



# wwPDB X-ray Structure Validation Summary Report ⓘ

Jun 3, 2020 – 11:35 am BST

PDB ID : 6ND6  
Title : Crystal structure of the *Thermus thermophilus* 70S ribosome in complex with erythromycin and bound to mRNA and A-, P-, and E-site tRNAs at 2.85Å resolution  
Authors : Svetlov, M.S.; Plessa, E.; Chen, C.-W.; Bougas, A.; Krokidis, M.G.; Dinos, G.P.; Polikanov, Y.S.  
Deposited on : 2018-12-13  
Resolution : 2.85 Å(reported)

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

We welcome your comments at [validation@mail.wwpdb.org](mailto: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.

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

MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.11  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.11

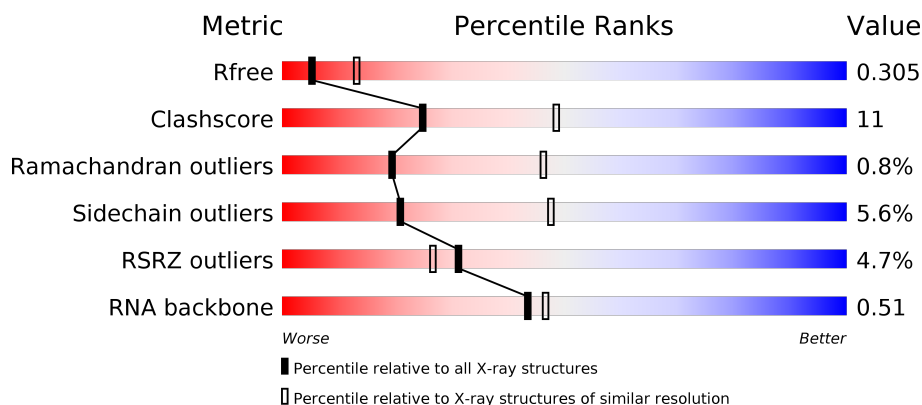
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.85 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.
















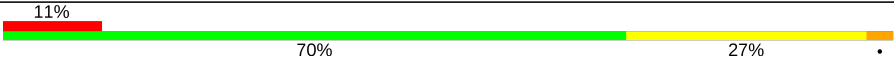

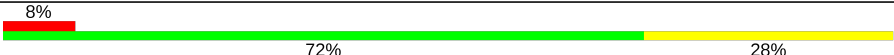


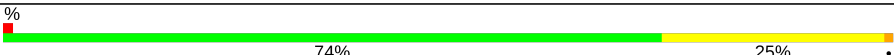
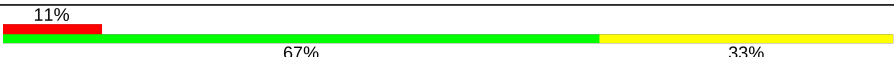
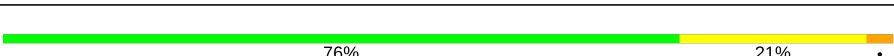


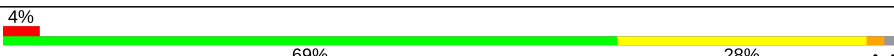
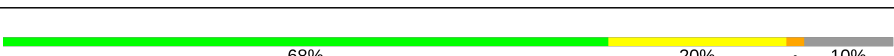
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	130704	3168 (2.90-2.82)
Clashscore	141614	3438 (2.90-2.82)
Ramachandran outliers	138981	3348 (2.90-2.82)
Sidechain outliers	138945	3351 (2.90-2.82)
RSRZ outliers	127900	3103 (2.90-2.82)
RNA backbone	3102	1088 (3.12-2.60)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	1A	2915	<div> <div>54%</div> <div>37%</div> <div>7%</div> <div>.</div> </div>
1	2A	2915	<div> <div>47%</div> <div>40%</div> <div>8%</div> <div>.</div> </div>
2	1B	121	<div> <div>58%</div> <div>39%</div> <div>..</div> </div>
2	2B	121	<div> <div>44%</div> <div>46%</div> <div>9%</div> <div>.</div> </div>

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Mol	Chain	Length	Quality of chain
3	1D	276	
3	2D	276	
4	1E	206	
4	2E	206	
5	1F	210	
5	2F	210	
6	1G	182	
6	2G	182	
7	1H	180	
7	2H	180	
8	1I	148	
8	2I	148	
9	1N	140	
9	2N	140	
10	1O	122	
10	2O	122	
11	1P	150	
11	2P	150	
12	1Q	141	
12	2Q	141	
13	1R	118	
13	2R	118	
14	1S	112	
14	2S	112	
15	1T	146	

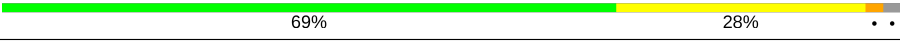

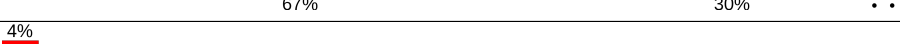

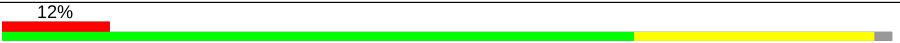
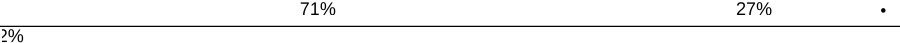

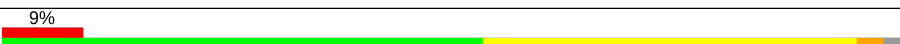





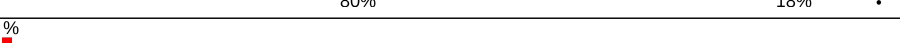





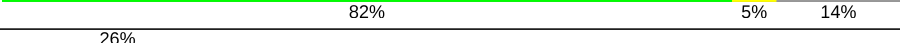


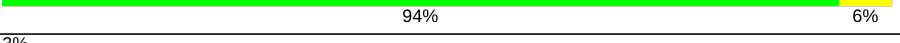

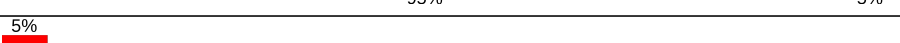
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Mol	Chain	Length	Quality of chain
15	2T	146	
16	1U	118	
16	2U	118	
17	1V	101	
17	2V	101	
18	1W	113	
18	2W	113	
19	1X	96	
19	2X	96	
20	1Y	110	
20	2Y	110	
21	1Z	206	
21	2Z	206	
22	10	85	
22	20	85	
23	11	98	
23	21	98	
24	12	72	
24	22	72	
25	13	60	
25	23	60	
26	14	71	
26	24	71	
27	15	60	
27	25	60	

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Mol	Chain	Length	Quality of chain
28	16	54	
28	26	54	
29	17	49	
29	27	49	
30	18	65	
30	28	65	
31	19	37	
31	29	37	
32	1a	1521	
32	2a	1521	
33	1b	256	
33	2b	256	
34	1c	239	
34	2c	239	
35	1d	209	
35	2d	209	
36	1e	162	
36	2e	162	
37	1f	101	
37	2f	101	
38	1g	156	
38	2g	156	
39	1h	138	
39	2h	138	
40	1i	128	

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Mol	Chain	Length	Quality of chain
40	2i	128	
41	1j	105	
41	2j	105	
42	1k	129	
42	2k	129	
43	1l	132	
43	2l	132	
44	1m	126	
44	2m	126	
45	1n	61	
45	2n	61	
46	1o	89	
46	2o	89	
47	1p	88	
47	2p	88	
48	1q	105	
48	2q	105	
49	1r	88	
49	2r	88	
50	1s	93	
50	2s	93	
51	1t	106	
51	2t	106	
52	1u	27	
52	2u	27	

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Mol	Chain	Length	Quality of chain
53	1v	27	
53	2v	27	
54	1w	76	
54	1y	76	
54	2w	76	
54	2y	76	
55	1x	77	
55	2x	77	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
54	6MZ	2y	37	-	-	-	X
56	MG	1A	3348	-	-	-	X
56	MG	1A	4073	-	-	-	X
56	MG	1F	314	-	-	-	X
56	MG	2A	3316	-	-	-	X
56	MG	2A	3359	-	-	-	X
56	MG	2A	3773	-	-	-	X
56	MG	2A	3774	-	-	-	X
56	MG	2A	3801	-	-	-	X
56	MG	2T	202	-	-	-	X

## 2 Entry composition

There are 60 unique types of molecules in this entry. The entry contains 300104 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	C	N	O	S	0	0	0
			933	588	171	170	4			

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

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

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

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

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

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
17	1V	101	Total	C	N	O	S	0	0	0
			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
			276	124	48	91	13			
53	2v	13	Total	C	N	O	P	0	0	0
			276	124	48	91	13			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
54	1w	73	Total	C	N	O	P	S	0	0
			1568	700	282	512	73	1		
54	1y	74	Total	C	N	O	P	S	0	0
			1591	710	287	519	74	1		
54	2w	73	Total	C	N	O	P	S	0	0
			1568	700	282	512	73	1		
54	2y	73	Total	C	N	O	P	S	0	0
			1568	700	282	512	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
			1625	725	294	529	76	1		
55	2x	76	Total	C	N	O	P	S	0	0
			1625	725	294	529	76	1		

- Molecule 56 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
56	2r	1	Total	Mg	0	0
			1	1		
56	1T	2	Total	Mg	0	0
			2	2		
56	20	2	Total	Mg	0	0
			2	2		
56	1Y	1	Total	Mg	0	0
			1	1		
56	2F	7	Total	Mg	0	0
			7	7		
56	1n	1	Total	Mg	0	0
			1	1		
56	2w	1	Total	Mg	0	0
			1	1		
56	1S	2	Total	Mg	0	0
			2	2		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
56	25	3	Total 3	Mg 3	0	0
56	1D	13	Total 13	Mg 13	0	0
56	1I	1	Total 1	Mg 1	0	0
56	2X	2	Total 2	Mg 2	0	0
56	1w	6	Total 6	Mg 6	0	0
56	1x	13	Total 13	Mg 13	0	0
56	1m	1	Total 1	Mg 1	0	0
56	2t	1	Total 1	Mg 1	0	0
56	2g	1	Total 1	Mg 1	0	0
56	2R	3	Total 3	Mg 3	0	0
56	14	1	Total 1	Mg 1	0	0
56	1r	1	Total 1	Mg 1	0	0
56	19	3	Total 3	Mg 3	0	0
56	2y	4	Total 4	Mg 4	0	0
56	2d	1	Total 1	Mg 1	0	0
56	1N	4	Total 4	Mg 4	0	0
56	2W	1	Total 1	Mg 1	0	0
56	13	6	Total 6	Mg 6	0	0
56	2B	21	Total 21	Mg 21	0	0
56	1b	1	Total 1	Mg 1	0	0
56	1W	8	Total 8	Mg 8	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
56	2I	1	Total 1	Mg 1	0	0
56	1X	5	Total 5	Mg 5	0	0
56	2i	2	Total 2	Mg 2	0	0
56	2T	3	Total 3	Mg 3	0	0
56	2G	1	Total 1	Mg 1	0	0
56	1a	229	Total 229	Mg 229	0	0
56	2p	1	Total 1	Mg 1	0	0
56	1R	2	Total 2	Mg 2	0	0
56	26	2	Total 2	Mg 2	0	0
56	1G	3	Total 3	Mg 3	0	0
56	1v	1	Total 1	Mg 1	0	0
56	2D	7	Total 7	Mg 7	0	0
56	1l	3	Total 3	Mg 3	0	0
56	1Q	8	Total 8	Mg 8	0	0
56	1B	35	Total 35	Mg 35	0	0
56	17	5	Total 5	Mg 5	0	0
56	18	2	Total 2	Mg 2	0	0
56	1f	1	Total 1	Mg 1	0	0
56	28	1	Total 1	Mg 1	0	0
56	2e	1	Total 1	Mg 1	0	0
56	1A	1073	Total 1073	Mg 1073	0	0

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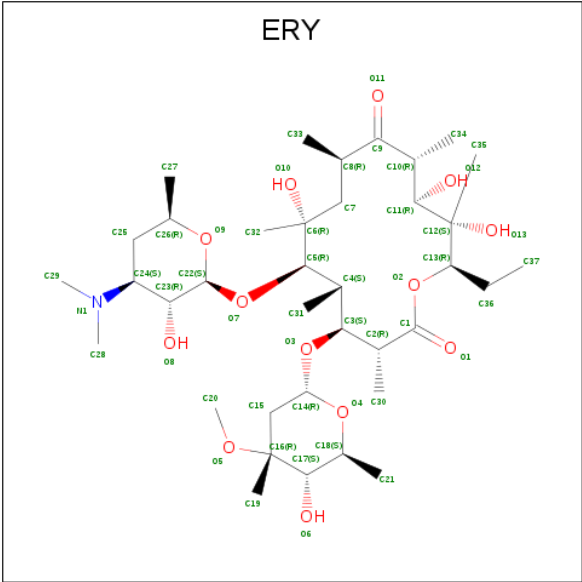
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
56	2P	2	Total 2	Mg 2	0	0
56	12	2	Total 2	Mg 2	0	0
56	1p	1	Total 1	Mg 1	0	0
56	2N	1	Total 1	Mg 1	0	0
56	1e	2	Total 2	Mg 2	0	0
56	1V	8	Total 8	Mg 8	0	0
56	22	1	Total 1	Mg 1	0	0
56	2j	2	Total 2	Mg 2	0	0
56	2U	3	Total 3	Mg 3	0	0
56	11	1	Total 1	Mg 1	0	0
56	2q	3	Total 3	Mg 3	0	0
56	1U	10	Total 10	Mg 10	0	0
56	27	2	Total 2	Mg 2	0	0
56	1F	14	Total 14	Mg 14	0	0
56	2Z	1	Total 1	Mg 1	0	0
56	2E	8	Total 8	Mg 8	0	0
56	2v	2	Total 2	Mg 2	0	0
56	1P	8	Total 8	Mg 8	0	0
56	2a	233	Total 233	Mg 233	0	0
56	1E	15	Total 15	Mg 15	0	0
56	2l	5	Total 5	Mg 5	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
56	16	4	Total 4	Mg 4	0	0
56	1t	1	Total 1	Mg 1	0	0
56	1y	5	Total 5	Mg 5	0	0
56	2f	2	Total 2	Mg 2	0	0
56	2Q	5	Total 5	Mg 5	0	0
56	15	7	Total 7	Mg 7	0	0
56	1s	1	Total 1	Mg 1	0	0
56	2O	1	Total 1	Mg 1	0	0
56	1d	1	Total 1	Mg 1	0	0
56	23	3	Total 3	Mg 3	0	0
56	2x	5	Total 5	Mg 5	0	0
56	1Z	3	Total 3	Mg 3	0	0
56	2k	1	Total 1	Mg 1	0	0
56	1O	2	Total 2	Mg 2	0	0
56	2V	1	Total 1	Mg 1	0	0
56	10	7	Total 7	Mg 7	0	0
56	2A	874	Total 874	Mg 874	0	0

- Molecule 57 is ERYTHROMYCIN A (three-letter code: ERY) (formula: C<sub>37</sub>H<sub>67</sub>NO<sub>13</sub>).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
57	1A	1	Total	C	N	O	0	0
			51	37	1	13		
57	2A	1	Total	C	N	O	0	0
			51	37	1	13		

- Molecule 58 is ZINC ION (three-letter code: ZN) (formula: Zn).

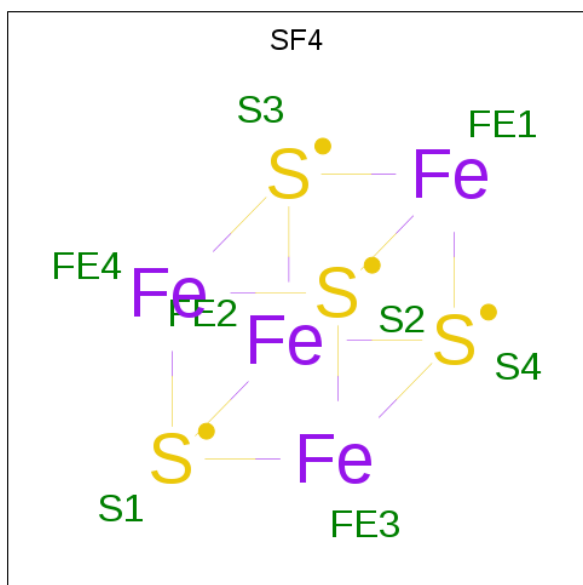
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
58	1Y	1	Total	Zn	0	0
			1	1		
58	14	1	Total	Zn	0	0
			1	1		
58	1n	1	Total	Zn	0	0
			1	1		
58	15	1	Total	Zn	0	0
			1	1		
58	29	1	Total	Zn	0	0
			1	1		
58	19	1	Total	Zn	0	0
			1	1		
58	26	1	Total	Zn	0	0
			1	1		
58	25	1	Total	Zn	0	0
			1	1		
58	24	1	Total	Zn	0	0
			1	1		
58	2n	1	Total	Zn	0	0
			1	1		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
58	2Y	1	Total	Zn	0	0
			1	1		
58	16	1	Total	Zn	0	0
			1	1		

- Molecule 59 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe<sub>4</sub>S<sub>4</sub>).



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

- Molecule 60 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
60	1A	3	Total	O	0	0
			3	3		
60	1A	1	Total	O	0	0
			1	1		
60	1A	5	Total	O	0	0
			5	5		
60	1A	5	Total	O	0	0
			5	5		
60	1A	2	Total	O	0	0
			2	2		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
60	1A	4	Total 4	O 4	0	0
60	1A	1	Total 1	O 1	0	0
60	1A	2	Total 2	O 2	0	0
60	1A	4	Total 4	O 4	0	0
60	1A	2	Total 2	O 2	0	0
60	1A	2	Total 2	O 2	0	0
60	1A	2	Total 2	O 2	0	0
60	1A	2	Total 2	O 2	0	0
60	1A	2	Total 2	O 2	0	0
60	1A	4	Total 4	O 4	0	0
60	1A	1	Total 1	O 1	0	0
60	1A	6	Total 6	O 6	0	0
60	1A	1	Total 1	O 1	0	0
60	1A	2	Total 2	O 2	0	0
60	1A	1	Total 1	O 1	0	0
60	1A	1	Total 1	O 1	0	0
60	1A	5	Total 5	O 5	0	0
60	1A	2	Total 2	O 2	0	0
60	1A	2	Total 2	O 2	0	0
60	1A	5	Total 5	O 5	0	0
60	1A	4	Total 4	O 4	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
60	1A	5	Total 5	O 5	0	0
60	1A	5	Total 5	O 5	0	0
60	1A	4	Total 4	O 4	0	0
60	1A	5	Total 5	O 5	0	0
60	1A	5	Total 5	O 5	0	0
60	1A	2	Total 2	O 2	0	0
60	1A	4	Total 4	O 4	0	0
60	1A	2	Total 2	O 2	0	0
60	1A	2	Total 2	O 2	0	0
60	1A	2	Total 2	O 2	0	0
60	1A	2	Total 2	O 2	0	0
60	1A	2	Total 2	O 2	0	0
60	1A	1	Total 1	O 1	0	0
60	1A	4	Total 4	O 4	0	0
60	1A	2	Total 2	O 2	0	0
60	1A	1	Total 1	O 1	0	0
60	1A	5	Total 5	O 5	0	0
60	1A	1	Total 1	O 1	0	0
60	1A	4	Total 4	O 4	0	0
60	1A	1	Total 1	O 1	0	0
60	1A	2	Total 2	O 2	0	0
60	1A	1	Total 1	O 1	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
60	1A	1	Total 1	O 1	0	0
60	1A	2	Total 2	O 2	0	0
60	1A	1	Total 1	O 1	0	0
60	1A	4	Total 4	O 4	0	0
60	1A	3	Total 3	O 3	0	0
60	1A	4	Total 4	O 4	0	0
60	1A	1	Total 1	O 1	0	0
60	1A	2	Total 2	O 2	0	0
60	1A	1	Total 1	O 1	0	0
60	1A	1	Total 1	O 1	0	0
60	1A	2	Total 2	O 2	0	0
60	1A	4	Total 4	O 4	0	0
60	1A	5	Total 5	O 5	0	0
60	1A	3	Total 3	O 3	0	0
60	1A	2	Total 2	O 2	0	0
60	1A	5	Total 5	O 5	0	0
60	1A	4	Total 4	O 4	0	0
60	1A	5	Total 5	O 5	0	0
60	1A	4	Total 4	O 4	0	0
60	1A	3	Total 3	O 3	0	0
60	1A	4	Total 4	O 4	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
60	1A	5	Total 5	O 5	0	0
60	1A	4	Total 4	O 4	0	0
60	1A	4	Total 4	O 4	0	0
60	1A	4	Total 4	O 4	0	0
60	1A	4	Total 4	O 4	0	0
60	1A	5	Total 5	O 5	0	0
60	1A	5	Total 5	O 5	0	0
60	1A	1	Total 1	O 1	0	0
60	1A	2	Total 2	O 2	0	0
60	1A	3	Total 3	O 3	0	0
60	1A	1	Total 1	O 1	0	0
60	1A	5	Total 5	O 5	0	0
60	1A	1	Total 1	O 1	0	0
60	1A	4	Total 4	O 4	0	0
60	1A	1	Total 1	O 1	0	0
60	1A	5	Total 5	O 5	0	0
60	1A	5	Total 5	O 5	0	0
60	1A	2	Total 2	O 2	0	0
60	1A	4	Total 4	O 4	0	0
60	1A	4	Total 4	O 4	0	0
60	1A	3	Total 3	O 3	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
60	1A	3	Total 3	O 3	0	0
60	1A	4	Total 4	O 4	0	0
60	1A	4	Total 4	O 4	0	0
60	1A	3	Total 3	O 3	0	0
60	1A	2	Total 2	O 2	0	0
60	1A	1	Total 1	O 1	0	0
60	1A	1	Total 1	O 1	0	0
60	1A	4	Total 4	O 4	0	0
60	1A	5	Total 5	O 5	0	0
60	1A	1	Total 1	O 1	0	0
60	1A	1	Total 1	O 1	0	0
60	1A	2	Total 2	O 2	0	0
60	1A	3	Total 3	O 3	0	0
60	1A	1	Total 1	O 1	0	0
60	1A	2	Total 2	O 2	0	0
60	1A	1	Total 1	O 1	0	0
60	1A	2	Total 2	O 2	0	0
60	1A	1	Total 1	O 1	0	0
60	1A	4	Total 4	O 4	0	0
60	1A	1	Total 1	O 1	0	0
60	1A	2	Total 2	O 2	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
60	1A	2	Total	O	0	0
			2	2		
60	1A	2	Total	O	0	0
			2	2		
60	1A	2	Total	O	0	0
			2	2		
60	1A	1	Total	O	0	0
			1	1		
60	1A	2	Total	O	0	0
			2	2		
60	1A	2	Total	O	0	0
			2	2		
60	1A	6	Total	O	0	0
			6	6		
60	1A	3	Total	O	0	0
			3	3		
60	1A	2	Total	O	0	0
			2	2		
60	1A	1	Total	O	0	0
			1	1		
60	1A	5	Total	O	0	0
			5	5		
60	1A	2	Total	O	0	0
			2	2		
60	1A	3	Total	O	0	0
			3	3		
60	1A	2	Total	O	0	0
			2	2		
60	1A	6	Total	O	0	0
			6	6		
60	1A	6	Total	O	0	0
			6	6		
60	1A	2	Total	O	0	0
			2	2		
60	1A	3	Total	O	0	0
			3	3		
60	1A	3	Total	O	0	0
			3	3		
60	1A	3	Total	O	0	0
			3	3		
60	1A	3	Total	O	0	0
			3	3		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
60	1A	2	Total 2	O 2	0	0
60	1A	1	Total 1	O 1	0	0
60	1A	2	Total 2	O 2	0	0
60	1A	6	Total 6	O 6	0	0
60	1A	3	Total 3	O 3	0	0
60	1A	3	Total 3	O 3	0	0
60	1A	1	Total 1	O 1	0	0
60	1A	5	Total 5	O 5	0	0
60	1A	2	Total 2	O 2	0	0
60	1A	2	Total 2	O 2	0	0
60	1A	2	Total 2	O 2	0	0
60	1A	1	Total 1	O 1	0	0
60	1A	5	Total 5	O 5	0	0
60	1A	3	Total 3	O 3	0	0
60	1A	5	Total 5	O 5	0	0
60	1A	6	Total 6	O 6	0	0
60	1A	6	Total 6	O 6	0	0
60	1A	4	Total 4	O 4	0	0
60	1A	2	Total 2	O 2	0	0
60	1A	3	Total 3	O 3	0	0
60	1A	4	Total 4	O 4	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
60	1A	2	Total 2	O 2	0	0
60	1A	6	Total 6	O 6	0	0
60	1A	3	Total 3	O 3	0	0
60	1A	2	Total 2	O 2	0	0
60	1A	5	Total 5	O 5	0	0
60	1A	2	Total 2	O 2	0	0
60	1A	4	Total 4	O 4	0	0
60	1A	2	Total 2	O 2	0	0
60	1A	2	Total 2	O 2	0	0
60	1A	5	Total 5	O 5	0	0
60	1A	4	Total 4	O 4	0	0
60	1A	4	Total 4	O 4	0	0
60	1A	4	Total 4	O 4	0	0
60	1A	5	Total 5	O 5	0	0
60	1A	4	Total 4	O 4	0	0
60	1A	4	Total 4	O 4	0	0
60	1A	3	Total 3	O 3	0	0
60	1A	5	Total 5	O 5	0	0
60	1A	2	Total 2	O 2	0	0
60	1A	2	Total 2	O 2	0	0
60	1A	2	Total 2	O 2	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
60	1A	1	Total 1	O 1	0	0
60	1A	5	Total 5	O 5	0	0
60	1A	4	Total 4	O 4	0	0
60	1A	1	Total 1	O 1	0	0
60	1A	5	Total 5	O 5	0	0
60	1A	5	Total 5	O 5	0	0
60	1A	5	Total 5	O 5	0	0
60	1A	2	Total 2	O 2	0	0
60	1A	1	Total 1	O 1	0	0
60	1A	2	Total 2	O 2	0	0
60	1A	5	Total 5	O 5	0	0
60	1A	6	Total 6	O 6	0	0
60	1A	4	Total 4	O 4	0	0
60	1A	3	Total 3	O 3	0	0
60	1A	3	Total 3	O 3	0	0
60	1A	3	Total 3	O 3	0	0
60	1A	5	Total 5	O 5	0	0
60	1A	2	Total 2	O 2	0	0
60	1A	2	Total 2	O 2	0	0
60	1A	6	Total 6	O 6	0	0
60	1A	2	Total 2	O 2	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
60	1A	1	Total 1	O 1	0	0
60	1A	3	Total 3	O 3	0	0
60	1A	1	Total 1	O 1	0	0
60	1A	5	Total 5	O 5	0	0
60	1A	3	Total 3	O 3	0	0
60	1A	1	Total 1	O 1	0	0
60	1A	1	Total 1	O 1	0	0
60	1A	2	Total 2	O 2	0	0
60	1A	1	Total 1	O 1	0	0
60	1A	2	Total 2	O 2	0	0
60	1A	1	Total 1	O 1	0	0
60	1A	1	Total 1	O 1	0	0
60	1A	1	Total 1	O 1	0	0
60	1A	1	Total 1	O 1	0	0
60	1A	1	Total 1	O 1	0	0
60	1A	1	Total 1	O 1	0	0
60	1A	1	Total 1	O 1	0	0
60	1A	1	Total 1	O 1	0	0
60	1A	1	Total 1	O 1	0	0
60	1A	1	Total 1	O 1	0	0
60	1A	2	Total 2	O 2	0	0
60	1A	1	Total 1	O 1	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
60	1A	2	Total 2	O 2	0	0
60	1A	3	Total 3	O 3	0	0
60	1A	1	Total 1	O 1	0	0
60	1A	1	Total 1	O 1	0	0
60	1A	1	Total 1	O 1	0	0
60	1A	4	Total 4	O 4	0	0
60	1A	1	Total 1	O 1	0	0
60	1A	1	Total 1	O 1	0	0
60	1A	3	Total 3	O 3	0	0
60	1A	3	Total 3	O 3	0	0
60	1A	2	Total 2	O 2	0	0
60	1A	3	Total 3	O 3	0	0
60	1A	3	Total 3	O 3	0	0
60	1A	2	Total 2	O 2	0	0
60	1A	2	Total 2	O 2	0	0
60	1A	2	Total 2	O 2	0	0
60	1A	5	Total 5	O 5	0	0
60	1A	1	Total 1	O 1	0	0
60	1A	2	Total 2	O 2	0	0
60	1A	3	Total 3	O 3	0	0
60	1A	1	Total 1	O 1	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
60	1A	2	Total 2	O 2	0	0
60	1A	1	Total 1	O 1	0	0
60	1A	5	Total 5	O 5	0	0
60	1A	1	Total 1	O 1	0	0
60	1A	2	Total 2	O 2	0	0
60	1A	1	Total 1	O 1	0	0
60	1A	2	Total 2	O 2	0	0
60	1A	3	Total 3	O 3	0	0
60	1A	1	Total 1	O 1	0	0
60	1A	1	Total 1	O 1	0	0
60	1A	1	Total 1	O 1	0	0
60	1A	5	Total 5	O 5	0	0
60	1A	1	Total 1	O 1	0	0
60	1A	1	Total 1	O 1	0	0
60	1A	1	Total 1	O 1	0	0
60	1A	1	Total 1	O 1	0	0
60	1A	1	Total 1	O 1	0	0
60	1A	1	Total 1	O 1	0	0
60	1A	1	Total 1	O 1	0	0
60	1A	1	Total 1	O 1	0	0
60	1A	4	Total 4	O 4	0	0
60	1A	1	Total 1	O 1	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
60	1A	3	Total 3	O 3	0	0
60	1A	5	Total 5	O 5	0	0
60	1A	6	Total 6	O 6	0	0
60	1A	2	Total 2	O 2	0	0
60	1A	2	Total 2	O 2	0	0
60	1A	5	Total 5	O 5	0	0
60	1A	4	Total 4	O 4	0	0
60	1A	4	Total 4	O 4	0	0
60	1A	4	Total 4	O 4	0	0
60	1A	5	Total 5	O 5	0	0
60	1A	2	Total 2	O 2	0	0
60	1A	1	Total 1	O 1	0	0
60	1A	1	Total 1	O 1	0	0
60	1A	2	Total 2	O 2	0	0
60	1A	1	Total 1	O 1	0	0
60	1A	5	Total 5	O 5	0	0
60	1A	2	Total 2	O 2	0	0
60	1A	1	Total 1	O 1	0	0
60	1A	1	Total 1	O 1	0	0
60	1A	2	Total 2	O 2	0	0
60	1A	3	Total 3	O 3	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
60	1A	6	Total 6	O 6	0	0
60	1A	1	Total 1	O 1	0	0
60	1A	1	Total 1	O 1	0	0
60	1A	1	Total 1	O 1	0	0
60	1A	1	Total 1	O 1	0	0
60	1A	6	Total 6	O 6	0	0
60	1A	6	Total 6	O 6	0	0
60	1A	2	Total 2	O 2	0	0
60	1A	2	Total 2	O 2	0	0
60	1A	1	Total 1	O 1	0	0
60	1A	6	Total 6	O 6	0	0
60	1A	6	Total 6	O 6	0	0
60	1A	6	Total 6	O 6	0	0
60	1A	2	Total 2	O 2	0	0
60	1A	4	Total 4	O 4	0	0
60	1A	6	Total 6	O 6	0	0
60	1A	5	Total 5	O 5	0	0
60	1A	4	Total 4	O 4	0	0
60	1A	4	Total 4	O 4	0	0
60	1A	5	Total 5	O 5	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
60	1A	3	Total 3	O 3	0	0
60	1A	3	Total 3	O 3	0	0
60	1A	3	Total 3	O 3	0	0
60	1A	6	Total 6	O 6	0	0
60	1A	6	Total 6	O 6	0	0
60	1A	6	Total 6	O 6	0	0
60	1A	5	Total 5	O 5	0	0
60	1A	4	Total 4	O 4	0	0
60	1A	5	Total 5	O 5	0	0
60	1A	4	Total 4	O 4	0	0
60	1A	2	Total 2	O 2	0	0
60	1A	4	Total 4	O 4	0	0
60	1A	5	Total 5	O 5	0	0
60	1A	2	Total 2	O 2	0	0
60	1A	4	Total 4	O 4	0	0
60	1A	5	Total 5	O 5	0	0
60	1A	6	Total 6	O 6	0	0
60	1A	5	Total 5	O 5	0	0
60	1A	2	Total 2	O 2	0	0
60	1A	2	Total 2	O 2	0	0
60	1A	3	Total 3	O 3	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
60	1A	5	Total 5	O 5	0	0
60	1A	5	Total 5	O 5	0	0
60	1A	4	Total 4	O 4	0	0
60	1A	2	Total 2	O 2	0	0
60	1A	4	Total 4	O 4	0	0
60	1A	3	Total 3	O 3	0	0
60	1A	5	Total 5	O 5	0	0
60	1A	3	Total 3	O 3	0	0
60	1A	3	Total 3	O 3	0	0
60	1A	2	Total 2	O 2	0	0
60	1A	2	Total 2	O 2	0	0
60	1A	4	Total 4	O 4	0	0
60	1A	1	Total 1	O 1	0	0
60	1A	2	Total 2	O 2	0	0
60	1A	6	Total 6	O 6	0	0
60	1A	2	Total 2	O 2	0	0
60	1A	5	Total 5	O 5	0	0
60	1A	6	Total 6	O 6	0	0
60	1A	6	Total 6	O 6	0	0
60	1A	3	Total 3	O 3	0	0
60	1A	5	Total 5	O 5	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
60	1A	3	Total 3	O 3	0	0
60	1A	2	Total 2	O 2	0	0
60	1A	3	Total 3	O 3	0	0
60	1A	6	Total 6	O 6	0	0
60	1A	5	Total 5	O 5	0	0
60	1A	2	Total 2	O 2	0	0
60	1A	5	Total 5	O 5	0	0
60	1A	4	Total 4	O 4	0	0
60	1A	4	Total 4	O 4	0	0
60	1A	3	Total 3	O 3	0	0
60	1A	6	Total 6	O 6	0	0
60	1A	4	Total 4	O 4	0	0
60	1A	3	Total 3	O 3	0	0
60	1A	5	Total 5	O 5	0	0
60	1A	5	Total 5	O 5	0	0
60	1A	4	Total 4	O 4	0	0
60	1A	2	Total 2	O 2	0	0
60	1A	2	Total 2	O 2	0	0
60	1A	2	Total 2	O 2	0	0
60	1A	1	Total 1	O 1	0	0
60	1A	2	Total 2	O 2	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
60	1A	6	Total 6	O 6	0	0
60	1A	2	Total 2	O 2	0	0
60	1A	6	Total 6	O 6	0	0
60	1A	4	Total 4	O 4	0	0
60	1A	4	Total 4	O 4	0	0
60	1A	3	Total 3	O 3	0	0
60	1A	6	Total 6	O 6	0	0
60	1A	3	Total 3	O 3	0	0
60	1A	5	Total 5	O 5	0	0
60	1A	4	Total 4	O 4	0	0
60	1A	6	Total 6	O 6	0	0
60	1A	5	Total 5	O 5	0	0
60	1A	2	Total 2	O 2	0	0
60	1A	1	Total 1	O 1	0	0
60	1A	2	Total 2	O 2	0	0
60	1A	3	Total 3	O 3	0	0
60	1A	6	Total 6	O 6	0	0
60	1A	4	Total 4	O 4	0	0
60	1A	3	Total 3	O 3	0	0
60	1A	4	Total 4	O 4	0	0
60	1A	6	Total 6	O 6	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
60	1A	3	Total 3	O 3	0	0
60	1A	5	Total 5	O 5	0	0
60	1A	6	Total 6	O 6	0	0
60	1A	5	Total 5	O 5	0	0
60	1A	2	Total 2	O 2	0	0
60	1A	5	Total 5	O 5	0	0
60	1A	6	Total 6	O 6	0	0
60	1A	2	Total 2	O 2	0	0
60	1A	4	Total 4	O 4	0	0
60	1A	5	Total 5	O 5	0	0
60	1A	2	Total 2	O 2	0	0
60	1A	2	Total 2	O 2	0	0
60	1A	3	Total 3	O 3	0	0
60	1A	1	Total 1	O 1	0	0
60	1A	3	Total 3	O 3	0	0
60	1A	3	Total 3	O 3	0	0
60	1A	2	Total 2	O 2	0	0
60	1A	4	Total 4	O 4	0	0
60	1A	4	Total 4	O 4	0	0
60	1A	4	Total 4	O 4	0	0
60	1A	3	Total 3	O 3	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
60	1A	2	Total 2	O 2	0	0
60	1A	5	Total 5	O 5	0	0
60	1A	2	Total 2	O 2	0	0
60	1A	3	Total 3	O 3	0	0
60	1A	1	Total 1	O 1	0	0
60	1A	4	Total 4	O 4	0	0
60	1A	3	Total 3	O 3	0	0
60	1A	5	Total 5	O 5	0	0
60	1A	2	Total 2	O 2	0	0
60	1A	6	Total 6	O 6	0	0
60	1A	4	Total 4	O 4	0	0
60	1A	1	Total 1	O 1	0	0
60	1A	6	Total 6	O 6	0	0
60	1A	1	Total 1	O 1	0	0
60	1A	6	Total 6	O 6	0	0
60	1A	1	Total 1	O 1	0	0
60	1A	4	Total 4	O 4	0	0
60	1A	2	Total 2	O 2	0	0
60	1A	1	Total 1	O 1	0	0
60	1A	2	Total 2	O 2	0	0
60	1A	2	Total 2	O 2	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
60	1A	6	Total 6	O 6	0	0
60	1A	1	Total 1	O 1	0	0
60	1A	1	Total 1	O 1	0	0
60	1A	1	Total 1	O 1	0	0
60	1A	1	Total 1	O 1	0	0
60	1A	1	Total 1	O 1	0	0
60	1A	1	Total 1	O 1	0	0
60	1A	2	Total 2	O 2	0	0
60	1A	2	Total 2	O 2	0	0
60	1A	1	Total 1	O 1	0	0
60	1A	1	Total 1	O 1	0	0
60	1A	1	Total 1	O 1	0	0
60	1A	1	Total 1	O 1	0	0
60	1A	1	Total 1	O 1	0	0
60	1A	1	Total 1	O 1	0	0
60	1A	2	Total 2	O 2	0	0
60	1A	1	Total 1	O 1	0	0
60	1A	2	Total 2	O 2	0	0
60	1A	1	Total 1	O 1	0	0
60	1A	1	Total 1	O 1	0	0
60	1A	2	Total 2	O 2	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
60	1A	2	Total 2	O 2	0	0
60	1A	1	Total 1	O 1	0	0
60	1A	6	Total 6	O 6	0	0
60	1A	384	Total 384	O 384	0	0
60	1B	1	Total 1	O 1	0	0
60	1B	5	Total 5	O 5	0	0
60	1B	3	Total 3	O 3	0	0
60	1B	3	Total 3	O 3	0	0
60	1B	1	Total 1	O 1	0	0
60	1B	1	Total 1	O 1	0	0
60	1B	1	Total 1	O 1	0	0
60	1B	1	Total 1	O 1	0	0
60	1B	1	Total 1	O 1	0	0
60	1B	2	Total 2	O 2	0	0
60	1B	2	Total 2	O 2	0	0
60	1B	2	Total 2	O 2	0	0
60	1B	1	Total 1	O 1	0	0
60	1B	4	Total 4	O 4	0	0
60	1B	1	Total 1	O 1	0	0
60	1B	1	Total 1	O 1	0	0
60	1B	1	Total 1	O 1	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
60	1B	2	Total 2	O 2	0	0
60	1B	1	Total 1	O 1	0	0
60	1B	1	Total 1	O 1	0	0
60	1B	2	Total 2	O 2	0	0
60	1B	1	Total 1	O 1	0	0
60	1B	5	Total 5	O 5	0	0
60	1B	1	Total 1	O 1	0	0
60	1B	15	Total 15	O 15	0	0
60	1D	4	Total 4	O 4	0	0
60	1D	1	Total 1	O 1	0	0
60	1D	1	Total 1	O 1	0	0
60	1D	10	Total 10	O 10	0	0
60	1E	2	Total 2	O 2	0	0
60	1E	5	Total 5	O 5	0	0
60	1E	1	Total 1	O 1	0	0
60	1E	5	Total 5	O 5	0	0
60	1E	8	Total 8	O 8	0	0
60	1F	1	Total 1	O 1	0	0
60	1F	6	Total 6	O 6	0	0
60	1G	2	Total 2	O 2	0	0
60	1G	2	Total 2	O 2	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
60	1H	1	Total 1	O 1	0	0
60	1I	2	Total 2	O 2	0	0
60	1N	5	Total 5	O 5	0	0
60	1O	1	Total 1	O 1	0	0
60	1O	1	Total 1	O 1	0	0
60	1O	5	Total 5	O 5	0	0
60	1P	4	Total 4	O 4	0	0
60	1P	1	Total 1	O 1	0	0
60	1P	2	Total 2	O 2	0	0
60	1P	4	Total 4	O 4	0	0
60	1Q	4	Total 4	O 4	0	0
60	1Q	1	Total 1	O 1	0	0
60	1Q	5	Total 5	O 5	0	0
60	1R	1	Total 1	O 1	0	0
60	1R	7	Total 7	O 7	0	0
60	1S	1	Total 1	O 1	0	0
60	1S	4	Total 4	O 4	0	0
60	1T	1	Total 1	O 1	0	0
60	1T	1	Total 1	O 1	0	0
60	1U	6	Total 6	O 6	0	0
60	1V	1	Total 1	O 1	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
60	1V	9	Total 9	O 9	0	0
60	1W	8	Total 8	O 8	0	0
60	1X	2	Total 2	O 2	0	0
60	1X	4	Total 4	O 4	0	0
60	1X	2	Total 2	O 2	0	0
60	1Y	4	Total 4	O 4	0	0
60	1Z	1	Total 1	O 1	0	0
60	10	3	Total 3	O 3	0	0
60	10	2	Total 2	O 2	0	0
60	10	4	Total 4	O 4	0	0
60	11	1	Total 1	O 1	0	0
60	11	9	Total 9	O 9	0	0
60	12	3	Total 3	O 3	0	0
60	13	1	Total 1	O 1	0	0
60	13	1	Total 1	O 1	0	0
60	14	2	Total 2	O 2	0	0
60	15	3	Total 3	O 3	0	0
60	16	1	Total 1	O 1	0	0
60	16	2	Total 2	O 2	0	0
60	17	2	Total 2	O 2	0	0
60	17	7	Total 7	O 7	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
60	18	2	Total 2	O 2	0	0
60	18	3	Total 3	O 3	0	0
60	19	2	Total 2	O 2	0	0
60	1a	2	Total 2	O 2	0	0
60	1a	3	Total 3	O 3	0	0
60	1a	4	Total 4	O 4	0	0
60	1a	1	Total 1	O 1	0	0
60	1a	2	Total 2	O 2	0	0
60	1a	2	Total 2	O 2	0	0
60	1a	1	Total 1	O 1	0	0
60	1a	5	Total 5	O 5	0	0
60	1a	4	Total 4	O 4	0	0
60	1a	4	Total 4	O 4	0	0
60	1a	5	Total 5	O 5	0	0
60	1a	2	Total 2	O 2	0	0
60	1a	4	Total 4	O 4	0	0
60	1a	1	Total 1	O 1	0	0
60	1a	2	Total 2	O 2	0	0
60	1a	1	Total 1	O 1	0	0
60	1a	1	Total 1	O 1	0	0
60	1a	2	Total 2	O 2	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
60	1a	2	Total 2	O 2	0	0
60	1a	5	Total 5	O 5	0	0
60	1a	6	Total 6	O 6	0	0
60	1a	1	Total 1	O 1	0	0
60	1a	3	Total 3	O 3	0	0
60	1a	3	Total 3	O 3	0	0
60	1a	5	Total 5	O 5	0	0
60	1a	5	Total 5	O 5	0	0
60	1a	4	Total 4	O 4	0	0
60	1a	1	Total 1	O 1	0	0
60	1a	1	Total 1	O 1	0	0
60	1a	5	Total 5	O 5	0	0
60	1a	2	Total 2	O 2	0	0
60	1a	4	Total 4	O 4	0	0
60	1a	1	Total 1	O 1	0	0
60	1a	6	Total 6	O 6	0	0
60	1a	5	Total 5	O 5	0	0
60	1a	4	Total 4	O 4	0	0
60	1a	4	Total 4	O 4	0	0
60	1a	3	Total 3	O 3	0	0
60	1a	1	Total 1	O 1	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
60	1a	1	Total 1	O 1	0	0
60	1a	1	Total 1	O 1	0	0
60	1a	6	Total 6	O 6	0	0
60	1a	3	Total 3	O 3	0	0
60	1a	3	Total 3	O 3	0	0
60	1a	1	Total 1	O 1	0	0
60	1a	3	Total 3	O 3	0	0
60	1a	4	Total 4	O 4	0	0
60	1a	2	Total 2	O 2	0	0
60	1a	4	Total 4	O 4	0	0
60	1a	5	Total 5	O 5	0	0
60	1a	5	Total 5	O 5	0	0
60	1a	6	Total 6	O 6	0	0
60	1a	4	Total 4	O 4	0	0
60	1a	5	Total 5	O 5	0	0
60	1a	4	Total 4	O 4	0	0
60	1a	3	Total 3	O 3	0	0
60	1a	3	Total 3	O 3	0	0
60	1a	6	Total 6	O 6	0	0
60	1a	3	Total 3	O 3	0	0
60	1a	3	Total 3	O 3	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
60	1a	4	Total 4	O 4	0	0
60	1a	6	Total 6	O 6	0	0
60	1a	6	Total 6	O 6	0	0
60	1a	6	Total 6	O 6	0	0
60	1a	6	Total 6	O 6	0	0
60	1a	5	Total 5	O 5	0	0
60	1a	4	Total 4	O 4	0	0
60	1a	5	Total 5	O 5	0	0
60	1a	6	Total 6	O 6	0	0
60	1a	6	Total 6	O 6	0	0
60	1a	6	Total 6	O 6	0	0
60	1a	6	Total 6	O 6	0	0
60	1a	6	Total 6	O 6	0	0
60	1a	2	Total 2	O 2	0	0
60	1a	4	Total 4	O 4	0	0
60	1a	5	Total 5	O 5	0	0
60	1a	6	Total 6	O 6	0	0
60	1a	6	Total 6	O 6	0	0
60	1a	3	Total 3	O 3	0	0
60	1a	6	Total 6	O 6	0	0
60	1a	5	Total 5	O 5	0	0
60	1a	6	Total 6	O 6	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
60	1a	1	Total 1	O 1	0	0
60	1a	1	Total 1	O 1	0	0
60	1a	2	Total 2	O 2	0	0
60	1a	1	Total 1	O 1	0	0
60	1a	2	Total 2	O 2	0	0
60	1a	2	Total 2	O 2	0	0
60	1a	71	Total 71	O 71	0	0
60	1b	1	Total 1	O 1	0	0
60	1g	1	Total 1	O 1	0	0
60	1k	1	Total 1	O 1	0	0
60	1l	2	Total 2	O 2	0	0
60	1q	4	Total 4	O 4	0	0
60	1v	1	Total 1	O 1	0	0
60	1w	2	Total 2	O 2	0	0
60	1x	1	Total 1	O 1	0	0
60	1x	1	Total 1	O 1	0	0
60	1x	1	Total 1	O 1	0	0
60	1x	2	Total 2	O 2	0	0
60	1x	2	Total 2	O 2	0	0
60	1x	1	Total 1	O 1	0	0
60	1x	1	Total 1	O 1	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
60	1x	1	Total 1	O 1	0	0
60	1x	5	Total 5	O 5	0	0
60	1y	2	Total 2	O 2	0	0
60	2A	6	Total 6	O 6	0	0
60	2A	5	Total 5	O 5	0	0
60	2A	6	Total 6	O 6	0	0
60	2A	1	Total 1	O 1	0	0
60	2A	5	Total 5	O 5	0	0
60	2A	4	Total 4	O 4	0	0
60	2A	3	Total 3	O 3	0	0
60	2A	1	Total 1	O 1	0	0
60	2A	3	Total 3	O 3	0	0
60	2A	1	Total 1	O 1	0	0
60	2A	1	Total 1	O 1	0	0
60	2A	5	Total 5	O 5	0	0
60	2A	3	Total 3	O 3	0	0
60	2A	1	Total 1	O 1	0	0
60	2A	6	Total 6	O 6	0	0
60	2A	1	Total 1	O 1	0	0
60	2A	5	Total 5	O 5	0	0
60	2A	3	Total 3	O 3	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
60	2A	1	Total 1	O 1	0	0
60	2A	1	Total 1	O 1	0	0
60	2A	2	Total 2	O 2	0	0
60	2A	5	Total 5	O 5	0	0
60	2A	1	Total 1	O 1	0	0
60	2A	1	Total 1	O 1	0	0
60	2A	4	Total 4	O 4	0	0
60	2A	5	Total 5	O 5	0	0
60	2A	2	Total 2	O 2	0	0
60	2A	5	Total 5	O 5	0	0
60	2A	5	Total 5	O 5	0	0
60	2A	5	Total 5	O 5	0	0
60	2A	2	Total 2	O 2	0	0
60	2A	1	Total 1	O 1	0	0
60	2A	1	Total 1	O 1	0	0
60	2A	1	Total 1	O 1	0	0
60	2A	2	Total 2	O 2	0	0
60	2A	2	Total 2	O 2	0	0
60	2A	2	Total 2	O 2	0	0
60	2A	2	Total 2	O 2	0	0
60	2A	1	Total 1	O 1	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
60	2A	1	Total 1	O 1	0	0
60	2A	1	Total 1	O 1	0	0
60	2A	3	Total 3	O 3	0	0
60	2A	5	Total 5	O 5	0	0
60	2A	4	Total 4	O 4	0	0
60	2A	5	Total 5	O 5	0	0
60	2A	5	Total 5	O 5	0	0
60	2A	3	Total 3	O 3	0	0
60	2A	1	Total 1	O 1	0	0
60	2A	4	Total 4	O 4	0	0
60	2A	5	Total 5	O 5	0	0
60	2A	5	Total 5	O 5	0	0
60	2A	3	Total 3	O 3	0	0
60	2A	4	Total 4	O 4	0	0
60	2A	4	Total 4	O 4	0	0
60	2A	3	Total 3	O 3	0	0
60	2A	1	Total 1	O 1	0	0
60	2A	4	Total 4	O 4	0	0
60	2A	4	Total 4	O 4	0	0
60	2A	3	Total 3	O 3	0	0
60	2A	5	Total 5	O 5	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
60	2A	5	Total 5	O 5	0	0
60	2A	3	Total 3	O 3	0	0
60	2A	2	Total 2	O 2	0	0
60	2A	3	Total 3	O 3	0	0
60	2A	4	Total 4	O 4	0	0
60	2A	5	Total 5	O 5	0	0
60	2A	4	Total 4	O 4	0	0
60	2A	4	Total 4	O 4	0	0
60	2A	5	Total 5	O 5	0	0
60	2A	2	Total 2	O 2	0	0
60	2A	1	Total 1	O 1	0	0
60	2A	4	Total 4	O 4	0	0
60	2A	2	Total 2	O 2	0	0
60	2A	4	Total 4	O 4	0	0
60	2A	3	Total 3	O 3	0	0
60	2A	5	Total 5	O 5	0	0
60	2A	3	Total 3	O 3	0	0
60	2A	2	Total 2	O 2	0	0
60	2A	1	Total 1	O 1	0	0
60	2A	1	Total 1	O 1	0	0
60	2A	1	Total 1	O 1	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
60	2A	1	Total 1	O 1	0	0
60	2A	2	Total 2	O 2	0	0
60	2A	1	Total 1	O 1	0	0
60	2A	1	Total 1	O 1	0	0
60	2A	2	Total 2	O 2	0	0
60	2A	2	Total 2	O 2	0	0
60	2A	6	Total 6	O 6	0	0
60	2A	1	Total 1	O 1	0	0
60	2A	5	Total 5	O 5	0	0
60	2A	1	Total 1	O 1	0	0
60	2A	4	Total 4	O 4	0	0
60	2A	2	Total 2	O 2	0	0
60	2A	6	Total 6	O 6	0	0
60	2A	6	Total 6	O 6	0	0
60	2A	2	Total 2	O 2	0	0
60	2A	1	Total 1	O 1	0	0
60	2A	1	Total 1	O 1	0	0
60	2A	1	Total 1	O 1	0	0
60	2A	2	Total 2	O 2	0	0
60	2A	2	Total 2	O 2	0	0
60	2A	4	Total 4	O 4	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
60	2A	2	Total	O	0	0
			2	2		
60	2A	2	Total	O	0	0
			2	2		
60	2A	1	Total	O	0	0
			1	1		
60	2A	2	Total	O	0	0
			2	2		
60	2A	1	Total	O	0	0
			1	1		
60	2A	1	Total	O	0	0
			1	1		
60	2A	6	Total	O	0	0
			6	6		
60	2A	5	Total	O	0	0
			5	5		
60	2A	4	Total	O	0	0
			4	4		
60	2A	3	Total	O	0	0
			3	3		
60	2A	2	Total	O	0	0
			2	2		
60	2A	4	Total	O	0	0
			4	4		
60	2A	4	Total	O	0	0
			4	4		
60	2A	4	Total	O	0	0
			4	4		
60	2A	4	Total	O	0	0
			4	4		
60	2A	3	Total	O	0	0
			3	3		
60	2A	5	Total	O	0	0
			5	5		
60	2A	2	Total	O	0	0
			2	2		
60	2A	1	Total	O	0	0
			1	1		
60	2A	3	Total	O	0	0
			3	3		
60	2A	1	Total	O	0	0
			1	1		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
60	2A	5	Total 5	O 5	0	0
60	2A	5	Total 5	O 5	0	0
60	2A	1	Total 1	O 1	0	0
60	2A	1	Total 1	O 1	0	0
60	2A	3	Total 3	O 3	0	0
60	2A	1	Total 1	O 1	0	0
60	2A	1	Total 1	O 1	0	0
60	2A	3	Total 3	O 3	0	0
60	2A	4	Total 4	O 4	0	0
60	2A	3	Total 3	O 3	0	0
60	2A	2	Total 2	O 2	0	0
60	2A	5	Total 5	O 5	0	0
60	2A	1	Total 1	O 1	0	0
60	2A	1	Total 1	O 1	0	0
60	2A	5	Total 5	O 5	0	0
60	2A	4	Total 4	O 4	0	0
60	2A	4	Total 4	O 4	0	0
60	2A	1	Total 1	O 1	0	0
60	2A	2	Total 2	O 2	0	0
60	2A	2	Total 2	O 2	0	0
60	2A	4	Total 4	O 4	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
60	2A	1	Total 1	O 1	0	0
60	2A	2	Total 2	O 2	0	0
60	2A	1	Total 1	O 1	0	0
60	2A	1	Total 1	O 1	0	0
60	2A	5	Total 5	O 5	0	0
60	2A	2	Total 2	O 2	0	0
60	2A	1	Total 1	O 1	0	0
60	2A	1	Total 1	O 1	0	0
60	2A	2	Total 2	O 2	0	0
60	2A	1	Total 1	O 1	0	0
60	2A	3	Total 3	O 3	0	0
60	2A	3	Total 3	O 3	0	0
60	2A	2	Total 2	O 2	0	0
60	2A	1	Total 1	O 1	0	0
60	2A	2	Total 2	O 2	0	0
60	2A	1	Total 1	O 1	0	0
60	2A	1	Total 1	O 1	0	0
60	2A	2	Total 2	O 2	0	0
60	2A	3	Total 3	O 3	0	0
60	2A	1	Total 1	O 1	0	0
60	2A	1	Total 1	O 1	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
60	2A	2	Total 2	O 2	0	0
60	2A	2	Total 2	O 2	0	0
60	2A	1	Total 1	O 1	0	0
60	2A	1	Total 1	O 1	0	0
60	2A	3	Total 3	O 3	0	0
60	2A	1	Total 1	O 1	0	0
60	2A	2	Total 2	O 2	0	0
60	2A	2	Total 2	O 2	0	0
60	2A	1	Total 1	O 1	0	0
60	2A	1	Total 1	O 1	0	0
60	2A	1	Total 1	O 1	0	0
60	2A	2	Total 2	O 2	0	0
60	2A	4	Total 4	O 4	0	0
60	2A	3	Total 3	O 3	0	0
60	2A	2	Total 2	O 2	0	0
60	2A	2	Total 2	O 2	0	0
60	2A	2	Total 2	O 2	0	0
60	2A	1	Total 1	O 1	0	0
60	2A	5	Total 5	O 5	0	0
60	2A	1	Total 1	O 1	0	0
60	2A	4	Total 4	O 4	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
60	2A	2	Total	O	0	0
			2	2		
60	2A	2	Total	O	0	0
			2	2		
60	2A	1	Total	O	0	0
			1	1		
60	2A	2	Total	O	0	0
			2	2		
60	2A	1	Total	O	0	0
			1	1		
60	2A	2	Total	O	0	0
			2	2		
60	2A	2	Total	O	0	0
			2	2		
60	2A	1	Total	O	0	0
			1	1		
60	2A	4	Total	O	0	0
			4	4		
60	2A	4	Total	O	0	0
			4	4		
60	2A	2	Total	O	0	0
			2	2		
60	2A	2	Total	O	0	0
			2	2		
60	2A	3	Total	O	0	0
			3	3		
60	2A	3	Total	O	0	0
			3	3		
60	2A	1	Total	O	0	0
			1	1		
60	2A	2	Total	O	0	0
			2	2		
60	2A	2	Total	O	0	0
			2	2		
60	2A	6	Total	O	0	0
			6	6		
60	2A	3	Total	O	0	0
			3	3		
60	2A	4	Total	O	0	0
			4	4		
60	2A	2	Total	O	0	0
			2	2		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
60	2A	1	Total 1	O 1	0	0
60	2A	4	Total 4	O 4	0	0
60	2A	3	Total 3	O 3	0	0
60	2A	3	Total 3	O 3	0	0
60	2A	6	Total 6	O 6	0	0
60	2A	4	Total 4	O 4	0	0
60	2A	2	Total 2	O 2	0	0
60	2A	2	Total 2	O 2	0	0
60	2A	1	Total 1	O 1	0	0
60	2A	2	Total 2	O 2	0	0
60	2A	2	Total 2	O 2	0	0
60	2A	6	Total 6	O 6	0	0
60	2A	4	Total 4	O 4	0	0
60	2A	1	Total 1	O 1	0	0
60	2A	5	Total 5	O 5	0	0
60	2A	4	Total 4	O 4	0	0
60	2A	1	Total 1	O 1	0	0
60	2A	1	Total 1	O 1	0	0
60	2A	2	Total 2	O 2	0	0
60	2A	2	Total 2	O 2	0	0
60	2A	6	Total 6	O 6	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
60	2A	2	Total 2	O 2	0	0
60	2A	1	Total 1	O 1	0	0
60	2A	3	Total 3	O 3	0	0
60	2A	1	Total 1	O 1	0	0
60	2A	2	Total 2	O 2	0	0
60	2A	2	Total 2	O 2	0	0
60	2A	2	Total 2	O 2	0	0
60	2A	3	Total 3	O 3	0	0
60	2A	4	Total 4	O 4	0	0
60	2A	1	Total 1	O 1	0	0
60	2A	2	Total 2	O 2	0	0
60	2A	1	Total 1	O 1	0	0
60	2A	1	Total 1	O 1	0	0
60	2A	6	Total 6	O 6	0	0
60	2A	1	Total 1	O 1	0	0
60	2A	3	Total 3	O 3	0	0
60	2A	1	Total 1	O 1	0	0
60	2A	1	Total 1	O 1	0	0
60	2A	2	Total 2	O 2	0	0
60	2A	2	Total 2	O 2	0	0
60	2A	1	Total 1	O 1	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
60	2A	2	Total 2	O 2	0	0
60	2A	2	Total 2	O 2	0	0
60	2A	3	Total 3	O 3	0	0
60	2A	3	Total 3	O 3	0	0
60	2A	1	Total 1	O 1	0	0
60	2A	4	Total 4	O 4	0	0
60	2A	1	Total 1	O 1	0	0
60	2A	1	Total 1	O 1	0	0
60	2A	1	Total 1	O 1	0	0
60	2A	1	Total 1	O 1	0	0
60	2A	1	Total 1	O 1	0	0
60	2A	1	Total 1	O 1	0	0
60	2A	2	Total 2	O 2	0	0
60	2A	4	Total 4	O 4	0	0
60	2A	1	Total 1	O 1	0	0
60	2A	1	Total 1	O 1	0	0
60	2A	3	Total 3	O 3	0	0
60	2A	1	Total 1	O 1	0	0
60	2A	1	Total 1	O 1	0	0
60	2A	2	Total 2	O 2	0	0
60	2A	2	Total 2	O 2	0	0
60	2A	5	Total 5	O 5	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
60	2A	4	Total 4	O 4	0	0
60	2A	1	Total 1	O 1	0	0
60	2A	1	Total 1	O 1	0	0
60	2A	1	Total 1	O 1	0	0
60	2A	3	Total 3	O 3	0	0
60	2A	2	Total 2	O 2	0	0
60	2A	1	Total 1	O 1	0	0
60	2A	5	Total 5	O 5	0	0
60	2A	1	Total 1	O 1	0	0
60	2A	2	Total 2	O 2	0	0
60	2A	6	Total 6	O 6	0	0
60	2A	5	Total 5	O 5	0	0
60	2A	6	Total 6	O 6	0	0
60	2A	3	Total 3	O 3	0	0
60	2A	6	Total 6	O 6	0	0
60	2A	6	Total 6	O 6	0	0
60	2A	5	Total 5	O 5	0	0
60	2A	3	Total 3	O 3	0	0
60	2A	6	Total 6	O 6	0	0
60	2A	6	Total 6	O 6	0	0
60	2A	3	Total 3	O 3	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
60	2A	4	Total 4	O 4	0	0
60	2A	3	Total 3	O 3	0	0
60	2A	1	Total 1	O 1	0	0
60	2A	6	Total 6	O 6	0	0
60	2A	6	Total 6	O 6	0	0
60	2A	6	Total 6	O 6	0	0
60	2A	5	Total 5	O 5	0	0
60	2A	4	Total 4	O 4	0	0
60	2A	5	Total 5	O 5	0	0
60	2A	6	Total 6	O 6	0	0
60	2A	4	Total 4	O 4	0	0
60	2A	6	Total 6	O 6	0	0
60	2A	5	Total 5	O 5	0	0
60	2A	3	Total 3	O 3	0	0
60	2A	3	Total 3	O 3	0	0
60	2A	5	Total 5	O 5	0	0
60	2A	5	Total 5	O 5	0	0
60	2A	4	Total 4	O 4	0	0
60	2A	5	Total 5	O 5	0	0
60	2A	2	Total 2	O 2	0	0
60	2A	3	Total 3	O 3	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
60	2A	4	Total 4	O 4	0	0
60	2A	5	Total 5	O 5	0	0
60	2A	6	Total 6	O 6	0	0
60	2A	4	Total 4	O 4	0	0
60	2A	4	Total 4	O 4	0	0
60	2A	3	Total 3	O 3	0	0
60	2A	3	Total 3	O 3	0	0
60	2A	5	Total 5	O 5	0	0
60	2A	6	Total 6	O 6	0	0
60	2A	6	Total 6	O 6	0	0
60	2A	6	Total 6	O 6	0	0
60	2A	4	Total 4	O 4	0	0
60	2A	6	Total 6	O 6	0	0
60	2A	4	Total 4	O 4	0	0
60	2A	6	Total 6	O 6	0	0
60	2A	5	Total 5	O 5	0	0
60	2A	4	Total 4	O 4	0	0
60	2A	4	Total 4	O 4	0	0
60	2A	4	Total 4	O 4	0	0
60	2A	6	Total 6	O 6	0	0
60	2A	5	Total 5	O 5	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
60	2A	5	Total	O	0	0
			5	5		
60	2A	5	Total	O	0	0
			5	5		
60	2A	4	Total	O	0	0
			4	4		
60	2A	5	Total	O	0	0
			5	5		
60	2A	5	Total	O	0	0
			5	5		
60	2A	4	Total	O	0	0
			4	4		
60	2A	6	Total	O	0	0
			6	6		
60	2A	4	Total	O	0	0
			4	4		
60	2A	4	Total	O	0	0
			4	4		
60	2A	6	Total	O	0	0
			6	6		
60	2A	5	Total	O	0	0
			5	5		
60	2A	5	Total	O	0	0
			5	5		
60	2A	6	Total	O	0	0
			6	6		
60	2A	6	Total	O	0	0
			6	6		
60	2A	6	Total	O	0	0
			6	6		
60	2A	4	Total	O	0	0
			4	4		
60	2A	6	Total	O	0	0
			6	6		
60	2A	5	Total	O	0	0
			5	5		
60	2A	4	Total	O	0	0
			4	4		
60	2A	3	Total	O	0	0
			3	3		
60	2A	5	Total	O	0	0
			5	5		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
60	2A	5	Total	O	0	0
			5	5		
60	2A	5	Total	O	0	0
			5	5		
60	2A	4	Total	O	0	0
			4	4		
60	2A	6	Total	O	0	0
			6	6		
60	2A	6	Total	O	0	0
			6	6		
60	2A	6	Total	O	0	0
			6	6		
60	2A	5	Total	O	0	0
			5	5		
60	2A	5	Total	O	0	0
			5	5		
60	2A	5	Total	O	0	0
			5	5		
60	2A	6	Total	O	0	0
			6	6		
60	2A	5	Total	O	0	0
			5	5		
60	2A	3	Total	O	0	0
			3	3		
60	2A	6	Total	O	0	0
			6	6		
60	2A	6	Total	O	0	0
			6	6		
60	2A	4	Total	O	0	0
			4	4		
60	2A	2	Total	O	0	0
			2	2		
60	2A	1	Total	O	0	0
			1	1		
60	2A	1	Total	O	0	0
			1	1		
60	2A	4	Total	O	0	0
			4	4		
60	2A	2	Total	O	0	0
			2	2		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
60	2A	3	Total 3	O 3	0	0
60	2A	2	Total 2	O 2	0	0
60	2A	1	Total 1	O 1	0	0
60	2A	1	Total 1	O 1	0	0
60	2A	2	Total 2	O 2	0	0
60	2A	1	Total 1	O 1	0	0
60	2A	1	Total 1	O 1	0	0
60	2A	1	Total 1	O 1	0	0
60	2A	2	Total 2	O 2	0	0
60	2A	1	Total 1	O 1	0	0
60	2A	2	Total 2	O 2	0	0
60	2A	2	Total 2	O 2	0	0
60	2A	2	Total 2	O 2	0	0
60	2A	1	Total 1	O 1	0	0
60	2A	6	Total 6	O 6	0	0
60	2A	214	Total 214	O 214	0	0
60	2B	2	Total 2	O 2	0	0
60	2B	3	Total 3	O 3	0	0
60	2B	3	Total 3	O 3	0	0
60	2B	1	Total 1	O 1	0	0
60	2B	2	Total 2	O 2	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
60	2B	2	Total 2	O 2	0	0
60	2B	1	Total 1	O 1	0	0
60	2B	12	Total 12	O 12	0	0
60	2D	1	Total 1	O 1	0	0
60	2D	5	Total 5	O 5	0	0
60	2D	8	Total 8	O 8	0	0
60	2E	4	Total 4	O 4	0	0
60	2E	2	Total 2	O 2	0	0
60	2E	3	Total 3	O 3	0	0
60	2F	8	Total 8	O 8	0	0
60	2I	4	Total 4	O 4	0	0
60	2N	1	Total 1	O 1	0	0
60	2O	1	Total 1	O 1	0	0
60	2P	2	Total 2	O 2	0	0
60	2P	3	Total 3	O 3	0	0
60	2Q	1	Total 1	O 1	0	0
60	2Q	1	Total 1	O 1	0	0
60	2R	1	Total 1	O 1	0	0
60	2R	1	Total 1	O 1	0	0
60	2T	4	Total 4	O 4	0	0
60	2U	2	Total 2	O 2	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
60	2W	4	Total 4	O 4	0	0
60	2X	4	Total 4	O 4	0	0
60	2Z	1	Total 1	O 1	0	0
60	20	6	Total 6	O 6	0	0
60	20	2	Total 2	O 2	0	0
60	20	1	Total 1	O 1	0	0
60	21	8	Total 8	O 8	0	0
60	22	1	Total 1	O 1	0	0
60	22	1	Total 1	O 1	0	0
60	23	1	Total 1	O 1	0	0
60	25	4	Total 4	O 4	0	0
60	27	1	Total 1	O 1	0	0
60	27	2	Total 2	O 2	0	0
60	28	4	Total 4	O 4	0	0
60	29	1	Total 1	O 1	0	0
60	2a	6	Total 6	O 6	0	0
60	2a	4	Total 4	O 4	0	0
60	2a	5	Total 5	O 5	0	0
60	2a	3	Total 3	O 3	0	0
60	2a	2	Total 2	O 2	0	0
60	2a	6	Total 6	O 6	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
60	2a	6	Total 6	O 6	0	0
60	2a	3	Total 3	O 3	0	0
60	2a	5	Total 5	O 5	0	0
60	2a	3	Total 3	O 3	0	0
60	2a	3	Total 3	O 3	0	0
60	2a	5	Total 5	O 5	0	0
60	2a	6	Total 6	O 6	0	0
60	2a	2	Total 2	O 2	0	0
60	2a	2	Total 2	O 2	0	0
60	2a	2	Total 2	O 2	0	0
60	2a	2	Total 2	O 2	0	0
60	2a	5	Total 5	O 5	0	0
60	2a	2	Total 2	O 2	0	0
60	2a	5	Total 5	O 5	0	0
60	2a	2	Total 2	O 2	0	0
60	2a	6	Total 6	O 6	0	0
60	2a	5	Total 5	O 5	0	0
60	2a	4	Total 4	O 4	0	0
60	2a	2	Total 2	O 2	0	0
60	2a	4	Total 4	O 4	0	0
60	2a	6	Total 6	O 6	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
60	2a	6	Total 6	O 6	0	0
60	2a	5	Total 5	O 5	0	0
60	2a	5	Total 5	O 5	0	0
60	2a	2	Total 2	O 2	0	0
60	2a	4	Total 4	O 4	0	0
60	2a	4	Total 4	O 4	0	0
60	2a	4	Total 4	O 4	0	0
60	2a	5	Total 5	O 5	0	0
60	2a	4	Total 4	O 4	0	0
60	2a	2	Total 2	O 2	0	0
60	2a	2	Total 2	O 2	0	0
60	2a	3	Total 3	O 3	0	0
60	2a	6	Total 6	O 6	0	0
60	2a	3	Total 3	O 3	0	0
60	2a	6	Total 6	O 6	0	0
60	2a	2	Total 2	O 2	0	0
60	2a	3	Total 3	O 3	0	0
60	2a	2	Total 2	O 2	0	0
60	2a	2	Total 2	O 2	0	0
60	2a	4	Total 4	O 4	0	0
60	2a	2	Total 2	O 2	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
60	2a	2	Total 2	O 2	0	0
60	2a	1	Total 1	O 1	0	0
60	2a	2	Total 2	O 2	0	0
60	2a	1	Total 1	O 1	0	0
60	2a	5	Total 5	O 5	0	0
60	2a	1	Total 1	O 1	0	0
60	2a	3	Total 3	O 3	0	0
60	2a	1	Total 1	O 1	0	0
60	2a	2	Total 2	O 2	0	0
60	2a	1	Total 1	O 1	0	0
60	2a	2	Total 2	O 2	0	0
60	2a	2	Total 2	O 2	0	0
60	2a	1	Total 1	O 1	0	0
60	2a	1	Total 1	O 1	0	0
60	2a	3	Total 3	O 3	0	0
60	2a	1	Total 1	O 1	0	0
60	2a	3	Total 3	O 3	0	0
60	2a	1	Total 1	O 1	0	0
60	2a	3	Total 3	O 3	0	0
60	2a	3	Total 3	O 3	0	0
60	2a	1	Total 1	O 1	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
60	2a	1	Total 1	O 1	0	0
60	2a	4	Total 4	O 4	0	0
60	2a	4	Total 4	O 4	0	0
60	2a	2	Total 2	O 2	0	0
60	2a	2	Total 2	O 2	0	0
60	2a	2	Total 2	O 2	0	0
60	2a	1	Total 1	O 1	0	0
60	2a	1	Total 1	O 1	0	0
60	2a	1	Total 1	O 1	0	0
60	2a	1	Total 1	O 1	0	0
60	2a	1	Total 1	O 1	0	0
60	2a	1	Total 1	O 1	0	0
60	2a	1	Total 1	O 1	0	0
60	2a	1	Total 1	O 1	0	0
60	2a	2	Total 2	O 2	0	0
60	2a	2	Total 2	O 2	0	0
60	2a	2	Total 2	O 2	0	0
60	2a	2	Total 2	O 2	0	0
60	2a	1	Total 1	O 1	0	0
60	2a	2	Total 2	O 2	0	0
60	2a	2	Total 2	O 2	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
60	2a	1	Total 1	O 1	0	0
60	2a	1	Total 1	O 1	0	0
60	2a	2	Total 2	O 2	0	0
60	2a	1	Total 1	O 1	0	0
60	2a	1	Total 1	O 1	0	0
60	2a	1	Total 1	O 1	0	0
60	2a	1	Total 1	O 1	0	0
60	2a	1	Total 1	O 1	0	0
60	2a	39	Total 39	O 39	0	0
60	2d	1	Total 1	O 1	0	0
60	2g	1	Total 1	O 1	0	0
60	2g	1	Total 1	O 1	0	0
60	2h	1	Total 1	O 1	0	0
60	2i	1	Total 1	O 1	0	0
60	2i	1	Total 1	O 1	0	0
60	2i	1	Total 1	O 1	0	0
60	2j	2	Total 2	O 2	0	0
60	2j	1	Total 1	O 1	0	0
60	2j	1	Total 1	O 1	0	0
60	2l	1	Total 1	O 1	0	0
60	2l	3	Total 3	O 3	0	0

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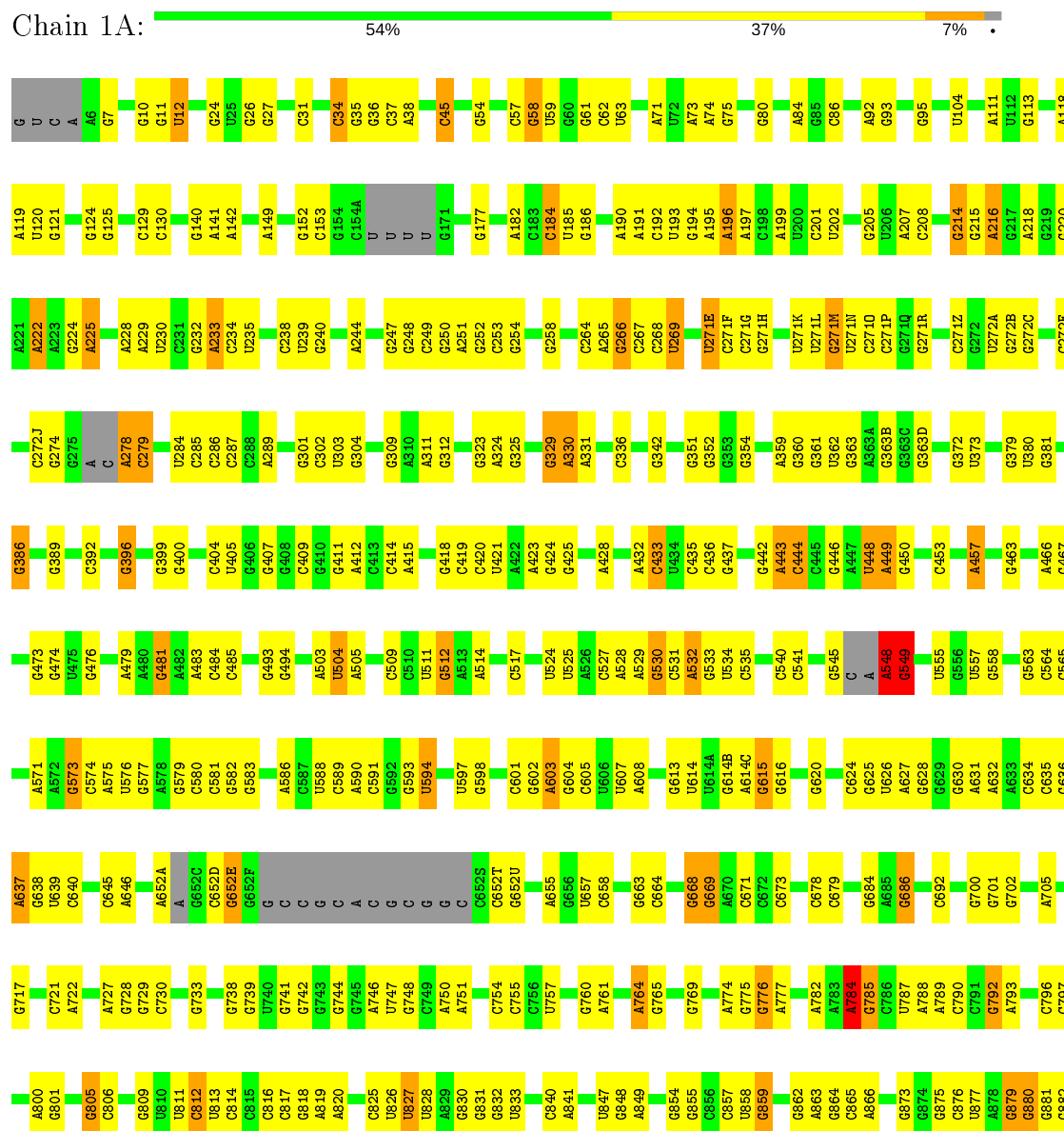
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
60	2p	1	Total 1	O 1	0	0
60	2r	1	Total 1	O 1	0	0
60	2t	2	Total 2	O 2	0	0
60	2v	1	Total 1	O 1	0	0
60	2x	2	Total 2	O 2	0	0
60	2x	2	Total 2	O 2	0	0
60	2x	4	Total 4	O 4	0	0
60	2y	1	Total 1	O 1	0	0
60	2y	10	Total 10	O 10	0	0

### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ( $RSRZ > 2$ ). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: 23S Ribosomal RNA



G2141	A2060	U1955	G1850	A1749	A1641	G1525	G1422	U1329	U1188	G1112	A1050	G974	C883
C2142	G2061	U1955	A1853	G1750	A1642	G1525	G1423	U1329	A1189	U1113	G1051	C974	C884
C2143	A2062	C1958	A1854	G1753	A1642	G1532	G1423	U1329	C1200	G1114	C1052	C975	C885
U2144	C2065	C1958	A1854	G1753	G1646	G1532	G1426	G1337	G1200	G1115	C1053	G975A	C886
C2145	C2066	U1963	G1858	A1754	G1647	U	A1427	G1338	C1201	G1116	A1054	A983	A887
C2146	G2067	G1964	A1859	A1755	G1648	A	G1428	G1339	C1202	G1117	G1055	A983	C888
G2147	U2068	G1860	G1860	G1756	G1649	C	G1429	U1342	G1206	G1118	C889	C889	C889
G2149	G2069	C1967	G1861	A1762	G1650	G1537	G1430	A1342	G1206	C1119	G1058	G987	A890
U2150	G2070	A1970	U1864	G1763	G1651	G1541	U1438	G1343	A1210	C1123	U1060	C992	C894
G2151	A2071	A1971	G1865	G1764	A1652	A1542	G1441	G1344	U1211	G1126	G1062	G993	U895
G2152	C2078	A1972	G1866	G1765	G1653	A1542	G1441	U1352	G1212	A1127	G1063	C994	A896
G2153	U2079	G1973	A1876	G1769	A1654	C1546	G1442	U1358	C1218	A1128	C1064	C995	C897
G2154	G2080	A1877	A1877	A1773	A1658	C1546	A1445	G1359	G1223	A1129	U1065	A996	
G2155	C2081	U1991	G1878	A1773	U1659	A1554	A1448	A1360	G1223	U1130	U1066	A1000	C902
G2156		G1992	A1878	U1778	A1665	G1555	G1448	G1361	G1223	G1135	A1067	A1001	C903
G2157	U2086	U1993	C1879	U1779	A1665	G1555	A1449	C1362	A1226	G1144	G1068	G1002	C904
G2158	G2087	C1994	G1883	A1780	A1667	A1558	G1450	G1363	G1230	G1136	A1069	G1003	U907
G2159		G1997	A1889	C1781	G1667	G1559	G1450	G1364	C1230	G1137	A1070	C1006	A909
G2160		G1998	A1890	A1782	A1668	A1566	U1453	A1365	G1231	G1138	G1071	C1007	A910
G2161	U2092	G1999	G1891	A1784	A1669	A1566	G1455	A1366	G1236	G1145	A1073	C1008	A911
C2095	G2095	C1999	C1892	A1784	G1674	A1567	G1459	G1371	G1236	C1145	G1074	A1009	
U2096	G2096	A2001	G1892	A1786	G1675	A1570	A1460	U1372	G1239	G1146	C1075	A1010	G916
G2099	U2099	G2002	U1687	A1788	A1676	A1571	G1461	G1373	U1240	C1147	G1076	G1011	A917
G2100	G2100	U1689	A1899	A1789	C1686	A1572	G1466	C1376	G1252	G1151	U1078	G1012	A918
G2101	U2011	A1900	A1900	G1790	C1684	A1572	C1467	U1379	A1253	G1152	C1080	G1013	G919
G2102	C2102	G1906		G1792	C1686	A1578	C1467	A1380	G1256	G1153	U1081	G1014	U922
C2103	A2013				C1687	U1578	A1471	G1379	G1256	G1154	U1082	G1015	U923
G2104	A2014				A1687	A1579	A1471	A1384	G1266	A1156	U1083	C1018	G927
A2171			A1913	U1796	U1688	A1580	G1478	A1384	A1267	U1159	A1085	A1021	U930
C2172			A1914	C1797	A1689	C1584	G1478	G1385	A1268	G1160	A1086	G931	G928
C2173	G2018	U1915	U1915	U1798	A1690	A1586	G1482	U1390	A1269	G1161	G1087	G1024	G932
A2176	U2109	A2020	G1799	G1799	C1691	A1587	A1486	U1391	C1270	G1164	U1088	G1025	A933
C2177	G2021	G2021	A1918	C1800	U1692	C1589	G1487	A1392	G1271	U1165	G1089	U1026	G934
C2178	U2022	G2023	A1919	G1801	U1693	C1589	A1490	U1392	A1272	C1166	U1090	A1027	C935
U2113	G2112	G2023	G1920	C1804	G1695	G1593	A1490	A1393	U1273	G1167	G1093	G1030	
A2117			G1921	C1804		G1594	C1493	U1394	U1273	U1167	U1094	G1031	G942
G2181	G2029	U1923	G1923	A1810	A1700	G1594	A1494	A1395	A1286	G1168	A1095	A1032	U943
G2182	A2030	C1924	C1924	G1811	G1703	G1595	A1494	U1396	U1292	G1169	U1096	U1033	G944
C2183	A2031	G1925	C1925	A1812		A1603	A1495	U1397	C1293	G1170	A1097	G1034	A945
G2184	G2124	A2033	U1926	A1815	C1710	A1603	U1496	U1397	U1293	G1171	U1097	G1034	G946
C2185	G2125	G2032	A1927	G1816	C1711	A1608	U1497	U1405	C1293	G1173	A1098	U1035	G947
A2126	C2126	G2037	A1928	G1817	C1712	A1609		U1406	G1297	A1175	G1099	G1036	G948
G2187	G2127	G1929	G1929	G1817		A1610	C1504	U1406	U1297	U1175	C1100	G1039	
U2189	C2128	U2041	G1930			C1611	C1505	C1407	U1300	G1176	U1101	G1039	A953
G2190	C2129	A2042	U1931	A1825	U1720	C1612	C1506	C1408	A1301	A1177	C1102	C1040	G956
	U2130	C2043	A1932	G1826	A1722	G1613	A1507	C1409	A1302	G1178	A1103	G1041	A957
G2193	G2131	G1933	G1933	C1827	G1722	A1614	A1508	G1410	A1302	C1179	C1104	G1042	U958
G2194	U2132	G1934	C1934	G1830	U1739	C1615	C1509	C1411	G1310	C1180	U1105	C1043	U958
	G2046	G1935	G1935	C1830	A1741	A1509A	A1509A	C1411			G1106	G1044	A959
A2134	A2134	G2053	A1936	C1834	G1742	G1622	A1509B	G1416			G1107	A1045	A960
C2136	A2136	G2055	A1937	C1844	G1746	G1628	U1514	C1417	U1313	G1183	G1107	A1046	C961
G2137	G2056	C1938	C1844	C1844	G1747	U1629	G1514	A1419	G1314	G1184	U1108	A1046	G967
C2138	C2138	A2057	U1939	A1847	G1748	G1629	U1514	A1419	C1315	G1185	G1109	G1047	C967
G2139	C2139	G2058	U1939	A1848	G1749	U1629	U1518	U1420	G1315	G1186	G1110	A1048	C967
C2140	C2140	A2059	U1942	C1848	G1749A	G1629	U1518	C1421	C1316	G1187	A1111	C1049	C968



Response	Percentage
Yes	47%
No	40%
Don't know	8%
Refuse to answer	5%

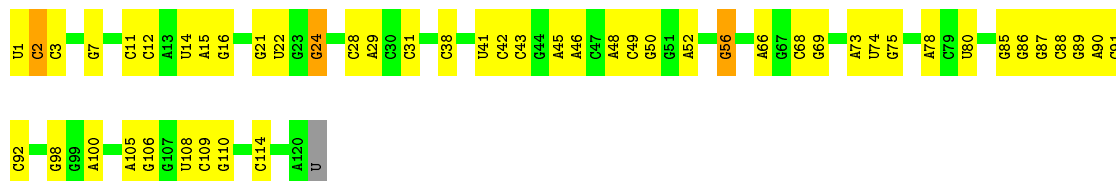


C1557	A1469	G1206	C1135	G1011	A941	A861	G785	A706	G652	C581	A503
A1558	G1470	A1210	G1156	U1012	G942	G862	A788	G707	A652A	G582	U504
A1566	A1471	G1211	G1137	C1013	G943	A863	A789	U709	A652B	A586	A505
G1567	G1400	G1212	G1138	U1014	A945	G864	G790	G708	G652C	G587	G506
A1569	G1401	A1213	C1139	G1015	A946	C865	C791	G710	C652D	U588	C509
U1570	U1405	A1214	U1141	G1016	G947	A866	G792	G711	G652E	C589	C510
A1571	U1406	C1215	U1142	C1017	G948	G869	A793	G715	G	G592	U511
U1578	C1407	G1218	A1142A	U1019	A953	G874	G796	A716	G	G	G512
A1579	C1408	G1223	A1143	G1022	G954	G875	C797	G717	C	C	A513
A1580	C1409	G1224	A1144	U1023	C955	G876	A800	C720	G	G	A514
G1581	G1410	G1225	G1149	G1024	G956	U877	G801	C721	A	A	C517
C1584	C1411	A1226	C1150	G1025	A957	A878	A802	A722	C	C	G521
A1586	G1416	G1325	G1151	U1026	U958	G879	G805	C723	G	G	U524
U1590	C1417	G1326	G1152	A1027	A959	G880	C806	U607	C	C	U525
G1591	U1420	C1327	C1153	G1028	G960	G881	G805	G602	G	G	A603
G1592	G1421	C1333	G1154	A1029	C961	G882	U807	A604	G	G	A604
G1593	G1422	U1334	A1155	G1030	G966	G883	G807	C605	C	C	A526
A1594	G1423	U1335	C1156	G1031	G967	C884	U811	U606	C	C	C527
G1595	G1424	G1336	U1157	A1032	C968	C885	C812	U607	A	A	A528
A1596	A1427	C1345	C1158	U1033	C969	C886	G818	U607	G852U	G	A529
C1599	G1428	U1342	G1159	G1034	C970	A887	C819	C732	C652V	A	G530
G1603	G1429	C1343	U1160	U1035	G971	C888	G817	G733	A653	C	C531
C1604	C1430	C1351	C1161	G1036	G972	C889	G818	A734	A654	A	A532
A1608	G1431	U1352	U1162	G1037	A973	A890	A819	U614A	G856	U	G533
A1609	U1434	G1355	G1163	C1038	C975	G892	A820	G741	G857	U	U534
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A1614	G1443	U1358	U1166	G1043	G979	C895	U827	U747	G660	C	G545
G1615	A1444	A1253	C1167	A	A980	C896	U828	U747	G661	A	C
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G1633	G1448	C1259	C1171	A	C984	C903	U834	C753	C665	U	U554
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G1635	G1450	U1263	U1173	A	C986	G987	G836	C755	G669	U	G556
C1636	C1451	U1264	C1174	A	A987	C988	U837	G760	G674	U	G561
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G1647	G1453	C1266	C1176	A	C989	A990	G839	G764	A676	G	G563
C1648	U1454	U1267	U1177	A	C990	A901	U840	G765	C679	U	U566
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A1652	G1456	A1272	C1179	A	C992	C915	U842	C767	C683	U	U568
G1653	G1457	U1273	C1180	A	C993	G916	U843	G771	G684	U	U569
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A1655	C1459	G1275	U1182	A	C995	A918	C845	G775	G686	U	A571
C1656	G1460	A1276	C1183	A	C996	G919	U846	G776	G687	U	G573
C1662	A1461	C1277	U1184	A	C997	U922	G847	A777	G688	U	C574
C1663	G1462	A1278	G1185	A	C998	C923	U848	G778	A675	C	G575
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	A1464	A1287	U1187	A	C1000	G928	C850	U779	C689	U	A577
	G1465	U1288	C1188	A	C1001	G929	U851	G780	G690	U	A578
	G1466	C1292	U1189	A	C1002	G930	G852	A781	G691	U	G577
	G1467	G1293	U1190	A	C1003	C931	U853	A782	G701	U	A579
	C1468	U1205	G1191	A	C1004	C932	G854	A783	A705	U	C580
			U1206	A	C1005	C933	G855				
				A	C1006	C934	G856				
				A	C1007	C935	G857				
				A	C1008	C936	G858				
				A	C1009	C937	G859				
				C	A1010	G938	U860				

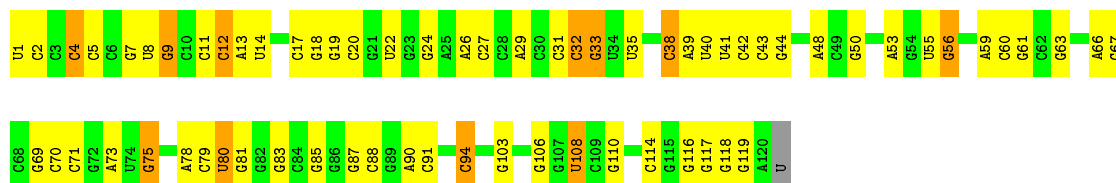




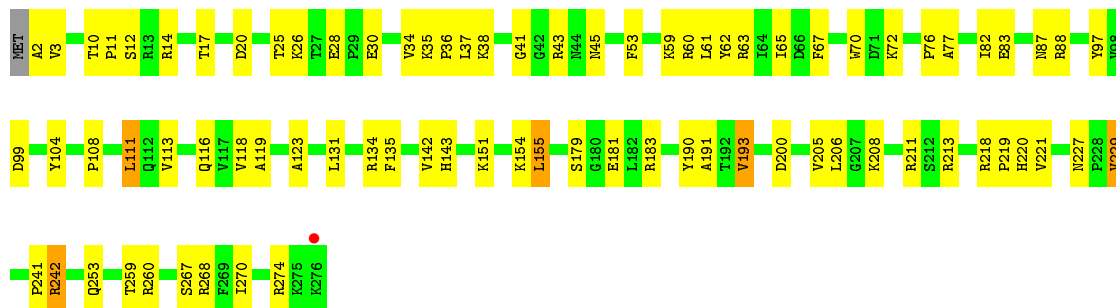
• Molecule 2: 5S Ribosomal RNA



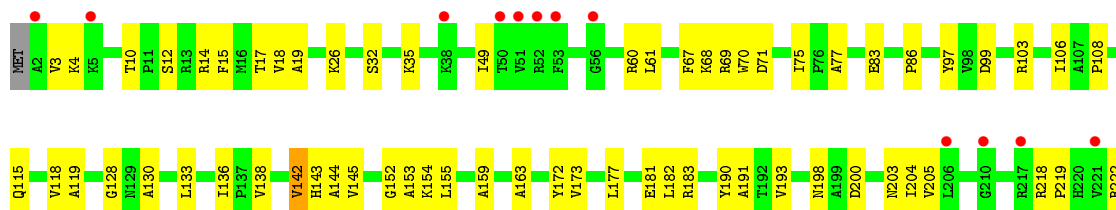
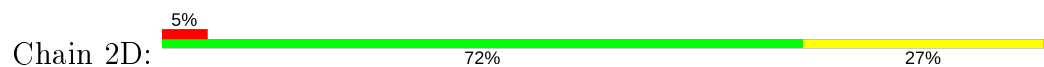
• Molecule 2: 5S Ribosomal RNA



• Molecule 3: 50S ribosomal protein L2



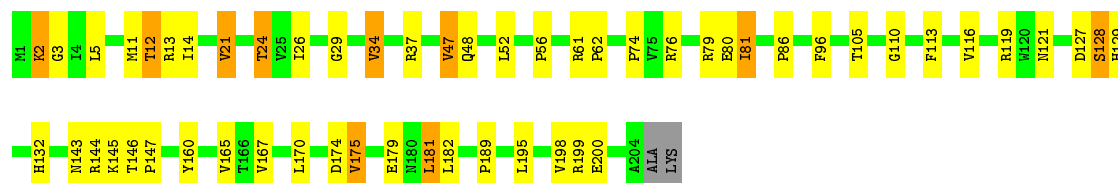
• Molecule 3: 50S ribosomal protein L2





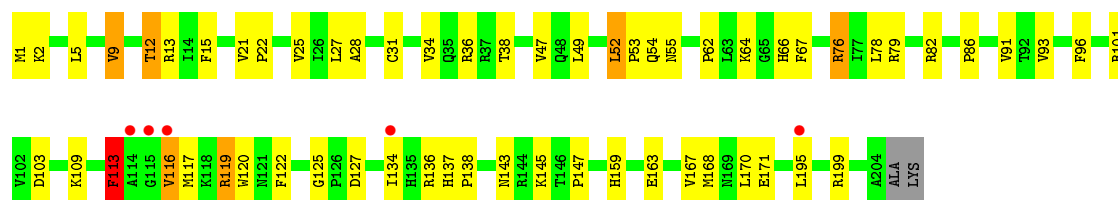
• Molecule 4: 50S ribosomal protein L3

Chain 1E: 72% 22% 5%



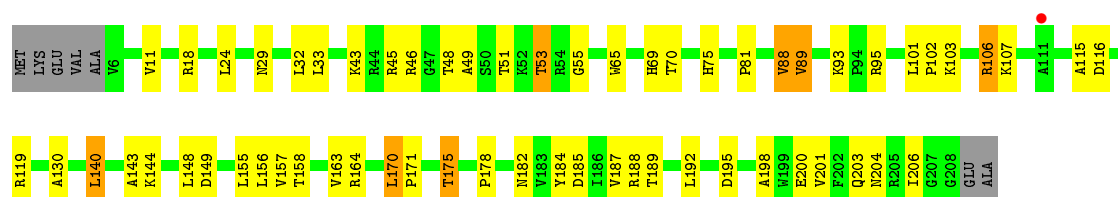
• Molecule 4: 50S ribosomal protein L3

Chain 2E: 2% 70% 26%



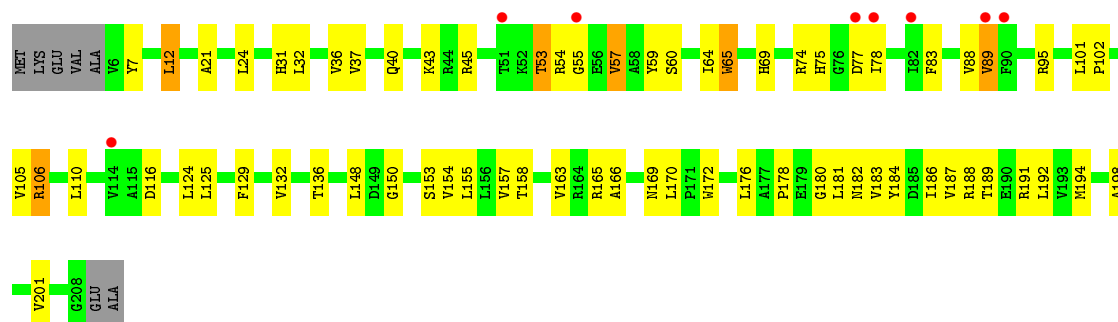
• Molecule 5: 50S ribosomal protein L4

Chain 1F: 68% 26%



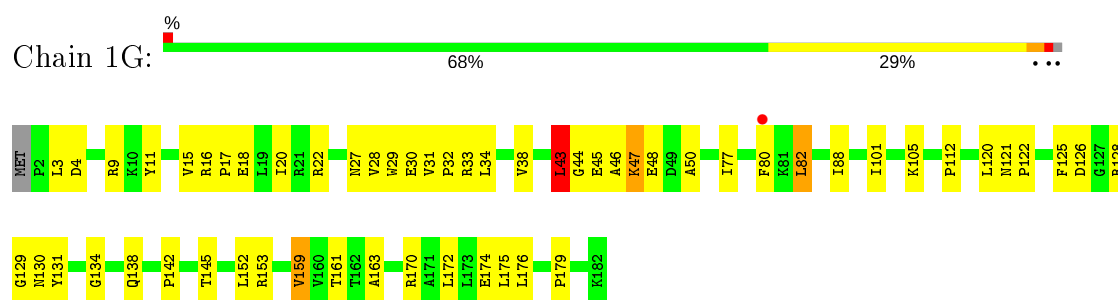
• Molecule 5: 50S ribosomal protein L4

Chain 2F: 4% 64% 30%

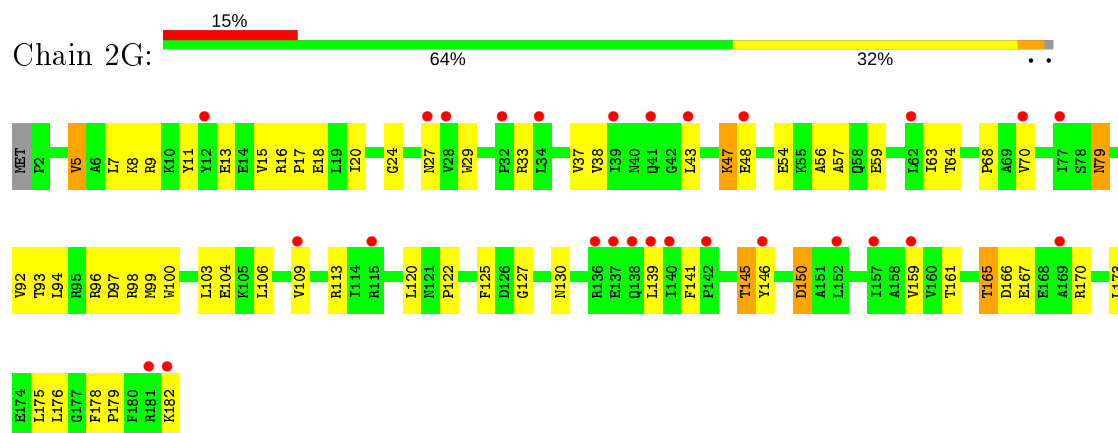


• Molecule 6: 50S ribosomal protein L5

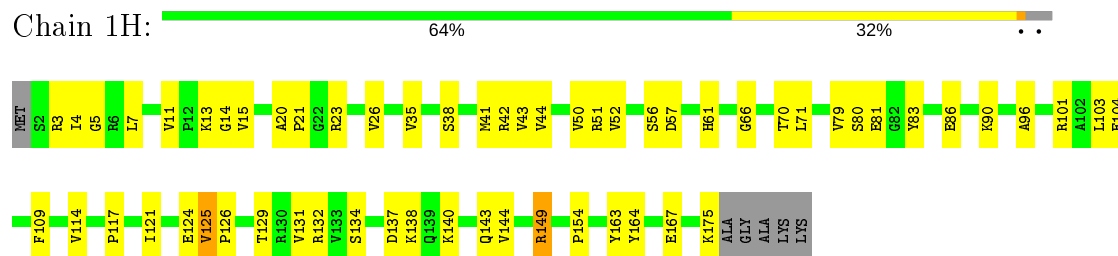




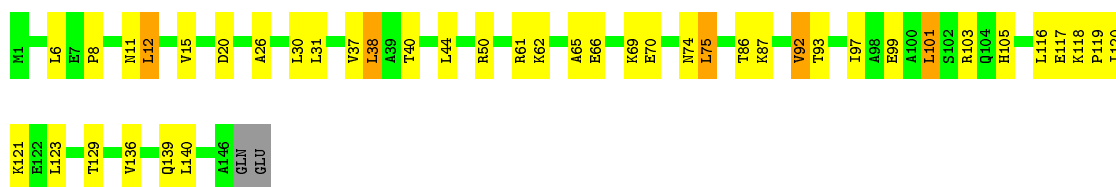
• Molecule 6: 50S ribosomal protein L5



• Molecule 7: 50S ribosomal protein L6

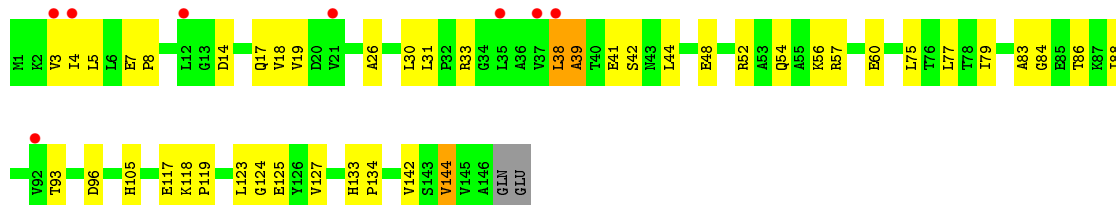


Chain 1I:  70% 25% ..




- Molecule 8: 50S ribosomal protein L9

Chain 2I:  5% 68% 28% ..



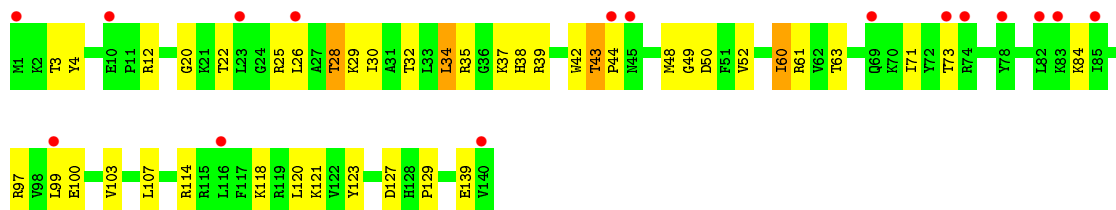
- Molecule 9: 50S ribosomal protein L13

Chain 1N:  82% 16% .



- Molecule 9: 50S ribosomal protein L13

Chain 2N:  11% 70% 27% .



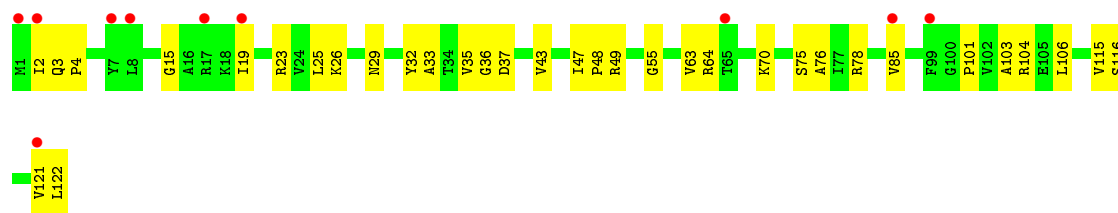
- Molecule 10: 50S ribosomal protein L14

Chain 1O:  76% 22% .

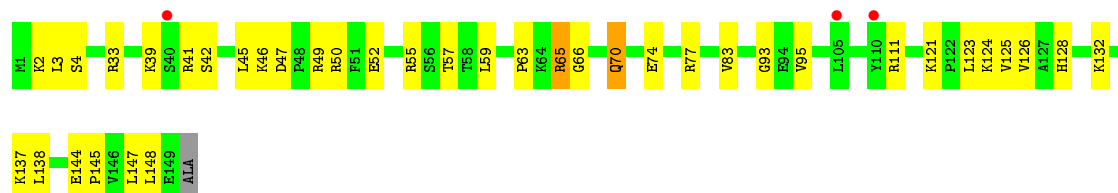
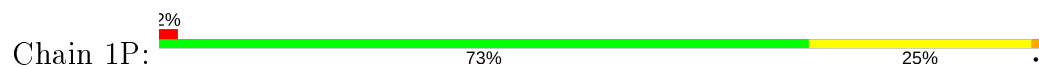


- Molecule 10: 50S ribosomal protein L14

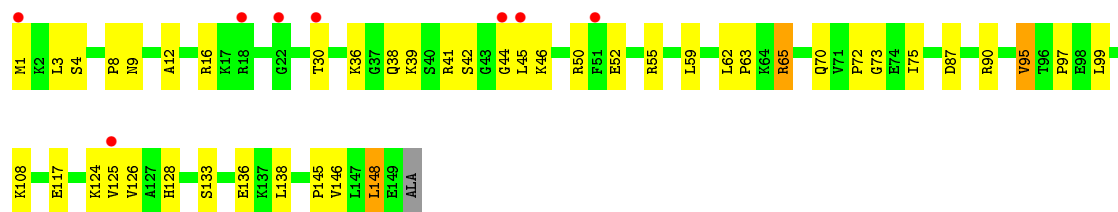
Chain 2O:  8% 72% 28%



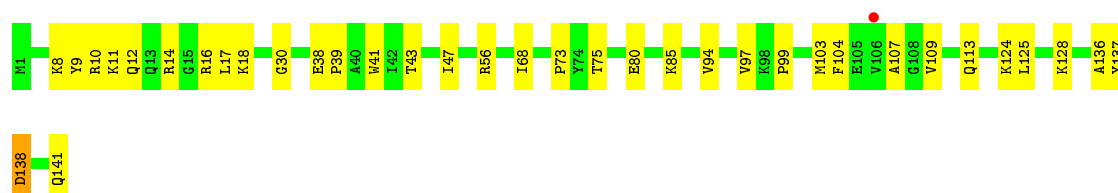
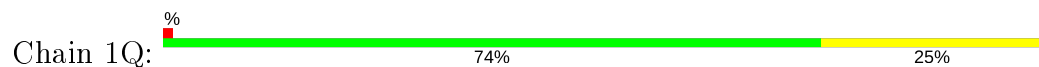
• Molecule 11: 50S ribosomal protein L15



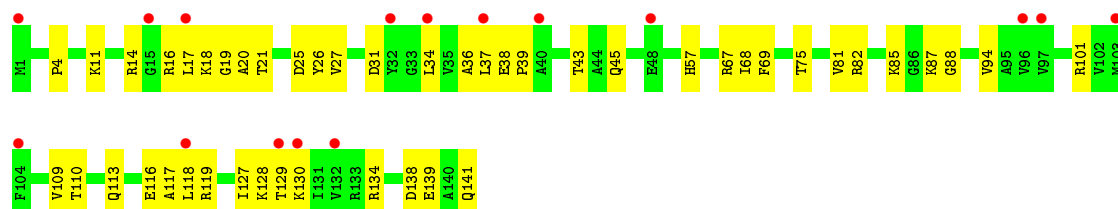
• Molecule 11: 50S ribosomal protein L15




• Molecule 12: 50S ribosomal protein L16

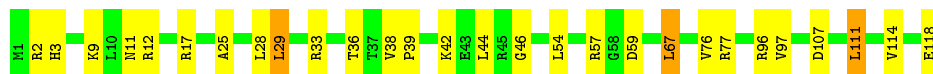


• Molecule 12: 50S ribosomal protein L16



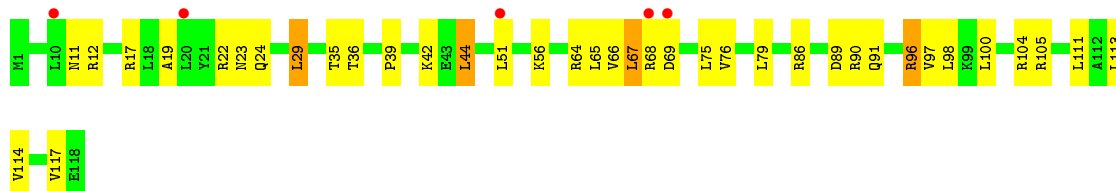
- Molecule 13: 50S ribosomal protein L17

Chain 1R:  76% 21% .



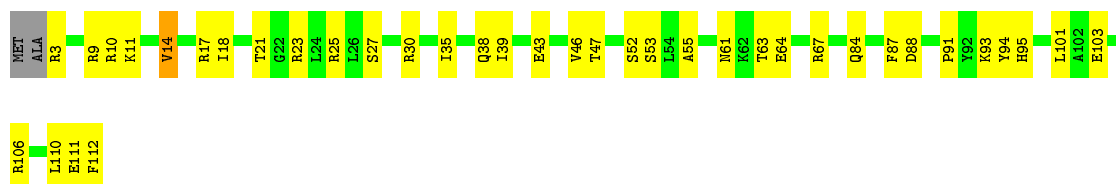
- Molecule 13: 50S ribosomal protein L17

Chain 2R:  4% 68% 29% .



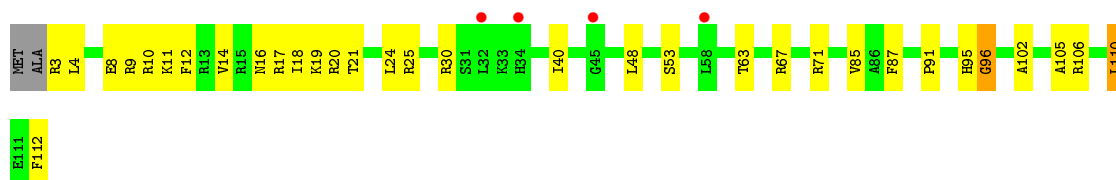
- Molecule 14: 50S ribosomal protein L18

Chain 1S:  64% 33% ..



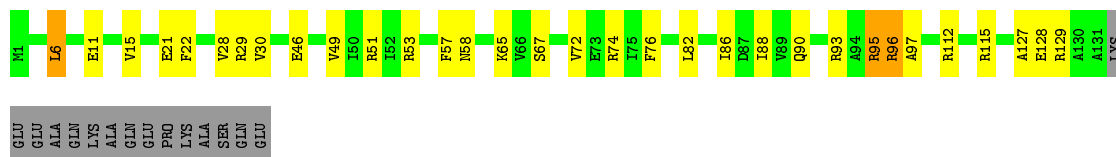
- Molecule 14: 50S ribosomal protein L18

Chain 2S:  4% 69% 28% ..



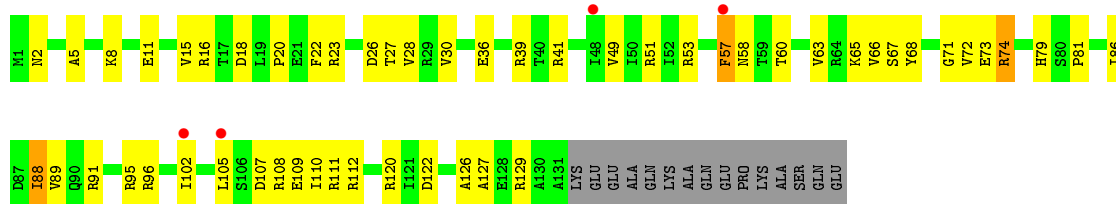
- Molecule 15: 50S ribosomal protein L19

Chain 1T:  68% 20% 10% .

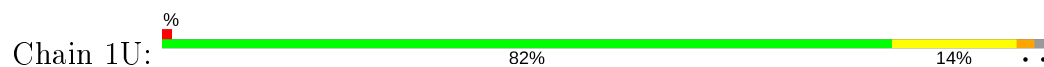


- Molecule 15: 50S ribosomal protein L19

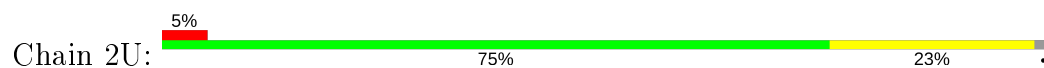
Chain 2T:  3% 53% 34% 10% .



- Molecule 16: 50S ribosomal protein L20



- Molecule 16: 50S ribosomal protein L20



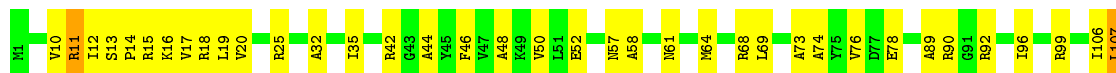
- Molecule 17: 50S ribosomal protein L21



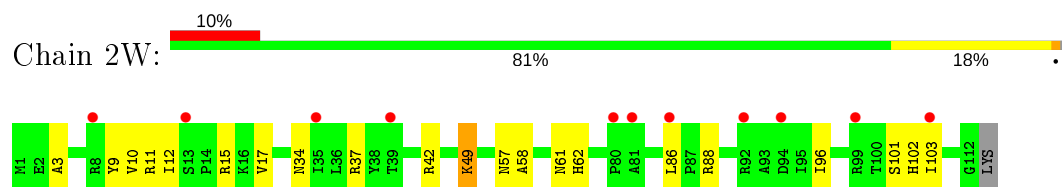
- Molecule 17: 50S ribosomal protein L21



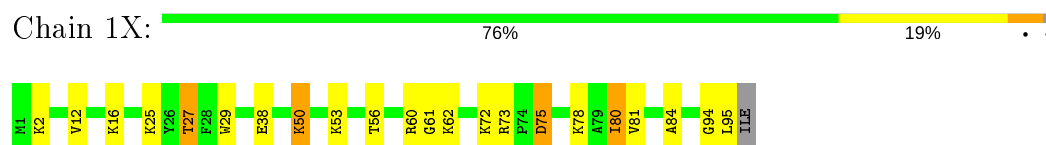
- Molecule 18: 50S ribosomal protein L22



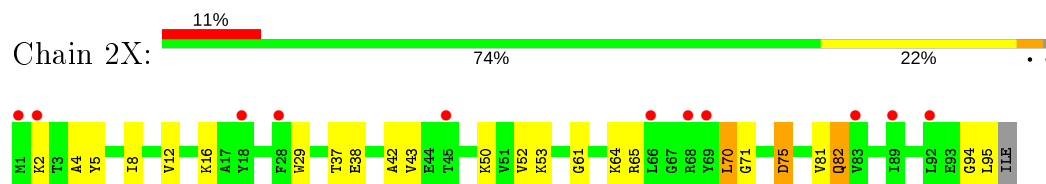
- Molecule 18: 50S ribosomal protein L22



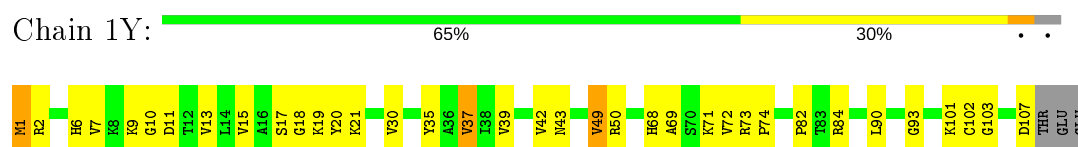
- Molecule 19: 50S ribosomal protein L23



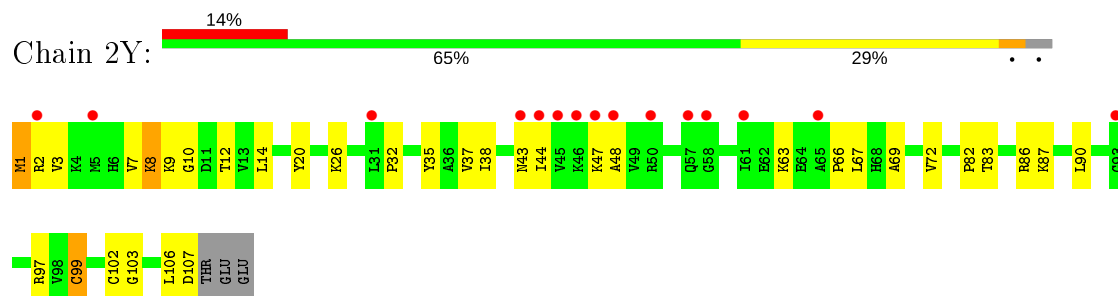
- Molecule 19: 50S ribosomal protein L23



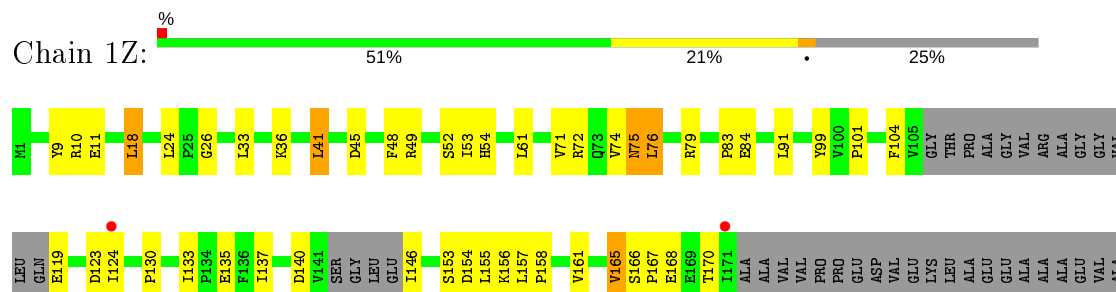
- Molecule 20: 50S ribosomal protein L24



- Molecule 20: 50S ribosomal protein L24

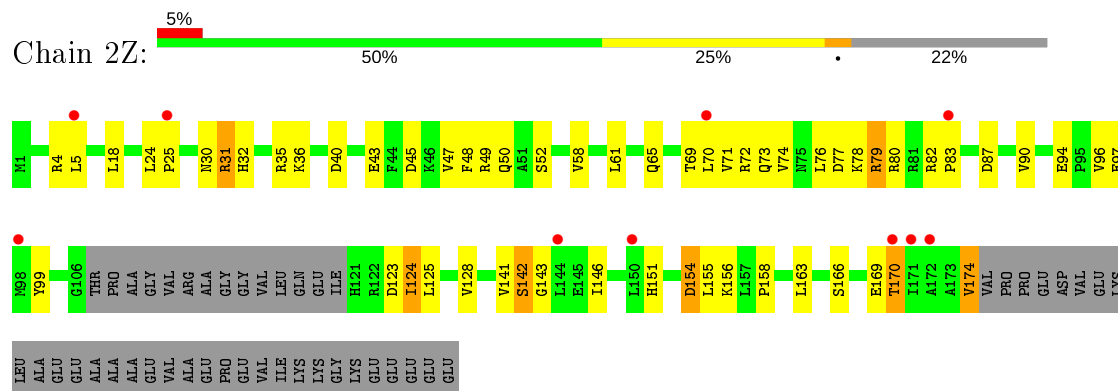


- Molecule 21: 50S ribosomal protein L25

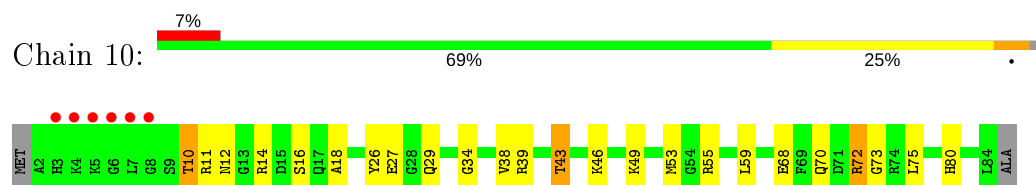


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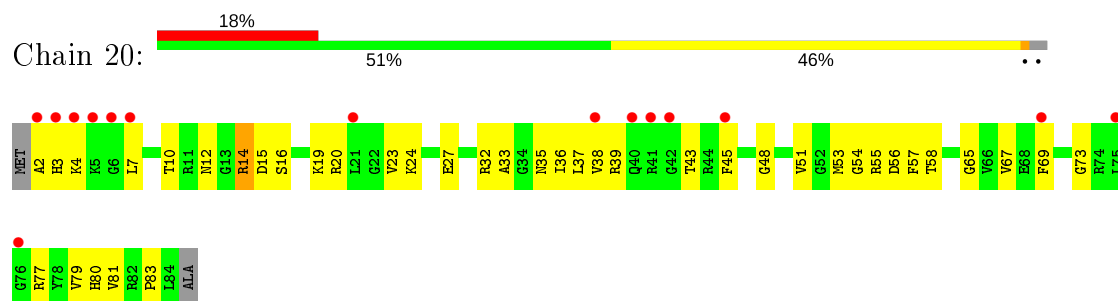
- Molecule 21: 50S ribosomal protein L25



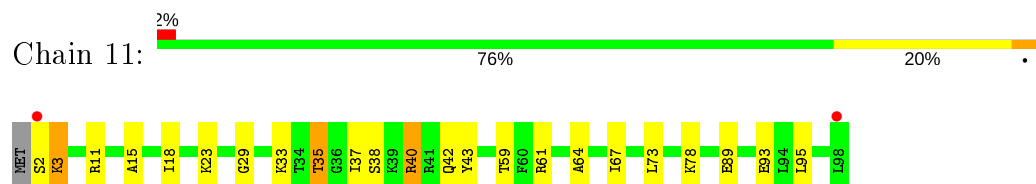
- Molecule 22: 50S ribosomal protein L27



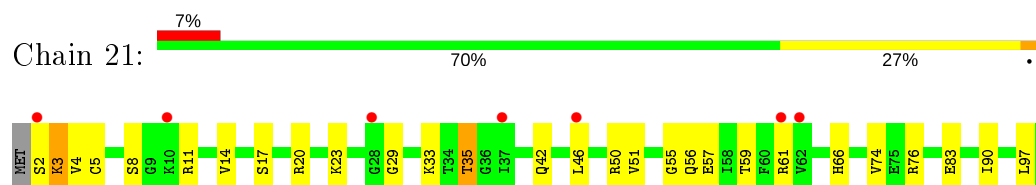
- Molecule 22: 50S ribosomal protein L27



- Molecule 23: 50S ribosomal protein L28

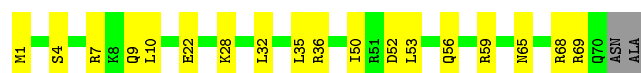


- Molecule 23: 50S ribosomal protein L28




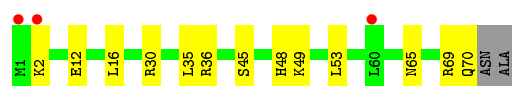
- Molecule 24: 50S ribosomal protein L29

Chain 12:  72% 25%



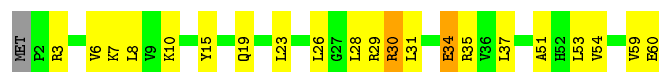
- Molecule 24: 50S ribosomal protein L29

Chain 22:  4% 79% 18%



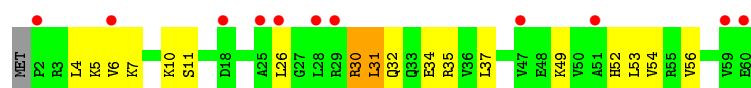
- Molecule 25: 50S ribosomal protein L30

Chain 13:  63% 32%



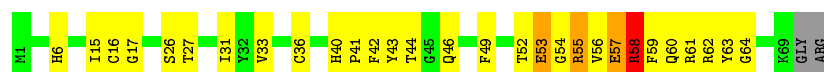
- Molecule 25: 50S ribosomal protein L30

Chain 23:  18% 68% 27%



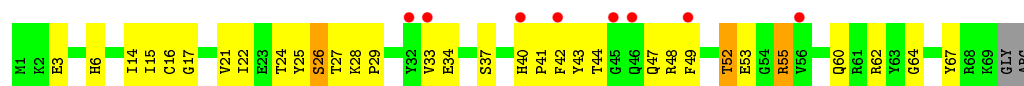
- Molecule 26: 50S ribosomal protein L31

Chain 14:  56% 35%



- Molecule 26: 50S ribosomal protein L31

Chain 24:  11% 52% 41%



- Molecule 27: 50S ribosomal protein L32

Chain 15:  80% 13% 5%



- Molecule 27: 50S ribosomal protein L32





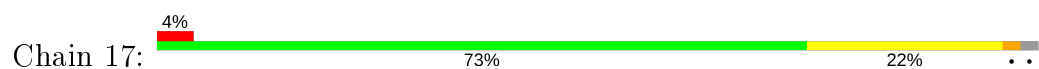
- Molecule 28: 50S ribosomal protein L33



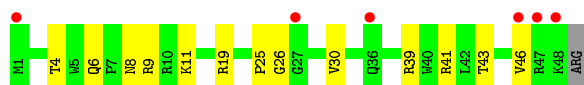
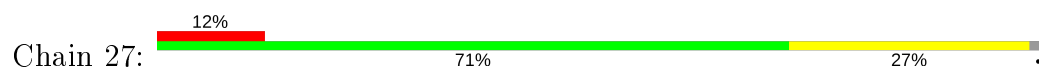
- Molecule 28: 50S ribosomal protein L33



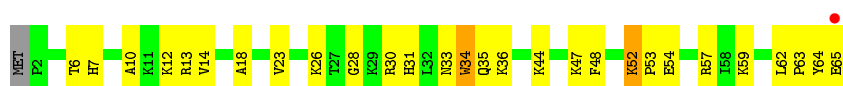
- Molecule 29: 50S ribosomal protein L34



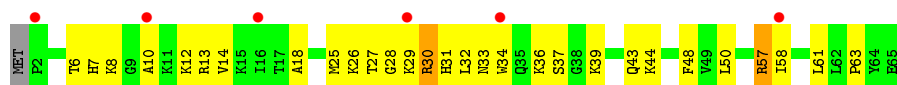
- Molecule 29: 50S ribosomal protein L34




- Molecule 30: 50S ribosomal protein L35

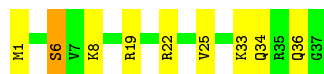


- Molecule 30: 50S ribosomal protein L35



- Molecule 31: 50S ribosomal protein L36

Chain 19:  76% 22%




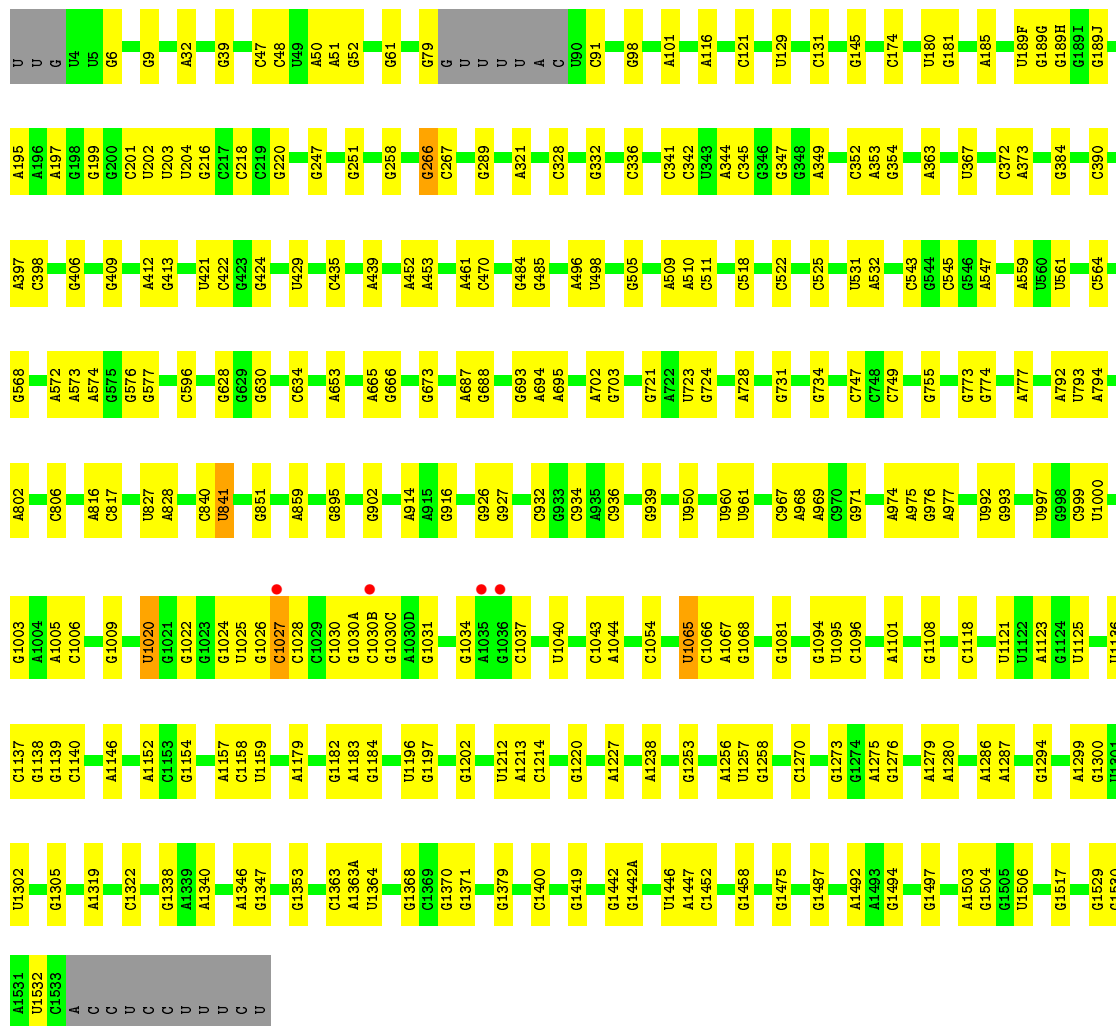
- Molecule 31: 50S ribosomal protein L36

Chain 29:  32% 62% 38%

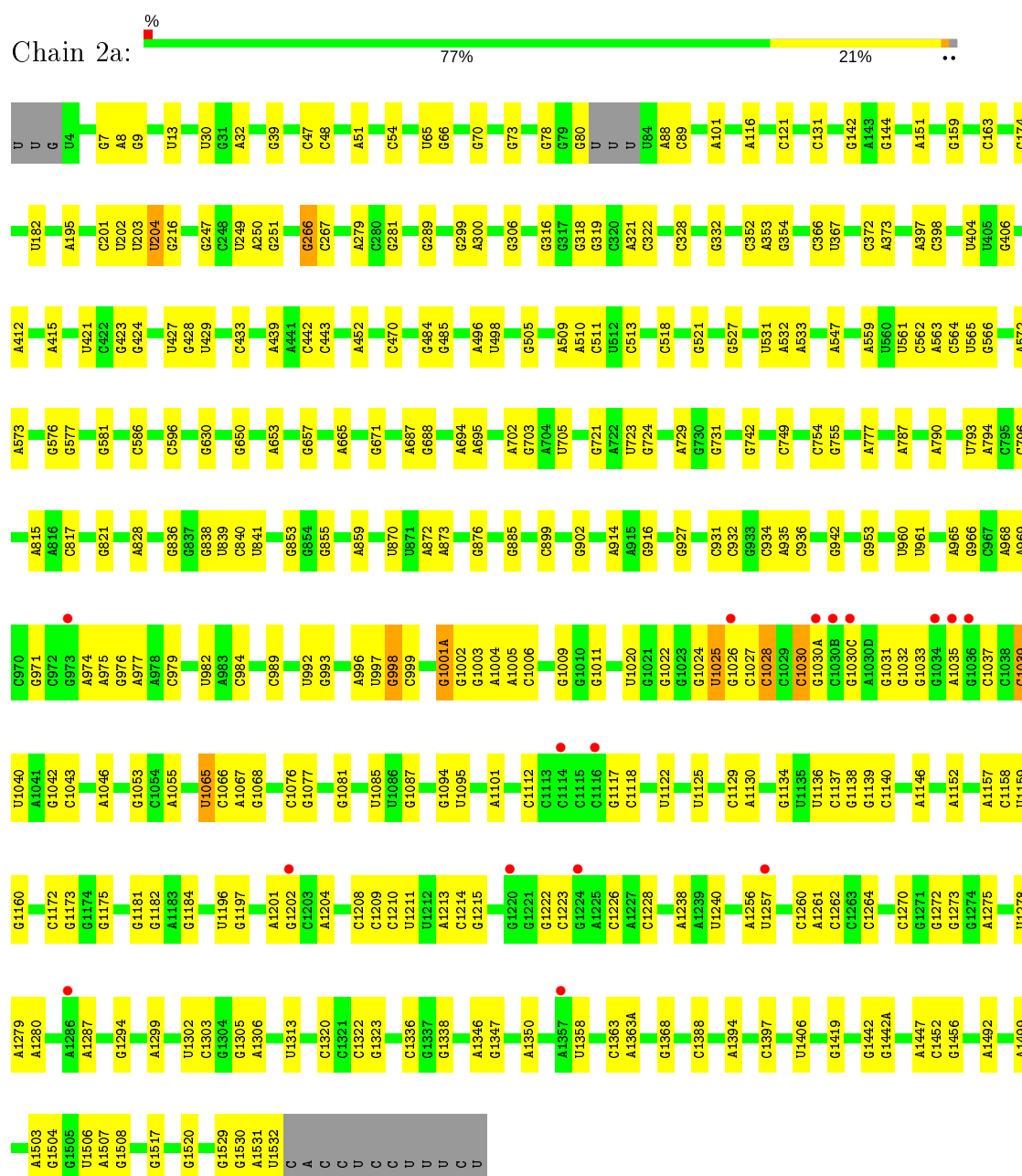


- Molecule 32: 16S Ribosomal RNA

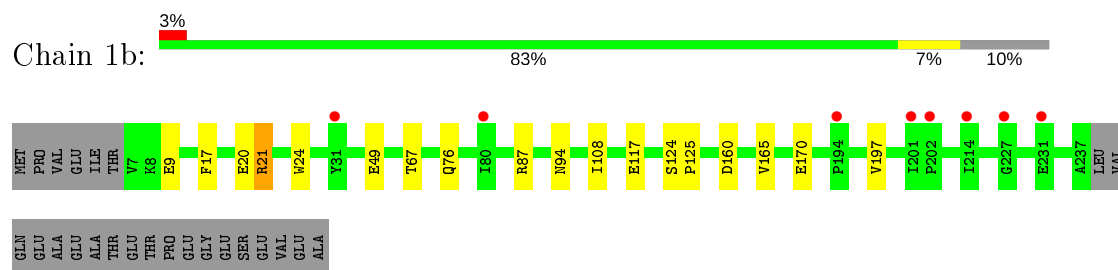
Chain 1a:  80% 18%



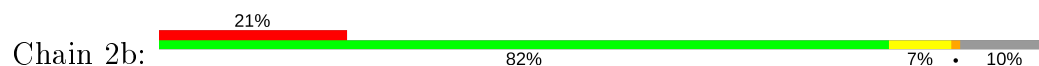
- Molecule 32: 16S Ribosomal RNA

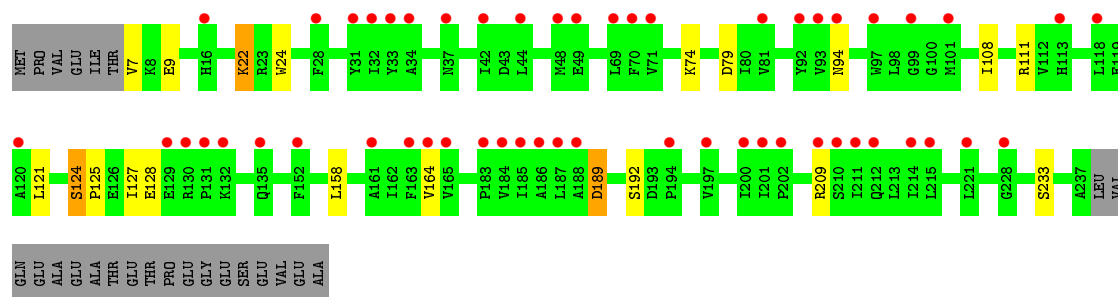


• Molecule 33: 30S ribosomal protein S2

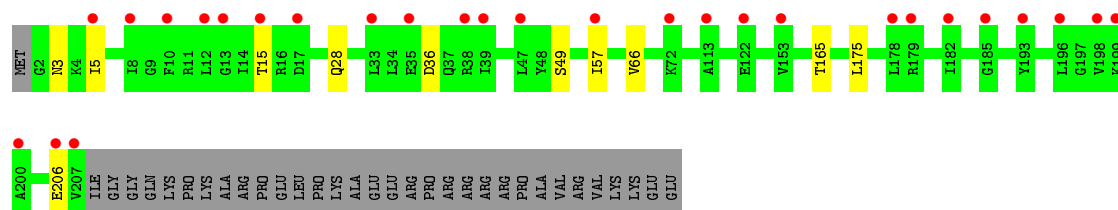
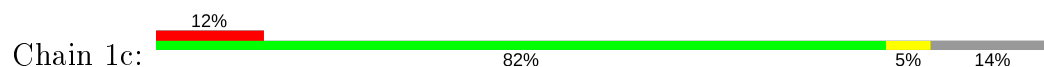


• Molecule 33: 30S ribosomal protein S2

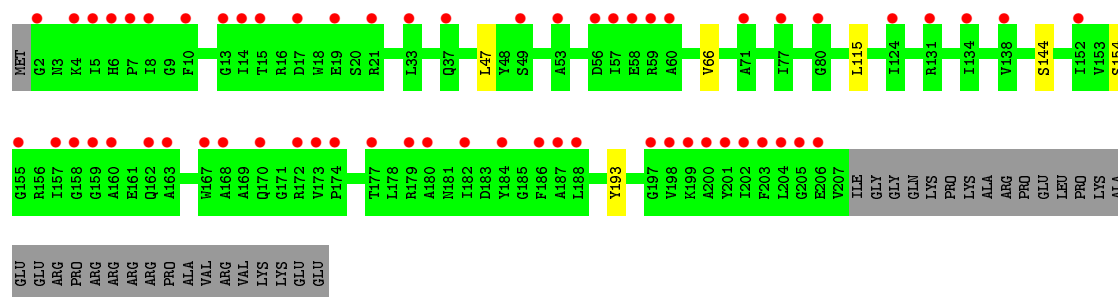
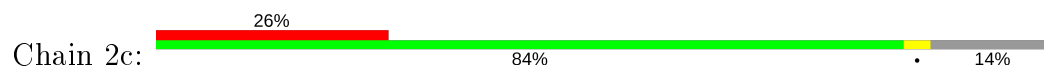




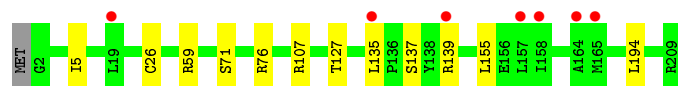
- Molecule 34: 30S ribosomal protein S3



- Molecule 34: 30S ribosomal protein S3



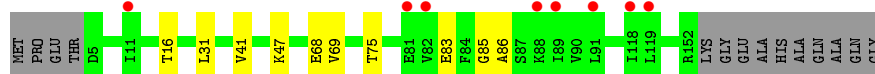
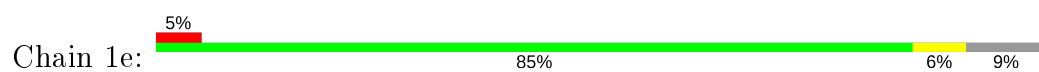
- Molecule 35: 30S ribosomal protein S4



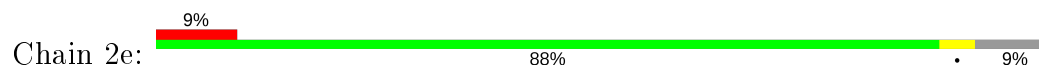
- Molecule 35: 30S ribosomal protein S4



- Molecule 36: 30S ribosomal protein S5



- Molecule 36: 30S ribosomal protein S5



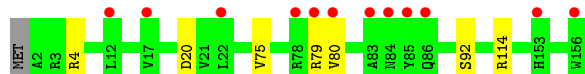
- Molecule 37: 30S ribosomal protein S6



- Molecule 37: 30S ribosomal protein S6



- Molecule 38: 30S ribosomal protein S7



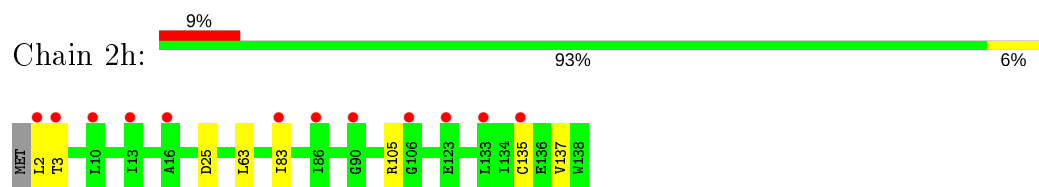
- Molecule 38: 30S ribosomal protein S7



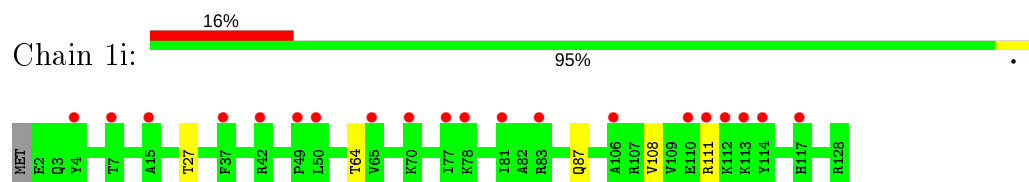
- Molecule 39: 30S ribosomal protein S8



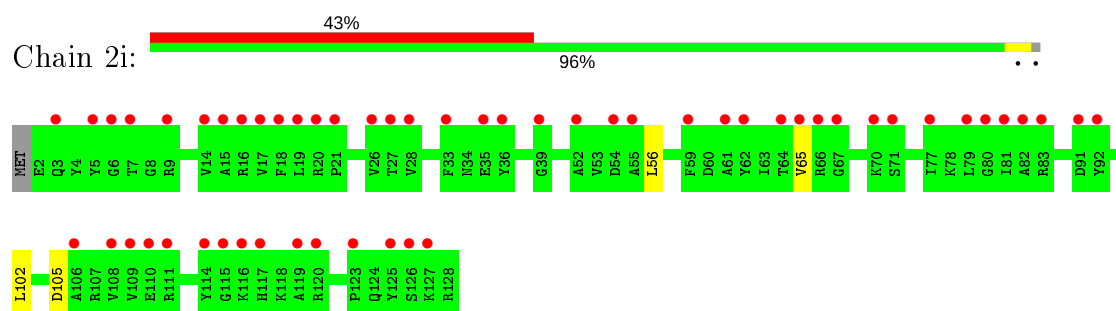
- Molecule 39: 30S ribosomal protein S8



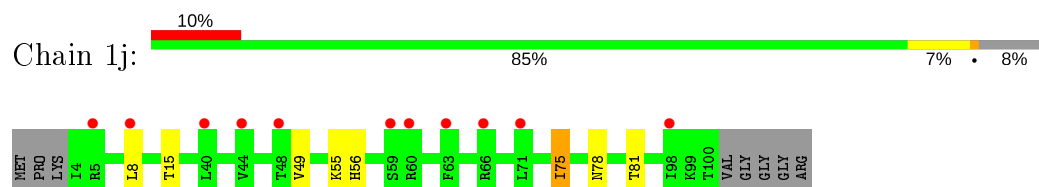
- Molecule 40: 30S ribosomal protein S9



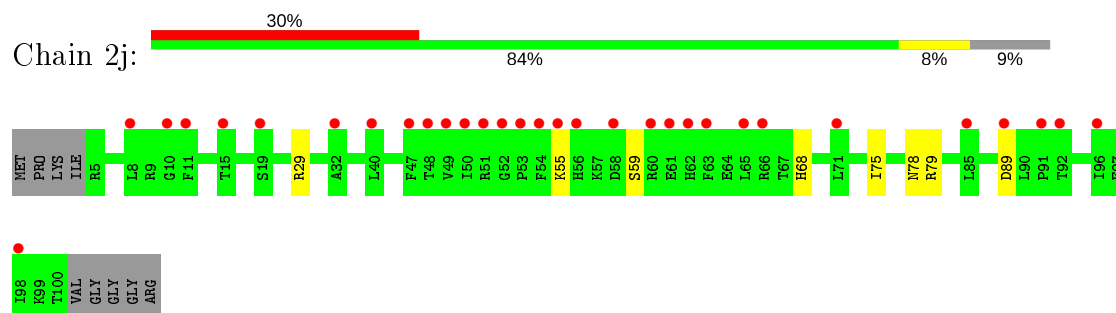
- Molecule 40: 30S ribosomal protein S9



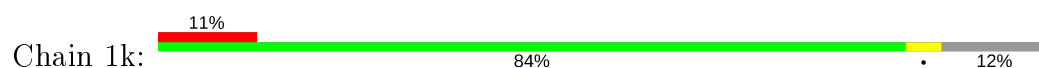
- Molecule 41: 30S ribosomal protein S10

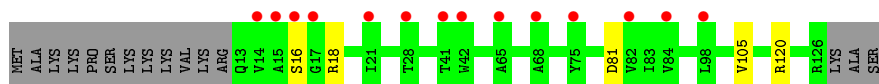


- Molecule 41: 30S ribosomal protein S10

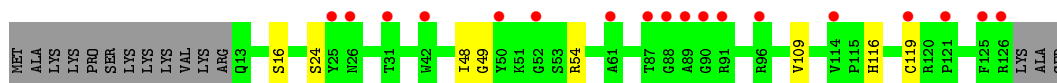
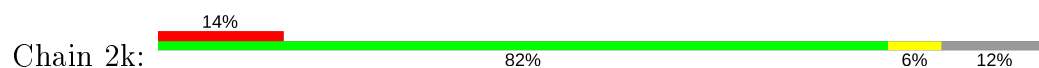


- Molecule 42: 30S ribosomal protein S11

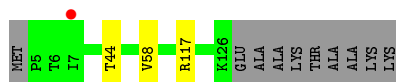
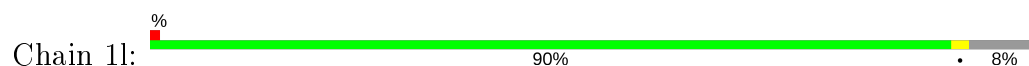




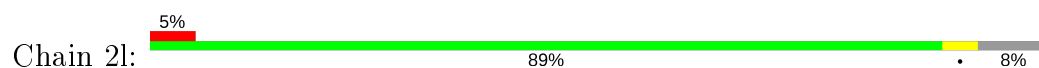
- Molecule 42: 30S ribosomal protein S11



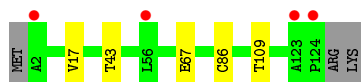
- Molecule 43: 30S ribosomal protein S12



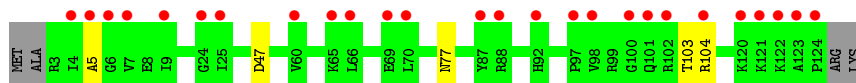
- Molecule 43: 30S ribosomal protein S12



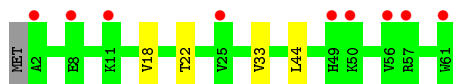
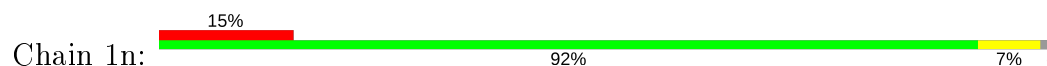
- Molecule 44: 30S ribosomal protein S13



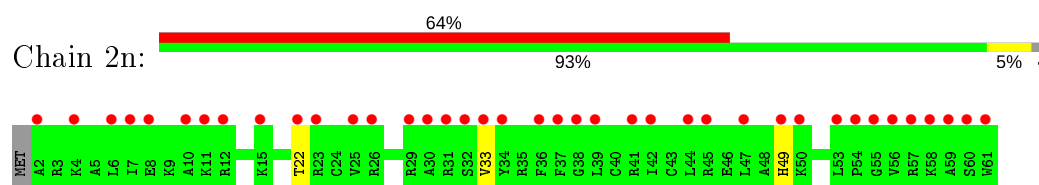
- Molecule 44: 30S ribosomal protein S13



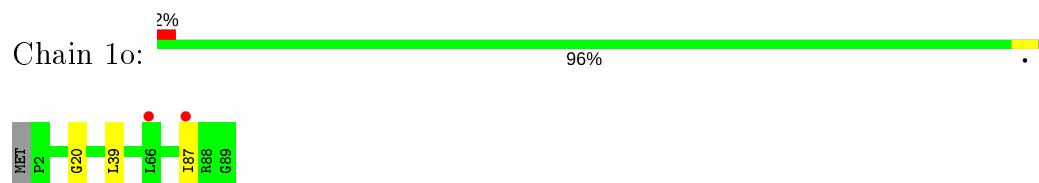
- Molecule 45: 30S ribosomal protein S14 type Z



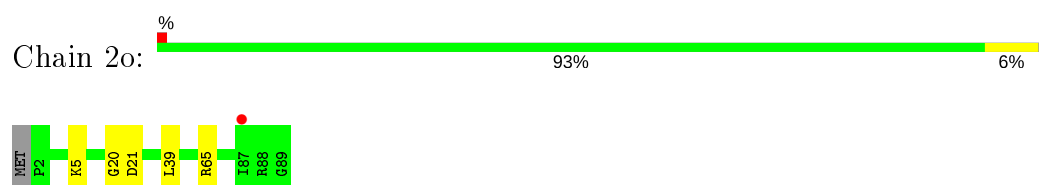
- Molecule 45: 30S ribosomal protein S14 type Z



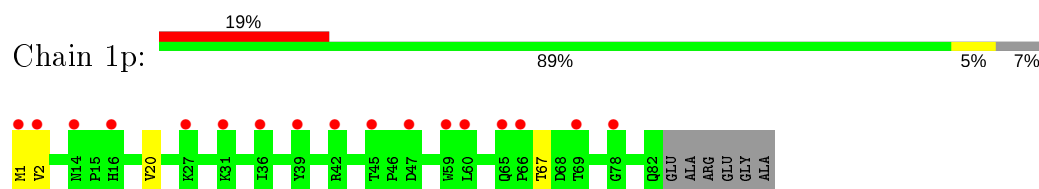
- Molecule 46: 30S ribosomal protein S15



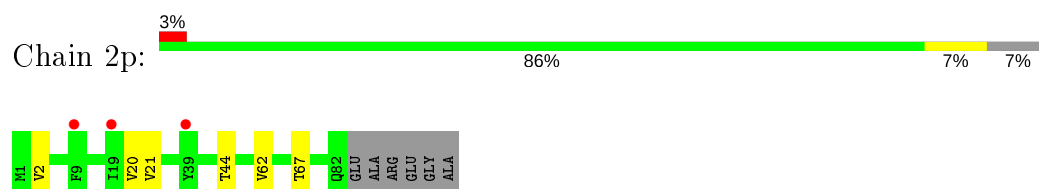
- Molecule 46: 30S ribosomal protein S15



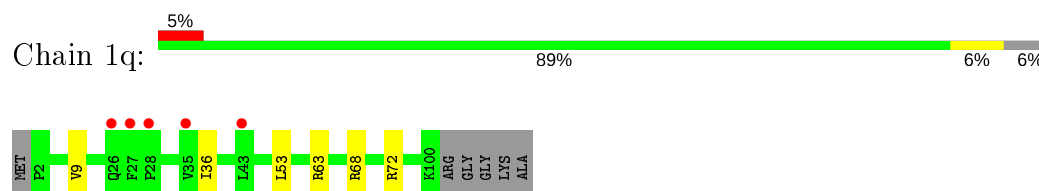
- Molecule 47: 30S ribosomal protein S16



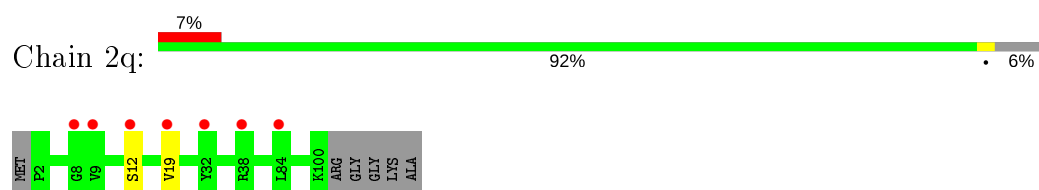
- Molecule 47: 30S ribosomal protein S16



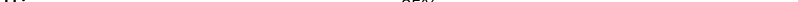
- Molecule 48: 30S ribosomal protein S17

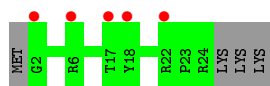


- Molecule 48: 30S ribosomal protein S17

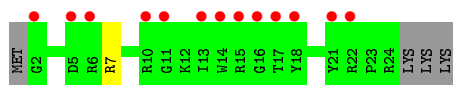
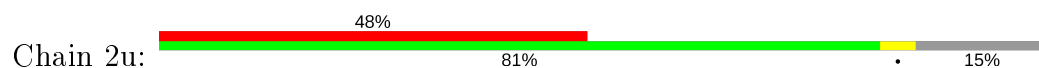




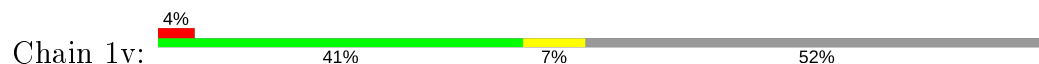
- Chain 1u: 



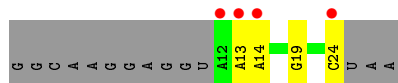
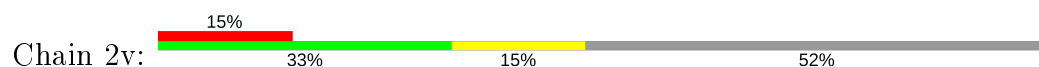
- Molecule 52: 30S ribosomal protein Thx



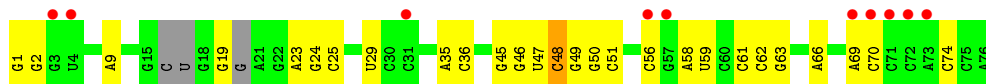
- Molecule 53: mRNA



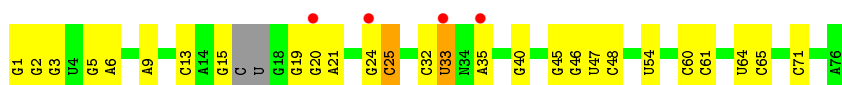
- Molecule 53: mRNA



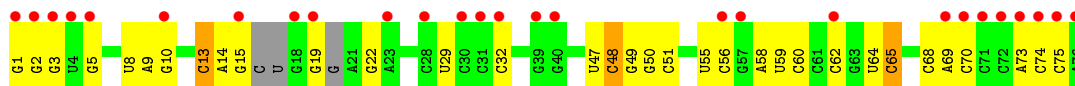
- Molecule 54: A-site and E-site tRNAs



- Molecule 54: A-site and E-site tRNAs

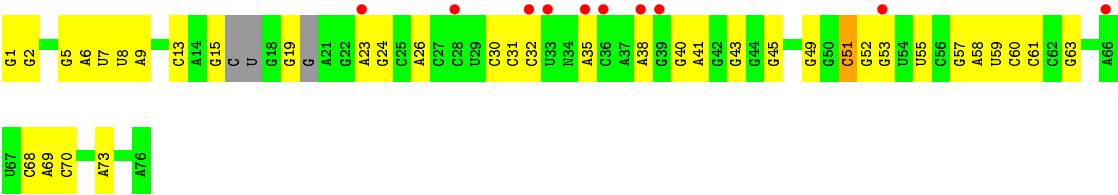


- Molecule 54: A-site and E-site tRNAs

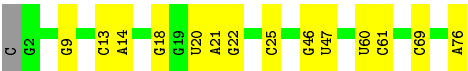
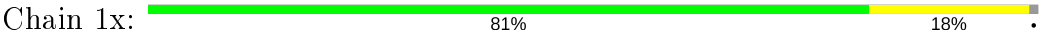


- Molecule 54: A-site and E-site tRNAs

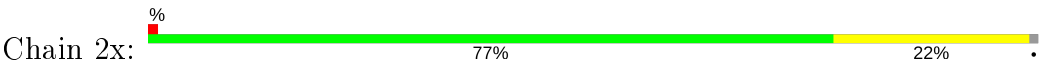




• Molecule 55: P-site tRNA



• Molecule 55: P-site tRNA



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	210.05Å 448.09Å 621.49Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	224.04 – 2.85 224.04 – 2.85	Depositor EDS
% Data completeness (in resolution range)	98.7 (224.04-2.85) 98.7 (224.04-2.85)	Depositor EDS
$R_{merge}$	0.19	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.19 (at 2.86Å)	Xtriage
Refinement program	PHENIX 1.8.2	Depositor
R, $R_{free}$	0.249 , 0.305 0.250 , 0.305	Depositor DCC
$R_{free}$ test set	66731 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	54.2	Xtriage
Anisotropy	0.151	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.27 , 59.2	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.34$ , $\langle L^2 \rangle = 0.17$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.87	EDS
Total number of atoms	300104	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	52.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.61% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

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

## 5 Model quality ⓘ

### 5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: 5MU, PSU, ZN, M2G, OMG, 2MU, SF4, 0TD, MG, ERY, 2MA, 6MZ, 2MG, 5MC, UR3, MA6, 4OC, 4SU, 7MG, CM0

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  $|Z| > 5$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
1	1A	0.33	0/69009	0.82	26/107712 (0.0%)
1	2A	0.26	0/67293	0.80	19/105034 (0.0%)
2	1B	0.33	1/2882 (0.0%)	0.78	0/4494
2	2B	0.31	1/2879 (0.0%)	0.80	1/4487 (0.0%)
3	1D	0.31	0/2186	0.49	0/2944
3	2D	0.29	0/2186	0.48	0/2944
4	1E	0.29	0/1592	0.49	0/2149
4	2E	0.27	0/1592	0.47	0/2149
5	1F	0.28	0/1619	0.47	0/2193
5	2F	0.27	0/1615	0.44	0/2188
6	1G	0.26	0/1448	0.44	0/1957
6	2G	0.26	0/1453	0.44	0/1963
7	1H	0.27	0/1356	0.46	0/1834
7	2H	0.26	0/1356	0.44	0/1834
8	1I	0.26	0/1112	0.45	0/1514
8	2I	0.25	0/1079	0.46	0/1475
9	1N	0.28	0/1144	0.45	0/1543
9	2N	0.26	0/1144	0.45	0/1543
10	1O	0.29	0/943	0.49	0/1269
10	2O	0.28	0/943	0.48	0/1269
11	1P	0.28	0/1152	0.53	1/1533 (0.1%)
11	2P	0.28	0/1152	0.47	0/1533
12	1Q	0.29	0/1143	0.46	0/1527
12	2Q	0.26	0/1143	0.46	0/1527
13	1R	0.27	0/982	0.48	0/1312
13	2R	0.24	0/982	0.45	0/1312
14	1S	0.26	0/883	0.45	0/1176
14	2S	0.25	0/880	0.44	0/1172
15	1T	0.27	0/1105	0.46	0/1477
15	2T	0.26	0/1097	0.44	0/1468
16	1U	0.28	0/977	0.43	0/1301

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
16	2U	0.26	0/977	0.39	0/1301
17	1V	0.30	0/782	0.53	0/1049
17	2V	0.28	0/782	0.50	0/1049
18	1W	0.29	0/897	0.48	0/1205
18	2W	0.26	0/897	0.45	0/1205
19	1X	0.28	0/764	0.48	0/1025
19	2X	0.27	0/764	0.45	0/1025
20	1Y	0.28	0/819	0.48	0/1095
20	2Y	0.27	0/819	0.47	0/1095
21	1Z	0.27	0/1267	0.48	0/1717
21	2Z	0.28	0/1299	0.50	0/1763
22	10	0.30	0/662	0.47	0/881
22	20	0.28	0/662	0.47	0/881
23	11	0.28	0/762	0.46	0/1014
23	21	0.28	0/762	0.44	0/1014
24	12	0.26	0/590	0.41	0/781
24	22	0.24	0/590	0.38	0/781
25	13	0.27	0/474	0.44	0/635
25	23	0.24	0/469	0.42	0/630
26	14	0.28	0/565	0.56	0/761
26	24	0.27	0/545	0.53	0/737
27	15	0.29	0/469	0.47	0/635
27	25	0.27	0/469	0.45	0/635
28	16	0.29	0/460	0.47	0/613
28	26	0.27	0/456	0.46	0/608
29	17	0.26	0/426	0.45	0/561
29	27	0.25	0/426	0.46	0/561
30	18	0.28	0/525	0.47	0/691
30	28	0.25	0/525	0.46	0/691
31	19	0.30	0/310	0.46	0/407
31	29	0.26	0/310	0.49	0/407
32	1a	0.26	0/35795	0.82	25/55864 (0.0%)
32	2a	0.26	0/35886	0.84	46/56005 (0.1%)
33	1b	0.26	0/1881	0.45	0/2542
33	2b	0.25	0/1860	0.45	0/2518
34	1c	0.26	0/1572	0.45	0/2126
34	2c	0.25	0/1566	0.44	0/2119
35	1d	0.26	0/1685	0.45	0/2262
35	2d	0.31	1/1704 (0.1%)	0.44	0/2284
36	1e	0.26	0/1145	0.46	0/1543
36	2e	0.27	0/1149	0.48	0/1548
37	1f	0.26	0/823	0.46	0/1115
37	2f	0.27	0/829	0.46	0/1123

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
38	1g	0.26	0/1250	0.41	0/1679
38	2g	0.25	0/1254	0.40	0/1683
39	1h	0.24	0/1108	0.44	0/1494
39	2h	0.25	0/1108	0.45	0/1494
40	1i	0.27	0/1002	0.45	0/1346
40	2i	0.27	0/997	0.51	0/1343
41	1j	0.24	0/722	0.48	1/982 (0.1%)
41	2j	0.24	0/727	0.47	0/988
42	1k	0.25	0/844	0.44	0/1145
42	2k	0.25	0/848	0.45	0/1149
43	1l	0.27	0/937	0.48	0/1260
43	2l	0.27	0/937	0.46	0/1260
44	1m	0.26	0/969	0.49	0/1302
44	2m	0.25	0/961	0.46	0/1291
45	1n	0.25	0/501	0.40	0/664
45	2n	0.25	0/501	0.42	0/664
46	1o	0.23	0/739	0.40	0/985
46	2o	0.25	0/739	0.44	0/985
47	1p	0.25	0/697	0.45	0/939
47	2p	0.25	0/693	0.45	0/935
48	1q	0.26	0/836	0.45	0/1117
48	2q	0.26	0/836	0.47	0/1117
49	1r	0.25	0/560	0.43	0/746
49	2r	0.24	0/560	0.42	0/746
50	1s	0.25	0/667	0.49	0/900
50	2s	0.27	0/661	0.52	0/893
51	1t	0.25	0/730	0.42	0/965
51	2t	0.24	0/729	0.46	0/965
52	1u	0.25	0/203	0.50	0/266
52	2u	0.25	0/203	0.48	0/266
53	1v	0.29	0/308	0.82	0/477
53	2v	0.30	0/308	0.83	0/477
54	1w	0.45	1/1600 (0.1%)	1.05	5/2482 (0.2%)
54	1y	0.43	1/1627 (0.1%)	1.01	3/2527 (0.1%)
54	2w	0.46	1/1600 (0.1%)	1.16	10/2482 (0.4%)
54	2y	0.47	1/1600 (0.1%)	1.11	6/2482 (0.2%)
55	1x	0.38	0/1725	0.98	7/2689 (0.3%)
55	2x	0.35	0/1725	1.02	2/2689 (0.1%)
All	All	0.29	7/316758 (0.0%)	0.75	152/474209 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a

sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
26	14	0	1
26	24	0	2
33	1b	0	1
33	2b	0	1
51	1t	0	1
All	All	0	6

The worst 5 of 7 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
54	2w	1	G	OP3-P	-10.58	1.48	1.61
2	2B	1	U	OP3-P	-10.49	1.48	1.61
54	1y	1	G	OP3-P	-10.45	1.48	1.61
54	1w	1	G	OP3-P	-10.42	1.48	1.61
54	2y	1	G	OP3-P	-10.40	1.48	1.61

The worst 5 of 152 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	2A	2136	C	N1-C2-O2	11.11	125.56	118.90
32	1a	1027	C	N3-C4-C5	-9.53	118.09	121.90
32	1a	1030(B)	C	C2-N1-C1'	9.04	128.74	118.80
2	2B	80	U	O4'-C1'-N1	8.80	115.24	108.20
1	2A	2155	G	N3-C2-N2	8.55	125.88	119.90

There are no chirality outliers.

5 of 6 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
26	14	57	GLU	Peptide
33	1b	124	SER	Peptide
51	1t	99	LEU	Peptide
26	24	53	GLU	Peptide
26	24	55	ARG	Peptide

## 5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within



the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	1A	61852	0	31191	819	0
1	2A	60322	0	30418	967	0
2	1B	2577	0	1305	33	0
2	2B	2575	0	1303	41	0
3	1D	2136	0	2218	66	0
3	2D	2136	0	2218	54	0
4	1E	1559	0	1617	37	0
4	2E	1559	0	1618	41	0
5	1F	1584	0	1625	38	0
5	2F	1580	0	1618	44	0
6	1G	1423	0	1436	42	0
6	2G	1428	0	1438	45	0
7	1H	1330	0	1407	32	0
7	2H	1330	0	1407	38	0
8	1I	1097	0	1140	22	0
8	2I	1064	0	1082	23	0
9	1N	1117	0	1184	13	0
9	2N	1117	0	1184	25	0
10	1O	933	0	996	21	0
10	2O	933	0	996	27	0
11	1P	1135	0	1212	33	0
11	2P	1135	0	1212	38	0
12	1Q	1122	0	1179	27	0
12	2Q	1122	0	1179	34	0
13	1R	968	0	1033	17	0
13	2R	968	0	1033	24	0
14	1S	873	0	927	26	0
14	2S	870	0	923	26	0
15	1T	1091	0	1151	21	0
15	2T	1083	0	1136	40	0
16	1U	959	0	1019	15	0
16	2U	959	0	1018	20	0
17	1V	771	0	830	17	0
17	2V	771	0	830	23	0
18	1W	886	0	939	24	0
18	2W	886	0	940	15	0
19	1X	750	0	814	14	0
19	2X	750	0	814	15	0
20	1Y	806	0	881	22	0
20	2Y	806	0	881	18	0
21	1Z	1240	0	1240	28	0
21	2Z	1271	0	1273	42	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
22	10	653	0	674	18	0
22	20	653	0	674	33	0
23	11	755	0	826	18	0
23	21	755	0	826	22	0
24	12	588	0	643	13	0
24	22	588	0	643	11	0
25	13	469	0	518	14	0
25	23	464	0	514	11	0
26	14	552	0	533	26	0
26	24	532	0	503	17	0
27	15	455	0	465	9	0
27	25	455	0	465	15	0
28	16	453	0	472	9	0
28	26	449	0	469	8	0
29	17	418	0	467	8	0
29	27	418	0	467	8	0
30	18	517	0	582	22	0
30	28	517	0	582	25	0
31	19	307	0	335	10	0
31	29	307	0	335	11	0
32	1a	32246	0	16294	0	0
32	2a	32327	0	16338	0	0
33	1b	1846	0	1867	0	0
33	2b	1825	0	1828	0	0
34	1c	1548	0	1535	0	0
34	2c	1542	0	1517	0	0
35	1d	1655	0	1672	0	0
35	2d	1674	0	1714	0	0
36	1e	1129	0	1185	0	0
36	2e	1133	0	1191	0	0
37	1f	810	0	804	0	0
37	2f	816	0	808	0	0
38	1g	1231	0	1238	0	0
38	2g	1235	0	1249	0	0
39	1h	1088	0	1126	0	0
39	2h	1088	0	1126	0	0
40	1i	983	0	986	0	0
40	2i	978	0	966	0	0
41	1j	709	0	650	0	0
41	2j	714	0	672	0	0
42	1k	829	0	825	0	0
42	2k	833	0	836	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
43	1l	932	0	981	0	0
43	2l	932	0	981	0	0
44	1m	958	0	1002	0	0
44	2m	950	0	988	0	0
45	1n	492	0	529	0	0
45	2n	492	0	529	0	0
46	1o	728	0	760	0	0
46	2o	728	0	760	0	0
47	1p	681	0	697	0	0
47	2p	677	0	686	0	0
48	1q	823	0	891	0	0
48	2q	823	0	891	0	0
49	1r	555	0	618	0	0
49	2r	555	0	618	0	0
50	1s	652	0	662	0	0
50	2s	646	0	644	0	0
51	1t	728	0	798	0	0
51	2t	727	0	796	0	0
52	1u	199	0	208	0	0
52	2u	199	0	208	0	0
53	1v	276	0	139	0	0
53	2v	276	0	139	0	0
54	1w	1568	0	801	0	0
54	1y	1591	0	812	0	0
54	2w	1568	0	802	0	0
54	2y	1568	0	802	0	0
55	1x	1625	0	829	0	0
55	2x	1625	0	829	0	0
56	10	7	0	0	0	0
56	11	1	0	0	0	0
56	12	2	0	0	0	0
56	13	6	0	0	0	0
56	14	1	0	0	0	0
56	15	7	0	0	0	0
56	16	4	0	0	0	0
56	17	5	0	0	0	0
56	18	2	0	0	0	0
56	19	3	0	0	0	0
56	1A	1073	0	0	0	0
56	1B	35	0	0	0	0
56	1D	13	0	0	0	0
56	1E	15	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
56	1F	14	0	0	0	0
56	1G	3	0	0	0	0
56	1I	1	0	0	0	0
56	1N	4	0	0	0	0
56	1O	2	0	0	0	0
56	1P	8	0	0	0	0
56	1Q	8	0	0	0	0
56	1R	2	0	0	0	0
56	1S	2	0	0	0	0
56	1T	2	0	0	0	0
56	1U	10	0	0	0	0
56	1V	8	0	0	0	0
56	1W	8	0	0	0	0
56	1X	5	0	0	0	0
56	1Y	1	0	0	0	0
56	1Z	3	0	0	0	0
56	1a	229	0	0	0	0
56	1b	1	0	0	0	0
56	1d	1	0	0	0	0
56	1e	2	0	0	0	0
56	1f	1	0	0	0	0
56	1l	3	0	0	0	0
56	1m	1	0	0	0	0
56	1n	1	0	0	0	0
56	1p	1	0	0	0	0
56	1r	1	0	0	0	0
56	1s	1	0	0	0	0
56	1t	1	0	0	0	0
56	1v	1	0	0	0	0
56	1w	6	0	0	0	0
56	1x	13	0	0	0	0
56	1y	5	0	0	0	0
56	20	2	0	0	0	0
56	21	1	0	0	0	0
56	22	1	0	0	0	0
56	23	3	0	0	0	0
56	25	3	0	0	0	0
56	26	2	0	0	0	0
56	27	2	0	0	0	0
56	28	1	0	0	0	0
56	2A	874	0	0	0	0
56	2B	21	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
56	2D	7	0	0	0	0
56	2E	8	0	0	0	0
56	2F	7	0	0	0	0
56	2G	1	0	0	0	0
56	2N	1	0	0	0	0
56	2O	1	0	0	0	0
56	2P	2	0	0	0	0
56	2Q	5	0	0	0	0
56	2R	3	0	0	0	0
56	2T	3	0	0	0	0
56	2U	3	0	0	0	0
56	2V	1	0	0	0	0
56	2W	1	0	0	0	0
56	2X	2	0	0	0	0
56	2Z	1	0	0	0	0
56	2a	233	0	0	0	0
56	2d	1	0	0	0	0
56	2e	1	0	0	0	0
56	2f	2	0	0	0	0
56	2g	1	0	0	0	0
56	2i	2	0	0	0	0
56	2j	2	0	0	0	0
56	2k	1	0	0	0	0
56	2l	5	0	0	0	0
56	2p	1	0	0	0	0
56	2q	3	0	0	0	0
56	2r	1	0	0	0	0
56	2t	1	0	0	0	0
56	2v	2	0	0	0	0
56	2w	1	0	0	0	0
56	2x	5	0	0	0	0
56	2y	4	0	0	0	0
57	1A	51	0	67	3	0
57	2A	51	0	67	3	0
58	14	1	0	0	0	0
58	15	1	0	0	0	0
58	16	1	0	0	0	0
58	19	1	0	0	0	0
58	1Y	1	0	0	0	0
58	1n	1	0	0	0	0
58	24	1	0	0	0	0
58	25	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
58	26	1	0	0	0	0
58	29	1	0	0	0	0
58	2Y	1	0	0	0	0
58	2n	1	0	0	0	0
59	1d	8	0	0	0	0
59	2d	8	0	0	0	0
60	10	9	0	0	0	0
60	11	10	0	0	0	0
60	12	3	0	0	0	0
60	13	2	0	0	0	0
60	14	2	0	0	0	0
60	15	3	0	0	0	0
60	16	3	0	0	0	0
60	17	9	0	0	0	0
60	18	5	0	0	1	0
60	19	2	0	0	0	0
60	1A	1719	0	0	66	0
60	1B	59	0	0	0	0
60	1D	16	0	0	1	0
60	1E	21	0	0	3	0
60	1F	7	0	0	0	0
60	1G	4	0	0	3	0
60	1H	1	0	0	0	0
60	1I	2	0	0	0	0
60	1N	5	0	0	0	0
60	1O	7	0	0	0	0
60	1P	11	0	0	1	0
60	1Q	10	0	0	0	0
60	1R	8	0	0	0	0
60	1S	5	0	0	0	0
60	1T	2	0	0	0	0
60	1U	6	0	0	0	0
60	1V	10	0	0	0	0
60	1W	8	0	0	0	0
60	1X	8	0	0	0	0
60	1Y	4	0	0	0	0
60	1Z	1	0	0	0	0
60	1a	381	0	0	0	0
60	1b	1	0	0	0	0
60	1g	1	0	0	0	0
60	1k	1	0	0	0	0
60	1l	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
60	1q	4	0	0	0	0
60	1v	1	0	0	0	0
60	1w	2	0	0	0	0
60	1x	15	0	0	0	0
60	1y	2	0	0	0	0
60	20	9	0	0	2	0
60	21	8	0	0	0	0
60	22	2	0	0	0	0
60	23	1	0	0	0	0
60	25	4	0	0	0	0
60	27	3	0	0	0	0
60	28	4	0	0	2	0
60	29	1	0	0	0	0
60	2A	1401	0	0	84	0
60	2B	26	0	0	0	0
60	2D	14	0	0	1	0
60	2E	9	0	0	0	0
60	2F	8	0	0	0	0
60	2I	4	0	0	0	0
60	2N	1	0	0	0	0
60	2O	1	0	0	0	0
60	2P	5	0	0	0	0
60	2Q	2	0	0	0	0
60	2R	2	0	0	0	0
60	2T	4	0	0	0	0
60	2U	2	0	0	1	0
60	2W	4	0	0	0	0
60	2X	4	0	0	0	0
60	2Z	1	0	0	0	0
60	2a	306	0	0	0	0
60	2d	1	0	0	0	0
60	2g	2	0	0	0	0
60	2h	1	0	0	0	0
60	2i	3	0	0	0	0
60	2j	4	0	0	0	0
60	2l	4	0	0	0	0
60	2p	1	0	0	0	0
60	2r	1	0	0	0	0
60	2t	2	0	0	0	0
60	2v	1	0	0	0	0
60	2x	8	0	0	0	0
60	2y	11	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	300104	0	196819	2823	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 11.

The worst 5 of 2823 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1A:2136:C:N4	1:1A:2155:G:H1	1.44	1.15
1:2A:1002:G:H1	1:2A:1038:C:N4	42.20	1.11
1:1A:1082:U:O4	1:1A:1086:A:N1	1.95	1.00
1:1A:1054:A:H61	1:1A:1105:U:H3	1.07	0.99
1:2A:2138:C:H42	1:2A:2153:G:H1	1.02	0.98

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	1D	273/276 (99%)	256 (94%)	16 (6%)	1 (0%)	34	62
3	2D	273/276 (99%)	256 (94%)	17 (6%)	0	100	100
4	1E	202/206 (98%)	188 (93%)	13 (6%)	1 (0%)	29	57
4	2E	202/206 (98%)	190 (94%)	10 (5%)	2 (1%)	15	40
5	1F	201/210 (96%)	196 (98%)	3 (2%)	2 (1%)	15	40
5	2F	201/210 (96%)	193 (96%)	7 (4%)	1 (0%)	29	57
6	1G	179/182 (98%)	166 (93%)	11 (6%)	2 (1%)	14	38
6	2G	179/182 (98%)	159 (89%)	18 (10%)	2 (1%)	14	38
7	1H	172/180 (96%)	163 (95%)	8 (5%)	1 (1%)	25	53

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
7	2H	172/180 (96%)	158 (92%)	11 (6%)	3 (2%)	9	27
8	1I	144/148 (97%)	130 (90%)	13 (9%)	1 (1%)	22	50
8	2I	144/148 (97%)	131 (91%)	12 (8%)	1 (1%)	22	50
9	1N	138/140 (99%)	132 (96%)	6 (4%)	0	100	100
9	2N	138/140 (99%)	133 (96%)	5 (4%)	0	100	100
10	1O	120/122 (98%)	113 (94%)	7 (6%)	0	100	100
10	2O	120/122 (98%)	108 (90%)	12 (10%)	0	100	100
11	1P	147/150 (98%)	143 (97%)	4 (3%)	0	100	100
11	2P	147/150 (98%)	138 (94%)	9 (6%)	0	100	100
12	1Q	139/141 (99%)	130 (94%)	9 (6%)	0	100	100
12	2Q	139/141 (99%)	133 (96%)	6 (4%)	0	100	100
13	1R	116/118 (98%)	108 (93%)	8 (7%)	0	100	100
13	2R	116/118 (98%)	110 (95%)	6 (5%)	0	100	100
14	1S	108/112 (96%)	102 (94%)	5 (5%)	1 (1%)	17	43
14	2S	108/112 (96%)	101 (94%)	6 (6%)	1 (1%)	17	43
15	1T	129/146 (88%)	122 (95%)	6 (5%)	1 (1%)	19	46
15	2T	129/146 (88%)	120 (93%)	9 (7%)	0	100	100
16	1U	114/118 (97%)	114 (100%)	0	0	100	100
16	2U	114/118 (97%)	112 (98%)	2 (2%)	0	100	100
17	1V	99/101 (98%)	91 (92%)	7 (7%)	1 (1%)	15	40
17	2V	99/101 (98%)	92 (93%)	5 (5%)	2 (2%)	7	23
18	1W	110/113 (97%)	105 (96%)	4 (4%)	1 (1%)	17	43
18	2W	110/113 (97%)	106 (96%)	4 (4%)	0	100	100
19	1X	93/96 (97%)	89 (96%)	4 (4%)	0	100	100
19	2X	93/96 (97%)	90 (97%)	3 (3%)	0	100	100
20	1Y	105/110 (96%)	97 (92%)	8 (8%)	0	100	100
20	2Y	105/110 (96%)	99 (94%)	5 (5%)	1 (1%)	15	40
21	1Z	148/206 (72%)	135 (91%)	12 (8%)	1 (1%)	22	50
21	2Z	156/206 (76%)	131 (84%)	22 (14%)	3 (2%)	8	24
22	10	81/85 (95%)	79 (98%)	2 (2%)	0	100	100
22	20	81/85 (95%)	75 (93%)	6 (7%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
23	11	95/98 (97%)	92 (97%)	2 (2%)	1 (1%)	14	38
23	21	95/98 (97%)	94 (99%)	1 (1%)	0	100	100
24	12	68/72 (94%)	66 (97%)	2 (3%)	0	100	100
24	22	68/72 (94%)	67 (98%)	1 (2%)	0	100	100
25	13	57/60 (95%)	56 (98%)	1 (2%)	0	100	100
25	23	57/60 (95%)	54 (95%)	3 (5%)	0	100	100
26	14	67/71 (94%)	48 (72%)	15 (22%)	4 (6%)	1	4
26	24	67/71 (94%)	51 (76%)	13 (19%)	3 (4%)	2	7
27	15	57/60 (95%)	54 (95%)	3 (5%)	0	100	100
27	25	57/60 (95%)	52 (91%)	5 (9%)	0	100	100
28	16	51/54 (94%)	47 (92%)	4 (8%)	0	100	100
28	26	51/54 (94%)	50 (98%)	1 (2%)	0	100	100
29	17	46/49 (94%)	45 (98%)	1 (2%)	0	100	100
29	27	46/49 (94%)	46 (100%)	0	0	100	100
30	18	62/65 (95%)	61 (98%)	1 (2%)	0	100	100
30	28	62/65 (95%)	60 (97%)	2 (3%)	0	100	100
31	19	35/37 (95%)	32 (91%)	3 (9%)	0	100	100
31	29	35/37 (95%)	33 (94%)	2 (6%)	0	100	100
33	1b	229/256 (90%)	195 (85%)	28 (12%)	6 (3%)	5	17
33	2b	229/256 (90%)	199 (87%)	24 (10%)	6 (3%)	5	17
34	1c	204/239 (85%)	189 (93%)	14 (7%)	1 (0%)	29	57
34	2c	204/239 (85%)	185 (91%)	18 (9%)	1 (0%)	29	57
35	1d	206/209 (99%)	193 (94%)	13 (6%)	0	100	100
35	2d	206/209 (99%)	195 (95%)	10 (5%)	1 (0%)	29	57
36	1e	146/162 (90%)	129 (88%)	14 (10%)	3 (2%)	7	22
36	2e	146/162 (90%)	134 (92%)	10 (7%)	2 (1%)	11	31
37	1f	98/101 (97%)	93 (95%)	5 (5%)	0	100	100
37	2f	98/101 (97%)	90 (92%)	8 (8%)	0	100	100
38	1g	153/156 (98%)	137 (90%)	13 (8%)	3 (2%)	7	23
38	2g	153/156 (98%)	142 (93%)	8 (5%)	3 (2%)	7	23
39	1h	135/138 (98%)	131 (97%)	4 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
39	2h	135/138 (98%)	130 (96%)	5 (4%)	0	100	100
40	1i	125/128 (98%)	111 (89%)	14 (11%)	0	100	100
40	2i	125/128 (98%)	115 (92%)	9 (7%)	1 (1%)	19	46
41	1j	95/105 (90%)	83 (87%)	8 (8%)	4 (4%)	3	8
41	2j	94/105 (90%)	81 (86%)	8 (8%)	5 (5%)	2	5
42	1k	112/129 (87%)	106 (95%)	5 (4%)	1 (1%)	17	43
42	2k	112/129 (87%)	102 (91%)	8 (7%)	2 (2%)	8	25
43	1l	119/132 (90%)	113 (95%)	6 (5%)	0	100	100
43	2l	119/132 (90%)	114 (96%)	5 (4%)	0	100	100
44	1m	121/126 (96%)	113 (93%)	7 (6%)	1 (1%)	19	46
44	2m	120/126 (95%)	107 (89%)	11 (9%)	2 (2%)	9	27
45	1n	58/61 (95%)	54 (93%)	4 (7%)	0	100	100
45	2n	58/61 (95%)	52 (90%)	6 (10%)	0	100	100
46	1o	86/89 (97%)	82 (95%)	3 (4%)	1 (1%)	13	35
46	2o	86/89 (97%)	81 (94%)	4 (5%)	1 (1%)	13	35
47	1p	80/88 (91%)	72 (90%)	8 (10%)	0	100	100
47	2p	80/88 (91%)	74 (92%)	6 (8%)	0	100	100
48	1q	97/105 (92%)	92 (95%)	4 (4%)	1 (1%)	15	40
48	2q	97/105 (92%)	92 (95%)	5 (5%)	0	100	100
49	1r	66/88 (75%)	62 (94%)	4 (6%)	0	100	100
49	2r	66/88 (75%)	66 (100%)	0	0	100	100
50	1s	81/93 (87%)	74 (91%)	6 (7%)	1 (1%)	13	35
50	2s	81/93 (87%)	73 (90%)	8 (10%)	0	100	100
51	1t	94/106 (89%)	86 (92%)	5 (5%)	3 (3%)	4	13
51	2t	94/106 (89%)	80 (85%)	7 (7%)	7 (7%)	1	2
52	1u	21/27 (78%)	19 (90%)	2 (10%)	0	100	100
52	2u	21/27 (78%)	20 (95%)	1 (5%)	0	100	100
All	All	11370/12128 (94%)	10568 (93%)	709 (6%)	93 (1%)	19	46

5 of 93 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
7	1H	126	PRO

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Mol	Chain	Res	Type
26	14	55	ARG
41	1j	56	HIS
5	2F	89	VAL
26	24	55	ARG

### 5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	1D	215/218 (99%)	208 (97%)	7 (3%)	38	68
3	2D	215/218 (99%)	204 (95%)	11 (5%)	24	52
4	1E	164/166 (99%)	151 (92%)	13 (8%)	12	31
4	2E	164/166 (99%)	152 (93%)	12 (7%)	14	35
5	1F	160/166 (96%)	147 (92%)	13 (8%)	11	30
5	2F	159/166 (96%)	147 (92%)	12 (8%)	13	34
6	1G	143/156 (92%)	137 (96%)	6 (4%)	30	60
6	2G	143/156 (92%)	133 (93%)	10 (7%)	15	37
7	1H	144/148 (97%)	134 (93%)	10 (7%)	15	38
7	2H	144/148 (97%)	140 (97%)	4 (3%)	43	73
8	1I	113/124 (91%)	103 (91%)	10 (9%)	10	26
8	2I	105/124 (85%)	99 (94%)	6 (6%)	20	47
9	1N	118/119 (99%)	110 (93%)	8 (7%)	16	38
9	2N	118/119 (99%)	109 (92%)	9 (8%)	13	33
10	1O	100/100 (100%)	95 (95%)	5 (5%)	24	53
10	2O	100/100 (100%)	99 (99%)	1 (1%)	76	91
11	1P	115/116 (99%)	108 (94%)	7 (6%)	18	43
11	2P	115/116 (99%)	108 (94%)	7 (6%)	18	43
12	1Q	111/111 (100%)	108 (97%)	3 (3%)	44	74
12	2Q	111/111 (100%)	109 (98%)	2 (2%)	59	82

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
13	1R	101/101 (100%)	92 (91%)	9 (9%)	9	26
13	2R	101/101 (100%)	91 (90%)	10 (10%)	8	21
14	1S	86/88 (98%)	81 (94%)	5 (6%)	20	46
14	2S	85/88 (97%)	80 (94%)	5 (6%)	19	45
15	1T	115/127 (91%)	107 (93%)	8 (7%)	15	37
15	2T	113/127 (89%)	109 (96%)	4 (4%)	36	67
16	1U	93/94 (99%)	90 (97%)	3 (3%)	39	69
16	2U	93/94 (99%)	92 (99%)	1 (1%)	73	90
17	1V	80/82 (98%)	73 (91%)	7 (9%)	10	26
17	2V	80/82 (98%)	77 (96%)	3 (4%)	33	64
18	1W	90/92 (98%)	87 (97%)	3 (3%)	38	68
18	2W	90/92 (98%)	89 (99%)	1 (1%)	73	90
19	1X	77/78 (99%)	73 (95%)	4 (5%)	23	51
19	2X	77/78 (99%)	72 (94%)	5 (6%)	17	41
20	1Y	85/91 (93%)	79 (93%)	6 (7%)	14	36
20	2Y	85/91 (93%)	80 (94%)	5 (6%)	19	45
21	1Z	135/179 (75%)	123 (91%)	12 (9%)	9	26
21	2Z	137/179 (76%)	131 (96%)	6 (4%)	28	58
22	10	65/67 (97%)	61 (94%)	4 (6%)	18	43
22	20	65/67 (97%)	61 (94%)	4 (6%)	18	43
23	11	80/83 (96%)	73 (91%)	7 (9%)	10	26
23	21	80/83 (96%)	77 (96%)	3 (4%)	33	64
24	12	65/67 (97%)	65 (100%)	0	100	100
24	22	65/67 (97%)	65 (100%)	0	100	100
25	13	51/52 (98%)	49 (96%)	2 (4%)	32	63
25	23	50/52 (96%)	47 (94%)	3 (6%)	19	45
26	14	59/63 (94%)	55 (93%)	4 (7%)	16	38
26	24	53/63 (84%)	48 (91%)	5 (9%)	8	23
27	15	50/52 (96%)	46 (92%)	4 (8%)	12	31
27	25	50/52 (96%)	45 (90%)	5 (10%)	7	21
28	16	51/52 (98%)	48 (94%)	3 (6%)	19	45

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
28	26	50/52 (96%)	45 (90%)	5 (10%)	7	21
29	17	41/42 (98%)	37 (90%)	4 (10%)	8	21
29	27	41/42 (98%)	37 (90%)	4 (10%)	8	21
30	18	54/55 (98%)	49 (91%)	5 (9%)	9	24
30	28	54/55 (98%)	48 (89%)	6 (11%)	6	16
31	19	34/34 (100%)	33 (97%)	1 (3%)	42	72
31	29	34/34 (100%)	34 (100%)	0	100	100
33	1b	192/220 (87%)	180 (94%)	12 (6%)	18	42
33	2b	187/220 (85%)	171 (91%)	16 (9%)	10	27
34	1c	142/188 (76%)	132 (93%)	10 (7%)	15	37
34	2c	140/188 (74%)	135 (96%)	5 (4%)	35	66
35	1d	169/181 (93%)	157 (93%)	12 (7%)	14	36
35	2d	173/181 (96%)	165 (95%)	8 (5%)	27	56
36	1e	113/123 (92%)	106 (94%)	7 (6%)	18	43
36	2e	114/123 (93%)	110 (96%)	4 (4%)	36	67
37	1f	84/90 (93%)	81 (96%)	3 (4%)	35	66
37	2f	85/90 (94%)	81 (95%)	4 (5%)	26	56
38	1g	119/127 (94%)	115 (97%)	4 (3%)	37	67
38	2g	120/127 (94%)	116 (97%)	4 (3%)	38	68
39	1h	114/119 (96%)	109 (96%)	5 (4%)	28	58
39	2h	114/119 (96%)	106 (93%)	8 (7%)	15	37
40	1i	90/99 (91%)	85 (94%)	5 (6%)	21	47
40	2i	89/99 (90%)	86 (97%)	3 (3%)	37	67
41	1j	66/92 (72%)	62 (94%)	4 (6%)	18	43
41	2j	69/92 (75%)	66 (96%)	3 (4%)	29	59
42	1k	82/99 (83%)	78 (95%)	4 (5%)	25	54
42	2k	83/99 (84%)	77 (93%)	6 (7%)	14	35
43	1l	96/108 (89%)	93 (97%)	3 (3%)	40	71
43	2l	96/108 (89%)	91 (95%)	5 (5%)	23	51
44	1m	93/101 (92%)	89 (96%)	4 (4%)	29	59
44	2m	92/101 (91%)	89 (97%)	3 (3%)	38	68

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
45	1n	49/50 (98%)	45 (92%)	4 (8%)	11	29
45	2n	49/50 (98%)	46 (94%)	3 (6%)	18	43
46	1o	78/80 (98%)	76 (97%)	2 (3%)	46	75
46	2o	78/80 (98%)	74 (95%)	4 (5%)	24	52
47	1p	69/74 (93%)	65 (94%)	4 (6%)	20	46
47	2p	68/74 (92%)	62 (91%)	6 (9%)	10	26
48	1q	94/97 (97%)	89 (95%)	5 (5%)	22	50
48	2q	94/97 (97%)	92 (98%)	2 (2%)	53	79
49	1r	59/77 (77%)	57 (97%)	2 (3%)	37	67
49	2r	59/77 (77%)	55 (93%)	4 (7%)	16	38
50	1s	69/80 (86%)	61 (88%)	8 (12%)	5	14
50	2s	67/80 (84%)	61 (91%)	6 (9%)	9	25
51	1t	70/82 (85%)	69 (99%)	1 (1%)	67	86
51	2t	70/82 (85%)	67 (96%)	3 (4%)	29	59
52	1u	18/22 (82%)	18 (100%)	0	100	100
52	2u	18/22 (82%)	17 (94%)	1 (6%)	21	47
All	All	9303/10064 (92%)	8784 (94%)	519 (6%)	21	47

5 of 519 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
41	1j	81	THR
4	2E	113	PHE
42	2k	109	VAL
43	1l	117	ARG
50	1s	12	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 97 such sidechains are listed below:

Mol	Chain	Res	Type
40	1i	87	GLN
3	2D	116	GLN
41	2j	21	GLN
40	1i	124	GLN
50	1s	14	HIS

### 5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	1A	2861/2915 (98%)	492 (17%)	23 (0%)
1	2A	2788/2915 (95%)	540 (19%)	19 (0%)
2	1B	119/121 (98%)	10 (8%)	0
2	2B	118/121 (97%)	33 (27%)	0
32	1a	1494/1521 (98%)	276 (18%)	0
32	2a	1498/1521 (98%)	319 (21%)	0
53	1v	12/27 (44%)	2 (16%)	0
53	2v	12/27 (44%)	4 (33%)	0
54	1w	68/76 (89%)	25 (36%)	0
54	1y	70/76 (92%)	25 (35%)	0
54	2w	68/76 (89%)	29 (42%)	0
54	2y	68/76 (89%)	32 (47%)	0
55	1x	75/77 (97%)	11 (14%)	0
55	2x	75/77 (97%)	15 (20%)	0
All	All	9326/9626 (96%)	1813 (19%)	42 (0%)

5 of 1813 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	1A	10	G
1	1A	34	C
1	1A	45	C
1	1A	58	G
1	1A	59	U

5 of 42 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	1A	1992	G
1	2A	228	A
1	2A	1790	C
1	1A	2134	A
1	1A	2183	C

## 5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The



Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
32	UR3	1a	1498	32	14,22,23	0.74	0	15,32,35	0.66	0
43	0TD	1l	92	43	4,9,10	3.14	1 (25%)	3,11,13	11.35	1 (33%)
1	PSU	2A	1911	1	17,21,22	1.51	2 (11%)	20,30,33	3.17	6 (30%)
1	PSU	1A	1917	1	17,21,22	1.63	2 (11%)	20,30,33	3.07	6 (30%)
55	5MC	1x	32	55	15,22,23	1.32	1 (6%)	19,32,35	1.39	3 (15%)
1	PSU	2A	1917	1,56	17,21,22	1.56	2 (11%)	20,30,33	3.14	6 (30%)
54	6MZ	1y	37	54	18,25,26	0.99	1 (5%)	16,36,39	2.21	4 (25%)
32	UR3	2a	1498	32	14,22,23	0.80	1 (7%)	15,32,35	0.70	0
32	7MG	2a	527	32,56	22,26,27	1.75	4 (18%)	28,39,42	2.74	9 (32%)
32	5MC	1a	1404	32	15,22,23	1.28	1 (6%)	19,32,35	1.36	3 (15%)
32	PSU	2a	516	32	17,21,22	1.45	2 (11%)	20,30,33	3.08	6 (30%)
32	5MC	2a	967	32	15,22,23	1.37	1 (6%)	19,32,35	1.33	3 (15%)
54	5MU	1y	54	54	15,22,23	1.06	1 (6%)	16,32,35	1.74	2 (12%)
1	PSU	1A	1911	1	17,21,22	1.54	3 (17%)	20,30,33	3.10	6 (30%)
1	PSU	1A	2605	1,56	17,21,22	1.53	3 (17%)	20,30,33	3.15	6 (30%)
32	2MG	2a	1207	32,56	19,26,27	1.25	2 (10%)	21,38,41	2.13	6 (28%)
32	PSU	1a	516	32,56	17,21,22	1.53	3 (17%)	20,30,33	3.03	6 (30%)
1	2MU	2A	2552	1,56	14,22,24	0.90	0	14,31,36	0.85	0
32	5MC	2a	1404	32	15,22,23	1.23	1 (6%)	19,32,35	1.52	4 (21%)
32	7MG	1a	527	32	22,26,27	1.77	3 (13%)	28,39,42	2.84	9 (32%)
54	4SU	1w	8	54	14,21,22	1.33	1 (7%)	15,30,33	1.42	2 (13%)
1	PSU	2A	2605	1	17,21,22	1.54	3 (17%)	20,30,33	3.17	6 (30%)
32	4OC	2a	1402	32,56	16,23,24	0.62	0	17,32,35	1.24	1 (5%)
1	5MU	1A	1939	1	15,22,23	1.07	1 (6%)	16,32,35	1.90	2 (12%)
32	MA6	2a	1518	32	19,26,27	0.99	1 (5%)	18,38,41	1.73	6 (33%)
32	MA6	1a	1518	32	19,26,27	0.99	1 (5%)	18,38,41	1.74	6 (33%)
54	CM0	2w	34	54	16,26,27	1.09	1 (6%)	18,37,40	1.93	4 (22%)
1	2MA	2A	2503	1	17,25,26	1.36	2 (11%)	19,37,40	2.13	3 (15%)
55	PSU	2x	55	55	17,21,22	1.47	2 (11%)	20,30,33	3.12	6 (30%)
54	6MZ	2w	37	54	18,25,26	0.96	1 (5%)	16,36,39	1.72	3 (18%)
1	4OC	1A	1920	1	15,22,24	0.64	0	17,31,35	1.59	2 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
32	2MG	1a	1207	32,56	19,26,27	1.28	2 (10%)	21,38,41	2.42	8 (38%)
54	PSU	1w	55	54	17,21,22	1.37	2 (11%)	20,30,33	3.34	6 (30%)
32	5MC	2a	1407	32,56	15,22,23	1.31	1 (6%)	19,32,35	1.35	3 (15%)
1	5MC	2A	1962	1,56	15,22,23	1.32	1 (6%)	19,32,35	1.36	3 (15%)
32	5MC	1a	1407	32	15,22,23	1.34	1 (6%)	19,32,35	1.34	3 (15%)
32	5MC	1a	1400	32	15,22,23	1.32	1 (6%)	19,32,35	1.39	3 (15%)
32	4OC	1a	1402	32	16,23,24	0.67	0	17,32,35	1.15	1 (5%)
1	OMG	2A	2251	1,55,56	18,26,27	1.21	2 (11%)	20,38,41	2.09	6 (30%)
1	4OC	2A	1920	1	15,22,24	0.64	0	17,31,35	1.47	2 (11%)
54	4SU	1y	8	54	14,21,22	1.24	1 (7%)	15,30,33	1.80	3 (20%)
32	MA6	2a	1519	32	19,26,27	0.99	1 (5%)	18,38,41	1.66	5 (27%)
1	OMG	1A	2251	1,55,56	18,26,27	1.15	2 (11%)	20,38,41	2.16	6 (30%)
1	2MU	1A	2552	1,56	14,22,24	0.86	0	14,31,36	0.68	1 (7%)
55	PSU	1x	55	55	17,21,22	1.58	2 (11%)	20,30,33	3.14	6 (30%)
54	4SU	2w	8	54	14,21,22	1.30	1 (7%)	15,30,33	1.33	2 (13%)
54	7MG	1w	46	54	22,26,27	1.80	4 (18%)	28,39,42	2.75	9 (32%)
1	5MC	2A	1942	1	15,22,23	1.30	1 (6%)	19,32,35	1.32	3 (15%)
54	5MU	1w	54	54	15,22,23	1.00	1 (6%)	16,32,35	1.85	2 (12%)
1	5MU	1A	1915	1	15,22,23	1.08	1 (6%)	16,32,35	2.01	1 (6%)
54	5MU	2y	54	54	15,22,23	1.03	1 (6%)	16,32,35	1.72	2 (12%)
1	5MC	1A	1962	1,56	15,22,23	1.29	1 (6%)	19,32,35	1.34	3 (15%)
1	5MU	2A	1915	1	15,22,23	1.07	1 (6%)	16,32,35	1.85	2 (12%)
54	PSU	1y	55	54	17,21,22	1.54	3 (17%)	20,30,33	3.14	6 (30%)
54	PSU	2w	55	54	17,21,22	1.33	2 (11%)	20,30,33	3.17	6 (30%)
55	4SU	1x	8	55	14,21,22	1.40	2 (14%)	15,30,33	2.22	2 (13%)
54	PSU	2y	55	54	17,21,22	1.60	3 (17%)	20,30,33	3.16	6 (30%)
54	6MZ	2y	37	54,32	18,25,26	0.95	1 (5%)	16,36,39	2.02	4 (25%)
54	7MG	2y	46	54	22,26,27	1.79	3 (13%)	28,39,42	3.15	11 (39%)
54	CM0	1w	34	54	16,26,27	1.07	2 (12%)	18,37,40	1.92	3 (16%)
32	M2G	1a	966	32	20,27,28	1.40	3 (15%)	22,40,43	2.14	5 (22%)
54	7MG	1y	46	54	22,26,27	1.81	3 (13%)	28,39,42	2.88	9 (32%)
54	4SU	2y	8	54	14,21,22	1.34	1 (7%)	15,30,33	1.40	3 (20%)
1	5MC	1A	1942	1	15,22,23	1.31	1 (6%)	19,32,35	1.34	3 (15%)
1	2MA	1A	2503	1,56	17,25,26	1.32	2 (11%)	19,37,40	2.14	4 (21%)
55	5MU	1x	54	55	15,22,23	1.04	1 (6%)	16,32,35	2.15	1 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
1	5MU	2A	1939	1,56	15,22,23	1.08	1 (6%)	16,32,35	1.77	2 (12%)
54	6MZ	1w	37	54	18,25,26	0.96	1 (5%)	16,36,39	2.04	4 (25%)
32	5MC	1a	967	32	15,22,23	1.30	1 (6%)	19,32,35	1.32	3 (15%)
54	5MU	2w	54	54	15,22,23	1.04	1 (6%)	16,32,35	2.06	2 (12%)
54	CM0	1y	34	54	16,26,27	1.13	1 (6%)	18,37,40	1.90	4 (22%)
54	7MG	2w	46	54	22,26,27	1.81	4 (18%)	28,39,42	2.57	8 (28%)
32	M2G	2a	966	32	20,27,28	1.42	3 (15%)	22,40,43	2.17	7 (31%)
32	MA6	1a	1519	32	19,26,27	1.04	1 (5%)	18,38,41	1.75	6 (33%)
55	5MC	2x	32	55	15,22,23	1.35	1 (6%)	19,32,35	1.35	3 (15%)
43	0TD	2l	92	43	4,9,10	3.09	1 (25%)	3,11,13	1.94	1 (33%)
55	4SU	2x	8	55	14,21,22	1.38	2 (14%)	15,30,33	2.09	2 (13%)
54	CM0	2y	34	54	16,26,27	1.14	2 (12%)	18,37,40	1.97	3 (16%)
55	5MU	2x	54	55	15,22,23	1.10	1 (6%)	16,32,35	1.94	2 (12%)
32	5MC	2a	1400	32	15,22,23	1.41	1 (6%)	19,32,35	1.42	3 (15%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
32	UR3	1a	1498	32	-	1/5/25/26	0/2/2/2
43	0TD	1l	92	43	-	2/3/12/14	-
1	PSU	2A	1911	1	-	0/7/25/26	0/2/2/2
1	PSU	1A	1917	1	-	0/7/25/26	0/2/2/2
55	5MC	1x	32	55	-	0/5/25/26	0/2/2/2
1	PSU	2A	1917	1,56	-	0/7/25/26	0/2/2/2
54	6MZ	1y	37	54	-	0/5/27/28	0/3/3/3
32	UR3	2a	1498	32	-	1/5/25/26	0/2/2/2
32	7MG	2a	527	32,56	-	3/7/37/38	0/3/3/3
32	5MC	1a	1404	32	-	0/5/25/26	0/2/2/2
32	PSU	2a	516	32	-	0/7/25/26	0/2/2/2
32	5MC	2a	967	32	-	2/5/25/26	0/2/2/2
54	5MU	1y	54	54	-	2/5/25/26	0/2/2/2
1	PSU	1A	1911	1	-	0/7/25/26	0/2/2/2
1	PSU	1A	2605	1,56	-	0/7/25/26	0/2/2/2
32	2MG	2a	1207	32,56	-	2/5/27/28	0/3/3/3
32	PSU	1a	516	32,56	-	0/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	2MU	2A	2552	1,56	-	0/7/27/28	0/2/2/2
32	5MC	2a	1404	32	-	0/5/25/26	0/2/2/2
32	7MG	1a	527	32	-	1/7/37/38	0/3/3/3
54	4SU	1w	8	54	-	0/5/25/26	0/2/2/2
1	PSU	2A	2605	1	-	0/7/25/26	0/2/2/2
32	4OC	2a	1402	32,56	-	2/9/29/30	0/2/2/2
1	5MU	1A	1939	1	-	0/5/25/26	0/2/2/2
32	MA6	2a	1518	32	-	1/7/29/30	0/3/3/3
32	MA6	1a	1518	32	-	1/7/29/30	0/3/3/3
54	CM0	2w	34	54	-	3/8/30/31	0/2/2/2
1	2MA	2A	2503	1	-	2/3/25/26	0/3/3/3
55	PSU	2x	55	55	-	0/7/25/26	0/2/2/2
54	6MZ	2w	37	54	-	2/5/27/28	0/3/3/3
1	4OC	1A	1920	1	-	0/7/27/30	0/2/2/2
32	2MG	1a	1207	32,56	-	0/5/27/28	0/3/3/3
54	PSU	1w	55	54	-	0/7/25/26	0/2/2/2
32	5MC	2a	1407	32,56	-	0/5/25/26	0/2/2/2
1	5MC	2A	1962	1,56	-	2/5/25/26	0/2/2/2
32	5MC	1a	1407	32	-	0/5/25/26	0/2/2/2
32	5MC	1a	1400	32	-	2/5/25/26	0/2/2/2
32	4OC	1a	1402	32	-	4/9/29/30	0/2/2/2
1	OMG	2A	2251	1,55,56	-	0/5/27/28	0/3/3/3
1	4OC	2A	1920	1	-	0/7/27/30	0/2/2/2
54	4SU	1y	8	54	-	2/5/25/26	0/2/2/2
32	MA6	2a	1519	32	-	4/7/29/30	0/3/3/3
1	OMG	1A	2251	1,55,56	-	0/5/27/28	0/3/3/3
1	2MU	1A	2552	1,56	-	0/7/27/28	0/2/2/2
55	PSU	1x	55	55	-	0/7/25/26	0/2/2/2
54	4SU	2w	8	54	-	1/5/25/26	0/2/2/2
54	7MG	1w	46	54	-	2/7/37/38	0/3/3/3
1	5MC	2A	1942	1	-	0/5/25/26	0/2/2/2
54	5MU	1w	54	54	-	0/5/25/26	0/2/2/2
1	5MU	1A	1915	1	-	3/5/25/26	0/2/2/2
54	5MU	2y	54	54	-	3/5/25/26	0/2/2/2
1	5MC	1A	1962	1,56	-	2/5/25/26	0/2/2/2
1	5MU	2A	1915	1	-	0/5/25/26	0/2/2/2
54	PSU	1y	55	54	-	0/7/25/26	0/2/2/2
54	PSU	2w	55	54	-	0/7/25/26	0/2/2/2
55	4SU	1x	8	55	-	0/5/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
54	PSU	2y	55	54	-	0/7/25/26	0/2/2/2
54	6MZ	2y	37	54,32	-	1/5/27/28	0/3/3/3
54	7MG	2y	46	54	-	2/7/37/38	0/3/3/3
54	CM0	1w	34	54	-	5/8/30/31	0/2/2/2
32	M2G	1a	966	32	-	4/7/29/30	0/3/3/3
54	7MG	1y	46	54	-	5/7/37/38	0/3/3/3
54	4SU	2y	8	54	-	1/5/25/26	0/2/2/2
1	5MC	1A	1942	1	-	0/5/25/26	0/2/2/2
1	2MA	1A	2503	1,56	-	2/3/25/26	0/3/3/3
55	5MU	1x	54	55	-	0/5/25/26	0/2/2/2
1	5MU	2A	1939	1,56	-	2/5/25/26	0/2/2/2
54	6MZ	1w	37	54	-	0/5/27/28	0/3/3/3
32	5MC	1a	967	32	-	2/5/25/26	0/2/2/2
54	5MU	2w	54	54	-	0/5/25/26	0/2/2/2
54	CM0	1y	34	54	-	1/8/30/31	0/2/2/2
54	7MG	2w	46	54	-	2/7/37/38	0/3/3/3
32	M2G	2a	966	32	-	4/7/29/30	0/3/3/3
32	MA6	1a	1519	32	-	3/7/29/30	0/3/3/3
55	5MC	2x	32	55	-	1/5/25/26	0/2/2/2
43	0TD	2l	92	43	-	1/3/12/14	-
55	4SU	2x	8	55	-	1/5/25/26	0/2/2/2
54	CM0	2y	34	54	-	4/8/30/31	0/2/2/2
55	5MU	2x	54	55	-	0/5/25/26	0/2/2/2
32	5MC	2a	1400	32	-	3/5/25/26	0/2/2/2

The worst 5 of 122 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
43	1l	92	0TD	CB-SB	-6.03	1.69	1.84
43	2l	92	0TD	CB-SB	-5.93	1.69	1.84
54	2w	46	7MG	C6-C5	5.44	1.48	1.41
54	1y	46	7MG	C6-C5	5.04	1.48	1.41
32	2a	1400	5MC	C5-C4	5.04	1.49	1.41

The worst 5 of 320 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
43	1l	92	0TD	CSB-SB-CB	-19.61	63.27	101.85
54	2y	46	7MG	N3-C4-N9	10.11	139.90	126.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	1a	527	7MG	N3-C4-N9	9.64	139.29	126.91
54	1y	46	7MG	N3-C4-N9	9.51	139.12	126.91
32	2a	527	7MG	N3-C4-N9	9.05	138.54	126.91

There are no chirality outliers.

5 of 94 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
32	1a	1498	UR3	O4'-C1'-N1-C6
32	2a	1402	4OC	O4'-C4'-C5'-O5'
32	2a	1498	UR3	O4'-C1'-N1-C6
54	1y	54	5MU	C3'-C4'-C5'-O5'
54	1y	54	5MU	O4'-C4'-C5'-O5'

There are no ring outliers.

12 monomers are involved in 14 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	2A	1917	PSU	1	0
1	2A	2552	2MU	2	0
1	2A	2605	PSU	1	0
1	1A	1939	5MU	1	0
1	2A	2503	2MA	1	0
1	2A	2251	OMG	1	0
1	2A	1920	4OC	1	0
1	1A	2251	OMG	1	0
1	1A	2552	2MU	1	0
1	2A	1942	5MC	1	0
1	2A	1915	5MU	2	0
1	1A	1942	5MC	1	0

## 5.5 Carbohydrates

There are no carbohydrates in this entry.

## 5.6 Ligand geometry

Of 2761 ligands modelled in this entry, 2757 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
57	ERY	1A	4074	-	53,53,53	0.93	2 (3%)	82,82,82	1.73	23 (28%)
59	SF4	1d	302	35	0,12,12	0.00	-	-		
59	SF4	2d	302	35	0,12,12	0.00	-	-		
57	ERY	2A	3875	-	53,53,53	0.93	2 (3%)	82,82,82	1.65	16 (19%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
57	ERY	1A	4074	-	-	5/72/107/107	0/3/3/3
59	SF4	1d	302	35	-	-	0/6/5/5
59	SF4	2d	302	35	-	-	0/6/5/5
57	ERY	2A	3875	-	-	12/72/107/107	0/3/3/3

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
57	2A	3875	ERY	O2-C1	4.88	1.45	1.34
57	1A	4074	ERY	O2-C1	4.85	1.45	1.34
57	1A	4074	ERY	O2-C13	-2.12	1.42	1.46
57	2A	3875	ERY	O2-C13	-2.05	1.42	1.46

The worst 5 of 39 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
57	1A	4074	ERY	C25-C24-C23	4.73	116.78	109.97
57	1A	4074	ERY	O5-C16-C15	-4.27	106.11	112.96
57	2A	3875	ERY	C13-O2-C1	-4.04	111.00	118.18
57	2A	3875	ERY	O5-C16-C15	-4.00	106.55	112.96
57	2A	3875	ERY	O2-C1-C2	3.93	120.18	111.56

There are no chirality outliers.

5 of 17 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
57	2A	3875	ERY	C9-C10-C11-C12
57	2A	3875	ERY	C34-C10-C11-C12
57	2A	3875	ERY	C15-C16-O5-C20
57	2A	3875	ERY	C17-C16-O5-C20
57	2A	3875	ERY	C19-C16-O5-C20

There are no ring outliers.

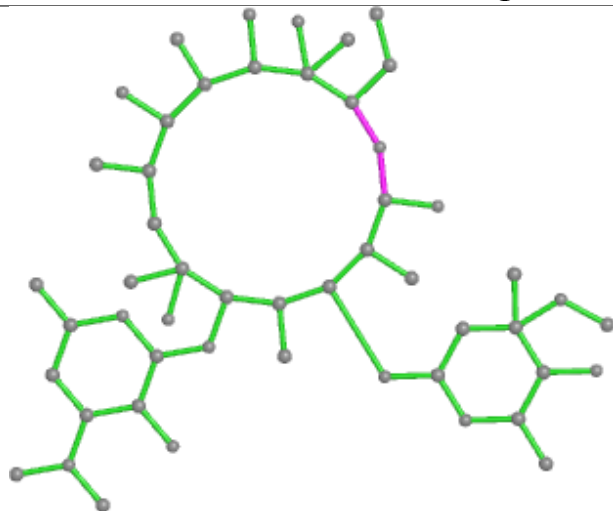
2 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
57	1A	4074	ERY	3	0
57	2A	3875	ERY	3	0

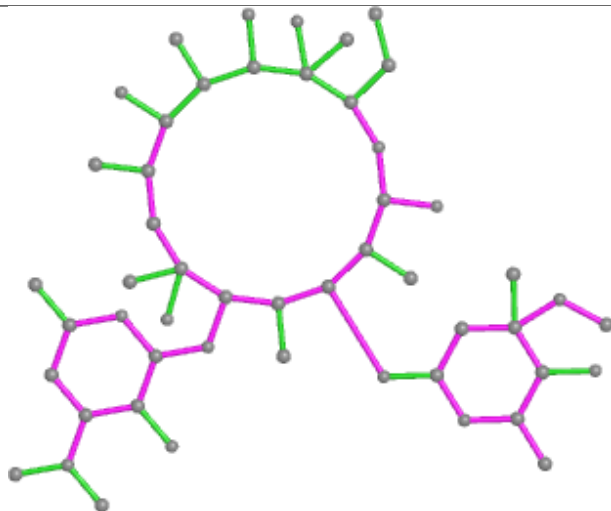
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



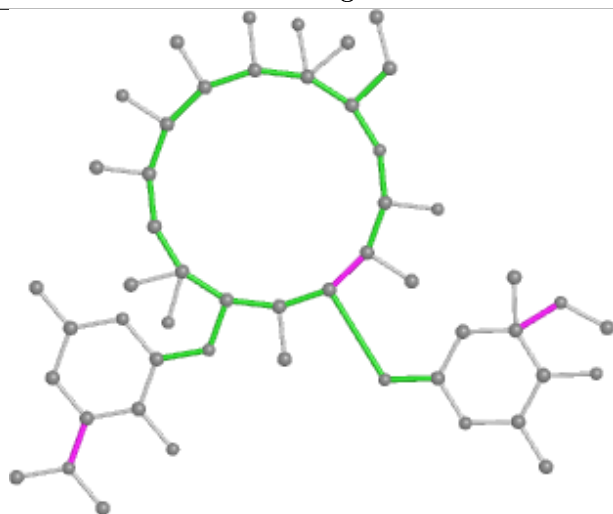
## Ligand ERY 1A 4074



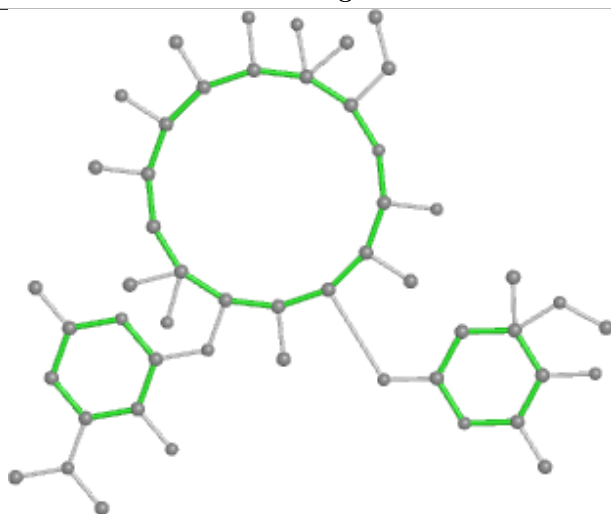
Bond lengths



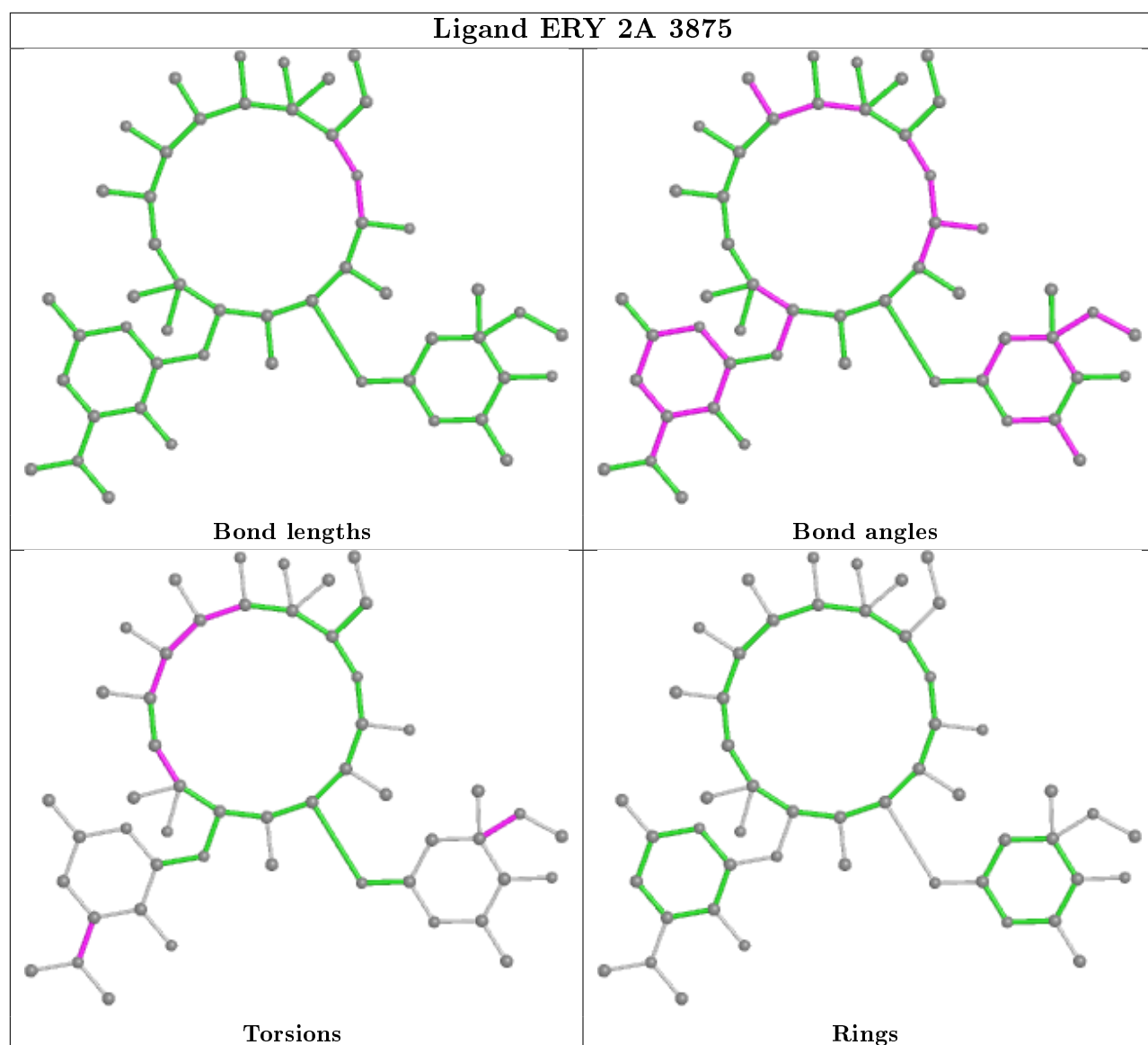
Bond angles



Torsions



Rings



## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	1A	2860/2915 (98%)	0.08	12 (0%) 92 92	10, 28, 83, 100	0
1	2A	2789/2915 (95%)	0.00	9 (0%) 94 94	28, 51, 82, 99	0
2	1B	120/121 (99%)	-0.10	0 100 100	19, 42, 58, 77	0
2	2B	120/121 (99%)	-0.11	0 100 100	53, 72, 81, 86	0
3	1D	275/276 (99%)	0.03	1 (0%) 92 92	13, 30, 43, 72	0
3	2D	275/276 (99%)	0.64	15 (5%) 25 20	25, 44, 58, 68	0
4	1E	204/206 (99%)	0.08	0 100 100	11, 33, 48, 71	0
4	2E	204/206 (99%)	0.32	5 (2%) 57 54	27, 54, 65, 72	0
5	1F	203/210 (96%)	0.17	1 (0%) 91 90	13, 33, 57, 76	0
5	2F	203/210 (96%)	0.41	8 (3%) 39 34	29, 56, 70, 79	0
6	1G	181/182 (99%)	0.02	1 (0%) 89 89	32, 51, 66, 76	0
6	2G	181/182 (99%)	0.95	27 (14%) 2 1	61, 72, 79, 89	0
7	1H	174/180 (96%)	-0.13	0 100 100	27, 44, 55, 61	0
7	2H	174/180 (96%)	1.15	34 (19%) 1 1	62, 73, 81, 89	0
8	1I	146/148 (98%)	-0.10	0 100 100	39, 62, 73, 79	0
8	2I	146/148 (98%)	0.22	8 (5%) 25 20	45, 65, 77, 83	0
9	1N	140/140 (100%)	0.01	0 100 100	14, 32, 49, 60	0
9	2N	140/140 (100%)	0.74	16 (11%) 5 3	43, 58, 69, 77	0
10	1O	122/122 (100%)	0.23	0 100 100	22, 33, 51, 56	0
10	2O	122/122 (100%)	0.67	10 (8%) 11 8	36, 52, 62, 70	0
11	1P	149/150 (99%)	0.25	3 (2%) 65 62	13, 38, 59, 67	0
11	2P	149/150 (99%)	0.42	8 (5%) 25 21	34, 56, 71, 86	0
12	1Q	141/141 (100%)	0.14	1 (0%) 87 87	20, 34, 46, 70	0
12	2Q	141/141 (100%)	0.89	16 (11%) 5 3	42, 58, 68, 75	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
13	1R	118/118 (100%)	0.11	0 100 100	16, 26, 38, 56	0
13	2R	118/118 (100%)	0.45	5 (4%) 36 31	32, 46, 56, 66	0
14	1S	110/112 (98%)	-0.05	0 100 100	29, 41, 53, 56	0
14	2S	110/112 (98%)	0.38	4 (3%) 42 37	56, 67, 75, 78	0
15	1T	131/146 (89%)	0.09	0 100 100	26, 38, 56, 70	0
15	2T	131/146 (89%)	0.37	4 (3%) 49 44	43, 55, 68, 76	0
16	1U	116/118 (98%)	0.21	1 (0%) 84 84	13, 21, 38, 53	0
16	2U	116/118 (98%)	0.59	6 (5%) 27 22	35, 56, 65, 71	0
17	1V	101/101 (100%)	-0.01	0 100 100	16, 29, 48, 57	0
17	2V	101/101 (100%)	0.55	7 (6%) 16 12	42, 61, 71, 76	0
18	1W	112/113 (99%)	0.06	0 100 100	13, 22, 37, 61	0
18	2W	112/113 (99%)	0.57	11 (9%) 7 5	33, 43, 56, 79	0
19	1X	95/96 (98%)	-0.06	0 100 100	16, 31, 46, 64	0
19	2X	95/96 (98%)	0.81	11 (11%) 4 3	34, 53, 63, 78	0
20	1Y	107/110 (97%)	0.04	0 100 100	23, 40, 58, 71	0
20	2Y	107/110 (97%)	0.85	15 (14%) 2 2	45, 60, 74, 81	0
21	1Z	154/206 (74%)	0.31	2 (1%) 77 76	31, 53, 75, 81	0
21	2Z	160/206 (77%)	0.60	10 (6%) 20 15	60, 72, 83, 87	0
22	10	83/85 (97%)	0.40	6 (7%) 15 11	19, 29, 53, 72	0
22	20	83/85 (97%)	1.18	15 (18%) 1 1	43, 57, 68, 75	0
23	11	97/98 (98%)	0.17	2 (2%) 63 60	15, 37, 62, 70	0
23	21	97/98 (98%)	0.69	7 (7%) 15 11	37, 50, 63, 70	0
24	12	70/72 (97%)	0.14	0 100 100	25, 37, 49, 65	0
24	22	70/72 (97%)	0.30	3 (4%) 35 30	45, 60, 70, 71	0
25	13	59/60 (98%)	0.07	0 100 100	15, 27, 55, 70	0
25	23	59/60 (98%)	1.22	11 (18%) 1 1	49, 58, 68, 75	0
26	14	69/71 (97%)	-0.05	0 100 100	48, 67, 79, 85	0
26	24	69/71 (97%)	0.57	8 (11%) 4 3	69, 79, 86, 90	0
27	15	59/60 (98%)	0.06	0 100 100	11, 22, 40, 53	0
27	25	59/60 (98%)	0.27	2 (3%) 45 39	33, 43, 59, 68	0
28	16	53/54 (98%)	-0.05	0 100 100	24, 35, 49, 57	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
28	26	53/54 (98%)	0.63	5 (9%) 8 5	42, 53, 64, 69	0
29	17	48/49 (97%)	0.17	2 (4%) 36 31	14, 20, 43, 59	0
29	27	48/49 (97%)	1.09	6 (12%) 3 2	25, 36, 57, 75	0
30	18	64/65 (98%)	0.23	1 (1%) 72 70	20, 26, 33, 47	0
30	28	64/65 (98%)	0.85	6 (9%) 8 5	38, 49, 58, 63	0
31	19	37/37 (100%)	0.16	0 100 100	22, 32, 44, 53	0
31	29	37/37 (100%)	1.47	12 (32%) 0 0	51, 61, 71, 75	0
32	1a	1488/1521 (97%)	-0.06	4 (0%) 94 94	28, 60, 83, 97	0
32	2a	1491/1521 (98%)	0.05	16 (1%) 80 80	45, 68, 87, 97	0
33	1b	231/256 (90%)	0.31	8 (3%) 44 38	54, 69, 78, 88	0
33	2b	231/256 (90%)	1.21	53 (22%) 0 0	60, 77, 86, 92	0
34	1c	206/239 (86%)	0.93	28 (13%) 3 2	53, 65, 74, 81	0
34	2c	206/239 (86%)	1.32	61 (29%) 0 0	58, 75, 83, 100	0
35	1d	208/209 (99%)	0.27	7 (3%) 45 39	52, 64, 72, 80	0
35	2d	208/209 (99%)	0.38	6 (2%) 51 47	43, 60, 68, 79	0
36	1e	148/162 (91%)	0.42	8 (5%) 25 21	48, 58, 66, 71	0
36	2e	148/162 (91%)	0.78	14 (9%) 8 5	58, 69, 77, 83	0
37	1f	100/101 (99%)	0.04	1 (1%) 82 81	45, 59, 67, 70	0
37	2f	100/101 (99%)	-0.07	1 (1%) 82 81	53, 63, 69, 74	0
38	1g	155/156 (99%)	0.34	12 (7%) 13 10	52, 62, 72, 80	0
38	2g	155/156 (99%)	0.72	22 (14%) 2 2	58, 70, 79, 88	0
39	1h	137/138 (99%)	0.44	9 (6%) 18 14	48, 58, 67, 70	0
39	2h	137/138 (99%)	0.69	12 (8%) 10 6	55, 67, 74, 75	0
40	1i	127/128 (99%)	0.98	20 (15%) 2 1	51, 68, 78, 86	0
40	2i	127/128 (99%)	1.95	55 (43%) 0 0	60, 76, 83, 88	0
41	1j	97/105 (92%)	0.69	11 (11%) 5 3	56, 70, 79, 84	0
41	2j	96/105 (91%)	1.47	31 (32%) 0 0	65, 75, 84, 89	0
42	1k	114/129 (88%)	0.80	14 (12%) 4 2	36, 57, 67, 71	0
42	2k	114/129 (88%)	0.99	18 (15%) 2 1	50, 65, 73, 77	0
43	1l	121/132 (91%)	0.09	1 (0%) 86 85	41, 52, 63, 70	0
43	2l	121/132 (91%)	0.44	7 (5%) 23 18	49, 62, 72, 75	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
44	1m	123/126 (97%)	0.23	4 (3%) 46 41	49, 61, 73, 82	0
44	2m	122/126 (96%)	1.34	26 (21%) 0 0	64, 75, 84, 89	0
45	1n	60/61 (98%)	0.99	9 (15%) 2 1	52, 62, 70, 75	0
45	2n	60/61 (98%)	2.68	39 (65%) 0 0	68, 76, 82, 84	0
46	1o	88/89 (98%)	0.10	2 (2%) 60 57	42, 55, 68, 73	0
46	2o	88/89 (98%)	0.33	1 (1%) 80 80	53, 64, 74, 78	0
47	1p	82/88 (93%)	1.28	17 (20%) 1 0	50, 62, 74, 76	0
47	2p	82/88 (93%)	0.51	3 (3%) 41 36	48, 59, 66, 78	0
48	1q	99/105 (94%)	0.41	5 (5%) 28 23	42, 55, 67, 73	0
48	2q	99/105 (94%)	0.55	7 (7%) 16 12	54, 63, 72, 77	0
49	1r	68/88 (77%)	0.32	3 (4%) 34 29	47, 58, 68, 73	0
49	2r	68/88 (77%)	0.33	1 (1%) 73 72	57, 62, 72, 76	0
50	1s	83/93 (89%)	0.15	2 (2%) 59 56	52, 63, 72, 77	0
50	2s	83/93 (89%)	0.81	10 (12%) 4 3	66, 76, 83, 92	0
51	1t	96/106 (90%)	0.41	4 (4%) 36 31	45, 61, 69, 72	0
51	2t	96/106 (90%)	0.55	9 (9%) 8 5	44, 60, 74, 79	0
52	1u	23/27 (85%)	1.03	5 (21%) 0 0	57, 63, 67, 72	0
52	2u	23/27 (85%)	2.50	13 (56%) 0 0	65, 74, 78, 79	0
53	1v	13/27 (48%)	0.77	1 (7%) 13 10	40, 63, 82, 88	0
53	2v	13/27 (48%)	1.12	4 (30%) 0 0	61, 75, 87, 90	0
54	1w	67/76 (88%)	0.99	10 (14%) 2 1	54, 83, 92, 98	0
54	1y	68/76 (89%)	0.52	4 (5%) 22 17	33, 86, 92, 98	0
54	2w	67/76 (88%)	1.88	27 (40%) 0 0	65, 89, 93, 98	0
54	2y	67/76 (88%)	1.04	10 (14%) 2 1	50, 89, 94, 96	0
55	1x	72/77 (93%)	-0.02	0 100 100	36, 61, 72, 78	0
55	2x	72/77 (93%)	0.05	1 (1%) 75 74	49, 73, 82, 92	0
All	All	20879/21754 (95%)	0.30	973 (4%) 31 27	10, 56, 81, 100	0

The worst 5 of 973 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
44	2m	124	PRO	13.8
45	2n	25	VAL	9.7

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Mol	Chain	Res	Type	RSRZ
44	2m	102	ARG	8.8
44	2m	6	GLY	8.7
44	2m	123	ALA	8.4

## 6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
54	PSU	2w	55	20/21	0.48	0.35	82,96,107,108	0
54	6MZ	2y	37	23/24	0.72	0.44	71,85,103,113	0
54	4SU	2y	8	20/21	0.75	0.19	82,92,104,109	0
54	PSU	1w	55	20/21	0.75	0.24	72,82,89,91	0
54	7MG	2y	46	24/25	0.75	0.25	75,93,100,110	0
54	4SU	1y	8	20/21	0.76	0.16	81,86,90,99	0
54	CM0	2y	34	25/26	0.77	0.39	76,88,100,116	0
54	5MU	2y	54	21/22	0.78	0.30	72,85,94,106	0
54	7MG	2w	46	24/25	0.82	0.28	79,92,98,107	0
54	7MG	1y	46	24/25	0.83	0.21	79,89,97,106	0
54	CM0	1y	34	25/26	0.83	0.32	59,84,89,100	0
54	4SU	1w	8	20/21	0.83	0.20	70,83,99,103	0
54	4SU	2w	8	20/21	0.83	0.26	89,95,100,101	0
54	5MU	1y	54	21/22	0.84	0.27	75,82,94,96	0
54	7MG	1w	46	24/25	0.84	0.19	75,83,91,102	0
54	PSU	2y	55	20/21	0.85	0.20	75,83,91,100	0
54	6MZ	1y	37	23/24	0.85	0.17	77,82,90,98	0
54	5MU	2w	54	21/22	0.86	0.20	75,83,90,98	0
1	5MU	2A	1915	21/22	0.86	0.17	62,69,78,91	0
55	4SU	2x	8	20/21	0.87	0.14	58,74,79,80	0
54	PSU	1y	55	20/21	0.88	0.23	74,82,94,99	0
54	CM0	2w	34	25/26	0.89	0.24	67,82,89,101	0
32	2MG	2a	1207	24/25	0.89	0.16	65,76,81,84	0
54	5MU	1w	54	21/22	0.89	0.22	68,74,81,86	0
54	CM0	1w	34	25/26	0.90	0.20	58,70,74,78	0
32	PSU	2a	516	20/21	0.90	0.13	60,64,69,69	0
32	M2G	2a	966	25/26	0.90	0.24	54,67,78,82	0
54	6MZ	1w	37	23/24	0.90	0.23	55,64,71,73	0
55	PSU	2x	55	20/21	0.90	0.12	70,78,86,93	0
55	4SU	1x	8	20/21	0.91	0.16	55,63,69,69	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
1	PSU	2A	1911	20/21	0.92	0.14	47,60,70,71	0
32	5MC	2a	1404	21/22	0.92	0.15	45,53,57,60	0
54	6MZ	2w	37	23/24	0.92	0.20	70,77,83,86	0
32	5MC	2a	967	21/22	0.92	0.23	54,67,73,79	0
43	0TD	1l	92	10/11	0.92	0.16	46,52,54,68	0
55	5MU	2x	54	21/22	0.92	0.15	71,78,83,85	0
43	0TD	2l	92	10/11	0.93	0.16	57,62,65,66	0
1	4OC	2A	1920	21/23	0.93	0.18	57,64,67,72	0
1	5MC	2A	1942	21/22	0.93	0.17	48,62,68,77	0
55	PSU	1x	55	20/21	0.93	0.15	54,59,74,77	0
32	MA6	2a	1518	24/25	0.93	0.21	49,60,64,66	0
32	4OC	2a	1402	22/23	0.94	0.15	48,60,64,65	0
1	5MU	1A	1915	21/22	0.94	0.15	40,51,57,58	0
32	UR3	2a	1498	21/22	0.94	0.20	42,52,58,62	0
32	7MG	2a	527	24/25	0.94	0.14	57,67,69,71	0
55	5MC	2x	32	21/22	0.94	0.21	63,69,74,76	0
32	PSU	1a	516	20/21	0.94	0.14	51,60,66,73	0
55	5MU	1x	54	21/22	0.94	0.15	48,61,64,74	0
1	PSU	2A	1917	20/21	0.94	0.15	51,60,66,71	0
32	5MC	1a	1400	21/22	0.95	0.17	41,49,54,59	0
1	PSU	1A	1911	20/21	0.95	0.16	29,39,51,52	0
32	2MG	1a	1207	24/25	0.95	0.17	48,60,66,66	0
1	PSU	1A	1917	20/21	0.95	0.15	32,52,55,56	0
32	MA6	2a	1519	24/25	0.95	0.24	41,56,60,62	0
1	5MC	2A	1962	21/22	0.95	0.15	30,47,54,66	0
32	5MC	2a	1400	21/22	0.95	0.20	61,66,68,71	0
1	5MU	2A	1939	21/22	0.96	0.19	35,41,47,47	0
1	PSU	1A	2605	20/21	0.96	0.20	14,20,26,27	0
32	5MC	1a	967	21/22	0.96	0.22	49,56,65,68	0
1	OMG	2A	2251	24/25	0.96	0.21	33,39,44,46	0
55	5MC	1x	32	21/22	0.96	0.20	47,56,62,64	0
1	PSU	2A	2605	20/21	0.96	0.16	27,34,40,43	0
32	5MC	2a	1407	21/22	0.96	0.15	45,51,54,56	0
32	5MC	1a	1404	21/22	0.96	0.18	30,34,39,40	0
32	M2G	1a	966	25/26	0.96	0.20	46,52,60,65	0
32	MA6	1a	1518	24/25	0.96	0.17	32,36,40,43	0
32	5MC	1a	1407	21/22	0.96	0.16	25,36,40,42	0
1	5MC	1A	1942	21/22	0.96	0.17	29,38,46,52	0
1	2MU	2A	2552	21/23	0.96	0.19	35,42,50,58	0
32	UR3	1a	1498	21/22	0.97	0.20	31,35,39,43	0
32	MA6	1a	1519	24/25	0.97	0.17	34,37,47,51	0
1	2MA	2A	2503	23/24	0.97	0.20	24,31,38,40	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
1	5MC	1A	1962	21/22	0.97	0.20	26,31,35,36	0
32	4OC	1a	1402	22/23	0.97	0.16	33,40,46,55	0
1	5MU	1A	1939	21/22	0.97	0.20	21,26,32,34	0
32	7MG	1a	527	24/25	0.97	0.15	32,41,45,46	0
1	4OC	1A	1920	21/23	0.97	0.18	31,40,45,46	0
1	2MU	1A	2552	21/23	0.98	0.15	16,22,26,27	0
1	OMG	1A	2251	24/25	0.98	0.18	10,15,22,23	0
1	2MA	1A	2503	23/24	0.98	0.20	6,12,15,18	0

### 6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

### 6.4 Ligands ⓘ

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	1A	3959	1/1	0.30	0.16	50,50,50,50	0
56	MG	2A	3670	1/1	0.35	0.22	67,67,67,67	0
56	MG	2A	3819	1/1	0.42	0.16	76,76,76,76	0
56	MG	2A	3766	1/1	0.42	0.38	80,80,80,80	0
56	MG	1A	3923	1/1	0.43	0.12	68,68,68,68	0
56	MG	2a	1777	1/1	0.43	0.11	69,69,69,69	0
56	MG	2A	3775	1/1	0.44	0.26	83,83,83,83	0
56	MG	1A	4073	1/1	0.45	0.40	66,66,66,66	0
56	MG	2A	3826	1/1	0.48	0.16	70,70,70,70	0
56	MG	2A	3786	1/1	0.49	0.25	67,67,67,67	0
56	MG	2A	3794	1/1	0.50	0.36	68,68,68,68	0
56	MG	1A	3912	1/1	0.51	0.18	60,60,60,60	0
56	MG	1A	3624	1/1	0.54	0.11	31,31,31,31	0
56	MG	2A	3219	1/1	0.58	0.21	57,57,57,57	0
56	MG	1m	201	1/1	0.60	0.20	64,64,64,64	0
56	MG	1a	3218	1/1	0.60	0.15	65,65,65,65	0
56	MG	2A	3643	1/1	0.60	0.16	71,71,71,71	0
56	MG	1A	4010	1/1	0.62	0.14	51,51,51,51	0
56	MG	2A	3469	1/1	0.62	0.35	61,61,61,61	0
56	MG	2A	3784	1/1	0.63	0.11	58,58,58,58	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	2A	3693	1/1	0.63	0.33	55,55,55,55	0
56	MG	2A	3372	1/1	0.63	0.18	57,57,57,57	0
56	MG	2T	202	1/1	0.63	0.49	55,55,55,55	0
56	MG	26	101	1/1	0.63	0.27	54,54,54,54	0
56	MG	2A	3390	1/1	0.64	0.35	53,53,53,53	0
56	MG	1A	3971	1/1	0.64	0.18	27,27,27,27	0
56	MG	2A	3521	1/1	0.64	0.13	60,60,60,60	0
56	MG	2a	1788	1/1	0.64	0.14	70,70,70,70	0
56	MG	2A	3698	1/1	0.65	0.08	51,51,51,51	0
56	MG	2a	1749	1/1	0.65	0.18	68,68,68,68	0
56	MG	2a	1612	1/1	0.66	0.15	62,62,62,62	0
56	MG	2A	3206	1/1	0.66	0.18	48,48,48,48	0
56	MG	2A	3632	1/1	0.66	0.28	61,61,61,61	0
56	MG	2A	3477	1/1	0.66	0.35	56,56,56,56	0
56	MG	2A	3243	1/1	0.66	0.33	59,59,59,59	0
56	MG	1A	3309	1/1	0.67	0.18	35,35,35,35	0
56	MG	2a	1603	1/1	0.67	0.17	50,50,50,50	0
56	MG	2A	3115	1/1	0.67	0.14	61,61,61,61	0
56	MG	2A	3491	1/1	0.67	0.12	33,33,33,33	0
56	MG	1A	3690	1/1	0.67	0.18	21,21,21,21	0
56	MG	2B	216	1/1	0.67	0.15	61,61,61,61	0
56	MG	2A	3678	1/1	0.68	0.12	76,76,76,76	0
56	MG	1A	3706	1/1	0.68	0.18	26,26,26,26	0
56	MG	1A	3270	1/1	0.69	0.22	61,61,61,61	0
56	MG	2A	3256	1/1	0.70	0.29	58,58,58,58	0
56	MG	1d	301	1/1	0.70	0.19	56,56,56,56	0
56	MG	1A	3343	1/1	0.71	0.14	43,43,43,43	0
56	MG	2A	3656	1/1	0.71	0.38	45,45,45,45	0
56	MG	2a	1752	1/1	0.71	0.06	64,64,64,64	0
56	MG	1a	3207	1/1	0.71	0.07	46,46,46,46	0
56	MG	1A	3795	1/1	0.72	0.07	69,69,69,69	0
56	MG	2A	3787	1/1	0.72	0.15	46,46,46,46	0
56	MG	2a	1758	1/1	0.72	0.09	70,70,70,70	0
56	MG	1A	3957	1/1	0.72	0.07	57,57,57,57	0
56	MG	1F	314	1/1	0.72	0.58	45,45,45,45	0
56	MG	1a	3104	1/1	0.72	0.12	72,72,72,72	0
56	MG	2A	3597	1/1	0.72	0.12	34,34,34,34	0
56	MG	1A	3472	1/1	0.72	0.24	60,60,60,60	0
56	MG	2A	3505	1/1	0.72	0.12	36,36,36,36	0
56	MG	2A	3821	1/1	0.72	0.18	26,26,26,26	0
56	MG	2a	1721	1/1	0.73	0.25	55,55,55,55	0
56	MG	2A	3789	1/1	0.73	0.20	74,74,74,74	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	2a	1832	1/1	0.73	0.17	51,51,51,51	0
56	MG	1a	3151	1/1	0.74	0.12	62,62,62,62	0
56	MG	2a	1649	1/1	0.74	0.16	54,54,54,54	0
56	MG	2a	1710	1/1	0.74	0.14	70,70,70,70	0
56	MG	1a	3075	1/1	0.74	0.29	63,63,63,63	0
56	MG	2A	3359	1/1	0.74	0.45	57,57,57,57	0
56	MG	2A	3183	1/1	0.74	0.13	35,35,35,35	0
56	MG	2A	3864	1/1	0.74	0.37	49,49,49,49	0
56	MG	1A	3626	1/1	0.74	0.15	17,17,17,17	0
56	MG	1A	3438	1/1	0.74	0.16	51,51,51,51	0
56	MG	2A	3528	1/1	0.74	0.10	66,66,66,66	0
56	MG	2A	3285	1/1	0.75	0.26	66,66,66,66	0
56	MG	2a	1685	1/1	0.75	0.15	49,49,49,49	0
56	MG	2A	3462	1/1	0.75	0.22	41,41,41,41	0
56	MG	2A	3818	1/1	0.75	0.26	56,56,56,56	0
56	MG	2A	3058	1/1	0.75	0.14	67,67,67,67	0
56	MG	2i	201	1/1	0.75	0.17	60,60,60,60	0
56	MG	1A	3116	1/1	0.75	0.22	36,36,36,36	0
56	MG	2a	1763	1/1	0.76	0.06	70,70,70,70	0
56	MG	2a	1748	1/1	0.76	0.11	59,59,59,59	0
56	MG	2a	1706	1/1	0.76	0.13	67,67,67,67	0
56	MG	1x	106	1/1	0.76	0.15	66,66,66,66	0
56	MG	2A	3026	1/1	0.76	0.11	40,40,40,40	0
56	MG	2P	202	1/1	0.76	0.23	55,55,55,55	0
56	MG	2A	3358	1/1	0.76	0.25	51,51,51,51	0
56	MG	1A	3085	1/1	0.76	0.18	16,16,16,16	0
56	MG	1A	3539	1/1	0.76	0.19	25,25,25,25	0
56	MG	2A	3840	1/1	0.77	0.09	41,41,41,41	0
56	MG	2A	3375	1/1	0.77	0.30	59,59,59,59	0
56	MG	2A	3839	1/1	0.77	0.12	47,47,47,47	0
56	MG	1A	3981	1/1	0.77	0.31	29,29,29,29	0
56	MG	2a	1759	1/1	0.77	0.20	61,61,61,61	0
56	MG	1A	3348	1/1	0.77	0.41	33,33,33,33	0
56	MG	1A	3067	1/1	0.77	0.26	44,44,44,44	0
56	MG	2A	3480	1/1	0.77	0.09	58,58,58,58	0
56	MG	2A	3498	1/1	0.77	0.17	51,51,51,51	0
56	MG	1A	4046	1/1	0.77	0.13	43,43,43,43	0
56	MG	2A	3776	1/1	0.77	0.28	74,74,74,74	0
56	MG	2A	3741	1/1	0.77	0.12	49,49,49,49	0
56	MG	2A	3277	1/1	0.77	0.31	55,55,55,55	0
56	MG	1A	3953	1/1	0.77	0.23	12,12,12,12	0
56	MG	1A	3939	1/1	0.77	0.23	47,47,47,47	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	2A	3222	1/1	0.78	0.20	29,29,29,29	0
56	MG	1A	3888	1/1	0.78	0.15	62,62,62,62	0
56	MG	2A	3502	1/1	0.78	0.32	53,53,53,53	0
56	MG	1a	3133	1/1	0.78	0.16	53,53,53,53	0
56	MG	2A	3396	1/1	0.78	0.15	50,50,50,50	0
56	MG	1a	3084	1/1	0.78	0.31	56,56,56,56	0
56	MG	2A	3771	1/1	0.78	0.14	50,50,50,50	0
56	MG	1A	3473	1/1	0.78	0.18	51,51,51,51	0
56	MG	2A	3569	1/1	0.78	0.10	62,62,62,62	0
56	MG	1A	3941	1/1	0.78	0.15	32,32,32,32	0
56	MG	2A	3806	1/1	0.78	0.15	50,50,50,50	0
56	MG	2A	3801	1/1	0.79	0.40	63,63,63,63	0
56	MG	2A	3812	1/1	0.79	0.16	59,59,59,59	0
56	MG	2A	3860	1/1	0.79	0.18	62,62,62,62	0
56	MG	2A	3316	1/1	0.79	0.50	48,48,48,48	0
56	MG	1A	3388	1/1	0.79	0.16	53,53,53,53	0
56	MG	2A	3428	1/1	0.79	0.15	66,66,66,66	0
56	MG	1A	4034	1/1	0.79	0.07	44,44,44,44	0
56	MG	1A	3497	1/1	0.79	0.16	33,33,33,33	0
56	MG	2A	3709	1/1	0.79	0.19	60,60,60,60	0
56	MG	1a	3167	1/1	0.79	0.07	54,54,54,54	0
56	MG	2A	3797	1/1	0.79	0.07	78,78,78,78	0
56	MG	2A	3405	1/1	0.79	0.12	50,50,50,50	0
56	MG	2A	3634	1/1	0.79	0.16	68,68,68,68	0
56	MG	2A	3774	1/1	0.79	0.59	66,66,66,66	0
56	MG	2A	3762	1/1	0.79	0.10	57,57,57,57	0
56	MG	1A	3676	1/1	0.79	0.21	28,28,28,28	0
56	MG	2A	3781	1/1	0.79	0.11	51,51,51,51	0
56	MG	2a	1698	1/1	0.80	0.14	43,43,43,43	0
56	MG	2A	3848	1/1	0.80	0.05	55,55,55,55	0
56	MG	2A	3665	1/1	0.80	0.09	48,48,48,48	0
56	MG	2A	3773	1/1	0.80	0.73	71,71,71,71	0
56	MG	2A	3750	1/1	0.80	0.15	28,28,28,28	0
56	MG	2A	3289	1/1	0.80	0.11	60,60,60,60	0
56	MG	1A	3835	1/1	0.80	0.13	22,22,22,22	0
56	MG	2a	1695	1/1	0.80	0.15	63,63,63,63	0
56	MG	2a	1720	1/1	0.80	0.21	55,55,55,55	0
56	MG	1A	3867	1/1	0.80	0.20	13,13,13,13	0
56	MG	1A	3713	1/1	0.80	0.17	22,22,22,22	0
56	MG	2a	1738	1/1	0.80	0.20	76,76,76,76	0
56	MG	2A	3783	1/1	0.80	0.08	53,53,53,53	0
56	MG	1A	3364	1/1	0.80	0.22	31,31,31,31	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	2a	1736	1/1	0.80	0.15	65,65,65,65	0
56	MG	2A	3525	1/1	0.80	0.08	33,33,33,33	0
56	MG	1A	3509	1/1	0.80	0.19	23,23,23,23	0
56	MG	1A	3827	1/1	0.80	0.36	38,38,38,38	0
56	MG	1a	3188	1/1	0.80	0.13	48,48,48,48	0
56	MG	1a	3153	1/1	0.80	0.12	27,27,27,27	0
56	MG	2a	1627	1/1	0.80	0.51	53,53,53,53	0
56	MG	2A	3779	1/1	0.81	0.09	47,47,47,47	0
56	MG	2A	3749	1/1	0.81	0.25	41,41,41,41	0
56	MG	1A	3893	1/1	0.81	0.12	48,48,48,48	0
56	MG	2A	3339	1/1	0.81	0.17	68,68,68,68	0
56	MG	2A	3853	1/1	0.81	0.12	33,33,33,33	0
56	MG	2A	3843	1/1	0.81	0.08	40,40,40,40	0
56	MG	1a	3191	1/1	0.81	0.10	42,42,42,42	0
56	MG	1A	3175	1/1	0.81	0.20	19,19,19,19	0
56	MG	2A	3745	1/1	0.81	0.26	49,49,49,49	0
56	MG	2A	3208	1/1	0.81	0.24	48,48,48,48	0
56	MG	2A	3716	1/1	0.81	0.22	56,56,56,56	0
56	MG	1A	3999	1/1	0.81	0.20	39,39,39,39	0
56	MG	2A	3842	1/1	0.81	0.18	62,62,62,62	0
56	MG	1a	3138	1/1	0.81	0.16	58,58,58,58	0
56	MG	2A	3600	1/1	0.81	0.11	69,69,69,69	0
56	MG	17	105	1/1	0.81	0.20	22,22,22,22	0
56	MG	1a	3113	1/1	0.81	0.13	41,41,41,41	0
56	MG	2A	3851	1/1	0.81	0.16	37,37,37,37	0
56	MG	2A	3701	1/1	0.81	0.11	40,40,40,40	0
56	MG	2A	3829	1/1	0.81	0.06	42,42,42,42	0
56	MG	1y	103	1/1	0.81	0.33	66,66,66,66	0
56	MG	1A	3016	1/1	0.82	0.14	26,26,26,26	0
56	MG	1A	3440	1/1	0.82	0.20	38,38,38,38	0
56	MG	2A	3799	1/1	0.82	0.47	68,68,68,68	0
56	MG	1A	4071	1/1	0.82	0.30	52,52,52,52	0
56	MG	1A	3426	1/1	0.82	0.17	28,28,28,28	0
56	MG	2A	3644	1/1	0.82	0.16	54,54,54,54	0
56	MG	1A	3292	1/1	0.82	0.14	35,35,35,35	0
56	MG	2A	3676	1/1	0.82	0.21	64,64,64,64	0
56	MG	2A	3804	1/1	0.82	0.11	60,60,60,60	0
56	MG	2R	202	1/1	0.82	0.15	46,46,46,46	0
56	MG	1a	3068	1/1	0.82	0.30	57,57,57,57	0
56	MG	1A	3708	1/1	0.82	0.10	25,25,25,25	0
56	MG	2a	1795	1/1	0.82	0.17	53,53,53,53	0
56	MG	2G	201	1/1	0.82	0.09	59,59,59,59	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	1a	3195	1/1	0.82	0.16	47,47,47,47	0
56	MG	1A	3446	1/1	0.82	0.12	43,43,43,43	0
56	MG	1a	3175	1/1	0.82	0.22	66,66,66,66	0
56	MG	1y	104	1/1	0.82	0.14	61,61,61,61	0
56	MG	1A	3288	1/1	0.82	0.25	32,32,32,32	0
56	MG	1A	3911	1/1	0.82	0.16	59,59,59,59	0
56	MG	1A	3389	1/1	0.82	0.16	39,39,39,39	0
56	MG	2A	3778	1/1	0.82	0.16	61,61,61,61	0
56	MG	2A	3499	1/1	0.82	0.12	50,50,50,50	0
56	MG	1A	3505	1/1	0.82	0.12	44,44,44,44	0
56	MG	2A	3800	1/1	0.82	0.06	47,47,47,47	0
56	MG	2A	3593	1/1	0.82	0.11	31,31,31,31	0
56	MG	2a	1769	1/1	0.82	0.08	60,60,60,60	0
56	MG	2A	3347	1/1	0.82	0.13	41,41,41,41	0
56	MG	1A	3997	1/1	0.82	0.18	57,57,57,57	0
56	MG	1P	203	1/1	0.82	0.96	27,27,27,27	0
56	MG	2A	3571	1/1	0.83	0.19	53,53,53,53	0
56	MG	1A	3353	1/1	0.83	0.40	41,41,41,41	0
56	MG	2A	3751	1/1	0.83	0.32	37,37,37,37	0
56	MG	1a	3109	1/1	0.83	0.20	40,40,40,40	0
56	MG	1a	3131	1/1	0.83	0.22	53,53,53,53	0
56	MG	1a	3080	1/1	0.83	0.17	62,62,62,62	0
56	MG	1B	201	1/1	0.83	0.18	40,40,40,40	0
56	MG	2A	3796	1/1	0.83	0.20	45,45,45,45	0
56	MG	1A	4035	1/1	0.83	0.10	39,39,39,39	0
56	MG	2a	1652	1/1	0.83	0.35	60,60,60,60	0
56	MG	1A	3966	1/1	0.83	0.17	15,15,15,15	0
56	MG	1A	3772	1/1	0.83	0.17	12,12,12,12	0
56	MG	2I	101	1/1	0.83	0.16	57,57,57,57	0
56	MG	2a	1606	1/1	0.83	0.11	59,59,59,59	0
56	MG	2A	3129	1/1	0.83	0.09	43,43,43,43	0
56	MG	2A	3618	1/1	0.83	0.20	39,39,39,39	0
56	MG	2A	3217	1/1	0.83	0.42	47,47,47,47	0
56	MG	2A	3270	1/1	0.83	0.26	50,50,50,50	0
56	MG	2A	3541	1/1	0.83	0.13	53,53,53,53	0
56	MG	1A	3704	1/1	0.83	0.09	34,34,34,34	0
56	MG	2A	3424	1/1	0.83	0.28	42,42,42,42	0
56	MG	1A	3272	1/1	0.83	0.21	24,24,24,24	0
56	MG	2A	3664	1/1	0.83	0.41	54,54,54,54	0
56	MG	1A	3915	1/1	0.83	0.10	29,29,29,29	0
56	MG	2E	307	1/1	0.83	0.12	25,25,25,25	0
56	MG	1a	3193	1/1	0.83	0.07	57,57,57,57	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	2a	1645	1/1	0.83	0.20	44,44,44,44	0
56	MG	1A	3276	1/1	0.83	0.14	38,38,38,38	0
56	MG	2A	3287	1/1	0.83	0.17	58,58,58,58	0
56	MG	1B	223	1/1	0.83	0.16	43,43,43,43	0
56	MG	2a	1674	1/1	0.83	0.46	55,55,55,55	0
56	MG	2A	3197	1/1	0.83	0.15	32,32,32,32	0
56	MG	22	101	1/1	0.83	0.12	42,42,42,42	0
56	MG	2p	101	1/1	0.83	0.14	43,43,43,43	0
56	MG	1A	3186	1/1	0.83	0.39	31,31,31,31	0
56	MG	1A	3238	1/1	0.83	0.14	27,27,27,27	0
56	MG	2y	102	1/1	0.83	0.13	51,51,51,51	0
56	MG	1x	111	1/1	0.83	0.20	49,49,49,49	0
56	MG	1A	3841	1/1	0.83	0.11	34,34,34,34	0
56	MG	2A	3795	1/1	0.83	0.27	61,61,61,61	0
56	MG	1A	3325	1/1	0.83	0.24	42,42,42,42	0
56	MG	2A	3410	1/1	0.83	0.13	48,48,48,48	0
56	MG	1A	3910	1/1	0.84	0.06	58,58,58,58	0
56	MG	1a	3031	1/1	0.84	0.14	53,53,53,53	0
56	MG	1a	3206	1/1	0.84	0.11	52,52,52,52	0
56	MG	2A	3090	1/1	0.84	0.13	59,59,59,59	0
56	MG	1A	3220	1/1	0.84	0.14	53,53,53,53	0
56	MG	1B	222	1/1	0.84	0.13	53,53,53,53	0
56	MG	1A	3836	1/1	0.84	0.19	47,47,47,47	0
56	MG	1A	3684	1/1	0.84	0.21	16,16,16,16	0
56	MG	2a	1666	1/1	0.84	0.20	50,50,50,50	0
56	MG	2a	1711	1/1	0.84	0.12	47,47,47,47	0
56	MG	1A	3490	1/1	0.84	0.13	18,18,18,18	0
56	MG	1A	3659	1/1	0.84	0.17	12,12,12,12	0
56	MG	2a	1681	1/1	0.84	0.24	51,51,51,51	0
56	MG	1A	3423	1/1	0.84	0.17	50,50,50,50	0
56	MG	2A	3566	1/1	0.84	0.17	44,44,44,44	0
56	MG	2A	3614	1/1	0.84	0.11	23,23,23,23	0
56	MG	2A	3540	1/1	0.84	0.10	28,28,28,28	0
56	MG	1a	3106	1/1	0.84	0.16	20,20,20,20	0
56	MG	19	101	1/1	0.84	0.23	43,43,43,43	0
56	MG	2D	303	1/1	0.84	0.40	61,61,61,61	0
56	MG	2A	3071	1/1	0.84	0.24	30,30,30,30	0
56	MG	1A	3200	1/1	0.84	0.21	37,37,37,37	0
56	MG	2A	3770	1/1	0.84	0.34	65,65,65,65	0
56	MG	1A	4021	1/1	0.84	0.10	32,32,32,32	0
56	MG	2a	1762	1/1	0.84	0.10	66,66,66,66	0
56	MG	1A	3179	1/1	0.84	0.35	60,60,60,60	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	1a	3214	1/1	0.84	0.08	49,49,49,49	0
56	MG	1A	3046	1/1	0.84	0.30	44,44,44,44	0
56	MG	1A	3435	1/1	0.84	0.23	50,50,50,50	0
56	MG	1a	3202	1/1	0.84	0.14	46,46,46,46	0
56	MG	2A	3239	1/1	0.84	0.22	45,45,45,45	0
56	MG	2A	3556	1/1	0.84	0.08	44,44,44,44	0
56	MG	1A	3326	1/1	0.84	0.28	29,29,29,29	0
56	MG	1A	3728	1/1	0.84	0.15	54,54,54,54	0
56	MG	2A	3014	1/1	0.85	0.18	38,38,38,38	0
56	MG	2a	1639	1/1	0.85	0.24	60,60,60,60	0
56	MG	2A	3327	1/1	0.85	0.63	44,44,44,44	0
56	MG	1w	104	1/1	0.85	0.15	51,51,51,51	0
56	MG	1A	3640	1/1	0.85	0.17	31,31,31,31	0
56	MG	2A	3765	1/1	0.85	0.30	62,62,62,62	0
56	MG	1A	4072	1/1	0.85	0.14	52,52,52,52	0
56	MG	2A	3160	1/1	0.85	0.10	50,50,50,50	0
56	MG	2a	1665	1/1	0.85	0.10	48,48,48,48	0
56	MG	2a	1770	1/1	0.85	0.16	51,51,51,51	0
56	MG	2a	1608	1/1	0.85	0.16	55,55,55,55	0
56	MG	2A	3568	1/1	0.85	0.17	46,46,46,46	0
56	MG	2a	1754	1/1	0.85	0.11	52,52,52,52	0
56	MG	1a	3107	1/1	0.85	0.13	34,34,34,34	0
56	MG	2A	3387	1/1	0.85	0.18	72,72,72,72	0
56	MG	1a	3119	1/1	0.85	0.30	42,42,42,42	0
56	MG	2B	209	1/1	0.85	0.12	41,41,41,41	0
56	MG	2a	1664	1/1	0.85	0.16	49,49,49,49	0
56	MG	2A	3074	1/1	0.85	0.41	42,42,42,42	0
56	MG	1A	3159	1/1	0.85	0.14	23,23,23,23	0
56	MG	2A	3356	1/1	0.85	0.14	55,55,55,55	0
56	MG	1a	3194	1/1	0.85	0.09	58,58,58,58	0
56	MG	2A	3294	1/1	0.85	0.11	44,44,44,44	0
56	MG	2a	1773	1/1	0.85	0.13	71,71,71,71	0
56	MG	1a	3204	1/1	0.85	0.08	49,49,49,49	0
56	MG	1a	3066	1/1	0.85	0.16	44,44,44,44	0
56	MG	2A	3120	1/1	0.85	0.45	48,48,48,48	0
56	MG	1A	3683	1/1	0.85	0.11	28,28,28,28	0
56	MG	2E	301	1/1	0.85	0.10	45,45,45,45	0
56	MG	2a	1724	1/1	0.85	0.23	64,64,64,64	0
56	MG	1A	3074	1/1	0.85	0.16	36,36,36,36	0
56	MG	2B	208	1/1	0.85	0.34	57,57,57,57	0
56	MG	2A	3446	1/1	0.85	0.12	39,39,39,39	0
56	MG	1A	3460	1/1	0.85	0.15	25,25,25,25	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	2A	3345	1/1	0.85	0.84	61,61,61,61	0
56	MG	1A	3824	1/1	0.85	0.15	25,25,25,25	0
56	MG	2A	3104	1/1	0.85	0.15	48,48,48,48	0
56	MG	2A	3245	1/1	0.85	0.37	58,58,58,58	0
56	MG	2A	3838	1/1	0.85	0.11	61,61,61,61	0
56	MG	1A	3333	1/1	0.85	0.26	42,42,42,42	0
56	MG	2a	1653	1/1	0.85	0.18	71,71,71,71	0
56	MG	1A	3437	1/1	0.85	0.14	39,39,39,39	0
56	MG	2A	3034	1/1	0.85	0.36	37,37,37,37	0
56	MG	1A	3133	1/1	0.85	0.47	19,19,19,19	0
56	MG	2a	1784	1/1	0.85	0.13	60,60,60,60	0
56	MG	1B	216	1/1	0.85	0.15	60,60,60,60	0
56	MG	1A	3409	1/1	0.85	0.26	30,30,30,30	0
56	MG	2A	3046	1/1	0.85	0.13	59,59,59,59	0
56	MG	2a	1619	1/1	0.85	0.20	44,44,44,44	0
56	MG	2A	3021	1/1	0.85	1.13	52,52,52,52	0
56	MG	1w	105	1/1	0.85	0.16	51,51,51,51	0
56	MG	1A	3420	1/1	0.85	0.79	47,47,47,47	0
56	MG	2A	3379	1/1	0.85	0.62	49,49,49,49	0
56	MG	1a	3128	1/1	0.85	0.18	34,34,34,34	0
56	MG	1A	3595	1/1	0.85	0.34	40,40,40,40	0
56	MG	1A	3566	1/1	0.85	0.25	38,38,38,38	0
56	MG	2A	3099	1/1	0.85	0.26	51,51,51,51	0
56	MG	1A	3598	1/1	0.86	0.17	36,36,36,36	0
56	MG	2A	3708	1/1	0.86	0.33	55,55,55,55	0
56	MG	2A	3538	1/1	0.86	0.14	33,33,33,33	0
56	MG	1A	3958	1/1	0.86	0.05	63,63,63,63	0
56	MG	2A	3095	1/1	0.86	0.10	66,66,66,66	0
56	MG	2A	3154	1/1	0.86	0.13	50,50,50,50	0
56	MG	2A	3035	1/1	0.86	0.13	59,59,59,59	0
56	MG	1a	3139	1/1	0.86	0.13	58,58,58,58	0
56	MG	2A	3176	1/1	0.86	0.13	43,43,43,43	0
56	MG	2A	3397	1/1	0.86	0.10	53,53,53,53	0
56	MG	1a	3054	1/1	0.86	0.19	46,46,46,46	0
56	MG	2A	3343	1/1	0.86	0.17	60,60,60,60	0
56	MG	2a	1679	1/1	0.86	0.13	58,58,58,58	0
56	MG	1Z	302	1/1	0.86	0.24	50,50,50,50	0
56	MG	2A	3391	1/1	0.86	0.40	57,57,57,57	0
56	MG	2A	3512	1/1	0.86	0.27	36,36,36,36	0
56	MG	2a	1783	1/1	0.86	0.09	42,42,42,42	0
56	MG	2i	202	1/1	0.86	0.13	42,42,42,42	0
56	MG	2A	3207	1/1	0.86	0.45	61,61,61,61	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	2A	3743	1/1	0.86	0.47	62,62,62,62	0
56	MG	1A	3075	1/1	0.86	0.24	34,34,34,34	0
56	MG	1A	3494	1/1	0.86	0.21	35,35,35,35	0
56	MG	2a	1705	1/1	0.86	0.14	51,51,51,51	0
56	MG	2A	3551	1/1	0.86	0.08	35,35,35,35	0
56	MG	1A	3890	1/1	0.86	0.16	17,17,17,17	0
56	MG	1A	3165	1/1	0.86	0.15	23,23,23,23	0
56	MG	2A	3049	1/1	0.86	0.12	54,54,54,54	0
56	MG	1A	3926	1/1	0.86	0.10	28,28,28,28	0
56	MG	2A	3330	1/1	0.86	0.11	47,47,47,47	0
56	MG	1A	3826	1/1	0.86	0.18	29,29,29,29	0
56	MG	1A	3103	1/1	0.86	0.13	46,46,46,46	0
56	MG	1A	3993	1/1	0.86	0.12	33,33,33,33	0
56	MG	1A	3662	1/1	0.86	0.14	44,44,44,44	0
56	MG	2A	3576	1/1	0.86	0.12	40,40,40,40	0
56	MG	2A	3788	1/1	0.86	0.13	40,40,40,40	0
56	MG	2a	1807	1/1	0.86	0.14	60,60,60,60	0
58	ZN	14	102	1/1	0.86	0.10	99,99,99,99	0
56	MG	1A	3094	1/1	0.86	0.26	27,27,27,27	0
56	MG	1A	3056	1/1	0.86	0.24	40,40,40,40	0
56	MG	2A	3501	1/1	0.86	0.07	42,42,42,42	0
56	MG	2A	3608	1/1	0.86	0.09	50,50,50,50	0
56	MG	2A	3312	1/1	0.86	0.10	32,32,32,32	0
56	MG	2A	3439	1/1	0.86	0.12	43,43,43,43	0
56	MG	2a	1620	1/1	0.86	0.22	46,46,46,46	0
56	MG	2A	3640	1/1	0.86	0.14	72,72,72,72	0
56	MG	2a	1617	1/1	0.86	0.11	31,31,31,31	0
56	MG	2A	3273	1/1	0.86	0.28	40,40,40,40	0
56	MG	1a	3055	1/1	0.86	0.20	58,58,58,58	0
56	MG	1a	3215	1/1	0.86	0.09	55,55,55,55	0
56	MG	2A	3533	1/1	0.86	0.10	33,33,33,33	0
56	MG	2A	3373	1/1	0.86	0.66	52,52,52,52	0
56	MG	1A	3856	1/1	0.86	0.11	28,28,28,28	0
56	MG	1A	3129	1/1	0.86	0.10	29,29,29,29	0
56	MG	2a	1663	1/1	0.86	0.09	33,33,33,33	0
56	MG	1A	3844	1/1	0.86	0.08	29,29,29,29	0
56	MG	2A	3303	1/1	0.86	0.20	56,56,56,56	0
56	MG	2A	3558	1/1	0.86	0.25	58,58,58,58	0
56	MG	1A	3526	1/1	0.86	0.17	31,31,31,31	0
56	MG	2A	3591	1/1	0.86	0.07	62,62,62,62	0
56	MG	1A	3605	1/1	0.86	0.14	35,35,35,35	0
56	MG	1A	3714	1/1	0.86	0.11	25,25,25,25	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	1a	3177	1/1	0.86	0.11	37,37,37,37	0
56	MG	2A	3736	1/1	0.86	0.25	48,48,48,48	0
56	MG	2A	3723	1/1	0.86	0.09	60,60,60,60	0
56	MG	2A	3802	1/1	0.86	0.07	54,54,54,54	0
56	MG	2a	1648	1/1	0.86	0.13	46,46,46,46	0
56	MG	2A	3032	1/1	0.86	0.14	54,54,54,54	0
56	MG	1A	3406	1/1	0.86	0.14	35,35,35,35	0
56	MG	2A	3820	1/1	0.87	0.12	32,32,32,32	0
56	MG	1B	231	1/1	0.87	0.13	41,41,41,41	0
56	MG	1a	3095	1/1	0.87	0.19	40,40,40,40	0
56	MG	2B	214	1/1	0.87	0.09	63,63,63,63	0
56	MG	2A	3650	1/1	0.87	0.19	47,47,47,47	0
56	MG	1A	3770	1/1	0.87	0.16	46,46,46,46	0
56	MG	2A	3559	1/1	0.87	0.17	39,39,39,39	0
56	MG	2a	1722	1/1	0.87	0.19	53,53,53,53	0
56	MG	2a	1669	1/1	0.87	0.18	41,41,41,41	0
56	MG	2a	1730	1/1	0.87	0.15	52,52,52,52	0
56	MG	2v	101	1/1	0.87	0.12	51,51,51,51	0
56	MG	1A	3508	1/1	0.87	0.20	31,31,31,31	0
56	MG	2A	3822	1/1	0.87	0.24	44,44,44,44	0
56	MG	2v	102	1/1	0.87	0.31	71,71,71,71	0
56	MG	1A	3397	1/1	0.87	0.13	33,33,33,33	0
56	MG	1A	3319	1/1	0.87	0.45	41,41,41,41	0
56	MG	2A	3663	1/1	0.87	0.10	41,41,41,41	0
56	MG	2A	3308	1/1	0.87	0.12	50,50,50,50	0
56	MG	2A	3833	1/1	0.87	0.09	48,48,48,48	0
56	MG	2A	3268	1/1	0.87	0.16	57,57,57,57	0
56	MG	2A	3699	1/1	0.87	0.09	39,39,39,39	0
56	MG	1A	3139	1/1	0.87	0.32	34,34,34,34	0
56	MG	2A	3365	1/1	0.87	0.15	48,48,48,48	0
56	MG	1F	306	1/1	0.87	0.21	42,42,42,42	0
56	MG	1A	3564	1/1	0.87	0.14	28,28,28,28	0
56	MG	2A	3269	1/1	0.87	0.43	44,44,44,44	0
56	MG	1A	3710	1/1	0.87	0.16	17,17,17,17	0
56	MG	1A	3569	1/1	0.87	0.20	26,26,26,26	0
56	MG	1a	3224	1/1	0.87	0.13	40,40,40,40	0
56	MG	1A	3028	1/1	0.87	0.17	32,32,32,32	0
56	MG	2A	3484	1/1	0.87	0.27	55,55,55,55	0
56	MG	1y	101	1/1	0.87	1.09	43,43,43,43	0
56	MG	2a	1709	1/1	0.87	0.20	60,60,60,60	0
56	MG	2a	1632	1/1	0.87	0.31	62,62,62,62	0
56	MG	2a	1640	1/1	0.87	0.11	56,56,56,56	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	2A	3265	1/1	0.87	0.60	46,46,46,46	0
56	MG	2A	3201	1/1	0.87	0.15	40,40,40,40	0
56	MG	2A	3156	1/1	0.87	0.14	46,46,46,46	0
56	MG	1a	3003	1/1	0.87	0.13	55,55,55,55	0
56	MG	2A	3825	1/1	0.87	0.15	31,31,31,31	0
56	MG	2A	3596	1/1	0.87	0.10	37,37,37,37	0
56	MG	2A	3153	1/1	0.87	0.21	47,47,47,47	0
56	MG	1A	3782	1/1	0.87	0.13	18,18,18,18	0
56	MG	2a	1737	1/1	0.87	0.10	52,52,52,52	0
56	MG	2A	3506	1/1	0.87	0.24	56,56,56,56	0
56	MG	1a	3226	1/1	0.87	0.07	63,63,63,63	0
56	MG	2A	3555	1/1	0.87	0.09	33,33,33,33	0
56	MG	1A	3877	1/1	0.87	0.14	43,43,43,43	0
56	MG	2A	3769	1/1	0.87	0.12	68,68,68,68	0
56	MG	1A	3155	1/1	0.87	0.12	29,29,29,29	0
56	MG	2A	3147	1/1	0.87	0.19	41,41,41,41	0
56	MG	2a	1610	1/1	0.87	0.23	64,64,64,64	0
56	MG	2A	3531	1/1	0.87	0.36	49,49,49,49	0
56	MG	2q	202	1/1	0.87	0.14	58,58,58,58	0
56	MG	1A	4004	1/1	0.87	0.20	45,45,45,45	0
56	MG	1A	3982	1/1	0.88	0.20	15,15,15,15	0
56	MG	1A	3976	1/1	0.88	0.13	24,24,24,24	0
56	MG	1A	3273	1/1	0.88	0.16	28,28,28,28	0
56	MG	1A	3453	1/1	0.88	0.15	54,54,54,54	0
56	MG	2a	1817	1/1	0.88	0.15	38,38,38,38	0
56	MG	1A	3889	1/1	0.88	0.11	35,35,35,35	0
56	MG	2A	3378	1/1	0.88	0.12	53,53,53,53	0
56	MG	1A	3935	1/1	0.88	0.13	34,34,34,34	0
56	MG	1A	3861	1/1	0.88	0.16	29,29,29,29	0
56	MG	1A	4070	1/1	0.88	0.17	43,43,43,43	0
56	MG	2A	3174	1/1	0.88	0.13	47,47,47,47	0
56	MG	1a	3166	1/1	0.88	0.13	53,53,53,53	0
56	MG	2A	3240	1/1	0.88	0.20	40,40,40,40	0
56	MG	1A	3631	1/1	0.88	0.17	24,24,24,24	0
56	MG	1A	3879	1/1	0.88	0.10	16,16,16,16	0
56	MG	2A	3260	1/1	0.88	0.19	37,37,37,37	0
56	MG	1a	3213	1/1	0.88	0.09	66,66,66,66	0
56	MG	2A	3667	1/1	0.88	0.11	53,53,53,53	0
56	MG	1a	3086	1/1	0.88	0.10	46,46,46,46	0
56	MG	1A	3677	1/1	0.88	0.16	18,18,18,18	0
56	MG	1A	3184	1/1	0.88	0.05	46,46,46,46	0
56	MG	1V	202	1/1	0.88	0.42	24,24,24,24	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	1A	3145	1/1	0.88	0.41	40,40,40,40	0
56	MG	1A	3798	1/1	0.88	0.08	31,31,31,31	0
56	MG	2a	1734	1/1	0.88	0.12	63,63,63,63	0
56	MG	1V	201	1/1	0.88	0.33	17,17,17,17	0
56	MG	1A	3495	1/1	0.88	0.15	29,29,29,29	0
56	MG	2A	3858	1/1	0.88	0.23	43,43,43,43	0
56	MG	1A	3819	1/1	0.88	0.17	42,42,42,42	0
56	MG	1A	3448	1/1	0.88	0.39	30,30,30,30	0
56	MG	2A	3098	1/1	0.88	0.12	43,43,43,43	0
56	MG	2A	3227	1/1	0.88	0.26	36,36,36,36	0
56	MG	2A	3068	1/1	0.88	0.09	31,31,31,31	0
56	MG	1l	201	1/1	0.88	0.14	22,22,22,22	0
56	MG	1A	3771	1/1	0.88	0.17	30,30,30,30	0
56	MG	2Z	301	1/1	0.88	0.11	61,61,61,61	0
56	MG	1Q	205	1/1	0.88	0.41	44,44,44,44	0
56	MG	2A	3482	1/1	0.88	0.10	40,40,40,40	0
56	MG	1A	3354	1/1	0.88	0.19	29,29,29,29	0
56	MG	1B	207	1/1	0.88	0.13	29,29,29,29	0
56	MG	1A	3673	1/1	0.88	0.23	49,49,49,49	0
56	MG	10	102	1/1	0.88	0.17	38,38,38,38	0
56	MG	2A	3325	1/1	0.88	0.32	60,60,60,60	0
56	MG	2a	1655	1/1	0.88	0.10	58,58,58,58	0
56	MG	2A	3792	1/1	0.88	0.25	52,52,52,52	0
56	MG	1a	3098	1/1	0.88	0.17	38,38,38,38	0
56	MG	2A	3096	1/1	0.88	0.11	38,38,38,38	0
56	MG	2A	3768	1/1	0.88	0.37	60,60,60,60	0
56	MG	1w	101	1/1	0.88	0.11	49,49,49,49	0
56	MG	2a	1701	1/1	0.88	0.16	64,64,64,64	0
56	MG	2A	3871	1/1	0.88	0.16	34,34,34,34	0
56	MG	2a	1678	1/1	0.88	0.10	57,57,57,57	0
56	MG	2A	3478	1/1	0.88	0.17	59,59,59,59	0
56	MG	1A	3909	1/1	0.88	0.13	19,19,19,19	0
56	MG	1A	3032	1/1	0.88	0.22	44,44,44,44	0
56	MG	2A	3406	1/1	0.88	0.08	37,37,37,37	0
56	MG	1A	3863	1/1	0.88	0.11	20,20,20,20	0
56	MG	2A	3076	1/1	0.88	0.30	42,42,42,42	0
56	MG	1A	3347	1/1	0.88	0.21	9,9,9,9	0
56	MG	2A	3193	1/1	0.88	0.16	40,40,40,40	0
56	MG	2A	3019	1/1	0.88	0.07	47,47,47,47	0
56	MG	2A	3304	1/1	0.88	0.39	50,50,50,50	0
56	MG	2A	3487	1/1	0.88	0.16	49,49,49,49	0
56	MG	1A	3807	1/1	0.88	0.16	40,40,40,40	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	1A	3534	1/1	0.88	0.51	50,50,50,50	0
56	MG	2A	3218	1/1	0.88	0.12	52,52,52,52	0
56	MG	1A	3206	1/1	0.88	0.24	16,16,16,16	0
56	MG	1a	3033	1/1	0.88	0.17	52,52,52,52	0
56	MG	1A	3480	1/1	0.88	0.16	49,49,49,49	0
56	MG	2A	3290	1/1	0.88	0.17	39,39,39,39	0
56	MG	1A	3039	1/1	0.88	0.46	29,29,29,29	0
56	MG	1A	3282	1/1	0.88	0.40	22,22,22,22	0
56	MG	2A	3023	1/1	0.88	0.08	42,42,42,42	0
56	MG	1A	3787	1/1	0.88	0.13	36,36,36,36	0
56	MG	2A	3344	1/1	0.88	0.21	49,49,49,49	0
56	MG	2A	3182	1/1	0.88	0.18	40,40,40,40	0
56	MG	2A	3435	1/1	0.88	0.24	51,51,51,51	0
56	MG	25	101	1/1	0.88	0.12	33,33,33,33	0
56	MG	2A	3173	1/1	0.88	0.13	33,33,33,33	0
56	MG	1A	3107	1/1	0.88	0.19	40,40,40,40	0
56	MG	1A	3471	1/1	0.88	0.20	50,50,50,50	0
56	MG	2A	3468	1/1	0.88	0.75	45,45,45,45	0
56	MG	1A	3111	1/1	0.88	0.13	28,28,28,28	0
56	MG	1A	3946	1/1	0.88	0.12	35,35,35,35	0
56	MG	1A	3823	1/1	0.88	0.17	30,30,30,30	0
56	MG	2A	3371	1/1	0.88	0.58	43,43,43,43	0
56	MG	2A	3728	1/1	0.88	0.28	66,66,66,66	0
56	MG	1A	4014	1/1	0.88	0.15	21,21,21,21	0
56	MG	2A	3144	1/1	0.88	0.08	43,43,43,43	0
56	MG	1F	305	1/1	0.88	0.22	35,35,35,35	0
56	MG	1a	3203	1/1	0.89	0.13	32,32,32,32	0
56	MG	1A	3474	1/1	0.89	0.11	38,38,38,38	0
56	MG	1A	3244	1/1	0.89	0.13	38,38,38,38	0
56	MG	2a	1672	1/1	0.89	0.27	43,43,43,43	0
56	MG	1W	203	1/1	0.89	0.15	36,36,36,36	0
56	MG	2a	1614	1/1	0.89	0.08	53,53,53,53	0
56	MG	1A	3830	1/1	0.89	0.09	28,28,28,28	0
56	MG	2A	3180	1/1	0.89	0.31	48,48,48,48	0
56	MG	2A	3291	1/1	0.89	0.08	32,32,32,32	0
56	MG	2A	3697	1/1	0.89	0.11	53,53,53,53	0
56	MG	1A	4043	1/1	0.89	0.14	30,30,30,30	0
56	MG	1A	3514	1/1	0.89	0.14	15,15,15,15	0
56	MG	1a	3053	1/1	0.89	0.10	62,62,62,62	0
56	MG	1A	3203	1/1	0.89	0.26	17,17,17,17	0
56	MG	1A	3596	1/1	0.89	0.37	43,43,43,43	0
56	MG	1A	3044	1/1	0.89	0.37	37,37,37,37	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	1A	3721	1/1	0.89	0.18	24,24,24,24	0
56	MG	1A	3498	1/1	0.89	0.17	57,57,57,57	0
56	MG	2A	3686	1/1	0.89	0.15	41,41,41,41	0
56	MG	2A	3340	1/1	0.89	0.11	38,38,38,38	0
56	MG	2A	3472	1/1	0.89	0.72	64,64,64,64	0
56	MG	1A	3178	1/1	0.89	0.10	45,45,45,45	0
56	MG	2A	3319	1/1	0.89	0.09	32,32,32,32	0
56	MG	2A	3199	1/1	0.89	0.14	27,27,27,27	0
56	MG	2A	3810	1/1	0.89	0.23	49,49,49,49	0
56	MG	2A	3658	1/1	0.89	0.19	61,61,61,61	0
56	MG	1A	3352	1/1	0.89	0.13	28,28,28,28	0
56	MG	1A	3314	1/1	0.89	0.12	39,39,39,39	0
56	MG	2A	3724	1/1	0.89	0.15	45,45,45,45	0
56	MG	1A	3395	1/1	0.89	0.16	32,32,32,32	0
56	MG	1A	4030	1/1	0.89	0.08	20,20,20,20	0
56	MG	1E	302	1/1	0.89	0.41	30,30,30,30	0
56	MG	1A	3392	1/1	0.89	0.22	24,24,24,24	0
56	MG	1a	3176	1/1	0.89	0.10	45,45,45,45	0
56	MG	2x	101	1/1	0.89	0.11	55,55,55,55	0
56	MG	2A	3250	1/1	0.89	0.18	46,46,46,46	0
56	MG	1a	3093	1/1	0.89	0.23	40,40,40,40	0
56	MG	1A	3425	1/1	0.89	0.16	43,43,43,43	0
56	MG	2A	3823	1/1	0.89	0.16	38,38,38,38	0
56	MG	1A	3170	1/1	0.89	0.12	30,30,30,30	0
56	MG	1A	3049	1/1	0.89	0.11	17,17,17,17	0
56	MG	2A	3445	1/1	0.89	0.68	57,57,57,57	0
56	MG	1A	3038	1/1	0.89	0.13	27,27,27,27	0
56	MG	1x	105	1/1	0.89	0.10	60,60,60,60	0
56	MG	2A	3328	1/1	0.89	0.40	51,51,51,51	0
56	MG	2a	1765	1/1	0.89	0.10	45,45,45,45	0
56	MG	1A	3653	1/1	0.89	0.12	19,19,19,19	0
56	MG	2A	3213	1/1	0.89	0.30	38,38,38,38	0
56	MG	1A	3645	1/1	0.89	0.15	19,19,19,19	0
56	MG	1A	3791	1/1	0.89	0.16	25,25,25,25	0
56	MG	2a	1779	1/1	0.89	0.09	51,51,51,51	0
58	ZN	24	501	1/1	0.89	0.07	108,108,108,108	0
56	MG	11	101	1/1	0.89	0.09	39,39,39,39	0
56	MG	1A	3887	1/1	0.89	0.10	21,21,21,21	0
56	MG	2A	3594	1/1	0.89	0.16	42,42,42,42	0
56	MG	1A	3592	1/1	0.89	0.28	33,33,33,33	0
56	MG	1a	3178	1/1	0.89	0.14	45,45,45,45	0
56	MG	2Q	202	1/1	0.89	0.36	39,39,39,39	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	1A	3949	1/1	0.89	0.13	40,40,40,40	0
56	MG	2a	1696	1/1	0.89	0.14	33,33,33,33	0
56	MG	1A	3927	1/1	0.89	0.10	54,54,54,54	0
56	MG	1x	110	1/1	0.89	0.10	43,43,43,43	0
56	MG	2A	3684	1/1	0.89	0.06	64,64,64,64	0
56	MG	1r	101	1/1	0.89	0.10	48,48,48,48	0
56	MG	1a	3105	1/1	0.89	0.14	51,51,51,51	0
56	MG	1A	3307	1/1	0.89	0.14	41,41,41,41	0
56	MG	2a	1755	1/1	0.89	0.10	40,40,40,40	0
56	MG	1B	213	1/1	0.89	0.08	57,57,57,57	0
56	MG	2A	3847	1/1	0.89	0.17	62,62,62,62	0
56	MG	2A	3305	1/1	0.89	0.11	44,44,44,44	0
56	MG	1A	3355	1/1	0.89	0.15	42,42,42,42	0
56	MG	1A	3847	1/1	0.89	0.10	38,38,38,38	0
56	MG	1A	3298	1/1	0.89	0.11	32,32,32,32	0
56	MG	1P	206	1/1	0.89	0.13	17,17,17,17	0
56	MG	2A	3192	1/1	0.89	0.15	38,38,38,38	0
56	MG	2A	3072	1/1	0.89	0.19	52,52,52,52	0
56	MG	1A	3729	1/1	0.89	0.26	39,39,39,39	0
56	MG	2A	3121	1/1	0.89	0.20	49,49,49,49	0
56	MG	1A	3970	1/1	0.89	0.12	19,19,19,19	0
56	MG	1A	3222	1/1	0.89	0.13	25,25,25,25	0
56	MG	2A	3386	1/1	0.89	0.16	41,41,41,41	0
56	MG	1A	3189	1/1	0.89	0.14	18,18,18,18	0
56	MG	1a	3085	1/1	0.89	0.10	41,41,41,41	0
56	MG	1a	3196	1/1	0.89	0.07	38,38,38,38	0
56	MG	1A	3903	1/1	0.89	0.21	18,18,18,18	0
56	MG	2a	1716	1/1	0.89	0.14	44,44,44,44	0
56	MG	1A	3664	1/1	0.89	0.17	20,20,20,20	0
56	MG	1A	3386	1/1	0.89	0.17	38,38,38,38	0
56	MG	1a	3100	1/1	0.89	0.12	42,42,42,42	0
56	MG	1A	3257	1/1	0.89	0.14	33,33,33,33	0
56	MG	2a	1719	1/1	0.89	0.10	49,49,49,49	0
56	MG	1a	3137	1/1	0.89	0.13	43,43,43,43	0
56	MG	15	101	1/1	0.89	0.28	34,34,34,34	0
56	MG	2A	3279	1/1	0.89	0.14	32,32,32,32	0
56	MG	1A	3775	1/1	0.89	0.26	10,10,10,10	0
56	MG	2a	1827	1/1	0.90	0.11	45,45,45,45	0
56	MG	2F	303	1/1	0.90	0.24	30,30,30,30	0
56	MG	2A	3275	1/1	0.90	0.24	44,44,44,44	0
56	MG	1A	3559	1/1	0.90	0.20	42,42,42,42	0
56	MG	2A	3720	1/1	0.90	0.11	46,46,46,46	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	1A	3617	1/1	0.90	0.31	18,18,18,18	0
56	MG	1A	3808	1/1	0.90	0.09	28,28,28,28	0
56	MG	1A	3384	1/1	0.90	0.14	37,37,37,37	0
56	MG	2A	3611	1/1	0.90	0.09	27,27,27,27	0
56	MG	2A	3623	1/1	0.90	0.15	44,44,44,44	0
56	MG	2A	3313	1/1	0.90	0.26	52,52,52,52	0
56	MG	2a	1731	1/1	0.90	0.14	42,42,42,42	0
56	MG	1A	3284	1/1	0.90	0.19	16,16,16,16	0
56	MG	2a	1796	1/1	0.90	0.22	48,48,48,48	0
56	MG	2A	3574	1/1	0.90	0.09	36,36,36,36	0
56	MG	2A	3426	1/1	0.90	0.15	42,42,42,42	0
56	MG	1a	3112	1/1	0.90	0.11	48,48,48,48	0
56	MG	1A	3973	1/1	0.90	0.13	37,37,37,37	0
56	MG	2A	3170	1/1	0.90	0.08	64,64,64,64	0
56	MG	2a	1707	1/1	0.90	0.20	52,52,52,52	0
56	MG	1a	3059	1/1	0.90	0.07	48,48,48,48	0
56	MG	1E	307	1/1	0.90	0.45	36,36,36,36	0
56	MG	1a	3123	1/1	0.90	0.15	53,53,53,53	0
56	MG	1A	3454	1/1	0.90	0.21	31,31,31,31	0
56	MG	2A	3230	1/1	0.90	0.26	36,36,36,36	0
56	MG	1A	3463	1/1	0.90	0.39	25,25,25,25	0
56	MG	1A	3619	1/1	0.90	0.19	25,25,25,25	0
56	MG	2A	3845	1/1	0.90	0.10	49,49,49,49	0
56	MG	1a	3162	1/1	0.90	0.07	30,30,30,30	0
56	MG	2a	1715	1/1	0.90	0.21	51,51,51,51	0
56	MG	1A	3919	1/1	0.90	0.12	38,38,38,38	0
56	MG	1A	3871	1/1	0.90	0.32	16,16,16,16	0
56	MG	2A	3733	1/1	0.90	0.68	73,73,73,73	0
56	MG	1F	304	1/1	0.90	0.26	31,31,31,31	0
56	MG	2A	3249	1/1	0.90	0.26	54,54,54,54	0
56	MG	1W	201	1/1	0.90	0.23	24,24,24,24	0
56	MG	1A	4064	1/1	0.90	0.24	36,36,36,36	0
56	MG	1A	3380	1/1	0.90	0.21	32,32,32,32	0
56	MG	1a	3143	1/1	0.90	0.08	48,48,48,48	0
56	MG	2a	1623	1/1	0.90	0.18	44,44,44,44	0
56	MG	2a	1708	1/1	0.90	0.09	54,54,54,54	0
56	MG	2A	3688	1/1	0.90	0.12	58,58,58,58	0
56	MG	2A	3543	1/1	0.90	0.09	47,47,47,47	0
56	MG	1A	4013	1/1	0.90	0.09	40,40,40,40	0
56	MG	2a	1703	1/1	0.90	0.12	69,69,69,69	0
56	MG	1A	3868	1/1	0.90	0.10	30,30,30,30	0
56	MG	1A	3885	1/1	0.90	0.09	9,9,9,9	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	2A	3355	1/1	0.90	0.19	42,42,42,42	0
56	MG	2A	3467	1/1	0.90	0.11	50,50,50,50	0
56	MG	2A	3107	1/1	0.90	0.41	44,44,44,44	0
56	MG	2a	1812	1/1	0.90	0.18	42,42,42,42	0
56	MG	1A	3788	1/1	0.90	0.12	27,27,27,27	0
56	MG	1A	3932	1/1	0.90	0.12	37,37,37,37	0
56	MG	2a	1775	1/1	0.90	0.08	49,49,49,49	0
56	MG	1y	105	1/1	0.90	0.25	53,53,53,53	0
56	MG	2A	3836	1/1	0.90	0.09	33,33,33,33	0
56	MG	2a	1616	1/1	0.90	0.16	55,55,55,55	0
56	MG	1b	301	1/1	0.90	0.10	52,52,52,52	0
56	MG	1A	3637	1/1	0.90	0.12	34,34,34,34	0
56	MG	1a	3056	1/1	0.90	0.13	45,45,45,45	0
56	MG	1A	3017	1/1	0.90	0.14	17,17,17,17	0
56	MG	1A	3313	1/1	0.90	0.14	31,31,31,31	0
56	MG	1A	3377	1/1	0.90	0.11	38,38,38,38	0
56	MG	1A	3269	1/1	0.90	0.18	22,22,22,22	0
56	MG	1a	3145	1/1	0.90	0.14	32,32,32,32	0
56	MG	2A	3451	1/1	0.90	0.10	37,37,37,37	0
56	MG	1A	3623	1/1	0.90	0.14	20,20,20,20	0
56	MG	2D	306	1/1	0.90	0.12	35,35,35,35	0
56	MG	1A	3567	1/1	0.90	0.22	37,37,37,37	0
56	MG	1A	3756	1/1	0.90	0.16	31,31,31,31	0
56	MG	1a	3174	1/1	0.90	0.06	48,48,48,48	0
56	MG	2A	3434	1/1	0.90	0.14	30,30,30,30	0
56	MG	1A	4026	1/1	0.90	0.13	24,24,24,24	0
56	MG	2A	3780	1/1	0.90	0.13	48,48,48,48	0
56	MG	1A	3033	1/1	0.90	0.10	21,21,21,21	0
56	MG	1A	3229	1/1	0.90	0.15	29,29,29,29	0
56	MG	1A	3093	1/1	0.90	0.51	32,32,32,32	0
56	MG	1A	3914	1/1	0.90	0.19	44,44,44,44	0
56	MG	2A	3496	1/1	0.90	0.12	28,28,28,28	0
56	MG	2a	1615	1/1	0.90	0.20	37,37,37,37	0
56	MG	1w	103	1/1	0.90	0.14	44,44,44,44	0
56	MG	2A	3409	1/1	0.90	0.14	41,41,41,41	0
56	MG	1a	3011	1/1	0.90	0.14	49,49,49,49	0
56	MG	2A	3807	1/1	0.90	0.14	46,46,46,46	0
56	MG	2A	3336	1/1	0.90	0.62	47,47,47,47	0
56	MG	1A	3235	1/1	0.90	0.12	47,47,47,47	0
56	MG	2B	212	1/1	0.90	0.09	68,68,68,68	0
56	MG	2A	3619	1/1	0.90	0.08	46,46,46,46	0
56	MG	1B	220	1/1	0.90	0.15	32,32,32,32	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	1a	3186	1/1	0.90	0.08	66,66,66,66	0
56	MG	2A	3366	1/1	0.90	0.40	39,39,39,39	0
56	MG	2A	3513	1/1	0.90	0.10	32,32,32,32	0
56	MG	2A	3729	1/1	0.90	0.46	66,66,66,66	0
56	MG	2A	3306	1/1	0.90	0.09	35,35,35,35	0
56	MG	1A	4044	1/1	0.90	0.17	29,29,29,29	0
56	MG	2a	1713	1/1	0.90	0.13	59,59,59,59	0
56	MG	1A	3724	1/1	0.90	0.10	33,33,33,33	0
56	MG	10	101	1/1	0.90	0.30	32,32,32,32	0
56	MG	1A	3657	1/1	0.90	0.23	24,24,24,24	0
56	MG	26	102	1/1	0.90	0.31	58,58,58,58	0
56	MG	2A	3715	1/1	0.90	0.17	48,48,48,48	0
56	MG	1A	3279	1/1	0.90	0.17	40,40,40,40	0
56	MG	2E	305	1/1	0.90	0.10	36,36,36,36	0
56	MG	2A	3186	1/1	0.90	0.19	36,36,36,36	0
56	MG	1a	3168	1/1	0.90	0.08	47,47,47,47	0
56	MG	2a	1631	1/1	0.90	0.18	54,54,54,54	0
56	MG	2a	1776	1/1	0.90	0.12	53,53,53,53	0
56	MG	2a	1647	1/1	0.90	0.10	52,52,52,52	0
56	MG	2a	1609	1/1	0.90	0.16	50,50,50,50	0
56	MG	2A	3626	1/1	0.90	0.13	51,51,51,51	0
56	MG	1V	203	1/1	0.90	0.55	24,24,24,24	0
56	MG	1N	203	1/1	0.90	0.21	34,34,34,34	0
56	MG	2A	3746	1/1	0.90	0.10	34,34,34,34	0
56	MG	2A	3015	1/1	0.90	0.34	30,30,30,30	0
56	MG	2A	3570	1/1	0.90	0.17	56,56,56,56	0
56	MG	1A	3574	1/1	0.90	0.41	21,21,21,21	0
56	MG	1A	3980	1/1	0.90	0.08	18,18,18,18	0
56	MG	1x	107	1/1	0.90	0.12	59,59,59,59	0
56	MG	1A	3339	1/1	0.90	0.08	21,21,21,21	0
56	MG	1A	3984	1/1	0.90	0.09	60,60,60,60	0
56	MG	1A	3963	1/1	0.90	0.17	36,36,36,36	0
56	MG	1A	3225	1/1	0.90	0.15	46,46,46,46	0
56	MG	1A	3948	1/1	0.90	0.10	17,17,17,17	0
56	MG	1w	102	1/1	0.90	0.25	48,48,48,48	0
56	MG	1A	3693	1/1	0.90	0.17	5,5,5,5	0
56	MG	2A	3598	1/1	0.90	0.07	47,47,47,47	0
56	MG	2A	3668	1/1	0.90	0.10	38,38,38,38	0
56	MG	2l	203	1/1	0.90	0.12	59,59,59,59	0
56	MG	2A	3782	1/1	0.90	0.07	53,53,53,53	0
56	MG	2A	3383	1/1	0.90	0.12	34,34,34,34	0
56	MG	19	103	1/1	0.90	0.09	42,42,42,42	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	2A	3145	1/1	0.90	0.23	42,42,42,42	0
56	MG	2A	3874	1/1	0.90	0.09	53,53,53,53	0
56	MG	2A	3683	1/1	0.90	0.08	53,53,53,53	0
56	MG	2A	3368	1/1	0.90	0.15	30,30,30,30	0
56	MG	2A	3164	1/1	0.90	0.13	54,54,54,54	0
56	MG	1a	3070	1/1	0.90	0.21	47,47,47,47	0
56	MG	1A	3301	1/1	0.91	0.15	38,38,38,38	0
56	MG	2A	3338	1/1	0.91	0.09	64,64,64,64	0
56	MG	2A	3546	1/1	0.91	0.11	22,22,22,22	0
56	MG	1B	226	1/1	0.91	0.08	51,51,51,51	0
56	MG	2a	1626	1/1	0.91	0.40	56,56,56,56	0
56	MG	1A	3271	1/1	0.91	0.20	28,28,28,28	0
56	MG	2A	3108	1/1	0.91	0.16	50,50,50,50	0
56	MG	1a	3010	1/1	0.91	0.13	58,58,58,58	0
56	MG	1A	3516	1/1	0.91	0.13	26,26,26,26	0
56	MG	1A	3003	1/1	0.91	0.12	15,15,15,15	0
56	MG	2A	3353	1/1	0.91	0.28	51,51,51,51	0
56	MG	2A	3586	1/1	0.91	0.17	43,43,43,43	0
56	MG	2A	3844	1/1	0.91	0.11	58,58,58,58	0
56	MG	1a	3155	1/1	0.91	0.11	29,29,29,29	0
56	MG	1a	3142	1/1	0.91	0.10	49,49,49,49	0
56	MG	2B	201	1/1	0.91	0.10	57,57,57,57	0
56	MG	2A	3003	1/1	0.91	0.14	41,41,41,41	0
56	MG	2A	3204	1/1	0.91	0.12	39,39,39,39	0
56	MG	1A	3875	1/1	0.91	0.19	33,33,33,33	0
56	MG	1a	3081	1/1	0.91	0.14	43,43,43,43	0
56	MG	2A	3577	1/1	0.91	0.13	41,41,41,41	0
56	MG	2A	3631	1/1	0.91	0.16	41,41,41,41	0
56	MG	2A	3258	1/1	0.91	0.55	41,41,41,41	0
56	MG	2a	1802	1/1	0.91	0.14	40,40,40,40	0
56	MG	1A	3553	1/1	0.91	0.19	36,36,36,36	0
56	MG	1A	3053	1/1	0.91	0.19	45,45,45,45	0
56	MG	2A	3349	1/1	0.91	0.13	43,43,43,43	0
56	MG	1A	3502	1/1	0.91	0.23	44,44,44,44	0
56	MG	1y	102	1/1	0.91	0.17	60,60,60,60	0
56	MG	1A	3156	1/1	0.91	0.09	30,30,30,30	0
56	MG	1A	3647	1/1	0.91	0.08	27,27,27,27	0
56	MG	1A	3620	1/1	0.91	0.23	29,29,29,29	0
56	MG	1A	3810	1/1	0.91	0.07	28,28,28,28	0
56	MG	2A	3109	1/1	0.91	0.12	36,36,36,36	0
56	MG	1F	307	1/1	0.91	0.11	23,23,23,23	0
56	MG	1A	4065	1/1	0.91	0.18	14,14,14,14	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	2A	3869	1/1	0.91	0.16	49,49,49,49	0
56	MG	1e	202	1/1	0.91	0.18	45,45,45,45	0
56	MG	2A	3760	1/1	0.91	0.12	35,35,35,35	0
56	MG	2A	3228	1/1	0.91	0.80	42,42,42,42	0
56	MG	2A	3567	1/1	0.91	0.08	35,35,35,35	0
56	MG	1a	3014	1/1	0.91	0.10	48,48,48,48	0
56	MG	2A	3324	1/1	0.91	0.27	45,45,45,45	0
56	MG	25	103	1/1	0.91	0.14	25,25,25,25	0
56	MG	1A	3142	1/1	0.91	0.11	44,44,44,44	0
56	MG	2A	3717	1/1	0.91	0.13	44,44,44,44	0
56	MG	1A	3334	1/1	0.91	0.11	35,35,35,35	0
56	MG	1O	202	1/1	0.91	0.12	41,41,41,41	0
56	MG	1A	3115	1/1	0.91	0.36	13,13,13,13	0
56	MG	2A	3575	1/1	0.91	0.11	43,43,43,43	0
56	MG	2A	3834	1/1	0.91	0.08	24,24,24,24	0
56	MG	1A	3697	1/1	0.91	0.18	36,36,36,36	0
56	MG	2a	1782	1/1	0.91	0.08	40,40,40,40	0
56	MG	1A	3382	1/1	0.91	0.14	36,36,36,36	0
56	MG	2A	3803	1/1	0.91	0.15	54,54,54,54	0
56	MG	1A	3194	1/1	0.91	0.35	28,28,28,28	0
56	MG	2a	1745	1/1	0.91	0.12	62,62,62,62	0
58	ZN	2Y	501	1/1	0.91	0.13	83,83,83,83	0
56	MG	2a	1677	1/1	0.91	0.10	60,60,60,60	0
56	MG	2A	3067	1/1	0.91	0.28	36,36,36,36	0
56	MG	2A	3500	1/1	0.91	0.16	53,53,53,53	0
56	MG	2a	1792	1/1	0.91	0.22	66,66,66,66	0
56	MG	1E	305	1/1	0.91	0.26	26,26,26,26	0
56	MG	1A	3335	1/1	0.91	0.17	23,23,23,23	0
56	MG	2A	3292	1/1	0.91	0.16	31,31,31,31	0
56	MG	1a	3006	1/1	0.91	0.10	29,29,29,29	0
56	MG	1a	3078	1/1	0.91	0.08	35,35,35,35	0
56	MG	1A	3052	1/1	0.91	0.14	48,48,48,48	0
56	MG	2a	1641	1/1	0.91	0.11	47,47,47,47	0
56	MG	2a	1806	1/1	0.91	0.11	63,63,63,63	0
56	MG	1A	3351	1/1	0.91	0.37	25,25,25,25	0
56	MG	1A	3933	1/1	0.91	0.20	58,58,58,58	0
56	MG	2a	1789	1/1	0.91	0.13	54,54,54,54	0
56	MG	17	103	1/1	0.91	0.25	28,28,28,28	0
56	MG	1a	3029	1/1	0.91	0.14	33,33,33,33	0
56	MG	1a	3228	1/1	0.91	0.10	51,51,51,51	0
56	MG	2a	1825	1/1	0.91	0.10	58,58,58,58	0
56	MG	2A	3385	1/1	0.91	0.15	52,52,52,52	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	1F	301	1/1	0.91	0.49	25,25,25,25	0
56	MG	2A	3481	1/1	0.91	0.12	44,44,44,44	0
56	MG	2A	3128	1/1	0.91	0.65	44,44,44,44	0
56	MG	1A	3688	1/1	0.91	0.12	19,19,19,19	0
56	MG	1a	3074	1/1	0.91	0.09	55,55,55,55	0
56	MG	1A	3778	1/1	0.91	0.13	26,26,26,26	0
56	MG	1B	208	1/1	0.91	0.12	44,44,44,44	0
56	MG	1P	204	1/1	0.91	0.18	18,18,18,18	0
56	MG	1A	3635	1/1	0.91	0.10	26,26,26,26	0
56	MG	2a	1732	1/1	0.91	0.12	52,52,52,52	0
56	MG	2A	3341	1/1	0.91	0.08	52,52,52,52	0
56	MG	10	103	1/1	0.91	0.18	32,32,32,32	0
56	MG	2A	3430	1/1	0.91	0.25	45,45,45,45	0
56	MG	2A	3830	1/1	0.91	0.13	58,58,58,58	0
56	MG	1a	3158	1/1	0.91	0.12	51,51,51,51	0
56	MG	1A	3372	1/1	0.91	0.13	37,37,37,37	0
56	MG	1A	3609	1/1	0.91	0.40	54,54,54,54	0
56	MG	2A	3050	1/1	0.91	0.13	53,53,53,53	0
56	MG	2A	3008	1/1	0.91	0.08	49,49,49,49	0
56	MG	2A	3011	1/1	0.91	0.10	36,36,36,36	0
56	MG	1A	3800	1/1	0.91	0.11	31,31,31,31	0
56	MG	1a	3094	1/1	0.91	0.17	29,29,29,29	0
56	MG	2A	3059	1/1	0.91	0.12	34,34,34,34	0
56	MG	1A	3461	1/1	0.91	0.25	36,36,36,36	0
56	MG	1a	3041	1/1	0.91	0.10	52,52,52,52	0
56	MG	2A	3233	1/1	0.91	0.20	47,47,47,47	0
56	MG	1A	3994	1/1	0.91	0.07	50,50,50,50	0
56	MG	2A	3791	1/1	0.91	0.18	46,46,46,46	0
56	MG	1A	3413	1/1	0.91	0.14	21,21,21,21	0
56	MG	2A	3873	1/1	0.91	0.18	44,44,44,44	0
56	MG	2A	3856	1/1	0.91	0.07	45,45,45,45	0
56	MG	2Q	205	1/1	0.91	0.50	50,50,50,50	0
56	MG	20	102	1/1	0.91	0.21	68,68,68,68	0
56	MG	2A	3685	1/1	0.91	0.07	27,27,27,27	0
56	MG	1G	201	1/1	0.91	0.10	34,34,34,34	0
56	MG	2A	3136	1/1	0.91	0.09	43,43,43,43	0
56	MG	2a	1688	1/1	0.91	0.11	42,42,42,42	0
56	MG	2A	3532	1/1	0.91	0.06	31,31,31,31	0
56	MG	1A	3317	1/1	0.91	0.19	44,44,44,44	0
56	MG	1Z	301	1/1	0.91	0.22	32,32,32,32	0
56	MG	1A	3330	1/1	0.91	0.23	17,17,17,17	0
56	MG	2A	3758	1/1	0.91	0.11	47,47,47,47	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	1B	219	1/1	0.91	0.15	53,53,53,53	0
56	MG	2A	3642	1/1	0.91	0.13	56,56,56,56	0
56	MG	2a	1741	1/1	0.91	0.12	55,55,55,55	0
56	MG	1A	3610	1/1	0.91	0.13	27,27,27,27	0
56	MG	1A	4055	1/1	0.91	0.09	41,41,41,41	0
56	MG	1a	3220	1/1	0.91	0.10	46,46,46,46	0
56	MG	2A	3298	1/1	0.91	0.15	68,68,68,68	0
56	MG	2D	307	1/1	0.91	0.10	34,34,34,34	0
56	MG	2A	3617	1/1	0.91	0.11	36,36,36,36	0
56	MG	1A	3964	1/1	0.91	0.21	63,63,63,63	0
56	MG	2a	1739	1/1	0.91	0.10	48,48,48,48	0
56	MG	1a	3071	1/1	0.91	0.14	36,36,36,36	0
56	MG	1A	3898	1/1	0.91	0.20	42,42,42,42	0
56	MG	1A	3315	1/1	0.91	0.13	42,42,42,42	0
56	MG	2a	1735	1/1	0.91	0.23	46,46,46,46	0
56	MG	1A	3095	1/1	0.91	0.11	26,26,26,26	0
56	MG	2a	1793	1/1	0.91	0.23	55,55,55,55	0
56	MG	1P	208	1/1	0.91	0.19	45,45,45,45	0
56	MG	2A	3185	1/1	0.91	0.27	41,41,41,41	0
56	MG	1A	3799	1/1	0.91	0.06	30,30,30,30	0
56	MG	1A	3295	1/1	0.91	0.14	30,30,30,30	0
56	MG	2A	3772	1/1	0.91	0.09	55,55,55,55	0
56	MG	1A	3660	1/1	0.91	0.14	60,60,60,60	0
56	MG	1a	3110	1/1	0.91	0.14	56,56,56,56	0
56	MG	2A	3131	1/1	0.91	0.10	58,58,58,58	0
56	MG	1E	301	1/1	0.91	0.17	25,25,25,25	0
56	MG	1A	3081	1/1	0.91	0.15	40,40,40,40	0
56	MG	1A	3813	1/1	0.91	0.06	24,24,24,24	0
56	MG	2A	3431	1/1	0.91	0.17	37,37,37,37	0
56	MG	1A	3573	1/1	0.91	0.10	40,40,40,40	0
56	MG	2A	3495	1/1	0.91	0.13	55,55,55,55	0
56	MG	2a	1761	1/1	0.91	0.04	68,68,68,68	0
56	MG	23	101	1/1	0.91	0.30	43,43,43,43	0
56	MG	1A	3549	1/1	0.91	0.13	21,21,21,21	0
56	MG	2A	3816	1/1	0.91	0.12	40,40,40,40	0
56	MG	2a	1808	1/1	0.91	0.21	52,52,52,52	0
56	MG	15	106	1/1	0.91	0.38	30,30,30,30	0
56	MG	1A	4056	1/1	0.91	0.12	43,43,43,43	0
56	MG	2A	3868	1/1	0.91	0.10	32,32,32,32	0
56	MG	1a	3082	1/1	0.91	0.12	51,51,51,51	0
56	MG	1A	4059	1/1	0.91	0.12	30,30,30,30	0
56	MG	1a	3024	1/1	0.91	0.25	50,50,50,50	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	2A	3401	1/1	0.91	0.10	33,33,33,33	0
56	MG	1a	3049	1/1	0.92	0.09	47,47,47,47	0
56	MG	1A	3154	1/1	0.92	0.22	25,25,25,25	0
56	MG	2A	3016	1/1	0.92	0.12	43,43,43,43	0
56	MG	1A	3369	1/1	0.92	0.14	37,37,37,37	0
56	MG	2F	305	1/1	0.92	0.10	46,46,46,46	0
56	MG	2A	3607	1/1	0.92	0.20	32,32,32,32	0
56	MG	1A	3323	1/1	0.92	0.18	45,45,45,45	0
56	MG	2A	3022	1/1	0.92	0.23	49,49,49,49	0
56	MG	1A	3456	1/1	0.92	0.20	40,40,40,40	0
56	MG	1a	3134	1/1	0.92	0.29	45,45,45,45	0
56	MG	2A	3692	1/1	0.92	0.14	29,29,29,29	0
56	MG	2A	3194	1/1	0.92	0.16	38,38,38,38	0
56	MG	1A	3558	1/1	0.92	0.33	21,21,21,21	0
56	MG	1A	3031	1/1	0.92	0.35	20,20,20,20	0
56	MG	28	101	1/1	0.92	0.12	58,58,58,58	0
56	MG	1A	3680	1/1	0.92	0.11	18,18,18,18	0
56	MG	1A	3510	1/1	0.92	0.29	26,26,26,26	0
56	MG	1a	3126	1/1	0.92	0.14	39,39,39,39	0
56	MG	2A	3062	1/1	0.92	0.09	60,60,60,60	0
56	MG	1A	3251	1/1	0.92	0.09	32,32,32,32	0
56	MG	1A	3499	1/1	0.92	0.10	50,50,50,50	0
56	MG	2A	3606	1/1	0.92	0.15	45,45,45,45	0
56	MG	2A	3043	1/1	0.92	0.18	35,35,35,35	0
56	MG	1A	3760	1/1	0.92	0.12	14,14,14,14	0
56	MG	1F	302	1/1	0.92	0.38	22,22,22,22	0
56	MG	1A	3530	1/1	0.92	0.15	33,33,33,33	0
56	MG	1A	4052	1/1	0.92	0.21	55,55,55,55	0
56	MG	1a	3099	1/1	0.92	0.08	39,39,39,39	0
56	MG	1A	3162	1/1	0.92	0.15	18,18,18,18	0
56	MG	1A	4045	1/1	0.92	0.16	35,35,35,35	0
56	MG	2A	3342	1/1	0.92	0.18	55,55,55,55	0
56	MG	1A	3293	1/1	0.92	0.13	28,28,28,28	0
56	MG	2A	3630	1/1	0.92	0.36	37,37,37,37	0
56	MG	1A	3666	1/1	0.92	0.13	39,39,39,39	0
56	MG	1A	3318	1/1	0.92	0.15	45,45,45,45	0
56	MG	2A	3680	1/1	0.92	0.15	50,50,50,50	0
56	MG	1A	3904	1/1	0.92	0.35	19,19,19,19	0
56	MG	1A	3507	1/1	0.92	0.12	35,35,35,35	0
56	MG	1A	3152	1/1	0.92	0.09	18,18,18,18	0
56	MG	2F	302	1/1	0.92	0.33	53,53,53,53	0
56	MG	2A	3731	1/1	0.92	0.21	45,45,45,45	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	2A	3711	1/1	0.92	0.18	51,51,51,51	0
56	MG	2a	1634	1/1	0.92	0.09	50,50,50,50	0
56	MG	2A	3517	1/1	0.92	0.08	37,37,37,37	0
56	MG	2A	3318	1/1	0.92	0.27	45,45,45,45	0
56	MG	2B	218	1/1	0.92	0.12	61,61,61,61	0
56	MG	1D	306	1/1	0.92	0.10	22,22,22,22	0
56	MG	1A	3097	1/1	0.92	0.18	31,31,31,31	0
56	MG	2A	3866	1/1	0.92	0.17	37,37,37,37	0
56	MG	1A	3491	1/1	0.92	0.17	24,24,24,24	0
56	MG	1A	3897	1/1	0.92	0.12	55,55,55,55	0
56	MG	1A	3985	1/1	0.92	0.10	39,39,39,39	0
56	MG	1D	301	1/1	0.92	0.17	19,19,19,19	0
56	MG	2a	1733	1/1	0.92	0.06	66,66,66,66	0
56	MG	2A	3790	1/1	0.92	0.16	48,48,48,48	0
56	MG	2A	3808	1/1	0.92	0.10	55,55,55,55	0
56	MG	1A	3342	1/1	0.92	0.24	19,19,19,19	0
56	MG	2A	3404	1/1	0.92	0.26	44,44,44,44	0
56	MG	1A	3202	1/1	0.92	0.23	26,26,26,26	0
56	MG	1A	3102	1/1	0.92	0.16	18,18,18,18	0
56	MG	1A	3757	1/1	0.92	0.18	9,9,9,9	0
56	MG	1A	3401	1/1	0.92	0.27	38,38,38,38	0
56	MG	2A	3389	1/1	0.92	0.24	38,38,38,38	0
56	MG	1A	3715	1/1	0.92	0.09	34,34,34,34	0
56	MG	2A	3150	1/1	0.92	0.10	47,47,47,47	0
56	MG	2a	1621	1/1	0.92	0.18	65,65,65,65	0
56	MG	1A	3452	1/1	0.92	0.14	22,22,22,22	0
56	MG	1A	3122	1/1	0.92	0.30	14,14,14,14	0
56	MG	13	105	1/1	0.92	0.12	48,48,48,48	0
56	MG	2A	3629	1/1	0.92	0.14	36,36,36,36	0
56	MG	1A	3267	1/1	0.92	0.15	33,33,33,33	0
56	MG	1A	4008	1/1	0.92	0.11	37,37,37,37	0
56	MG	1A	3500	1/1	0.92	0.31	27,27,27,27	0
56	MG	1A	3193	1/1	0.92	0.16	24,24,24,24	0
56	MG	19	102	1/1	0.92	0.18	33,33,33,33	0
56	MG	1A	3300	1/1	0.92	0.12	28,28,28,28	0
56	MG	1A	3486	1/1	0.92	0.10	24,24,24,24	0
56	MG	2E	306	1/1	0.92	0.24	40,40,40,40	0
56	MG	1Q	208	1/1	0.92	0.15	15,15,15,15	0
56	MG	2Q	201	1/1	0.92	0.10	33,33,33,33	0
56	MG	1D	312	1/1	0.92	0.20	36,36,36,36	0
56	MG	2x	102	1/1	0.92	0.12	59,59,59,59	0
56	MG	1a	3009	1/1	0.92	0.08	48,48,48,48	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	2A	3438	1/1	0.92	0.11	32,32,32,32	0
56	MG	2A	3416	1/1	0.92	0.14	45,45,45,45	0
56	MG	2A	3205	1/1	0.92	0.10	33,33,33,33	0
56	MG	1A	3851	1/1	0.92	0.44	36,36,36,36	0
56	MG	1a	3163	1/1	0.92	0.10	33,33,33,33	0
56	MG	1A	3362	1/1	0.92	0.15	28,28,28,28	0
56	MG	2A	3246	1/1	0.92	0.06	54,54,54,54	0
56	MG	16	101	1/1	0.92	0.23	35,35,35,35	0
56	MG	1A	3968	1/1	0.92	0.14	20,20,20,20	0
56	MG	1A	3026	1/1	0.92	0.45	17,17,17,17	0
56	MG	2A	3622	1/1	0.92	0.09	37,37,37,37	0
56	MG	1A	3529	1/1	0.92	0.41	27,27,27,27	0
56	MG	1A	3488	1/1	0.92	0.17	44,44,44,44	0
56	MG	2A	3357	1/1	0.92	0.13	43,43,43,43	0
56	MG	2A	3143	1/1	0.92	0.16	33,33,33,33	0
56	MG	1A	3922	1/1	0.92	0.07	24,24,24,24	0
56	MG	1A	3632	1/1	0.92	0.14	38,38,38,38	0
56	MG	1A	3297	1/1	0.92	0.21	28,28,28,28	0
56	MG	2A	3394	1/1	0.92	0.31	50,50,50,50	0
56	MG	2A	3105	1/1	0.92	0.15	50,50,50,50	0
56	MG	2l	201	1/1	0.92	0.12	48,48,48,48	0
56	MG	20	101	1/1	0.92	0.11	50,50,50,50	0
56	MG	1A	3185	1/1	0.92	0.10	39,39,39,39	0
56	MG	2a	1699	1/1	0.92	0.23	54,54,54,54	0
56	MG	1n	101	1/1	0.92	0.08	52,52,52,52	0
56	MG	1a	3125	1/1	0.92	0.14	35,35,35,35	0
56	MG	2A	3278	1/1	0.92	0.12	26,26,26,26	0
56	MG	2a	1650	1/1	0.92	0.37	63,63,63,63	0
56	MG	1A	3023	1/1	0.92	0.12	13,13,13,13	0
56	MG	2x	103	1/1	0.92	0.09	46,46,46,46	0
56	MG	1A	3806	1/1	0.92	0.13	16,16,16,16	0
56	MG	2A	3053	1/1	0.92	0.13	53,53,53,53	0
56	MG	1a	3223	1/1	0.92	0.08	40,40,40,40	0
56	MG	1A	3214	1/1	0.92	0.13	32,32,32,32	0
56	MG	2a	1781	1/1	0.92	0.34	41,41,41,41	0
56	MG	1A	3008	1/1	0.92	0.18	16,16,16,16	0
56	MG	1A	4012	1/1	0.92	0.24	42,42,42,42	0
56	MG	1A	3952	1/1	0.92	0.10	19,19,19,19	0
56	MG	2A	3286	1/1	0.92	0.28	46,46,46,46	0
56	MG	1A	3503	1/1	0.92	0.16	21,21,21,21	0
56	MG	1A	3541	1/1	0.92	0.14	14,14,14,14	0
56	MG	1a	3051	1/1	0.92	0.14	44,44,44,44	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	2A	3091	1/1	0.92	0.21	36,36,36,36	0
56	MG	1a	3173	1/1	0.92	0.10	44,44,44,44	0
56	MG	1A	3360	1/1	0.92	0.30	27,27,27,27	0
56	MG	1A	3266	1/1	0.92	0.19	25,25,25,25	0
56	MG	1A	3703	1/1	0.92	0.11	38,38,38,38	0
56	MG	1A	3580	1/1	0.92	0.11	40,40,40,40	0
56	MG	2a	1799	1/1	0.92	0.21	45,45,45,45	0
56	MG	1X	102	1/1	0.92	0.13	29,29,29,29	0
56	MG	1A	3537	1/1	0.92	0.16	31,31,31,31	0
56	MG	1a	3002	1/1	0.92	0.12	42,42,42,42	0
56	MG	2A	3553	1/1	0.92	0.08	27,27,27,27	0
56	MG	2a	1712	1/1	0.92	0.14	48,48,48,48	0
56	MG	2a	1751	1/1	0.92	0.07	72,72,72,72	0
56	MG	2A	3545	1/1	0.92	0.10	32,32,32,32	0
56	MG	2A	3657	1/1	0.92	0.06	38,38,38,38	0
56	MG	1a	3222	1/1	0.92	0.09	41,41,41,41	0
56	MG	2A	3595	1/1	0.92	0.07	34,34,34,34	0
56	MG	2A	3563	1/1	0.92	0.19	50,50,50,50	0
56	MG	2a	1611	1/1	0.92	0.32	51,51,51,51	0
56	MG	1a	3047	1/1	0.92	0.17	39,39,39,39	0
56	MG	1E	306	1/1	0.92	0.24	22,22,22,22	0
56	MG	2a	1717	1/1	0.92	0.14	52,52,52,52	0
56	MG	2A	3604	1/1	0.92	0.09	33,33,33,33	0
56	MG	2A	3235	1/1	0.92	0.26	31,31,31,31	0
56	MG	1B	211	1/1	0.92	0.25	54,54,54,54	0
56	MG	1B	218	1/1	0.92	0.10	21,21,21,21	0
56	MG	1a	3038	1/1	0.92	0.11	56,56,56,56	0
56	MG	2q	203	1/1	0.92	0.12	41,41,41,41	0
56	MG	1A	3761	1/1	0.92	0.23	39,39,39,39	0
56	MG	1A	4027	1/1	0.92	0.10	48,48,48,48	0
56	MG	1A	3825	1/1	0.92	0.07	30,30,30,30	0
56	MG	1A	3797	1/1	0.92	0.07	19,19,19,19	0
56	MG	2A	3057	1/1	0.92	0.14	29,29,29,29	0
56	MG	1A	3837	1/1	0.92	0.14	27,27,27,27	0
56	MG	1A	3687	1/1	0.92	0.10	21,21,21,21	0
56	MG	1A	3236	1/1	0.92	0.14	28,28,28,28	0
56	MG	2A	3674	1/1	0.92	0.05	53,53,53,53	0
56	MG	1A	3691	1/1	0.92	0.14	16,16,16,16	0
56	MG	1Q	206	1/1	0.92	0.14	26,26,26,26	0
56	MG	1A	3884	1/1	0.92	0.11	15,15,15,15	0
56	MG	1B	204	1/1	0.92	0.20	30,30,30,30	0
56	MG	2E	303	1/1	0.92	0.09	15,15,15,15	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	1A	3470	1/1	0.92	0.12	36,36,36,36	0
56	MG	1x	104	1/1	0.92	0.11	67,67,67,67	0
56	MG	1t	201	1/1	0.92	0.09	40,40,40,40	0
56	MG	2A	3393	1/1	0.92	0.20	42,42,42,42	0
56	MG	1E	304	1/1	0.92	0.25	25,25,25,25	0
56	MG	2A	3702	1/1	0.92	0.10	29,29,29,29	0
56	MG	2A	3284	1/1	0.92	0.16	29,29,29,29	0
56	MG	2A	3223	1/1	0.92	0.13	41,41,41,41	0
56	MG	2a	1651	1/1	0.92	0.11	43,43,43,43	0
56	MG	1A	3493	1/1	0.92	0.36	55,55,55,55	0
56	MG	1A	3224	1/1	0.92	0.14	23,23,23,23	0
56	MG	1A	3117	1/1	0.92	0.75	38,38,38,38	0
56	MG	2a	1800	1/1	0.92	0.08	56,56,56,56	0
56	MG	16	104	1/1	0.93	0.20	33,33,33,33	0
56	MG	1A	3227	1/1	0.93	0.09	56,56,56,56	0
56	MG	1A	3765	1/1	0.93	0.13	33,33,33,33	0
56	MG	2A	3361	1/1	0.93	0.09	33,33,33,33	0
56	MG	2A	3101	1/1	0.93	0.14	39,39,39,39	0
56	MG	1A	3290	1/1	0.93	0.13	12,12,12,12	0
56	MG	2A	3861	1/1	0.93	0.08	33,33,33,33	0
56	MG	1a	3090	1/1	0.93	0.21	29,29,29,29	0
56	MG	1A	3698	1/1	0.93	0.13	41,41,41,41	0
56	MG	2A	3463	1/1	0.93	0.28	45,45,45,45	0
56	MG	2A	3464	1/1	0.93	0.61	41,41,41,41	0
56	MG	1B	232	1/1	0.93	0.11	35,35,35,35	0
56	MG	1A	3164	1/1	0.93	0.11	26,26,26,26	0
56	MG	2V	201	1/1	0.93	0.71	44,44,44,44	0
56	MG	2A	3583	1/1	0.93	0.08	39,39,39,39	0
56	MG	1a	3205	1/1	0.93	0.10	39,39,39,39	0
56	MG	1x	108	1/1	0.93	0.12	38,38,38,38	0
56	MG	2A	3241	1/1	0.93	0.20	38,38,38,38	0
56	MG	2A	3615	1/1	0.93	0.17	28,28,28,28	0
56	MG	2A	3510	1/1	0.93	0.17	49,49,49,49	0
56	MG	1A	3088	1/1	0.93	0.18	21,21,21,21	0
56	MG	1a	3136	1/1	0.93	0.16	44,44,44,44	0
56	MG	2A	3001	1/1	0.93	0.15	41,41,41,41	0
56	MG	2A	3764	1/1	0.93	0.20	54,54,54,54	0
56	MG	1A	3277	1/1	0.93	0.17	36,36,36,36	0
56	MG	1a	3150	1/1	0.93	0.09	43,43,43,43	0
56	MG	1a	3077	1/1	0.93	0.16	50,50,50,50	0
56	MG	1A	3478	1/1	0.93	0.27	22,22,22,22	0
56	MG	1A	3496	1/1	0.93	0.13	28,28,28,28	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	1A	3769	1/1	0.93	0.16	21,21,21,21	0
56	MG	1A	3918	1/1	0.93	0.15	27,27,27,27	0
56	MG	1A	3535	1/1	0.93	0.15	31,31,31,31	0
56	MG	2A	3456	1/1	0.93	0.23	37,37,37,37	0
56	MG	2A	3603	1/1	0.93	0.08	39,39,39,39	0
56	MG	2A	3146	1/1	0.93	0.21	29,29,29,29	0
56	MG	2X	102	1/1	0.93	0.11	45,45,45,45	0
56	MG	2A	3400	1/1	0.93	0.12	62,62,62,62	0
56	MG	2A	3537	1/1	0.93	0.13	27,27,27,27	0
56	MG	1A	3965	1/1	0.93	0.10	44,44,44,44	0
56	MG	2A	3189	1/1	0.93	0.11	46,46,46,46	0
56	MG	1P	207	1/1	0.93	0.35	29,29,29,29	0
56	MG	1a	3034	1/1	0.93	0.13	42,42,42,42	0
56	MG	1A	3733	1/1	0.93	0.17	45,45,45,45	0
56	MG	2A	3190	1/1	0.93	0.14	26,26,26,26	0
56	MG	1A	3331	1/1	0.93	0.32	42,42,42,42	0
56	MG	2A	3381	1/1	0.93	0.21	36,36,36,36	0
56	MG	1A	3527	1/1	0.93	0.20	22,22,22,22	0
56	MG	2A	3479	1/1	0.93	0.24	49,49,49,49	0
56	MG	2A	3646	1/1	0.93	0.21	34,34,34,34	0
56	MG	1a	3147	1/1	0.93	0.09	54,54,54,54	0
56	MG	1A	4032	1/1	0.93	0.08	43,43,43,43	0
56	MG	1A	3385	1/1	0.93	0.10	29,29,29,29	0
56	MG	2A	3677	1/1	0.93	0.22	36,36,36,36	0
56	MG	1a	3101	1/1	0.93	0.16	43,43,43,43	0
56	MG	2A	3504	1/1	0.93	0.18	59,59,59,59	0
56	MG	2A	3562	1/1	0.93	0.44	65,65,65,65	0
56	MG	1A	3718	1/1	0.93	0.08	22,22,22,22	0
56	MG	1A	3990	1/1	0.93	0.11	43,43,43,43	0
56	MG	1F	311	1/1	0.93	0.19	29,29,29,29	0
56	MG	1A	3130	1/1	0.93	0.08	21,21,21,21	0
56	MG	1A	3656	1/1	0.93	0.11	36,36,36,36	0
56	MG	1A	3045	1/1	0.93	0.25	41,41,41,41	0
56	MG	1A	3705	1/1	0.93	0.14	15,15,15,15	0
56	MG	1A	3764	1/1	0.93	0.11	20,20,20,20	0
56	MG	1x	112	1/1	0.93	0.12	58,58,58,58	0
56	MG	1X	104	1/1	0.93	0.12	43,43,43,43	0
56	MG	1a	3058	1/1	0.93	0.12	58,58,58,58	0
56	MG	1A	3363	1/1	0.93	0.16	34,34,34,34	0
56	MG	1A	3264	1/1	0.93	0.17	26,26,26,26	0
56	MG	2A	3188	1/1	0.93	0.24	36,36,36,36	0
56	MG	27	102	1/1	0.93	0.81	51,51,51,51	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	2E	304	1/1	0.93	0.30	57,57,57,57	0
56	MG	1A	3907	1/1	0.93	0.18	10,10,10,10	0
56	MG	2A	3581	1/1	0.93	0.12	30,30,30,30	0
56	MG	1A	4019	1/1	0.93	0.23	9,9,9,9	0
56	MG	2A	3660	1/1	0.93	0.27	56,56,56,56	0
56	MG	1A	3242	1/1	0.93	0.28	13,13,13,13	0
56	MG	1a	3149	1/1	0.93	0.07	33,33,33,33	0
56	MG	1A	3961	1/1	0.93	0.10	57,57,57,57	0
56	MG	1A	3258	1/1	0.93	0.57	39,39,39,39	0
56	MG	1A	3741	1/1	0.93	0.09	51,51,51,51	0
56	MG	1A	3492	1/1	0.93	0.09	26,26,26,26	0
56	MG	1A	3247	1/1	0.93	0.22	19,19,19,19	0
56	MG	1A	3801	1/1	0.93	0.16	46,46,46,46	0
56	MG	2A	3584	1/1	0.93	0.14	44,44,44,44	0
56	MG	1A	3862	1/1	0.93	0.09	29,29,29,29	0
56	MG	1D	309	1/1	0.93	0.14	30,30,30,30	0
56	MG	1A	3374	1/1	0.93	0.21	40,40,40,40	0
56	MG	2a	1697	1/1	0.93	0.19	55,55,55,55	0
56	MG	1A	3250	1/1	0.93	0.29	31,31,31,31	0
56	MG	2a	1602	1/1	0.93	0.33	49,49,49,49	0
56	MG	2a	1816	1/1	0.93	0.20	38,38,38,38	0
56	MG	2A	3645	1/1	0.93	0.12	38,38,38,38	0
56	MG	2A	3212	1/1	0.93	0.15	38,38,38,38	0
56	MG	2f	201	1/1	0.93	0.14	37,37,37,37	0
56	MG	2A	3579	1/1	0.93	0.14	46,46,46,46	0
56	MG	1A	3432	1/1	0.93	0.30	21,21,21,21	0
56	MG	1A	3506	1/1	0.93	0.16	43,43,43,43	0
56	MG	1A	4024	1/1	0.93	0.17	28,28,28,28	0
56	MG	1A	3090	1/1	0.93	0.62	28,28,28,28	0
56	MG	2A	3039	1/1	0.93	0.09	35,35,35,35	0
56	MG	1V	206	1/1	0.93	0.16	31,31,31,31	0
56	MG	1a	3154	1/1	0.93	0.19	34,34,34,34	0
56	MG	2A	3346	1/1	0.93	0.14	33,33,33,33	0
56	MG	2A	3740	1/1	0.93	0.22	55,55,55,55	0
56	MG	1F	303	1/1	0.93	0.55	23,23,23,23	0
56	MG	1B	228	1/1	0.93	0.10	35,35,35,35	0
56	MG	1a	3044	1/1	0.93	0.08	53,53,53,53	0
56	MG	2A	3508	1/1	0.93	0.09	43,43,43,43	0
56	MG	1A	3365	1/1	0.93	0.51	28,28,28,28	0
56	MG	2w	101	1/1	0.93	0.09	50,50,50,50	0
56	MG	1A	3987	1/1	0.93	0.11	16,16,16,16	0
56	MG	2A	3148	1/1	0.93	0.33	41,41,41,41	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	1a	3199	1/1	0.93	0.06	45,45,45,45	0
56	MG	1A	3296	1/1	0.93	0.13	16,16,16,16	0
56	MG	1a	3190	1/1	0.93	0.14	37,37,37,37	0
56	MG	2a	1637	1/1	0.93	0.23	45,45,45,45	0
56	MG	2A	3547	1/1	0.93	0.11	18,18,18,18	0
56	MG	1A	3956	1/1	0.93	0.10	50,50,50,50	0
56	MG	2a	1668	1/1	0.93	0.09	48,48,48,48	0
56	MG	1w	106	1/1	0.93	0.13	32,32,32,32	0
56	MG	2A	3123	1/1	0.93	0.07	34,34,34,34	0
56	MG	2d	301	1/1	0.93	0.08	51,51,51,51	0
56	MG	1A	3444	1/1	0.93	0.17	25,25,25,25	0
56	MG	2A	3633	1/1	0.93	0.10	41,41,41,41	0
56	MG	1A	3134	1/1	0.93	0.31	22,22,22,22	0
56	MG	1A	3943	1/1	0.93	0.09	24,24,24,24	0
56	MG	1A	3665	1/1	0.93	0.12	23,23,23,23	0
56	MG	1A	3263	1/1	0.93	0.28	24,24,24,24	0
56	MG	1a	3164	1/1	0.93	0.08	49,49,49,49	0
56	MG	1A	3294	1/1	0.93	0.18	37,37,37,37	0
56	MG	2A	3020	1/1	0.93	0.11	44,44,44,44	0
56	MG	1A	4025	1/1	0.93	0.09	42,42,42,42	0
56	MG	1A	3518	1/1	0.93	0.45	30,30,30,30	0
56	MG	1A	3750	1/1	0.93	0.13	43,43,43,43	0
56	MG	1A	3127	1/1	0.93	0.44	23,23,23,23	0
56	MG	2y	103	1/1	0.93	0.06	41,41,41,41	0
56	MG	1A	3367	1/1	0.93	0.12	18,18,18,18	0
56	MG	2A	3093	1/1	0.93	0.08	29,29,29,29	0
56	MG	1A	3018	1/1	0.93	0.14	17,17,17,17	0
56	MG	2A	3455	1/1	0.93	0.12	63,63,63,63	0
56	MG	1a	3069	1/1	0.93	0.16	54,54,54,54	0
56	MG	2A	3139	1/1	0.93	0.34	44,44,44,44	0
56	MG	2B	213	1/1	0.93	0.13	35,35,35,35	0
56	MG	1A	3084	1/1	0.93	0.08	31,31,31,31	0
56	MG	2A	3450	1/1	0.93	0.08	52,52,52,52	0
56	MG	2A	3524	1/1	0.93	0.12	31,31,31,31	0
56	MG	1a	3130	1/1	0.93	0.13	52,52,52,52	0
56	MG	1A	3148	1/1	0.93	0.40	29,29,29,29	0
56	MG	2A	3403	1/1	0.93	0.10	51,51,51,51	0
56	MG	1A	3433	1/1	0.93	0.27	22,22,22,22	0
56	MG	1A	3641	1/1	0.93	0.11	18,18,18,18	0
56	MG	2A	3841	1/1	0.93	0.08	39,39,39,39	0
56	MG	2a	1768	1/1	0.93	0.14	48,48,48,48	0
56	MG	1A	3532	1/1	0.93	0.23	42,42,42,42	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	1A	3255	1/1	0.93	0.19	20,20,20,20	0
56	MG	2A	3402	1/1	0.93	0.17	42,42,42,42	0
56	MG	1A	4023	1/1	0.93	0.09	46,46,46,46	0
56	MG	2A	3625	1/1	0.93	0.19	53,53,53,53	0
56	MG	1A	3783	1/1	0.93	0.11	17,17,17,17	0
56	MG	2A	3488	1/1	0.93	0.12	43,43,43,43	0
56	MG	1A	3368	1/1	0.93	0.10	18,18,18,18	0
56	MG	1A	3411	1/1	0.93	0.08	36,36,36,36	0
56	MG	2A	3310	1/1	0.93	0.45	24,24,24,24	0
56	MG	18	101	1/1	0.93	0.27	36,36,36,36	0
56	MG	1A	3832	1/1	0.93	0.12	35,35,35,35	0
56	MG	2a	1607	1/1	0.93	0.11	31,31,31,31	0
56	MG	2A	3689	1/1	0.93	0.14	48,48,48,48	0
56	MG	1a	3116	1/1	0.93	0.12	40,40,40,40	0
56	MG	1A	3860	1/1	0.93	0.08	25,25,25,25	0
56	MG	2B	221	1/1	0.93	0.13	56,56,56,56	0
56	MG	1R	202	1/1	0.93	0.12	23,23,23,23	0
56	MG	1A	3709	1/1	0.93	0.14	31,31,31,31	0
56	MG	2A	3549	1/1	0.93	0.27	58,58,58,58	0
56	MG	2B	211	1/1	0.93	0.13	61,61,61,61	0
56	MG	2a	1675	1/1	0.93	0.07	55,55,55,55	0
56	MG	1A	3398	1/1	0.93	0.47	33,33,33,33	0
56	MG	1A	3101	1/1	0.93	0.32	36,36,36,36	0
56	MG	1A	3696	1/1	0.93	0.16	24,24,24,24	0
56	MG	1A	3419	1/1	0.93	0.15	47,47,47,47	0
56	MG	1A	3048	1/1	0.93	0.08	27,27,27,27	0
56	MG	1A	3327	1/1	0.93	0.44	31,31,31,31	0
56	MG	1A	3177	1/1	0.93	0.19	21,21,21,21	0
56	MG	2A	3010	1/1	0.93	0.08	39,39,39,39	0
56	MG	1A	3063	1/1	0.93	0.21	26,26,26,26	0
56	MG	2A	3288	1/1	0.93	0.12	51,51,51,51	0
56	MG	1a	3189	1/1	0.93	0.11	60,60,60,60	0
56	MG	1a	3192	1/1	0.93	0.08	42,42,42,42	0
56	MG	1A	3969	1/1	0.93	0.13	13,13,13,13	0
56	MG	1a	3025	1/1	0.93	0.18	40,40,40,40	0
56	MG	1T	202	1/1	0.93	0.37	50,50,50,50	0
56	MG	2a	1774	1/1	0.93	0.18	65,65,65,65	0
56	MG	2A	3069	1/1	0.93	0.31	41,41,41,41	0
56	MG	2A	3635	1/1	0.93	0.18	59,59,59,59	0
56	MG	2a	1813	1/1	0.93	0.12	60,60,60,60	0
56	MG	1U	204	1/1	0.93	0.52	27,27,27,27	0
56	MG	2A	3216	1/1	0.93	0.13	39,39,39,39	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	2A	3624	1/1	0.93	0.29	58,58,58,58	0
56	MG	2A	3511	1/1	0.93	0.21	39,39,39,39	0
56	MG	1a	3043	1/1	0.93	0.09	36,36,36,36	0
56	MG	2A	3169	1/1	0.93	0.21	35,35,35,35	0
56	MG	1A	3883	1/1	0.93	0.10	30,30,30,30	0
56	MG	1A	3991	1/1	0.93	0.15	24,24,24,24	0
56	MG	1A	3457	1/1	0.93	0.18	24,24,24,24	0
56	MG	2A	3761	1/1	0.93	0.10	42,42,42,42	0
56	MG	1A	3428	1/1	0.93	0.31	55,55,55,55	0
56	MG	2A	3835	1/1	0.93	0.07	51,51,51,51	0
56	MG	1A	3515	1/1	0.93	0.09	38,38,38,38	0
56	MG	1a	3148	1/1	0.93	0.13	46,46,46,46	0
56	MG	1a	3007	1/1	0.93	0.19	54,54,54,54	0
56	MG	1a	3135	1/1	0.93	0.21	33,33,33,33	0
56	MG	17	101	1/1	0.93	0.15	21,21,21,21	0
56	MG	2A	3088	1/1	0.93	0.07	47,47,47,47	0
56	MG	2A	3203	1/1	0.93	0.32	34,34,34,34	0
56	MG	2A	3497	1/1	0.93	0.34	72,72,72,72	0
56	MG	2A	3333	1/1	0.93	0.08	37,37,37,37	0
56	MG	1A	3237	1/1	0.93	0.13	29,29,29,29	0
56	MG	2A	3332	1/1	0.93	0.10	59,59,59,59	0
56	MG	1A	3223	1/1	0.93	0.13	29,29,29,29	0
56	MG	2a	1659	1/1	0.93	0.10	49,49,49,49	0
56	MG	2A	3202	1/1	0.93	0.16	22,22,22,22	0
56	MG	1U	208	1/1	0.93	0.34	25,25,25,25	0
56	MG	1A	3579	1/1	0.93	0.18	32,32,32,32	0
56	MG	1a	3045	1/1	0.93	0.16	48,48,48,48	0
56	MG	1a	3165	1/1	0.93	0.14	63,63,63,63	0
56	MG	1F	312	1/1	0.93	0.10	28,28,28,28	0
56	MG	2A	3086	1/1	0.93	0.11	34,34,34,34	0
56	MG	2A	3671	1/1	0.93	0.09	35,35,35,35	0
56	MG	1A	3468	1/1	0.93	0.19	25,25,25,25	0
56	MG	1A	3361	1/1	0.94	0.07	43,43,43,43	0
56	MG	2a	1742	1/1	0.94	0.09	60,60,60,60	0
56	MG	1A	3310	1/1	0.94	0.21	19,19,19,19	0
56	MG	1A	3901	1/1	0.94	0.14	32,32,32,32	0
56	MG	1A	3199	1/1	0.94	0.12	32,32,32,32	0
56	MG	2A	3309	1/1	0.94	0.26	41,41,41,41	0
56	MG	1A	3132	1/1	0.94	0.11	35,35,35,35	0
56	MG	1A	3891	1/1	0.94	0.09	37,37,37,37	0
56	MG	2A	3752	1/1	0.94	0.12	47,47,47,47	0
56	MG	2a	1683	1/1	0.94	0.14	41,41,41,41	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	2A	3255	1/1	0.94	0.11	30,30,30,30	0
56	MG	2A	3247	1/1	0.94	0.10	32,32,32,32	0
56	MG	1A	3763	1/1	0.94	0.10	25,25,25,25	0
56	MG	1B	209	1/1	0.94	0.16	43,43,43,43	0
56	MG	2A	3756	1/1	0.94	0.47	51,51,51,51	0
56	MG	10	105	1/1	0.94	0.13	32,32,32,32	0
56	MG	2A	3655	1/1	0.94	0.30	39,39,39,39	0
56	MG	15	103	1/1	0.94	0.40	21,21,21,21	0
56	MG	1A	3654	1/1	0.94	0.07	10,10,10,10	0
56	MG	15	105	1/1	0.94	0.26	13,13,13,13	0
56	MG	2A	3264	1/1	0.94	0.38	38,38,38,38	0
56	MG	1A	3727	1/1	0.94	0.18	31,31,31,31	0
56	MG	1A	3538	1/1	0.94	0.19	20,20,20,20	0
56	MG	1x	103	1/1	0.94	0.10	57,57,57,57	0
56	MG	2A	3215	1/1	0.94	0.10	31,31,31,31	0
56	MG	1A	3306	1/1	0.94	0.11	27,27,27,27	0
56	MG	1A	3752	1/1	0.94	0.10	26,26,26,26	0
56	MG	2a	1805	1/1	0.94	0.27	54,54,54,54	0
56	MG	2A	3399	1/1	0.94	0.07	40,40,40,40	0
56	MG	1A	3588	1/1	0.94	0.10	27,27,27,27	0
56	MG	2a	1822	1/1	0.94	0.13	50,50,50,50	0
56	MG	2A	3785	1/1	0.94	0.10	70,70,70,70	0
56	MG	2A	3195	1/1	0.94	0.17	38,38,38,38	0
56	MG	1A	3719	1/1	0.94	0.09	50,50,50,50	0
56	MG	2A	3055	1/1	0.94	0.10	47,47,47,47	0
56	MG	2A	3539	1/1	0.94	0.09	56,56,56,56	0
56	MG	2a	1656	1/1	0.94	0.16	43,43,43,43	0
56	MG	2A	3659	1/1	0.94	0.18	57,57,57,57	0
56	MG	2A	3364	1/1	0.94	0.14	23,23,23,23	0
56	MG	1A	3390	1/1	0.94	0.11	25,25,25,25	0
56	MG	2A	3687	1/1	0.94	0.14	36,36,36,36	0
56	MG	2A	3599	1/1	0.94	0.08	44,44,44,44	0
56	MG	1A	3210	1/1	0.94	0.33	18,18,18,18	0
56	MG	1A	3485	1/1	0.94	0.13	43,43,43,43	0
56	MG	1A	3051	1/1	0.94	0.12	15,15,15,15	0
56	MG	1A	3781	1/1	0.94	0.14	21,21,21,21	0
56	MG	1a	3209	1/1	0.94	0.15	68,68,68,68	0
56	MG	1A	3850	1/1	0.94	0.11	23,23,23,23	0
56	MG	1A	3695	1/1	0.94	0.14	16,16,16,16	0
56	MG	1A	3421	1/1	0.94	0.09	28,28,28,28	0
56	MG	2a	1684	1/1	0.94	0.18	45,45,45,45	0
56	MG	1a	3079	1/1	0.94	0.14	48,48,48,48	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	2A	3436	1/1	0.94	0.11	44,44,44,44	0
56	MG	2A	3085	1/1	0.94	0.22	37,37,37,37	0
56	MG	1A	3843	1/1	0.94	0.12	32,32,32,32	0
56	MG	1A	3651	1/1	0.94	0.12	8,8,8,8	0
56	MG	2A	3360	1/1	0.94	0.12	49,49,49,49	0
56	MG	2A	3163	1/1	0.94	0.16	71,71,71,71	0
56	MG	2R	201	1/1	0.94	0.12	27,27,27,27	0
56	MG	2U	203	1/1	0.94	0.43	36,36,36,36	0
56	MG	1a	3039	1/1	0.94	0.13	42,42,42,42	0
56	MG	1A	3287	1/1	0.94	0.16	28,28,28,28	0
56	MG	2g	201	1/1	0.94	0.09	57,57,57,57	0
56	MG	1A	3379	1/1	0.94	0.09	32,32,32,32	0
56	MG	2A	3276	1/1	0.94	0.28	43,43,43,43	0
56	MG	2a	1821	1/1	0.94	0.13	54,54,54,54	0
56	MG	2A	3509	1/1	0.94	0.14	19,19,19,19	0
56	MG	2a	1766	1/1	0.94	0.16	53,53,53,53	0
56	MG	2A	3165	1/1	0.94	0.08	30,30,30,30	0
56	MG	2A	3433	1/1	0.94	0.15	20,20,20,20	0
56	MG	1A	3552	1/1	0.94	0.18	23,23,23,23	0
56	MG	2Q	204	1/1	0.94	0.11	38,38,38,38	0
56	MG	2A	3044	1/1	0.94	0.11	44,44,44,44	0
56	MG	2A	3030	1/1	0.94	0.29	41,41,41,41	0
57	ERY	1A	4074	51/51	0.94	0.27	15,23,34,44	0
56	MG	2A	3158	1/1	0.94	0.09	39,39,39,39	0
56	MG	2A	3271	1/1	0.94	0.10	36,36,36,36	0
56	MG	1A	4040	1/1	0.94	0.13	12,12,12,12	0
56	MG	1A	3583	1/1	0.94	0.18	23,23,23,23	0
56	MG	2A	3314	1/1	0.94	0.16	54,54,54,54	0
56	MG	1A	3644	1/1	0.94	0.13	46,46,46,46	0
56	MG	2A	3002	1/1	0.94	0.16	35,35,35,35	0
56	MG	1A	3716	1/1	0.94	0.14	26,26,26,26	0
56	MG	1x	109	1/1	0.94	0.21	47,47,47,47	0
56	MG	2A	3094	1/1	0.94	0.13	40,40,40,40	0
56	MG	2a	1644	1/1	0.94	0.16	47,47,47,47	0
56	MG	2A	3317	1/1	0.94	0.51	47,47,47,47	0
56	MG	2A	3706	1/1	0.94	0.16	34,34,34,34	0
56	MG	2A	3125	1/1	0.94	0.43	44,44,44,44	0
56	MG	1A	3050	1/1	0.94	0.10	22,22,22,22	0
56	MG	2A	3859	1/1	0.94	0.07	60,60,60,60	0
56	MG	1A	3855	1/1	0.94	0.13	10,10,10,10	0
56	MG	1a	3170	1/1	0.94	0.07	52,52,52,52	0
56	MG	1A	3195	1/1	0.94	0.13	41,41,41,41	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	1A	3519	1/1	0.94	0.28	20,20,20,20	0
56	MG	1A	3930	1/1	0.94	0.09	43,43,43,43	0
56	MG	1A	3921	1/1	0.94	0.14	14,14,14,14	0
56	MG	2A	3523	1/1	0.94	0.09	38,38,38,38	0
56	MG	1A	3831	1/1	0.94	0.11	22,22,22,22	0
56	MG	1a	3200	1/1	0.94	0.09	53,53,53,53	0
56	MG	1A	3092	1/1	0.94	0.22	26,26,26,26	0
56	MG	2A	3757	1/1	0.94	0.09	19,19,19,19	0
56	MG	2A	3710	1/1	0.94	0.16	51,51,51,51	0
56	MG	1A	3281	1/1	0.94	0.40	39,39,39,39	0
56	MG	1V	208	1/1	0.94	0.19	42,42,42,42	0
56	MG	1A	3622	1/1	0.94	0.10	22,22,22,22	0
56	MG	1A	3245	1/1	0.94	0.25	22,22,22,22	0
56	MG	2A	3272	1/1	0.94	0.14	35,35,35,35	0
56	MG	1A	3443	1/1	0.94	0.20	37,37,37,37	0
56	MG	1A	3570	1/1	0.94	0.18	30,30,30,30	0
56	MG	1A	3211	1/1	0.94	0.22	33,33,33,33	0
56	MG	2A	3297	1/1	0.94	0.12	27,27,27,27	0
56	MG	2A	3065	1/1	0.94	0.37	37,37,37,37	0
56	MG	2A	3653	1/1	0.94	0.20	57,57,57,57	0
56	MG	1A	3234	1/1	0.94	0.38	35,35,35,35	0
56	MG	2A	3522	1/1	0.94	0.10	51,51,51,51	0
56	MG	2A	3122	1/1	0.94	0.13	50,50,50,50	0
56	MG	1A	3663	1/1	0.94	0.20	46,46,46,46	0
56	MG	2A	3681	1/1	0.94	0.07	43,43,43,43	0
56	MG	2A	3048	1/1	0.94	0.10	48,48,48,48	0
56	MG	1A	3773	1/1	0.94	0.18	30,30,30,30	0
56	MG	1V	207	1/1	0.94	0.53	22,22,22,22	0
56	MG	2A	3529	1/1	0.94	0.10	35,35,35,35	0
56	MG	1A	3020	1/1	0.94	0.12	21,21,21,21	0
56	MG	2A	3196	1/1	0.94	0.17	33,33,33,33	0
56	MG	1A	3960	1/1	0.94	0.28	52,52,52,52	0
56	MG	2F	307	1/1	0.94	0.14	50,50,50,50	0
56	MG	1A	4048	1/1	0.94	0.11	27,27,27,27	0
56	MG	1A	3675	1/1	0.94	0.17	44,44,44,44	0
56	MG	2A	3535	1/1	0.94	0.10	55,55,55,55	0
56	MG	1A	3427	1/1	0.94	0.16	38,38,38,38	0
56	MG	1A	3483	1/1	0.94	0.28	33,33,33,33	0
56	MG	1A	3246	1/1	0.94	0.40	22,22,22,22	0
56	MG	1A	3057	1/1	0.94	0.12	29,29,29,29	0
56	MG	1A	3208	1/1	0.94	0.25	19,19,19,19	0
56	MG	1A	4009	1/1	0.94	0.11	25,25,25,25	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	1A	3459	1/1	0.94	0.13	30,30,30,30	0
56	MG	2a	1787	1/1	0.94	0.06	59,59,59,59	0
56	MG	1W	208	1/1	0.94	0.52	36,36,36,36	0
56	MG	1U	206	1/1	0.94	0.22	25,25,25,25	0
56	MG	1a	3057	1/1	0.94	0.16	38,38,38,38	0
56	MG	2A	3422	1/1	0.94	0.21	43,43,43,43	0
56	MG	1A	3359	1/1	0.94	0.38	30,30,30,30	0
56	MG	1P	202	1/1	0.94	0.40	21,21,21,21	0
56	MG	2A	3734	1/1	0.94	0.12	20,20,20,20	0
56	MG	1a	3146	1/1	0.94	0.17	38,38,38,38	0
56	MG	2A	3013	1/1	0.94	0.40	41,41,41,41	0
56	MG	1A	3302	1/1	0.94	0.08	21,21,21,21	0
56	MG	2A	3507	1/1	0.94	0.09	29,29,29,29	0
56	MG	14	101	1/1	0.94	0.12	30,30,30,30	0
56	MG	1a	3048	1/1	0.94	0.08	54,54,54,54	0
56	MG	1A	3404	1/1	0.94	0.14	18,18,18,18	0
56	MG	1A	3942	1/1	0.94	0.06	51,51,51,51	0
56	MG	1A	3138	1/1	0.94	0.09	31,31,31,31	0
56	MG	2a	1613	1/1	0.94	0.08	50,50,50,50	0
56	MG	2A	3465	1/1	0.94	0.09	31,31,31,31	0
56	MG	2A	3282	1/1	0.94	0.64	36,36,36,36	0
56	MG	2A	3142	1/1	0.94	0.07	55,55,55,55	0
56	MG	2A	3089	1/1	0.94	0.14	35,35,35,35	0
56	MG	1A	3329	1/1	0.94	0.16	39,39,39,39	0
56	MG	1A	3015	1/1	0.94	0.18	31,31,31,31	0
56	MG	2A	3077	1/1	0.94	0.20	32,32,32,32	0
56	MG	2A	3311	1/1	0.94	0.28	34,34,34,34	0
56	MG	2a	1801	1/1	0.94	0.09	40,40,40,40	0
56	MG	12	102	1/1	0.94	0.49	28,28,28,28	0
56	MG	13	101	1/1	0.94	0.32	36,36,36,36	0
56	MG	1A	3601	1/1	0.94	0.24	43,43,43,43	0
56	MG	1A	3036	1/1	0.94	0.20	14,14,14,14	0
56	MG	1a	3050	1/1	0.94	0.09	46,46,46,46	0
56	MG	2A	3798	1/1	0.94	0.09	55,55,55,55	0
56	MG	2A	3009	1/1	0.94	0.24	45,45,45,45	0
56	MG	1a	3067	1/1	0.94	0.17	43,43,43,43	0
56	MG	1A	3996	1/1	0.94	0.15	37,37,37,37	0
56	MG	2A	3135	1/1	0.94	0.08	47,47,47,47	0
56	MG	1A	3260	1/1	0.94	0.22	27,27,27,27	0
56	MG	1A	3324	1/1	0.94	0.28	23,23,23,23	0
56	MG	1A	3793	1/1	0.94	0.09	50,50,50,50	0
56	MG	2A	3362	1/1	0.94	0.12	39,39,39,39	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	1A	3814	1/1	0.94	0.57	26,26,26,26	0
56	MG	1A	3007	1/1	0.94	0.08	16,16,16,16	0
56	MG	1A	3418	1/1	0.94	0.25	25,25,25,25	0
56	MG	2A	3612	1/1	0.94	0.11	40,40,40,40	0
56	MG	2a	1823	1/1	0.94	0.11	51,51,51,51	0
56	MG	1S	201	1/1	0.94	0.13	34,34,34,34	0
56	MG	2a	1803	1/1	0.94	0.10	55,55,55,55	0
56	MG	2A	3382	1/1	0.94	0.19	44,44,44,44	0
56	MG	1A	3174	1/1	0.94	0.14	30,30,30,30	0
56	MG	1a	3212	1/1	0.94	0.10	34,34,34,34	0
56	MG	1A	3646	1/1	0.94	0.09	28,28,28,28	0
56	MG	1a	3083	1/1	0.94	0.12	42,42,42,42	0
56	MG	2A	3814	1/1	0.94	0.15	30,30,30,30	0
56	MG	2l	205	1/1	0.94	0.07	33,33,33,33	0
56	MG	1A	3840	1/1	0.94	0.10	28,28,28,28	0
56	MG	1A	3513	1/1	0.94	0.31	23,23,23,23	0
56	MG	1A	3944	1/1	0.94	0.12	55,55,55,55	0
56	MG	10	107	1/1	0.94	0.10	34,34,34,34	0
56	MG	2a	1628	1/1	0.94	0.23	35,35,35,35	0
56	MG	1A	3407	1/1	0.94	0.11	42,42,42,42	0
56	MG	1A	3866	1/1	0.94	0.13	31,31,31,31	0
56	MG	2B	205	1/1	0.94	0.07	40,40,40,40	0
56	MG	2A	3315	1/1	0.94	0.21	45,45,45,45	0
56	MG	2a	1791	1/1	0.94	0.08	53,53,53,53	0
56	MG	2A	3300	1/1	0.94	0.15	49,49,49,49	0
56	MG	1A	3582	1/1	0.94	0.11	29,29,29,29	0
56	MG	1A	3424	1/1	0.94	0.10	50,50,50,50	0
56	MG	2a	1714	1/1	0.94	0.18	51,51,51,51	0
56	MG	2A	3133	1/1	0.94	0.14	27,27,27,27	0
56	MG	2A	3855	1/1	0.94	0.11	30,30,30,30	0
56	MG	2Q	203	1/1	0.94	0.24	44,44,44,44	0
56	MG	1A	3396	1/1	0.94	0.10	21,21,21,21	0
56	MG	2A	3721	1/1	0.94	0.06	43,43,43,43	0
56	MG	1A	3169	1/1	0.94	0.15	13,13,13,13	0
56	MG	2A	3047	1/1	0.94	0.07	49,49,49,49	0
56	MG	2A	3157	1/1	0.94	0.12	57,57,57,57	0
56	MG	1A	3006	1/1	0.94	0.12	7,7,7,7	0
56	MG	1A	3120	1/1	0.94	0.14	39,39,39,39	0
56	MG	1a	3185	1/1	0.94	0.15	64,64,64,64	0
56	MG	1A	3686	1/1	0.94	0.12	6,6,6,6	0
56	MG	2A	3588	1/1	0.94	0.05	48,48,48,48	0
56	MG	1A	3209	1/1	0.94	0.28	15,15,15,15	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	2a	1670	1/1	0.94	0.09	40,40,40,40	0
56	MG	2A	3209	1/1	0.94	0.42	38,38,38,38	0
56	MG	1A	3305	1/1	0.94	0.16	19,19,19,19	0
56	MG	2A	3637	1/1	0.94	0.13	50,50,50,50	0
56	MG	1A	3005	1/1	0.94	0.20	30,30,30,30	0
56	MG	2A	3542	1/1	0.94	0.11	50,50,50,50	0
56	MG	1A	3876	1/1	0.94	0.17	56,56,56,56	0
56	MG	1A	3726	1/1	0.94	0.10	32,32,32,32	0
56	MG	2A	3536	1/1	0.94	0.07	42,42,42,42	0
56	MG	1A	3280	1/1	0.94	0.19	28,28,28,28	0
56	MG	1A	3043	1/1	0.94	0.17	13,13,13,13	0
56	MG	1N	201	1/1	0.94	0.43	32,32,32,32	0
56	MG	2A	3251	1/1	0.94	0.15	48,48,48,48	0
56	MG	2a	1654	1/1	0.94	0.23	50,50,50,50	0
56	MG	2a	1636	1/1	0.94	0.18	54,54,54,54	0
56	MG	2A	3392	1/1	0.94	0.24	47,47,47,47	0
56	MG	2A	3471	1/1	0.94	0.18	34,34,34,34	0
56	MG	2a	1740	1/1	0.94	0.07	60,60,60,60	0
56	MG	2A	3420	1/1	0.94	0.14	36,36,36,36	0
56	MG	1a	3061	1/1	0.94	0.51	38,38,38,38	0
56	MG	2A	3295	1/1	0.94	0.16	54,54,54,54	0
56	MG	1A	3937	1/1	0.94	0.09	58,58,58,58	0
56	MG	2A	3038	1/1	0.94	0.15	29,29,29,29	0
56	MG	1A	3681	1/1	0.94	0.15	37,37,37,37	0
56	MG	1P	201	1/1	0.94	0.35	20,20,20,20	0
56	MG	1A	3113	1/1	0.94	0.07	47,47,47,47	0
56	MG	1A	3839	1/1	0.94	0.17	29,29,29,29	0
56	MG	1A	3241	1/1	0.94	0.17	32,32,32,32	0
56	MG	1A	3231	1/1	0.94	0.16	22,22,22,22	0
56	MG	2A	3857	1/1	0.94	0.08	46,46,46,46	0
56	MG	1E	308	1/1	0.94	0.10	26,26,26,26	0
56	MG	1a	3208	1/1	0.94	0.08	34,34,34,34	0
56	MG	2A	3824	1/1	0.94	0.10	37,37,37,37	0
56	MG	1A	3815	1/1	0.94	0.13	26,26,26,26	0
56	MG	2A	3457	1/1	0.94	0.20	24,24,24,24	0
56	MG	2A	3494	1/1	0.94	0.12	42,42,42,42	0
56	MG	1A	3066	1/1	0.94	0.18	26,26,26,26	0
56	MG	1p	101	1/1	0.94	0.24	51,51,51,51	0
56	MG	1a	3114	1/1	0.94	0.16	34,34,34,34	0
56	MG	2a	1694	1/1	0.94	0.09	44,44,44,44	0
56	MG	2a	1667	1/1	0.94	0.17	27,27,27,27	0
56	MG	2A	3815	1/1	0.94	0.15	36,36,36,36	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	16	102	1/1	0.94	0.14	23,23,23,23	0
56	MG	1A	3204	1/1	0.94	0.26	16,16,16,16	0
56	MG	1A	4039	1/1	0.94	0.11	28,28,28,28	0
56	MG	1A	3873	1/1	0.94	0.27	17,17,17,17	0
56	MG	1A	3989	1/1	0.94	0.06	29,29,29,29	0
56	MG	1A	3114	1/1	0.94	0.14	19,19,19,19	0
56	MG	2A	3602	1/1	0.94	0.26	45,45,45,45	0
56	MG	2A	3544	1/1	0.94	0.09	44,44,44,44	0
56	MG	2a	1764	1/1	0.94	0.13	46,46,46,46	0
56	MG	2a	1704	1/1	0.94	0.16	52,52,52,52	0
56	MG	1A	3655	1/1	0.94	0.16	33,33,33,33	0
56	MG	1A	3065	1/1	0.94	0.22	26,26,26,26	0
56	MG	2A	3244	1/1	0.94	0.13	39,39,39,39	0
56	MG	2A	3263	1/1	0.94	0.11	30,30,30,30	0
56	MG	2A	3041	1/1	0.94	0.61	34,34,34,34	0
56	MG	1A	3820	1/1	0.94	0.22	31,31,31,31	0
56	MG	2t	201	1/1	0.94	0.15	29,29,29,29	0
56	MG	2A	3118	1/1	0.94	0.53	67,67,67,67	0
56	MG	1A	3183	1/1	0.94	0.08	26,26,26,26	0
56	MG	2A	3033	1/1	0.94	0.24	39,39,39,39	0
56	MG	1A	3408	1/1	0.94	0.17	36,36,36,36	0
56	MG	1a	3052	1/1	0.94	0.11	40,40,40,40	0
56	MG	1S	202	1/1	0.94	0.14	51,51,51,51	0
56	MG	1A	3268	1/1	0.94	0.11	30,30,30,30	0
56	MG	2A	3703	1/1	0.94	0.08	34,34,34,34	0
56	MG	2a	1625	1/1	0.94	0.12	25,25,25,25	0
56	MG	1A	3599	1/1	0.95	0.12	25,25,25,25	0
56	MG	2A	3084	1/1	0.95	0.11	45,45,45,45	0
56	MG	1A	3451	1/1	0.95	0.17	16,16,16,16	0
56	MG	2A	3237	1/1	0.95	0.13	32,32,32,32	0
56	MG	2A	3747	1/1	0.95	0.10	45,45,45,45	0
56	MG	2A	3103	1/1	0.95	0.11	38,38,38,38	0
56	MG	1A	3602	1/1	0.95	0.29	20,20,20,20	0
56	MG	2A	3682	1/1	0.95	0.07	39,39,39,39	0
56	MG	1A	3391	1/1	0.95	0.12	32,32,32,32	0
56	MG	1W	202	1/1	0.95	0.13	18,18,18,18	0
56	MG	1a	3172	1/1	0.95	0.06	57,57,57,57	0
56	MG	1A	3226	1/1	0.95	0.28	37,37,37,37	0
56	MG	1a	3102	1/1	0.95	0.15	53,53,53,53	0
56	MG	1a	3198	1/1	0.95	0.11	44,44,44,44	0
56	MG	1A	3737	1/1	0.95	0.11	14,14,14,14	0
56	MG	1A	3320	1/1	0.95	0.08	23,23,23,23	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	2A	3018	1/1	0.95	0.24	54,54,54,54	0
56	MG	1B	225	1/1	0.95	0.11	33,33,33,33	0
56	MG	2a	1718	1/1	0.95	0.13	39,39,39,39	0
56	MG	2A	3548	1/1	0.95	0.07	32,32,32,32	0
56	MG	2A	3161	1/1	0.95	0.12	47,47,47,47	0
56	MG	2A	3178	1/1	0.95	0.09	45,45,45,45	0
56	MG	1E	310	1/1	0.95	0.14	41,41,41,41	0
56	MG	1a	3180	1/1	0.95	0.08	52,52,52,52	0
56	MG	1A	4049	1/1	0.95	0.21	35,35,35,35	0
56	MG	2U	201	1/1	0.95	0.48	38,38,38,38	0
56	MG	1A	3720	1/1	0.95	0.11	19,19,19,19	0
56	MG	1a	3035	1/1	0.95	0.09	32,32,32,32	0
56	MG	1A	3062	1/1	0.95	0.14	38,38,38,38	0
56	MG	1A	3083	1/1	0.95	0.15	42,42,42,42	0
56	MG	1A	3865	1/1	0.95	0.30	29,29,29,29	0
56	MG	1A	3143	1/1	0.95	0.12	30,30,30,30	0
56	MG	1A	3304	1/1	0.95	0.13	25,25,25,25	0
56	MG	1A	3577	1/1	0.95	0.10	16,16,16,16	0
56	MG	1A	3012	1/1	0.95	0.12	26,26,26,26	0
56	MG	1B	234	1/1	0.95	0.13	30,30,30,30	0
56	MG	2A	3331	1/1	0.95	0.12	28,28,28,28	0
56	MG	2A	3592	1/1	0.95	0.09	35,35,35,35	0
56	MG	1A	3707	1/1	0.95	0.12	4,4,4,4	0
56	MG	1A	3098	1/1	0.95	0.19	16,16,16,16	0
56	MG	1A	3233	1/1	0.95	0.18	27,27,27,27	0
56	MG	2a	1767	1/1	0.95	0.07	47,47,47,47	0
56	MG	1A	3484	1/1	0.95	0.28	34,34,34,34	0
56	MG	2A	3449	1/1	0.95	0.07	35,35,35,35	0
56	MG	1A	4054	1/1	0.95	0.16	24,24,24,24	0
56	MG	1A	3802	1/1	0.95	0.12	28,28,28,28	0
56	MG	2A	3514	1/1	0.95	0.24	48,48,48,48	0
56	MG	1A	3805	1/1	0.95	0.17	10,10,10,10	0
56	MG	1A	3219	1/1	0.95	0.34	28,28,28,28	0
56	MG	1A	3753	1/1	0.95	0.17	23,23,23,23	0
56	MG	2B	215	1/1	0.95	0.17	40,40,40,40	0
56	MG	1A	4020	1/1	0.95	0.12	36,36,36,36	0
56	MG	1a	3064	1/1	0.95	0.09	33,33,33,33	0
56	MG	1A	3874	1/1	0.95	0.11	47,47,47,47	0
56	MG	1A	3557	1/1	0.95	0.14	28,28,28,28	0
56	MG	1A	3504	1/1	0.95	0.18	24,24,24,24	0
56	MG	2A	3662	1/1	0.95	0.14	55,55,55,55	0
56	MG	1A	3086	1/1	0.95	0.30	25,25,25,25	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	1A	3678	1/1	0.95	0.09	18,18,18,18	0
56	MG	1A	3422	1/1	0.95	0.26	36,36,36,36	0
56	MG	2A	3141	1/1	0.95	0.38	47,47,47,47	0
56	MG	2A	3811	1/1	0.95	0.10	33,33,33,33	0
56	MG	2a	1624	1/1	0.95	0.24	31,31,31,31	0
56	MG	1A	3578	1/1	0.95	0.13	12,12,12,12	0
56	MG	1s	101	1/1	0.95	0.16	46,46,46,46	0
56	MG	1a	3115	1/1	0.95	0.19	19,19,19,19	0
56	MG	1A	3071	1/1	0.95	0.11	17,17,17,17	0
56	MG	1A	3252	1/1	0.95	0.15	32,32,32,32	0
56	MG	2B	203	1/1	0.95	0.06	50,50,50,50	0
56	MG	2A	3636	1/1	0.95	0.21	49,49,49,49	0
56	MG	1A	4036	1/1	0.95	0.17	10,10,10,10	0
56	MG	1A	3896	1/1	0.95	0.17	23,23,23,23	0
56	MG	1a	3132	1/1	0.95	0.08	27,27,27,27	0
56	MG	1A	3465	1/1	0.95	0.50	34,34,34,34	0
56	MG	1A	3004	1/1	0.95	0.09	39,39,39,39	0
56	MG	2a	1635	1/1	0.95	0.10	44,44,44,44	0
56	MG	1A	3816	1/1	0.95	0.10	31,31,31,31	0
56	MG	2A	3452	1/1	0.95	0.23	43,43,43,43	0
56	MG	1A	3878	1/1	0.95	0.15	12,12,12,12	0
56	MG	2E	308	1/1	0.95	0.11	38,38,38,38	0
56	MG	1A	3979	1/1	0.95	0.20	22,22,22,22	0
56	MG	1A	3674	1/1	0.95	0.10	24,24,24,24	0
56	MG	23	102	1/1	0.95	0.17	31,31,31,31	0
56	MG	2X	101	1/1	0.95	0.90	57,57,57,57	0
56	MG	1A	3079	1/1	0.95	0.15	58,58,58,58	0
56	MG	2A	3191	1/1	0.95	0.13	31,31,31,31	0
56	MG	2A	3398	1/1	0.95	0.13	40,40,40,40	0
56	MG	1A	3068	1/1	0.95	0.25	22,22,22,22	0
56	MG	1A	3479	1/1	0.95	0.18	25,25,25,25	0
56	MG	1a	3117	1/1	0.95	0.19	30,30,30,30	0
56	MG	1A	4061	1/1	0.95	0.10	58,58,58,58	0
56	MG	1A	3755	1/1	0.95	0.09	30,30,30,30	0
56	MG	2A	3587	1/1	0.95	0.07	47,47,47,47	0
56	MG	2A	3429	1/1	0.95	0.18	43,43,43,43	0
56	MG	17	104	1/1	0.95	0.14	26,26,26,26	0
56	MG	1A	3594	1/1	0.95	0.19	24,24,24,24	0
56	MG	1A	3667	1/1	0.95	0.20	44,44,44,44	0
56	MG	1a	3160	1/1	0.95	0.15	51,51,51,51	0
56	MG	2A	3732	1/1	0.95	0.06	31,31,31,31	0
56	MG	2y	101	1/1	0.95	0.07	46,46,46,46	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	1f	201	1/1	0.95	0.16	36,36,36,36	0
56	MG	2A	3754	1/1	0.95	0.11	48,48,48,48	0
56	MG	1A	4015	1/1	0.95	0.23	41,41,41,41	0
56	MG	1N	202	1/1	0.95	0.10	27,27,27,27	0
56	MG	1A	3215	1/1	0.95	0.19	16,16,16,16	0
56	MG	1A	3905	1/1	0.95	0.12	9,9,9,9	0
56	MG	2A	3672	1/1	0.95	0.08	42,42,42,42	0
56	MG	1A	3341	1/1	0.95	0.16	16,16,16,16	0
56	MG	1x	101	1/1	0.95	0.16	22,22,22,22	0
56	MG	1A	3606	1/1	0.95	0.29	32,32,32,32	0
56	MG	1A	3700	1/1	0.95	0.16	14,14,14,14	0
56	MG	2a	1798	1/1	0.95	0.12	44,44,44,44	0
56	MG	1A	3950	1/1	0.95	0.07	42,42,42,42	0
56	MG	2A	3620	1/1	0.95	0.17	48,48,48,48	0
56	MG	2A	3117	1/1	0.95	0.07	38,38,38,38	0
56	MG	2A	3060	1/1	0.95	0.09	24,24,24,24	0
56	MG	1A	3955	1/1	0.95	0.06	23,23,23,23	0
56	MG	1A	3322	1/1	0.95	0.22	23,23,23,23	0
56	MG	2A	3078	1/1	0.95	0.07	39,39,39,39	0
56	MG	1B	229	1/1	0.95	0.08	28,28,28,28	0
56	MG	2A	3064	1/1	0.95	0.08	30,30,30,30	0
56	MG	1A	3047	1/1	0.95	0.16	6,6,6,6	0
56	MG	1x	113	1/1	0.95	0.10	42,42,42,42	0
56	MG	1A	3512	1/1	0.95	0.11	13,13,13,13	0
56	MG	2A	3299	1/1	0.95	0.07	11,11,11,11	0
56	MG	2A	3850	1/1	0.95	0.29	44,44,44,44	0
56	MG	2D	302	1/1	0.95	0.22	39,39,39,39	0
56	MG	1B	210	1/1	0.95	0.13	39,39,39,39	0
56	MG	2F	306	1/1	0.95	0.41	40,40,40,40	0
56	MG	1a	3088	1/1	0.95	0.19	46,46,46,46	0
57	ERY	2A	3875	51/51	0.95	0.37	29,41,51,56	0
56	MG	2A	3527	1/1	0.95	0.10	44,44,44,44	0
56	MG	2A	3045	1/1	0.95	0.09	52,52,52,52	0
56	MG	2B	204	1/1	0.95	0.09	52,52,52,52	0
56	MG	1a	3103	1/1	0.95	0.13	37,37,37,37	0
56	MG	2a	1700	1/1	0.95	0.15	56,56,56,56	0
56	MG	1B	212	1/1	0.95	0.18	26,26,26,26	0
56	MG	1A	3934	1/1	0.95	0.11	29,29,29,29	0
56	MG	1B	235	1/1	0.95	0.15	40,40,40,40	0
56	MG	1A	3061	1/1	0.95	0.09	5,5,5,5	0
56	MG	1A	3299	1/1	0.95	0.12	6,6,6,6	0
56	MG	1A	3191	1/1	0.95	0.24	30,30,30,30	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	2a	1725	1/1	0.95	0.08	43,43,43,43	0
56	MG	1A	3394	1/1	0.95	0.10	31,31,31,31	0
56	MG	1A	3925	1/1	0.95	0.08	21,21,21,21	0
56	MG	1a	3129	1/1	0.95	0.21	51,51,51,51	0
56	MG	1A	3387	1/1	0.95	0.28	40,40,40,40	0
56	MG	1W	205	1/1	0.95	0.10	15,15,15,15	0
56	MG	2A	3054	1/1	0.95	0.17	35,35,35,35	0
56	MG	1A	4058	1/1	0.95	0.11	42,42,42,42	0
56	MG	2A	3301	1/1	0.95	0.08	28,28,28,28	0
56	MG	1B	206	1/1	0.95	0.12	26,26,26,26	0
56	MG	1A	4067	1/1	0.95	0.17	31,31,31,31	0
56	MG	2A	3012	1/1	0.95	0.20	44,44,44,44	0
56	MG	1A	3358	1/1	0.95	0.46	23,23,23,23	0
56	MG	1A	3286	1/1	0.95	0.18	27,27,27,27	0
56	MG	1A	3974	1/1	0.95	0.07	41,41,41,41	0
56	MG	1A	3857	1/1	0.95	0.13	45,45,45,45	0
56	MG	1A	3540	1/1	0.95	0.11	20,20,20,20	0
56	MG	1a	3005	1/1	0.95	0.14	54,54,54,54	0
56	MG	2A	3042	1/1	0.95	0.14	40,40,40,40	0
56	MG	2F	301	1/1	0.95	0.14	34,34,34,34	0
56	MG	2a	1729	1/1	0.95	0.13	46,46,46,46	0
56	MG	1A	3311	1/1	0.95	0.38	28,28,28,28	0
56	MG	2a	1790	1/1	0.95	0.08	41,41,41,41	0
56	MG	1A	3767	1/1	0.95	0.12	19,19,19,19	0
56	MG	2A	3259	1/1	0.95	0.06	44,44,44,44	0
56	MG	1A	3524	1/1	0.95	0.08	40,40,40,40	0
56	MG	1A	3144	1/1	0.95	0.21	23,23,23,23	0
56	MG	1A	3739	1/1	0.95	0.11	21,21,21,21	0
56	MG	2A	3337	1/1	0.95	0.13	48,48,48,48	0
56	MG	1D	313	1/1	0.95	0.20	17,17,17,17	0
56	MG	2A	3110	1/1	0.95	0.35	33,33,33,33	0
56	MG	2x	105	1/1	0.95	0.06	33,33,33,33	0
56	MG	2A	3793	1/1	0.95	0.09	46,46,46,46	0
56	MG	2a	1820	1/1	0.95	0.13	52,52,52,52	0
56	MG	1a	3001	1/1	0.95	0.09	49,49,49,49	0
56	MG	2A	3252	1/1	0.95	0.07	41,41,41,41	0
56	MG	2A	3651	1/1	0.95	0.21	59,59,59,59	0
56	MG	1F	308	1/1	0.95	0.08	27,27,27,27	0
56	MG	2A	3719	1/1	0.95	0.18	29,29,29,29	0
56	MG	1A	3259	1/1	0.95	0.16	20,20,20,20	0
56	MG	2A	3582	1/1	0.95	0.17	59,59,59,59	0
56	MG	1A	3658	1/1	0.95	0.11	28,28,28,28	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	2A	3155	1/1	0.95	0.17	41,41,41,41	0
56	MG	2A	3395	1/1	0.95	0.46	43,43,43,43	0
56	MG	1A	4028	1/1	0.95	0.13	35,35,35,35	0
56	MG	1A	3611	1/1	0.95	0.19	36,36,36,36	0
58	ZN	1n	102	1/1	0.95	0.13	59,59,59,59	0
56	MG	1A	3135	1/1	0.95	0.16	27,27,27,27	0
56	MG	2A	3198	1/1	0.95	0.13	48,48,48,48	0
56	MG	1l	202	1/1	0.95	0.12	25,25,25,25	0
56	MG	2B	202	1/1	0.95	0.11	50,50,50,50	0
56	MG	1A	3166	1/1	0.95	0.33	18,18,18,18	0
56	MG	2A	3695	1/1	0.95	0.25	39,39,39,39	0
56	MG	1A	3682	1/1	0.95	0.12	37,37,37,37	0
56	MG	1A	3346	1/1	0.95	0.18	24,24,24,24	0
56	MG	2A	3214	1/1	0.95	0.16	34,34,34,34	0
56	MG	2A	3557	1/1	0.95	0.14	41,41,41,41	0
56	MG	1A	3701	1/1	0.95	0.13	38,38,38,38	0
56	MG	2a	1771	1/1	0.95	0.07	44,44,44,44	0
56	MG	2A	3735	1/1	0.95	0.15	28,28,28,28	0
56	MG	1A	3393	1/1	0.95	0.18	17,17,17,17	0
56	MG	1a	3111	1/1	0.95	0.10	37,37,37,37	0
56	MG	1A	3804	1/1	0.95	0.10	14,14,14,14	0
56	MG	2A	3565	1/1	0.95	0.09	25,25,25,25	0
56	MG	1A	3702	1/1	0.95	0.14	14,14,14,14	0
56	MG	2A	3087	1/1	0.95	0.08	60,60,60,60	0
56	MG	1A	3321	1/1	0.95	0.13	34,34,34,34	0
56	MG	1A	4042	1/1	0.95	0.10	31,31,31,31	0
56	MG	1A	3776	1/1	0.95	0.14	13,13,13,13	0
56	MG	1D	307	1/1	0.95	0.40	24,24,24,24	0
56	MG	2T	201	1/1	0.95	0.22	47,47,47,47	0
56	MG	1A	3108	1/1	0.95	0.19	24,24,24,24	0
56	MG	2A	3530	1/1	0.95	0.11	19,19,19,19	0
56	MG	2A	3027	1/1	0.95	0.12	32,32,32,32	0
56	MG	1A	3962	1/1	0.95	0.20	38,38,38,38	0
56	MG	1A	3607	1/1	0.95	0.25	31,31,31,31	0
56	MG	1A	3400	1/1	0.95	0.17	21,21,21,21	0
56	MG	1A	3118	1/1	0.95	0.14	16,16,16,16	0
56	MG	1A	3274	1/1	0.95	0.12	24,24,24,24	0
56	MG	2A	3320	1/1	0.95	0.30	47,47,47,47	0
56	MG	2A	3827	1/1	0.95	0.09	36,36,36,36	0
56	MG	1A	3308	1/1	0.95	0.26	24,24,24,24	0
56	MG	2a	1819	1/1	0.95	0.16	67,67,67,67	0
56	MG	2A	3419	1/1	0.95	0.17	38,38,38,38	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	1A	3589	1/1	0.95	0.09	36,36,36,36	0
56	MG	1A	3141	1/1	0.95	0.09	15,15,15,15	0
56	MG	2A	3159	1/1	0.95	0.05	42,42,42,42	0
56	MG	2A	3274	1/1	0.95	0.14	25,25,25,25	0
56	MG	2a	1690	1/1	0.95	0.14	53,53,53,53	0
56	MG	1a	3210	1/1	0.95	0.05	61,61,61,61	0
56	MG	2A	3242	1/1	0.95	0.10	55,55,55,55	0
56	MG	1F	310	1/1	0.95	0.31	15,15,15,15	0
56	MG	1A	4063	1/1	0.95	0.15	52,52,52,52	0
56	MG	2A	3140	1/1	0.95	0.08	45,45,45,45	0
56	MG	1A	3853	1/1	0.95	0.14	28,28,28,28	0
56	MG	1A	3521	1/1	0.95	0.35	24,24,24,24	0
56	MG	1A	3253	1/1	0.95	0.09	30,30,30,30	0
56	MG	2A	3070	1/1	0.95	0.23	27,27,27,27	0
56	MG	2a	1746	1/1	0.95	0.11	57,57,57,57	0
56	MG	1A	3291	1/1	0.95	0.10	23,23,23,23	0
56	MG	2a	1728	1/1	0.95	0.10	46,46,46,46	0
56	MG	1A	3125	1/1	0.95	0.68	25,25,25,25	0
56	MG	1A	3576	1/1	0.95	0.15	28,28,28,28	0
56	MG	10	106	1/1	0.95	0.17	37,37,37,37	0
56	MG	1A	3758	1/1	0.95	0.14	12,12,12,12	0
56	MG	2a	1780	1/1	0.95	0.09	47,47,47,47	0
56	MG	1A	3059	1/1	0.95	0.09	10,10,10,10	0
56	MG	1E	309	1/1	0.95	0.19	26,26,26,26	0
56	MG	2A	3149	1/1	0.95	0.55	50,50,50,50	0
56	MG	18	102	1/1	0.95	0.09	20,20,20,20	0
56	MG	2A	3229	1/1	0.95	0.36	31,31,31,31	0
56	MG	1a	3171	1/1	0.95	0.14	39,39,39,39	0
56	MG	2a	1622	1/1	0.95	0.06	47,47,47,47	0
56	MG	2a	1760	1/1	0.95	0.20	60,60,60,60	0
56	MG	1A	3010	1/1	0.95	0.23	21,21,21,21	0
56	MG	2A	3112	1/1	0.95	0.10	26,26,26,26	0
56	MG	1a	3073	1/1	0.95	0.10	65,65,65,65	0
56	MG	1a	3030	1/1	0.95	0.13	52,52,52,52	0
56	MG	1A	3285	1/1	0.95	0.14	24,24,24,24	0
56	MG	2a	1605	1/1	0.95	0.21	36,36,36,36	0
56	MG	1A	3336	1/1	0.95	0.31	27,27,27,27	0
56	MG	1A	3881	1/1	0.95	0.13	17,17,17,17	0
56	MG	1A	3604	1/1	0.95	0.30	18,18,18,18	0
56	MG	2A	3281	1/1	0.95	0.29	33,33,33,33	0
56	MG	2A	3177	1/1	0.95	0.09	37,37,37,37	0
56	MG	1A	3986	1/1	0.95	0.09	35,35,35,35	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	1A	4041	1/1	0.95	0.15	43,43,43,43	0
56	MG	1A	3445	1/1	0.96	0.12	32,32,32,32	0
56	MG	1l	203	1/1	0.96	0.09	48,48,48,48	0
56	MG	2A	3025	1/1	0.96	0.14	38,38,38,38	0
56	MG	1E	303	1/1	0.96	0.24	25,25,25,25	0
56	MG	13	104	1/1	0.96	0.10	26,26,26,26	0
56	MG	2A	3609	1/1	0.96	0.20	33,33,33,33	0
56	MG	1a	3122	1/1	0.96	0.10	36,36,36,36	0
56	MG	1a	3219	1/1	0.96	0.08	61,61,61,61	0
56	MG	2A	3138	1/1	0.96	0.13	30,30,30,30	0
56	MG	1A	3417	1/1	0.96	0.10	18,18,18,18	0
56	MG	1A	3590	1/1	0.96	0.14	39,39,39,39	0
56	MG	2A	3453	1/1	0.96	0.11	33,33,33,33	0
56	MG	2A	3200	1/1	0.96	0.09	33,33,33,33	0
56	MG	1A	3261	1/1	0.96	0.27	31,31,31,31	0
56	MG	1A	3520	1/1	0.96	0.39	22,22,22,22	0
56	MG	1A	3228	1/1	0.96	0.08	50,50,50,50	0
56	MG	1A	3892	1/1	0.96	0.11	15,15,15,15	0
56	MG	1A	3197	1/1	0.96	0.12	17,17,17,17	0
56	MG	2a	1723	1/1	0.96	0.28	38,38,38,38	0
56	MG	1A	3240	1/1	0.96	0.40	29,29,29,29	0
56	MG	1A	3415	1/1	0.96	0.12	31,31,31,31	0
56	MG	2A	3031	1/1	0.96	0.08	26,26,26,26	0
56	MG	2A	3561	1/1	0.96	0.17	27,27,27,27	0
56	MG	2A	3321	1/1	0.96	0.14	20,20,20,20	0
56	MG	2A	3437	1/1	0.96	0.15	42,42,42,42	0
56	MG	1a	3229	1/1	0.96	0.17	41,41,41,41	0
56	MG	1A	3858	1/1	0.96	0.15	10,10,10,10	0
56	MG	1A	3669	1/1	0.96	0.10	19,19,19,19	0
56	MG	1A	3501	1/1	0.96	0.17	29,29,29,29	0
56	MG	1A	3128	1/1	0.96	0.26	17,17,17,17	0
56	MG	1A	3745	1/1	0.96	0.14	13,13,13,13	0
56	MG	1a	3157	1/1	0.96	0.38	49,49,49,49	0
56	MG	2A	3388	1/1	0.96	0.09	41,41,41,41	0
56	MG	2A	3443	1/1	0.96	0.12	34,34,34,34	0
56	MG	1A	3749	1/1	0.96	0.23	47,47,47,47	0
56	MG	1A	3608	1/1	0.96	0.15	36,36,36,36	0
56	MG	2A	3694	1/1	0.96	0.17	47,47,47,47	0
56	MG	1A	3205	1/1	0.96	0.11	20,20,20,20	0
56	MG	1R	201	1/1	0.96	0.08	26,26,26,26	0
56	MG	2A	3124	1/1	0.96	0.25	41,41,41,41	0
56	MG	1A	4000	1/1	0.96	0.08	43,43,43,43	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	1A	3350	1/1	0.96	0.80	33,33,33,33	0
56	MG	1A	3846	1/1	0.96	0.11	29,29,29,29	0
56	MG	1A	3786	1/1	0.96	0.13	16,16,16,16	0
56	MG	2A	3648	1/1	0.96	0.09	44,44,44,44	0
56	MG	2A	3116	1/1	0.96	0.10	61,61,61,61	0
56	MG	2A	3073	1/1	0.96	0.57	47,47,47,47	0
56	MG	2A	3162	1/1	0.96	0.14	43,43,43,43	0
56	MG	2f	202	1/1	0.96	0.13	47,47,47,47	0
56	MG	2a	1660	1/1	0.96	0.09	37,37,37,37	0
56	MG	1A	3854	1/1	0.96	0.13	42,42,42,42	0
56	MG	1a	3072	1/1	0.96	0.10	41,41,41,41	0
56	MG	2a	1629	1/1	0.96	0.17	37,37,37,37	0
56	MG	1A	3833	1/1	0.96	0.19	42,42,42,42	0
56	MG	1A	3489	1/1	0.96	0.22	17,17,17,17	0
56	MG	1a	3065	1/1	0.96	0.07	34,34,34,34	0
56	MG	2a	1815	1/1	0.96	0.12	56,56,56,56	0
56	MG	1A	3160	1/1	0.96	0.14	13,13,13,13	0
56	MG	1A	3789	1/1	0.96	0.12	21,21,21,21	0
56	MG	2A	3181	1/1	0.96	0.13	21,21,21,21	0
56	MG	1A	3517	1/1	0.96	0.53	33,33,33,33	0
56	MG	1A	4016	1/1	0.96	0.15	24,24,24,24	0
56	MG	1A	3565	1/1	0.96	0.12	11,11,11,11	0
56	MG	2A	3638	1/1	0.96	0.08	36,36,36,36	0
56	MG	2A	3712	1/1	0.96	0.12	34,34,34,34	0
56	MG	23	103	1/1	0.96	0.21	44,44,44,44	0
56	MG	1a	3037	1/1	0.96	0.14	41,41,41,41	0
56	MG	27	101	1/1	0.96	0.33	32,32,32,32	0
56	MG	1A	3722	1/1	0.96	0.10	16,16,16,16	0
56	MG	1a	3118	1/1	0.96	0.09	43,43,43,43	0
56	MG	2e	201	1/1	0.96	0.08	52,52,52,52	0
56	MG	1A	3256	1/1	0.96	0.12	26,26,26,26	0
58	ZN	29	501	1/1	0.96	0.08	66,66,66,66	0
56	MG	2P	201	1/1	0.96	0.31	40,40,40,40	0
56	MG	2a	1630	1/1	0.96	0.09	51,51,51,51	0
56	MG	2A	3515	1/1	0.96	0.09	48,48,48,48	0
56	MG	2A	3590	1/1	0.96	0.07	36,36,36,36	0
56	MG	2A	3470	1/1	0.96	0.10	33,33,33,33	0
56	MG	1A	3723	1/1	0.96	0.14	26,26,26,26	0
56	MG	1A	3467	1/1	0.96	0.13	14,14,14,14	0
56	MG	2A	3518	1/1	0.96	0.10	63,63,63,63	0
56	MG	1A	3151	1/1	0.96	0.18	23,23,23,23	0
56	MG	1U	205	1/1	0.96	0.09	28,28,28,28	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	1a	3096	1/1	0.96	0.12	38,38,38,38	0
56	MG	2A	3334	1/1	0.96	0.13	32,32,32,32	0
56	MG	1A	4001	1/1	0.96	0.17	29,29,29,29	0
56	MG	2A	3029	1/1	0.96	0.08	32,32,32,32	0
56	MG	1A	3838	1/1	0.96	0.09	27,27,27,27	0
56	MG	1A	3533	1/1	0.96	0.17	36,36,36,36	0
56	MG	2A	3564	1/1	0.96	0.19	36,36,36,36	0
56	MG	1A	4033	1/1	0.96	0.08	34,34,34,34	0
56	MG	2A	3863	1/1	0.96	0.13	27,27,27,27	0
56	MG	1A	3593	1/1	0.96	0.14	30,30,30,30	0
56	MG	2D	304	1/1	0.96	0.09	25,25,25,25	0
56	MG	2A	3350	1/1	0.96	0.47	34,34,34,34	0
56	MG	1Q	203	1/1	0.96	0.24	20,20,20,20	0
56	MG	2A	3738	1/1	0.96	0.22	54,54,54,54	0
56	MG	2A	3307	1/1	0.96	0.05	52,52,52,52	0
56	MG	2A	3024	1/1	0.96	0.08	33,33,33,33	0
56	MG	1U	207	1/1	0.96	0.42	24,24,24,24	0
56	MG	1A	3469	1/1	0.96	0.12	27,27,27,27	0
56	MG	2A	3493	1/1	0.96	0.10	20,20,20,20	0
56	MG	1A	3629	1/1	0.96	0.10	18,18,18,18	0
56	MG	1A	3812	1/1	0.96	0.15	25,25,25,25	0
56	MG	1A	3785	1/1	0.96	0.10	14,14,14,14	0
56	MG	2A	3560	1/1	0.96	0.09	61,61,61,61	0
56	MG	1A	4050	1/1	0.96	0.15	38,38,38,38	0
56	MG	1A	3571	1/1	0.96	0.23	23,23,23,23	0
56	MG	2A	3210	1/1	0.96	0.16	23,23,23,23	0
56	MG	2a	1833	1/1	0.96	0.12	58,58,58,58	0
56	MG	1B	202	1/1	0.96	0.24	48,48,48,48	0
56	MG	1a	3040	1/1	0.96	0.10	51,51,51,51	0
56	MG	1A	4069	1/1	0.96	0.07	37,37,37,37	0
56	MG	2A	3805	1/1	0.96	0.07	41,41,41,41	0
56	MG	2a	1692	1/1	0.96	0.19	52,52,52,52	0
56	MG	1A	3025	1/1	0.96	0.31	13,13,13,13	0
56	MG	1A	3977	1/1	0.96	0.14	27,27,27,27	0
56	MG	2A	3184	1/1	0.96	0.14	32,32,32,32	0
56	MG	1A	3124	1/1	0.96	0.25	35,35,35,35	0
56	MG	1A	3099	1/1	0.96	0.11	22,22,22,22	0
56	MG	2A	3466	1/1	0.96	0.15	19,19,19,19	0
56	MG	2D	305	1/1	0.96	0.47	39,39,39,39	0
56	MG	1A	3176	1/1	0.96	0.13	22,22,22,22	0
56	MG	1a	3124	1/1	0.96	0.07	33,33,33,33	0
56	MG	2A	3870	1/1	0.96	0.22	48,48,48,48	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	1a	3004	1/1	0.96	0.44	47,47,47,47	0
56	MG	2a	1772	1/1	0.96	0.14	50,50,50,50	0
56	MG	2a	1756	1/1	0.96	0.11	74,74,74,74	0
56	MG	1N	204	1/1	0.96	0.68	31,31,31,31	0
56	MG	15	107	1/1	0.96	0.28	33,33,33,33	0
56	MG	2a	1786	1/1	0.96	0.08	50,50,50,50	0
56	MG	2a	1743	1/1	0.96	0.14	56,56,56,56	0
56	MG	1A	3822	1/1	0.96	0.13	35,35,35,35	0
56	MG	2A	3063	1/1	0.96	0.13	35,35,35,35	0
56	MG	2A	3707	1/1	0.96	0.08	20,20,20,20	0
56	MG	1a	3216	1/1	0.96	0.07	33,33,33,33	0
56	MG	1A	3087	1/1	0.96	0.13	16,16,16,16	0
56	MG	1A	3900	1/1	0.96	0.16	34,34,34,34	0
56	MG	1T	201	1/1	0.96	0.17	35,35,35,35	0
56	MG	2A	3351	1/1	0.96	0.14	30,30,30,30	0
56	MG	1A	3366	1/1	0.96	0.22	29,29,29,29	0
56	MG	1A	3751	1/1	0.96	0.07	25,25,25,25	0
56	MG	1A	3112	1/1	0.96	0.23	22,22,22,22	0
56	MG	2A	3061	1/1	0.96	0.43	66,66,66,66	0
56	MG	1A	3642	1/1	0.96	0.15	17,17,17,17	0
56	MG	1A	3972	1/1	0.96	0.07	39,39,39,39	0
56	MG	2A	3075	1/1	0.96	0.12	38,38,38,38	0
56	MG	2A	3854	1/1	0.96	0.17	43,43,43,43	0
56	MG	1A	3042	1/1	0.96	0.21	14,14,14,14	0
56	MG	2A	3639	1/1	0.96	0.09	36,36,36,36	0
56	MG	1A	3829	1/1	0.96	0.26	18,18,18,18	0
56	MG	2A	3092	1/1	0.96	0.10	34,34,34,34	0
56	MG	2A	3005	1/1	0.96	0.11	39,39,39,39	0
56	MG	1A	3568	1/1	0.96	0.12	16,16,16,16	0
56	MG	2A	3232	1/1	0.96	0.13	46,46,46,46	0
56	MG	1A	4017	1/1	0.96	0.11	28,28,28,28	0
56	MG	1A	3945	1/1	0.96	0.11	31,31,31,31	0
56	MG	1A	3157	1/1	0.96	0.12	36,36,36,36	0
56	MG	1G	202	1/1	0.96	0.15	19,19,19,19	0
56	MG	1A	3104	1/1	0.96	0.30	21,21,21,21	0
56	MG	2A	3367	1/1	0.96	0.37	41,41,41,41	0
56	MG	2A	3621	1/1	0.96	0.14	31,31,31,31	0
56	MG	2A	3739	1/1	0.96	0.11	34,34,34,34	0
56	MG	1a	3062	1/1	0.96	0.07	56,56,56,56	0
56	MG	2A	3254	1/1	0.96	0.17	30,30,30,30	0
56	MG	2A	3127	1/1	0.96	0.49	42,42,42,42	0
56	MG	2A	3627	1/1	0.96	0.29	40,40,40,40	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	1A	3475	1/1	0.96	0.13	32,32,32,32	0
56	MG	1A	3091	1/1	0.96	0.36	17,17,17,17	0
56	MG	1X	105	1/1	0.96	0.13	20,20,20,20	0
56	MG	1B	230	1/1	0.96	0.10	38,38,38,38	0
56	MG	2A	3040	1/1	0.96	0.09	16,16,16,16	0
56	MG	2A	3231	1/1	0.96	0.11	41,41,41,41	0
56	MG	1a	3127	1/1	0.96	0.06	20,20,20,20	0
56	MG	1A	3035	1/1	0.96	0.20	20,20,20,20	0
56	MG	1A	4057	1/1	0.96	0.12	22,22,22,22	0
56	MG	1A	3163	1/1	0.96	0.14	24,24,24,24	0
56	MG	1A	4022	1/1	0.96	0.07	34,34,34,34	0
56	MG	1B	205	1/1	0.96	0.23	33,33,33,33	0
56	MG	2A	3384	1/1	0.96	0.10	34,34,34,34	0
56	MG	2A	3726	1/1	0.96	0.07	50,50,50,50	0
56	MG	2A	3004	1/1	0.96	0.11	32,32,32,32	0
56	MG	2O	8400	1/1	0.96	0.23	40,40,40,40	0
56	MG	1A	3430	1/1	0.96	0.16	48,48,48,48	0
56	MG	2A	3238	1/1	0.96	0.23	50,50,50,50	0
56	MG	2B	206	1/1	0.96	0.16	42,42,42,42	0
56	MG	1A	3192	1/1	0.96	0.25	23,23,23,23	0
58	ZN	2n	501	1/1	0.96	0.08	95,95,95,95	0
56	MG	1A	3312	1/1	0.96	0.12	22,22,22,22	0
56	MG	1a	3169	1/1	0.96	0.14	35,35,35,35	0
56	MG	1A	3938	1/1	0.96	0.23	47,47,47,47	0
56	MG	1E	314	1/1	0.96	0.40	29,29,29,29	0
56	MG	2a	1826	1/1	0.96	0.09	43,43,43,43	0
56	MG	1A	3902	1/1	0.96	0.06	36,36,36,36	0
56	MG	2A	3503	1/1	0.96	0.33	33,33,33,33	0
56	MG	1A	3442	1/1	0.96	0.26	33,33,33,33	0
56	MG	1A	3774	1/1	0.96	0.11	27,27,27,27	0
56	MG	1A	3936	1/1	0.96	0.07	35,35,35,35	0
56	MG	1A	3615	1/1	0.96	0.14	31,31,31,31	0
56	MG	1A	3848	1/1	0.96	0.05	38,38,38,38	0
56	MG	1A	3232	1/1	0.96	0.31	20,20,20,20	0
56	MG	2A	3442	1/1	0.96	0.17	39,39,39,39	0
56	MG	2A	3475	1/1	0.96	0.10	37,37,37,37	0
56	MG	1A	3531	1/1	0.96	0.23	25,25,25,25	0
56	MG	2a	1829	1/1	0.96	0.06	45,45,45,45	0
56	MG	1a	3121	1/1	0.96	0.10	42,42,42,42	0
56	MG	1A	3544	1/1	0.96	0.14	13,13,13,13	0
56	MG	2A	3725	1/1	0.96	0.25	34,34,34,34	0
56	MG	1A	3613	1/1	0.96	0.26	21,21,21,21	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	1A	3572	1/1	0.96	0.17	36,36,36,36	0
56	MG	2A	3370	1/1	0.96	0.07	35,35,35,35	0
56	MG	1A	3416	1/1	0.96	0.08	39,39,39,39	0
56	MG	2T	203	1/1	0.96	0.20	34,34,34,34	0
56	MG	1A	3119	1/1	0.96	0.12	11,11,11,11	0
56	MG	2a	1811	1/1	0.96	0.11	50,50,50,50	0
56	MG	1A	3792	1/1	0.96	0.14	29,29,29,29	0
56	MG	2j	201	1/1	0.96	0.10	47,47,47,47	0
56	MG	2A	3846	1/1	0.96	0.26	46,46,46,46	0
56	MG	1A	3685	1/1	0.96	0.16	15,15,15,15	0
56	MG	1A	3150	1/1	0.96	0.11	20,20,20,20	0
56	MG	1A	3872	1/1	0.96	0.11	13,13,13,13	0
56	MG	2A	3413	1/1	0.96	0.11	39,39,39,39	0
56	MG	1Q	204	1/1	0.96	0.09	13,13,13,13	0
56	MG	2A	3713	1/1	0.96	0.07	34,34,34,34	0
56	MG	1A	3414	1/1	0.96	0.18	10,10,10,10	0
56	MG	1A	3168	1/1	0.96	0.11	32,32,32,32	0
56	MG	1A	3545	1/1	0.96	0.11	30,30,30,30	0
56	MG	2A	3649	1/1	0.96	0.18	28,28,28,28	0
56	MG	2a	1747	1/1	0.96	0.06	67,67,67,67	0
56	MG	1a	3032	1/1	0.96	0.07	32,32,32,32	0
56	MG	1A	3439	1/1	0.96	0.14	25,25,25,25	0
56	MG	1A	3040	1/1	0.96	0.12	20,20,20,20	0
56	MG	1D	303	1/1	0.96	0.08	25,25,25,25	0
56	MG	1a	3015	1/1	0.96	0.10	28,28,28,28	0
56	MG	2x	104	1/1	0.96	0.11	42,42,42,42	0
56	MG	2a	1657	1/1	0.96	0.12	48,48,48,48	0
56	MG	2k	201	1/1	0.96	0.12	51,51,51,51	0
56	MG	16	103	1/1	0.96	0.15	39,39,39,39	0
56	MG	1D	310	1/1	0.96	0.49	18,18,18,18	0
56	MG	2A	3137	1/1	0.96	0.14	24,24,24,24	0
56	MG	1A	3147	1/1	0.96	0.10	27,27,27,27	0
56	MG	2a	1638	1/1	0.96	0.17	39,39,39,39	0
56	MG	2A	3266	1/1	0.96	0.07	42,42,42,42	0
56	MG	1a	3018	1/1	0.96	0.21	49,49,49,49	0
56	MG	1A	3849	1/1	0.96	0.10	27,27,27,27	0
56	MG	2A	3418	1/1	0.96	0.15	21,21,21,21	0
56	MG	1W	207	1/1	0.96	0.27	4,4,4,4	0
56	MG	1A	3551	1/1	0.96	0.17	14,14,14,14	0
56	MG	1A	3880	1/1	0.96	0.12	20,20,20,20	0
56	MG	1A	3037	1/1	0.96	0.10	9,9,9,9	0
56	MG	1A	3633	1/1	0.96	0.10	30,30,30,30	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	1A	3182	1/1	0.96	0.15	22,22,22,22	0
56	MG	2A	3483	1/1	0.96	0.11	38,38,38,38	0
56	MG	1A	3717	1/1	0.96	0.14	17,17,17,17	0
56	MG	2A	3363	1/1	0.96	0.17	48,48,48,48	0
56	MG	2a	1797	1/1	0.96	0.11	37,37,37,37	0
56	MG	2A	3225	1/1	0.96	0.38	39,39,39,39	0
56	MG	2a	1757	1/1	0.96	0.05	54,54,54,54	0
56	MG	1a	3019	1/1	0.96	0.08	45,45,45,45	0
56	MG	2A	3102	1/1	0.96	0.12	44,44,44,44	0
56	MG	1A	3694	1/1	0.96	0.15	14,14,14,14	0
56	MG	2a	1809	1/1	0.96	0.07	44,44,44,44	0
56	MG	2A	3817	1/1	0.96	0.07	28,28,28,28	0
56	MG	1A	3600	1/1	0.96	0.13	44,44,44,44	0
56	MG	2A	3151	1/1	0.96	0.21	43,43,43,43	0
56	MG	1I	201	1/1	0.96	0.08	36,36,36,36	0
56	MG	1O	201	1/1	0.96	0.10	29,29,29,29	0
56	MG	2A	3578	1/1	0.96	0.30	44,44,44,44	0
56	MG	1A	3201	1/1	0.96	0.18	38,38,38,38	0
56	MG	1A	3511	1/1	0.96	0.11	21,21,21,21	0
56	MG	1A	3221	1/1	0.96	0.18	19,19,19,19	0
56	MG	1A	3920	1/1	0.96	0.10	31,31,31,31	0
56	MG	1A	3928	1/1	0.96	0.11	26,26,26,26	0
56	MG	1A	3523	1/1	0.96	0.14	36,36,36,36	0
56	MG	2a	1753	1/1	0.96	0.07	51,51,51,51	0
56	MG	1A	3692	1/1	0.96	0.12	10,10,10,10	0
56	MG	2a	1794	1/1	0.96	0.21	58,58,58,58	0
56	MG	25	102	1/1	0.96	0.44	40,40,40,40	0
56	MG	2A	3534	1/1	0.96	0.13	30,30,30,30	0
56	MG	1a	3028	1/1	0.96	0.12	48,48,48,48	0
56	MG	1A	3376	1/1	0.96	0.07	35,35,35,35	0
56	MG	1A	3603	1/1	0.96	0.29	16,16,16,16	0
56	MG	2A	3322	1/1	0.96	0.35	45,45,45,45	0
56	MG	2A	3302	1/1	0.96	0.10	22,22,22,22	0
56	MG	1A	3041	1/1	0.96	0.14	37,37,37,37	0
56	MG	2A	3111	1/1	0.96	0.08	52,52,52,52	0
56	MG	2A	3080	1/1	0.96	0.12	51,51,51,51	0
56	MG	1A	3345	1/1	0.96	0.16	19,19,19,19	0
56	MG	2a	1818	1/1	0.96	0.12	48,48,48,48	0
56	MG	2A	3700	1/1	0.96	0.10	55,55,55,55	0
56	MG	2A	3616	1/1	0.96	0.16	32,32,32,32	0
56	MG	2a	1702	1/1	0.96	0.14	40,40,40,40	0
56	MG	2N	201	1/1	0.96	0.08	32,32,32,32	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	1Q	202	1/1	0.97	0.14	16,16,16,16	0
56	MG	2A	3187	1/1	0.97	0.12	39,39,39,39	0
56	MG	2A	3641	1/1	0.97	0.22	49,49,49,49	0
56	MG	1A	3522	1/1	0.97	0.10	21,21,21,21	0
56	MG	1A	3213	1/1	0.97	0.23	35,35,35,35	0
56	MG	2a	1824	1/1	0.97	0.18	26,26,26,26	0
56	MG	1V	205	1/1	0.97	0.24	19,19,19,19	0
56	MG	1A	3983	1/1	0.97	0.10	10,10,10,10	0
56	MG	2A	3744	1/1	0.97	0.11	29,29,29,29	0
56	MG	2a	1831	1/1	0.97	0.14	39,39,39,39	0
56	MG	1A	3988	1/1	0.97	0.16	20,20,20,20	0
56	MG	1A	3349	1/1	0.97	0.27	23,23,23,23	0
56	MG	2A	3849	1/1	0.97	0.09	30,30,30,30	0
56	MG	2A	3421	1/1	0.97	0.10	22,22,22,22	0
56	MG	1A	3870	1/1	0.97	0.29	23,23,23,23	0
56	MG	1A	3378	1/1	0.97	0.17	35,35,35,35	0
56	MG	2A	3867	1/1	0.97	0.09	46,46,46,46	0
56	MG	1A	3441	1/1	0.97	0.18	27,27,27,27	0
56	MG	2A	3552	1/1	0.97	0.07	56,56,56,56	0
56	MG	2l	202	1/1	0.97	0.39	45,45,45,45	0
56	MG	2A	3017	1/1	0.97	0.14	30,30,30,30	0
56	MG	1A	3638	1/1	0.97	0.12	30,30,30,30	0
56	MG	2A	3432	1/1	0.97	0.16	41,41,41,41	0
56	MG	1A	3383	1/1	0.97	0.11	22,22,22,22	0
56	MG	1A	3370	1/1	0.97	0.10	33,33,33,33	0
56	MG	2a	1691	1/1	0.97	0.09	44,44,44,44	0
56	MG	2a	1828	1/1	0.97	0.21	37,37,37,37	0
56	MG	1A	3100	1/1	0.97	0.21	22,22,22,22	0
56	MG	1A	3554	1/1	0.97	0.29	12,12,12,12	0
56	MG	1v	101	1/1	0.97	0.24	61,61,61,61	0
56	MG	1A	3627	1/1	0.97	0.11	27,27,27,27	0
56	MG	2A	3714	1/1	0.97	0.09	38,38,38,38	0
56	MG	1A	3748	1/1	0.97	0.09	34,34,34,34	0
56	MG	1A	3373	1/1	0.97	0.17	20,20,20,20	0
56	MG	1a	3042	1/1	0.97	0.11	37,37,37,37	0
56	MG	1A	3455	1/1	0.97	0.18	28,28,28,28	0
56	MG	2a	1673	1/1	0.97	0.11	48,48,48,48	0
56	MG	2A	3380	1/1	0.97	0.07	33,33,33,33	0
56	MG	2A	3460	1/1	0.97	0.14	48,48,48,48	0
56	MG	2A	3412	1/1	0.97	0.12	41,41,41,41	0
56	MG	1A	4066	1/1	0.97	0.15	21,21,21,21	0
56	MG	2A	3376	1/1	0.97	0.06	44,44,44,44	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	1A	3940	1/1	0.97	0.06	49,49,49,49	0
56	MG	1A	3283	1/1	0.97	0.17	36,36,36,36	0
56	MG	1A	3105	1/1	0.97	0.19	11,11,11,11	0
56	MG	2a	1643	1/1	0.97	0.16	29,29,29,29	0
56	MG	13	103	1/1	0.97	0.30	26,26,26,26	0
56	MG	1A	3381	1/1	0.97	0.07	23,23,23,23	0
56	MG	1A	3784	1/1	0.97	0.09	28,28,28,28	0
56	MG	1A	3803	1/1	0.97	0.20	29,29,29,29	0
56	MG	2A	3261	1/1	0.97	0.09	26,26,26,26	0
56	MG	1A	3064	1/1	0.97	0.09	13,13,13,13	0
56	MG	1A	3995	1/1	0.97	0.17	32,32,32,32	0
56	MG	2A	3589	1/1	0.97	0.07	38,38,38,38	0
56	MG	1A	3029	1/1	0.97	0.12	11,11,11,11	0
56	MG	1A	3429	1/1	0.97	0.11	27,27,27,27	0
56	MG	1A	4007	1/1	0.97	0.13	36,36,36,36	0
56	MG	1a	3012	1/1	0.97	0.13	49,49,49,49	0
56	MG	2a	1604	1/1	0.97	0.10	39,39,39,39	0
56	MG	2A	3862	1/1	0.97	0.38	45,45,45,45	0
56	MG	1A	3450	1/1	0.97	0.08	20,20,20,20	0
56	MG	1A	3180	1/1	0.97	0.15	18,18,18,18	0
56	MG	1A	3060	1/1	0.97	0.20	18,18,18,18	0
56	MG	1A	3371	1/1	0.97	0.20	10,10,10,10	0
56	MG	1A	3916	1/1	0.97	0.10	40,40,40,40	0
56	MG	2A	3130	1/1	0.97	0.07	28,28,28,28	0
56	MG	1e	201	1/1	0.97	0.09	48,48,48,48	0
56	MG	1A	4051	1/1	0.97	0.08	16,16,16,16	0
56	MG	2A	3051	1/1	0.97	0.15	34,34,34,34	0
56	MG	1A	3375	1/1	0.97	0.08	37,37,37,37	0
56	MG	2A	3323	1/1	0.97	0.27	63,63,63,63	0
56	MG	2A	3132	1/1	0.97	0.14	40,40,40,40	0
56	MG	1A	3073	1/1	0.97	0.22	29,29,29,29	0
56	MG	1A	3464	1/1	0.97	0.38	25,25,25,25	0
56	MG	2a	1658	1/1	0.97	0.10	30,30,30,30	0
56	MG	2A	3722	1/1	0.97	0.28	39,39,39,39	0
56	MG	2a	1618	1/1	0.97	0.13	36,36,36,36	0
56	MG	1A	3555	1/1	0.97	0.21	23,23,23,23	0
56	MG	1E	313	1/1	0.97	0.18	10,10,10,10	0
56	MG	1A	3548	1/1	0.97	0.29	27,27,27,27	0
56	MG	1A	3616	1/1	0.97	0.16	19,19,19,19	0
56	MG	1a	3161	1/1	0.97	0.15	53,53,53,53	0
56	MG	1A	3462	1/1	0.97	0.28	38,38,38,38	0
56	MG	1A	3648	1/1	0.97	0.07	18,18,18,18	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	2A	3459	1/1	0.97	0.18	35,35,35,35	0
56	MG	1A	3869	1/1	0.97	0.24	31,31,31,31	0
56	MG	1U	203	1/1	0.97	0.55	23,23,23,23	0
56	MG	1A	3908	1/1	0.97	0.10	23,23,23,23	0
56	MG	1A	3338	1/1	0.97	0.09	13,13,13,13	0
56	MG	2A	3006	1/1	0.97	0.11	42,42,42,42	0
56	MG	1A	4029	1/1	0.97	0.20	19,19,19,19	0
56	MG	2a	1726	1/1	0.97	0.27	32,32,32,32	0
56	MG	2A	3220	1/1	0.97	0.45	32,32,32,32	0
56	MG	1P	205	1/1	0.97	0.07	15,15,15,15	0
56	MG	1A	3173	1/1	0.97	0.12	21,21,21,21	0
56	MG	1A	3009	1/1	0.97	0.11	16,16,16,16	0
56	MG	2A	3865	1/1	0.97	0.13	28,28,28,28	0
56	MG	1A	3882	1/1	0.97	0.09	26,26,26,26	0
56	MG	1A	3230	1/1	0.97	0.08	24,24,24,24	0
56	MG	15	102	1/1	0.97	0.21	10,10,10,10	0
56	MG	1B	227	1/1	0.97	0.19	37,37,37,37	0
56	MG	1A	3001	1/1	0.97	0.15	35,35,35,35	0
56	MG	1a	3017	1/1	0.97	0.21	26,26,26,26	0
56	MG	1A	3137	1/1	0.97	0.19	35,35,35,35	0
56	MG	1Q	201	1/1	0.97	0.22	30,30,30,30	0
56	MG	2B	217	1/1	0.97	0.05	47,47,47,47	0
56	MG	2A	3554	1/1	0.97	0.08	45,45,45,45	0
56	MG	2A	3759	1/1	0.97	0.08	39,39,39,39	0
56	MG	1A	3399	1/1	0.97	0.17	16,16,16,16	0
56	MG	1A	3249	1/1	0.97	0.16	28,28,28,28	0
56	MG	1A	3089	1/1	0.97	0.25	28,28,28,28	0
56	MG	1A	3458	1/1	0.97	0.20	37,37,37,37	0
56	MG	2A	3248	1/1	0.97	0.14	47,47,47,47	0
56	MG	1a	3141	1/1	0.97	0.16	48,48,48,48	0
56	MG	1a	3087	1/1	0.97	0.09	39,39,39,39	0
56	MG	2A	3082	1/1	0.97	0.47	38,38,38,38	0
56	MG	2A	3415	1/1	0.97	0.09	34,34,34,34	0
56	MG	1A	3780	1/1	0.97	0.06	29,29,29,29	0
56	MG	1A	3030	1/1	0.97	0.22	17,17,17,17	0
56	MG	1a	3201	1/1	0.97	0.09	55,55,55,55	0
56	MG	2A	3175	1/1	0.97	0.14	28,28,28,28	0
56	MG	2A	3486	1/1	0.97	0.09	33,33,33,33	0
56	MG	1A	3217	1/1	0.97	0.28	42,42,42,42	0
56	MG	1A	3967	1/1	0.97	0.13	18,18,18,18	0
56	MG	1A	3110	1/1	0.97	0.38	24,24,24,24	0
56	MG	2A	3730	1/1	0.97	0.18	48,48,48,48	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	1a	3089	1/1	0.97	0.06	33,33,33,33	0
56	MG	1A	3019	1/1	0.97	0.24	26,26,26,26	0
56	MG	2A	3767	1/1	0.97	0.10	43,43,43,43	0
56	MG	1E	312	1/1	0.97	0.12	26,26,26,26	0
56	MG	1A	3679	1/1	0.97	0.13	10,10,10,10	0
56	MG	1A	3563	1/1	0.97	0.22	16,16,16,16	0
56	MG	1A	3082	1/1	0.97	0.13	20,20,20,20	0
56	MG	1A	3403	1/1	0.97	0.15	20,20,20,20	0
56	MG	1a	3076	1/1	0.97	0.06	35,35,35,35	0
56	MG	1A	3586	1/1	0.97	0.23	25,25,25,25	0
56	MG	2A	3852	1/1	0.97	0.07	24,24,24,24	0
56	MG	1A	3731	1/1	0.97	0.12	27,27,27,27	0
56	MG	1A	3431	1/1	0.97	0.29	24,24,24,24	0
56	MG	1A	3357	1/1	0.97	0.12	17,17,17,17	0
56	MG	1A	3002	1/1	0.97	0.11	22,22,22,22	0
56	MG	1D	308	1/1	0.97	0.12	29,29,29,29	0
56	MG	1A	3998	1/1	0.97	0.08	26,26,26,26	0
56	MG	2A	3476	1/1	0.97	0.10	40,40,40,40	0
56	MG	1a	3182	1/1	0.97	0.09	51,51,51,51	0
56	MG	1a	3221	1/1	0.97	0.08	47,47,47,47	0
56	MG	1a	3120	1/1	0.97	0.14	42,42,42,42	0
56	MG	1A	3817	1/1	0.97	0.12	28,28,28,28	0
56	MG	1A	3743	1/1	0.97	0.11	16,16,16,16	0
56	MG	2A	3119	1/1	0.97	0.32	34,34,34,34	0
56	MG	2a	1646	1/1	0.97	0.08	51,51,51,51	0
56	MG	1A	3649	1/1	0.97	0.11	12,12,12,12	0
56	MG	1A	3547	1/1	0.97	0.21	9,9,9,9	0
56	MG	1W	204	1/1	0.97	0.21	25,25,25,25	0
56	MG	1A	3161	1/1	0.97	0.12	26,26,26,26	0
56	MG	1A	3278	1/1	0.97	0.11	16,16,16,16	0
56	MG	1A	3198	1/1	0.97	0.22	20,20,20,20	0
56	MG	1A	3906	1/1	0.97	0.14	9,9,9,9	0
56	MG	1A	3562	1/1	0.97	0.26	7,7,7,7	0
56	MG	2A	3628	1/1	0.97	0.06	33,33,33,33	0
56	MG	1A	3072	1/1	0.97	0.13	18,18,18,18	0
56	MG	2A	3097	1/1	0.97	0.09	37,37,37,37	0
56	MG	1A	3158	1/1	0.97	0.19	37,37,37,37	0
56	MG	1a	3023	1/1	0.97	0.12	17,17,17,17	0
56	MG	1a	3060	1/1	0.97	0.07	48,48,48,48	0
56	MG	1A	3634	1/1	0.97	0.18	14,14,14,14	0
56	MG	1A	3661	1/1	0.97	0.17	34,34,34,34	0
56	MG	2A	3007	1/1	0.97	0.09	27,27,27,27	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	2a	1778	1/1	0.97	0.14	54,54,54,54	0
56	MG	1A	3779	1/1	0.97	0.23	15,15,15,15	0
56	MG	1A	3894	1/1	0.97	0.17	27,27,27,27	0
56	MG	2a	1804	1/1	0.97	0.06	37,37,37,37	0
56	MG	1a	3046	1/1	0.97	0.16	19,19,19,19	0
56	MG	1W	206	1/1	0.97	0.10	20,20,20,20	0
56	MG	1A	3794	1/1	0.97	0.13	12,12,12,12	0
56	MG	1A	3481	1/1	0.97	0.10	26,26,26,26	0
56	MG	1A	3842	1/1	0.97	0.13	37,37,37,37	0
56	MG	1A	4011	1/1	0.97	0.17	34,34,34,34	0
56	MG	1A	3744	1/1	0.97	0.11	25,25,25,25	0
56	MG	2A	3679	1/1	0.97	0.19	51,51,51,51	0
56	MG	2a	1687	1/1	0.97	0.13	51,51,51,51	0
56	MG	1a	3179	1/1	0.97	0.07	47,47,47,47	0
56	MG	2a	1689	1/1	0.97	0.11	47,47,47,47	0
56	MG	2A	3126	1/1	0.97	0.12	44,44,44,44	0
56	MG	2A	3837	1/1	0.97	0.11	18,18,18,18	0
56	MG	1A	3670	1/1	0.97	0.11	20,20,20,20	0
56	MG	1A	3818	1/1	0.97	0.12	31,31,31,31	0
56	MG	1A	3536	1/1	0.97	0.16	31,31,31,31	0
56	MG	1E	311	1/1	0.97	0.16	30,30,30,30	0
56	MG	2A	3425	1/1	0.97	0.31	34,34,34,34	0
56	MG	1A	3895	1/1	0.97	0.16	30,30,30,30	0
56	MG	1A	3725	1/1	0.97	0.08	40,40,40,40	0
56	MG	2A	3666	1/1	0.97	0.10	30,30,30,30	0
56	MG	2A	3226	1/1	0.97	0.20	31,31,31,31	0
56	MG	2A	3601	1/1	0.97	0.07	42,42,42,42	0
56	MG	2A	3704	1/1	0.97	0.18	33,33,33,33	0
56	MG	2A	3326	1/1	0.97	0.23	31,31,31,31	0
56	MG	1A	3821	1/1	0.97	0.09	31,31,31,31	0
56	MG	1A	3190	1/1	0.97	0.11	17,17,17,17	0
56	MG	2A	3280	1/1	0.97	0.25	39,39,39,39	0
56	MG	1a	3156	1/1	0.97	0.11	34,34,34,34	0
56	MG	2A	3516	1/1	0.97	0.13	36,36,36,36	0
56	MG	1A	3550	1/1	0.97	0.11	4,4,4,4	0
56	MG	1a	3036	1/1	0.97	0.10	32,32,32,32	0
56	MG	2a	1662	1/1	0.97	0.13	43,43,43,43	0
56	MG	1A	3275	1/1	0.97	0.15	36,36,36,36	0
56	MG	2A	3152	1/1	0.97	0.30	42,42,42,42	0
56	MG	2A	3166	1/1	0.97	0.15	35,35,35,35	0
56	MG	1A	3525	1/1	0.97	0.08	30,30,30,30	0
56	MG	2A	3832	1/1	0.97	0.14	35,35,35,35	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	1A	3080	1/1	0.97	0.11	17,17,17,17	0
56	MG	1D	302	1/1	0.97	0.69	35,35,35,35	0
56	MG	1A	3332	1/1	0.97	0.13	22,22,22,22	0
56	MG	1A	3405	1/1	0.97	0.08	38,38,38,38	0
56	MG	1a	3159	1/1	0.97	0.15	46,46,46,46	0
56	MG	2A	3221	1/1	0.97	0.17	51,51,51,51	0
56	MG	2A	3444	1/1	0.97	0.12	36,36,36,36	0
56	MG	2A	3179	1/1	0.97	0.06	33,33,33,33	0
56	MG	1A	3947	1/1	0.97	0.12	22,22,22,22	0
56	MG	1a	3184	1/1	0.97	0.11	49,49,49,49	0
56	MG	1a	3108	1/1	0.97	0.07	24,24,24,24	0
56	MG	1a	3187	1/1	0.97	0.16	29,29,29,29	0
56	MG	2a	1744	1/1	0.97	0.16	65,65,65,65	0
56	MG	1A	3614	1/1	0.97	0.25	35,35,35,35	0
56	MG	2A	3831	1/1	0.97	0.14	68,68,68,68	0
56	MG	1A	3076	1/1	0.97	0.12	32,32,32,32	0
56	MG	1A	3575	1/1	0.97	0.09	23,23,23,23	0
56	MG	2a	1830	1/1	0.97	0.18	38,38,38,38	0
56	MG	2A	3447	1/1	0.97	0.15	39,39,39,39	0
56	MG	2A	3573	1/1	0.97	0.10	28,28,28,28	0
56	MG	1G	203	1/1	0.97	0.12	34,34,34,34	0
56	MG	2B	220	1/1	0.97	0.16	57,57,57,57	0
56	MG	2A	3763	1/1	0.97	0.11	41,41,41,41	0
56	MG	2A	3374	1/1	0.97	0.06	50,50,50,50	0
56	MG	1A	3014	1/1	0.97	0.16	32,32,32,32	0
56	MG	1a	3097	1/1	0.97	0.20	34,34,34,34	0
56	MG	2A	3872	1/1	0.97	0.07	42,42,42,42	0
56	MG	1A	3131	1/1	0.97	0.11	16,16,16,16	0
56	MG	1A	3612	1/1	0.97	0.25	26,26,26,26	0
56	MG	2A	3296	1/1	0.97	0.08	46,46,46,46	0
56	MG	1A	3069	1/1	0.97	0.44	33,33,33,33	0
56	MG	1a	3016	1/1	0.97	0.12	43,43,43,43	0
56	MG	1A	3013	1/1	0.97	0.11	11,11,11,11	0
56	MG	1A	3239	1/1	0.97	0.20	9,9,9,9	0
56	MG	1A	3123	1/1	0.97	0.11	6,6,6,6	0
56	MG	2A	3354	1/1	0.97	0.25	41,41,41,41	0
56	MG	1A	3621	1/1	0.97	0.10	30,30,30,30	0
56	MG	1A	3218	1/1	0.97	0.12	19,19,19,19	0
56	MG	1A	3734	1/1	0.97	0.13	30,30,30,30	0
56	MG	2A	3613	1/1	0.97	0.28	58,58,58,58	0
56	MG	1A	3466	1/1	0.97	0.22	23,23,23,23	0
56	MG	2A	3461	1/1	0.97	0.37	29,29,29,29	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	2A	3234	1/1	0.97	0.49	37,37,37,37	0
56	MG	1a	3197	1/1	0.97	0.06	49,49,49,49	0
56	MG	2A	3526	1/1	0.97	0.17	42,42,42,42	0
56	MG	1A	3449	1/1	0.97	0.28	19,19,19,19	0
56	MG	1B	224	1/1	0.97	0.14	36,36,36,36	0
56	MG	1A	3790	1/1	0.97	0.14	10,10,10,10	0
56	MG	1A	3929	1/1	0.97	0.11	34,34,34,34	0
56	MG	1A	3924	1/1	0.97	0.09	9,9,9,9	0
56	MG	1A	3811	1/1	0.97	0.08	20,20,20,20	0
56	MG	2a	1750	1/1	0.97	0.10	51,51,51,51	0
56	MG	1A	3747	1/1	0.97	0.07	35,35,35,35	0
56	MG	2A	3224	1/1	0.97	0.42	45,45,45,45	0
56	MG	2A	3675	1/1	0.97	0.12	37,37,37,37	0
56	MG	2D	301	1/1	0.97	0.14	37,37,37,37	0
56	MG	1a	3144	1/1	0.97	0.14	61,61,61,61	0
56	MG	2A	3490	1/1	0.97	0.08	52,52,52,52	0
56	MG	2A	3369	1/1	0.97	0.27	53,53,53,53	0
56	MG	1A	3899	1/1	0.97	0.10	23,23,23,23	0
56	MG	1A	3011	1/1	0.97	0.07	25,25,25,25	0
56	MG	1A	3689	1/1	0.97	0.08	19,19,19,19	0
56	MG	1F	309	1/1	0.97	0.34	21,21,21,21	0
56	MG	1A	3070	1/1	0.97	0.27	23,23,23,23	0
56	MG	2a	1686	1/1	0.97	0.07	34,34,34,34	0
56	MG	1A	3768	1/1	0.97	0.12	22,22,22,22	0
56	MG	1A	3356	1/1	0.97	0.42	12,12,12,12	0
56	MG	1A	3034	1/1	0.97	0.18	15,15,15,15	0
56	MG	2B	210	1/1	0.97	0.15	72,72,72,72	0
56	MG	1A	3410	1/1	0.97	0.10	17,17,17,17	0
56	MG	1A	3917	1/1	0.97	0.17	34,34,34,34	0
56	MG	2A	3114	1/1	0.97	0.09	32,32,32,32	0
56	MG	1B	233	1/1	0.97	0.08	41,41,41,41	0
56	MG	1A	3975	1/1	0.97	0.05	25,25,25,25	0
56	MG	2A	3654	1/1	0.97	0.28	30,30,30,30	0
56	MG	2A	3171	1/1	0.97	0.12	27,27,27,27	0
56	MG	1A	3181	1/1	0.97	0.15	35,35,35,35	0
56	MG	2A	3100	1/1	0.97	0.20	41,41,41,41	0
56	MG	1X	101	1/1	0.97	0.23	28,28,28,28	0
56	MG	2a	1642	1/1	0.97	0.10	38,38,38,38	0
56	MG	1A	3243	1/1	0.97	0.22	16,16,16,16	0
56	MG	2A	3052	1/1	0.97	0.15	58,58,58,58	0
56	MG	12	101	1/1	0.97	0.20	28,28,28,28	0
56	MG	1A	3978	1/1	0.97	0.14	24,24,24,24	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	1A	3528	1/1	0.97	0.16	27,27,27,27	0
56	MG	2A	3669	1/1	0.97	0.13	31,31,31,31	0
56	MG	1a	3181	1/1	0.97	0.06	39,39,39,39	0
56	MG	13	106	1/1	0.97	0.20	15,15,15,15	0
56	MG	1a	3026	1/1	0.98	0.19	28,28,28,28	0
56	MG	1A	3078	1/1	0.98	0.22	30,30,30,30	0
56	MG	2a	1601	1/1	0.98	0.30	59,59,59,59	0
56	MG	2A	3492	1/1	0.98	0.14	37,37,37,37	0
56	MG	2A	3167	1/1	0.98	0.17	51,51,51,51	0
56	MG	1A	3054	1/1	0.98	0.13	23,23,23,23	0
56	MG	2A	3691	1/1	0.98	0.07	43,43,43,43	0
56	MG	2F	304	1/1	0.98	0.09	32,32,32,32	0
56	MG	2A	3414	1/1	0.98	0.11	38,38,38,38	0
56	MG	1A	3859	1/1	0.98	0.08	22,22,22,22	0
56	MG	1A	3712	1/1	0.98	0.10	28,28,28,28	0
56	MG	1A	3951	1/1	0.98	0.12	22,22,22,22	0
56	MG	1A	3585	1/1	0.98	0.25	25,25,25,25	0
56	MG	1A	3188	1/1	0.98	0.10	19,19,19,19	0
56	MG	2A	3377	1/1	0.98	0.12	29,29,29,29	0
56	MG	2a	1785	1/1	0.98	0.23	63,63,63,63	0
56	MG	2R	203	1/1	0.98	0.15	23,23,23,23	0
56	MG	1A	4003	1/1	0.98	0.08	18,18,18,18	0
56	MG	1a	3140	1/1	0.98	0.21	34,34,34,34	0
56	MG	2A	3454	1/1	0.98	0.12	31,31,31,31	0
56	MG	2A	3056	1/1	0.98	0.08	28,28,28,28	0
56	MG	1A	3762	1/1	0.98	0.07	37,37,37,37	0
56	MG	2A	3257	1/1	0.98	0.06	30,30,30,30	0
56	MG	1A	3216	1/1	0.98	0.15	37,37,37,37	0
56	MG	1A	3628	1/1	0.98	0.19	19,19,19,19	0
56	MG	1A	3476	1/1	0.98	0.13	26,26,26,26	0
58	ZN	16	105	1/1	0.98	0.19	31,31,31,31	0
56	MG	1A	3625	1/1	0.98	0.14	19,19,19,19	0
56	MG	1A	3487	1/1	0.98	0.19	14,14,14,14	0
56	MG	2a	1693	1/1	0.98	0.23	40,40,40,40	0
56	MG	2A	3727	1/1	0.98	0.07	33,33,33,33	0
56	MG	2a	1810	1/1	0.98	0.10	50,50,50,50	0
56	MG	2A	3352	1/1	0.98	0.18	9,9,9,9	0
56	MG	1V	204	1/1	0.98	0.32	25,25,25,25	0
56	MG	1A	3447	1/1	0.98	0.19	23,23,23,23	0
56	MG	2A	3696	1/1	0.98	0.09	34,34,34,34	0
56	MG	1A	3477	1/1	0.98	0.13	22,22,22,22	0
56	MG	2A	3673	1/1	0.98	0.12	27,27,27,27	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	2A	3828	1/1	0.98	0.08	39,39,39,39	0
56	MG	1D	305	1/1	0.98	0.14	36,36,36,36	0
56	MG	1a	3183	1/1	0.98	0.06	49,49,49,49	0
56	MG	2A	3661	1/1	0.98	0.09	56,56,56,56	0
56	MG	1A	3587	1/1	0.98	0.26	13,13,13,13	0
56	MG	1A	3561	1/1	0.98	0.10	10,10,10,10	0
56	MG	1A	3289	1/1	0.98	0.20	25,25,25,25	0
56	MG	1A	4037	1/1	0.98	0.18	5,5,5,5	0
56	MG	2a	1727	1/1	0.98	0.20	44,44,44,44	0
56	MG	2A	3211	1/1	0.98	0.12	31,31,31,31	0
56	MG	1A	3738	1/1	0.98	0.12	46,46,46,46	0
56	MG	1A	3055	1/1	0.98	0.07	19,19,19,19	0
56	MG	2a	1676	1/1	0.98	0.09	36,36,36,36	0
56	MG	1A	3212	1/1	0.98	0.13	23,23,23,23	0
56	MG	1A	3618	1/1	0.98	0.37	16,16,16,16	0
56	MG	1A	4047	1/1	0.98	0.16	19,19,19,19	0
56	MG	2A	3652	1/1	0.98	0.20	35,35,35,35	0
56	MG	2A	3718	1/1	0.98	0.07	32,32,32,32	0
56	MG	1A	3254	1/1	0.98	0.17	10,10,10,10	0
56	MG	2A	3813	1/1	0.98	0.10	25,25,25,25	0
56	MG	1a	3225	1/1	0.98	0.12	41,41,41,41	0
56	MG	1A	3591	1/1	0.98	0.07	34,34,34,34	0
56	MG	1a	3021	1/1	0.98	0.13	47,47,47,47	0
56	MG	2A	3293	1/1	0.98	0.08	46,46,46,46	0
56	MG	2j	202	1/1	0.98	0.12	59,59,59,59	0
56	MG	1a	3092	1/1	0.98	0.21	40,40,40,40	0
56	MG	1a	3013	1/1	0.98	0.10	33,33,33,33	0
56	MG	1A	3024	1/1	0.98	0.11	9,9,9,9	0
56	MG	1A	3845	1/1	0.98	0.13	37,37,37,37	0
56	MG	1Q	207	1/1	0.98	0.10	25,25,25,25	0
56	MG	1A	3109	1/1	0.98	0.15	37,37,37,37	0
56	MG	1a	3027	1/1	0.98	0.09	49,49,49,49	0
56	MG	1B	215	1/1	0.98	0.12	29,29,29,29	0
56	MG	1A	3809	1/1	0.98	0.08	32,32,32,32	0
56	MG	2A	3585	1/1	0.98	0.12	34,34,34,34	0
56	MG	1A	3886	1/1	0.98	0.17	14,14,14,14	0
56	MG	2A	3605	1/1	0.98	0.12	33,33,33,33	0
56	MG	1D	311	1/1	0.98	0.14	16,16,16,16	0
56	MG	1A	3126	1/1	0.98	0.22	18,18,18,18	0
56	MG	2A	3474	1/1	0.98	0.34	38,38,38,38	0
56	MG	1A	3265	1/1	0.98	0.10	4,4,4,4	0
56	MG	1A	4018	1/1	0.98	0.13	10,10,10,10	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	1A	3630	1/1	0.98	0.11	30,30,30,30	0
56	MG	1a	3091	1/1	0.98	0.20	24,24,24,24	0
56	MG	1A	3542	1/1	0.98	0.10	31,31,31,31	0
56	MG	1A	4005	1/1	0.98	0.07	28,28,28,28	0
56	MG	2A	3440	1/1	0.98	0.16	36,36,36,36	0
56	MG	1a	3008	1/1	0.98	0.10	17,17,17,17	0
56	MG	2B	207	1/1	0.98	0.08	48,48,48,48	0
56	MG	1A	3650	1/1	0.98	0.12	13,13,13,13	0
56	MG	1U	202	1/1	0.98	0.37	21,21,21,21	0
56	MG	1B	221	1/1	0.98	0.08	18,18,18,18	0
56	MG	2A	3407	1/1	0.98	0.31	47,47,47,47	0
56	MG	1A	3402	1/1	0.98	0.19	12,12,12,12	0
56	MG	2r	101	1/1	0.98	0.07	58,58,58,58	0
56	MG	2A	3408	1/1	0.98	0.13	41,41,41,41	0
56	MG	2A	3520	1/1	0.98	0.13	42,42,42,42	0
59	SF4	2d	302	8/8	0.98	0.15	45,64,68,72	0
56	MG	2q	201	1/1	0.98	0.11	55,55,55,55	0
56	MG	13	102	1/1	0.98	0.12	12,12,12,12	0
56	MG	2A	3748	1/1	0.98	0.07	34,34,34,34	0
56	MG	1A	4060	1/1	0.98	0.09	24,24,24,24	0
56	MG	1a	3063	1/1	0.98	0.12	48,48,48,48	0
56	MG	1B	217	1/1	0.98	0.14	17,17,17,17	0
56	MG	1A	3556	1/1	0.98	0.14	10,10,10,10	0
56	MG	1A	3436	1/1	0.98	0.08	29,29,29,29	0
56	MG	1A	3730	1/1	0.98	0.09	15,15,15,15	0
56	MG	1B	214	1/1	0.98	0.11	36,36,36,36	0
56	MG	1A	3746	1/1	0.98	0.09	13,13,13,13	0
56	MG	2A	3168	1/1	0.98	0.12	23,23,23,23	0
56	MG	2A	3550	1/1	0.98	0.09	37,37,37,37	0
56	MG	2a	1682	1/1	0.98	0.12	66,66,66,66	0
56	MG	2A	3028	1/1	0.98	0.10	20,20,20,20	0
56	MG	1A	3077	1/1	0.98	0.17	10,10,10,10	0
56	MG	1A	3759	1/1	0.98	0.10	36,36,36,36	0
56	MG	2A	3079	1/1	0.98	0.12	23,23,23,23	0
56	MG	1A	3597	1/1	0.98	0.11	11,11,11,11	0
56	MG	2A	3777	1/1	0.98	0.11	36,36,36,36	0
56	MG	1A	3732	1/1	0.98	0.13	10,10,10,10	0
56	MG	1A	3153	1/1	0.98	0.08	25,25,25,25	0
56	MG	1A	3140	1/1	0.98	0.28	22,22,22,22	0
56	MG	1A	3412	1/1	0.98	0.21	16,16,16,16	0
56	MG	2A	3262	1/1	0.98	0.16	42,42,42,42	0
56	MG	1A	3146	1/1	0.98	0.10	26,26,26,26	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	10	104	1/1	0.98	0.34	36,36,36,36	0
56	MG	1A	3172	1/1	0.98	0.25	24,24,24,24	0
56	MG	2a	1661	1/1	0.98	0.08	51,51,51,51	0
56	MG	1A	3852	1/1	0.98	0.17	13,13,13,13	0
56	MG	2B	219	1/1	0.98	0.09	52,52,52,52	0
56	MG	1A	3735	1/1	0.98	0.11	27,27,27,27	0
56	MG	1x	102	1/1	0.98	0.11	24,24,24,24	0
56	MG	2E	302	1/1	0.98	0.16	46,46,46,46	0
56	MG	1A	3058	1/1	0.98	0.09	26,26,26,26	0
56	MG	1A	4002	1/1	0.98	0.10	25,25,25,25	0
56	MG	1A	3796	1/1	0.98	0.16	47,47,47,47	0
56	MG	2A	3335	1/1	0.98	0.24	53,53,53,53	0
56	MG	2A	3742	1/1	0.98	0.15	40,40,40,40	0
56	MG	1A	3167	1/1	0.98	0.05	32,32,32,32	0
56	MG	2A	3755	1/1	0.98	0.10	40,40,40,40	0
56	MG	1A	3639	1/1	0.98	0.08	42,42,42,42	0
56	MG	2A	3485	1/1	0.98	0.13	40,40,40,40	0
56	MG	1A	3652	1/1	0.98	0.16	32,32,32,32	0
56	MG	2a	1633	1/1	0.98	0.16	36,36,36,36	0
56	MG	1A	4053	1/1	0.98	0.05	48,48,48,48	0
56	MG	1F	313	1/1	0.98	0.21	20,20,20,20	0
56	MG	2A	3737	1/1	0.98	0.05	21,21,21,21	0
56	MG	1A	3931	1/1	0.98	0.12	36,36,36,36	0
56	MG	1A	3581	1/1	0.98	0.21	20,20,20,20	0
56	MG	1A	3584	1/1	0.98	0.20	31,31,31,31	0
56	MG	1A	3207	1/1	0.98	0.13	22,22,22,22	0
56	MG	2A	3519	1/1	0.98	0.11	19,19,19,19	0
56	MG	1A	3337	1/1	0.98	0.12	23,23,23,23	0
56	MG	2A	3458	1/1	0.98	0.17	60,60,60,60	0
58	ZN	1Y	202	1/1	0.98	0.13	57,57,57,57	0
56	MG	1a	3022	1/1	0.98	0.09	22,22,22,22	0
56	MG	1U	201	1/1	0.98	0.22	20,20,20,20	0
56	MG	2A	3580	1/1	0.98	0.14	39,39,39,39	0
56	MG	1A	4062	1/1	0.98	0.08	21,21,21,21	0
56	MG	1A	3303	1/1	0.98	0.17	25,25,25,25	0
56	MG	1A	3328	1/1	0.98	0.15	21,21,21,21	0
56	MG	1A	3913	1/1	0.98	0.15	38,38,38,38	0
56	MG	2A	3427	1/1	0.98	0.13	23,23,23,23	0
56	MG	1D	304	1/1	0.98	0.09	18,18,18,18	0
56	MG	1a	3211	1/1	0.98	0.09	27,27,27,27	0
56	MG	1Y	201	1/1	0.98	0.22	39,39,39,39	0
56	MG	2A	3081	1/1	0.98	0.05	33,33,33,33	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	15	104	1/1	0.98	0.40	25,25,25,25	0
56	MG	1a	3227	1/1	0.98	0.08	39,39,39,39	0
56	MG	2A	3423	1/1	0.98	0.08	22,22,22,22	0
56	MG	2A	3411	1/1	0.98	0.12	28,28,28,28	0
56	MG	1B	203	1/1	0.98	0.36	32,32,32,32	0
56	MG	1A	3096	1/1	0.98	0.24	20,20,20,20	0
56	MG	2A	3489	1/1	0.98	0.07	37,37,37,37	0
56	MG	1A	3992	1/1	0.98	0.11	20,20,20,20	0
56	MG	1A	3434	1/1	0.98	0.19	39,39,39,39	0
56	MG	1A	3766	1/1	0.98	0.10	22,22,22,22	0
56	MG	2A	3690	1/1	0.98	0.14	35,35,35,35	0
56	MG	1U	209	1/1	0.98	0.21	18,18,18,18	0
56	MG	2A	3134	1/1	0.98	0.15	37,37,37,37	0
56	MG	1A	3742	1/1	0.98	0.12	29,29,29,29	0
56	MG	2a	1680	1/1	0.98	0.16	44,44,44,44	0
56	MG	2A	3267	1/1	0.98	0.11	26,26,26,26	0
56	MG	1A	3740	1/1	0.98	0.07	45,45,45,45	0
56	MG	1A	3671	1/1	0.98	0.15	36,36,36,36	0
56	MG	1A	3777	1/1	0.98	0.11	9,9,9,9	0
56	MG	2A	3417	1/1	0.98	0.17	36,36,36,36	0
56	MG	2A	3753	1/1	0.98	0.07	47,47,47,47	0
56	MG	1A	3106	1/1	0.98	0.15	25,25,25,25	0
56	MG	1X	103	1/1	0.98	0.11	26,26,26,26	0
56	MG	1A	3546	1/1	0.98	0.15	21,21,21,21	0
56	MG	1a	3217	1/1	0.98	0.08	65,65,65,65	0
56	MG	2A	3172	1/1	0.98	0.06	33,33,33,33	0
56	MG	1A	3864	1/1	0.98	0.07	17,17,17,17	0
56	MG	2A	3283	1/1	0.98	0.14	32,32,32,32	0
56	MG	2A	3236	1/1	0.99	0.26	40,40,40,40	0
56	MG	1A	3699	1/1	0.99	0.12	38,38,38,38	0
56	MG	2A	3113	1/1	0.99	0.09	36,36,36,36	0
56	MG	1A	3482	1/1	0.99	0.09	12,12,12,12	0
56	MG	2A	3610	1/1	0.99	0.11	54,54,54,54	0
56	MG	1A	3560	1/1	0.99	0.13	11,11,11,11	0
58	ZN	15	108	1/1	0.99	0.19	33,33,33,33	0
56	MG	1E	315	1/1	0.99	0.05	23,23,23,23	0
56	MG	1A	3344	1/1	0.99	0.07	21,21,21,21	0
56	MG	2A	3473	1/1	0.99	0.14	46,46,46,46	0
56	MG	2A	3036	1/1	0.99	0.09	41,41,41,41	0
56	MG	1A	3736	1/1	0.99	0.14	17,17,17,17	0
56	MG	1A	4006	1/1	0.99	0.07	15,15,15,15	0
56	MG	1A	3543	1/1	0.99	0.14	12,12,12,12	0

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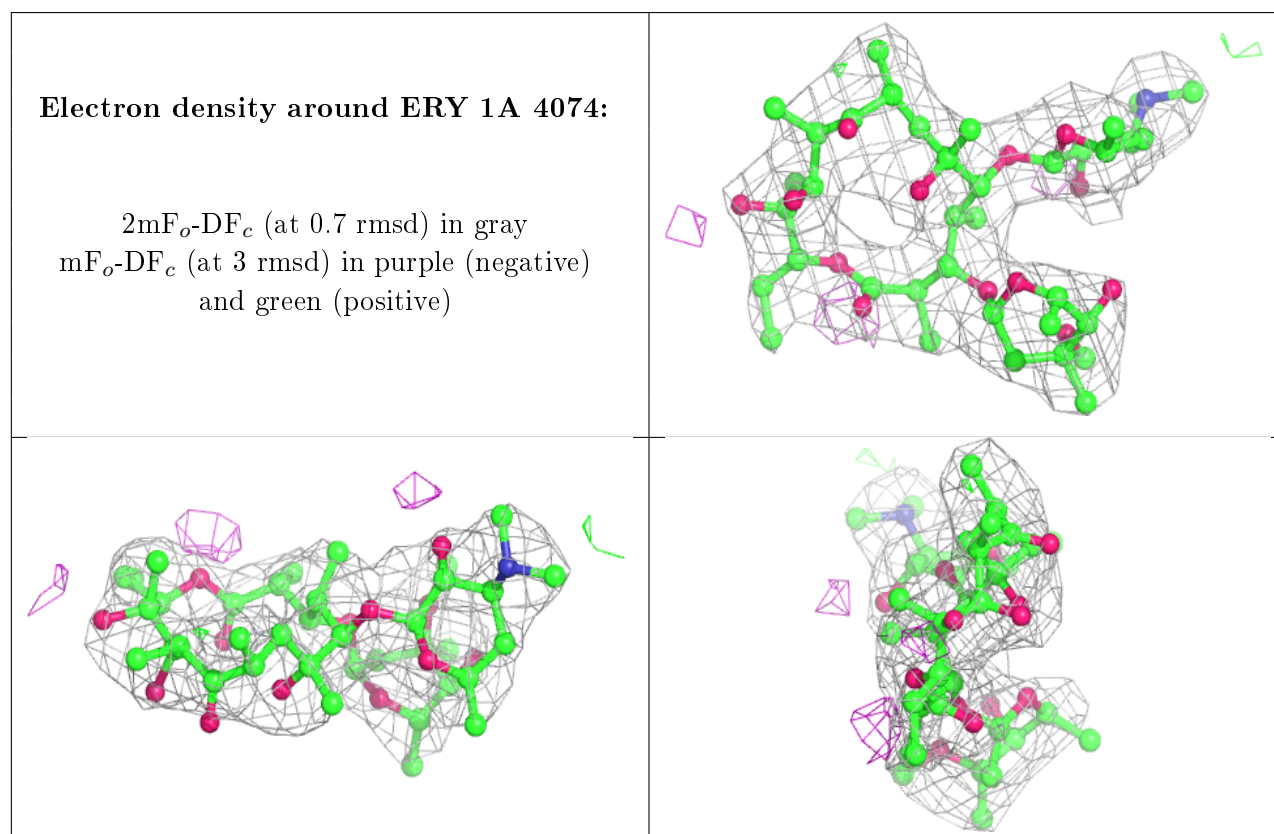
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	1A	3021	1/1	0.99	0.15	16,16,16,16	0
58	ZN	26	103	1/1	0.99	0.17	55,55,55,55	0
56	MG	17	102	1/1	0.99	0.10	14,14,14,14	0
56	MG	1A	3136	1/1	0.99	0.20	19,19,19,19	0
56	MG	1A	3022	1/1	0.99	0.09	26,26,26,26	0
56	MG	2A	3253	1/1	0.99	0.31	46,46,46,46	0
56	MG	1A	3754	1/1	0.99	0.08	35,35,35,35	0
56	MG	2A	3572	1/1	0.99	0.10	34,34,34,34	0
56	MG	1A	3828	1/1	0.99	0.07	30,30,30,30	0
56	MG	2A	3448	1/1	0.99	0.18	34,34,34,34	0
56	MG	2A	3647	1/1	0.99	0.21	38,38,38,38	0
56	MG	1A	3187	1/1	0.99	0.18	19,19,19,19	0
56	MG	2A	3809	1/1	0.99	0.13	37,37,37,37	0
56	MG	1a	3020	1/1	0.99	0.06	48,48,48,48	0
59	SF4	1d	302	8/8	0.99	0.15	39,58,69,70	0
56	MG	1A	3711	1/1	0.99	0.14	10,10,10,10	0
56	MG	1A	4038	1/1	0.99	0.11	30,30,30,30	0
56	MG	2A	3037	1/1	0.99	0.12	48,48,48,48	0
56	MG	1A	3672	1/1	0.99	0.11	20,20,20,20	0
56	MG	2y	104	1/1	0.99	0.03	39,39,39,39	0
56	MG	2A	3348	1/1	0.99	0.21	26,26,26,26	0
56	MG	2W	201	1/1	0.99	0.16	40,40,40,40	0
56	MG	2l	204	1/1	0.99	0.20	49,49,49,49	0
56	MG	1A	3668	1/1	0.99	0.10	15,15,15,15	0
56	MG	2U	202	1/1	0.99	0.22	48,48,48,48	0
56	MG	1A	3027	1/1	0.99	0.08	16,16,16,16	0
56	MG	2A	3083	1/1	0.99	0.28	44,44,44,44	0
56	MG	1A	3171	1/1	0.99	0.12	10,10,10,10	0
56	MG	1A	3636	1/1	0.99	0.13	4,4,4,4	0
56	MG	1A	3340	1/1	0.99	0.10	23,23,23,23	0
58	ZN	19	104	1/1	0.99	0.14	36,36,36,36	0
56	MG	2A	3441	1/1	0.99	0.14	41,41,41,41	0
56	MG	1A	3121	1/1	0.99	0.13	12,12,12,12	0
56	MG	1A	3643	1/1	0.99	0.10	15,15,15,15	0
56	MG	1A	3834	1/1	0.99	0.12	20,20,20,20	0
56	MG	2a	1671	1/1	0.99	0.11	46,46,46,46	0
56	MG	2A	3705	1/1	0.99	0.21	41,41,41,41	0
56	MG	1A	4068	1/1	0.99	0.11	34,34,34,34	0
56	MG	1a	3152	1/1	0.99	0.09	32,32,32,32	0
56	MG	2a	1814	1/1	0.99	0.13	26,26,26,26	0
56	MG	1A	4031	1/1	0.99	0.06	21,21,21,21	0
56	MG	1A	3316	1/1	0.99	0.18	20,20,20,20	0

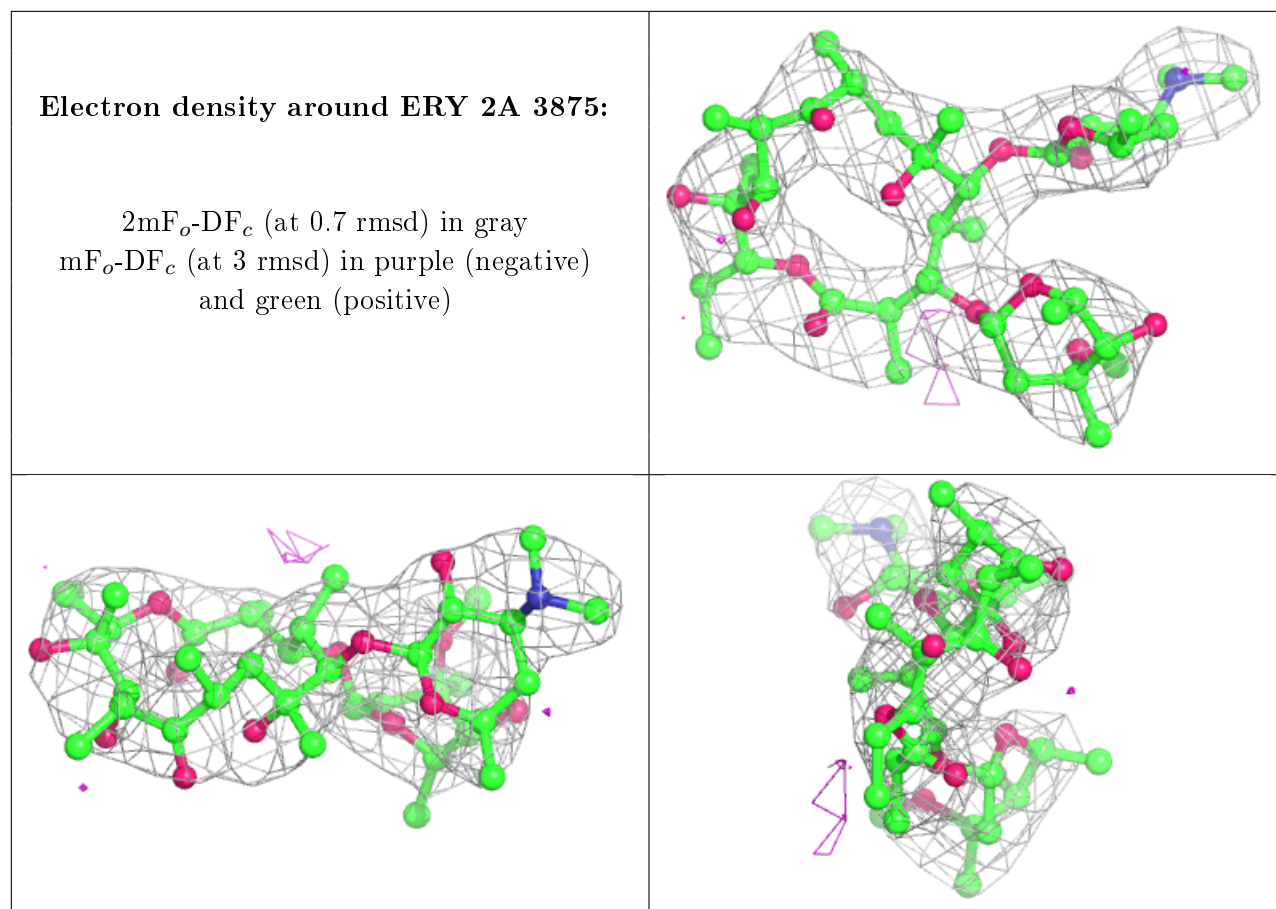
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	1A	3954	1/1	0.99	0.10	31,31,31,31	0
56	MG	1A	3248	1/1	0.99	0.10	30,30,30,30	0
58	ZN	25	104	1/1	0.99	0.17	44,44,44,44	0
56	MG	1A	3262	1/1	0.99	0.28	16,16,16,16	0
56	MG	1A	3196	1/1	0.99	0.23	23,23,23,23	0
56	MG	1Z	303	1/1	0.99	0.10	29,29,29,29	0
56	MG	1A	3149	1/1	0.99	0.23	19,19,19,19	0
56	MG	2A	3329	1/1	0.99	0.12	37,37,37,37	0
56	MG	2A	3106	1/1	0.99	0.09	35,35,35,35	0
56	MG	1U	210	1/1	0.99	0.37	15,15,15,15	0
56	MG	2A	3066	1/1	0.99	0.15	28,28,28,28	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.





## 6.5 Other polymers ⓘ

There are no such residues in this entry.