,29,29	0
56	MG	1A	3216	1/1	0.97	0.09	42,42,42,42	0
56	MG	1A	3273	1/1	0.97	0.09	46,46,46,46	0
56	MG	1A	3166	1/1	0.97	0.27	22,22,22,22	0
56	MG	1A	3133	1/1	0.97	0.06	17,17,17,17	0
56	MG	1A	3759	1/1	0.97	0.12	35,35,35,35	0
56	MG	2A	3824	1/1	0.97	0.10	43,43,43,43	0
56	MG	2A	3568	1/1	0.97	0.07	42,42,42,42	0
56	MG	2A	3569	1/1	0.97	0.07	31,31,31,31	0
56	MG	2A	3101	1/1	0.97	0.14	34,34,34,34	0
56	MG	2A	3317	1/1	0.97	0.04	55,55,55,55	0
56	MG	2A	3102	1/1	0.97	0.15	33,33,33,33	0
56	MG	1A	3341	1/1	0.97	0.10	29,29,29,29	0
56	MG	2A	3104	1/1	0.97	0.09	30,30,30,30	0
56	MG	1A	3903	1/1	0.97	0.05	34,34,34,34	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	1A	3219	1/1	0.97	0.09	24,24,24,24	0
56	MG	1A	3908	1/1	0.97	0.04	18,18,18,18	0
56	MG	1A	3499	1/1	0.97	0.09	21,21,21,21	0
56	MG	2a	3159	1/1	0.97	0.05	58,58,58,58	0
56	MG	1A	3500	1/1	0.97	0.17	27,27,27,27	0
56	MG	1A	3170	1/1	0.97	0.05	13,13,13,13	0
56	MG	1A	3419	1/1	0.97	0.12	23,23,23,23	0
56	MG	1A	3620	1/1	0.97	0.10	26,26,26,26	0
56	MG	1A	3503	1/1	0.97	0.14	30,30,30,30	0
56	MG	1A	3917	1/1	0.97	0.14	52,52,52,52	0
56	MG	1A	3279	1/1	0.97	0.13	12,12,12,12	0
56	MG	1A	3919	1/1	0.97	0.05	35,35,35,35	0
56	MG	2a	3168	1/1	0.97	0.09	61,61,61,61	0
56	MG	1A	3626	1/1	0.97	0.08	19,19,19,19	0
56	MG	1A	3771	1/1	0.97	0.04	13,13,13,13	0
56	MG	1A	3627	1/1	0.97	0.06	15,15,15,15	0
56	MG	15	103	1/1	0.97	0.10	17,17,17,17	0
56	MG	2A	3848	1/1	0.97	0.09	33,33,33,33	0
56	MG	2a	3174	1/1	0.97	0.20	47,47,47,47	0
56	MG	1A	3171	1/1	0.97	0.05	21,21,21,21	0
56	MG	2A	3340	1/1	0.97	0.04	48,48,48,48	0
56	MG	1A	3775	1/1	0.97	0.28	19,19,19,19	0
56	MG	1A	3629	1/1	0.97	0.06	13,13,13,13	0
56	MG	17	101	1/1	0.97	0.07	15,15,15,15	0
56	MG	1A	3135	1/1	0.97	0.07	42,42,42,42	0
56	MG	1A	3024	1/1	0.97	0.04	26,26,26,26	0
56	MG	18	102	1/1	0.97	0.11	19,19,19,19	0
56	MG	1A	3058	1/1	0.97	0.11	36,36,36,36	0
56	MG	2A	3860	1/1	0.97	0.12	38,38,38,38	0
56	MG	2A	3129	1/1	0.97	0.11	31,31,31,31	0
56	MG	1A	3425	1/1	0.97	0.07	21,21,21,21	0
56	MG	19	103	1/1	0.97	0.06	26,26,26,26	0
56	MG	1A	3933	1/1	0.97	0.05	46,46,46,46	0
56	MG	1A	3512	1/1	0.97	0.15	30,30,30,30	0
56	MG	2A	3868	1/1	0.97	0.07	35,35,35,35	0
56	MG	1A	3785	1/1	0.97	0.27	21,21,21,21	0
56	MG	2A	3354	1/1	0.97	0.07	43,43,43,43	0
56	MG	1A	3070	1/1	0.97	0.04	23,23,23,23	0
56	MG	1A	3350	1/1	0.97	0.08	34,34,34,34	0
56	MG	1a	3195	1/1	0.97	0.07	51,51,51,51	0
56	MG	1A	3286	1/1	0.97	0.20	38,38,38,38	0
56	MG	1A	3643	1/1	0.97	0.08	15,15,15,15	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	1a	3008	1/1	0.97	0.10	37,37,37,37	0
56	MG	1a	3199	1/1	0.97	0.08	61,61,61,61	0
56	MG	1a	3009	1/1	0.97	0.24	44,44,44,44	0
56	MG	1A	3517	1/1	0.97	0.05	37,37,37,37	0
56	MG	2A	3144	1/1	0.97	0.08	42,42,42,42	0
56	MG	1a	3210	1/1	0.97	0.05	57,57,57,57	0
56	MG	1A	3943	1/1	0.97	0.05	52,52,52,52	0
56	MG	1A	3352	1/1	0.97	0.05	34,34,34,34	0
56	MG	1a	3216	1/1	0.97	0.05	62,62,62,62	0
56	MG	1a	3014	1/1	0.97	0.06	36,36,36,36	0
56	MG	1A	3110	1/1	0.97	0.17	22,22,22,22	0
56	MG	1A	3289	1/1	0.97	0.12	33,33,33,33	0
56	MG	1A	3522	1/1	0.97	0.05	26,26,26,26	0
56	MG	1A	3653	1/1	0.97	0.06	9,9,9,9	0
56	MG	1A	3432	1/1	0.97	0.04	25,25,25,25	0
56	MG	2A	3630	1/1	0.97	0.06	49,49,49,49	0
56	MG	1a	3020	1/1	0.97	0.10	33,33,33,33	0
56	MG	1a	3021	1/1	0.97	0.06	43,43,43,43	0
56	MG	1A	3799	1/1	0.97	0.09	32,32,32,32	0
56	MG	1A	3433	1/1	0.97	0.05	12,12,12,12	0
56	MG	1A	3953	1/1	0.97	0.09	36,36,36,36	0
56	MG	1A	3111	1/1	0.97	0.16	15,15,15,15	0
56	MG	1A	4134	1/1	0.97	0.15	31,31,31,31	0
56	MG	1A	4136	1/1	0.97	0.27	28,28,28,28	0
56	MG	1a	3233	1/1	0.97	0.17	32,32,32,32	0
56	MG	2A	3642	1/1	0.97	0.09	37,37,37,37	0
56	MG	1A	3657	1/1	0.97	0.06	17,17,17,17	0
56	MG	1A	4140	1/1	0.97	0.19	21,21,21,21	0
56	MG	1A	4141	1/1	0.97	0.08	27,27,27,27	0
56	MG	1A	3436	1/1	0.97	0.17	24,24,24,24	0
56	MG	2A	3391	1/1	0.97	0.22	36,36,36,36	0
56	MG	1A	3291	1/1	0.97	0.10	36,36,36,36	0
56	MG	1A	3228	1/1	0.97	0.12	18,18,18,18	0
56	MG	1f	3001	1/1	0.97	0.12	34,34,34,34	0
56	MG	2A	3652	1/1	0.97	0.08	50,50,50,50	0
56	MG	2A	3173	1/1	0.97	0.10	39,39,39,39	0
56	MG	1A	3358	1/1	0.97	0.17	21,21,21,21	0
56	MG	2F	302	1/1	0.97	0.08	39,39,39,39	0
56	MG	1l	201	1/1	0.97	0.16	29,29,29,29	0
56	MG	1l	202	1/1	0.97	0.05	61,61,61,61	0
56	MG	2A	3657	1/1	0.97	0.06	45,45,45,45	0
56	MG	2A	3177	1/1	0.97	0.11	42,42,42,42	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	1A	3051	1/1	0.97	0.06	25,25,25,25	0
56	MG	1A	3808	1/1	0.97	0.06	29,29,29,29	0
56	MG	1B	3005	1/1	0.97	0.23	50,50,50,50	0
56	MG	1n	503	1/1	0.97	0.08	43,43,43,43	0
56	MG	2A	3405	1/1	0.97	0.03	34,34,34,34	0
56	MG	2T	3002	1/1	0.97	0.06	38,38,38,38	0
56	MG	1A	3090	1/1	0.97	0.12	22,22,22,22	0
56	MG	2U	201	1/1	0.97	0.18	39,39,39,39	0
56	MG	1A	3295	1/1	0.97	0.07	42,42,42,42	0
56	MG	1A	3073	1/1	0.97	0.05	19,19,19,19	0
56	MG	1A	3812	1/1	0.97	0.05	38,38,38,38	0
56	MG	1w	101	1/1	0.97	0.08	67,67,67,67	0
56	MG	2U	206	1/1	0.97	0.04	32,32,32,32	0
56	MG	1A	3445	1/1	0.97	0.07	33,33,33,33	0
56	MG	2A	3413	1/1	0.97	0.16	50,50,50,50	0
56	MG	1A	3971	1/1	0.97	0.06	43,43,43,43	0
56	MG	1A	3814	1/1	0.97	0.07	38,38,38,38	0
56	MG	1B	3013	1/1	0.97	0.04	31,31,31,31	0
56	MG	1A	3365	1/1	0.97	0.11	17,17,17,17	0
56	MG	2A	3419	1/1	0.97	0.18	28,28,28,28	0
56	MG	1A	3236	1/1	0.97	0.23	23,23,23,23	0
56	MG	1B	3017	1/1	0.97	0.03	19,19,19,19	0
56	MG	1A	3539	1/1	0.97	0.04	27,27,27,27	0
56	MG	2A	3196	1/1	0.97	0.08	38,38,38,38	0
56	MG	2A	3424	1/1	0.97	0.07	35,35,35,35	0
56	MG	1B	3019	1/1	0.97	0.07	34,34,34,34	0
56	MG	1A	3145	1/1	0.97	0.05	18,18,18,18	0
56	MG	27	101	1/1	0.97	0.13	32,32,32,32	0
56	MG	2A	3199	1/1	0.97	0.11	44,44,44,44	0
56	MG	1A	3369	1/1	0.97	0.14	44,44,44,44	0
56	MG	1A	3820	1/1	0.97	0.10	27,27,27,27	0
56	MG	1A	3982	1/1	0.97	0.06	31,31,31,31	0
56	MG	1x	104	1/1	0.97	0.13	51,51,51,51	0
56	MG	1A	3122	1/1	0.98	0.08	24,24,24,24	0
56	MG	1A	3508	1/1	0.98	0.10	13,13,13,13	0
56	MG	1A	3560	1/1	0.98	0.08	21,21,21,21	0
56	MG	1A	4057	1/1	0.98	0.08	50,50,50,50	0
56	MG	1B	3035	1/1	0.98	0.07	21,21,21,21	0
56	MG	1A	3561	1/1	0.98	0.08	16,16,16,16	0
56	MG	1a	3139	1/1	0.98	0.09	31,31,31,31	0
56	MG	1A	3695	1/1	0.98	0.04	24,24,24,24	0
56	MG	1A	3621	1/1	0.98	0.07	34,34,34,34	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	1D	303	1/1	0.98	0.04	23,23,23,23	0
56	MG	2A	3479	1/1	0.98	0.04	37,37,37,37	0
56	MG	1A	3778	1/1	0.98	0.04	22,22,22,22	0
56	MG	1A	4062	1/1	0.98	0.07	23,23,23,23	0
56	MG	1D	306	1/1	0.98	0.06	14,14,14,14	0
56	MG	1A	3780	1/1	0.98	0.07	41,41,41,41	0
56	MG	1A	3954	1/1	0.98	0.07	50,50,50,50	0
56	MG	1a	3148	1/1	0.98	0.06	31,31,31,31	0
56	MG	1A	3465	1/1	0.98	0.12	22,22,22,22	0
56	MG	1A	3234	1/1	0.98	0.04	25,25,25,25	0
56	MG	2A	3167	1/1	0.98	0.08	44,44,44,44	0
56	MG	1A	3957	1/1	0.98	0.07	37,37,37,37	0
56	MG	1A	3191	1/1	0.98	0.16	14,14,14,14	0
56	MG	2A	3857	1/1	0.98	0.05	51,51,51,51	0
56	MG	2A	3020	1/1	0.98	0.11	26,26,26,26	0
56	MG	2A	3859	1/1	0.98	0.23	38,38,38,38	0
56	MG	1A	3192	1/1	0.98	0.07	20,20,20,20	0
56	MG	2A	3861	1/1	0.98	0.06	51,51,51,51	0
56	MG	2A	3172	1/1	0.98	0.18	44,44,44,44	0
56	MG	1A	3960	1/1	0.98	0.05	25,25,25,25	0
56	MG	1A	4071	1/1	0.98	0.06	34,34,34,34	0
56	MG	2A	3327	1/1	0.98	0.12	40,40,40,40	0
56	MG	1E	302	1/1	0.98	0.06	16,16,16,16	0
56	MG	1E	303	1/1	0.98	0.05	23,23,23,23	0
56	MG	1A	3384	1/1	0.98	0.06	33,33,33,33	0
56	MG	2a	3109	1/1	0.98	0.12	43,43,43,43	0
56	MG	2A	3027	1/1	0.98	0.07	30,30,30,30	0
56	MG	2A	3502	1/1	0.98	0.08	35,35,35,35	0
56	MG	1A	3786	1/1	0.98	0.05	42,42,42,42	0
56	MG	2A	3333	1/1	0.98	0.09	33,33,33,33	0
56	MG	1A	3288	1/1	0.98	0.06	17,17,17,17	0
56	MG	1A	4075	1/1	0.98	0.05	39,39,39,39	0
56	MG	1A	3867	1/1	0.98	0.06	18,18,18,18	0
56	MG	1A	3049	1/1	0.98	0.06	24,24,24,24	0
56	MG	1A	3516	1/1	0.98	0.13	37,37,37,37	0
56	MG	2a	3119	1/1	0.98	0.04	59,59,59,59	0
56	MG	1A	3870	1/1	0.98	0.04	25,25,25,25	0
56	MG	1A	3570	1/1	0.98	0.07	16,16,16,16	0
56	MG	1A	3969	1/1	0.98	0.12	33,33,33,33	0
56	MG	1A	3064	1/1	0.98	0.14	6,6,6,6	0
56	MG	2A	3189	1/1	0.98	0.04	38,38,38,38	0
56	MG	1F	304	1/1	0.98	0.22	28,28,28,28	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	1A	3074	1/1	0.98	0.05	37,37,37,37	0
56	MG	2A	3040	1/1	0.98	0.04	38,38,38,38	0
56	MG	1A	3321	1/1	0.98	0.04	16,16,16,16	0
56	MG	1A	3520	1/1	0.98	0.16	55,55,55,55	0
56	MG	1A	3640	1/1	0.98	0.06	12,12,12,12	0
56	MG	1A	3641	1/1	0.98	0.10	9,9,9,9	0
56	MG	2a	3133	1/1	0.98	0.04	69,69,69,69	0
56	MG	1A	3196	1/1	0.98	0.07	21,21,21,21	0
56	MG	2A	3524	1/1	0.98	0.04	44,44,44,44	0
56	MG	2a	3136	1/1	0.98	0.05	60,60,60,60	0
56	MG	1A	3112	1/1	0.98	0.14	29,29,29,29	0
56	MG	1A	3645	1/1	0.98	0.06	14,14,14,14	0
56	MG	2a	3139	1/1	0.98	0.04	41,41,41,41	0
56	MG	2A	3527	1/1	0.98	0.15	41,41,41,41	0
56	MG	1A	3882	1/1	0.98	0.04	25,25,25,25	0
56	MG	2A	3531	1/1	0.98	0.12	51,51,51,51	0
56	MG	1A	4095	1/1	0.98	0.04	19,19,19,19	0
56	MG	1a	3181	1/1	0.98	0.10	68,68,68,68	0
56	MG	2D	302	1/1	0.98	0.09	38,38,38,38	0
56	MG	2a	3147	1/1	0.98	0.10	45,45,45,45	0
56	MG	1A	3267	1/1	0.98	0.12	16,16,16,16	0
56	MG	2A	3713	1/1	0.98	0.04	55,55,55,55	0
56	MG	1N	3002	1/1	0.98	0.03	25,25,25,25	0
56	MG	1A	3720	1/1	0.98	0.05	19,19,19,19	0
56	MG	2A	3055	1/1	0.98	0.10	24,24,24,24	0
56	MG	1N	3004	1/1	0.98	0.10	27,27,27,27	0
56	MG	1A	3075	1/1	0.98	0.15	14,14,14,14	0
56	MG	1A	3648	1/1	0.98	0.10	38,38,38,38	0
56	MG	2a	3157	1/1	0.98	0.05	73,73,73,73	0
56	MG	1A	3649	1/1	0.98	0.04	13,13,13,13	0
56	MG	1a	3190	1/1	0.98	0.05	44,44,44,44	0
56	MG	2A	3543	1/1	0.98	0.04	51,51,51,51	0
56	MG	1A	3243	1/1	0.98	0.06	38,38,38,38	0
56	MG	1A	4103	1/1	0.98	0.08	16,16,16,16	0
56	MG	1A	3990	1/1	0.98	0.04	19,19,19,19	0
56	MG	2A	3370	1/1	0.98	0.18	43,43,43,43	0
56	MG	2F	304	1/1	0.98	0.09	46,46,46,46	0
56	MG	1A	3889	1/1	0.98	0.04	57,57,57,57	0
56	MG	1A	3395	1/1	0.98	0.11	35,35,35,35	0
56	MG	2Q	201	1/1	0.98	0.04	43,43,43,43	0
56	MG	2A	3551	1/1	0.98	0.07	29,29,29,29	0
56	MG	1A	4107	1/1	0.98	0.17	17,17,17,17	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	1A	3396	1/1	0.98	0.04	29,29,29,29	0
56	MG	1A	3397	1/1	0.98	0.04	27,27,27,27	0
56	MG	1Q	3002	1/1	0.98	0.08	21,21,21,21	0
56	MG	1a	3200	1/1	0.98	0.05	42,42,42,42	0
56	MG	1A	3076	1/1	0.98	0.13	26,26,26,26	0
56	MG	1A	4111	1/1	0.98	0.07	20,20,20,20	0
56	MG	2A	3380	1/1	0.98	0.16	36,36,36,36	0
56	MG	1a	3204	1/1	0.98	0.06	27,27,27,27	0
56	MG	1a	3205	1/1	0.98	0.11	55,55,55,55	0
56	MG	1a	3206	1/1	0.98	0.04	54,54,54,54	0
56	MG	1a	3208	1/1	0.98	0.05	62,62,62,62	0
56	MG	1Q	3005	1/1	0.98	0.04	25,25,25,25	0
56	MG	1A	3895	1/1	0.98	0.05	61,61,61,61	0
56	MG	1A	3999	1/1	0.98	0.05	35,35,35,35	0
56	MG	2A	3567	1/1	0.98	0.06	45,45,45,45	0
56	MG	1a	3213	1/1	0.98	0.05	44,44,44,44	0
56	MG	1a	3215	1/1	0.98	0.04	49,49,49,49	0
56	MG	1A	4114	1/1	0.98	0.12	25,25,25,25	0
56	MG	1A	3130	1/1	0.98	0.29	30,30,30,30	0
56	MG	1A	3732	1/1	0.98	0.07	16,16,16,16	0
56	MG	1a	3072	1/1	0.98	0.06	36,36,36,36	0
56	MG	2A	3237	1/1	0.98	0.16	31,31,31,31	0
56	MG	1a	3220	1/1	0.98	0.04	42,42,42,42	0
56	MG	1A	3532	1/1	0.98	0.19	29,29,29,29	0
56	MG	1A	4119	1/1	0.98	0.26	27,27,27,27	0
56	MG	1A	3329	1/1	0.98	0.17	22,22,22,22	0
56	MG	1A	3361	1/1	0.98	0.05	25,25,25,25	0
56	MG	1A	3007	1/1	0.98	0.04	27,27,27,27	0
56	MG	1A	3008	1/1	0.98	0.04	9,9,9,9	0
56	MG	1A	4124	1/1	0.98	0.08	17,17,17,17	0
56	MG	1A	3364	1/1	0.98	0.24	23,23,23,23	0
56	MG	1a	3229	1/1	0.98	0.12	42,42,42,42	0
56	MG	2A	3096	1/1	0.98	0.06	33,33,33,33	0
56	MG	2A	3764	1/1	0.98	0.04	23,23,23,23	0
56	MG	1A	3904	1/1	0.98	0.06	6,6,6,6	0
56	MG	1U	206	1/1	0.98	0.16	24,24,24,24	0
56	MG	1A	3003	1/1	0.98	0.08	13,13,13,13	0
56	MG	2A	3410	1/1	0.98	0.04	22,22,22,22	0
56	MG	1A	4128	1/1	0.98	0.05	22,22,22,22	0
56	MG	1A	4130	1/1	0.98	0.10	20,20,20,20	0
56	MG	1A	3906	1/1	0.98	0.04	43,43,43,43	0
56	MG	2A	3772	1/1	0.98	0.04	30,30,30,30	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	1A	3366	1/1	0.98	0.31	24,24,24,24	0
56	MG	1A	3275	1/1	0.98	0.05	30,30,30,30	0
56	MG	1W	205	1/1	0.98	0.08	24,24,24,24	0
56	MG	2A	3417	1/1	0.98	0.13	22,22,22,22	0
56	MG	1W	206	1/1	0.98	0.09	17,17,17,17	0
56	MG	2A	3598	1/1	0.98	0.06	27,27,27,27	0
56	MG	1A	3541	1/1	0.98	0.12	29,29,29,29	0
56	MG	2A	3781	1/1	0.98	0.05	33,33,33,33	0
56	MG	1X	101	1/1	0.98	0.07	25,25,25,25	0
56	MG	1X	102	1/1	0.98	0.09	20,20,20,20	0
56	MG	1A	4135	1/1	0.98	0.11	20,20,20,20	0
56	MG	2A	3604	1/1	0.98	0.09	35,35,35,35	0
56	MG	2A	3787	1/1	0.98	0.04	48,48,48,48	0
56	MG	1A	3743	1/1	0.98	0.06	17,17,17,17	0
56	MG	1A	3824	1/1	0.98	0.10	10,10,10,10	0
56	MG	1A	4139	1/1	0.98	0.07	23,23,23,23	0
56	MG	2A	3426	1/1	0.98	0.04	39,39,39,39	0
56	MG	1A	3599	1/1	0.98	0.07	16,16,16,16	0
56	MG	2A	3793	1/1	0.98	0.03	19,19,19,19	0
56	MG	1Y	504	1/1	0.98	0.14	45,45,45,45	0
56	MG	2A	3795	1/1	0.98	0.05	34,34,34,34	0
56	MG	1A	3053	1/1	0.98	0.10	38,38,38,38	0
56	MG	1A	3747	1/1	0.98	0.05	18,18,18,18	0
56	MG	1A	3015	1/1	0.98	0.08	20,20,20,20	0
56	MG	1A	3669	1/1	0.98	0.05	15,15,15,15	0
56	MG	1A	3920	1/1	0.98	0.04	41,41,41,41	0
56	MG	1B	3002	1/1	0.98	0.12	27,27,27,27	0
56	MG	1A	3750	1/1	0.98	0.19	41,41,41,41	0
56	MG	1A	4028	1/1	0.98	0.05	24,24,24,24	0
56	MG	2A	3437	1/1	0.98	0.05	43,43,43,43	0
56	MG	1A	3107	1/1	0.98	0.06	25,25,25,25	0
56	MG	1A	3672	1/1	0.98	0.06	9,9,9,9	0
56	MG	1A	3371	1/1	0.98	0.18	32,32,32,32	0
56	MG	2A	3442	1/1	0.98	0.06	41,41,41,41	0
56	MG	1A	3208	1/1	0.98	0.09	24,24,24,24	0
56	MG	1A	3307	1/1	0.98	0.13	32,32,32,32	0
56	MG	2w	3001	1/1	0.98	0.15	34,34,34,34	0
56	MG	1A	3230	1/1	0.98	0.20	19,19,19,19	0
56	MG	2A	3446	1/1	0.98	0.04	30,30,30,30	0
56	MG	1A	3309	1/1	0.98	0.07	37,37,37,37	0
56	MG	1A	3930	1/1	0.98	0.06	40,40,40,40	0
56	MG	1A	4037	1/1	0.98	0.07	45,45,45,45	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	2A	3451	1/1	0.98	0.06	29,29,29,29	0
56	MG	1A	3310	1/1	0.98	0.21	43,43,43,43	0
56	MG	1A	3460	1/1	0.98	0.07	20,20,20,20	0
56	MG	2A	3634	1/1	0.98	0.06	54,54,54,54	0
56	MG	1A	3033	1/1	0.98	0.18	23,23,23,23	0
56	MG	1A	3553	1/1	0.98	0.07	32,32,32,32	0
56	MG	1A	3378	1/1	0.98	0.04	25,25,25,25	0
56	MG	2A	3638	1/1	0.98	0.06	48,48,48,48	0
56	MG	1A	3232	1/1	0.98	0.13	15,15,15,15	0
56	MG	1A	3937	1/1	0.98	0.10	33,33,33,33	0
56	MG	1A	4045	1/1	0.98	0.05	30,30,30,30	0
56	MG	2y	105	1/1	0.98	0.04	65,65,65,65	0
56	MG	1A	3938	1/1	0.98	0.05	32,32,32,32	0
56	MG	17	103	1/1	0.98	0.05	36,36,36,36	0
56	MG	1A	3684	1/1	0.98	0.05	24,24,24,24	0
56	MG	1A	3614	1/1	0.98	0.04	22,22,22,22	0
56	MG	1A	3506	1/1	0.98	0.16	18,18,18,18	0
59	ZN	14	501	1/1	0.98	0.04	71,71,71,71	0
56	MG	1A	3687	1/1	0.98	0.04	30,30,30,30	0
59	ZN	25	101	1/1	0.98	0.03	44,44,44,44	0
56	MG	1A	3688	1/1	0.98	0.10	20,20,20,20	0
56	MG	1A	3557	1/1	0.98	0.09	19,19,19,19	0
60	SF4	1d	501	8/8	0.98	0.06	51,59,62,71	0
60	SF4	2d	302	8/8	0.98	0.05	53,66,72,75	0
56	MG	1A	3972	1/1	0.99	0.05	35,35,35,35	0
56	MG	1A	3639	1/1	0.99	0.03	19,19,19,19	0
56	MG	1A	3974	1/1	0.99	0.07	8,8,8,8	0
56	MG	2A	3441	1/1	0.99	0.09	47,47,47,47	0
56	MG	1A	3210	1/1	0.99	0.19	37,37,37,37	0
56	MG	1A	3265	1/1	0.99	0.14	25,25,25,25	0
56	MG	2A	3365	1/1	0.99	0.07	23,23,23,23	0
56	MG	1A	4094	1/1	0.99	0.09	22,22,22,22	0
56	MG	2A	3878	1/1	0.99	0.08	36,36,36,36	0
56	MG	2A	3528	1/1	0.99	0.05	28,28,28,28	0
56	MG	2A	3529	1/1	0.99	0.06	31,31,31,31	0
56	MG	1B	3014	1/1	0.99	0.08	31,31,31,31	0
56	MG	1A	3977	1/1	0.99	0.03	17,17,17,17	0
56	MG	1A	3582	1/1	0.99	0.09	13,13,13,13	0
56	MG	2A	3449	1/1	0.99	0.09	53,53,53,53	0
56	MG	1A	3437	1/1	0.99	0.11	27,27,27,27	0
56	MG	1A	3716	1/1	0.99	0.04	25,25,25,25	0
56	MG	1A	3798	1/1	0.99	0.09	39,39,39,39	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	1A	3644	1/1	0.99	0.04	12,12,12,12	0
56	MG	1A	3179	1/1	0.99	0.10	24,24,24,24	0
56	MG	1A	3229	1/1	0.99	0.14	32,32,32,32	0
56	MG	1A	3167	1/1	0.99	0.16	20,20,20,20	0
56	MG	1a	3203	1/1	0.99	0.04	56,56,56,56	0
56	MG	1A	3137	1/1	0.99	0.11	24,24,24,24	0
56	MG	1B	3025	1/1	0.99	0.06	21,21,21,21	0
56	MG	2A	3544	1/1	0.99	0.09	40,40,40,40	0
56	MG	2a	3122	1/1	0.99	0.04	73,73,73,73	0
56	MG	1A	3987	1/1	0.99	0.03	21,21,21,21	0
56	MG	1a	3207	1/1	0.99	0.06	33,33,33,33	0
56	MG	2A	3462	1/1	0.99	0.05	20,20,20,20	0
56	MG	1A	3589	1/1	0.99	0.09	19,19,19,19	0
56	MG	1a	3209	1/1	0.99	0.04	44,44,44,44	0
56	MG	18	104	1/1	0.99	0.07	19,19,19,19	0
56	MG	1A	3169	1/1	0.99	0.07	18,18,18,18	0
56	MG	1A	4048	1/1	0.99	0.03	17,17,17,17	0
56	MG	1A	3183	1/1	0.99	0.14	24,24,24,24	0
56	MG	1a	3214	1/1	0.99	0.06	70,70,70,70	0
56	MG	1A	3012	1/1	0.99	0.05	14,14,14,14	0
56	MG	1A	3893	1/1	0.99	0.07	21,21,21,21	0
56	MG	1A	3993	1/1	0.99	0.04	30,30,30,30	0
56	MG	1A	3185	1/1	0.99	0.14	22,22,22,22	0
56	MG	1A	3850	1/1	0.99	0.05	33,33,33,33	0
56	MG	2A	3646	1/1	0.99	0.04	23,23,23,23	0
56	MG	1A	3996	1/1	0.99	0.02	50,50,50,50	0
56	MG	1A	3072	1/1	0.99	0.27	23,23,23,23	0
56	MG	1A	3595	1/1	0.99	0.03	32,32,32,32	0
56	MG	1A	3623	1/1	0.99	0.07	17,17,17,17	0
56	MG	1a	3011	1/1	0.99	0.10	19,19,19,19	0
56	MG	1A	3101	1/1	0.99	0.11	24,24,24,24	0
56	MG	2a	3145	1/1	0.99	0.05	64,64,64,64	0
56	MG	1A	3625	1/1	0.99	0.04	23,23,23,23	0
56	MG	1U	202	1/1	0.99	0.08	19,19,19,19	0
56	MG	2a	3148	1/1	0.99	0.04	65,65,65,65	0
56	MG	1A	3102	1/1	0.99	0.12	23,23,23,23	0
56	MG	1A	4003	1/1	0.99	0.05	33,33,33,33	0
56	MG	1A	3774	1/1	0.99	0.03	25,25,25,25	0
56	MG	1A	3257	1/1	0.99	0.04	18,18,18,18	0
56	MG	1A	3952	1/1	0.99	0.03	52,52,52,52	0
56	MG	1A	3124	1/1	0.99	0.16	17,17,17,17	0
56	MG	1A	4129	1/1	0.99	0.04	16,16,16,16	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	1A	3697	1/1	0.99	0.03	8,8,8,8	0
56	MG	1A	3103	1/1	0.99	0.12	18,18,18,18	0
56	MG	1a	3162	1/1	0.99	0.08	42,42,42,42	0
56	MG	1A	3779	1/1	0.99	0.08	25,25,25,25	0
56	MG	1W	204	1/1	0.99	0.03	21,21,21,21	0
56	MG	1A	4013	1/1	0.99	0.02	26,26,26,26	0
56	MG	1A	3909	1/1	0.99	0.02	23,23,23,23	0
56	MG	1A	3406	1/1	0.99	0.14	24,24,24,24	0
56	MG	2A	3498	1/1	0.99	0.04	39,39,39,39	0
56	MG	1A	3134	1/1	0.99	0.06	8,8,8,8	0
56	MG	1A	3207	1/1	0.99	0.14	25,25,25,25	0
56	MG	1A	4138	1/1	0.99	0.16	29,29,29,29	0
56	MG	1A	3633	1/1	0.99	0.06	24,24,24,24	0
56	MG	1A	3014	1/1	0.99	0.06	15,15,15,15	0
56	MG	2A	3504	1/1	0.99	0.03	41,41,41,41	0
56	MG	1A	3019	1/1	0.99	0.06	8,8,8,8	0
56	MG	1A	4142	1/1	0.99	0.04	16,16,16,16	0
56	MG	1E	312	1/1	0.99	0.05	20,20,20,20	0
56	MG	1A	3745	1/1	0.99	0.03	28,28,28,28	0
56	MG	1A	4079	1/1	0.99	0.04	29,29,29,29	0
56	MG	1A	3636	1/1	0.99	0.07	6,6,6,6	0
56	MG	1A	3707	1/1	0.99	0.06	40,40,40,40	0
56	MG	1A	3670	1/1	0.99	0.06	8,8,8,8	0
56	MG	1A	3921	1/1	0.99	0.04	45,45,45,45	0
56	MG	1A	3284	1/1	0.99	0.03	27,27,27,27	0
59	ZN	1Y	501	1/1	0.99	0.03	49,49,49,49	0
56	MG	1A	4027	1/1	0.99	0.08	59,59,59,59	0
59	ZN	15	101	1/1	0.99	0.04	37,37,37,37	0
59	ZN	16	101	1/1	0.99	0.04	33,33,33,33	0
59	ZN	1n	501	1/1	0.99	0.03	55,55,55,55	0
59	ZN	2Y	501	1/1	0.99	0.05	75,75,75,75	0
56	MG	2A	3052	1/1	0.99	0.06	37,37,37,37	0
56	MG	2A	3602	1/1	0.99	0.04	37,37,37,37	0
59	ZN	26	501	1/1	0.99	0.03	55,55,55,55	0
56	MG	1A	3875	1/1	0.99	0.03	22,22,22,22	0
56	MG	1A	3434	1/1	0.99	0.03	24,24,24,24	0
56	MG	2a	3186	1/1	0.99	0.10	37,37,37,37	0
56	MG	1a	3186	1/1	0.99	0.05	57,57,57,57	0
56	MG	1A	3689	1/1	1.00	0.06	12,12,12,12	0
56	MG	1A	4008	1/1	1.00	0.03	22,22,22,22	0
56	MG	1A	4098	1/1	1.00	0.05	14,14,14,14	0
56	MG	1A	3698	1/1	1.00	0.03	8,8,8,8	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	2A	3774	1/1	1.00	0.02	27,27,27,27	0
56	MG	1A	4087	1/1	1.00	0.03	14,14,14,14	0
59	ZN	19	102	1/1	1.00	0.02	31,31,31,31	0
56	MG	1A	3763	1/1	1.00	0.08	7,7,7,7	0
56	MG	1A	3854	1/1	1.00	0.04	18,18,18,18	0
56	MG	1A	4012	1/1	1.00	0.02	17,17,17,17	0
56	MG	1A	3728	1/1	1.00	0.06	27,27,27,27	0
56	MG	1A	3585	1/1	1.00	0.06	15,15,15,15	0
56	MG	1A	3914	1/1	1.00	0.02	26,26,26,26	0
56	MG	1A	3721	1/1	1.00	0.05	16,16,16,16	0
56	MG	1A	3907	1/1	1.00	0.08	11,11,11,11	0
56	MG	2A	3784	1/1	1.00	0.02	17,17,17,17	0

5.5 Other polymers (i)

There are no such residues in this entry.