



# Full wwPDB X-ray Structure Validation Report ⓘ

Aug 19, 2020 – 02:54 PM BST

PDB ID : 6XQD  
Title : Crystal structure of the *Thermus thermophilus* 70S ribosome in complex with sarecycline, UUC-mRNA, and deacylated P-site tRNA at 2.80Å resolution  
Authors : Batool, Z.; Lomakin, I.B.; Bunick, C.G.; Polikanov, Y.S.  
Deposited on : 2020-07-09  
Resolution : 2.80 Å(reported)

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

We welcome your comments at [validation@mail.wwpdb.org](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 : 2.13  
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) : 2.13

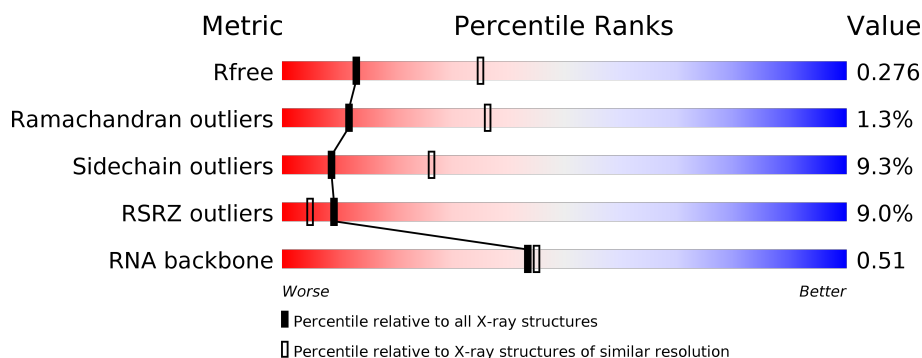
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.80 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	130704	3140 (2.80-2.80)
Ramachandran outliers	138981	3498 (2.80-2.80)
Sidechain outliers	138945	3500 (2.80-2.80)
RSRZ outliers	127900	3078 (2.80-2.80)
RNA backbone	3102	1227 (3.10-2.50)

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>2%</div> <div> <div></div> <div>81%</div> <div>17%</div> <div>..</div> </div> </div>
1	2A	2915	<div> <div>3%</div> <div> <div></div> <div>77%</div> <div>18%</div> <div>..</div> </div> </div>
2	1B	121	<div> <div></div> <div> <div></div> <div>88%</div> <div>10%</div> <div>..</div> </div> </div>
2	2B	121	<div> <div>6%</div> <div> <div></div> <div>71%</div> <div>28%</div> <div>.</div> </div> </div>
3	1D	276	<div> <div>3%</div> <div> <div></div> <div>95%</div> <div></div> <div>.</div> </div> </div>
3	2D	276	<div> <div>16%</div> <div> <div></div> <div>96%</div> <div></div> <div>.</div> </div> </div>

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Mol	Chain	Length	Quality of chain
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	
15	2T	146	
16	1U	118	

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Mol	Chain	Length	Quality of chain
16	2U	118	<div> <div>22%</div> <div>93%</div> <div>5%</div> </div>
17	1V	101	<div> <div>96%</div> </div>
17	2V	101	<div> <div>12%</div> <div>93%</div> <div>7%</div> </div>
18	1W	113	<div> <div>91%</div> <div>8%</div> </div>
18	2W	113	<div> <div>4%</div> <div>93%</div> <div>6%</div> </div>
19	1X	96	<div> <div>95%</div> </div>
19	2X	96	<div> <div>8%</div> <div>92%</div> <div>7%</div> </div>
20	1Y	110	<div> <div>87%</div> <div>10%</div> </div>
20	2Y	110	<div> <div>14%</div> <div>86%</div> <div>11%</div> </div>
21	1Z	206	<div> <div>67%</div> <div>8%</div> <div>25%</div> </div>
21	2Z	206	<div> <div>5%</div> <div>66%</div> <div>12%</div> <div>22%</div> </div>
22	10	85	<div> <div>12%</div> <div>93%</div> </div>
22	20	85	<div> <div>45%</div> <div>93%</div> <div>5%</div> </div>
23	11	98	<div> <div>4%</div> <div>95%</div> </div>
23	21	98	<div> <div>16%</div> <div>93%</div> <div>6%</div> </div>
24	12	72	<div> <div>88%</div> <div>10%</div> </div>
24	22	72	<div> <div>%</div> <div>89%</div> <div>8%</div> </div>
25	13	60	<div> <div>85%</div> <div>13%</div> </div>
25	23	60	<div> <div>12%</div> <div>90%</div> <div>8%</div> </div>
26	14	71	<div> <div>3%</div> <div>79%</div> <div>17%</div> </div>
26	24	71	<div> <div>10%</div> <div>85%</div> <div>13%</div> </div>
27	15	60	<div> <div>2%</div> <div>90%</div> <div>8%</div> </div>
27	25	60	<div> <div>8%</div> <div>92%</div> <div>7%</div> </div>
28	16	54	<div> <div>83%</div> <div>15%</div> </div>
28	26	54	<div> <div>7%</div> <div>89%</div> <div>9%</div> </div>

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Mol	Chain	Length	Quality of chain
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	
40	2i	128	
41	1j	105	

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Mol	Chain	Length	Quality of chain
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	
53	1v	24	
53	2v	24	

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Mol	Chain	Length	Quality of chain
54	1x	77	
54	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
55	MG	18	105	-	-	-	X
55	MG	1A	3120	-	-	-	X
55	MG	1A	3303	-	-	-	X
55	MG	1A	3347	-	-	-	X
55	MG	1A	3369	-	-	-	X
55	MG	1A	3450	-	-	-	X
55	MG	1A	4061	-	-	-	X
55	MG	1B	229	-	-	-	X
55	MG	1a	1643	-	-	-	X
55	MG	1n	102	-	-	-	X
55	MG	2A	3191	-	-	-	X
55	MG	2A	3192	-	-	-	X
55	MG	2A	3199	-	-	-	X
55	MG	2A	3200	-	-	-	X
55	MG	2A	3201	-	-	-	X
55	MG	2A	3222	-	-	-	X
55	MG	2A	3232	-	-	-	X
55	MG	2A	3289	-	-	-	X
55	MG	2A	3323	-	-	-	X
55	MG	2A	3369	-	-	-	X
55	MG	2A	3371	-	-	-	X
55	MG	2A	3457	-	-	-	X
55	MG	2A	3498	-	-	-	X
55	MG	2A	3653	-	-	-	X
55	MG	2A	3741	-	-	-	X
55	MG	2T	201	-	-	-	X
55	MG	2U	201	-	-	-	X
55	MG	2a	3021	-	-	-	X
55	MG	2x	101	-	-	-	X

## 2 Entry composition [i](#)

There are 59 unique types of molecules in this entry. The entry contains 292670 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	122	Total	C	N	O	S	0	0	0
			951	587	197	165	2			
44	2m	121	Total	C	N	O	S	0	0	0
			943	581	196	164	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	10	Total	C	N	O	P	0	0	0
			213	96	39	68	10			
53	2v	6	Total	C	N	O	P	0	0	0
			113	49	22	36	6			

- Molecule 54 is a RNA chain called P-site tRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
54	1x	76	Total	C	N	O	P	S	0	0
			1625	725	294	529	76	1		
54	2x	76	Total	C	N	O	P	S	0	0
			1625	725	294	529	76	1		

- Molecule 55 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
55	2E	9	Total	Mg	0	0
			9	9		
55	17	4	Total	Mg	0	0
			4	4		
55	2d	2	Total	Mg	0	0
			2	2		
55	1T	3	Total	Mg	0	0
			3	3		
55	1N	4	Total	Mg	0	0
			4	4		
55	20	1	Total	Mg	0	0
			1	1		
55	18	6	Total	Mg	0	0
			6	6		
55	2W	2	Total	Mg	0	0
			2	2		
55	1Y	4	Total	Mg	0	0
			4	4		
55	13	3	Total	Mg	0	0
			3	3		
55	1f	2	Total	Mg	0	0
			2	2		
55	1P	3	Total	Mg	0	0
			3	3		
55	2B	19	Total	Mg	0	0
			19	19		
55	2a	209	Total	Mg	0	0
			209	209		

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
55	1E	11	Total Mg 11 11	0	0
55	1b	1	Total Mg 1 1	0	0
55	2l	3	Total Mg 3 3	0	0
55	2F	6	Total Mg 6 6	0	0
55	16	1	Total Mg 1 1	0	0
55	28	3	Total Mg 3 3	0	0
55	2e	1	Total Mg 1 1	0	0
55	1W	5	Total Mg 5 5	0	0
55	1A	1117	Total Mg 1117 1117	0	0
55	1t	1	Total Mg 1 1	0	0
55	1n	2	Total Mg 2 2	0	0
55	2P	2	Total Mg 2 2	0	0
55	1X	6	Total Mg 6 6	0	0
55	12	2	Total Mg 2 2	0	0
55	2p	1	Total Mg 1 1	0	0
55	2i	1	Total Mg 1 1	0	0
55	1S	1	Total Mg 1 1	0	0
55	25	2	Total Mg 2 2	0	0
55	2T	3	Total Mg 3 3	0	0
55	1D	13	Total Mg 13 13	0	0
55	2N	2	Total Mg 2 2	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
55	1e	2	Total Mg 2 2	0	0
55	2G	1	Total Mg 1 1	0	0
55	2f	2	Total Mg 2 2	0	0
55	1V	4	Total Mg 4 4	0	0
55	2X	2	Total Mg 2 2	0	0
55	1a	234	Total Mg 234 234	0	0
55	2Q	4	Total Mg 4 4	0	0
55	15	5	Total Mg 5 5	0	0
55	1x	13	Total Mg 13 13	0	0
55	2j	2	Total Mg 2 2	0	0
55	1R	2	Total Mg 2 2	0	0
55	26	1	Total Mg 1 1	0	0
55	2U	2	Total Mg 2 2	0	0
55	1G	4	Total Mg 4 4	0	0
55	2O	2	Total Mg 2 2	0	0
55	11	4	Total Mg 4 4	0	0
55	2r	1	Total Mg 1 1	0	0
55	2g	1	Total Mg 1 1	0	0
55	1v	2	Total Mg 2 2	0	0
55	2x	5	Total Mg 5 5	0	0
55	2R	2	Total Mg 2 2	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
55	1Z	2	Total 2	Mg 2	0	0
55	2D	3	Total 3	Mg 3	0	0
55	2q	1	Total 1	Mg 1	0	0
55	1U	7	Total 7	Mg 7	0	0
55	1O	4	Total 4	Mg 4	0	0
55	27	1	Total 1	Mg 1	0	0
55	19	1	Total 1	Mg 1	0	0
55	1l	4	Total 4	Mg 4	0	0
55	2V	3	Total 3	Mg 3	0	0
55	1F	11	Total 11	Mg 11	0	0
55	10	5	Total 5	Mg 5	0	0
55	2t	1	Total 1	Mg 1	0	0
55	1Q	7	Total 7	Mg 7	0	0
55	2A	862	Total 862	Mg 862	0	0
55	23	1	Total 1	Mg 1	0	0
55	2Z	1	Total 1	Mg 1	0	0
55	1B	35	Total 35	Mg 35	0	0

- Molecule 56 is ZINC ION (three-letter code: ZN) (formula: Zn).

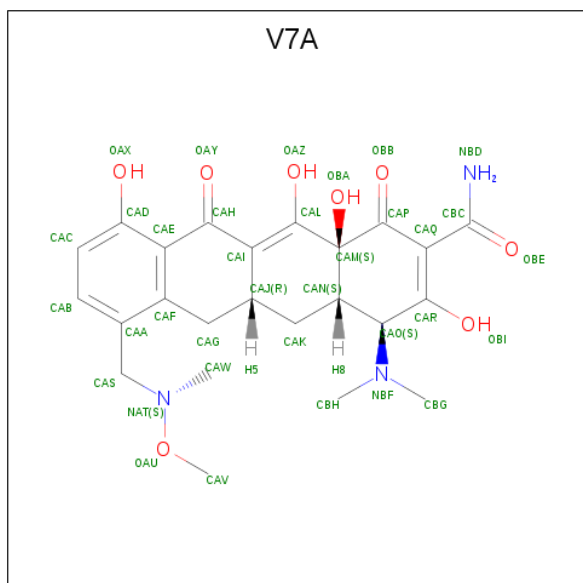
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
56	1Y	1	Total 1	Zn 1	0	0
56	14	1	Total 1	Zn 1	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
56	1n	1	Total	Zn	0	0
			1	1		
56	15	1	Total	Zn	0	0
			1	1		
56	29	1	Total	Zn	0	0
			1	1		
56	19	1	Total	Zn	0	0
			1	1		
56	26	1	Total	Zn	0	0
			1	1		
56	25	1	Total	Zn	0	0
			1	1		
56	24	1	Total	Zn	0	0
			1	1		
56	2n	1	Total	Zn	0	0
			1	1		
56	2Y	1	Total	Zn	0	0
			1	1		
56	16	1	Total	Zn	0	0
			1	1		

- Molecule 57 is Sarecycline (three-letter code: V7A) (formula:  $C_{24}H_{29}N_3O_8$ ).



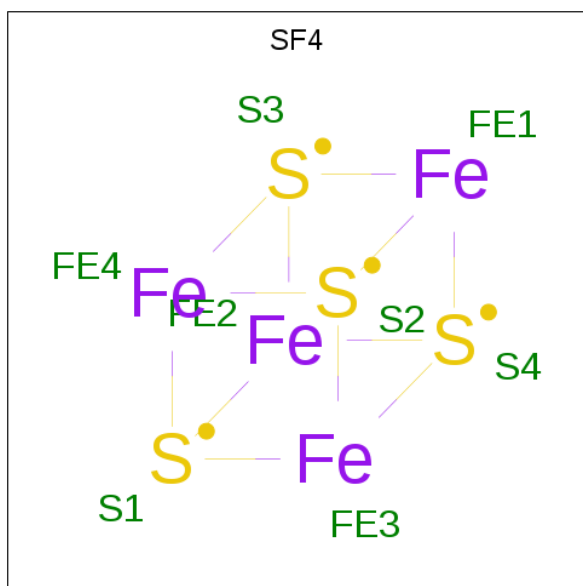
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
57	1a	1	Total	C	N	O	0	0
			35	24	3	8		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
57	2a	1	Total	C	N	O	0	0
			35	24	3	8		

- Molecule 58 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe<sub>4</sub>S<sub>4</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
58	1d	1	Total	Fe	S	0	0
			8	4	4		
58	2d	1	Total	Fe	S	0	0
			8	4	4		

- Molecule 59 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
59	1A	1716	Total	O	0	0
			1716	1716		
59	1B	47	Total	O	0	0
			47	47		
59	1D	21	Total	O	0	0
			21	21		
59	1E	25	Total	O	0	0
			25	25		
59	1F	13	Total	O	0	0
			13	13		
59	1G	2	Total	O	0	0
			2	2		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
59	1H	2	Total	O	0	0
			2	2		
59	1I	2	Total	O	0	0
			2	2		
59	1N	3	Total	O	0	0
			3	3		
59	1O	7	Total	O	0	0
			7	7		
59	1P	17	Total	O	0	0
			17	17		
59	1Q	6	Total	O	0	0
			6	6		
59	1R	9	Total	O	0	0
			9	9		
59	1S	1	Total	O	0	0
			1	1		
59	1T	8	Total	O	0	0
			8	8		
59	1U	13	Total	O	0	0
			13	13		
59	1V	9	Total	O	0	0
			9	9		
59	1W	8	Total	O	0	0
			8	8		
59	1X	6	Total	O	0	0
			6	6		
59	1Y	2	Total	O	0	0
			2	2		
59	10	8	Total	O	0	0
			8	8		
59	11	7	Total	O	0	0
			7	7		
59	12	1	Total	O	0	0
			1	1		
59	13	4	Total	O	0	0
			4	4		
59	15	7	Total	O	0	0
			7	7		
59	16	2	Total	O	0	0
			2	2		
59	17	6	Total	O	0	0
			6	6		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
59	18	9	Total 9	O 9	0	0
59	1a	294	Total 294	O 294	0	0
59	1b	1	Total 1	O 1	0	0
59	1d	3	Total 3	O 3	0	0
59	1e	1	Total 1	O 1	0	0
59	1i	1	Total 1	O 1	0	0
59	1j	1	Total 1	O 1	0	0
59	1l	4	Total 4	O 4	0	0
59	1m	1	Total 1	O 1	0	0
59	1o	1	Total 1	O 1	0	0
59	1q	2	Total 2	O 2	0	0
59	1v	4	Total 4	O 4	0	0
59	1x	17	Total 17	O 17	0	0
59	2A	867	Total 867	O 867	0	0
59	2B	14	Total 14	O 14	0	0
59	2D	16	Total 16	O 16	0	0
59	2E	8	Total 8	O 8	0	0
59	2F	13	Total 13	O 13	0	0
59	2I	1	Total 1	O 1	0	0
59	2N	1	Total 1	O 1	0	0
59	2O	1	Total 1	O 1	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
59	2P	4	Total 4	O 4	0	0
59	2Q	2	Total 2	O 2	0	0
59	2R	2	Total 2	O 2	0	0
59	2T	4	Total 4	O 4	0	0
59	2U	3	Total 3	O 3	0	0
59	2W	5	Total 5	O 5	0	0
59	2X	2	Total 2	O 2	0	0
59	2Z	1	Total 1	O 1	0	0
59	20	3	Total 3	O 3	0	0
59	21	8	Total 8	O 8	0	0
59	22	1	Total 1	O 1	0	0
59	25	1	Total 1	O 1	0	0
59	27	1	Total 1	O 1	0	0
59	28	3	Total 3	O 3	0	0
59	29	1	Total 1	O 1	0	0
59	2a	146	Total 146	O 146	0	0
59	2g	1	Total 1	O 1	0	0
59	2j	2	Total 2	O 2	0	0
59	2l	4	Total 4	O 4	0	0
59	2p	1	Total 1	O 1	0	0
59	2r	1	Total 1	O 1	0	0

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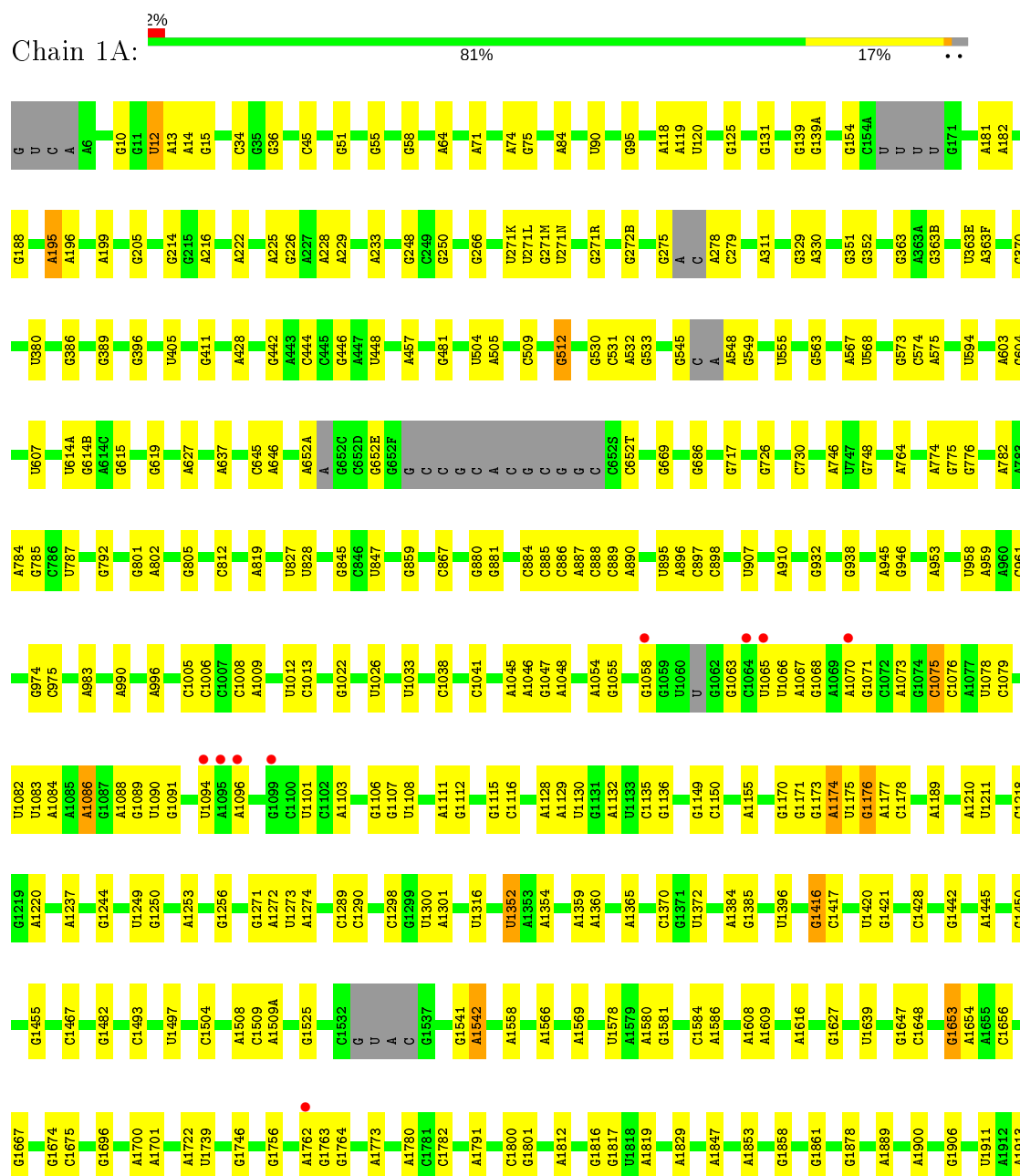
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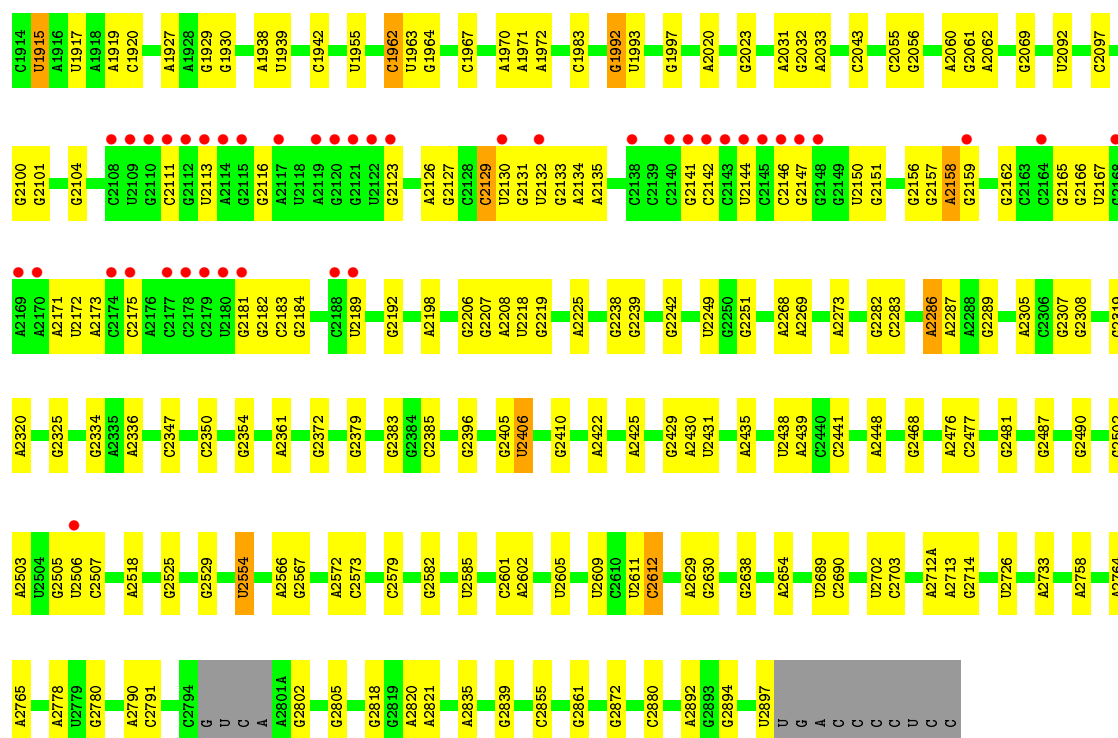
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
59	2t	1	Total	O	0	0
			1	1		
59	2v	1	Total	O	0	0
			1	1		
59	2x	6	Total	O	0	0
			6	6		

### 3 Residue-property plots

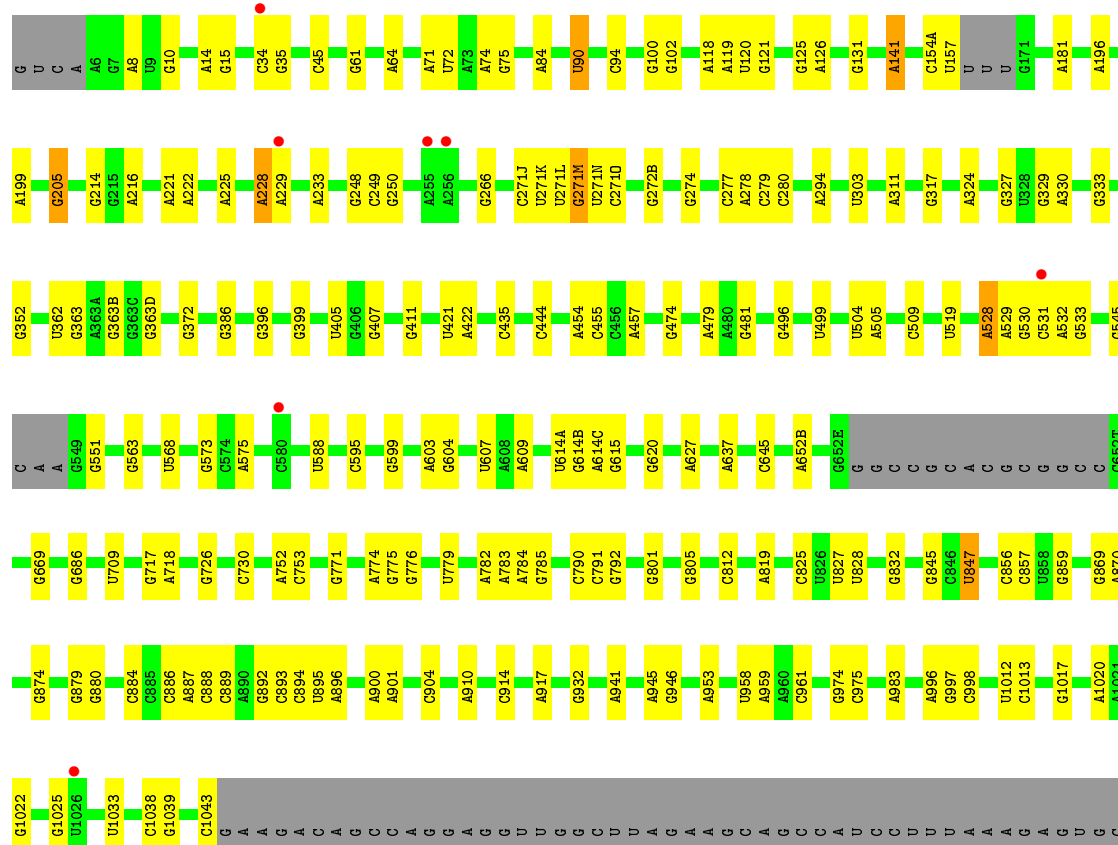
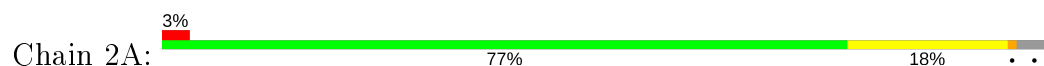
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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.

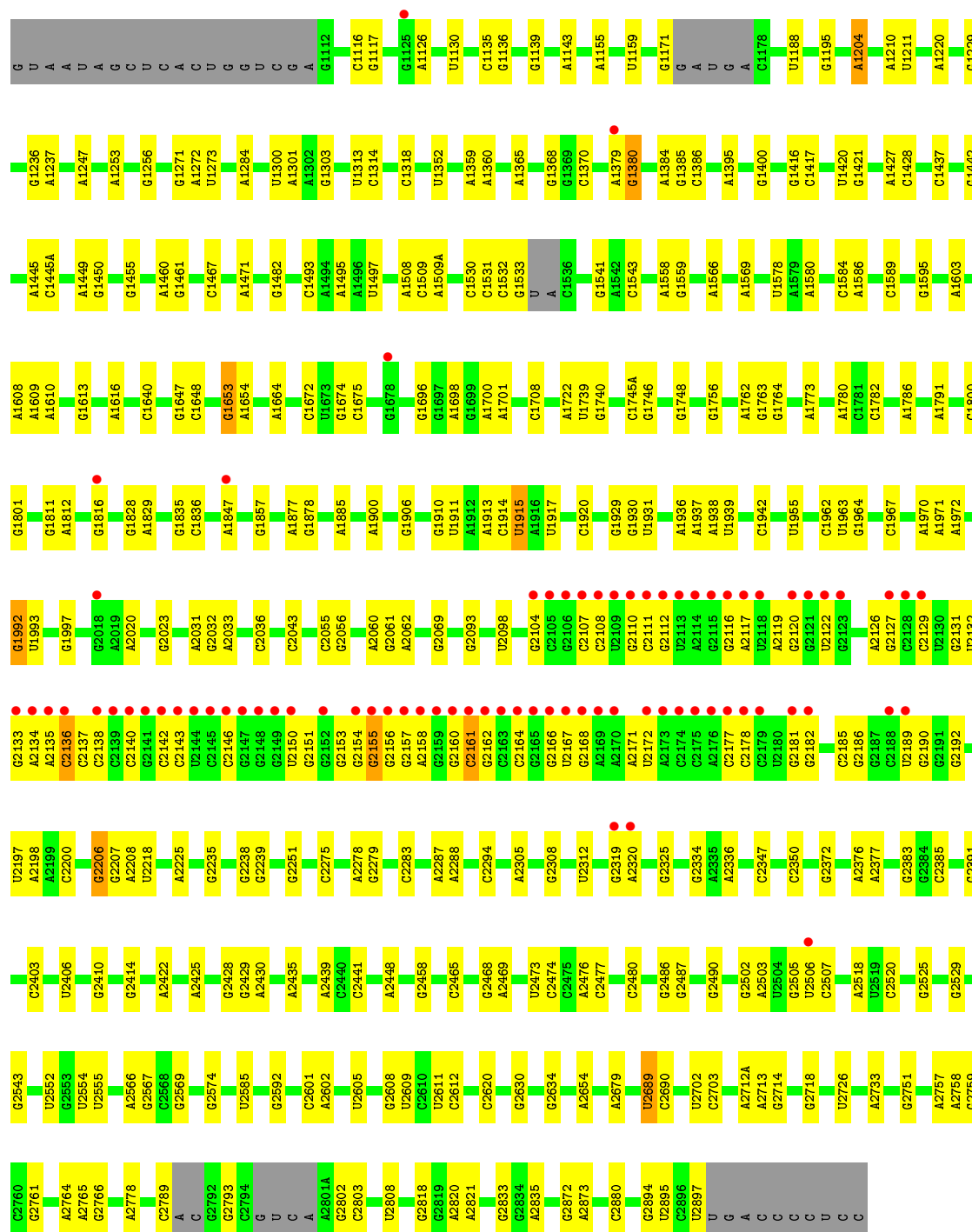
#### • Molecule 1: 23S Ribosomal RNA





• Molecule 1: 23S Ribosomal RNA



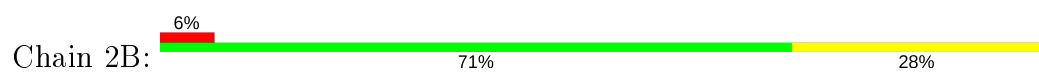


- Molecule 2: 5S Ribosomal RNA

Chain 1B:



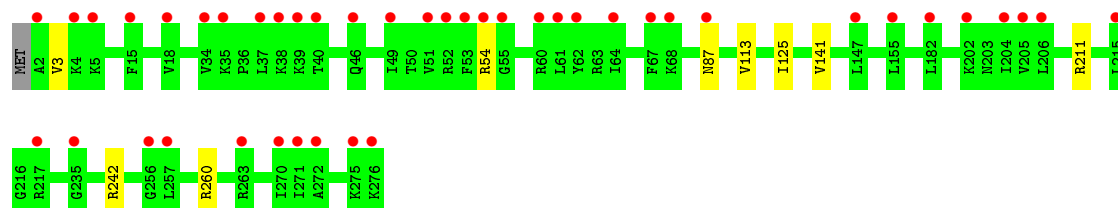
- Molecule 2: 5S Ribosomal RNA



- Molecule 3: 50S ribosomal protein L2



- Molecule 3: 50S ribosomal protein L2



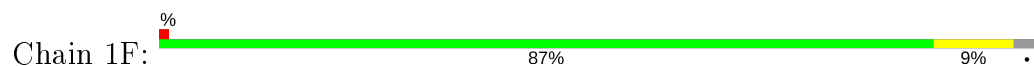
- Molecule 4: 50S ribosomal protein L3



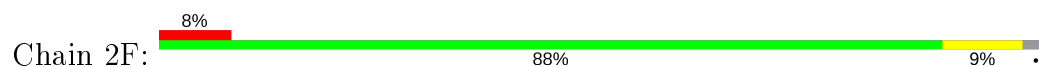
- Molecule 4: 50S ribosomal protein L3

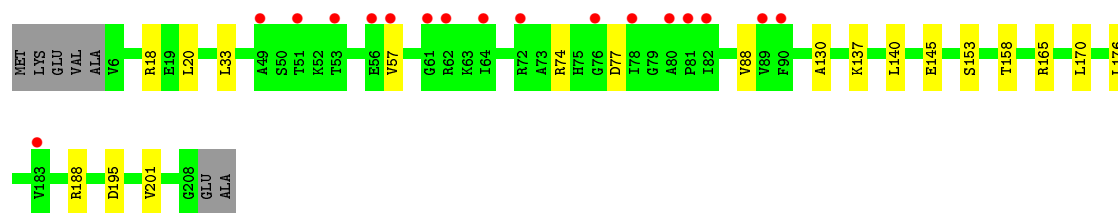


- Molecule 5: 50S ribosomal protein L4

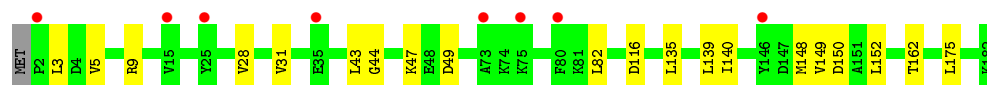
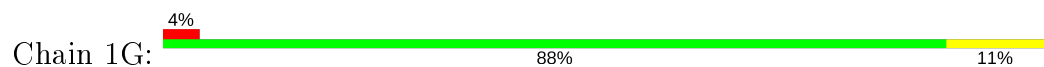


- Molecule 5: 50S ribosomal protein L4

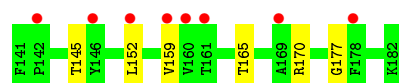
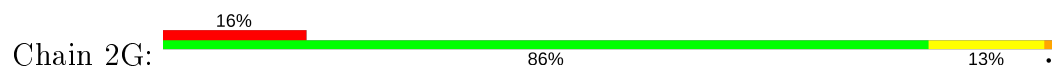




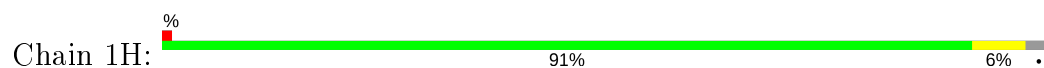
- Molecule 6: 50S ribosomal protein L5



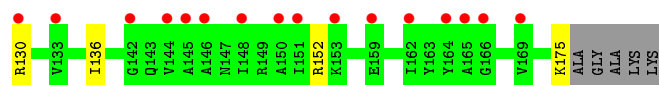
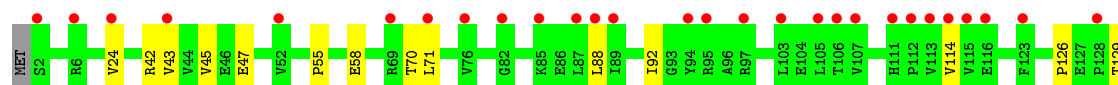
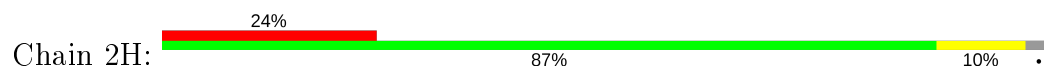
- Molecule 6: 50S ribosomal protein L5



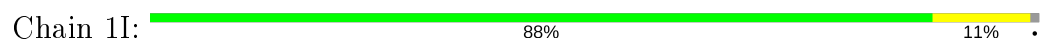
- Molecule 7: 50S ribosomal protein L6



- Molecule 7: 50S ribosomal protein L6

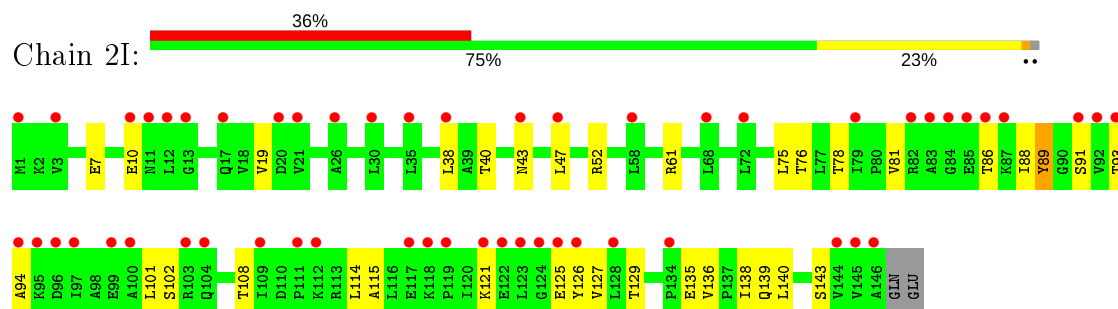


- Molecule 8: 50S ribosomal protein L9

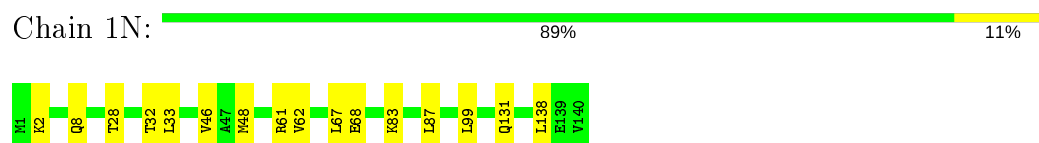




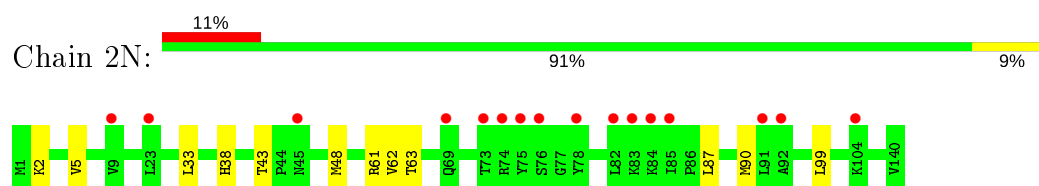
- Molecule 8: 50S ribosomal protein L9



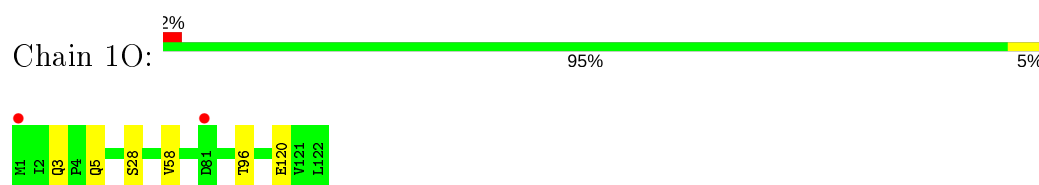
- Molecule 9: 50S ribosomal protein L13



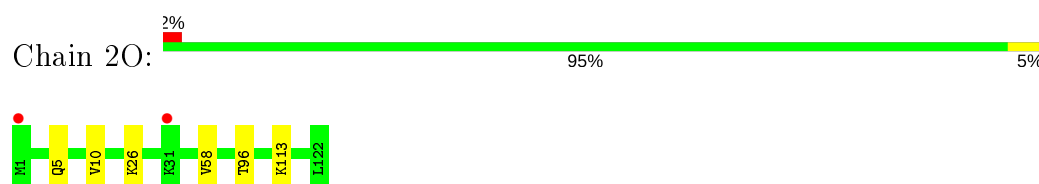
- Molecule 9: 50S ribosomal protein L13



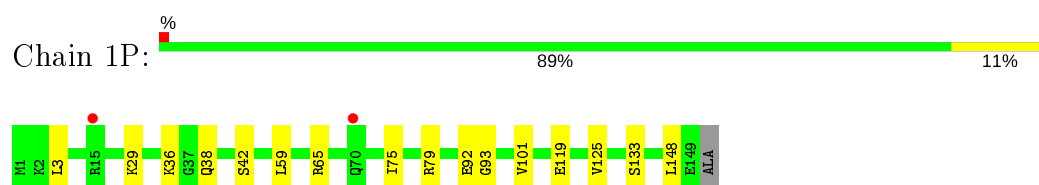
- Molecule 10: 50S ribosomal protein L14



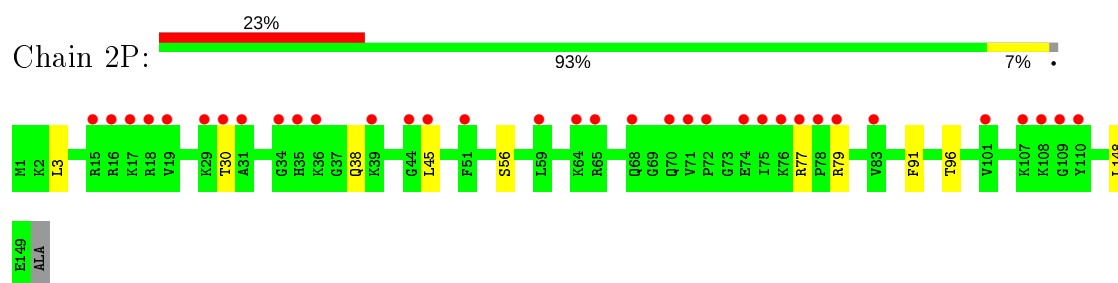
- Molecule 10: 50S ribosomal protein L14



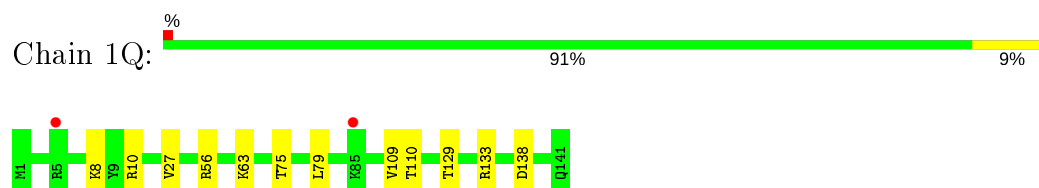
- Molecule 11: 50S ribosomal protein L15



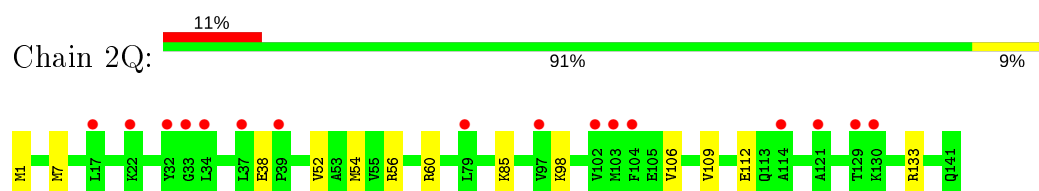
- Molecule 11: 50S ribosomal protein L15



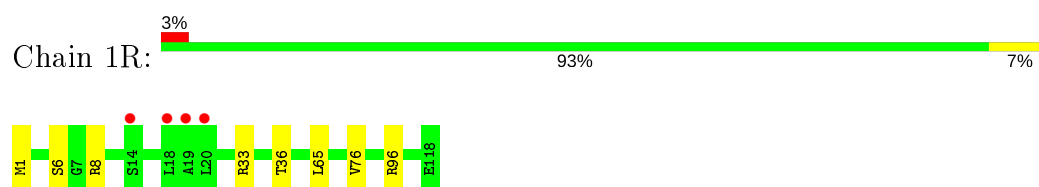
- Molecule 12: 50S ribosomal protein L16



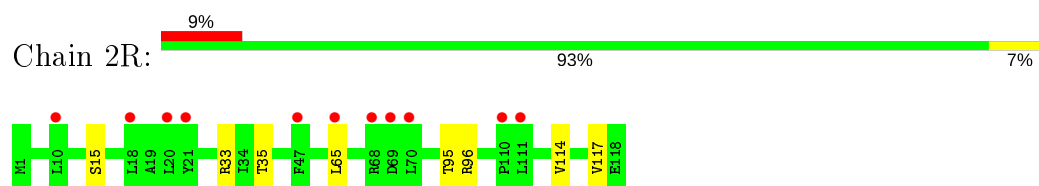
- Molecule 12: 50S ribosomal protein L16



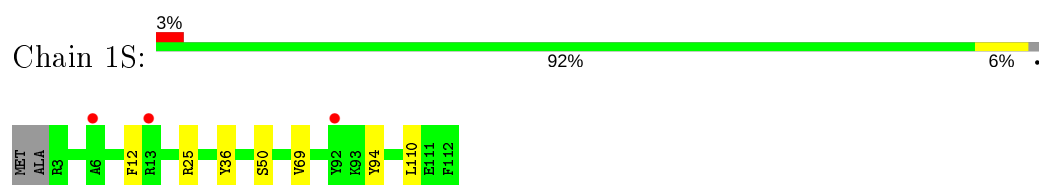
- Molecule 13: 50S ribosomal protein L17



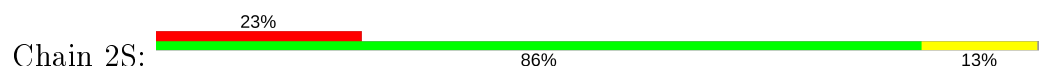
- Molecule 13: 50S ribosomal protein L17

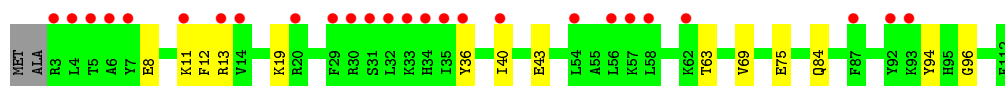


- Molecule 14: 50S ribosomal protein L18

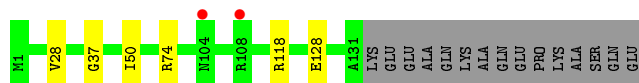
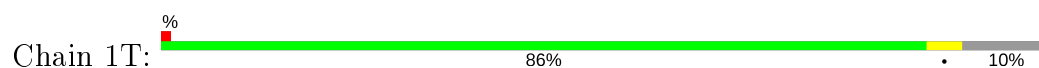


- Molecule 14: 50S ribosomal protein L18

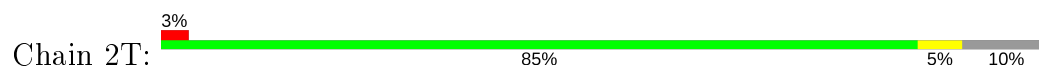




- Molecule 15: 50S ribosomal protein L19



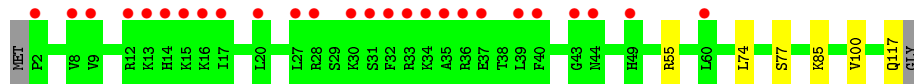
- Molecule 15: 50S ribosomal protein L19



- Molecule 16: 50S ribosomal protein L20



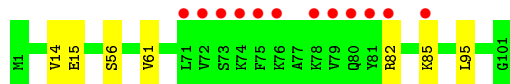
- Molecule 16: 50S ribosomal protein L20



- Molecule 17: 50S ribosomal protein L21

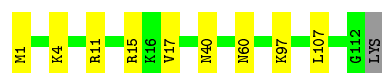


- Molecule 17: 50S ribosomal protein L21



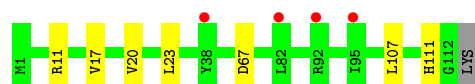
- Molecule 18: 50S ribosomal protein L22

Chain 1W:  91% 8%



- Molecule 18: 50S ribosomal protein L22

Chain 2W:  4% 93% 6%



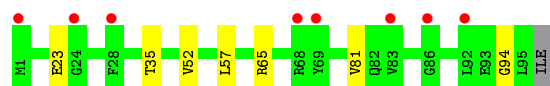
- Molecule 19: 50S ribosomal protein L23

Chain 1X:  95%



- Molecule 19: 50S ribosomal protein L23

Chain 2X:  8% 92% 7%




- Molecule 20: 50S ribosomal protein L24

Chain 1Y:  87% 10%



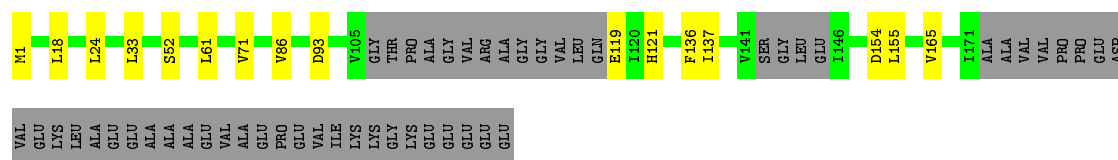
- Molecule 20: 50S ribosomal protein L24

Chain 2Y:  14% 86% 11%

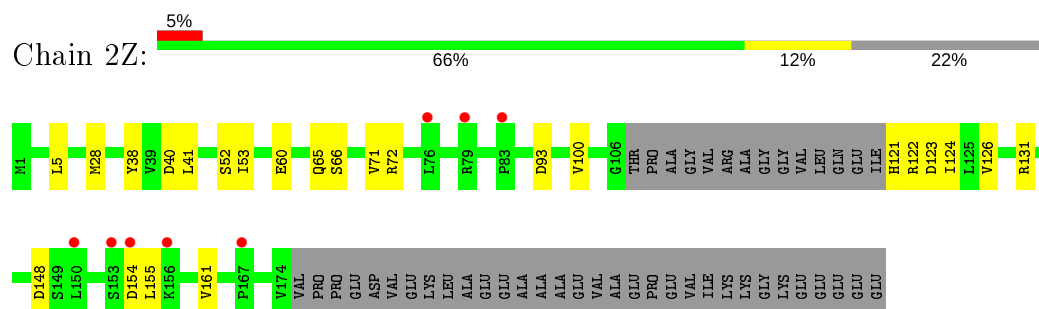


- Molecule 21: 50S ribosomal protein L25

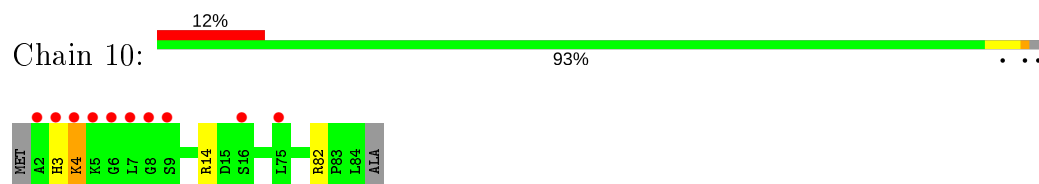
Chain 1Z:  67% 8% 25%



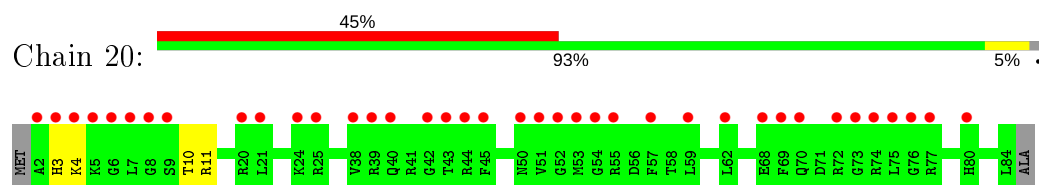
- Molecule 21: 50S ribosomal protein L25



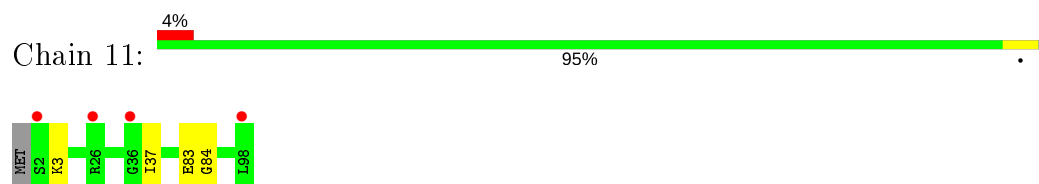
- Molecule 22: 50S ribosomal protein L27



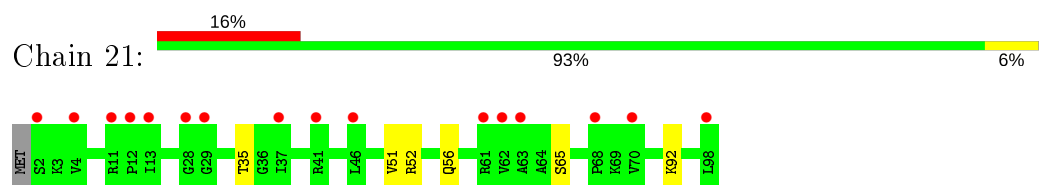
- Molecule 22: 50S ribosomal protein L27



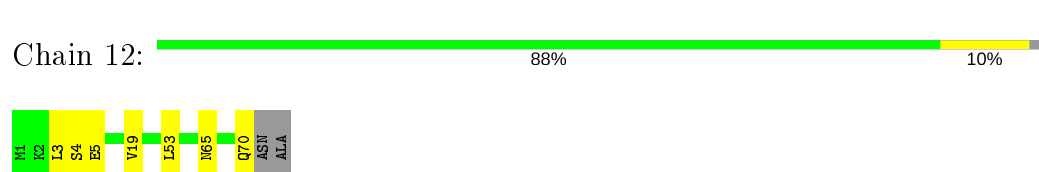
- Molecule 23: 50S ribosomal protein L28



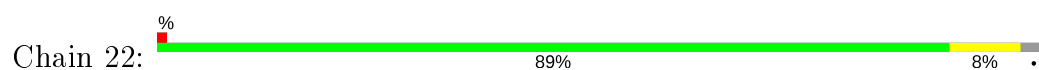
- Molecule 23: 50S ribosomal protein L28



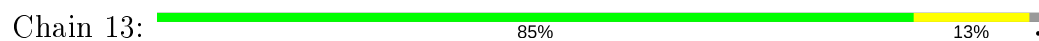
- Molecule 24: 50S ribosomal protein L29



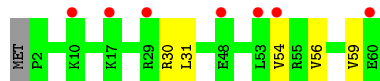
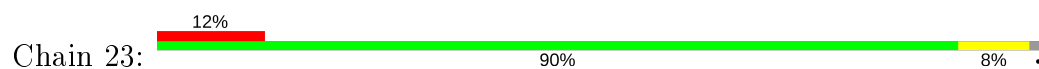
- Molecule 24: 50S ribosomal protein L29



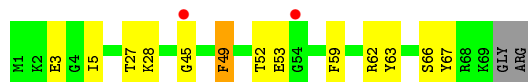
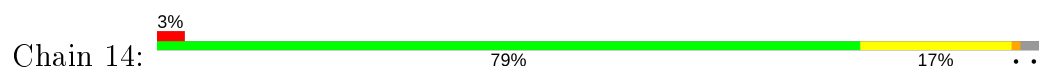
- Molecule 25: 50S ribosomal protein L30



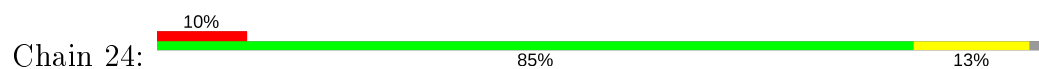
- Molecule 25: 50S ribosomal protein L30



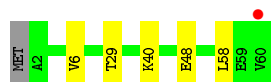
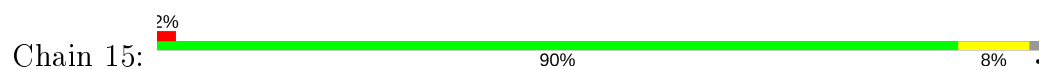
- Molecule 26: 50S ribosomal protein L31



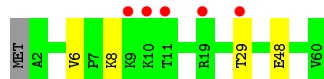
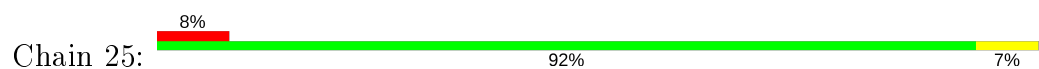
- Molecule 26: 50S ribosomal protein L31




- Molecule 27: 50S ribosomal protein L32



- Molecule 27: 50S ribosomal protein L32




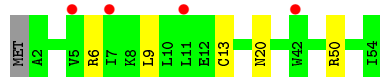
- Molecule 28: 50S ribosomal protein L33

Chain 16:  83% 15% .



- Molecule 28: 50S ribosomal protein L33

Chain 26:  7% 89% 9% .




- Molecule 29: 50S ribosomal protein L34

Chain 17:  10% 92% 6% .



- Molecule 29: 50S ribosomal protein L34

Chain 27:  14% 88% 10% .

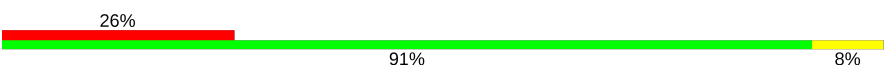


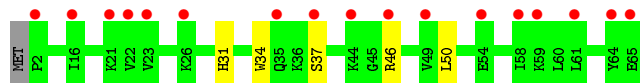
- Molecule 30: 50S ribosomal protein L35

Chain 18:  9% 92% 6% .



- Molecule 30: 50S ribosomal protein L35

Chain 28:  26% 91% 8% .

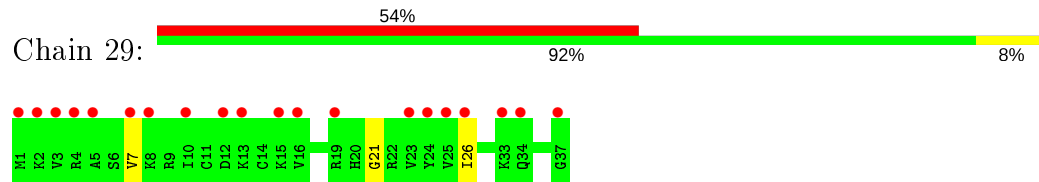


- Molecule 31: 50S ribosomal protein L36

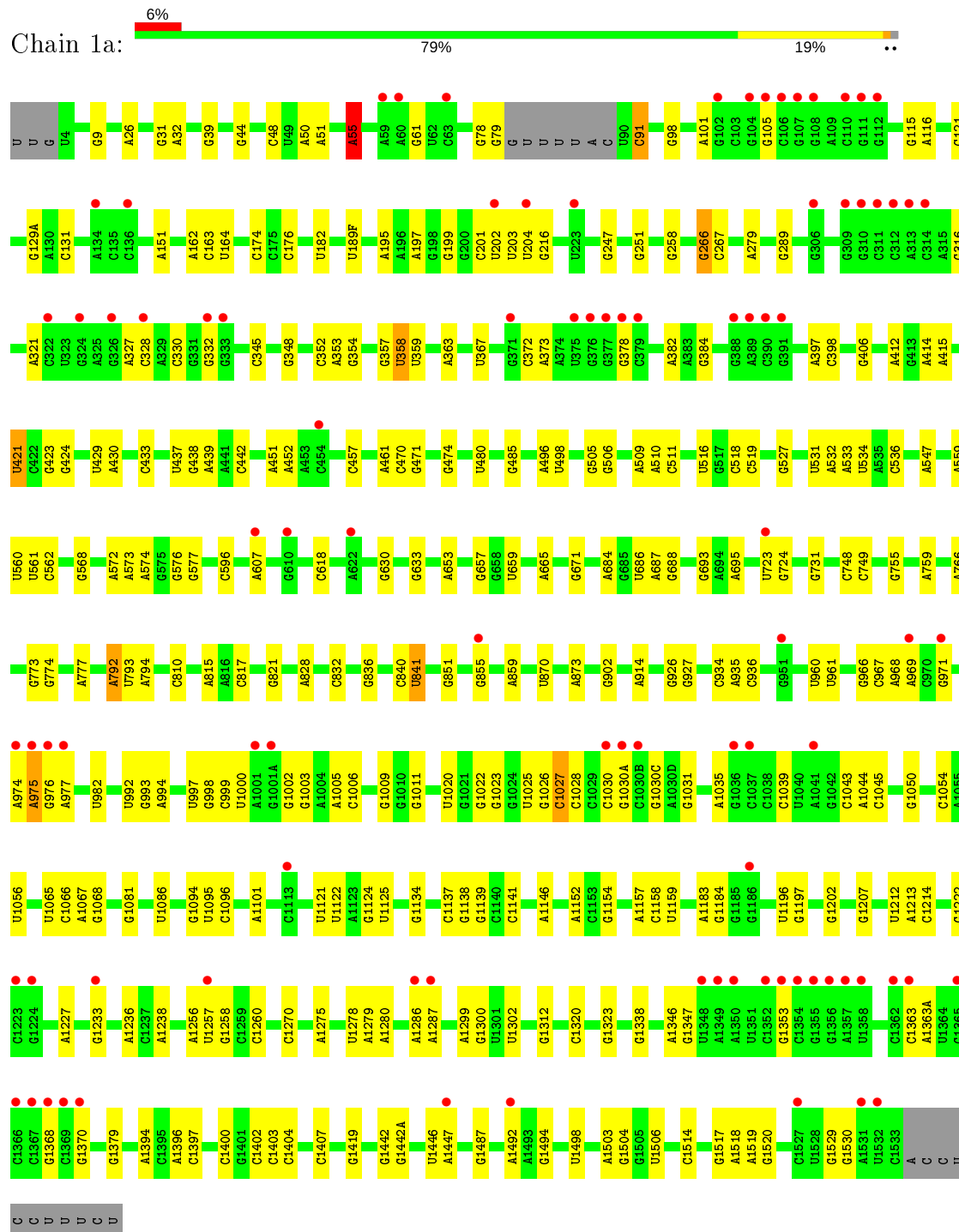
Chain 19:  97% .



• Molecule 31: 50S ribosomal protein L36

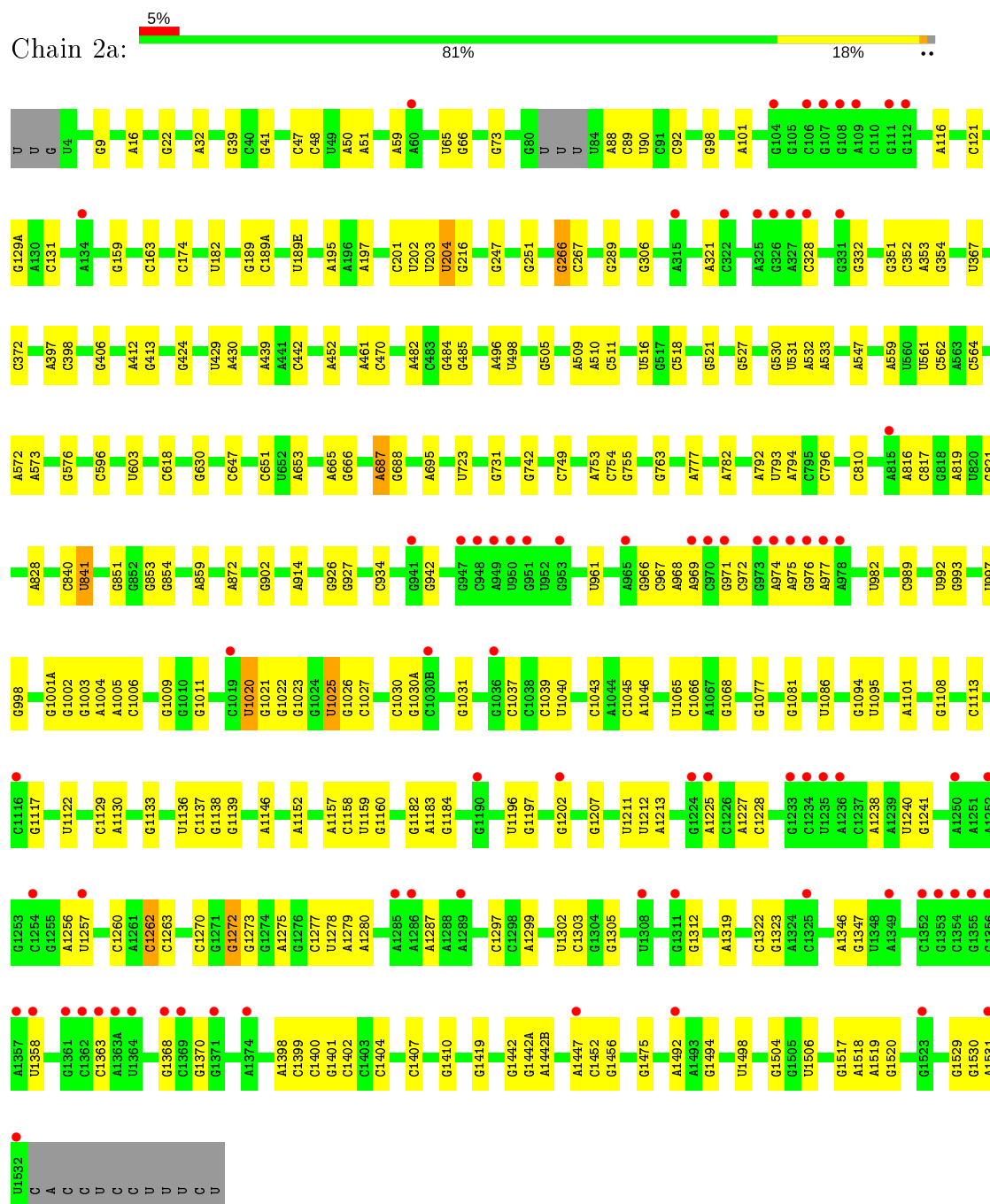


• Molecule 32: 16S Ribosomal RNA

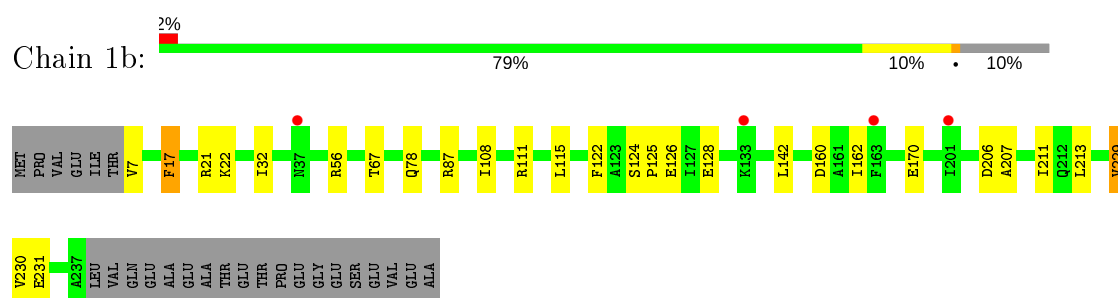




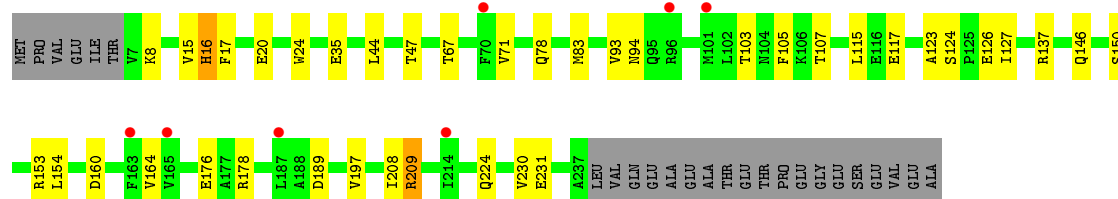
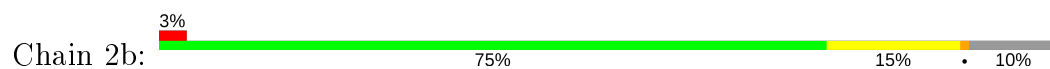
• Molecule 32: 16S Ribosomal RNA



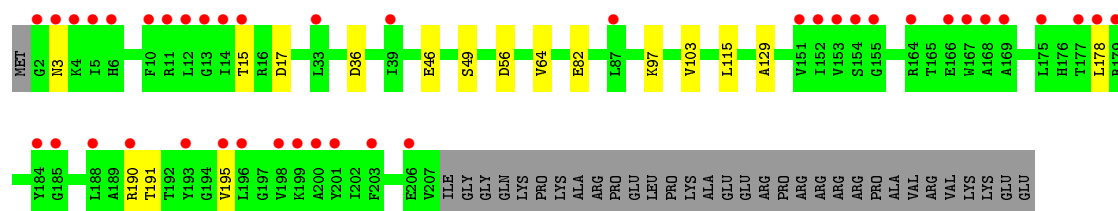
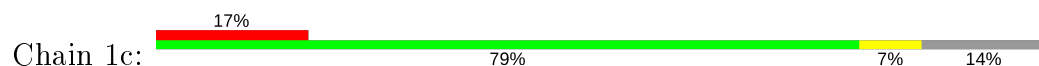
• Molecule 33: 30S ribosomal protein S2



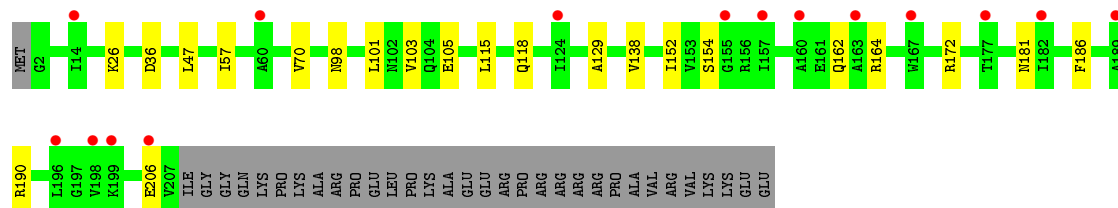
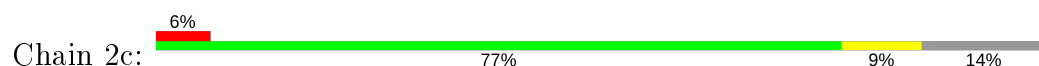
- Molecule 33: 30S ribosomal protein S2



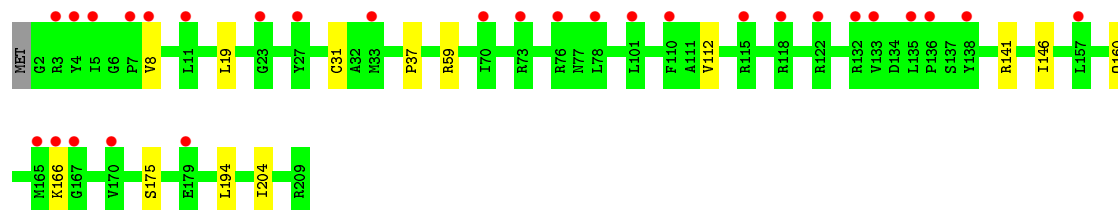
- Molecule 34: 30S ribosomal protein S3



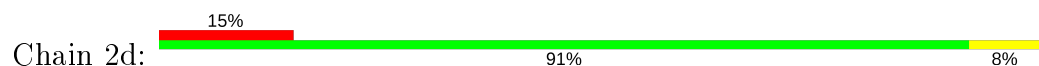
- Molecule 34: 30S ribosomal protein S3

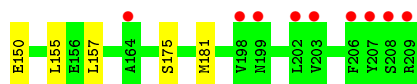


- Molecule 35: 30S ribosomal protein S4

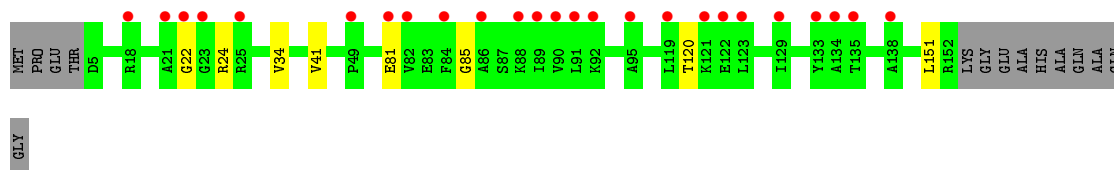
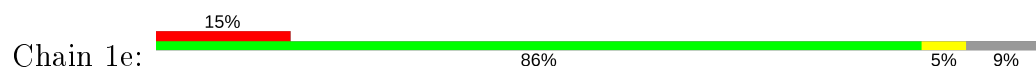


- Molecule 35: 30S ribosomal protein S4

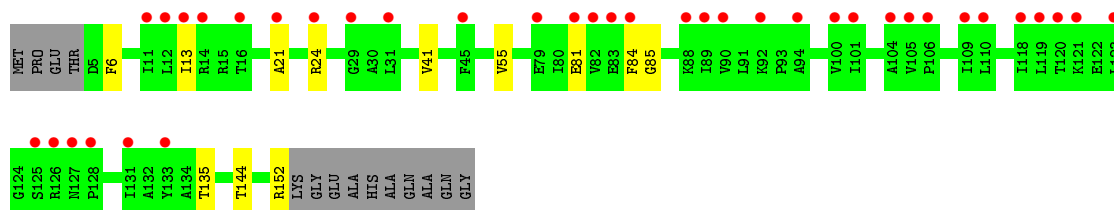
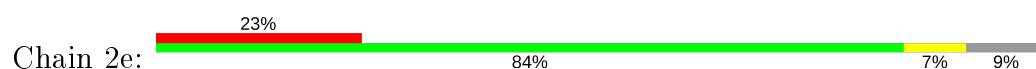




- Molecule 36: 30S ribosomal protein S5



- Molecule 36: 30S ribosomal protein S5



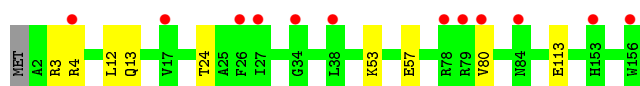
- Molecule 37: 30S ribosomal protein S6



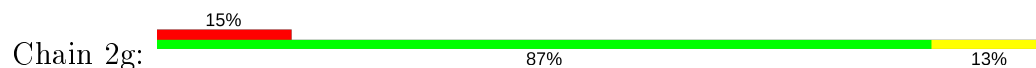
- Molecule 37: 30S ribosomal protein S6

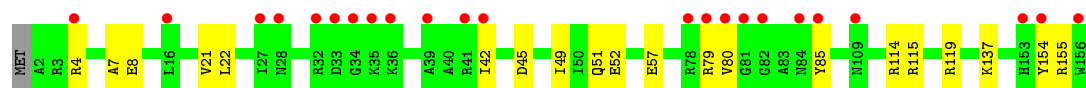


- Molecule 38: 30S ribosomal protein S7

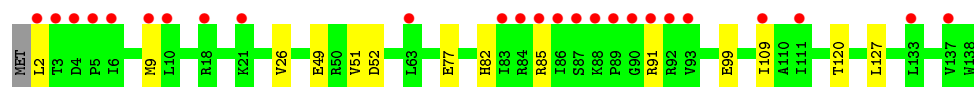
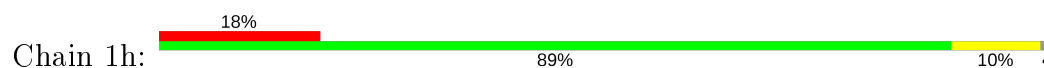


- Molecule 38: 30S ribosomal protein S7

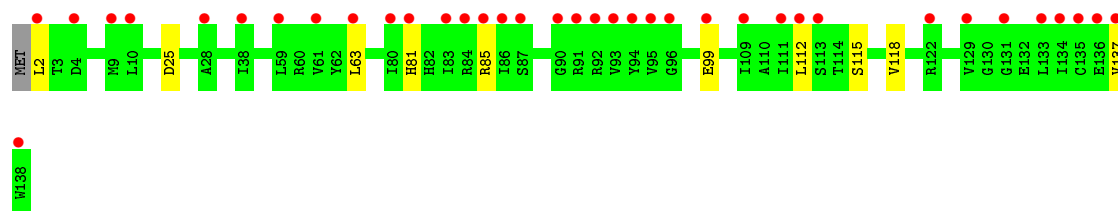
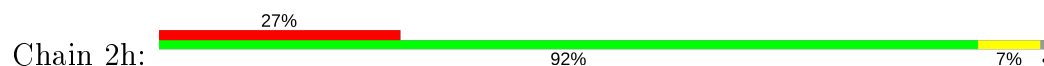




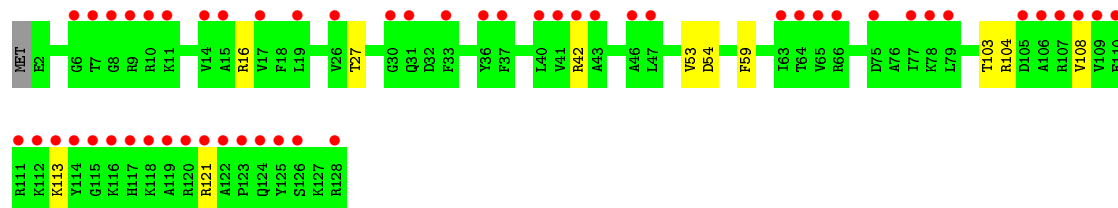
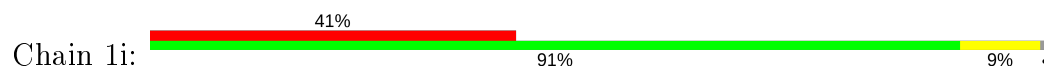
- Molecule 39: 30S ribosomal protein S8



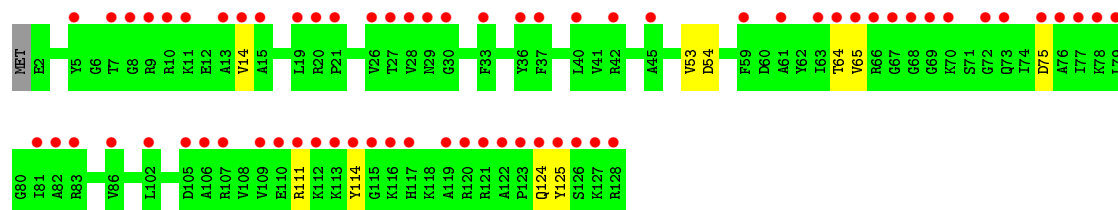
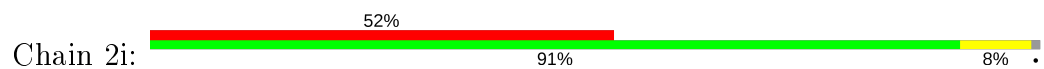
- Molecule 39: 30S ribosomal protein S8



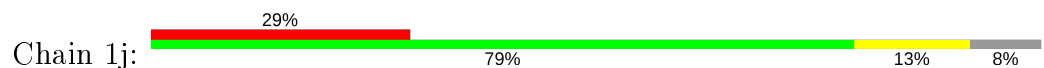
- Molecule 40: 30S ribosomal protein S9



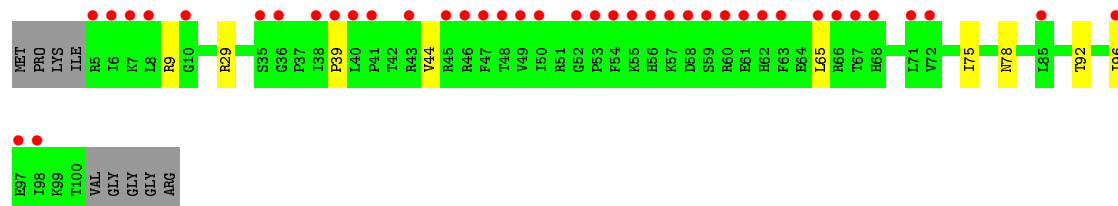
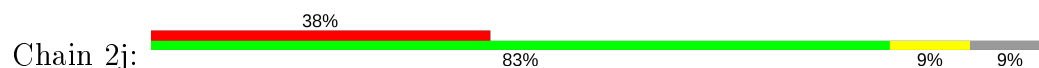
- Molecule 40: 30S ribosomal protein S9



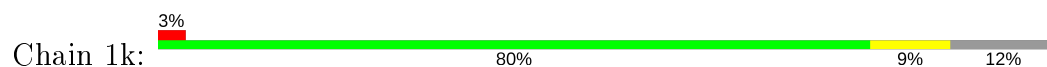
- Molecule 41: 30S ribosomal protein S10



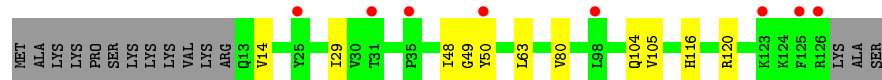
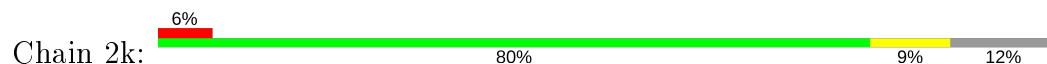
- Molecule 41: 30S ribosomal protein S10



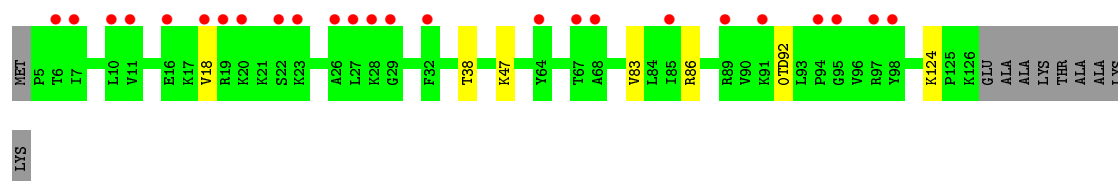
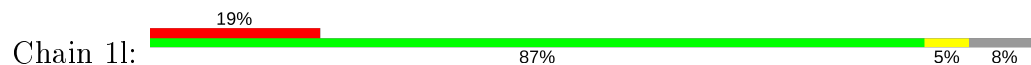
- Molecule 42: 30S ribosomal protein S11



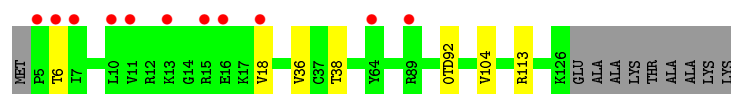
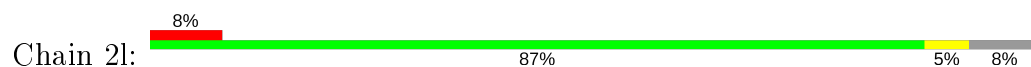
- Molecule 42: 30S ribosomal protein S11



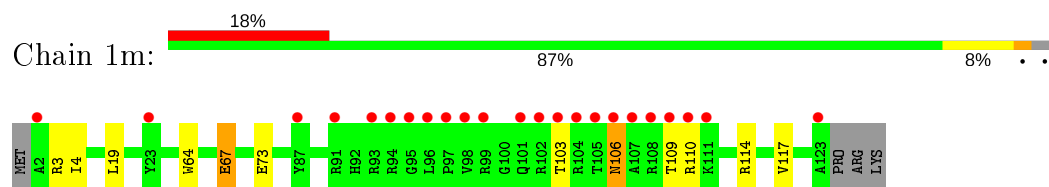
- Molecule 43: 30S ribosomal protein S12



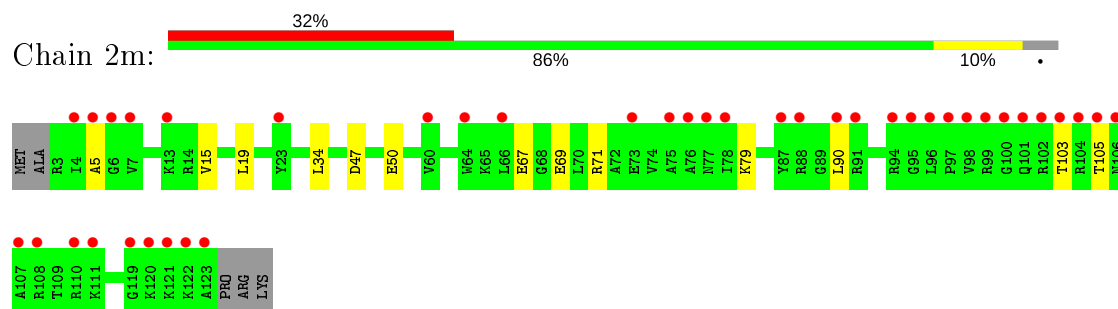
- Molecule 43: 30S ribosomal protein S12



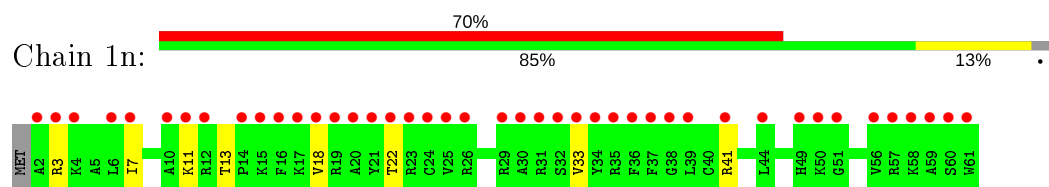
- Molecule 44: 30S ribosomal protein S13



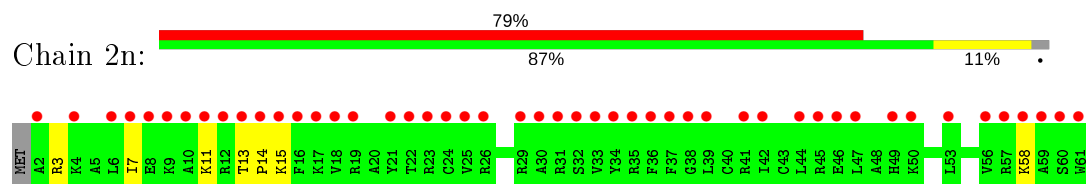
- Molecule 44: 30S ribosomal protein S13



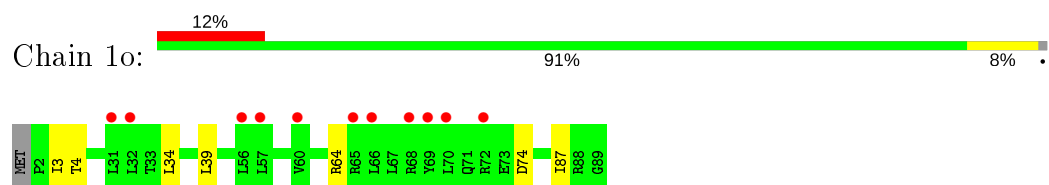
- Molecule 45: 30S ribosomal protein S14 type Z



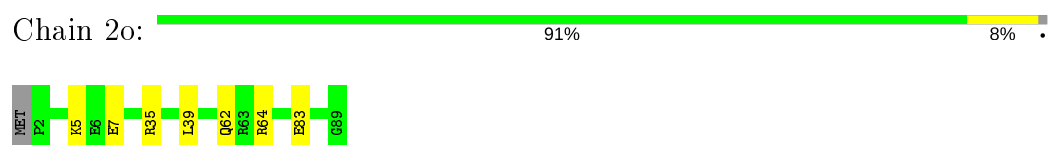
- Molecule 45: 30S ribosomal protein S14 type Z



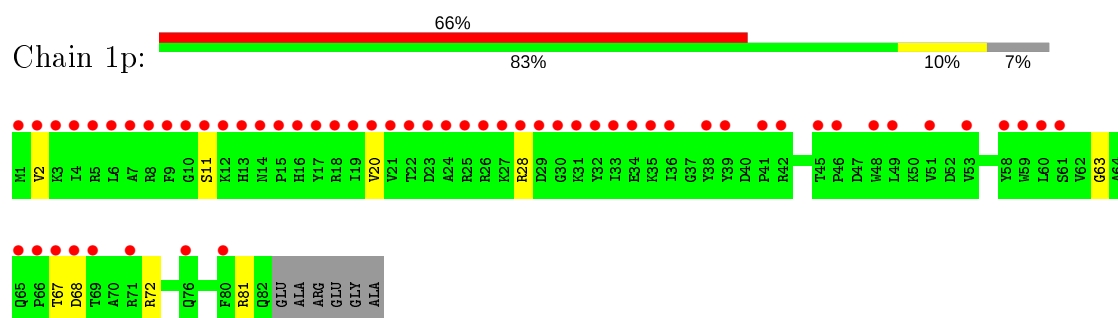
- Molecule 46: 30S ribosomal protein S15



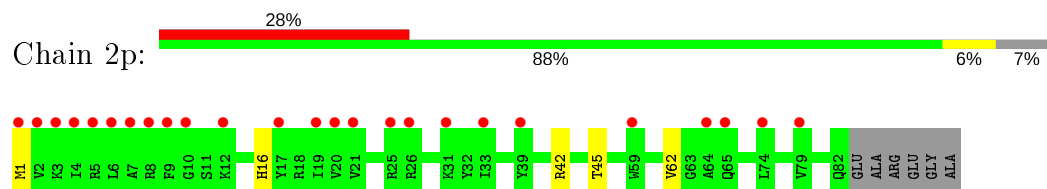
- Molecule 46: 30S ribosomal protein S15



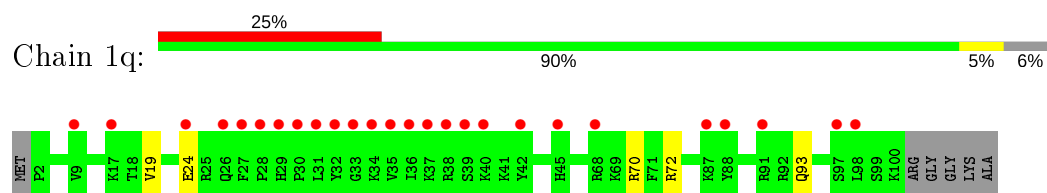
- Molecule 47: 30S ribosomal protein S16



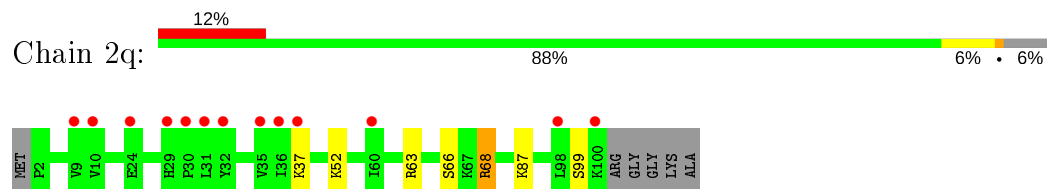
- Molecule 47: 30S ribosomal protein S16



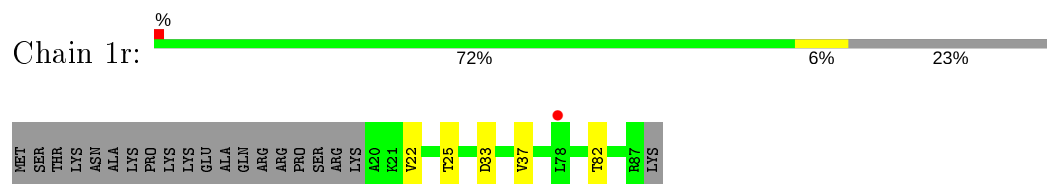
- Molecule 48: 30S ribosomal protein S17



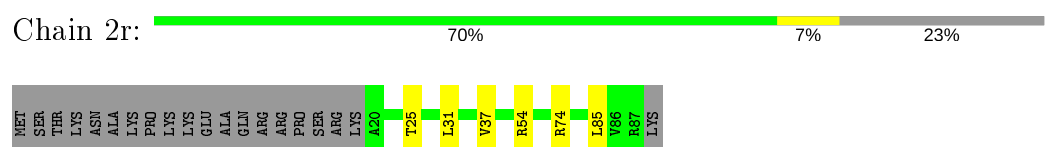
- Molecule 48: 30S ribosomal protein S17



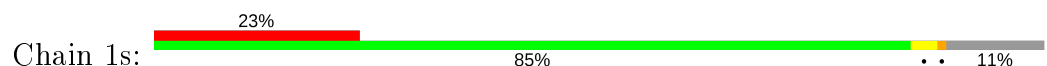
- Molecule 49: 30S ribosomal protein S18

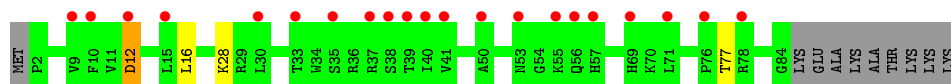


- Molecule 49: 30S ribosomal protein S18

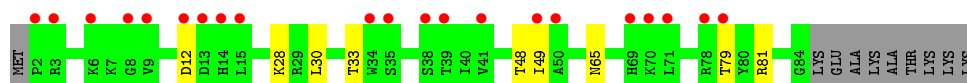
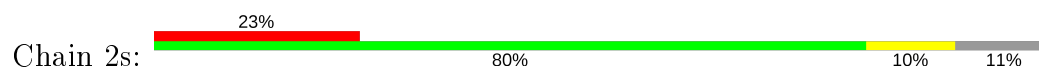


- Molecule 50: 30S ribosomal protein S19

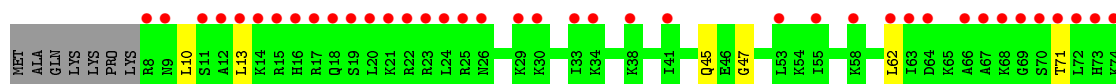
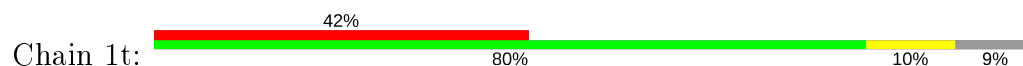




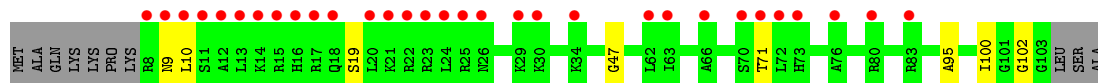
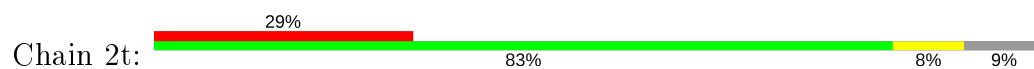
- Molecule 50: 30S ribosomal protein S19



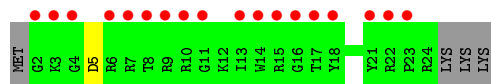
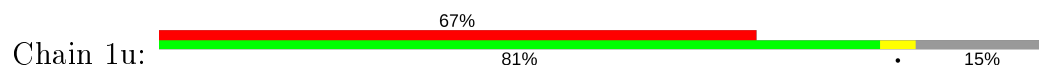
- Molecule 51: 30S ribosomal protein S20



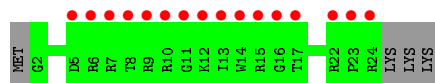
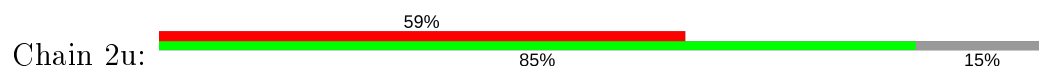
- Molecule 51: 30S ribosomal protein S20



- Molecule 52: 30S ribosomal protein Thx



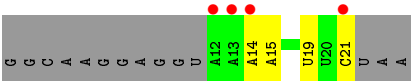
- Molecule 52: 30S ribosomal protein Thx



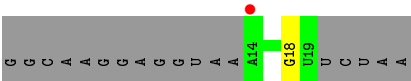
- Molecule 53: mRNA



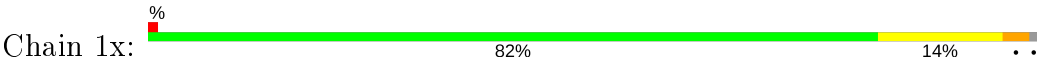




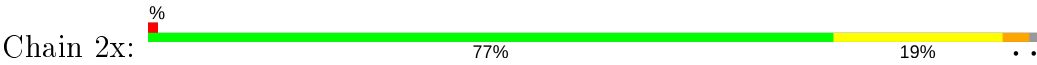
● Molecule 53: mRNA



● Molecule 54: P-site tRNA



● Molecule 54: P-site tRNA



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	208.33Å 447.60Å 612.33Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	75.46 – 2.80 210.20 – 2.80	Depositor EDS
% Data completeness (in resolution range)	98.3 (75.46-2.80) 98.4 (210.20-2.80)	Depositor EDS
$R_{merge}$	0.21	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.21 (at 2.82Å)	Xtriage
Refinement program	PHENIX 1.8.2	Depositor
R, $R_{free}$	0.225 , 0.276 0.225 , 0.276	Depositor DCC
$R_{free}$ test set	68487 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	54.7	Xtriage
Anisotropy	0.309	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.29 , 54.2	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.41$ , $\langle L^2 \rangle = 0.24$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.85	EDS
Total number of atoms	292670	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	59.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.59% 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, ZN, M2G, OMG, MA6, SF4, 0TD, MG, 2MA, 2MU, 2MG, 5MC, UR3, 4OC, 4SU, 7MG, V7A, PSU

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	0.53	0/69009	0.95	52/107712 (0.0%)
1	2A	0.41	0/67293	0.87	30/105034 (0.0%)
2	1B	0.47	1/2882 (0.0%)	0.87	0/4494
2	2B	0.40	1/2879 (0.0%)	0.89	4/4487 (0.1%)
3	1D	0.35	0/2186	0.54	0/2944
3	2D	0.33	0/2186	0.51	0/2944
4	1E	0.35	0/1592	0.54	0/2149
4	2E	0.32	0/1592	0.51	0/2149
5	1F	0.35	0/1619	0.51	0/2193
5	2F	0.31	0/1615	0.50	0/2188
6	1G	0.30	0/1448	0.51	0/1957
6	2G	0.28	0/1453	0.48	0/1963
7	1H	0.32	0/1356	0.50	0/1834
7	2H	0.28	0/1356	0.46	0/1834
8	1I	0.29	0/1112	0.49	0/1514
8	2I	4.40	4/1079 (0.4%)	1.10	6/1475 (0.4%)
9	1N	0.34	0/1144	0.50	0/1543
9	2N	0.27	0/1144	0.46	0/1543
10	1O	0.36	0/943	0.54	0/1269
10	2O	0.33	0/943	0.52	0/1269
11	1P	0.35	0/1152	0.57	0/1533
11	2P	0.31	0/1152	0.52	0/1533
12	1Q	0.36	0/1143	0.53	0/1527
12	2Q	0.30	0/1143	0.48	0/1527
13	1R	0.32	0/982	0.52	0/1312
13	2R	0.27	0/982	0.48	0/1312
14	1S	0.31	0/883	0.50	0/1176
14	2S	0.29	0/880	0.49	0/1172
15	1T	0.32	0/1105	0.51	0/1477
15	2T	0.32	0/1097	0.49	0/1468
16	1U	0.40	0/977	0.50	0/1301

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
16	2U	0.29	0/977	0.47	0/1301
17	1V	0.33	0/782	0.57	0/1049
17	2V	0.30	0/782	0.51	0/1049
18	1W	0.36	0/897	0.50	0/1205
18	2W	0.31	0/897	0.48	0/1205
19	1X	0.35	0/764	0.56	0/1025
19	2X	0.29	0/764	0.51	0/1025
20	1Y	0.35	0/819	0.52	0/1095
20	2Y	0.30	0/819	0.50	0/1095
21	1Z	0.31	0/1267	0.52	0/1717
21	2Z	0.29	0/1299	0.49	0/1763
22	10	0.37	0/662	0.55	0/881
22	20	0.32	0/662	0.49	0/881
23	11	0.33	0/762	0.52	0/1014
23	21	0.32	0/762	0.52	0/1014
24	12	0.31	0/590	0.47	0/781
24	22	0.29	0/590	0.40	0/781
25	13	0.32	0/474	0.52	0/635
25	23	0.29	0/469	0.46	0/630
26	14	0.33	0/565	0.57	0/761
26	24	0.32	0/545	0.53	0/737
27	15	0.35	0/469	0.56	0/635
27	25	0.31	0/469	0.47	0/635
28	16	0.37	0/460	0.53	0/613
28	26	0.31	0/456	0.48	0/608
29	17	0.35	0/426	0.54	0/561
29	27	0.30	0/426	0.47	0/561
30	18	0.33	0/525	0.55	0/691
30	28	0.31	0/525	0.49	0/691
31	19	0.32	0/310	0.53	0/407
31	29	0.28	0/310	0.52	0/407
32	1a	0.89	10/35795 (0.0%)	0.90	33/55864 (0.1%)
32	2a	0.35	2/35886 (0.0%)	0.88	33/56005 (0.1%)
33	1b	0.30	0/1881	0.50	0/2542
33	2b	0.30	0/1860	0.48	0/2518
34	1c	0.28	0/1572	0.45	0/2126
34	2c	0.29	0/1566	0.50	0/2119
35	1d	0.29	0/1685	0.47	0/2262
35	2d	0.29	0/1704	0.45	0/2284
36	1e	0.30	0/1145	0.50	0/1543
36	2e	0.30	0/1149	0.50	0/1548
37	1f	0.29	0/823	0.49	0/1115
37	2f	0.28	0/829	0.47	0/1123

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
38	1g	0.27	0/1250	0.44	0/1679
38	2g	0.27	0/1254	0.42	0/1683
39	1h	0.28	0/1108	0.48	0/1494
39	2h	0.27	0/1108	0.46	0/1494
40	1i	0.30	0/1002	0.49	0/1346
40	2i	0.29	0/997	0.49	0/1343
41	1j	0.28	0/722	0.48	0/982
41	2j	0.29	0/727	0.48	0/988
42	1k	0.29	0/844	0.49	0/1145
42	2k	0.28	0/848	0.48	0/1149
43	1l	0.29	0/937	0.50	0/1260
43	2l	0.29	0/937	0.48	0/1260
44	1m	0.29	0/961	0.48	0/1290
44	2m	0.27	0/953	0.49	0/1279
45	1n	0.29	0/501	0.48	0/664
45	2n	0.31	0/501	0.48	0/664
46	1o	0.28	0/739	0.41	0/985
46	2o	0.28	0/739	0.42	0/985
47	1p	0.30	0/697	0.48	0/939
47	2p	0.28	0/693	0.49	0/935
48	1q	0.28	0/836	0.50	0/1117
48	2q	0.29	0/836	0.47	0/1117
49	1r	0.29	0/560	0.48	0/746
49	2r	0.29	0/560	0.46	0/746
50	1s	0.28	0/667	0.55	0/900
50	2s	0.30	0/661	0.57	0/893
51	1t	0.27	0/730	0.44	0/965
51	2t	0.27	0/729	0.45	0/965
52	1u	0.27	0/203	0.44	0/266
52	2u	0.32	0/203	0.48	0/266
53	1v	0.43	0/238	0.90	0/368
53	2v	0.60	0/126	1.33	2/195 (1.0%)
54	1x	0.51	1/1725 (0.1%)	1.10	16/2689 (0.6%)
54	2x	0.42	0/1725	1.02	7/2689 (0.3%)
All	All	0.55	19/310063 (0.0%)	0.82	183/463821 (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
21	1Z	0	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
32	1a	0	1
33	1b	0	2
All	All	0	4

All (19) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	2I	89	TYR	CD2-CE2	102.02	2.92	1.39
8	2I	89	TYR	CE1-CZ	101.34	2.70	1.38
32	1a	55	A	C5-C4	100.44	2.09	1.38
32	1a	55	A	N7-C5	52.03	1.70	1.39
32	1a	55	A	N9-C4	47.12	1.66	1.37
32	1a	55	A	C8-N7	43.51	1.62	1.31
32	1a	55	A	N3-C4	42.16	1.60	1.34
32	1a	55	A	N9-C8	37.07	1.67	1.37
32	1a	55	A	C6-N1	36.11	1.60	1.35
32	1a	55	A	C5-C6	29.44	1.67	1.41
32	1a	55	A	N1-C2	27.70	1.59	1.34
32	1a	55	A	C2-N3	26.40	1.57	1.33
2	1B	1	U	OP3-P	-10.31	1.48	1.61
2	2B	1	U	OP3-P	-10.25	1.48	1.61
32	2a	1272	G	N1-C2	-7.03	1.32	1.37
8	2I	89	TYR	CE2-CZ	6.82	1.47	1.38
32	2a	1272	G	C6-N1	-6.31	1.35	1.39
54	1x	22	G	N7-C5	5.50	1.42	1.39
8	2I	89	TYR	CG-CD1	-5.09	1.32	1.39

All (183) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	2I	89	TYR	CZ-CE2-CD2	-22.98	99.12	119.80
8	2I	89	TYR	CD1-CE1-CZ	20.42	138.18	119.80
32	1a	55	A	C4-C5-N7	-19.94	100.73	110.70
32	1a	55	A	C2-N3-C4	18.92	120.06	110.60
32	2a	1263	C	N1-C2-O2	18.48	129.99	118.90
32	1a	55	A	C6-C5-N7	18.17	145.02	132.30
32	1a	55	A	C6-N1-C2	16.99	128.79	118.60
32	1a	55	A	C5-N7-C8	16.84	112.32	103.90
32	2a	1272	G	N3-C2-N2	16.82	131.68	119.90
8	2I	89	TYR	CG-CD2-CE2	16.62	134.59	121.30
32	2a	1272	G	C5-C6-O6	16.10	138.26	128.60
32	1a	55	A	C8-N9-C4	15.71	112.08	105.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	1a	55	A	N3-C4-N9	14.31	138.84	127.40
32	2a	1272	G	N1-C2-N2	-13.94	103.65	116.20
32	1a	55	A	N3-C4-C5	-13.24	117.53	126.80
32	2a	1272	G	C6-N1-C2	11.65	132.09	125.10
32	1a	55	A	N1-C2-N3	-11.46	123.57	129.30
1	1A	1075	C	N1-C2-O2	10.88	125.42	118.90
32	2a	1263	C	C2-N3-C4	10.85	125.33	119.90
32	2a	1272	G	C5-C6-N1	-10.75	106.13	111.50
32	1a	357	G	OP1-P-O3'	-10.55	81.98	105.20
2	2B	80	U	O4'-C1'-N1	10.44	116.55	108.20
32	1a	55	A	N9-C4-C5	-10.13	101.75	105.80
32	1a	55	A	C4-C5-C6	-9.38	112.31	117.00
32	2a	1263	C	N3-C2-O2	-9.29	115.40	121.90
32	2a	1263	C	C5-C6-N1	8.64	125.32	121.00
54	1x	46	G	C6-N1-C2	-8.62	119.93	125.10
1	1A	1075	C	C2-N3-C4	8.50	124.15	119.90
1	1A	1086	A	N1-C6-N6	-8.38	113.58	118.60
32	1a	357	G	OP2-P-O3'	-8.31	86.91	105.20
1	2A	2136	C	N1-C2-O2	8.26	123.86	118.90
8	2I	89	TYR	CE1-CZ-CE2	-7.97	107.04	119.80
32	1a	841	U	C2-N1-C1'	7.96	127.25	117.70
1	1A	2167	U	C2-N1-C1'	7.83	127.09	117.70
1	1A	512	G	O4'-C1'-N9	7.72	114.37	108.20
1	1A	1249	U	O5'-P-OP1	-7.71	98.76	105.70
54	1x	22	G	N1-C6-O6	-7.67	115.30	119.90
32	2a	754	C	N1-C2-O2	7.67	123.50	118.90
32	2a	1272	G	C4-N9-C1'	7.63	136.42	126.50
1	1A	1063	G	C6-N1-C2	7.56	129.64	125.10
1	1A	12	U	C2-N1-C1'	7.55	126.77	117.70
32	2a	754	C	C2-N1-C1'	7.51	127.06	118.80
1	2A	2473	U	C2-N1-C1'	7.40	126.58	117.70
32	2a	1272	G	C8-N9-C1'	-7.36	117.43	127.00
32	1a	841	U	C5-C6-N1	7.35	126.38	122.70
54	1x	22	G	C4-C5-C6	-7.33	114.40	118.80
32	2a	1272	G	N1-C6-O6	-7.19	115.59	119.90
1	1A	1075	C	N3-C2-O2	-7.11	116.92	121.90
1	1A	1063	G	C5-C6-O6	7.00	132.80	128.60
1	1A	2167	U	N3-C2-O2	-6.97	117.32	122.20
32	2a	1263	C	C2-N1-C1'	6.96	126.45	118.80
1	1A	226	G	O4'-C1'-N9	6.94	113.75	108.20
32	2a	1263	C	C4-C5-C6	-6.87	113.96	117.40
1	2A	1313	U	C2-N1-C1'	6.77	125.83	117.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	1x	14	A	C5-N7-C8	6.68	107.24	103.90
54	1x	22	G	C5-N7-C8	-6.67	100.97	104.30
1	1A	2319	G	C4-C5-N7	6.66	113.47	110.80
32	2a	1263	C	N1-C2-N3	-6.61	114.57	119.20
1	1A	2167	U	N1-C2-O2	6.60	127.42	122.80
32	1a	91	C	N1-C2-O2	6.57	122.84	118.90
32	2a	1158	C	C2-N1-C1'	6.53	125.98	118.80
53	2v	18	G	N3-C2-N2	6.43	124.40	119.90
1	1A	801	G	O5'-P-OP2	-6.40	99.94	105.70
32	1a	358	U	OP1-P-OP2	6.40	129.20	119.60
1	2A	2155	G	C6-N1-C2	6.39	128.94	125.10
1	1A	1075	C	C6-N1-C2	-6.37	117.75	120.30
54	2x	46	G	C6-N1-C2	-6.37	121.28	125.10
54	1x	22	G	N3-C4-N9	-6.34	122.20	126.00
54	2x	34	C	N1-C2-O2	6.34	122.70	118.90
32	1a	841	U	C6-N1-C2	-6.33	117.20	121.00
54	1x	14	A	C4-C5-C6	6.33	120.17	117.00
1	2A	2473	U	N1-C2-O2	6.33	127.23	122.80
1	1A	787	U	O5'-P-OP1	-6.33	100.00	105.70
32	1a	1514	C	C6-N1-C2	-6.32	117.77	120.30
54	2x	46	G	N3-C2-N2	-6.32	115.48	119.90
1	1A	2554	U	O5'-P-OP1	-6.31	100.02	105.70
8	2I	75	LEU	CA-CB-CG	6.24	129.66	115.30
54	1x	22	G	C8-N9-C1'	6.23	135.10	127.00
1	1A	2100	G	C5-C6-O6	-6.21	124.88	128.60
1	1A	1653	G	P-O3'-C3'	6.14	127.08	119.70
1	1A	1639	U	O5'-P-OP2	-6.13	100.18	105.70
1	2A	2473	U	N3-C2-O2	-6.11	117.92	122.20
32	1a	1158	C	C2-N1-C1'	6.08	125.49	118.80
32	2a	1272	G	C2-N3-C4	-6.07	108.86	111.90
54	2x	14	A	C4-C5-C6	6.07	120.03	117.00
32	2a	1020	U	N1-C2-O2	6.05	127.04	122.80
53	2v	18	G	N3-C4-N9	6.02	129.61	126.00
32	1a	266	G	P-O3'-C3'	5.97	126.86	119.70
1	1A	567	A	O5'-P-OP1	-5.97	100.33	105.70
1	2A	141	A	C8-N9-C4	-5.95	103.42	105.80
54	1x	22	G	C6-C5-N7	5.89	133.94	130.40
1	2A	845	G	C4-N9-C1'	5.88	134.14	126.50
1	1A	1150	C	C6-N1-C2	-5.83	117.97	120.30
54	2x	22	G	N1-C6-O6	-5.81	116.41	119.90
54	2x	14	A	C5-N7-C8	5.78	106.79	103.90
1	1A	1992	G	P-O3'-C3'	5.76	126.61	119.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1A	1075	C	C5-C4-N4	5.75	124.22	120.20
1	1A	1075	C	C2-N1-C1'	5.74	125.11	118.80
32	1a	841	U	N3-C2-O2	-5.74	118.18	122.20
32	2a	841	U	C5-C6-N1	5.74	125.57	122.70
1	1A	2129	C	C2-N3-C4	5.73	122.77	119.90
32	2a	754	C	N3-C2-O2	-5.69	117.92	121.90
32	1a	1002	G	N3-C4-N9	5.67	129.40	126.00
1	2A	2107	C	C2-N3-C4	5.66	122.73	119.90
32	2a	754	C	C6-N1-C1'	-5.66	114.01	120.80
1	2A	141	A	N7-C8-N9	5.65	116.63	113.80
1	2A	1992	G	P-O3'-C3'	5.64	126.47	119.70
1	1A	2406	U	O4'-C1'-N1	-5.62	103.70	108.20
1	1A	2612	C	N1-C2-O2	5.61	122.27	118.90
1	2A	205	G	C4-N9-C1'	-5.60	119.22	126.50
1	1A	2572	A	C8-N9-C4	5.59	108.04	105.80
1	2A	90	U	C2-N1-C1'	5.59	124.41	117.70
1	2A	1698	A	O4'-C1'-N9	5.59	112.67	108.20
1	2A	801	G	O5'-P-OP2	-5.58	100.68	105.70
1	1A	12	U	C5-C6-N1	5.58	125.49	122.70
32	1a	841	U	N1-C2-O2	5.58	126.70	122.80
32	2a	1025	U	C2-N1-C1'	5.49	124.28	117.70
1	2A	2136	C	N3-C2-O2	-5.48	118.07	121.90
1	1A	1542	A	O5'-P-OP1	-5.45	100.80	105.70
32	2a	1263	C	N3-C4-N4	-5.45	114.19	118.00
1	1A	2158	A	P-O3'-C3'	5.45	126.23	119.70
32	2a	1262	C	N1-C2-O2	5.44	122.17	118.90
1	1A	847	U	C2-N1-C1'	5.43	124.21	117.70
2	2B	3	C	N1-C2-O2	5.43	122.16	118.90
1	1A	2100	G	N1-C6-O6	5.43	123.16	119.90
1	2A	2155	G	N3-C2-N2	5.38	123.67	119.90
1	1A	1174	A	P-O3'-C3'	5.38	126.16	119.70
32	2a	266	G	P-O3'-C3'	5.38	126.16	119.70
1	1A	748	G	C8-N9-C1'	5.37	133.98	127.00
54	1x	46	G	N9-C4-C5	5.37	107.55	105.40
1	2A	847	U	C2-N1-C1'	5.36	124.13	117.70
32	1a	792	A	O4'-C1'-N9	5.35	112.48	108.20
32	1a	1067	A	P-O3'-C3'	5.34	126.11	119.70
1	2A	528	A	C2-N3-C4	-5.34	107.93	110.60
54	1x	22	G	C5-C6-N1	5.34	114.17	111.50
32	2a	1025	U	N1-C2-O2	5.34	126.54	122.80
1	1A	195	A	OP2-P-O3'	5.33	116.92	105.20
1	1A	2897	U	C2-N1-C1'	5.32	124.08	117.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1A	1075	C	C5-C6-N1	5.31	123.66	121.00
32	2a	1158	C	N1-C2-O2	5.31	122.09	118.90
32	1a	748	C	P-O3'-C3'	5.31	126.07	119.70
1	2A	228	A	P-O3'-C3'	5.31	126.07	119.70
1	1A	1176	G	OP1-P-O3'	5.31	116.87	105.20
1	2A	2155	G	C5-C6-O6	5.30	131.78	128.60
1	2A	1204	A	O4'-C1'-N9	5.30	112.44	108.20
1	2A	2161	C	C2-N1-C1'	5.29	124.62	118.80
1	2A	205	G	C8-N9-C4	5.29	108.52	106.40
2	2B	3	C	C2-N1-C1'	5.29	124.61	118.80
1	1A	2167	U	C6-N1-C2	-5.27	117.84	121.00
32	1a	1027	C	N3-C2-O2	-5.27	118.21	121.90
1	1A	1352	U	O5'-P-OP1	-5.26	100.96	105.70
54	1x	14	A	C5-C6-N1	-5.25	115.08	117.70
1	1A	195	A	P-O3'-C3'	5.24	125.99	119.70
32	2a	204	U	C2-N1-C1'	5.23	123.98	117.70
1	1A	2319	G	C6-C5-N7	-5.22	127.27	130.40
1	1A	2319	G	O4'-C1'-N9	5.20	112.36	108.20
32	1a	91	C	C2-N3-C4	5.20	122.50	119.90
1	2A	2206	G	C4-N9-C1'	-5.19	119.75	126.50
1	1A	568	U	C5-C4-O4	-5.18	122.79	125.90
32	2a	687	A	P-O3'-C3'	5.18	125.92	119.70
54	1x	46	G	N3-C2-N2	-5.17	116.28	119.90
32	1a	1002	G	C4-N9-C1'	5.16	133.21	126.50
1	2A	2689	U	P-O3'-C3'	5.16	125.90	119.70
54	1x	46	G	C5-C6-N1	5.16	114.08	111.50
32	2a	1225	A	C5-C6-N6	5.15	127.82	123.70
32	1a	975	A	O4'-C1'-N9	-5.15	104.08	108.20
32	2a	530	G	C4-N9-C1'	5.14	133.18	126.50
1	2A	205	G	N3-C4-C5	5.13	131.17	128.60
8	2I	89	TYR	CE1-CZ-OH	5.13	133.96	120.10
1	2A	271(M)	G	P-O3'-C3'	5.13	125.85	119.70
1	2A	1380	G	O5'-P-OP2	-5.10	101.11	105.70
32	1a	115	G	P-O3'-C3'	5.08	125.79	119.70
32	1a	421	U	N1-C2-O2	5.06	126.34	122.80
1	1A	1174	A	OP1-P-O3'	5.05	116.32	105.20
1	1A	1416	G	O4'-C1'-N9	5.05	112.24	108.20
1	1A	1063	G	C5-C6-N1	-5.03	108.98	111.50
54	2x	46	G	N9-C4-C5	5.03	107.41	105.40
1	1A	845	G	O4'-C1'-N9	5.03	112.22	108.20
54	1x	22	G	C4-N9-C1'	-5.02	119.97	126.50
54	1x	46	G	N1-C2-N3	5.02	126.91	123.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	2B	80	U	C5'-C4'-O4'	5.01	115.12	109.10
1	1A	2286	A	O4'-C1'-N9	-5.01	104.19	108.20
1	2A	1653	G	P-O3'-C3'	5.00	125.71	119.70

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
21	1Z	136	PHE	Peptide
32	1a	55	A	Sidechain
33	1b	122	PHE	Peptide
33	1b	126	GLU	Peptide

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

Due to software issues we are unable to calculate clashes - this section is therefore empty.

## 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%)	255 (93%)	18 (7%)	0	100	100
3	2D	273/276 (99%)	251 (92%)	21 (8%)	1 (0%)	34	66
4	1E	202/206 (98%)	188 (93%)	12 (6%)	2 (1%)	15	44
4	2E	202/206 (98%)	187 (93%)	13 (6%)	2 (1%)	15	44
5	1F	201/210 (96%)	194 (96%)	4 (2%)	3 (2%)	10	33
5	2F	201/210 (96%)	188 (94%)	12 (6%)	1 (0%)	29	61
6	1G	179/182 (98%)	162 (90%)	13 (7%)	4 (2%)	6	22
6	2G	179/182 (98%)	148 (83%)	24 (13%)	7 (4%)	3	10
7	1H	172/180 (96%)	158 (92%)	14 (8%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
7	2H	172/180 (96%)	151 (88%)	17 (10%)	4 (2%)	6	21
8	1I	144/148 (97%)	126 (88%)	16 (11%)	2 (1%)	11	34
8	2I	144/148 (97%)	112 (78%)	26 (18%)	6 (4%)	3	9
9	1N	138/140 (99%)	135 (98%)	2 (1%)	1 (1%)	22	53
9	2N	138/140 (99%)	131 (95%)	6 (4%)	1 (1%)	22	53
10	1O	120/122 (98%)	108 (90%)	11 (9%)	1 (1%)	19	49
10	2O	120/122 (98%)	107 (89%)	12 (10%)	1 (1%)	19	49
11	1P	147/150 (98%)	134 (91%)	10 (7%)	3 (2%)	7	24
11	2P	147/150 (98%)	133 (90%)	12 (8%)	2 (1%)	11	34
12	1Q	139/141 (99%)	128 (92%)	10 (7%)	1 (1%)	22	53
12	2Q	139/141 (99%)	124 (89%)	15 (11%)	0	100	100
13	1R	116/118 (98%)	108 (93%)	8 (7%)	0	100	100
13	2R	116/118 (98%)	108 (93%)	7 (6%)	1 (1%)	17	46
14	1S	108/112 (96%)	96 (89%)	11 (10%)	1 (1%)	17	46
14	2S	108/112 (96%)	101 (94%)	4 (4%)	3 (3%)	5	17
15	1T	129/146 (88%)	121 (94%)	7 (5%)	1 (1%)	19	49
15	2T	129/146 (88%)	121 (94%)	8 (6%)	0	100	100
16	1U	114/118 (97%)	112 (98%)	2 (2%)	0	100	100
16	2U	114/118 (97%)	112 (98%)	2 (2%)	0	100	100
17	1V	99/101 (98%)	90 (91%)	8 (8%)	1 (1%)	15	44
17	2V	99/101 (98%)	93 (94%)	6 (6%)	0	100	100
18	1W	110/113 (97%)	106 (96%)	3 (3%)	1 (1%)	17	46
18	2W	110/113 (97%)	108 (98%)	2 (2%)	0	100	100
19	1X	93/96 (97%)	85 (91%)	6 (6%)	2 (2%)	6	22
19	2X	93/96 (97%)	87 (94%)	5 (5%)	1 (1%)	14	41
20	1Y	105/110 (96%)	101 (96%)	4 (4%)	0	100	100
20	2Y	105/110 (96%)	93 (89%)	11 (10%)	1 (1%)	15	44
21	1Z	148/206 (72%)	130 (88%)	16 (11%)	2 (1%)	11	34
21	2Z	156/206 (76%)	128 (82%)	24 (15%)	4 (3%)	5	18
22	10	81/85 (95%)	76 (94%)	4 (5%)	1 (1%)	13	39
22	20	81/85 (95%)	76 (94%)	4 (5%)	1 (1%)	13	39

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
23	11	95/98 (97%)	91 (96%)	2 (2%)	2 (2%)	7	23
23	21	95/98 (97%)	91 (96%)	4 (4%)	0	100	100
24	12	68/72 (94%)	67 (98%)	1 (2%)	0	100	100
24	22	68/72 (94%)	60 (88%)	8 (12%)	0	100	100
25	13	57/60 (95%)	54 (95%)	3 (5%)	0	100	100
25	23	57/60 (95%)	52 (91%)	4 (7%)	1 (2%)	8	28
26	14	67/71 (94%)	56 (84%)	7 (10%)	4 (6%)	1	4
26	24	67/71 (94%)	53 (79%)	13 (19%)	1 (2%)	10	33
27	15	57/60 (95%)	55 (96%)	2 (4%)	0	100	100
27	25	57/60 (95%)	55 (96%)	2 (4%)	0	100	100
28	16	51/54 (94%)	49 (96%)	2 (4%)	0	100	100
28	26	51/54 (94%)	47 (92%)	4 (8%)	0	100	100
29	17	46/49 (94%)	46 (100%)	0	0	100	100
29	27	46/49 (94%)	46 (100%)	0	0	100	100
30	18	62/65 (95%)	59 (95%)	3 (5%)	0	100	100
30	28	62/65 (95%)	58 (94%)	4 (6%)	0	100	100
31	19	35/37 (95%)	35 (100%)	0	0	100	100
31	29	35/37 (95%)	30 (86%)	4 (11%)	1 (3%)	4	15
33	1b	229/256 (90%)	193 (84%)	29 (13%)	7 (3%)	4	14
33	2b	229/256 (90%)	199 (87%)	21 (9%)	9 (4%)	3	10
34	1c	204/239 (85%)	179 (88%)	24 (12%)	1 (0%)	29	61
34	2c	204/239 (85%)	179 (88%)	22 (11%)	3 (2%)	10	33
35	1d	206/209 (99%)	184 (89%)	21 (10%)	1 (0%)	29	61
35	2d	206/209 (99%)	191 (93%)	15 (7%)	0	100	100
36	1e	146/162 (90%)	128 (88%)	16 (11%)	2 (1%)	11	34
36	2e	146/162 (90%)	126 (86%)	18 (12%)	2 (1%)	11	34
37	1f	98/101 (97%)	89 (91%)	9 (9%)	0	100	100
37	2f	98/101 (97%)	91 (93%)	7 (7%)	0	100	100
38	1g	153/156 (98%)	134 (88%)	17 (11%)	2 (1%)	12	36
38	2g	153/156 (98%)	132 (86%)	18 (12%)	3 (2%)	7	24
39	1h	135/138 (98%)	125 (93%)	10 (7%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
39	2h	135/138 (98%)	124 (92%)	11 (8%)	0	100	100
40	1i	125/128 (98%)	106 (85%)	17 (14%)	2 (2%)	9	31
40	2i	125/128 (98%)	106 (85%)	18 (14%)	1 (1%)	19	49
41	1j	95/105 (90%)	77 (81%)	13 (14%)	5 (5%)	2	6
41	2j	94/105 (90%)	82 (87%)	8 (8%)	4 (4%)	2	8
42	1k	112/129 (87%)	101 (90%)	7 (6%)	4 (4%)	3	11
42	2k	112/129 (87%)	99 (88%)	11 (10%)	2 (2%)	8	28
43	1l	119/132 (90%)	107 (90%)	12 (10%)	0	100	100
43	2l	119/132 (90%)	105 (88%)	14 (12%)	0	100	100
44	1m	120/126 (95%)	107 (89%)	11 (9%)	2 (2%)	9	29
44	2m	119/126 (94%)	105 (88%)	11 (9%)	3 (2%)	5	19
45	1n	58/61 (95%)	52 (90%)	6 (10%)	0	100	100
45	2n	58/61 (95%)	54 (93%)	3 (5%)	1 (2%)	9	29
46	1o	86/89 (97%)	81 (94%)	5 (6%)	0	100	100
46	2o	86/89 (97%)	78 (91%)	8 (9%)	0	100	100
47	1p	80/88 (91%)	68 (85%)	9 (11%)	3 (4%)	3	10
47	2p	80/88 (91%)	71 (89%)	9 (11%)	0	100	100
48	1q	97/105 (92%)	87 (90%)	10 (10%)	0	100	100
48	2q	97/105 (92%)	86 (89%)	10 (10%)	1 (1%)	15	44
49	1r	66/88 (75%)	58 (88%)	7 (11%)	1 (2%)	10	33
49	2r	66/88 (75%)	65 (98%)	1 (2%)	0	100	100
50	1s	81/93 (87%)	67 (83%)	13 (16%)	1 (1%)	13	39
50	2s	81/93 (87%)	71 (88%)	8 (10%)	2 (2%)	5	19
51	1t	94/106 (89%)	82 (87%)	7 (7%)	5 (5%)	2	6
51	2t	94/106 (89%)	82 (87%)	7 (7%)	5 (5%)	2	6
52	1u	21/27 (78%)	18 (86%)	2 (10%)	1 (5%)	2	7
52	2u	21/27 (78%)	17 (81%)	4 (19%)	0	100	100
All	All	11368/12128 (94%)	10282 (90%)	942 (8%)	144 (1%)	12	36

All (144) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	1E	71	GLY

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Mol	Chain	Res	Type
5	1F	130	ALA
11	1P	36	LYS
11	1P	38	GLN
12	1Q	27	VAL
14	1S	94	TYR
26	14	62	ARG
33	1b	17	PHE
33	1b	125	PRO
38	1g	80	VAL
40	1i	54	ASP
44	1m	67	GLU
44	1m	106	ASN
5	2F	130	ALA
7	2H	126	PRO
8	2I	127	VAL
10	2O	5	GLN
11	2P	45	LEU
33	2b	16	HIS
33	2b	123	ALA
40	2i	54	ASP
42	2k	105	VAL
50	2s	12	ASP
51	2t	10	LEU
5	1F	168	ARG
6	1G	43	LEU
18	1W	40	ASN
21	1Z	52	SER
23	11	3	LYS
26	14	45	GLY
26	14	49	PHE
34	1c	129	ALA
36	1e	85	GLY
41	1j	56	HIS
41	1j	79	ARG
42	1k	49	GLY
42	1k	107	SER
4	2E	71	GLY
6	2G	45	GLU
6	2G	51	ARG
8	2I	108	THR
8	2I	115	ALA
11	2P	38	GLN

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Mol	Chain	Res	Type
14	2S	96	GLY
19	2X	94	GLY
21	2Z	65	GLN
21	2Z	66	SER
26	24	45	GLY
33	2b	126	GLU
36	2e	21	ALA
36	2e	85	GLY
42	2k	49	GLY
44	2m	67	GLU
48	2q	68	ARG
4	1E	52	LEU
6	1G	44	GLY
17	1V	43	GLU
19	1X	94	GLY
26	14	53	GLU
33	1b	124	SER
38	1g	4	ARG
42	1k	91	ARG
47	1p	28	ARG
47	1p	81	ARG
50	1s	12	ASP
51	1t	102	GLY
52	1u	5	ASP
6	2G	117	PHE
8	2I	135	GLU
9	2N	2	LYS
14	2S	94	TYR
21	2Z	52	SER
31	29	21	GLY
33	2b	78	GLN
33	2b	105	PHE
51	2t	9	ASN
51	2t	95	ALA
6	1G	47	LYS
23	11	84	GLY
33	1b	231	GLU
40	1i	42	ARG
42	1k	106	LYS
49	1r	33	ASP
51	1t	47	GLY
51	1t	95	ALA

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
51	1t	100	ILE
4	2E	52	LEU
7	2H	47	GLU
7	2H	55	PRO
7	2H	92	ILE
8	2I	94	ALA
14	2S	84	GLN
34	2c	129	ALA
34	2c	181	ASN
38	2g	7	ALA
38	2g	80	VAL
41	2j	29	ARG
41	2j	78	ASN
45	2n	14	PRO
5	1F	122	LYS
6	1G	49	ASP
8	1I	33	ARG
8	1I	42	SER
9	1N	2	LYS
10	1O	5	GLN
21	1Z	137	ILE
22	10	4	LYS
33	1b	22	LYS
47	1p	63	GLY
51	1t	96	GLY
8	2I	10	GLU
33	2b	17	PHE
33	2b	20	GLU
33	2b	209	ARG
38	2g	4	ARG
11	1P	93	GLY
19	1X	2	LYS
33	1b	207	ALA
41	1j	75	ILE
41	1j	78	ASN
6	2G	3	LEU
6	2G	44	GLY
20	2Y	21	LYS
21	2Z	93	ASP
22	20	4	LYS
33	2b	231	GLU
41	2j	39	PRO

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Mol	Chain	Res	Type
44	2m	5	ALA
44	2m	90	LEU
50	2s	33	THR
51	2t	47	GLY
15	1T	37	GLY
33	1b	229	VAL
41	1j	77	PRO
51	2t	102	GLY
36	1e	22	GLY
3	2D	125	ILE
34	2c	138	VAL
25	23	59	VAL
41	2j	75	ILE
35	1d	37	PRO
6	2G	109	VAL
6	2G	177	GLY
13	2R	117	VAL

### 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%)	203 (94%)	12 (6%)	21	51
3	2D	215/218 (99%)	207 (96%)	8 (4%)	34	68
4	1E	164/166 (99%)	153 (93%)	11 (7%)	16	43
4	2E	164/166 (99%)	151 (92%)	13 (8%)	12	34
5	1F	160/166 (96%)	142 (89%)	18 (11%)	6	18
5	2F	159/166 (96%)	141 (89%)	18 (11%)	6	18
6	1G	143/156 (92%)	127 (89%)	16 (11%)	6	18
6	2G	143/156 (92%)	123 (86%)	20 (14%)	3	11
7	1H	144/148 (97%)	134 (93%)	10 (7%)	15	41
7	2H	144/148 (97%)	130 (90%)	14 (10%)	8	24
8	1I	113/124 (91%)	99 (88%)	14 (12%)	4	14

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
8	2I	105/124 (85%)	78 (74%)	27 (26%)	0	1
9	1N	118/119 (99%)	103 (87%)	15 (13%)	4	14
9	2N	118/119 (99%)	107 (91%)	11 (9%)	9	26
10	1O	100/100 (100%)	95 (95%)	5 (5%)	24	56
10	2O	100/100 (100%)	95 (95%)	5 (5%)	24	56
11	1P	115/116 (99%)	102 (89%)	13 (11%)	6	18
11	2P	115/116 (99%)	107 (93%)	8 (7%)	15	40
12	1Q	111/111 (100%)	100 (90%)	11 (10%)	8	23
12	2Q	111/111 (100%)	98 (88%)	13 (12%)	5	16
13	1R	101/101 (100%)	93 (92%)	8 (8%)	12	34
13	2R	101/101 (100%)	94 (93%)	7 (7%)	15	41
14	1S	86/88 (98%)	80 (93%)	6 (7%)	15	40
14	2S	85/88 (97%)	74 (87%)	11 (13%)	4	13
15	1T	115/127 (91%)	110 (96%)	5 (4%)	29	62
15	2T	113/127 (89%)	106 (94%)	7 (6%)	18	47
16	1U	93/94 (99%)	87 (94%)	6 (6%)	17	44
16	2U	93/94 (99%)	87 (94%)	6 (6%)	17	44
17	1V	80/82 (98%)	77 (96%)	3 (4%)	33	67
17	2V	80/82 (98%)	73 (91%)	7 (9%)	10	29
18	1W	90/92 (98%)	82 (91%)	8 (9%)	9	28
18	2W	90/92 (98%)	83 (92%)	7 (8%)	12	35
19	1X	77/78 (99%)	75 (97%)	2 (3%)	46	79
19	2X	77/78 (99%)	71 (92%)	6 (8%)	12	35
20	1Y	85/91 (93%)	74 (87%)	11 (13%)	4	13
20	2Y	85/91 (93%)	74 (87%)	11 (13%)	4	13
21	1Z	135/179 (75%)	122 (90%)	13 (10%)	8	24
21	2Z	137/179 (76%)	116 (85%)	21 (15%)	2	8
22	10	65/67 (97%)	61 (94%)	4 (6%)	18	47
22	20	65/67 (97%)	62 (95%)	3 (5%)	27	60
23	11	80/83 (96%)	78 (98%)	2 (2%)	47	80
23	21	80/83 (96%)	74 (92%)	6 (8%)	13	37

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
24	12	65/67 (97%)	58 (89%)	7 (11%)	6	19
24	22	65/67 (97%)	59 (91%)	6 (9%)	9	27
25	13	51/52 (98%)	43 (84%)	8 (16%)	2	8
25	23	50/52 (96%)	46 (92%)	4 (8%)	12	34
26	14	59/63 (94%)	49 (83%)	10 (17%)	2	6
26	24	53/63 (84%)	45 (85%)	8 (15%)	3	9
27	15	50/52 (96%)	45 (90%)	5 (10%)	7	22
27	25	50/52 (96%)	46 (92%)	4 (8%)	12	34
28	16	51/52 (98%)	43 (84%)	8 (16%)	2	8
28	26	50/52 (96%)	45 (90%)	5 (10%)	7	22
29	17	41/42 (98%)	38 (93%)	3 (7%)	14	38
29	27	41/42 (98%)	36 (88%)	5 (12%)	5	15
30	18	54/55 (98%)	50 (93%)	4 (7%)	13	37
30	28	54/55 (98%)	49 (91%)	5 (9%)	9	26
31	19	34/34 (100%)	33 (97%)	1 (3%)	42	76
31	29	34/34 (100%)	32 (94%)	2 (6%)	19	49
33	1b	192/220 (87%)	171 (89%)	21 (11%)	6	19
33	2b	187/220 (85%)	154 (82%)	33 (18%)	2	5
34	1c	142/188 (76%)	126 (89%)	16 (11%)	6	18
34	2c	140/188 (74%)	121 (86%)	19 (14%)	3	11
35	1d	169/181 (93%)	157 (93%)	12 (7%)	14	39
35	2d	173/181 (96%)	156 (90%)	17 (10%)	8	24
36	1e	113/123 (92%)	107 (95%)	6 (5%)	22	54
36	2e	114/123 (93%)	104 (91%)	10 (9%)	10	29
37	1f	84/90 (93%)	79 (94%)	5 (6%)	19	48
37	2f	85/90 (94%)	80 (94%)	5 (6%)	19	49
38	1g	119/127 (94%)	112 (94%)	7 (6%)	19	49
38	2g	120/127 (94%)	103 (86%)	17 (14%)	3	10
39	1h	114/119 (96%)	100 (88%)	14 (12%)	4	15
39	2h	114/119 (96%)	104 (91%)	10 (9%)	10	29
40	1i	90/99 (91%)	81 (90%)	9 (10%)	7	22

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
40	2i	89/99 (90%)	80 (90%)	9 (10%)	7	22
41	1j	66/92 (72%)	57 (86%)	9 (14%)	3	11
41	2j	69/92 (75%)	64 (93%)	5 (7%)	14	38
42	1k	82/99 (83%)	75 (92%)	7 (8%)	10	31
42	2k	83/99 (84%)	74 (89%)	9 (11%)	6	19
43	1l	96/108 (89%)	90 (94%)	6 (6%)	18	46
43	2l	96/108 (89%)	90 (94%)	6 (6%)	18	46
44	1m	92/101 (91%)	80 (87%)	12 (13%)	4	13
44	2m	91/101 (90%)	81 (89%)	10 (11%)	6	19
45	1n	49/50 (98%)	41 (84%)	8 (16%)	2	7
45	2n	49/50 (98%)	43 (88%)	6 (12%)	5	15
46	1o	78/80 (98%)	71 (91%)	7 (9%)	9	28
46	2o	78/80 (98%)	71 (91%)	7 (9%)	9	28
47	1p	69/74 (93%)	63 (91%)	6 (9%)	10	30
47	2p	68/74 (92%)	63 (93%)	5 (7%)	13	37
48	1q	94/97 (97%)	89 (95%)	5 (5%)	22	54
48	2q	94/97 (97%)	87 (93%)	7 (7%)	13	37
49	1r	59/77 (77%)	55 (93%)	4 (7%)	16	42
49	2r	59/77 (77%)	53 (90%)	6 (10%)	7	22
50	1s	69/80 (86%)	65 (94%)	4 (6%)	20	50
50	2s	67/80 (84%)	60 (90%)	7 (10%)	7	21
51	1t	70/82 (85%)	64 (91%)	6 (9%)	10	30
51	2t	70/82 (85%)	67 (96%)	3 (4%)	29	62
52	1u	18/22 (82%)	18 (100%)	0	100	100
52	2u	18/22 (82%)	18 (100%)	0	100	100
All	All	9301/10064 (92%)	8439 (91%)	862 (9%)	9	26

All (862) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	1D	3	VAL
3	1D	27	THR
3	1D	30	GLU

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Mol	Chain	Res	Type
3	1D	32	SER
3	1D	34	VAL
3	1D	35	LYS
3	1D	61	LEU
3	1D	142	VAL
3	1D	193	VAL
3	1D	211	ARG
3	1D	229	VAL
3	1D	242	ARG
4	1E	19	ARG
4	1E	33	VAL
4	1E	49	LEU
4	1E	82	ARG
4	1E	89	ASP
4	1E	101	ARG
4	1E	116	VAL
4	1E	170	LEU
4	1E	181	LEU
4	1E	184	VAL
4	1E	195	LEU
5	1F	17	ARG
5	1F	18	ARG
5	1F	33	LEU
5	1F	53	THR
5	1F	57	VAL
5	1F	70	THR
5	1F	74	ARG
5	1F	106	ARG
5	1F	132	VAL
5	1F	158	THR
5	1F	168	ARG
5	1F	175	THR
5	1F	176	LEU
5	1F	183	VAL
5	1F	190	GLU
5	1F	192	LEU
5	1F	195	ASP
5	1F	197	ASP
6	1G	3	LEU
6	1G	5	VAL
6	1G	9	ARG
6	1G	28	VAL

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Mol	Chain	Res	Type
6	1G	31	VAL
6	1G	82	LEU
6	1G	116	ASP
6	1G	135	LEU
6	1G	139	LEU
6	1G	140	ILE
6	1G	148	MET
6	1G	149	VAL
6	1G	150	ASP
6	1G	152	LEU
6	1G	162	THR
6	1G	175	LEU
7	1H	18	GLU
7	1H	44	VAL
7	1H	56	SER
7	1H	84	SER
7	1H	95	ARG
7	1H	98	LEU
7	1H	114	VAL
7	1H	127	GLU
7	1H	129	THR
7	1H	164	TYR
8	1I	12	LEU
8	1I	20	ASP
8	1I	40	THR
8	1I	54	GLN
8	1I	74	ASN
8	1I	78	THR
8	1I	95	LYS
8	1I	104	GLN
8	1I	108	THR
8	1I	109	ILE
8	1I	116	LEU
8	1I	129	THR
8	1I	140	LEU
8	1I	142	VAL
9	1N	8	GLN
9	1N	28	THR
9	1N	32	THR
9	1N	33	LEU
9	1N	46	VAL
9	1N	48	MET

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Mol	Chain	Res	Type
9	1N	61	ARG
9	1N	62	VAL
9	1N	67	LEU
9	1N	68	GLU
9	1N	83	LYS
9	1N	87	LEU
9	1N	99	LEU
9	1N	131	GLN
9	1N	138	LEU
10	1O	3	GLN
10	1O	28	SER
10	1O	58	VAL
10	1O	96	THR
10	1O	120	GLU
11	1P	3	LEU
11	1P	29	LYS
11	1P	42	SER
11	1P	59	LEU
11	1P	65	ARG
11	1P	75	ILE
11	1P	79	ARG
11	1P	92	GLU
11	1P	101	VAL
11	1P	119	GLU
11	1P	125	VAL
11	1P	133	SER
11	1P	148	LEU
12	1Q	8	LYS
12	1Q	10	ARG
12	1Q	56	ARG
12	1Q	63	LYS
12	1Q	75	THR
12	1Q	79	LEU
12	1Q	109	VAL
12	1Q	110	THR
12	1Q	129	THR
12	1Q	133	ARG
12	1Q	138	ASP
13	1R	1	MET
13	1R	6	SER
13	1R	8	ARG
13	1R	33	ARG

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Mol	Chain	Res	Type
13	1R	36	THR
13	1R	65	LEU
13	1R	76	VAL
13	1R	96	ARG
14	1S	12	PHE
14	1S	25	ARG
14	1S	36	TYR
14	1S	50	SER
14	1S	69	VAL
14	1S	110	LEU
15	1T	28	VAL
15	1T	50	ILE
15	1T	74	ARG
15	1T	118	ARG
15	1T	128	GLU
16	1U	31	SER
16	1U	50	ARG
16	1U	74	LEU
16	1U	77	SER
16	1U	85	LYS
16	1U	100	VAL
17	1V	32	THR
17	1V	38	LEU
17	1V	82	ARG
18	1W	1	MET
18	1W	4	LYS
18	1W	11	ARG
18	1W	15	ARG
18	1W	17	VAL
18	1W	60	ASN
18	1W	97	LYS
18	1W	107	LEU
19	1X	23	GLU
19	1X	57	LEU
20	1Y	1	MET
20	1Y	43	ASN
20	1Y	50	ARG
20	1Y	64	GLU
20	1Y	67	LEU
20	1Y	70	SER
20	1Y	72	VAL
20	1Y	90	LEU

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Mol	Chain	Res	Type
20	1Y	91	GLU
20	1Y	99	CYS
20	1Y	106	LEU
21	1Z	1	MET
21	1Z	18	LEU
21	1Z	24	LEU
21	1Z	33	LEU
21	1Z	61	LEU
21	1Z	71	VAL
21	1Z	86	VAL
21	1Z	93	ASP
21	1Z	119	GLU
21	1Z	121	HIS
21	1Z	154	ASP
21	1Z	155	LEU
21	1Z	165	VAL
22	10	3	HIS
22	10	4	LYS
22	10	14	ARG
22	10	82	ARG
23	11	37	ILE
23	11	83	GLU
24	12	3	LEU
24	12	4	SER
24	12	5	GLU
24	12	19	VAL
24	12	53	LEU
24	12	65	ASN
24	12	70	GLN
25	13	6	VAL
25	13	18	ASP
25	13	23	LEU
25	13	36	VAL
25	13	54	VAL
25	13	56	VAL
25	13	58	VAL
25	13	60	GLU
26	14	3	GLU
26	14	5	ILE
26	14	27	THR
26	14	28	LYS
26	14	49	PHE

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Mol	Chain	Res	Type
26	14	52	THR
26	14	59	PHE
26	14	63	TYR
26	14	66	SER
26	14	67	TYR
27	15	6	VAL
27	15	29	THR
27	15	40	LYS
27	15	48	GLU
27	15	58	LEU
28	16	6	ARG
28	16	9	LEU
28	16	14	THR
28	16	19	ARG
28	16	38	LYS
28	16	48	VAL
28	16	49	HIS
28	16	53	LYS
29	17	1	MET
29	17	4	THR
29	17	48	LYS
30	18	14	VAL
30	18	29	LYS
30	18	31	HIS
30	18	34	TRP
31	19	13	LYS
33	1b	7	VAL
33	1b	17	PHE
33	1b	21	ARG
33	1b	32	ILE
33	1b	56	ARG
33	1b	67	THR
33	1b	78	GLN
33	1b	87	ARG
33	1b	108	ILE
33	1b	111	ARG
33	1b	115	LEU
33	1b	128	GLU
33	1b	142	LEU
33	1b	160	ASP
33	1b	162	ILE
33	1b	170	GLU

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Mol	Chain	Res	Type
33	1b	206	ASP
33	1b	211	ILE
33	1b	213	LEU
33	1b	229	VAL
33	1b	230	VAL
34	1c	3	ASN
34	1c	15	THR
34	1c	17	ASP
34	1c	36	ASP
34	1c	46	GLU
34	1c	49	SER
34	1c	56	ASP
34	1c	64	VAL
34	1c	82	GLU
34	1c	97	LYS
34	1c	103	VAL
34	1c	115	LEU
34	1c	178	LEU
34	1c	190	ARG
34	1c	191	THR
34	1c	195	VAL
35	1d	8	VAL
35	1d	19	LEU
35	1d	31	CYS
35	1d	59	ARG
35	1d	112	VAL
35	1d	141	ARG
35	1d	146	ILE
35	1d	160	GLN
35	1d	166	LYS
35	1d	175	SER
35	1d	194	LEU
35	1d	204	ILE
36	1e	24	ARG
36	1e	34	VAL
36	1e	41	VAL
36	1e	81	GLU
36	1e	120	THR
36	1e	151	LEU
37	1f	39	LYS
37	1f	43	LEU
37	1f	46	ARG

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Mol	Chain	Res	Type
37	1f	55	ASP
37	1f	70	ASP
38	1g	3	ARG
38	1g	12	LEU
38	1g	13	GLN
38	1g	24	THR
38	1g	53	LYS
38	1g	57	GLU
38	1g	113	GLU
39	1h	2	LEU
39	1h	9	MET
39	1h	26	VAL
39	1h	49	GLU
39	1h	51	VAL
39	1h	52	ASP
39	1h	77	GLU
39	1h	82	HIS
39	1h	85	ARG
39	1h	91	ARG
39	1h	99	GLU
39	1h	109	ILE
39	1h	120	THR
39	1h	127	LEU
40	1i	16	ARG
40	1i	27	THR
40	1i	53	VAL
40	1i	59	PHE
40	1i	103	THR
40	1i	104	ARG
40	1i	108	VAL
40	1i	113	LYS
40	1i	121	ARG
41	1j	17	ASP
41	1j	19	SER
41	1j	21	GLN
41	1j	30	SER
41	1j	38	ILE
41	1j	48	THR
41	1j	65	LEU
41	1j	81	THR
41	1j	98	ILE
42	1k	33	THR

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Mol	Chain	Res	Type
42	1k	48	ILE
42	1k	82	VAL
42	1k	87	THR
42	1k	110	ASP
42	1k	114	VAL
42	1k	117	ASN
43	1l	18	VAL
43	1l	38	THR
43	1l	47	LYS
43	1l	83	VAL
43	1l	86	ARG
43	1l	124	LYS
44	1m	3	ARG
44	1m	4	ILE
44	1m	19	LEU
44	1m	64	TRP
44	1m	67	GLU
44	1m	73	GLU
44	1m	103	THR
44	1m	106	ASN
44	1m	109	THR
44	1m	110	ARG
44	1m	114	ARG
44	1m	117	VAL
45	1n	3	ARG
45	1n	7	ILE
45	1n	11	LYS
45	1n	13	THR
45	1n	18	VAL
45	1n	22	THR
45	1n	33	VAL
45	1n	41	ARG
46	1o	3	ILE
46	1o	4	THR
46	1o	34	LEU
46	1o	39	LEU
46	1o	64	ARG
46	1o	74	ASP
46	1o	87	ILE
47	1p	2	VAL
47	1p	11	SER
47	1p	20	VAL

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Mol	Chain	Res	Type
47	1p	67	THR
47	1p	68	ASP
47	1p	72	ARG
48	1q	19	VAL
48	1q	24	GLU
48	1q	70	ARG
48	1q	72	ARG
48	1q	93	GLN
49	1r	22	VAL
49	1r	25	THR
49	1r	37	VAL
49	1r	82	THR
50	1s	12	ASP
50	1s	16	LEU
50	1s	28	LYS
50	1s	77	THR
51	1t	10	LEU
51	1t	13	LEU
51	1t	45	GLN
51	1t	62	LEU
51	1t	71	THR
51	1t	89	ARG
3	2D	3	VAL
3	2D	54	ARG
3	2D	87	ASN
3	2D	113	VAL
3	2D	141	VAL
3	2D	211	ARG
3	2D	242	ARG
3	2D	260	ARG
4	2E	1	MET
4	2E	12	THR
4	2E	27	LEU
4	2E	38	THR
4	2E	73	GLU
4	2E	82	ARG
4	2E	89	ASP
4	2E	90	THR
4	2E	101	ARG
4	2E	113	PHE
4	2E	116	VAL
4	2E	170	LEU

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Mol	Chain	Res	Type
4	2E	178	GLU
5	2F	18	ARG
5	2F	20	LEU
5	2F	33	LEU
5	2F	57	VAL
5	2F	74	ARG
5	2F	77	ASP
5	2F	88	VAL
5	2F	137	LYS
5	2F	140	LEU
5	2F	145	GLU
5	2F	153	SER
5	2F	158	THR
5	2F	165	ARG
5	2F	170	LEU
5	2F	176	LEU
5	2F	188	ARG
5	2F	195	ASP
5	2F	201	VAL
6	2G	3	LEU
6	2G	5	VAL
6	2G	15	VAL
6	2G	22	ARG
6	2G	28	VAL
6	2G	51	ARG
6	2G	79	ASN
6	2G	88	ILE
6	2G	91	ARG
6	2G	98	ARG
6	2G	106	LEU
6	2G	128	ARG
6	2G	135	LEU
6	2G	139	LEU
6	2G	140	ILE
6	2G	145	THR
6	2G	152	LEU
6	2G	159	VAL
6	2G	165	THR
6	2G	170	ARG
7	2H	24	VAL
7	2H	42	ARG
7	2H	43	VAL

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Mol	Chain	Res	Type
7	2H	45	VAL
7	2H	58	GLU
7	2H	70	THR
7	2H	71	LEU
7	2H	88	LEU
7	2H	114	VAL
7	2H	129	THR
7	2H	130	ARG
7	2H	136	ILE
7	2H	152	ARG
7	2H	175	LYS
8	2I	7	GLU
8	2I	19	VAL
8	2I	38	LEU
8	2I	40	THR
8	2I	43	ASN
8	2I	47	LEU
8	2I	52	ARG
8	2I	61	ARG
8	2I	76	THR
8	2I	78	THR
8	2I	81	VAL
8	2I	86	THR
8	2I	88	ILE
8	2I	91	SER
8	2I	93	THR
8	2I	101	LEU
8	2I	102	SER
8	2I	114	LEU
8	2I	121	LYS
8	2I	125	GLU
8	2I	126	TYR
8	2I	129	THR
8	2I	136	VAL
8	2I	138	ILE
8	2I	139	GLN
8	2I	140	LEU
8	2I	143	SER
9	2N	5	VAL
9	2N	33	LEU
9	2N	38	HIS
9	2N	43	THR

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Mol	Chain	Res	Type
9	2N	48	MET
9	2N	61	ARG
9	2N	62	VAL
9	2N	63	THR
9	2N	87	LEU
9	2N	90	MET
9	2N	99	LEU
10	2O	10	VAL
10	2O	26	LYS
10	2O	58	VAL
10	2O	96	THR
10	2O	113	LYS
11	2P	3	LEU
11	2P	30	THR
11	2P	56	SER
11	2P	77	ARG
11	2P	79	ARG
11	2P	91	PHE
11	2P	96	THR
11	2P	148	LEU
12	2Q	1	MET
12	2Q	7	MET
12	2Q	38	GLU
12	2Q	52	VAL
12	2Q	54	MET
12	2Q	56	ARG
12	2Q	60	ARG
12	2Q	85	LYS
12	2Q	98	LYS
12	2Q	106	VAL
12	2Q	109	VAL
12	2Q	112	GLU
12	2Q	133	ARG
13	2R	15	SER
13	2R	33	ARG
13	2R	35	THR
13	2R	65	LEU
13	2R	95	THR
13	2R	96	ARG
13	2R	114	VAL
14	2S	8	GLU
14	2S	11	LYS

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Mol	Chain	Res	Type
14	2S	12	PHE
14	2S	13	ARG
14	2S	19	LYS
14	2S	36	TYR
14	2S	40	ILE
14	2S	43	GLU
14	2S	63	THR
14	2S	69	VAL
14	2S	75	GLU
15	2T	6	LEU
15	2T	31	SER
15	2T	55	ASN
15	2T	89	VAL
15	2T	95	ARG
15	2T	96	ARG
15	2T	107	ASP
16	2U	55	ARG
16	2U	74	LEU
16	2U	77	SER
16	2U	85	LYS
16	2U	100	VAL
16	2U	117	GLN
17	2V	14	VAL
17	2V	15	GLU
17	2V	56	SER
17	2V	61	VAL
17	2V	82	ARG
17	2V	85	LYS
17	2V	95	LEU
18	2W	11	ARG
18	2W	17	VAL
18	2W	20	VAL
18	2W	23	LEU
18	2W	67	ASP
18	2W	107	LEU
18	2W	111	HIS
19	2X	23	GLU
19	2X	35	THR
19	2X	52	VAL
19	2X	57	LEU
19	2X	65	ARG
19	2X	81	VAL

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Mol	Chain	Res	Type
20	2Y	6	HIS
20	2Y	24	VAL
20	2Y	55	TYR
20	2Y	72	VAL
20	2Y	81	LYS
20	2Y	85	VAL
20	2Y	86	ARG
20	2Y	90	LEU
20	2Y	91	GLU
20	2Y	94	LYS
20	2Y	99	CYS
21	2Z	5	LEU
21	2Z	28	MET
21	2Z	38	TYR
21	2Z	40	ASP
21	2Z	41	LEU
21	2Z	53	ILE
21	2Z	60	GLU
21	2Z	71	VAL
21	2Z	72	ARG
21	2Z	100	VAL
21	2Z	121	HIS
21	2Z	122	ARG
21	2Z	123	ASP
21	2Z	124	ILE
21	2Z	126	VAL
21	2Z	131	ARG
21	2Z	136	PHE
21	2Z	148	ASP
21	2Z	154	ASP
21	2Z	155	LEU
21	2Z	161	VAL
22	20	3	HIS
22	20	10	THR
22	20	11	ARG
23	21	35	THR
23	21	51	VAL
23	21	52	ARG
23	21	56	GLN
23	21	65	SER
23	21	92	LYS
24	22	26	ARG

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Mol	Chain	Res	Type
24	22	30	ARG
24	22	34	GLU
24	22	35	LEU
24	22	53	LEU
24	22	70	GLN
25	23	30	ARG
25	23	31	LEU
25	23	54	VAL
25	23	56	VAL
26	24	13	ARG
26	24	33	VAL
26	24	34	GLU
26	24	48	ARG
26	24	49	PHE
26	24	56	VAL
26	24	62	ARG
26	24	63	TYR
27	25	6	VAL
27	25	8	LYS
27	25	29	THR
27	25	48	GLU
28	26	6	ARG
28	26	9	LEU
28	26	13	CYS
28	26	20	ASN
28	26	50	ARG
29	27	1	MET
29	27	4	THR
29	27	41	ARG
29	27	46	VAL
29	27	48	LYS
30	28	31	HIS
30	28	34	TRP
30	28	37	SER
30	28	46	ARG
30	28	50	LEU
31	29	7	VAL
31	29	26	ILE
33	2b	8	LYS
33	2b	15	VAL
33	2b	16	HIS
33	2b	24	TRP

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Mol	Chain	Res	Type
33	2b	35	GLU
33	2b	44	LEU
33	2b	47	THR
33	2b	67	THR
33	2b	71	VAL
33	2b	83	MET
33	2b	93	VAL
33	2b	94	ASN
33	2b	103	THR
33	2b	107	THR
33	2b	115	LEU
33	2b	117	GLU
33	2b	124	SER
33	2b	127	ILE
33	2b	137	ARG
33	2b	146	GLN
33	2b	150	SER
33	2b	153	ARG
33	2b	154	LEU
33	2b	160	ASP
33	2b	164	VAL
33	2b	176	GLU
33	2b	178	ARG
33	2b	189	ASP
33	2b	197	VAL
33	2b	208	ILE
33	2b	209	ARG
33	2b	224	GLN
33	2b	230	VAL
34	2c	26	LYS
34	2c	36	ASP
34	2c	47	LEU
34	2c	57	ILE
34	2c	70	VAL
34	2c	98	ASN
34	2c	101	LEU
34	2c	103	VAL
34	2c	105	GLU
34	2c	115	LEU
34	2c	118	GLN
34	2c	152	ILE
34	2c	154	SER

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Mol	Chain	Res	Type
34	2c	162	GLN
34	2c	164	ARG
34	2c	172	ARG
34	2c	186	PHE
34	2c	190	ARG
34	2c	206	GLU
35	2d	21	LEU
35	2d	27	TYR
35	2d	28	SER
35	2d	31	CYS
35	2d	38	TYR
35	2d	57	ARG
35	2d	60	GLU
35	2d	76	ARG
35	2d	102	ASP
35	2d	108	LEU
35	2d	127	THR
35	2d	135	LEU
35	2d	150	GLU
35	2d	155	LEU
35	2d	157	LEU
35	2d	175	SER
35	2d	181	MET
36	2e	6	PHE
36	2e	13	ILE
36	2e	24	ARG
36	2e	41	VAL
36	2e	55	VAL
36	2e	81	GLU
36	2e	84	PHE
36	2e	135	THR
36	2e	144	THR
36	2e	152	ARG
37	2f	61	LEU
37	2f	72	VAL
37	2f	81	ILE
37	2f	94	GLN
37	2f	95	GLU
38	2g	8	GLU
38	2g	21	VAL
38	2g	22	LEU
38	2g	42	ILE

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Mol	Chain	Res	Type
38	2g	45	ASP
38	2g	49	ILE
38	2g	51	GLN
38	2g	52	GLU
38	2g	57	GLU
38	2g	79	ARG
38	2g	85	TYR
38	2g	114	ARG
38	2g	115	ARG
38	2g	119	ARG
38	2g	137	LYS
38	2g	154	TYR
38	2g	155	ARG
39	2h	2	LEU
39	2h	25	ASP
39	2h	63	LEU
39	2h	81	HIS
39	2h	85	ARG
39	2h	99	GLU
39	2h	112	LEU
39	2h	115	SER
39	2h	118	VAL
39	2h	137	VAL
40	2i	14	VAL
40	2i	53	VAL
40	2i	64	THR
40	2i	65	VAL
40	2i	75	ASP
40	2i	111	ARG
40	2i	114	TYR
40	2i	124	GLN
40	2i	125	TYR
41	2j	9	ARG
41	2j	44	VAL
41	2j	65	LEU
41	2j	92	THR
41	2j	96	ILE
42	2k	14	VAL
42	2k	29	ILE
42	2k	48	ILE
42	2k	50	TYR
42	2k	63	LEU

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Mol	Chain	Res	Type
42	2k	80	VAL
42	2k	104	GLN
42	2k	116	HIS
42	2k	120	ARG
43	2l	6	THR
43	2l	18	VAL
43	2l	36	VAL
43	2l	38	THR
43	2l	104	VAL
43	2l	113	ARG
44	2m	15	VAL
44	2m	19	LEU
44	2m	34	LEU
44	2m	47	ASP
44	2m	50	GLU
44	2m	69	GLU
44	2m	71	ARG
44	2m	79	LYS
44	2m	103	THR
44	2m	105	THR
45	2n	3	ARG
45	2n	7	ILE
45	2n	11	LYS
45	2n	13	THR
45	2n	15	LYS
45	2n	58	LYS
46	2o	5	LYS
46	2o	7	GLU
46	2o	35	ARG
46	2o	39	LEU
46	2o	62	GLN
46	2o	64	ARG
46	2o	83	GLU
47	2p	1	MET
47	2p	16	HIS
47	2p	42	ARG
47	2p	45	THR
47	2p	62	VAL
48	2q	37	LYS
48	2q	52	LYS
48	2q	63	ARG
48	2q	66	SER

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Mol	Chain	Res	Type
48	2q	68	ARG
48	2q	87	LYS
48	2q	99	SER
49	2r	25	THR
49	2r	31	LEU
49	2r	37	VAL
49	2r	54	ARG
49	2r	74	ARG
49	2r	85	LEU
50	2s	28	LYS
50	2s	30	LEU
50	2s	48	THR
50	2s	49	ILE
50	2s	65	ASN
50	2s	79	THR
50	2s	81	ARG
51	2t	19	SER
51	2t	71	THR
51	2t	100	ILE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (105) such sidechains are listed below:

Mol	Chain	Res	Type
4	1E	48	GLN
5	1F	8	GLN
8	1I	139	GLN
9	1N	131	GLN
10	1O	3	GLN
10	1O	5	GLN
12	1Q	57	HIS
12	1Q	123	HIS
13	1R	13	HIS
13	1R	71	GLN
13	1R	91	GLN
14	1S	61	ASN
15	1T	58	ASN
16	1U	94	ASN
19	1X	31	HIS
19	1X	82	GLN
20	1Y	6	HIS
20	1Y	92	ASN
21	1Z	73	GLN

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Mol	Chain	Res	Type
21	1Z	151	HIS
22	10	3	HIS
23	11	56	GLN
24	12	38	GLN
33	1b	16	HIS
33	1b	78	GLN
33	1b	94	ASN
34	1c	6	HIS
34	1c	104	GLN
34	1c	110	ASN
35	1d	42	GLN
35	1d	116	GLN
35	1d	119	GLN
35	1d	123	HIS
36	1e	78	HIS
37	1f	13	ASN
37	1f	18	GLN
37	1f	100	ASN
38	1g	28	ASN
38	1g	64	GLN
39	1h	15	ASN
40	1i	3	GLN
40	1i	34	ASN
40	1i	58	HIS
40	1i	73	GLN
40	1i	124	GLN
41	1j	56	HIS
42	1k	99	GLN
44	1m	12	ASN
46	1o	28	GLN
46	1o	46	HIS
47	1p	16	HIS
47	1p	65	GLN
49	1r	63	GLN
50	1s	14	HIS
50	1s	23	ASN
50	1s	57	HIS
50	1s	69	HIS
50	1s	83	HIS
51	1t	90	GLN
4	2E	48	GLN
5	2F	69	HIS

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Mol	Chain	Res	Type
5	2F	75	HIS
6	2G	58	GLN
9	2N	8	GLN
14	2S	38	GLN
15	2T	43	GLN
15	2T	58	ASN
18	2W	60	ASN
19	2X	31	HIS
20	2Y	6	HIS
20	2Y	92	ASN
21	2Z	73	GLN
23	21	56	GLN
31	29	20	HIS
33	2b	19	HIS
33	2b	40	HIS
33	2b	224	GLN
34	2c	6	HIS
35	2d	74	GLN
35	2d	77	ASN
35	2d	116	GLN
35	2d	119	GLN
35	2d	123	HIS
35	2d	125	HIS
36	2e	78	HIS
38	2g	28	ASN
38	2g	86	GLN
38	2g	109	ASN
38	2g	122	HIS
38	2g	153	HIS
40	2i	3	GLN
40	2i	23	ASN
40	2i	31	GLN
40	2i	124	GLN
41	2j	33	GLN
42	2k	99	GLN
43	2l	99	HIS
44	2m	62	ASN
44	2m	77	ASN
46	2o	28	GLN
48	2q	16	GLN
48	2q	26	GLN
49	2r	63	GLN

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Mol	Chain	Res	Type
50	2s	23	ASN
51	2t	16	HIS

### 5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	1A	2861/2915 (98%)	479 (16%)	37 (1%)
1	2A	2788/2915 (95%)	530 (19%)	25 (0%)
2	1B	120/121 (99%)	12 (10%)	1 (0%)
2	2B	118/121 (97%)	31 (26%)	0
32	1a	1494/1521 (98%)	285 (19%)	0
32	2a	1498/1521 (98%)	259 (17%)	0
53	1v	9/24 (37%)	4 (44%)	0
53	2v	4/24 (16%)	0	0
54	1x	75/77 (97%)	8 (10%)	0
54	2x	75/77 (97%)	11 (14%)	0
All	All	9042/9316 (97%)	1619 (17%)	63 (0%)

All (1619) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	1A	10	G
1	1A	12	U
1	1A	13	A
1	1A	14	A
1	1A	15	G
1	1A	34	C
1	1A	36	G
1	1A	45	C
1	1A	51	G
1	1A	55	G
1	1A	58	G
1	1A	64	A
1	1A	71	A
1	1A	74	A
1	1A	75	G
1	1A	84	A
1	1A	95	G
1	1A	118	A
1	1A	119	A
1	1A	120	U

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Mol	Chain	Res	Type
1	1A	125	G
1	1A	131	G
1	1A	139	G
1	1A	139(A)	G
1	1A	154	G
1	1A	181	A
1	1A	182	A
1	1A	188	G
1	1A	196	A
1	1A	199	A
1	1A	205	G
1	1A	214	G
1	1A	216	A
1	1A	222	A
1	1A	225	A
1	1A	228	A
1	1A	229	A
1	1A	233	A
1	1A	248	G
1	1A	250	G
1	1A	271(L)	U
1	1A	271(M)	G
1	1A	271(N)	U
1	1A	271(R)	G
1	1A	272(B)	G
1	1A	275	G
1	1A	279	C
1	1A	311	A
1	1A	329	G
1	1A	330	A
1	1A	352	G
1	1A	363	G
1	1A	363(B)	G
1	1A	363(E)	U
1	1A	363(F)	A
1	1A	370	G
1	1A	380	U
1	1A	386	G
1	1A	389	G
1	1A	396	G
1	1A	405	U
1	1A	411	G

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Mol	Chain	Res	Type
1	1A	428	A
1	1A	442	G
1	1A	444	C
1	1A	446	G
1	1A	448	U
1	1A	457	A
1	1A	481	G
1	1A	504	U
1	1A	505	A
1	1A	509	C
1	1A	512	G
1	1A	530	G
1	1A	531	C
1	1A	532	A
1	1A	533	G
1	1A	545	G
1	1A	549	G
1	1A	555	U
1	1A	563	G
1	1A	573	G
1	1A	574	C
1	1A	575	A
1	1A	594	U
1	1A	603	A
1	1A	604	G
1	1A	607	U
1	1A	614(A)	U
1	1A	614(B)	G
1	1A	615	G
1	1A	619	G
1	1A	627	A
1	1A	637	A
1	1A	645	C
1	1A	646	A
1	1A	652(A)	A
1	1A	652(E)	G
1	1A	652(T)	C
1	1A	669	G
1	1A	686	G
1	1A	717	G
1	1A	726	G
1	1A	730	C

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Mol	Chain	Res	Type
1	1A	764	A
1	1A	775	G
1	1A	776	G
1	1A	782	A
1	1A	784	A
1	1A	785	G
1	1A	792	G
1	1A	802	A
1	1A	805	G
1	1A	812	C
1	1A	819	A
1	1A	827	U
1	1A	828	U
1	1A	859	G
1	1A	867	C
1	1A	880	G
1	1A	881	G
1	1A	884	C
1	1A	885	C
1	1A	886	C
1	1A	887	A
1	1A	888	C
1	1A	889	C
1	1A	890	A
1	1A	896	A
1	1A	897	C
1	1A	898	C
1	1A	907	U
1	1A	910	A
1	1A	932	G
1	1A	938	G
1	1A	945	A
1	1A	946	G
1	1A	953	A
1	1A	958	U
1	1A	959	A
1	1A	961	C
1	1A	974	G
1	1A	975	C
1	1A	983	A
1	1A	990	A
1	1A	996	A

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Mol	Chain	Res	Type
1	1A	1005	C
1	1A	1006	C
1	1A	1008	C
1	1A	1009	A
1	1A	1012	U
1	1A	1013	C
1	1A	1022	G
1	1A	1026	U
1	1A	1033	U
1	1A	1038	C
1	1A	1041	C
1	1A	1045	A
1	1A	1046	A
1	1A	1047	G
1	1A	1048	A
1	1A	1054	A
1	1A	1055	G
1	1A	1058	G
1	1A	1066	U
1	1A	1068	G
1	1A	1070	A
1	1A	1071	G
1	1A	1073	A
1	1A	1075	C
1	1A	1076	C
1	1A	1078	U
1	1A	1079	C
1	1A	1082	U
1	1A	1083	U
1	1A	1084	A
1	1A	1086	A
1	1A	1088	A
1	1A	1089	G
1	1A	1090	U
1	1A	1091	G
1	1A	1094	U
1	1A	1096	A
1	1A	1101	U
1	1A	1103	A
1	1A	1106	G
1	1A	1108	U
1	1A	1111	A

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Mol	Chain	Res	Type
1	1A	1112	G
1	1A	1115	G
1	1A	1116	C
1	1A	1128	A
1	1A	1129	A
1	1A	1130	U
1	1A	1132	A
1	1A	1135	C
1	1A	1136	G
1	1A	1149	G
1	1A	1155	A
1	1A	1170	G
1	1A	1171	G
1	1A	1173	G
1	1A	1174	A
1	1A	1175	U
1	1A	1176	G
1	1A	1177	A
1	1A	1178	C
1	1A	1189	A
1	1A	1211	U
1	1A	1218	C
1	1A	1220	A
1	1A	1237	A
1	1A	1244	G
1	1A	1250	G
1	1A	1253	A
1	1A	1256	G
1	1A	1271	G
1	1A	1272	A
1	1A	1273	U
1	1A	1274	A
1	1A	1289	C
1	1A	1290	C
1	1A	1298	C
1	1A	1300	U
1	1A	1301	A
1	1A	1316	U
1	1A	1352	U
1	1A	1354	A
1	1A	1359	A
1	1A	1360	A

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Mol	Chain	Res	Type
1	1A	1365	A
1	1A	1370	C
1	1A	1372	U
1	1A	1384	A
1	1A	1385	G
1	1A	1396	U
1	1A	1416	G
1	1A	1417	C
1	1A	1420	U
1	1A	1421	G
1	1A	1428	C
1	1A	1445	A
1	1A	1450	G
1	1A	1455	G
1	1A	1467	C
1	1A	1482	G
1	1A	1493	C
1	1A	1497	U
1	1A	1504	C
1	1A	1508	A
1	1A	1509	C
1	1A	1509(A)	A
1	1A	1525	G
1	1A	1541	G
1	1A	1542	A
1	1A	1558	A
1	1A	1566	A
1	1A	1569	A
1	1A	1578	U
1	1A	1580	A
1	1A	1581	G
1	1A	1584	C
1	1A	1586	A
1	1A	1608	A
1	1A	1609	A
1	1A	1616	A
1	1A	1627	G
1	1A	1647	G
1	1A	1648	C
1	1A	1654	A
1	1A	1656	C
1	1A	1667	G

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Mol	Chain	Res	Type
1	1A	1674	G
1	1A	1675	C
1	1A	1696	G
1	1A	1700	A
1	1A	1701	A
1	1A	1722	A
1	1A	1739	U
1	1A	1746	G
1	1A	1756	G
1	1A	1762	A
1	1A	1763	G
1	1A	1764	G
1	1A	1773	A
1	1A	1780	A
1	1A	1782	C
1	1A	1791	A
1	1A	1800	C
1	1A	1801	G
1	1A	1812	A
1	1A	1816	G
1	1A	1817	G
1	1A	1819	A
1	1A	1829	A
1	1A	1847	A
1	1A	1853	A
1	1A	1858	G
1	1A	1861	G
1	1A	1878	G
1	1A	1889	A
1	1A	1900	A
1	1A	1906	G
1	1A	1913	A
1	1A	1915	5MU
1	1A	1919	A
1	1A	1927	A
1	1A	1929	G
1	1A	1930	G
1	1A	1938	A
1	1A	1955	U
1	1A	1962	5MC
1	1A	1963	U
1	1A	1964	G

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Mol	Chain	Res	Type
1	1A	1967	C
1	1A	1970	A
1	1A	1971	A
1	1A	1972	A
1	1A	1983	C
1	1A	1993	U
1	1A	1997	G
1	1A	2020	A
1	1A	2023	G
1	1A	2031	A
1	1A	2032	G
1	1A	2033	A
1	1A	2043	C
1	1A	2055	C
1	1A	2056	G
1	1A	2060	A
1	1A	2061	G
1	1A	2062	A
1	1A	2069	G
1	1A	2092	U
1	1A	2097	C
1	1A	2101	G
1	1A	2104	G
1	1A	2111	C
1	1A	2113	U
1	1A	2116	G
1	1A	2123	G
1	1A	2126	A
1	1A	2127	G
1	1A	2129	C
1	1A	2130	U
1	1A	2131	G
1	1A	2132	U
1	1A	2133	G
1	1A	2134	A
1	1A	2135	A
1	1A	2141	G
1	1A	2142	C
1	1A	2144	U
1	1A	2146	C
1	1A	2147	G
1	1A	2150	U

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Mol	Chain	Res	Type
1	1A	2151	G
1	1A	2156	G
1	1A	2157	G
1	1A	2158	A
1	1A	2159	G
1	1A	2162	G
1	1A	2165	G
1	1A	2166	G
1	1A	2171	A
1	1A	2172	U
1	1A	2173	A
1	1A	2175	C
1	1A	2181	G
1	1A	2182	G
1	1A	2183	C
1	1A	2184	G
1	1A	2189	U
1	1A	2192	G
1	1A	2198	A
1	1A	2206	G
1	1A	2207	G
1	1A	2208	A
1	1A	2218	U
1	1A	2219	G
1	1A	2225	A
1	1A	2238	G
1	1A	2239	G
1	1A	2242	G
1	1A	2249	U
1	1A	2268	A
1	1A	2269	A
1	1A	2273	A
1	1A	2282	G
1	1A	2283	C
1	1A	2286	A
1	1A	2287	A
1	1A	2289	G
1	1A	2305	A
1	1A	2307	G
1	1A	2308	G
1	1A	2320	A
1	1A	2325	G

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Mol	Chain	Res	Type
1	1A	2334	G
1	1A	2336	A
1	1A	2347	C
1	1A	2350	C
1	1A	2354	G
1	1A	2361	A
1	1A	2372	G
1	1A	2379	G
1	1A	2383	G
1	1A	2385	C
1	1A	2396	G
1	1A	2405	G
1	1A	2406	U
1	1A	2410	G
1	1A	2422	A
1	1A	2425	A
1	1A	2429	G
1	1A	2430	A
1	1A	2431	U
1	1A	2435	A
1	1A	2438	U
1	1A	2439	A
1	1A	2441	C
1	1A	2448	A
1	1A	2468	G
1	1A	2476	A
1	1A	2477	C
1	1A	2481	G
1	1A	2487	G
1	1A	2490	G
1	1A	2502	G
1	1A	2505	G
1	1A	2506	U
1	1A	2507	C
1	1A	2518	A
1	1A	2525	G
1	1A	2529	G
1	1A	2554	U
1	1A	2566	A
1	1A	2567	G
1	1A	2573	C
1	1A	2579	C

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Mol	Chain	Res	Type
1	1A	2582	G
1	1A	2585	U
1	1A	2602	A
1	1A	2609	U
1	1A	2611	U
1	1A	2612	C
1	1A	2629	A
1	1A	2630	G
1	1A	2638	G
1	1A	2654	A
1	1A	2689	U
1	1A	2690	C
1	1A	2702	U
1	1A	2703	C
1	1A	2712(A)	A
1	1A	2713	A
1	1A	2714	G
1	1A	2726	U
1	1A	2733	A
1	1A	2758	A
1	1A	2764	A
1	1A	2765	A
1	1A	2778	A
1	1A	2780	G
1	1A	2790	A
1	1A	2791	C
1	1A	2802	G
1	1A	2805	G
1	1A	2818	G
1	1A	2820	A
1	1A	2821	A
1	1A	2835	A
1	1A	2839	G
1	1A	2855	C
1	1A	2861	G
1	1A	2872	G
1	1A	2880	C
1	1A	2892	A
1	1A	2894	G
2	1B	2	C
2	1B	13	A
2	1B	15	A

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Mol	Chain	Res	Type
2	1B	35	U
2	1B	50	G
2	1B	52	A
2	1B	56	G
2	1B	73	A
2	1B	85	G
2	1B	91	C
2	1B	106	G
2	1B	110	G
32	1a	9	G
32	1a	26	A
32	1a	31	G
32	1a	32	A
32	1a	39	G
32	1a	44	G
32	1a	48	C
32	1a	50	A
32	1a	51	A
32	1a	61	G
32	1a	78	G
32	1a	79	G
32	1a	91	C
32	1a	98	G
32	1a	101	A
32	1a	105	G
32	1a	116	A
32	1a	121	C
32	1a	129(A)	G
32	1a	131	C
32	1a	151	A
32	1a	162	A
32	1a	163	C
32	1a	164	U
32	1a	174	C
32	1a	176	C
32	1a	182	U
32	1a	189(F)	U
32	1a	195	A
32	1a	197	A
32	1a	199	G
32	1a	201	C
32	1a	202	U

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Mol	Chain	Res	Type
32	1a	203	U
32	1a	204	U
32	1a	216	G
32	1a	247	G
32	1a	251	G
32	1a	258	G
32	1a	266	G
32	1a	267	C
32	1a	279	A
32	1a	289	G
32	1a	316	G
32	1a	321	A
32	1a	327	A
32	1a	328	C
32	1a	330	C
32	1a	332	G
32	1a	345	C
32	1a	348	G
32	1a	352	C
32	1a	353	A
32	1a	354	G
32	1a	358	U
32	1a	359	U
32	1a	363	A
32	1a	367	U
32	1a	372	C
32	1a	373	A
32	1a	378	G
32	1a	382	A
32	1a	384	G
32	1a	397	A
32	1a	398	C
32	1a	406	G
32	1a	412	A
32	1a	414	A
32	1a	415	A
32	1a	421	U
32	1a	423	G
32	1a	424	G
32	1a	429	U
32	1a	430	A
32	1a	433	C

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Mol	Chain	Res	Type
32	1a	437	U
32	1a	438	G
32	1a	439	A
32	1a	442	C
32	1a	451	A
32	1a	452	A
32	1a	457	C
32	1a	461	A
32	1a	470	C
32	1a	471	G
32	1a	474	G
32	1a	480	U
32	1a	485	G
32	1a	496	A
32	1a	498	U
32	1a	505	G
32	1a	506	G
32	1a	509	A
32	1a	510	A
32	1a	511	C
32	1a	518	C
32	1a	519	C
32	1a	531	U
32	1a	532	A
32	1a	533	A
32	1a	534	U
32	1a	536	C
32	1a	547	A
32	1a	559	A
32	1a	560	U
32	1a	561	U
32	1a	562	C
32	1a	568	G
32	1a	572	A
32	1a	573	A
32	1a	574	A
32	1a	576	G
32	1a	577	G
32	1a	596	C
32	1a	607	A
32	1a	618	C
32	1a	630	G

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
32	1a	633	G
32	1a	653	A
32	1a	657	G
32	1a	659	U
32	1a	665	A
32	1a	671	G
32	1a	684	A
32	1a	686	U
32	1a	687	A
32	1a	688	G
32	1a	693	G
32	1a	695	A
32	1a	723	U
32	1a	724	G
32	1a	731	G
32	1a	749	C
32	1a	755	G
32	1a	759	A
32	1a	766	A
32	1a	773	G
32	1a	774	G
32	1a	777	A
32	1a	792	A
32	1a	793	U
32	1a	794	A
32	1a	810	C
32	1a	815	A
32	1a	817	C
32	1a	821	G
32	1a	828	A
32	1a	832	C
32	1a	836	G
32	1a	840	C
32	1a	841	U
32	1a	851	G
32	1a	855	G
32	1a	859	A
32	1a	870	U
32	1a	873	A
32	1a	902	G
32	1a	914	A
32	1a	926	G

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
32	1a	927	G
32	1a	934	C
32	1a	935	A
32	1a	936	C
32	1a	960	U
32	1a	961	U
32	1a	968	A
32	1a	969	A
32	1a	971	G
32	1a	974	A
32	1a	975	A
32	1a	976	G
32	1a	977	A
32	1a	982	U
32	1a	992	U
32	1a	993	G
32	1a	994	A
32	1a	997	U
32	1a	998	G
32	1a	999	C
32	1a	1000	U
32	1a	1003	G
32	1a	1005	A
32	1a	1006	C
32	1a	1009	G
32	1a	1011	G
32	1a	1020	U
32	1a	1022	G
32	1a	1023	G
32	1a	1025	U
32	1a	1026	G
32	1a	1027	C
32	1a	1028	C
32	1a	1030	C
32	1a	1030(A)	G
32	1a	1030(C)	G
32	1a	1031	G
32	1a	1035	A
32	1a	1039	C
32	1a	1043	C
32	1a	1044	A
32	1a	1045	C

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Mol	Chain	Res	Type
32	1a	1050	G
32	1a	1054	C
32	1a	1056	U
32	1a	1065	U
32	1a	1066	C
32	1a	1068	G
32	1a	1081	G
32	1a	1086	U
32	1a	1094	G
32	1a	1095	U
32	1a	1096	C
32	1a	1101	A
32	1a	1121	U
32	1a	1122	U
32	1a	1124	G
32	1a	1125	U
32	1a	1134	G
32	1a	1137	C
32	1a	1138	G
32	1a	1139	G
32	1a	1141	C
32	1a	1146	A
32	1a	1152	A
32	1a	1154	G
32	1a	1157	A
32	1a	1159	U
32	1a	1183	A
32	1a	1184	G
32	1a	1196	U
32	1a	1197	G
32	1a	1202	G
32	1a	1212	U
32	1a	1213	A
32	1a	1214	C
32	1a	1222	G
32	1a	1227	A
32	1a	1233	G
32	1a	1236	A
32	1a	1238	A
32	1a	1256	A
32	1a	1257	U
32	1a	1258	G

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Mol	Chain	Res	Type
32	1a	1260	C
32	1a	1270	C
32	1a	1275	A
32	1a	1278	U
32	1a	1279	A
32	1a	1280	A
32	1a	1286	A
32	1a	1287	A
32	1a	1299	A
32	1a	1300	G
32	1a	1302	U
32	1a	1312	G
32	1a	1320	C
32	1a	1323	G
32	1a	1338	G
32	1a	1346	A
32	1a	1347	G
32	1a	1353	G
32	1a	1363	C
32	1a	1363(A)	A
32	1a	1368	G
32	1a	1370	G
32	1a	1379	G
32	1a	1394	A
32	1a	1396	A
32	1a	1397	C
32	1a	1403	C
32	1a	1419	G
32	1a	1442	G
32	1a	1442(A)	G
32	1a	1446	U
32	1a	1447	A
32	1a	1487	G
32	1a	1492	A
32	1a	1494	G
32	1a	1503	A
32	1a	1504	G
32	1a	1506	U
32	1a	1517	G
32	1a	1520	G
32	1a	1529	G
32	1a	1530	G

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Mol	Chain	Res	Type
53	1v	14	A
53	1v	15	A
53	1v	19	U
53	1v	21	C
54	1x	9	G
54	1x	14	A
54	1x	18	G
54	1x	19	G
54	1x	21	A
54	1x	32	5MC
54	1x	47	U
54	1x	76	A
1	2A	8	A
1	2A	10	G
1	2A	14	A
1	2A	15	G
1	2A	34	C
1	2A	35	G
1	2A	45	C
1	2A	61	G
1	2A	64	A
1	2A	71	A
1	2A	72	U
1	2A	74	A
1	2A	75	G
1	2A	84	A
1	2A	90	U
1	2A	94	C
1	2A	100	G
1	2A	102	G
1	2A	118	A
1	2A	119	A
1	2A	120	U
1	2A	121	G
1	2A	125	G
1	2A	126	A
1	2A	131	G
1	2A	141	A
1	2A	154(A)	C
1	2A	157	U
1	2A	181	A
1	2A	196	A

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Mol	Chain	Res	Type
1	2A	199	A
1	2A	205	G
1	2A	214	G
1	2A	216	A
1	2A	221	A
1	2A	222	A
1	2A	225	A
1	2A	228	A
1	2A	229	A
1	2A	233	A
1	2A	248	G
1	2A	249	C
1	2A	250	G
1	2A	271(J)	C
1	2A	271(K)	U
1	2A	271(L)	U
1	2A	271(M)	G
1	2A	271(N)	U
1	2A	271(O)	C
1	2A	272(B)	G
1	2A	274	G
1	2A	277	C
1	2A	278	A
1	2A	279	C
1	2A	280	C
1	2A	294	A
1	2A	303	U
1	2A	311	A
1	2A	317	G
1	2A	324	A
1	2A	327	G
1	2A	329	G
1	2A	330	A
1	2A	333	G
1	2A	352	G
1	2A	362	U
1	2A	363	G
1	2A	363(B)	G
1	2A	363(D)	G
1	2A	372	G
1	2A	386	G
1	2A	396	G

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Mol	Chain	Res	Type
1	2A	399	G
1	2A	405	U
1	2A	407	G
1	2A	411	G
1	2A	421	U
1	2A	422	A
1	2A	435	C
1	2A	444	C
1	2A	454	A
1	2A	455	C
1	2A	457	A
1	2A	474	G
1	2A	479	A
1	2A	481	G
1	2A	496	G
1	2A	499	U
1	2A	504	U
1	2A	505	A
1	2A	509	C
1	2A	519	U
1	2A	529	A
1	2A	530	G
1	2A	531	C
1	2A	532	A
1	2A	533	G
1	2A	545	G
1	2A	551	G
1	2A	563	G
1	2A	568	U
1	2A	573	G
1	2A	575	A
1	2A	588	U
1	2A	595	C
1	2A	599	G
1	2A	603	A
1	2A	604	G
1	2A	607	U
1	2A	609	A
1	2A	614(A)	U
1	2A	614(B)	G
1	2A	614(C)	A
1	2A	615	G

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Mol	Chain	Res	Type
1	2A	620	G
1	2A	627	A
1	2A	637	A
1	2A	645	C
1	2A	652(B)	A
1	2A	669	G
1	2A	686	G
1	2A	709	U
1	2A	717	G
1	2A	718	A
1	2A	726	G
1	2A	730	C
1	2A	752	A
1	2A	753	C
1	2A	771	G
1	2A	775	G
1	2A	776	G
1	2A	779	U
1	2A	782	A
1	2A	783	A
1	2A	784	A
1	2A	785	G
1	2A	790	C
1	2A	791	C
1	2A	792	G
1	2A	805	G
1	2A	812	C
1	2A	819	A
1	2A	825	C
1	2A	827	U
1	2A	828	U
1	2A	832	G
1	2A	847	U
1	2A	857	C
1	2A	859	G
1	2A	869	G
1	2A	870	A
1	2A	874	G
1	2A	879	G
1	2A	880	G
1	2A	884	C
1	2A	886	C

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Mol	Chain	Res	Type
1	2A	887	A
1	2A	888	C
1	2A	889	C
1	2A	892	G
1	2A	893	C
1	2A	894	C
1	2A	895	U
1	2A	896	A
1	2A	900	A
1	2A	901	A
1	2A	904	C
1	2A	910	A
1	2A	914	C
1	2A	917	A
1	2A	932	G
1	2A	941	A
1	2A	945	A
1	2A	946	G
1	2A	953	A
1	2A	958	U
1	2A	959	A
1	2A	961	C
1	2A	974	G
1	2A	975	C
1	2A	983	A
1	2A	996	A
1	2A	997	G
1	2A	998	C
1	2A	1012	U
1	2A	1013	C
1	2A	1017	G
1	2A	1020	A
1	2A	1022	G
1	2A	1025	G
1	2A	1033	U
1	2A	1038	C
1	2A	1039	G
1	2A	1043	C
1	2A	1116	C
1	2A	1117	G
1	2A	1126	A
1	2A	1130	U

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Mol	Chain	Res	Type
1	2A	1135	C
1	2A	1136	G
1	2A	1139	G
1	2A	1143	A
1	2A	1155	A
1	2A	1159	U
1	2A	1171	G
1	2A	1188	U
1	2A	1195	G
1	2A	1204	A
1	2A	1211	U
1	2A	1220	A
1	2A	1229	G
1	2A	1236	G
1	2A	1237	A
1	2A	1247	A
1	2A	1253	A
1	2A	1256	G
1	2A	1271	G
1	2A	1272	A
1	2A	1273	U
1	2A	1284	A
1	2A	1300	U
1	2A	1301	A
1	2A	1303	G
1	2A	1314	C
1	2A	1318	C
1	2A	1352	U
1	2A	1359	A
1	2A	1360	A
1	2A	1365	A
1	2A	1368	G
1	2A	1370	C
1	2A	1380	G
1	2A	1384	A
1	2A	1385	G
1	2A	1386	C
1	2A	1395	A
1	2A	1400	G
1	2A	1416	G
1	2A	1417	C
1	2A	1420	U

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Mol	Chain	Res	Type
1	2A	1421	G
1	2A	1427	A
1	2A	1428	C
1	2A	1437	C
1	2A	1445	A
1	2A	1445(A)	C
1	2A	1449	A
1	2A	1450	G
1	2A	1455	G
1	2A	1460	A
1	2A	1461	G
1	2A	1467	C
1	2A	1471	A
1	2A	1482	G
1	2A	1493	C
1	2A	1495	A
1	2A	1497	U
1	2A	1508	A
1	2A	1509	C
1	2A	1509(A)	A
1	2A	1531	C
1	2A	1532	C
1	2A	1533	G
1	2A	1541	G
1	2A	1543	C
1	2A	1558	A
1	2A	1559	G
1	2A	1566	A
1	2A	1569	A
1	2A	1578	U
1	2A	1580	A
1	2A	1584	C
1	2A	1586	A
1	2A	1589	C
1	2A	1595	G
1	2A	1603	A
1	2A	1608	A
1	2A	1609	A
1	2A	1610	A
1	2A	1613	G
1	2A	1616	A
1	2A	1640	C

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Mol	Chain	Res	Type
1	2A	1647	G
1	2A	1648	C
1	2A	1654	A
1	2A	1664	A
1	2A	1672	C
1	2A	1674	G
1	2A	1675	C
1	2A	1696	G
1	2A	1700	A
1	2A	1701	A
1	2A	1708	C
1	2A	1722	A
1	2A	1739	U
1	2A	1740	G
1	2A	1745(A)	C
1	2A	1746	G
1	2A	1748	G
1	2A	1756	G
1	2A	1762	A
1	2A	1763	G
1	2A	1764	G
1	2A	1773	A
1	2A	1780	A
1	2A	1782	C
1	2A	1786	A
1	2A	1791	A
1	2A	1800	C
1	2A	1801	G
1	2A	1811	G
1	2A	1812	A
1	2A	1816	G
1	2A	1828	G
1	2A	1829	A
1	2A	1835	G
1	2A	1836	C
1	2A	1847	A
1	2A	1857	G
1	2A	1877	A
1	2A	1878	G
1	2A	1885	A
1	2A	1900	A
1	2A	1906	G

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Mol	Chain	Res	Type
1	2A	1910	G
1	2A	1913	A
1	2A	1914	C
1	2A	1915	5MU
1	2A	1929	G
1	2A	1930	G
1	2A	1931	U
1	2A	1936	A
1	2A	1937	A
1	2A	1938	A
1	2A	1955	U
1	2A	1963	U
1	2A	1964	G
1	2A	1967	C
1	2A	1970	A
1	2A	1971	A
1	2A	1972	A
1	2A	1993	U
1	2A	1997	G
1	2A	2020	A
1	2A	2023	G
1	2A	2031	A
1	2A	2032	G
1	2A	2033	A
1	2A	2036	C
1	2A	2043	C
1	2A	2055	C
1	2A	2056	G
1	2A	2060	A
1	2A	2061	G
1	2A	2062	A
1	2A	2069	G
1	2A	2093	G
1	2A	2098	U
1	2A	2104	G
1	2A	2108	C
1	2A	2110	G
1	2A	2111	C
1	2A	2112	G
1	2A	2116	G
1	2A	2117	A
1	2A	2119	A

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Mol	Chain	Res	Type
1	2A	2120	G
1	2A	2122	U
1	2A	2126	A
1	2A	2127	G
1	2A	2129	C
1	2A	2131	G
1	2A	2132	U
1	2A	2133	G
1	2A	2134	A
1	2A	2135	A
1	2A	2136	C
1	2A	2137	C
1	2A	2138	C
1	2A	2140	C
1	2A	2142	C
1	2A	2143	C
1	2A	2146	C
1	2A	2150	U
1	2A	2151	G
1	2A	2153	G
1	2A	2154	G
1	2A	2155	G
1	2A	2156	G
1	2A	2157	G
1	2A	2158	A
1	2A	2160	G
1	2A	2161	C
1	2A	2162	G
1	2A	2164	C
1	2A	2166	G
1	2A	2167	U
1	2A	2168	G
1	2A	2171	A
1	2A	2172	U
1	2A	2177	C
1	2A	2178	C
1	2A	2181	G
1	2A	2182	G
1	2A	2185	C
1	2A	2186	G
1	2A	2189	U
1	2A	2190	G

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Mol	Chain	Res	Type
1	2A	2192	G
1	2A	2197	U
1	2A	2198	A
1	2A	2200	C
1	2A	2206	G
1	2A	2207	G
1	2A	2208	A
1	2A	2218	U
1	2A	2225	A
1	2A	2235	G
1	2A	2238	G
1	2A	2239	G
1	2A	2275	C
1	2A	2278	A
1	2A	2279	G
1	2A	2283	C
1	2A	2287	A
1	2A	2288	A
1	2A	2294	C
1	2A	2305	A
1	2A	2308	G
1	2A	2312	U
1	2A	2319	G
1	2A	2320	A
1	2A	2325	G
1	2A	2334	G
1	2A	2336	A
1	2A	2347	C
1	2A	2350	C
1	2A	2372	G
1	2A	2376	A
1	2A	2377	A
1	2A	2383	G
1	2A	2385	C
1	2A	2391	G
1	2A	2403	C
1	2A	2406	U
1	2A	2410	G
1	2A	2414	G
1	2A	2422	A
1	2A	2425	A
1	2A	2428	G

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Mol	Chain	Res	Type
1	2A	2429	G
1	2A	2430	A
1	2A	2435	A
1	2A	2439	A
1	2A	2441	C
1	2A	2448	A
1	2A	2458	G
1	2A	2465	C
1	2A	2468	G
1	2A	2469	A
1	2A	2474	C
1	2A	2476	A
1	2A	2477	C
1	2A	2480	C
1	2A	2486	G
1	2A	2487	G
1	2A	2490	G
1	2A	2502	G
1	2A	2505	G
1	2A	2506	U
1	2A	2507	C
1	2A	2518	A
1	2A	2520	C
1	2A	2525	G
1	2A	2529	G
1	2A	2543	G
1	2A	2554	U
1	2A	2555	U
1	2A	2566	A
1	2A	2567	G
1	2A	2569	G
1	2A	2574	G
1	2A	2585	U
1	2A	2592	G
1	2A	2601	C
1	2A	2602	A
1	2A	2608	G
1	2A	2609	U
1	2A	2611	U
1	2A	2612	C
1	2A	2620	C
1	2A	2630	G

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Mol	Chain	Res	Type
1	2A	2634	G
1	2A	2654	A
1	2A	2679	A
1	2A	2689	U
1	2A	2690	C
1	2A	2702	U
1	2A	2703	C
1	2A	2712(A)	A
1	2A	2713	A
1	2A	2714	G
1	2A	2718	G
1	2A	2726	U
1	2A	2733	A
1	2A	2751	G
1	2A	2757	A
1	2A	2758	A
1	2A	2759	G
1	2A	2761	G
1	2A	2764	A
1	2A	2765	A
1	2A	2766	G
1	2A	2778	A
1	2A	2789	C
1	2A	2793	G
1	2A	2802	G
1	2A	2803	C
1	2A	2808	U
1	2A	2818	G
1	2A	2820	A
1	2A	2821	A
1	2A	2833	G
1	2A	2835	A
1	2A	2872	G
1	2A	2873	A
1	2A	2880	C
1	2A	2894	G
1	2A	2895	U
1	2A	2897	U
2	2B	2	C
2	2B	5	C
2	2B	8	U
2	2B	19	G

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Mol	Chain	Res	Type
2	2B	20	C
2	2B	25	A
2	2B	30	C
2	2B	41	U
2	2B	42	C
2	2B	52	A
2	2B	53	A
2	2B	56	G
2	2B	63	G
2	2B	67	G
2	2B	73	A
2	2B	74	U
2	2B	75	G
2	2B	85	G
2	2B	88	C
2	2B	89	G
2	2B	91	C
2	2B	94	C
2	2B	106	G
2	2B	108	U
2	2B	110	G
2	2B	111	G
2	2B	114	C
2	2B	116	G
2	2B	117	G
2	2B	119	G
2	2B	120	A
32	2a	9	G
32	2a	16	A
32	2a	22	G
32	2a	32	A
32	2a	39	G
32	2a	41	G
32	2a	47	C
32	2a	48	C
32	2a	50	A
32	2a	51	A
32	2a	59	A
32	2a	65	U
32	2a	66	G
32	2a	73	G
32	2a	88	A

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Mol	Chain	Res	Type
32	2a	89	C
32	2a	90	U
32	2a	92	C
32	2a	98	G
32	2a	101	A
32	2a	116	A
32	2a	121	C
32	2a	129(A)	G
32	2a	131	C
32	2a	159	G
32	2a	163	C
32	2a	174	C
32	2a	182	U
32	2a	189	G
32	2a	189(A)	C
32	2a	189(E)	U
32	2a	195	A
32	2a	197	A
32	2a	201	C
32	2a	202	U
32	2a	203	U
32	2a	204	U
32	2a	216	G
32	2a	247	G
32	2a	251	G
32	2a	266	G
32	2a	267	C
32	2a	289	G
32	2a	306	G
32	2a	321	A
32	2a	328	C
32	2a	332	G
32	2a	351	G
32	2a	352	C
32	2a	353	A
32	2a	354	G
32	2a	367	U
32	2a	372	C
32	2a	397	A
32	2a	398	C
32	2a	406	G
32	2a	412	A

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Mol	Chain	Res	Type
32	2a	413	G
32	2a	424	G
32	2a	429	U
32	2a	430	A
32	2a	439	A
32	2a	442	C
32	2a	452	A
32	2a	461	A
32	2a	470	C
32	2a	482	A
32	2a	484	G
32	2a	485	G
32	2a	496	A
32	2a	498	U
32	2a	505	G
32	2a	509	A
32	2a	510	A
32	2a	511	C
32	2a	518	C
32	2a	521	G
32	2a	531	U
32	2a	532	A
32	2a	533	A
32	2a	547	A
32	2a	559	A
32	2a	561	U
32	2a	562	C
32	2a	564	C
32	2a	572	A
32	2a	573	A
32	2a	576	G
32	2a	596	C
32	2a	603	U
32	2a	618	C
32	2a	630	G
32	2a	647	C
32	2a	651	C
32	2a	653	A
32	2a	665	A
32	2a	666	G
32	2a	687	A
32	2a	688	G

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Mol	Chain	Res	Type
32	2a	695	A
32	2a	723	U
32	2a	731	G
32	2a	742	G
32	2a	749	C
32	2a	753	A
32	2a	755	G
32	2a	763	G
32	2a	777	A
32	2a	782	A
32	2a	792	A
32	2a	793	U
32	2a	794	A
32	2a	796	C
32	2a	810	C
32	2a	816	A
32	2a	817	C
32	2a	819	A
32	2a	821	G
32	2a	828	A
32	2a	840	C
32	2a	841	U
32	2a	851	G
32	2a	853	G
32	2a	854	G
32	2a	859	A
32	2a	872	A
32	2a	902	G
32	2a	914	A
32	2a	926	G
32	2a	927	G
32	2a	934	C
32	2a	942	G
32	2a	961	U
32	2a	968	A
32	2a	969	A
32	2a	971	G
32	2a	972	C
32	2a	974	A
32	2a	975	A
32	2a	976	G
32	2a	977	A

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Mol	Chain	Res	Type
32	2a	982	U
32	2a	989	C
32	2a	992	U
32	2a	993	G
32	2a	997	U
32	2a	998	G
32	2a	1001(A)	G
32	2a	1002	G
32	2a	1003	G
32	2a	1004	A
32	2a	1005	A
32	2a	1006	C
32	2a	1009	G
32	2a	1011	G
32	2a	1020	U
32	2a	1021	G
32	2a	1022	G
32	2a	1023	G
32	2a	1025	U
32	2a	1026	G
32	2a	1027	C
32	2a	1030	C
32	2a	1030(A)	G
32	2a	1031	G
32	2a	1037	C
32	2a	1039	C
32	2a	1040	U
32	2a	1043	C
32	2a	1045	C
32	2a	1046	A
32	2a	1065	U
32	2a	1066	C
32	2a	1068	G
32	2a	1077	G
32	2a	1081	G
32	2a	1086	U
32	2a	1094	G
32	2a	1095	U
32	2a	1101	A
32	2a	1108	G
32	2a	1113	C
32	2a	1117	G

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Mol	Chain	Res	Type
32	2a	1122	U
32	2a	1129	C
32	2a	1130	A
32	2a	1133	G
32	2a	1136	U
32	2a	1137	C
32	2a	1138	G
32	2a	1139	G
32	2a	1146	A
32	2a	1152	A
32	2a	1157	A
32	2a	1159	U
32	2a	1160	G
32	2a	1182	G
32	2a	1183	A
32	2a	1184	G
32	2a	1196	U
32	2a	1197	G
32	2a	1202	G
32	2a	1211	U
32	2a	1212	U
32	2a	1213	A
32	2a	1227	A
32	2a	1228	C
32	2a	1238	A
32	2a	1240	U
32	2a	1241	G
32	2a	1256	A
32	2a	1257	U
32	2a	1260	C
32	2a	1262	C
32	2a	1270	C
32	2a	1272	G
32	2a	1273	G
32	2a	1275	A
32	2a	1277	C
32	2a	1278	U
32	2a	1279	A
32	2a	1280	A
32	2a	1287	A
32	2a	1297	C
32	2a	1299	A

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Mol	Chain	Res	Type
32	2a	1302	U
32	2a	1303	C
32	2a	1305	G
32	2a	1312	G
32	2a	1319	A
32	2a	1322	C
32	2a	1323	G
32	2a	1346	A
32	2a	1347	G
32	2a	1358	U
32	2a	1363	C
32	2a	1368	G
32	2a	1370	G
32	2a	1398	A
32	2a	1399	C
32	2a	1401	G
32	2a	1410	G
32	2a	1419	G
32	2a	1442	G
32	2a	1442(A)	G
32	2a	1442(B)	A
32	2a	1447	A
32	2a	1452	C
32	2a	1456	G
32	2a	1475	G
32	2a	1492	A
32	2a	1494	G
32	2a	1504	G
32	2a	1506	U
32	2a	1517	G
32	2a	1520	G
32	2a	1529	G
32	2a	1530	G
32	2a	1531	A
54	2x	8	4SU
54	2x	9	G
54	2x	19	G
54	2x	21	A
54	2x	22	G
54	2x	47	U
54	2x	52	G
54	2x	56	C

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Mol	Chain	Res	Type
54	2x	59	A
54	2x	68	C
54	2x	76	A

All (63) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	1A	90	U
1	1A	195	A
1	1A	266	G
1	1A	271(K)	U
1	1A	278	A
1	1A	351	G
1	1A	548	A
1	1A	574	C
1	1A	746	A
1	1A	774	A
1	1A	895	U
1	1A	974	G
1	1A	1047	G
1	1A	1065	U
1	1A	1067	A
1	1A	1078	U
1	1A	1107	G
1	1A	1174	A
1	1A	1175	U
1	1A	1176	G
1	1A	1210	A
1	1A	1384	A
1	1A	1442	G
1	1A	1508	A
1	1A	1608	A
1	1A	1653	G
1	1A	1992	G
1	1A	2134	A
1	1A	2156	G
1	1A	2158	A
1	1A	2181	G
1	1A	2183	C
1	1A	2406	U
1	1A	2422	A
1	1A	2430	A

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Mol	Chain	Res	Type
1	1A	2601	C
1	1A	2689	U
2	1B	1	U
1	2A	34	C
1	2A	196	A
1	2A	228	A
1	2A	266	G
1	2A	271(K)	U
1	2A	271(M)	G
1	2A	277	C
1	2A	528	A
1	2A	752	A
1	2A	774	A
1	2A	805	G
1	2A	856	C
1	2A	900	A
1	2A	1210	A
1	2A	1379	A
1	2A	1420	U
1	2A	1442	G
1	2A	1530	C
1	2A	1608	A
1	2A	1653	G
1	2A	1913	A
1	2A	1992	G
1	2A	2119	A
1	2A	2126	A
1	2A	2689	U

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
1	5MU	2A	1915	1	15,22,23	1.14	1 (6%)	16,32,35	1.87	1 (6%)
32	5MC	2a	1407	32	15,22,23	1.25	1 (6%)	19,32,35	1.38	2 (10%)
1	5MU	1A	1915	1	15,22,23	1.09	1 (6%)	16,32,35	1.80	1 (6%)
32	7MG	1a	527	55,32	22,26,27	1.77	4 (18%)	28,39,42	2.76	9 (32%)
54	PSU	2x	55	54	17,21,22	1.50	2 (11%)	20,30,33	3.07	6 (30%)
32	7MG	2a	527	55,32	22,26,27	1.75	4 (18%)	28,39,42	2.66	9 (32%)
54	PSU	1x	55	54	17,21,22	1.63	2 (11%)	20,30,33	3.30	6 (30%)
1	OMG	2A	2251	1,55,54	18,26,27	1.10	2 (11%)	20,38,41	1.98	5 (25%)
32	5MC	2a	967	32	15,22,23	1.35	1 (6%)	19,32,35	1.29	3 (15%)
1	PSU	1A	2605	1	17,21,22	1.79	4 (23%)	20,30,33	3.22	6 (30%)
32	5MC	1a	1404	32	15,22,23	1.45	1 (6%)	19,32,35	1.22	2 (10%)
54	5MC	1x	32	54	15,22,23	1.27	1 (6%)	19,32,35	1.59	4 (21%)
32	M2G	1a	966	55,32	20,27,28	1.41	3 (15%)	22,40,43	2.11	6 (27%)
32	5MC	2a	1404	32	15,22,23	1.26	1 (6%)	19,32,35	1.28	2 (10%)
32	MA6	2a	1518	32	19,26,27	0.96	1 (5%)	18,38,41	1.75	4 (22%)
1	PSU	1A	1917	1	17,21,22	1.62	3 (17%)	20,30,33	3.17	6 (30%)
32	5MC	1a	1407	32	15,22,23	1.33	1 (6%)	19,32,35	1.29	2 (10%)
43	0TD	1l	92	43	4,9,10	3.06	1 (25%)	3,11,13	4.99	1 (33%)
32	MA6	2a	1519	32	19,26,27	1.05	1 (5%)	18,38,41	1.70	4 (22%)
32	PSU	1a	516	55,32	17,21,22	1.42	3 (17%)	20,30,33	3.12	6 (30%)
32	MA6	1a	1518	32	19,26,27	0.89	1 (5%)	18,38,41	1.70	4 (22%)
32	4OC	1a	1402	32	16,23,24	0.72	0	17,32,35	1.56	1 (5%)
1	2MA	2A	2503	1,55	17,25,26	1.27	2 (11%)	19,37,40	2.06	3 (15%)
1	2MU	2A	2552	1,55	14,22,24	0.94	1 (7%)	14,31,36	0.91	0
1	5MC	2A	1942	1	15,22,23	1.32	1 (6%)	19,32,35	1.31	3 (15%)
54	5MU	1x	54	55,54	15,22,23	1.08	2 (13%)	16,32,35	2.07	2 (12%)
54	4SU	1x	8	54	14,21,22	1.52	2 (14%)	15,30,33	2.20	2 (13%)
1	PSU	1A	1911	1	17,21,22	1.51	2 (11%)	20,30,33	3.14	6 (30%)
43	0TD	2l	92	43	4,9,10	3.14	1 (25%)	3,11,13	8.37	1 (33%)
32	PSU	2a	516	55,32	17,21,22	1.50	3 (17%)	20,30,33	3.14	6 (30%)
32	UR3	1a	1498	32	14,22,23	0.81	1 (7%)	15,32,35	0.72	1 (6%)
1	5MC	2A	1962	1,55	15,22,23	1.25	1 (6%)	19,32,35	1.48	3 (15%)
1	2MU	1A	2552	1,55	14,22,24	0.88	0	14,31,36	0.68	0
54	5MU	2x	54	54	15,22,23	1.09	1 (6%)	16,32,35	1.87	1 (6%)
1	4OC	1A	1920	1	15,22,24	0.66	0	17,31,35	1.49	2 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
32	M2G	2a	966	55,32	20,27,28	1.46	3 (15%)	22,40,43	2.10	5 (22%)
1	4OC	2A	1920	1	15,22,24	0.68	0	17,31,35	1.42	2 (11%)
32	5MC	1a	967	32	15,22,23	1.21	1 (6%)	19,32,35	1.44	2 (10%)
1	OMG	1A	2251	1,55,54	18,26,27	1.18	2 (11%)	20,38,41	2.21	6 (30%)
32	2MG	2a	1207	32	19,26,27	1.31	2 (10%)	21,38,41	2.30	7 (33%)
1	5MU	2A	1939	1	15,22,23	1.14	2 (13%)	16,32,35	1.68	2 (12%)
1	2MA	1A	2503	1,55	17,25,26	1.30	2 (11%)	19,37,40	2.14	3 (15%)
32	4OC	2a	1402	55,32	16,23,24	0.71	0	17,32,35	1.38	1 (5%)
54	5MC	2x	32	54	15,22,23	1.36	1 (6%)	19,32,35	1.41	3 (15%)
1	5MC	1A	1962	1,55	15,22,23	1.27	1 (6%)	19,32,35	1.32	3 (15%)
32	MA6	1a	1519	32	19,26,27	1.04	1 (5%)	18,38,41	1.58	4 (22%)
1	PSU	2A	2605	1	17,21,22	1.59	3 (17%)	20,30,33	3.20	6 (30%)
54	4SU	2x	8	54	14,21,22	1.29	2 (14%)	15,30,33	2.37	2 (13%)
1	PSU	2A	1917	1,55	17,21,22	1.49	2 (11%)	20,30,33	3.17	6 (30%)
32	UR3	2a	1498	32	14,22,23	0.82	1 (7%)	15,32,35	0.78	1 (6%)
32	5MC	1a	1400	32	15,22,23	1.34	1 (6%)	19,32,35	1.38	3 (15%)
32	2MG	1a	1207	55,32	19,26,27	1.21	2 (10%)	21,38,41	2.28	8 (38%)
1	PSU	2A	1911	1	17,21,22	1.50	3 (17%)	20,30,33	3.08	6 (30%)
1	5MU	1A	1939	1,55	15,22,23	1.10	2 (13%)	16,32,35	1.91	2 (12%)
1	5MC	1A	1942	1,55	15,22,23	1.18	1 (6%)	19,32,35	1.48	4 (21%)
32	5MC	2a	1400	32,54	15,22,23	1.36	1 (6%)	19,32,35	1.49	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
1	5MU	2A	1915	1	-	0/5/25/26	0/2/2/2
32	5MC	2a	1407	32	-	0/5/25/26	0/2/2/2
1	5MU	1A	1915	1	-	2/5/25/26	0/2/2/2
32	7MG	1a	527	55,32	-	1/7/37/38	0/3/3/3
54	PSU	2x	55	54	-	0/7/25/26	0/2/2/2
32	7MG	2a	527	55,32	-	2/7/37/38	0/3/3/3
54	PSU	1x	55	54	-	0/7/25/26	0/2/2/2
1	OMG	2A	2251	1,55,54	-	0/5/27/28	0/3/3/3
32	5MC	2a	967	32	-	0/5/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	PSU	1A	2605	1	-	0/7/25/26	0/2/2/2
32	5MC	1a	1404	32	-	0/5/25/26	0/2/2/2
54	5MC	1x	32	54	-	0/5/25/26	0/2/2/2
32	M2G	1a	966	55,32	-	0/7/29/30	0/3/3/3
32	5MC	2a	1404	32	-	0/5/25/26	0/2/2/2
32	MA6	2a	1518	32	-	2/7/29/30	0/3/3/3
1	PSU	1A	1917	1	-	0/7/25/26	0/2/2/2
32	5MC	1a	1407	32	-	0/5/25/26	0/2/2/2
43	0TD	1l	92	43	-	1/3/12/14	-
32	MA6	2a	1519	32	-	4/7/29/30	0/3/3/3
32	PSU	1a	516	55,32	-	0/7/25/26	0/2/2/2
32	MA6	1a	1518	32	-	3/7/29/30	0/3/3/3
32	4OC	1a	1402	32	-	1/9/29/30	0/2/2/2
1	2MA	2A	2503	1,55	-	1/3/25/26	0/3/3/3
1	2MU	2A	2552	1,55	-	0/7/27/28	0/2/2/2
1	5MC	2A	1942	1	-	0/5/25/26	0/2/2/2
54	5MU	1x	54	55,54	-	0/5/25/26	0/2/2/2
54	4SU	1x	8	54	-	0/5/25/26	0/2/2/2
1	PSU	1A	1911	1	-	0/7/25/26	0/2/2/2
43	0TD	2l	92	43	-	1/3/12/14	-
32	PSU	2a	516	55,32	-	0/7/25/26	0/2/2/2
32	UR3	1a	1498	32	-	0/5/25/26	0/2/2/2
1	5MC	2A	1962	1,55	-	2/5/25/26	0/2/2/2
1	2MU	1A	2552	1,55	-	0/7/27/28	0/2/2/2
54	5MU	2x	54	54	-	0/5/25/26	0/2/2/2
1	4OC	1A	1920	1	-	0/7/27/30	0/2/2/2
32	M2G	2a	966	55,32	-	0/7/29/30	0/3/3/3
1	4OC	2A	1920	1	-	2/7/27/30	0/2/2/2
32	5MC	1a	967	32	-	2/5/25/26	0/2/2/2
1	OMG	1A	2251	1,55,54	-	0/5/27/28	0/3/3/3
32	2MG	2a	1207	32	-	0/5/27/28	0/3/3/3
1	5MU	2A	1939	1	-	2/5/25/26	0/2/2/2
1	2MA	1A	2503	1,55	-	2/3/25/26	0/3/3/3
32	4OC	2a	1402	55,32	-	2/9/29/30	0/2/2/2
54	5MC	2x	32	54	-	0/5/25/26	0/2/2/2
1	5MC	1A	1962	1,55	-	2/5/25/26	0/2/2/2
32	MA6	1a	1519	32	-	4/7/29/30	0/3/3/3
1	PSU	2A	2605	1	-	0/7/25/26	0/2/2/2
54	4SU	2x	8	54	-	0/5/25/26	0/2/2/2
1	PSU	2A	1917	1,55	-	0/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
32	UR3	2a	1498	32	-	0/5/25/26	0/2/2/2
32	5MC	1a	1400	32	-	0/5/25/26	0/2/2/2
32	2MG	1a	1207	55,32	-	0/5/27/28	0/3/3/3
1	PSU	2A	1911	1	-	0/7/25/26	0/2/2/2
1	5MU	1A	1939	1,55	-	0/5/25/26	0/2/2/2
1	5MC	1A	1942	1,55	-	0/5/25/26	0/2/2/2
32	5MC	2a	1400	32,54	-	2/5/25/26	0/2/2/2

All (89) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
43	2l	92	0TD	CB-SB	-6.03	1.69	1.84
43	1l	92	0TD	CB-SB	-5.84	1.70	1.84
1	1A	2605	PSU	C5-C1'	-5.28	1.47	1.52
32	1a	1404	5MC	C5-C4	5.19	1.49	1.41
32	1a	527	7MG	C6-C5	4.97	1.48	1.41
54	1x	55	PSU	C5-C1'	-4.93	1.48	1.52
32	2a	527	7MG	C6-C5	4.90	1.48	1.41
54	2x	32	5MC	C5-C4	4.83	1.48	1.41
32	1a	1400	5MC	C5-C4	4.81	1.48	1.41
32	2a	967	5MC	C5-C4	4.78	1.48	1.41
32	2a	1400	5MC	C5-C4	4.73	1.48	1.41
32	1a	1407	5MC	C5-C4	4.73	1.48	1.41
1	2A	1942	5MC	C5-C4	4.71	1.48	1.41
32	2a	1207	2MG	C6-C5	4.59	1.49	1.41
1	1A	1917	PSU	C5-C1'	-4.55	1.48	1.52
54	1x	32	5MC	C5-C4	4.55	1.48	1.41
1	1A	1962	5MC	C5-C4	4.51	1.48	1.41
32	2a	1404	5MC	C5-C4	4.47	1.48	1.41
32	2a	527	7MG	C5-C4	4.45	1.47	1.39
1	1A	2503	2MA	C6-C5	4.42	1.48	1.41
1	2A	1962	5MC	C5-C4	4.41	1.48	1.41
1	2A	2605	PSU	C5-C1'	-4.40	1.48	1.52
32	1a	527	7MG	C5-C4	4.37	1.47	1.39
32	2a	966	M2G	C6-C5	4.35	1.48	1.41
32	1a	967	5MC	C5-C4	4.35	1.48	1.41
32	2a	1407	5MC	C5-C4	4.31	1.48	1.41
32	1a	966	M2G	C6-C5	4.27	1.48	1.41
1	2A	2503	2MA	C6-C5	4.25	1.47	1.41
32	1a	1207	2MG	C6-C5	4.23	1.48	1.41
1	1A	1942	5MC	C5-C4	4.15	1.47	1.41
54	1x	8	4SU	C4-S4	-4.11	1.60	1.67

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	1A	1911	PSU	C5-C1'	-3.92	1.48	1.52
1	1A	2251	OMG	C6-C5	3.85	1.48	1.41
32	2a	516	PSU	C5-C1'	-3.84	1.49	1.52
1	2A	1911	PSU	C5-C1'	-3.77	1.49	1.52
1	2A	1915	5MU	C4-C5	3.75	1.49	1.41
54	2x	55	PSU	C5-C1'	-3.72	1.49	1.52
54	2x	8	4SU	C4-S4	-3.71	1.60	1.67
1	2A	1917	PSU	C4-C5	3.57	1.49	1.41
1	2A	2251	OMG	C6-C5	3.54	1.47	1.41
54	1x	8	4SU	C2-N3	-3.53	1.31	1.38
54	2x	55	PSU	C4-C5	3.51	1.49	1.41
32	2a	966	M2G	C2-N2	3.50	1.40	1.34
32	1a	516	PSU	C4-C5	3.50	1.49	1.41
1	2A	1939	5MU	C4-C5	3.48	1.48	1.41
1	1A	1915	5MU	C4-C5	3.48	1.48	1.41
1	2A	1917	PSU	C5-C1'	-3.47	1.49	1.52
54	2x	54	5MU	C4-C5	3.43	1.48	1.41
32	1a	527	7MG	C5-N7	-3.39	1.34	1.39
32	1a	966	M2G	C2-N2	3.31	1.40	1.34
32	2a	527	7MG	C5-N7	-3.27	1.34	1.39
1	1A	1911	PSU	C4-C5	3.27	1.48	1.41
54	1x	54	5MU	C4-C5	3.26	1.48	1.41
1	2A	2605	PSU	C4-C5	3.22	1.48	1.41
1	1A	1917	PSU	C4-C5	3.21	1.48	1.41
1	2A	1911	PSU	C4-C5	3.20	1.48	1.41
1	1A	1939	5MU	C4-C5	3.10	1.48	1.41
32	2a	516	PSU	C4-C5	3.10	1.48	1.41
54	1x	55	PSU	C4-C5	3.09	1.48	1.41
32	1a	516	PSU	C5-C1'	-2.95	1.49	1.52
1	1A	2605	PSU	C4-C5	2.87	1.47	1.41
54	2x	8	4SU	C2-N3	-2.68	1.32	1.38
32	2a	1207	2MG	C5-C4	2.68	1.48	1.40
32	2a	966	M2G	C5-C4	2.65	1.47	1.40
32	1a	966	M2G	C5-C4	2.61	1.47	1.40
32	1a	1519	MA6	C5-C4	2.58	1.47	1.40
32	2a	1519	MA6	C5-C4	2.58	1.47	1.40
32	2a	1518	MA6	C5-C4	2.53	1.47	1.40
1	2A	2251	OMG	C5-C4	2.51	1.47	1.40
1	1A	2605	PSU	C2-N3	-2.37	1.33	1.38
32	2a	516	PSU	O4'-C1'	-2.35	1.41	1.44
32	1a	1207	2MG	C5-C4	2.33	1.47	1.40
32	1a	1518	MA6	C5-C4	2.33	1.47	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	1a	527	7MG	C4-N9	-2.32	1.34	1.38
1	1A	2605	PSU	C2-N1	-2.32	1.33	1.38
1	1A	2251	OMG	C5-C4	2.29	1.47	1.40
32	1a	1498	UR3	C4-N3	2.27	1.41	1.38
1	1A	2503	2MA	C5-C4	2.27	1.46	1.40
32	2a	527	7MG	C4-N9	-2.26	1.34	1.38
1	2A	2503	2MA	C5-C4	2.26	1.46	1.40
32	2a	1498	UR3	C4-N3	2.23	1.41	1.38
1	2A	1939	5MU	C2-N3	-2.20	1.33	1.38
1	1A	1939	5MU	C2-N3	-2.16	1.33	1.38
1	2A	2552	2MU	C2-N3	-2.14	1.33	1.38
32	1a	516	PSU	O4'-C1'	-2.06	1.41	1.44
1	1A	1917	PSU	C2-N3	-2.06	1.34	1.38
1	2A	1911	PSU	C2-N1	-2.02	1.34	1.38
54	1x	54	5MU	C2-N3	-2.02	1.34	1.38
1	2A	2605	PSU	C2-N3	-2.01	1.34	1.38

All (199) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
43	2l	92	0TD	CSB-SB-CB	-14.44	73.45	101.85
32	1a	527	7MG	N3-C4-N9	9.12	138.62	126.91
32	2a	516	PSU	N1-C2-N3	-8.96	121.31	128.43
1	1A	2605	PSU	N1-C2-N3	-8.91	121.35	128.43
32	1a	516	PSU	N1-C2-N3	-8.80	121.44	128.43
54	1x	55	PSU	N1-C2-N3	-8.77	121.46	128.43
1	2A	1917	PSU	N1-C2-N3	-8.75	121.48	128.43
1	1A	1911	PSU	N1-C2-N3	-8.69	121.52	128.43
32	2a	527	7MG	N3-C4-N9	8.61	137.97	126.91
43	1l	92	0TD	CSB-SB-CB	-8.55	85.04	101.85
1	2A	2605	PSU	N1-C2-N3	-8.52	121.66	128.43
1	2A	1911	PSU	N1-C2-N3	-8.41	121.74	128.43
54	2x	55	PSU	N1-C2-N3	-8.39	121.76	128.43
1	1A	1917	PSU	N1-C2-N3	-8.35	121.79	128.43
54	2x	8	4SU	C2-N3-C4	7.89	126.58	115.15
54	1x	54	5MU	C4-N3-C2	7.82	121.75	115.14
54	1x	8	4SU	C2-N3-C4	7.46	125.97	115.15
1	2A	1917	PSU	C4-N3-C2	7.20	121.22	115.14
32	1a	516	PSU	C4-N3-C2	7.20	121.22	115.14
32	2a	516	PSU	C4-N3-C2	7.12	121.15	115.14
1	2A	1915	5MU	C4-N3-C2	6.96	121.02	115.14
54	2x	54	5MU	C4-N3-C2	6.90	120.97	115.14

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	2A	1911	PSU	C4-N3-C2	6.86	120.93	115.14
1	1A	1915	5MU	C4-N3-C2	6.72	120.82	115.14
54	1x	55	PSU	C4-N3-C2	6.70	120.80	115.14
1	1A	1911	PSU	C4-N3-C2	6.70	120.80	115.14
1	2A	2605	PSU	C4-N3-C2	6.62	120.73	115.14
1	1A	2605	PSU	C4-N3-C2	6.54	120.67	115.14
54	2x	55	PSU	C4-N3-C2	6.44	120.58	115.14
1	1A	2503	2MA	C2-N3-C4	6.25	120.60	115.52
1	2A	2503	2MA	C2-N3-C4	6.22	120.58	115.52
1	1A	1939	5MU	C4-N3-C2	6.08	120.28	115.14
1	1A	1917	PSU	C4-N3-C2	6.01	120.22	115.14
32	1a	1402	4OC	CM4-N4-C4	-5.47	118.27	122.97
1	2A	1917	PSU	C5-C4-N3	-5.39	118.41	125.36
54	1x	55	PSU	C5-C4-N3	-5.35	118.47	125.36
32	2a	516	PSU	C5-C4-N3	-5.33	118.49	125.36
1	2A	2605	PSU	C5-C4-N3	-5.32	118.51	125.36
32	1a	527	7MG	N7-C8-N9	-5.28	95.83	103.38
1	1A	1911	PSU	C5-C4-N3	-5.27	118.58	125.36
1	1A	2503	2MA	C5-C6-N1	-5.25	117.55	123.06
32	1a	516	PSU	C5-C4-N3	-5.24	118.61	125.36
32	1a	527	7MG	C5-C4-N3	-5.24	117.94	126.49
32	2a	527	7MG	C5-C4-N3	-5.18	118.03	126.49
1	2A	1911	PSU	C5-C4-N3	-5.16	118.72	125.36
32	2a	966	M2G	C2-N3-C4	5.15	121.13	115.28
1	2A	1939	5MU	C4-N3-C2	5.12	119.47	115.14
32	1a	966	M2G	C6-N1-C2	5.11	122.27	116.18
32	2a	527	7MG	N7-C8-N9	-5.08	96.11	103.38
54	2x	55	PSU	C5-C4-N3	-5.03	118.88	125.36
32	2a	966	M2G	C6-N1-C2	5.03	122.17	116.18
1	2A	2503	2MA	C5-C6-N1	-5.00	117.82	123.06
1	1A	2605	PSU	C5-C4-N3	-4.94	119.00	125.36
1	1A	1917	PSU	C5-C4-N3	-4.91	119.04	125.36
1	1A	1917	PSU	C5-C6-N1	-4.77	118.58	124.44
32	2a	1207	2MG	C5-C6-N1	-4.75	116.94	123.43
32	1a	1207	2MG	C2-N3-C4	4.71	120.62	115.28
32	2a	1207	2MG	C2-N3-C4	4.70	120.61	115.28
1	1A	2251	OMG	C2-N3-C4	4.59	120.60	115.36
32	1a	966	M2G	C2-N3-C4	4.53	120.42	115.28
32	2a	1402	4OC	CM4-N4-C4	-4.53	119.08	122.97
1	2A	2605	PSU	C5-C6-N1	-4.47	118.95	124.44
54	1x	55	PSU	C5-C6-N1	-4.45	118.98	124.44
54	1x	55	PSU	C5-C1'-C2'	-4.44	107.40	115.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1A	1917	PSU	C6-N1-C2	4.43	122.67	115.36
1	1A	2605	PSU	C6-N1-C2	4.41	122.63	115.36
32	1a	966	M2G	C5-C6-N1	-4.40	117.42	123.43
32	2a	527	7MG	C6-N1-C2	4.34	122.82	115.93
32	2a	1207	2MG	C6-N1-C2	4.34	122.94	115.18
1	1A	1920	4OC	C2-N3-C4	4.32	120.72	116.34
1	2A	2605	PSU	C6-N1-C2	4.31	122.48	115.36
32	1a	527	7MG	C6-N1-C2	4.30	122.76	115.93
1	2A	1920	4OC	C2-N3-C4	4.30	120.70	116.34
1	1A	2605	PSU	C5-C6-N1	-4.26	119.21	124.44
32	2a	966	M2G	C5-C6-N1	-4.21	117.67	123.43
54	2x	55	PSU	C5-C6-N1	-4.20	119.28	124.44
54	1x	55	PSU	C6-N1-C2	4.19	122.27	115.36
32	1a	1207	2MG	C6-C5-C4	-4.19	116.80	120.80
1	2A	2251	OMG	C5-C6-N1	-4.19	117.71	123.43
1	1A	2251	OMG	C6-N1-C2	4.18	122.58	115.93
54	2x	8	4SU	C5-C4-N3	-4.18	118.24	123.83
1	1A	1911	PSU	C6-N1-C2	4.18	122.25	115.36
32	1a	527	7MG	C6-C5-C4	4.17	119.68	115.20
54	2x	55	PSU	C6-N1-C2	4.16	122.22	115.36
1	2A	2251	OMG	C2-N3-C4	4.15	120.09	115.36
1	2A	1917	PSU	C6-N1-C2	4.10	122.13	115.36
1	1A	1917	PSU	C5-C1'-C2'	-4.07	108.05	115.32
1	1A	1911	PSU	C5-C6-N1	-4.05	119.46	124.44
32	1a	516	PSU	C6-N1-C2	4.04	122.03	115.36
1	2A	2251	OMG	C6-N1-C2	4.04	122.35	115.93
32	1a	1207	2MG	C6-N1-C2	4.01	122.37	115.18
1	1A	2251	OMG	C6-C5-C4	-4.01	116.97	120.80
32	1a	1207	2MG	C5-C6-N1	-4.00	117.96	123.43
32	2a	527	7MG	C6-C5-C4	3.93	119.42	115.20
32	1a	1518	MA6	C9-N6-C6	-3.93	107.61	119.51
1	2A	1911	PSU	C6-N1-C2	3.93	121.84	115.36
32	2a	516	PSU	C6-N1-C2	3.92	121.83	115.36
1	1A	2251	OMG	C5-C6-N1	-3.89	118.11	123.43
1	2A	1917	PSU	C5-C6-N1	-3.83	119.74	124.44
32	1a	967	5MC	C2-N3-C4	3.81	120.62	116.02
32	2a	1407	5MC	C2-N3-C4	3.79	120.59	116.02
32	1a	1407	5MC	C2-N3-C4	3.75	120.55	116.02
32	2a	1518	MA6	C9-N6-C6	-3.75	108.16	119.51
32	1a	1207	2MG	CM2-N2-C2	-3.72	119.10	123.59
32	2a	1207	2MG	CM2-N2-C2	-3.71	119.12	123.59
1	2A	1962	5MC	C2-N3-C4	3.69	120.47	116.02

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	2x	32	5MC	C2-N3-C4	3.68	120.46	116.02
1	2A	1939	5MU	C5-C6-N1	-3.68	118.23	122.19
32	2a	967	5MC	C2-N3-C4	3.67	120.45	116.02
54	1x	8	4SU	C5-C4-N3	-3.67	118.92	123.83
32	1a	1518	MA6	C4-C5-N7	-3.67	105.58	109.40
1	2A	1911	PSU	C5-C6-N1	-3.67	119.93	124.44
32	2a	1400	5MC	C2-N3-C4	3.64	120.41	116.02
32	1a	516	PSU	C5-C6-N1	-3.60	120.01	124.44
32	2a	1404	5MC	C2-N3-C4	3.60	120.36	116.02
32	1a	527	7MG	C5-C6-N1	-3.59	115.76	123.14
32	2a	1519	MA6	N1-C6-N6	3.57	120.81	117.06
32	2a	527	7MG	C5-C6-N1	-3.53	115.88	123.14
1	2A	1962	5MC	N4-C4-N3	3.53	122.03	117.03
1	1A	1962	5MC	C2-N3-C4	3.53	120.28	116.02
1	2A	2605	PSU	C5-C1'-C2'	-3.51	109.05	115.32
32	2a	1207	2MG	C6-C5-C4	-3.50	117.45	120.80
1	1A	1942	5MC	C2-N3-C4	3.46	120.20	116.02
1	2A	1942	5MC	C2-N3-C4	3.46	120.19	116.02
1	1A	2251	OMG	N3-C2-N1	-3.44	122.63	127.22
1	1A	2605	PSU	C5-C1'-C2'	-3.39	109.27	115.32
32	2a	516	PSU	C5-C6-N1	-3.38	120.29	124.44
54	1x	32	5MC	C2-N3-C4	3.36	120.08	116.02
32	1a	1400	5MC	C2-N3-C4	3.33	120.04	116.02
32	1a	1404	5MC	C2-N3-C4	3.30	120.00	116.02
1	1A	1939	5MU	C5-C6-N1	-3.28	118.66	122.19
32	1a	1518	MA6	N3-C2-N1	-3.28	123.56	128.68
32	2a	1518	MA6	N3-C2-N1	-3.26	123.59	128.68
32	1a	967	5MC	N4-C4-N3	3.24	121.61	117.03
32	2a	1518	MA6	C4-C5-N7	-3.24	106.02	109.40
32	1a	1519	MA6	N3-C2-N1	-3.22	123.64	128.68
1	2A	2251	OMG	C6-C5-C4	-3.18	117.76	120.80
32	2a	1207	2MG	C4-C5-N7	-3.18	106.09	109.40
32	1a	966	M2G	C6-C5-C4	-3.14	117.80	120.80
32	2a	1519	MA6	N3-C2-N1	-3.08	123.86	128.68
32	1a	1519	MA6	C9-N6-C6	-3.08	110.20	119.51
32	2a	1519	MA6	C9-N6-C6	-3.06	110.26	119.51
32	2a	1519	MA6	C4-C5-N7	-3.03	106.24	109.40
54	1x	32	5MC	C5-C6-N1	-2.94	119.02	122.19
1	1A	2251	OMG	C4-C5-N7	-2.92	106.35	109.40
32	1a	1519	MA6	C4-C5-N7	-2.92	106.36	109.40
32	1a	1400	5MC	N4-C4-N3	2.92	121.16	117.03
1	2A	1911	PSU	C5-C1'-C2'	-2.92	110.11	115.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	1x	32	5MC	N4-C4-N3	2.90	121.14	117.03
32	2a	1407	5MC	N4-C4-N3	2.90	121.13	117.03
1	1A	1942	5MC	N4-C4-N3	2.89	121.11	117.03
54	2x	55	PSU	C5-C1'-C2'	-2.88	110.18	115.32
32	1a	1207	2MG	C4-C5-N7	-2.88	106.40	109.40
1	2A	2503	2MA	C4-C5-N7	-2.87	106.41	109.40
1	2A	2251	OMG	N3-C2-N1	-2.85	123.42	127.22
32	1a	1404	5MC	C5-C6-N1	-2.81	119.16	122.19
32	1a	966	M2G	C4-C5-N7	-2.81	106.47	109.40
32	2a	966	M2G	C6-C5-C4	-2.81	118.11	120.80
1	1A	1962	5MC	N4-C4-N3	2.78	120.97	117.03
32	1a	527	7MG	C8-N7-C5	2.77	116.15	108.94
1	1A	1911	PSU	C5-C1'-C2'	-2.76	110.39	115.32
1	1A	1920	4OC	N4-C4-N3	2.74	120.83	116.49
1	1A	2503	2MA	C4-C5-N7	-2.73	106.56	109.40
32	1a	1400	5MC	C5-C6-N1	-2.71	119.27	122.19
32	1a	1519	MA6	N1-C6-N6	2.71	119.90	117.06
32	2a	1404	5MC	N4-C4-N3	2.70	120.85	117.03
32	2a	527	7MG	C8-N7-C5	2.70	115.96	108.94
32	2a	1518	MA6	C10-N6-C9	-2.69	107.44	116.12
1	2A	1942	5MC	N4-C4-N3	2.62	120.74	117.03
32	1a	1407	5MC	N4-C4-N3	2.61	120.72	117.03
54	2x	32	5MC	C5-C6-N1	-2.60	119.39	122.19
32	2a	1400	5MC	N4-C4-N3	2.57	120.66	117.03
32	2a	966	M2G	C4-C5-N7	-2.56	106.73	109.40
54	1x	32	5MC	CM5-C5-C4	-2.51	119.19	121.72
1	1A	1942	5MC	C5-C6-N1	-2.49	119.51	122.19
1	2A	1942	5MC	C5-C6-N1	-2.41	119.60	122.19
32	1a	966	M2G	CM2-N2-C2	-2.39	119.01	121.29
32	1a	1207	2MG	N2-C2-N1	2.39	119.26	116.96
1	2A	1962	5MC	C5-C6-N1	-2.34	119.67	122.19
32	2a	967	5MC	C5-C6-N1	-2.33	119.68	122.19
32	2a	1498	UR3	C3U-N3-C4	2.32	121.20	118.12
32	1a	1518	MA6	C10-N6-C9	-2.32	108.64	116.12
32	2a	1400	5MC	C5-C6-N1	-2.29	119.73	122.19
32	1a	527	7MG	C2-N3-C4	2.22	120.04	113.89
1	1A	1962	5MC	C5-C6-N1	-2.18	119.85	122.19
1	2A	1920	4OC	N4-C4-N3	2.16	119.91	116.49
32	1a	527	7MG	C5-C4-N9	-2.15	103.43	106.44
32	2a	527	7MG	C2-N3-C4	2.14	119.79	113.89
32	2a	516	PSU	O4'-C1'-C2'	2.13	108.11	104.66
32	2a	527	7MG	CM7-N7-C5	2.13	132.19	124.01

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	2x	32	5MC	N4-C4-N3	2.13	120.04	117.03
32	2a	967	5MC	N4-C4-N3	2.08	119.97	117.03
32	1a	1498	UR3	C3U-N3-C4	2.07	120.86	118.12
54	1x	54	5MU	C5-C6-N1	-2.05	119.98	122.19
1	1A	1942	5MC	CM5-C5-C4	-2.04	119.66	121.72
32	2a	1207	2MG	N2-C2-N1	2.02	118.90	116.96
32	1a	1207	2MG	N3-C2-N1	-2.01	123.05	126.23
32	1a	516	PSU	O4'-C1'-C2'	2.01	107.91	104.66
1	2A	1917	PSU	C5-C1'-C2'	-2.00	111.74	115.32

There are no chirality outliers.

All (38) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
32	2a	1518	MA6	C5-C6-N6-C10
32	2a	1519	MA6	O4'-C4'-C5'-O5'
32	1a	1518	MA6	C5-C6-N6-C9
1	2A	1962	5MC	O4'-C1'-N1-C6
1	2A	1962	5MC	C2'-C1'-N1-C6
1	2A	1920	4OC	C2'-C1'-N1-C6
32	1a	967	5MC	C3'-C4'-C5'-O5'
1	2A	1939	5MU	C2'-C1'-N1-C6
1	2A	1939	5MU	O4'-C1'-N1-C6
32	2a	1402	4OC	O4'-C4'-C5'-O5'
1	1A	1962	5MC	O4'-C1'-N1-C6
1	1A	1962	5MC	C2'-C1'-N1-C6
32	1a	1519	MA6	O4'-C4'-C5'-O5'
32	1a	1519	MA6	C3'-C4'-C5'-O5'
32	1a	1519	MA6	C5-C6-N6-C10
1	1A	1915	5MU	C3'-C4'-C5'-O5'
1	1A	1915	5MU	O4'-C4'-C5'-O5'
32	2a	1519	MA6	C3'-C4'-C5'-O5'
32	1a	967	5MC	O4'-C4'-C5'-O5'
32	2a	1402	4OC	C3'-C4'-C5'-O5'
32	1a	1518	MA6	N1-C6-N6-C9
32	2a	1518	MA6	C5-C6-N6-C9
32	1a	1518	MA6	C5-C6-N6-C10
32	1a	1519	MA6	C5-C6-N6-C9
32	2a	527	7MG	C3'-C4'-C5'-O5'
32	2a	1400	5MC	O4'-C4'-C5'-O5'
32	2a	1519	MA6	C5-C6-N6-C10
32	2a	527	7MG	O4'-C4'-C5'-O5'

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Mol	Chain	Res	Type	Atoms
1	2A	1920	4OC	C3'-C2'-O2'-CM2
32	1a	527	7MG	C3'-C4'-C5'-O5'
32	2a	1400	5MC	C3'-C4'-C5'-O5'
32	2a	1519	MA6	C4'-C5'-O5'-P
32	1a	1402	4OC	O4'-C4'-C5'-O5'
43	1l	92	0TD	CG-CB-SB-CSB
43	2l	92	0TD	CG-CB-SB-CSB
1	2A	2503	2MA	O4'-C4'-C5'-O5'
1	1A	2503	2MA	O4'-C4'-C5'-O5'
1	1A	2503	2MA	C4'-C5'-O5'-P

There are no ring outliers.

No monomer is involved in short contacts.

## 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 2715 ligands modelled in this entry, 2711 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	V7A	1a	1835	55	36,38,38	4.23	12 (33%)	40,60,60	2.10	10 (25%)
58	SF4	2d	303	35	0,12,12	0.00	-	-	-	-
57	V7A	2a	3210	55	36,38,38	4.01	12 (33%)	40,60,60	2.03	10 (25%)
58	SF4	1d	501	35	0,12,12	0.00	-	-	-	-

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	V7A	1a	1835	55	-	4/13/72/72	0/4/4/4
58	SF4	2d	303	35	-	-	0/6/5/5
57	V7A	2a	3210	55	-	4/13/72/72	0/4/4/4
58	SF4	1d	501	35	-	-	0/6/5/5

All (24) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
57	1a	1835	V7A	CAM-CAL	-14.48	1.39	1.52
57	2a	3210	V7A	CAM-CAL	-12.85	1.40	1.52
57	1a	1835	V7A	CAM-CAP	-11.46	1.39	1.55
57	1a	1835	V7A	CAJ-CAI	-11.05	1.40	1.51
57	2a	3210	V7A	CAJ-CAI	-10.51	1.40	1.51
57	2a	3210	V7A	CAM-CAP	-10.31	1.41	1.55
57	1a	1835	V7A	CAS-CAA	-7.40	1.39	1.51
57	2a	3210	V7A	CAS-CAA	-7.37	1.39	1.51
57	2a	3210	V7A	CAG-CAF	-6.38	1.41	1.51
57	1a	1835	V7A	CAG-CAF	-6.09	1.41	1.51
57	1a	1835	V7A	CAO-CAR	-5.27	1.41	1.51
57	2a	3210	V7A	CAO-CAR	-5.20	1.41	1.51
57	2a	3210	V7A	OAU-NAT	4.30	1.55	1.44
57	2a	3210	V7A	CAQ-CBC	-3.78	1.39	1.47
57	1a	1835	V7A	CAQ-CBC	-3.57	1.40	1.47
57	1a	1835	V7A	CAI-CAH	-3.24	1.39	1.47
57	2a	3210	V7A	CAI-CAL	3.17	1.40	1.36
57	2a	3210	V7A	CAI-CAH	-3.05	1.39	1.47
57	1a	1835	V7A	CAE-CAH	-3.05	1.38	1.46
57	2a	3210	V7A	CAE-CAH	-2.90	1.39	1.46
57	1a	1835	V7A	CAQ-CAP	-2.59	1.39	1.45
57	2a	3210	V7A	CAQ-CAP	-2.49	1.39	1.45
57	1a	1835	V7A	CAM-CAN	-2.42	1.51	1.53
57	1a	1835	V7A	CAI-CAL	2.14	1.38	1.36

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
57	2a	3210	V7A	CAV-OAU-NAT	6.17	121.36	108.11
57	1a	1835	V7A	CAV-OAU-NAT	5.77	120.49	108.11
57	1a	1835	V7A	OAZ-CAL-CAI	-5.57	116.27	123.90
57	2a	3210	V7A	OAZ-CAL-CAI	-5.40	116.51	123.90
57	1a	1835	V7A	CAJ-CAK-CAN	-3.84	103.74	110.49
57	2a	3210	V7A	OBI-CAR-CAQ	-3.57	116.69	122.96
57	1a	1835	V7A	OBI-CAR-CAQ	-3.47	116.88	122.96

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
57	2a	3210	V7A	CAJ-CAK-CAN	-3.45	104.42	110.49
57	1a	1835	V7A	CBG-NBF-CAO	-3.20	106.57	114.09
57	1a	1835	V7A	OAZ-CAL-CAM	3.19	117.99	113.37
57	2a	3210	V7A	CAM-CAP-CAQ	3.11	120.70	115.75
57	1a	1835	V7A	CAM-CAP-CAQ	2.90	120.35	115.75
57	2a	3210	V7A	OAZ-CAL-CAM	2.87	117.52	113.37
57	2a	3210	V7A	CAM-CAL-CAI	2.85	125.96	123.06
57	1a	1835	V7A	CAM-CAL-CAI	2.63	125.73	123.06
57	2a	3210	V7A	OAX-CAD-CAE	-2.40	116.66	121.14
57	1a	1835	V7A	OAX-CAD-CAE	-2.33	116.78	121.14
57	2a	3210	V7A	OBB-CAP-CAQ	-2.29	118.73	123.55
57	2a	3210	V7A	CBH-NBF-CAO	-2.25	108.81	114.09
57	1a	1835	V7A	OBB-CAP-CAQ	-2.07	119.21	123.55

There are no chirality outliers.

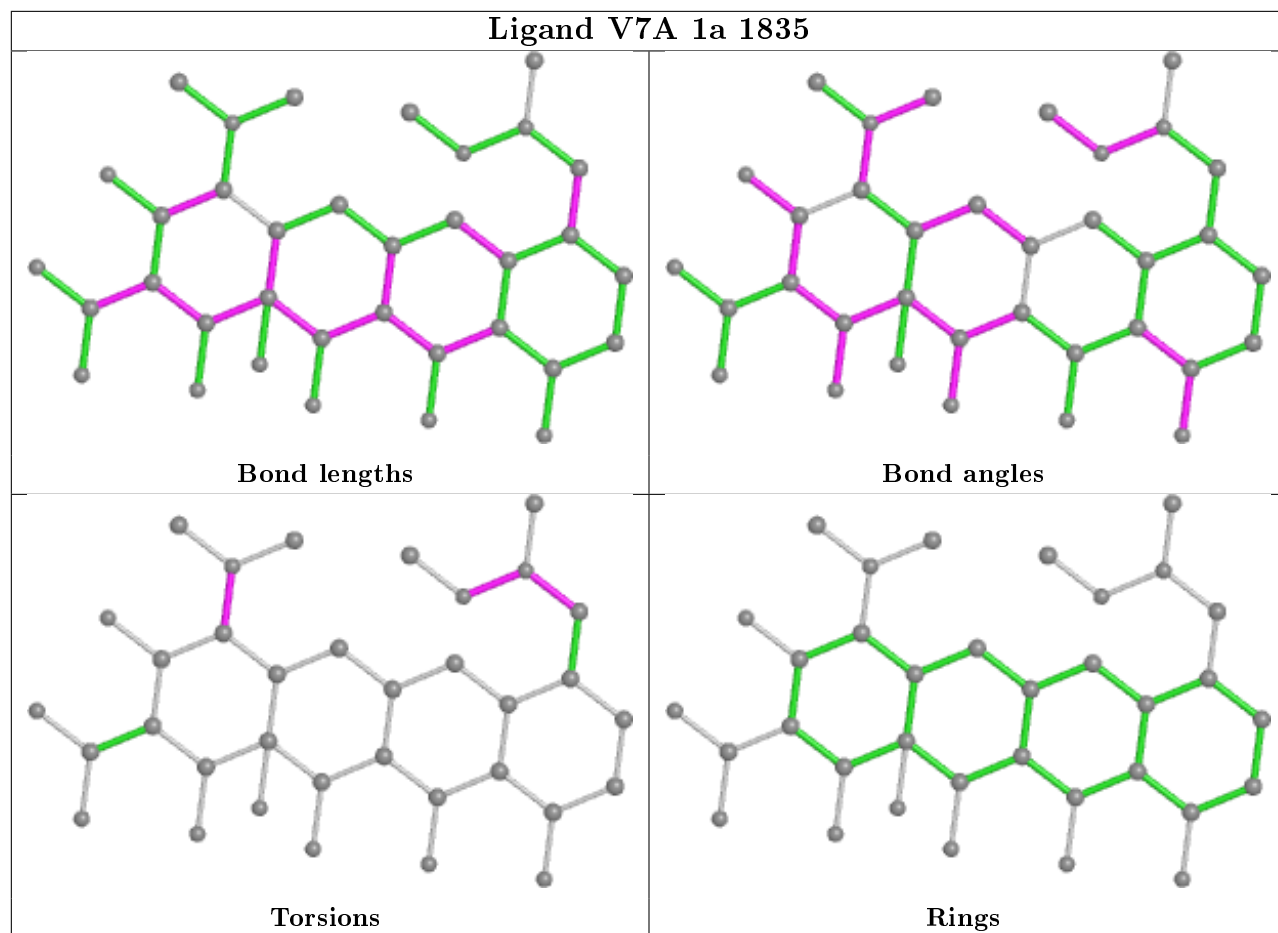
All (8) torsion outliers are listed below:

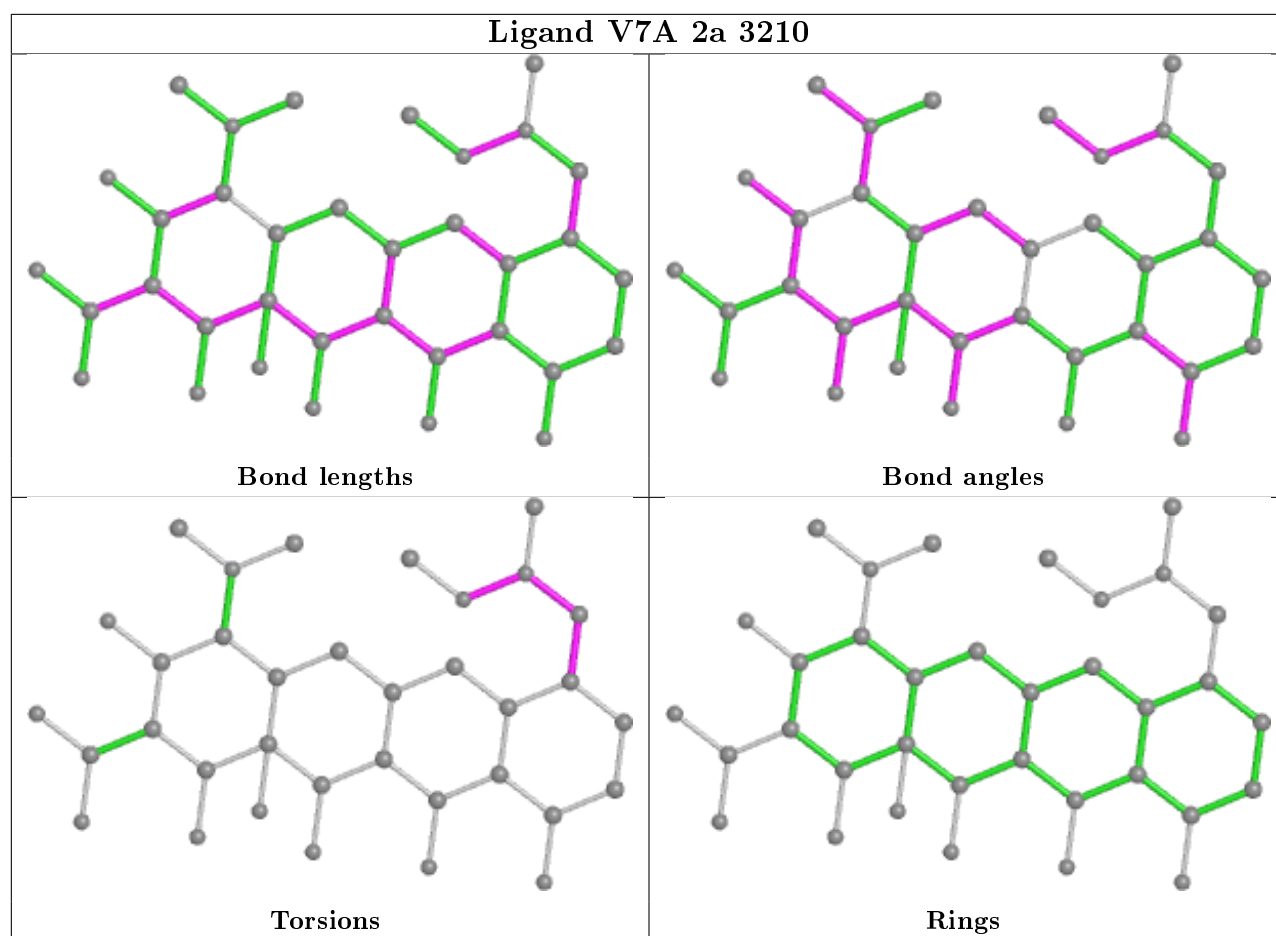
Mol	Chain	Res	Type	Atoms
57	1a	1835	V7A	CAN-CAO-NBF-CBH
57	1a	1835	V7A	CAA-CAS-NAT-CAW
57	1a	1835	V7A	CAA-CAS-NAT-OAU
57	1a	1835	V7A	CAW-NAT-OAU-CAV
57	2a	3210	V7A	CAA-CAS-NAT-CAW
57	2a	3210	V7A	CAA-CAS-NAT-OAU
57	2a	3210	V7A	CAW-NAT-OAU-CAV
57	2a	3210	V7A	CAF-CAA-CAS-NAT

There are no ring outliers.

No monomer is involved in short contacts.

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





## 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%)	0.43	50 (1%) 70 63	17, 35, 97, 111	0
1	2A	2789/2915 (95%)	0.40	85 (3%) 50 40	28, 55, 93, 117	0
2	1B	120/121 (99%)	0.18	0 100 100	25, 50, 67, 89	0
2	2B	120/121 (99%)	0.28	7 (5%) 23 15	58, 79, 89, 99	0
3	1D	275/276 (99%)	0.67	9 (3%) 46 36	19, 36, 50, 75	0
3	2D	275/276 (99%)	1.04	43 (15%) 2 1	28, 48, 62, 79	0
4	1E	204/206 (99%)	0.38	4 (1%) 65 56	18, 38, 58, 75	0
4	2E	204/206 (99%)	0.58	9 (4%) 34 24	32, 53, 69, 78	0
5	1F	203/210 (96%)	0.20	2 (0%) 82 77	19, 40, 65, 83	0
5	2F	203/210 (96%)	0.41	17 (8%) 11 5	33, 64, 80, 88	0
6	1G	181/182 (99%)	0.35	8 (4%) 34 24	37, 58, 72, 86	0
6	2G	181/182 (99%)	0.83	30 (16%) 1 1	63, 79, 86, 94	0
7	1H	174/180 (96%)	0.08	1 (0%) 89 86	35, 51, 64, 72	0
7	2H	174/180 (96%)	1.11	44 (25%) 0 0	67, 80, 89, 95	0
8	1I	146/148 (98%)	0.06	0 100 100	40, 70, 78, 83	0
8	2I	146/148 (98%)	1.76	53 (36%) 0 0	52, 87, 99, 104	0
9	1N	140/140 (100%)	0.36	0 100 100	22, 38, 60, 71	0
9	2N	140/140 (100%)	0.64	16 (11%) 5 3	44, 63, 78, 87	0
10	1O	122/122 (100%)	0.44	2 (1%) 72 66	28, 40, 55, 60	0
10	2O	122/122 (100%)	0.23	2 (1%) 72 66	40, 52, 64, 72	0
11	1P	149/150 (99%)	0.29	2 (1%) 77 72	18, 43, 64, 71	0
11	2P	149/150 (99%)	1.21	34 (22%) 0 0	37, 65, 80, 88	0
12	1Q	141/141 (100%)	0.41	2 (1%) 75 70	28, 39, 54, 69	0
12	2Q	141/141 (100%)	0.91	16 (11%) 5 3	46, 62, 74, 79	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
13	1R	118/118 (100%)	0.50	4 (3%) 45 35	24, 32, 47, 60	0
13	2R	118/118 (100%)	0.79	11 (9%) 8 4	37, 49, 61, 66	0
14	1S	110/112 (98%)	0.22	3 (2%) 54 44	35, 48, 58, 63	0
14	2S	110/112 (98%)	1.06	26 (23%) 0 0	59, 72, 80, 87	0
15	1T	131/146 (89%)	0.12	2 (1%) 73 68	30, 44, 68, 78	0
15	2T	131/146 (89%)	0.38	5 (3%) 40 30	47, 57, 73, 82	0
16	1U	116/118 (98%)	0.32	1 (0%) 84 80	20, 29, 43, 63	0
16	2U	116/118 (98%)	0.98	26 (22%) 0 0	40, 59, 72, 80	0
17	1V	101/101 (100%)	0.16	0 100 100	21, 36, 58, 67	0
17	2V	101/101 (100%)	0.48	12 (11%) 4 2	40, 68, 79, 84	0
18	1W	112/113 (99%)	0.21	0 100 100	19, 29, 46, 82	0
18	2W	112/113 (99%)	0.62	4 (3%) 42 32	39, 49, 66, 86	0
19	1X	95/96 (98%)	0.22	0 100 100	24, 36, 56, 75	0
19	2X	95/96 (98%)	0.76	8 (8%) 11 5	47, 59, 75, 81	0
20	1Y	107/110 (97%)	0.27	0 100 100	33, 47, 69, 79	0
20	2Y	107/110 (97%)	0.94	15 (14%) 2 1	56, 70, 80, 92	0
21	1Z	154/206 (74%)	0.08	0 100 100	38, 56, 70, 78	0
21	2Z	160/206 (77%)	0.38	10 (6%) 20 12	63, 74, 86, 94	0
22	10	83/85 (97%)	1.28	10 (12%) 4 2	25, 35, 69, 86	0
22	20	83/85 (97%)	2.20	38 (45%) 0 0	50, 61, 79, 89	0
23	11	97/98 (98%)	0.57	4 (4%) 37 27	23, 41, 68, 75	0
23	21	97/98 (98%)	1.09	16 (16%) 1 1	40, 54, 73, 81	0
24	12	70/72 (97%)	0.22	0 100 100	35, 47, 57, 76	0
24	22	70/72 (97%)	0.30	1 (1%) 75 70	56, 69, 80, 85	0
25	13	59/60 (98%)	0.21	0 100 100	23, 35, 54, 72	0
25	23	59/60 (98%)	0.98	7 (11%) 4 2	47, 58, 75, 83	0
26	14	69/71 (97%)	0.06	2 (2%) 51 41	56, 74, 88, 94	0
26	24	69/71 (97%)	0.24	7 (10%) 7 4	75, 86, 93, 98	0
27	15	59/60 (98%)	0.30	1 (1%) 70 63	18, 32, 51, 67	0
27	25	59/60 (98%)	0.50	5 (8%) 10 5	35, 50, 66, 83	0
28	16	53/54 (98%)	0.22	0 100 100	28, 38, 51, 59	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
28	26	53/54 (98%)	0.46	4 (7%) 14 8	49, 58, 69, 71	0
29	17	48/49 (97%)	0.87	5 (10%) 6 3	22, 26, 55, 59	0
29	27	48/49 (97%)	1.05	7 (14%) 2 1	31, 41, 62, 75	0
30	18	64/65 (98%)	0.89	6 (9%) 8 4	25, 31, 39, 53	0
30	28	64/65 (98%)	1.60	17 (26%) 0 0	44, 54, 61, 73	0
31	19	37/37 (100%)	0.69	0 100 100	28, 38, 56, 62	0
31	29	37/37 (100%)	2.74	20 (54%) 0 0	53, 64, 75, 77	0
32	1a	1488/1521 (97%)	0.51	92 (6%) 20 13	37, 71, 95, 109	0
32	2a	1491/1521 (98%)	0.41	78 (5%) 27 18	44, 75, 96, 111	0
33	1b	231/256 (90%)	0.08	4 (1%) 70 63	64, 78, 90, 97	0
33	2b	231/256 (90%)	0.04	7 (3%) 50 40	67, 83, 90, 100	0
34	1c	206/239 (86%)	0.84	41 (19%) 1 0	64, 76, 85, 90	0
34	2c	206/239 (86%)	0.44	15 (7%) 15 8	71, 82, 90, 93	0
35	1d	208/209 (99%)	0.72	29 (13%) 2 1	59, 74, 87, 97	0
35	2d	208/209 (99%)	0.83	32 (15%) 2 1	58, 70, 80, 85	0
36	1e	148/162 (91%)	0.88	25 (16%) 1 1	54, 66, 74, 77	0
36	2e	148/162 (91%)	1.07	38 (25%) 0 0	60, 71, 81, 85	0
37	1f	100/101 (99%)	-0.02	0 100 100	55, 69, 76, 79	0
37	2f	100/101 (99%)	-0.14	1 (1%) 82 77	63, 71, 79, 82	0
38	1g	155/156 (99%)	0.27	12 (7%) 13 7	63, 73, 86, 90	0
38	2g	155/156 (99%)	0.57	23 (14%) 2 1	69, 80, 91, 96	0
39	1h	137/138 (99%)	0.90	25 (18%) 1 1	56, 68, 76, 82	0
39	2h	137/138 (99%)	1.30	37 (27%) 0 0	61, 74, 80, 87	0
40	1i	127/128 (99%)	1.87	53 (41%) 0 0	61, 78, 84, 86	0
40	2i	127/128 (99%)	2.51	67 (52%) 0 0	70, 85, 92, 94	0
41	1j	97/105 (92%)	1.37	30 (30%) 0 0	64, 80, 90, 91	0
41	2j	96/105 (91%)	1.80	40 (41%) 0 0	75, 85, 93, 95	0
42	1k	114/129 (88%)	0.07	4 (3%) 44 34	44, 67, 78, 80	0
42	2k	114/129 (88%)	0.35	8 (7%) 16 9	55, 73, 80, 84	0
43	1l	121/132 (91%)	0.89	25 (20%) 1 0	49, 61, 70, 76	0
43	2l	121/132 (91%)	0.54	11 (9%) 9 5	53, 63, 73, 80	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
44	1m	122/126 (96%)	0.95	23 (18%) 1 1	61, 72, 82, 84	0
44	2m	121/126 (96%)	1.44	40 (33%) 0 0	73, 82, 87, 93	0
45	1n	60/61 (98%)	2.96	43 (71%) 0 0	67, 74, 80, 81	0
45	2n	60/61 (98%)	3.37	48 (80%) 0 0	72, 83, 87, 90	0
46	1o	88/89 (98%)	0.49	11 (12%) 3 2	48, 63, 76, 86	0
46	2o	88/89 (98%)	0.28	0 100 100	56, 69, 76, 81	0
47	1p	82/88 (93%)	3.36	58 (70%) 0 0	62, 75, 84, 87	0
47	2p	82/88 (93%)	1.26	25 (30%) 0 0	58, 68, 77, 82	0
48	1q	99/105 (94%)	1.26	26 (26%) 0 0	56, 65, 74, 79	0
48	2q	99/105 (94%)	0.78	13 (13%) 3 2	55, 68, 78, 84	0
49	1r	68/88 (77%)	0.10	1 (1%) 73 68	59, 69, 77, 81	0
49	2r	68/88 (77%)	0.09	0 100 100	62, 70, 79, 83	0
50	1s	83/93 (89%)	1.10	21 (25%) 0 0	63, 76, 85, 89	0
50	2s	83/93 (89%)	1.06	21 (25%) 0 0	75, 83, 91, 94	0
51	1t	96/106 (90%)	2.12	44 (45%) 0 0	61, 71, 80, 84	0
51	2t	96/106 (90%)	1.50	31 (32%) 0 0	58, 68, 76, 79	0
52	1u	23/27 (85%)	3.42	18 (78%) 0 0	66, 72, 77, 80	0
52	2u	23/27 (85%)	3.67	16 (69%) 0 0	75, 80, 82, 85	0
53	1v	10/24 (41%)	1.70	4 (40%) 0 0	54, 92, 98, 99	0
53	2v	6/24 (25%)	0.54	1 (16%) 1 1	67, 73, 86, 96	0
54	1x	72/77 (93%)	0.04	1 (1%) 75 70	38, 64, 78, 89	0
54	2x	72/77 (93%)	-0.04	1 (1%) 75 70	49, 77, 89, 93	0
All	All	20598/21444 (96%)	0.60	1856 (9%) 9 5	17, 63, 89, 117	0

All (1856) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
22	10	6	GLY	16.9
22	10	7	LEU	12.3
44	2m	102	ARG	12.0
8	2I	100	ALA	11.5
8	2I	119	PRO	10.9
31	29	37	GLY	10.8
47	1p	7	ALA	10.3

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Mol	Chain	Res	Type	RSRZ
38	2g	80	VAL	10.0
40	2i	115	GLY	9.9
8	2l	111	PRO	9.9
45	2n	34	TYR	9.8
52	2u	14	TRP	9.4
45	2n	22	THR	9.4
1	2A	2147	G	9.1
47	1p	6	LEU	9.0
22	20	7	LEU	9.0
44	2m	123	ALA	8.8
50	1s	39	THR	8.8
8	2l	117	GLU	8.8
8	2l	86	THR	8.7
23	2l	2	SER	8.6
40	2i	124	GLN	8.5
52	1u	17	THR	8.5
40	2i	125	TYR	8.2
47	1p	68	ASP	8.2
22	20	2	ALA	8.1
1	2A	2166	G	8.0
8	2l	124	GLY	7.9
41	2j	47	PHE	7.9
22	10	5	LYS	7.8
40	1i	106	ALA	7.8
1	1A	2145	C	7.8
38	2g	81	GLY	7.8
52	2u	6	ARG	7.7
44	1m	102	ARG	7.7
6	2G	28	VAL	7.6
40	2i	110	GLU	7.6
1	2A	2146	C	7.5
8	2l	118	LYS	7.5
1	2A	2155	G	7.5
52	2u	16	GLY	7.4
44	2m	122	LYS	7.4
41	2j	50	ILE	7.4
41	1j	47	PHE	7.4
40	1i	114	TYR	7.4
40	2i	128	ARG	7.3
40	2i	123	PRO	7.3
38	1g	79	ARG	7.2
45	2n	25	VAL	7.2

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Mol	Chain	Res	Type	RSRZ
41	2j	6	ILE	7.1
22	20	4	LYS	7.1
51	1t	18	GLN	7.0
41	1j	62	HIS	7.0
44	2m	98	VAL	7.0
22	20	8	GLY	7.0
21	2Z	143	GLY	7.0
52	2u	22	ARG	6.9
40	2i	116	LYS	6.9
45	2n	38	GLY	6.9
43	2l	18	VAL	6.9
51	1t	14	LYS	6.9
45	1n	21	TYR	6.9
45	2n	37	PHE	6.8
44	2m	121	LYS	6.8
47	1p	29	ASP	6.8
52	1u	14	TRP	6.8
1	2A	2148	G	6.8
22	10	3	HIS	6.8
8	2l	109	ILE	6.7
22	10	8	GLY	6.7
41	1j	60	ARG	6.7
47	1p	28	ARG	6.7
51	1t	9	ASN	6.7
29	27	48	LYS	6.6
51	2t	25	ARG	6.6
6	2G	29	TRP	6.6
41	2j	40	LEU	6.6
40	2i	36	TYR	6.6
47	1p	17	TYR	6.6
51	1t	13	LEU	6.6
8	2l	146	ALA	6.6
45	2n	29	ARG	6.6
44	2m	101	GLN	6.6
52	2u	17	THR	6.5
31	29	12	ASP	6.4
47	1p	22	THR	6.4
22	20	5	LYS	6.3
3	1D	276	LYS	6.3
40	2i	117	HIS	6.3
1	2A	2111	C	6.3
29	17	46	VAL	6.2

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Mol	Chain	Res	Type	RSRZ
41	2j	60	ARG	6.2
41	2j	46	ARG	6.2
47	1p	1	MET	6.2
45	2n	39	LEU	6.2
52	2u	15	ARG	6.1
41	2j	98	ILE	6.1
1	2A	2145	C	6.1
22	10	4	LYS	6.1
40	1i	117	HIS	6.1
44	1m	96	LEU	6.1
41	2j	55	LYS	6.0
8	2I	85	GLU	6.0
40	2i	14	VAL	6.0
47	1p	19	ILE	6.0
47	1p	10	GLY	6.0
22	10	9	SER	6.0
41	2j	48	THR	5.9
17	2V	73	SER	5.9
51	1t	70	SER	5.9
21	2Z	142	SER	5.9
51	2t	24	LEU	5.8
47	1p	36	ILE	5.8
45	1n	59	ALA	5.8
44	2m	120	LYS	5.8
41	2j	10	GLY	5.8
7	2H	115	VAL	5.7
47	1p	25	ARG	5.7
51	1t	22	ARG	5.7
51	1t	69	GLY	5.7
44	1m	107	ALA	5.7
51	1t	80	ARG	5.6
44	1m	97	PRO	5.6
40	1i	111	ARG	5.6
40	2i	127	LYS	5.6
45	2n	11	LYS	5.6
42	2k	126	ARG	5.6
40	1i	120	ARG	5.6
22	20	6	GLY	5.6
40	1i	125	TYR	5.5
44	2m	106	ASN	5.5
45	1n	30	ALA	5.5
3	2D	275	LYS	5.5

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Mol	Chain	Res	Type	RSRZ
41	1j	59	SER	5.5
51	1t	68	LYS	5.5
11	2P	79	ARG	5.5
47	1p	9	PHE	5.5
40	2i	114	TYR	5.5
40	1i	109	VAL	5.5
8	2I	84	GLY	5.5
1	2A	2122	U	5.5
45	1n	15	LYS	5.5
1	1A	2146	C	5.5
44	2m	6	GLY	5.4
32	1a	1257	U	5.4
51	2t	9	ASN	5.4
36	1e	23	GLY	5.4
40	1i	15	ALA	5.4
47	1p	66	PRO	5.4
38	2g	79	ARG	5.4
47	1p	5	ARG	5.3
39	1h	89	PRO	5.3
40	1i	113	LYS	5.3
52	2u	13	ILE	5.3
51	1t	24	LEU	5.3
45	2n	18	VAL	5.3
44	2m	105	THR	5.3
51	1t	72	LEU	5.3
40	1i	65	VAL	5.3
40	2i	66	ARG	5.3
39	2h	2	LEU	5.3
38	2g	33	ASP	5.3
22	20	75	LEU	5.2
51	1t	20	LEU	5.2
1	2A	2160	G	5.2
51	1t	71	THR	5.2
41	2j	49	VAL	5.2
32	2a	1532	U	5.2
45	1n	32	SER	5.2
39	2h	93	VAL	5.2
1	2A	2112	G	5.2
34	1c	178	LEU	5.2
48	1q	35	VAL	5.2
14	2S	32	LEU	5.1
44	1m	87	TYR	5.1

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Mol	Chain	Res	Type	RSRZ
51	1t	21	LYS	5.1
8	2I	145	VAL	5.1
7	2H	159	GLU	5.1
20	2Y	5	MET	5.1
40	1i	119	ALA	5.1
45	2n	35	ARG	5.1
40	2i	109	VAL	5.1
45	1n	18	VAL	5.1
8	2I	121	LYS	5.1
51	2t	80	ARG	5.1
14	2S	33	LYS	5.1
44	2m	5	ALA	5.1
1	2A	2165	G	5.1
1	2A	2138	C	5.1
22	10	2	ALA	5.1
35	1d	166	LYS	5.1
32	2a	1492	A	5.1
41	2j	63	PHE	5.1
1	2A	2159	G	5.1
40	1i	37	PHE	5.0
44	2m	103	THR	5.0
31	29	13	LYS	5.0
35	1d	179	GLU	5.0
40	2i	10	ARG	5.0
31	29	33	LYS	5.0
52	1u	3	LYS	5.0
52	1u	18	TYR	5.0
47	1p	67	THR	4.9
1	2A	2116	G	4.9
51	2t	13	LEU	4.9
38	1g	80	VAL	4.9
3	2D	270	ILE	4.9
47	1p	8	ARG	4.9
52	1u	15	ARG	4.9
8	2I	122	GLU	4.9
40	2i	126	SER	4.9
44	1m	105	THR	4.9
48	1q	33	GLY	4.9
41	1j	58	ASP	4.9
47	1p	30	GLY	4.9
32	2a	1286	A	4.9
44	2m	7	VAL	4.9

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Mol	Chain	Res	Type	RSRZ
47	2p	9	PHE	4.9
41	1j	55	LYS	4.9
21	2Z	153	SER	4.9
41	2j	54	PHE	4.9
44	2m	104	ARG	4.8
32	1a	1447	A	4.8
40	1i	107	ARG	4.8
40	1i	116	LYS	4.8
34	1c	153	VAL	4.8
44	2m	100	GLY	4.8
7	2H	113	VAL	4.8
1	1A	2113	U	4.8
44	1m	106	ASN	4.8
14	2S	20	ARG	4.8
34	1c	188	LEU	4.8
40	2i	37	PHE	4.8
47	1p	24	ALA	4.8
41	1j	98	ILE	4.8
45	1n	31	ARG	4.8
32	1a	1286	A	4.8
40	2i	79	LEU	4.8
40	2i	106	ALA	4.8
41	2j	8	LEU	4.8
47	1p	27	LYS	4.8
3	1D	37	LEU	4.8
36	2e	90	VAL	4.7
29	17	48	LYS	4.7
36	2e	88	LYS	4.7
47	1p	41	PRO	4.7
40	2i	5	TYR	4.7
45	1n	11	LYS	4.7
45	2n	33	VAL	4.7
35	2d	208	SER	4.7
1	2A	2161	C	4.7
11	2P	68	GLN	4.7
40	2i	15	ALA	4.7
31	29	16	VAL	4.7
45	1n	2	ALA	4.7
1	1A	2143	C	4.7
3	2D	276	LYS	4.7
51	1t	23	ARG	4.7
11	2P	78	PRO	4.7

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Mol	Chain	Res	Type	RSRZ
50	2s	41	VAL	4.7
41	2j	67	THR	4.7
39	2h	133	LEU	4.6
40	2i	121	ARG	4.6
34	2c	160	ALA	4.6
47	1p	32	TYR	4.6
29	17	47	ARG	4.6
41	1j	57	LYS	4.6
47	1p	65	GLN	4.6
51	1t	17	ARG	4.6
11	2P	109	GLY	4.6
50	1s	40	ILE	4.6
1	2A	2110	G	4.6
1	2A	2120	G	4.6
40	2i	29	ASN	4.6
48	2q	30	PRO	4.6
47	1p	2	VAL	4.6
38	2g	78	ARG	4.6
7	2H	107	VAL	4.6
17	2V	71	LEU	4.6
39	2h	134	ILE	4.6
41	1j	46	ARG	4.6
1	2A	2167	U	4.6
51	2t	29	LYS	4.6
45	2n	58	LYS	4.6
1	1A	2121	G	4.6
7	2H	89	ILE	4.6
51	2t	14	LYS	4.6
41	2j	5	ARG	4.5
8	2l	125	GLU	4.5
44	2m	99	ARG	4.5
7	2H	103	LEU	4.5
44	1m	123	ALA	4.5
8	2l	12	LEU	4.5
32	1a	1353	G	4.5
39	1h	93	VAL	4.5
8	2l	93	THR	4.5
35	2d	49	ARG	4.5
1	2A	2117	A	4.5
44	1m	2	ALA	4.5
22	20	3	HIS	4.5
52	1u	6	ARG	4.5

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
52	1u	22	ARG	4.5
34	1c	196	LEU	4.5
40	2i	7	THR	4.5
48	2q	32	TYR	4.5
32	2a	1030(B)	C	4.5
7	2H	164	TYR	4.5
36	2e	31	LEU	4.4
36	2e	81	GLU	4.4
44	2m	97	PRO	4.4
11	2P	108	LYS	4.4
40	2i	70	LYS	4.4
47	1p	4	ILE	4.4
35	1d	3	ARG	4.4
40	2i	122	ALA	4.4
45	2n	23	ARG	4.4
1	2A	2140	C	4.4
8	2I	3	VAL	4.4
43	1l	18	VAL	4.4
44	2m	95	GLY	4.4
52	2u	24	ARG	4.4
38	2g	156	TRP	4.4
22	20	53	MET	4.4
1	2A	2139	C	4.4
1	2A	2142	C	4.4
23	1l	2	SER	4.4
41	1j	48	THR	4.4
22	20	55	ARG	4.4
1	1A	2112	G	4.4
47	1p	35	LYS	4.4
40	1i	8	GLY	4.3
1	2A	2144	U	4.3
45	2n	61	TRP	4.3
40	1i	115	GLY	4.3
40	2i	67	GLY	4.3
5	2F	82	ILE	4.3
45	2n	31	ARG	4.3
7	2H	169	VAL	4.3
39	1h	3	THR	4.3
45	2n	56	VAL	4.3
47	1p	15	PRO	4.3
47	1p	48	TRP	4.3
3	2D	215	LEU	4.3

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Mol	Chain	Res	Type	RSRZ
45	1n	25	VAL	4.3
1	1A	2115	G	4.3
20	2Y	1	MET	4.3
40	1i	47	LEU	4.3
50	2s	12	ASP	4.3
16	2U	12	ARG	4.3
42	2k	25	TYR	4.2
35	1d	101	LEU	4.2
43	1l	64	TYR	4.2
6	2G	161	THR	4.2
34	1c	3	ASN	4.2
45	1n	36	PHE	4.2
47	1p	39	TYR	4.2
45	2n	17	LYS	4.2
16	2U	44	ASN	4.2
51	2t	18	GLN	4.2
3	2D	271	ILE	4.2
41	1j	66	ARG	4.2
48	1q	98	LEU	4.2
32	2a	1357	A	4.2
29	27	46	VAL	4.2
1	1A	2109	U	4.2
3	2D	272	ALA	4.2
48	1q	28	PRO	4.2
11	2P	45	LEU	4.2
31	29	15	LYS	4.2
50	2s	70	LYS	4.2
45	2n	41	ARG	4.2
39	2h	86	ILE	4.2
3	2D	55	GLY	4.2
50	1s	38	SER	4.1
51	1t	66	ALA	4.1
40	1i	42	ARG	4.1
41	2j	58	ASP	4.1
50	2s	2	PRO	4.1
48	2q	36	ILE	4.1
1	2A	2168	G	4.1
40	1i	64	THR	4.1
36	2e	126	ARG	4.1
34	1c	201	TYR	4.1
40	1i	33	PHE	4.1
43	2l	10	LEU	4.1

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
14	2S	34	HIS	4.1
8	2I	79	ILE	4.1
23	2I	61	ARG	4.1
41	1j	45	ARG	4.1
32	2a	1363(A)	A	4.1
45	1n	61	TRP	4.1
14	2S	58	LEU	4.1
45	2n	6	LEU	4.1
41	1j	63	PHE	4.1
43	2l	64	TYR	4.1
47	1p	33	ILE	4.1
1	2A	2121	G	4.1
44	2m	90	LEU	4.1
6	2G	2	PRO	4.0
1	1A	2110	G	4.0
20	2Y	45	VAL	4.0
48	1q	27	PHE	4.0
47	1p	20	VAL	4.0
45	1n	34	TYR	4.0
45	2n	42	ILE	4.0
1	2A	2109	U	4.0
22	20	76	GLY	4.0
44	1m	104	ARG	4.0
8	2I	35	LEU	4.0
51	2t	21	LYS	4.0
32	1a	204	U	4.0
51	2t	26	ASN	4.0
11	2P	76	LYS	4.0
45	1n	50	LYS	4.0
35	2d	78	LEU	4.0
44	1m	108	ARG	4.0
1	1A	2178	C	4.0
1	1A	2180	U	4.0
11	2P	110	TYR	4.0
41	1j	71	LEU	4.0
45	1n	57	ARG	4.0
40	1i	123	PRO	3.9
44	2m	4	ILE	3.9
32	2a	1353	G	3.9
34	1c	12	LEU	3.9
39	1h	92	ARG	3.9
45	1n	35	ARG	3.9

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Mol	Chain	Res	Type	RSRZ
35	2d	70	ILE	3.9
41	2j	41	PRO	3.9
40	1i	66	ARG	3.9
38	2g	82	GLY	3.9
36	2e	13	ILE	3.9
41	1j	49	VAL	3.9
1	1A	2117	A	3.9
11	2P	70	GLN	3.9
1	2A	2115	G	3.9
31	29	25	VAL	3.9
36	1e	89	ILE	3.9
40	1i	7	THR	3.9
36	2e	133	TYR	3.9
47	1p	31	LYS	3.9
1	2A	2156	G	3.9
41	1j	44	VAL	3.9
50	1s	15	LEU	3.9
41	2j	57	LYS	3.9
52	1u	16	GLY	3.9
43	1l	6	THR	3.9
47	1p	18	ARG	3.9
53	1v	21	C	3.9
36	2e	128	PRO	3.9
45	1n	37	PHE	3.9
51	2t	23	ARG	3.9
8	2I	96	ASP	3.9
13	2R	69	ASP	3.9
1	2A	2188	C	3.9
29	17	45	ALA	3.9
7	2H	94	TYR	3.8
22	20	9	SER	3.9
1	2A	2157	G	3.8
22	20	52	GLY	3.8
32	2a	1224	G	3.8
36	1e	129	ILE	3.8
40	2i	63	ILE	3.8
36	1e	138	ALA	3.8
11	2P	75	ILE	3.8
40	2i	30	GLY	3.8
35	2d	21	LEU	3.8
51	1t	62	LEU	3.8
30	28	2	PRO	3.8

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Mol	Chain	Res	Type	RSRZ
38	2g	32	ARG	3.8
32	2a	1116	C	3.8
51	1t	16	HIS	3.8
39	1h	2	LEU	3.8
45	2n	15	LYS	3.8
40	2i	119	ALA	3.8
22	20	43	THR	3.8
22	20	69	PHE	3.8
41	2j	65	LEU	3.8
32	2a	1202	G	3.8
45	2n	4	LYS	3.8
30	28	22	VAL	3.8
32	1a	1367	C	3.8
17	2V	75	PHE	3.8
40	1i	19	LEU	3.8
52	2u	5	ASP	3.8
6	1G	75	LYS	3.8
14	2S	29	PHE	3.8
50	2s	3	ARG	3.8
1	2A	2143	C	3.8
47	1p	11	SER	3.8
47	1p	42	ARG	3.8
6	2G	160	VAL	3.8
1	1A	2179	C	3.7
1	2A	2104	G	3.7
11	2P	74	GLU	3.7
52	1u	2	GLY	3.7
40	1i	121	ARG	3.7
45	1n	12	ARG	3.7
1	2A	2127	G	3.7
45	2n	16	PHE	3.7
33	2b	187	LEU	3.7
34	1c	152	ILE	3.7
36	2e	12	LEU	3.7
3	2D	35	LYS	3.7
23	11	98	LEU	3.7
34	1c	11	ARG	3.7
8	2I	94	ALA	3.7
40	1i	122	ALA	3.7
40	2i	64	THR	3.7
50	2s	79	THR	3.7
3	2D	155	LEU	3.7

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Mol	Chain	Res	Type	RSRZ
22	20	44	ARG	3.7
40	2i	83	ARG	3.7
14	2S	35	ILE	3.7
45	1n	23	ARG	3.7
45	1n	39	LEU	3.7
48	1q	34	LYS	3.7
51	2t	72	LEU	3.7
41	2j	59	SER	3.7
45	1n	7	ILE	3.7
11	1P	70	GLN	3.7
16	1U	117	GLN	3.7
50	2s	69	HIS	3.7
52	2u	10	ARG	3.7
45	2n	14	PRO	3.7
52	1u	21	TYR	3.7
41	1j	64	GLU	3.7
31	29	10	ILE	3.7
45	2n	7	ILE	3.7
53	1v	13	A	3.7
52	1u	13	ILE	3.7
45	1n	17	LYS	3.6
8	2I	123	LEU	3.6
43	1l	91	LYS	3.6
52	2u	11	GLY	3.6
1	1A	2181	G	3.6
1	1A	2111	C	3.6
16	2U	13	LYS	3.6
15	2T	99	LEU	3.6
12	2Q	104	PHE	3.6
36	1e	123	LEU	3.6
48	2q	31	LEU	3.6
31	29	2	LYS	3.6
40	1i	118	LYS	3.6
45	1n	58	LYS	3.6
41	2j	45	ARG	3.6
6	2G	19	LEU	3.6
40	1i	26	VAL	3.6
44	2m	66	LEU	3.6
45	2n	44	LEU	3.6
31	29	24	TYR	3.6
52	1u	9	ARG	3.6
1	2A	2164	C	3.6

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Mol	Chain	Res	Type	RSRZ
41	1j	50	ILE	3.6
35	1d	4	TYR	3.6
51	1t	15	ARG	3.6
12	2Q	22	LYS	3.6
33	1b	133	LYS	3.6
47	1p	21	VAL	3.6
19	2X	68	ARG	3.6
3	2D	38	LYS	3.6
8	2I	95	LYS	3.6
7	2H	116	GLU	3.6
26	24	56	VAL	3.6
52	2u	23	PRO	3.6
1	2A	1026	U	3.6
13	2R	68	ARG	3.6
51	1t	12	ALA	3.6
40	2i	19	LEU	3.6
41	1j	65	LEU	3.6
50	1s	71	LEU	3.6
11	2P	65	ARG	3.6
1	1A	2120	G	3.5
9	2N	73	THR	3.5
1	2A	2158	A	3.5
47	1p	12	LYS	3.5
32	2a	1364	U	3.5
22	20	74	ARG	3.5
39	1h	84	ARG	3.5
1	2A	2162	G	3.5
32	1a	1369	C	3.5
30	28	58	ILE	3.5
36	1e	88	LYS	3.5
45	1n	22	THR	3.5
47	1p	80	PHE	3.5
30	28	64	TYR	3.5
40	2i	72	GLY	3.5
34	1c	5	ILE	3.5
39	2h	122	ARG	3.5
32	1a	378	G	3.5
51	1t	55	ILE	3.5
51	1t	25	ARG	3.5
8	2I	134	PRO	3.5
47	1p	13	HIS	3.5
8	2I	1	MET	3.5

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Mol	Chain	Res	Type	RSRZ
47	2p	17	TYR	3.5
8	2I	83	ALA	3.5
33	2b	165	VAL	3.5
50	2s	9	VAL	3.5
48	1q	29	HIS	3.5
39	2h	112	LEU	3.5
3	2D	39	LYS	3.5
5	2F	90	PHE	3.5
14	2S	93	LYS	3.5
3	2D	2	ALA	3.5
23	2I	46	LEU	3.5
38	1g	4	ARG	3.5
51	1t	67	ALA	3.5
1	1A	2174	C	3.5
19	2X	92	LEU	3.4
45	1n	41	ARG	3.4
11	2P	44	GLY	3.4
34	1c	167	TRP	3.4
43	1l	28	LYS	3.4
7	2H	2	SER	3.4
8	2I	91	SER	3.4
45	1n	6	LEU	3.4
49	1r	78	LEU	3.4
34	1c	155	GLY	3.4
32	1a	975	A	3.4
34	2c	124	ILE	3.4
40	1i	124	GLN	3.4
44	2m	119	GLY	3.4
7	2H	88	LEU	3.4
51	1t	58	LYS	3.4
51	2t	11	SER	3.4
34	1c	184	TYR	3.4
46	1o	69	TYR	3.4
1	2A	2141	G	3.4
17	2V	74	LYS	3.4
42	2k	123	LYS	3.4
1	2A	2108	C	3.4
51	2t	20	LEU	3.4
48	1q	36	ILE	3.4
42	2k	125	PHE	3.4
7	2H	106	THR	3.4
32	2a	949	A	3.4

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Mol	Chain	Res	Type	RSRZ
50	2s	13	ASP	3.4
32	2a	112	G	3.4
32	2a	1361	G	3.4
41	2j	71	LEU	3.4
36	2e	14	ARG	3.4
6	2G	169	ALA	3.4
45	1n	20	ALA	3.4
23	2l	62	VAL	3.4
11	2P	39	LYS	3.4
16	2U	43	GLY	3.4
45	2n	36	PHE	3.4
3	2D	61	LEU	3.4
1	2A	2133	G	3.4
8	2I	11	ASN	3.4
43	1l	19	ARG	3.3
40	2i	112	LYS	3.3
36	2e	45	PHE	3.3
40	1i	108	VAL	3.3
40	2i	69	GLY	3.3
51	2t	63	ILE	3.3
30	18	23	VAL	3.3
39	2h	92	ARG	3.3
40	2i	9	ARG	3.3
7	2H	105	LEU	3.3
36	1e	91	LEU	3.3
50	2s	8	GLY	3.3
50	2s	14	HIS	3.3
32	1a	1001(A)	G	3.3
7	2H	166	GLY	3.3
34	2c	182	ILE	3.3
5	2F	89	VAL	3.3
22	20	45	PHE	3.3
38	1g	78	ARG	3.3
50	1s	78	ARG	3.3
26	24	63	TYR	3.3
32	2a	1257	U	3.3
40	1i	6	GLY	3.3
45	1n	38	GLY	3.3
51	2t	30	LYS	3.3
47	1p	34	GLU	3.3
51	2t	73	HIS	3.3
48	1q	87	LYS	3.3

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Mol	Chain	Res	Type	RSRZ
39	2h	95	VAL	3.3
1	1A	2147	G	3.3
7	2H	112	PRO	3.3
36	1e	81	GLU	3.3
1	2A	2135	A	3.3
6	2G	136	ARG	3.3
14	2S	92	TYR	3.3
16	2U	8	VAL	3.3
1	1A	2141	G	3.3
32	1a	111	G	3.3
52	1u	11	GLY	3.3
39	2h	83	ILE	3.3
3	2D	5	LYS	3.3
44	1m	103	THR	3.3
34	2c	155	GLY	3.3
25	23	60	GLU	3.2
32	2a	1225	A	3.2
34	1c	14	ILE	3.2
22	20	38	VAL	3.2
36	2e	94	ALA	3.2
43	1l	20	LYS	3.2
44	2m	111	LYS	3.2
41	1j	8	LEU	3.2
43	1l	27	LEU	3.2
11	2P	35	HIS	3.2
34	1c	154	SER	3.2
16	2U	17	ILE	3.2
47	1p	71	ARG	3.2
23	21	98	LEU	3.2
33	2b	96	ARG	3.2
5	2F	80	ALA	3.2
47	1p	14	ASN	3.2
32	1a	377	G	3.2
8	2I	112	LYS	3.2
1	2A	229	A	3.2
41	1j	52	GLY	3.2
36	2e	120	THR	3.2
39	2h	91	ARG	3.2
40	2i	81	ILE	3.2
39	2h	137	VAL	3.2
52	2u	12	LYS	3.2
41	1j	54	PHE	3.2

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Mol	Chain	Res	Type	RSRZ
13	2R	10	LEU	3.2
3	2D	64	ILE	3.2
32	1a	607	A	3.2
34	1c	200	ALA	3.2
40	1i	9	ARG	3.2
42	1k	126	ARG	3.2
44	1m	101	GLN	3.2
45	2n	32	SER	3.2
48	1q	31	LEU	3.2
43	1l	7	ILE	3.2
6	1G	73	ALA	3.2
6	2G	159	VAL	3.2
41	1j	10	GLY	3.2
6	2G	152	LEU	3.2
16	2U	20	LEU	3.2
47	1p	59	TRP	3.2
47	1p	16	HIS	3.1
1	1A	2170	A	3.1
26	14	54	GLY	3.1
16	2U	60	LEU	3.1
48	1q	97	SER	3.1
40	2i	105	ASP	3.1
3	1D	38	LYS	3.1
40	2i	11	LYS	3.1
51	1t	34	LYS	3.1
36	1e	82	VAL	3.1
45	2n	30	ALA	3.1
45	2n	59	ALA	3.1
14	2S	7	TYR	3.1
22	20	62	LEU	3.1
32	2a	1236	A	3.1
1	2A	2182	G	3.1
8	2I	99	GLU	3.1
34	1c	4	LYS	3.1
39	2h	80	ILE	3.1
40	1i	77	ILE	3.1
1	2A	2114	A	3.1
8	2I	20	ASP	3.1
16	2U	40	PHE	3.1
22	20	77	ARG	3.1
23	21	68	PRO	3.1
45	2n	2	ALA	3.1

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Mol	Chain	Res	Type	RSRZ
17	2V	82	ARG	3.1
45	1n	4	LYS	3.1
45	1n	49	HIS	3.1
40	1i	14	VAL	3.1
11	2P	17	LYS	3.1
38	2g	36	LYS	3.1
45	1n	29	ARG	3.1
20	2Y	12	THR	3.1
6	1G	146	TYR	3.1
14	2S	36	TYR	3.1
45	1n	14	PRO	3.1
35	1d	5	ILE	3.1
2	2B	53	A	3.1
47	2p	26	ARG	3.1
32	1a	112	G	3.1
39	2h	94	TYR	3.1
40	1i	36	TYR	3.1
40	1i	112	LYS	3.1
22	20	42	GLY	3.1
32	2a	1285	A	3.1
1	2A	2149	G	3.1
22	20	50	ASN	3.1
36	2e	131	ILE	3.1
28	26	5	VAL	3.1
40	1i	110	GLU	3.1
47	1p	53	VAL	3.1
32	2a	60	A	3.1
26	24	40	HIS	3.1
39	2h	84	ARG	3.1
34	1c	2	GLY	3.1
34	2c	177	THR	3.1
51	1t	63	ILE	3.1
16	2U	9	VAL	3.0
44	1m	111	LYS	3.0
51	1t	29	LYS	3.0
1	1A	1095	A	3.0
1	2A	2178	C	3.0
51	1t	26	ASN	3.0
9	2N	83	LYS	3.0
40	2i	26	VAL	3.0
13	2R	18	LEU	3.0
39	1h	91	ARG	3.0

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Mol	Chain	Res	Type	RSRZ
40	1i	79	LEU	3.0
41	2j	66	ARG	3.0
34	1c	185	GLY	3.0
39	2h	9	MET	3.0
21	2Z	167	PRO	3.0
14	2S	3	ARG	3.0
20	2Y	60	PHE	3.0
46	1o	57	LEU	3.0
39	2h	96	GLY	3.0
41	2j	7	LYS	3.0
22	20	70	GLN	3.0
32	2a	975	A	3.0
42	1k	25	TYR	3.0
41	1j	42	THR	3.0
3	2D	182	LEU	3.0
39	2h	87	SER	3.0
35	1d	167	GLY	3.0
40	2i	68	GLY	3.0
7	2H	151	ILE	3.0
17	2V	72	VAL	3.0
32	2a	1531	A	3.0
5	2F	53	THR	3.0
28	26	11	LEU	3.0
34	2c	196	LEU	3.0
51	1t	30	LYS	3.0
45	1n	51	GLY	3.0
21	2Z	154	ASP	3.0
9	2N	74	ARG	3.0
1	2A	2174	C	3.0
33	1b	37	ASN	3.0
30	28	61	LEU	3.0
43	1l	67	THR	3.0
19	2X	86	GLY	3.0
23	11	26	ARG	3.0
47	2p	25	ARG	3.0
24	22	1	MET	3.0
31	29	26	ILE	3.0
1	2A	2123	G	3.0
1	2A	2319	G	3.0
47	2p	64	ALA	3.0
4	2E	195	LEU	3.0
11	1P	15	ARG	3.0

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Mol	Chain	Res	Type	RSRZ
35	1d	118	ARG	3.0
51	1t	79	ARG	3.0
1	1A	2122	U	3.0
6	2G	34	LEU	3.0
7	2H	87	LEU	3.0
35	2d	4	TYR	3.0
39	1h	88	LYS	3.0
51	2t	71	THR	3.0
1	2A	2169	A	3.0
48	1q	26	GLN	3.0
33	1b	201	ILE	3.0
7	2H	144	VAL	3.0
3	2D	37	LEU	2.9
44	2m	108	ARG	2.9
43	1l	23	LYS	2.9
32	1a	328	C	2.9
36	1e	135	THR	2.9
31	29	1	MET	2.9
29	27	23	ARG	2.9
34	1c	6	HIS	2.9
40	2i	45	ALA	2.9
40	2i	111	ARG	2.9
2	2B	55	U	2.9
32	1a	1358	U	2.9
48	1q	40	LYS	2.9
40	2i	8	GLY	2.9
32	1a	976	G	2.9
29	27	47	ARG	2.9
43	1l	89	ARG	2.9
44	2m	60	VAL	2.9
50	1s	37	ARG	2.9
5	2F	81	PRO	2.9
9	2N	82	LEU	2.9
12	2Q	79	LEU	2.9
16	2U	27	LEU	2.9
40	1i	40	LEU	2.9
51	2t	66	ALA	2.9
35	1d	138	TYR	2.9
39	1h	4	ASP	2.9
43	2l	15	ARG	2.9
16	2U	39	LEU	2.9
21	2Z	150	LEU	2.9

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Mol	Chain	Res	Type	RSRZ
38	1g	38	LEU	2.9
41	2j	62	HIS	2.9
4	1E	151	TYR	2.9
17	2V	81	TYR	2.9
41	2j	38	ILE	2.9
39	2h	136	GLU	2.9
1	2A	2170	A	2.9
25	23	17	LYS	2.9
44	2m	87	TYR	2.9
50	2s	6	LYS	2.9
11	2P	71	VAL	2.9
51	1t	19	SER	2.9
8	2I	38	LEU	2.9
41	2j	85	LEU	2.9
1	2A	2113	U	2.9
48	1q	37	LYS	2.9
7	2H	97	ARG	2.9
41	2j	61	GLU	2.9
32	1a	1352	C	2.9
32	2a	1325	C	2.9
32	2a	1354	C	2.9
36	2e	119	LEU	2.9
6	2G	32	PRO	2.9
50	1s	56	GLN	2.9
51	1t	73	HIS	2.9
9	2N	85	ILE	2.9
14	2S	57	LYS	2.9
8	2I	13	GLY	2.9
23	11	36	GLY	2.9
34	1c	39	ILE	2.9
1	2A	2134	A	2.9
3	2D	34	VAL	2.9
51	2t	22	ARG	2.9
30	28	37	SER	2.8
47	1p	61	SER	2.8
4	2E	151	TYR	2.8
41	1j	61	GLU	2.8
26	24	49	PHE	2.8
38	1g	34	GLY	2.8
39	2h	61	VAL	2.8
45	1n	16	PHE	2.8
32	2a	327	A	2.8

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Mol	Chain	Res	Type	RSRZ
54	1x	76	A	2.8
32	2a	1356	G	2.8
43	2l	13	LYS	2.8
38	2g	4	ARG	2.8
40	2i	120	ARG	2.8
44	2m	78	ILE	2.8
34	1c	198	VAL	2.8
12	2Q	121	ALA	2.8
50	2s	15	LEU	2.8
32	2a	1250	A	2.8
1	2A	2179	C	2.8
2	2B	54	G	2.8
39	1h	18	ARG	2.8
47	1p	69	THR	2.8
5	2F	78	ILE	2.8
40	1i	63	ILE	2.8
13	2R	21	TYR	2.8
11	2P	83	VAL	2.8
17	2V	79	VAL	2.8
34	1c	199	LYS	2.8
45	1n	44	LEU	2.8
1	1A	1096	A	2.8
12	1Q	5	ARG	2.8
40	2i	27	THR	2.8
51	1t	33	ILE	2.8
11	2P	107	LYS	2.8
32	2a	328	C	2.8
34	1c	10	PHE	2.8
40	1i	41	VAL	2.8
41	2j	72	VAL	2.8
43	1l	26	ALA	2.8
44	2m	110	ARG	2.8
3	2D	202	LYS	2.8
48	2q	100	LYS	2.8
16	2U	49	HIS	2.8
22	20	80	HIS	2.8
23	21	13	ILE	2.8
32	2a	1289	A	2.8
1	2A	2129	C	2.8
21	2Z	79	ARG	2.8
36	2e	21	ALA	2.8
40	2i	76	ALA	2.8

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Mol	Chain	Res	Type	RSRZ
41	2j	43	ARG	2.8
52	2u	9	ARG	2.8
39	2h	135	CYS	2.8
45	2n	49	HIS	2.8
9	2N	75	TYR	2.8
31	29	23	VAL	2.8
32	1a	1357	A	2.8
32	1a	1531	A	2.8
32	1a	1223	C	2.8
38	1g	84	ASN	2.8
43	1l	29	GLY	2.8
33	2b	70	PHE	2.8
36	2e	84	PHE	2.8
38	1g	153	HIS	2.8
35	1d	157	LEU	2.8
35	1d	170	VAL	2.8
40	2i	28	VAL	2.8
1	2A	2107	C	2.8
17	2V	76	LYS	2.8
32	2a	1363	C	2.8
36	2e	121	LYS	2.8
36	1e	134	ALA	2.8
34	1c	203	PHE	2.8
7	2H	52	VAL	2.8
34	2c	198	VAL	2.8
23	2l	63	ALA	2.8
32	1a	1366	C	2.8
35	2d	207	TYR	2.8
40	1i	43	ALA	2.8
54	2x	76	A	2.7
1	1A	2144	U	2.7
18	2W	92	ARG	2.7
1	1A	2168	G	2.7
30	18	2	PRO	2.7
45	1n	33	VAL	2.7
47	2p	20	VAL	2.7
40	2i	107	ARG	2.7
30	28	16	ILE	2.7
6	2G	142	PRO	2.7
3	2D	206	LEU	2.7
20	2Y	31	LEU	2.7
41	2j	35	SER	2.7

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
32	2a	1368	G	2.7
48	1q	45	HIS	2.7
5	2F	62	ARG	2.7
11	2P	15	ARG	2.7
22	20	20	ARG	2.7
45	2n	13	THR	2.7
32	1a	106	C	2.7
40	1i	30	GLY	2.7
1	2A	2118	U	2.7
3	2D	15	PHE	2.7
40	2i	77	ILE	2.7
8	2I	87	LYS	2.7
14	2S	31	SER	2.7
35	2d	164	ALA	2.7
40	2i	82	ALA	2.7
47	1p	26	ARG	2.7
48	1q	38	ARG	2.7
1	1A	2159	G	2.7
32	1a	1036	G	2.7
1	2A	2105	C	2.7
32	1a	63	C	2.7
32	1a	1030(B)	C	2.7
38	2g	28	ASN	2.7
33	2b	214	ILE	2.7
39	1h	83	ILE	2.7
1	1A	2119	A	2.7
6	1G	2	PRO	2.7
34	2c	167	TRP	2.7
35	1d	135	LEU	2.7
7	2H	95	ARG	2.7
31	29	19	ARG	2.7
35	2d	57	ARG	2.7
45	1n	19	ARG	2.7
45	2n	60	SER	2.7
51	2t	15	ARG	2.7
51	2t	76	ALA	2.7
39	1h	90	GLY	2.7
1	2A	2175	C	2.7
40	2i	113	LYS	2.7
6	2G	26	GLN	2.7
23	21	4	VAL	2.7
35	1d	133	VAL	2.7

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Mol	Chain	Res	Type	RSRZ
35	2d	96	LEU	2.7
40	1i	128	ARG	2.7
40	2i	65	VAL	2.7
44	2m	91	ARG	2.7
48	2q	9	VAL	2.7
41	2j	97	GLU	2.7
34	1c	13	GLY	2.7
52	1u	4	GLY	2.7
52	1u	8	THR	2.7
35	2d	199	ASN	2.7
30	28	46	ARG	2.7
32	2a	973	G	2.7
51	2t	8	ARG	2.7
39	2h	59	LEU	2.7
47	2p	6	LEU	2.7
44	2m	73	GLU	2.7
39	1h	87	SER	2.7
40	1i	126	SER	2.7
1	1A	2189	U	2.7
7	2H	148	ILE	2.7
34	1c	190	ARG	2.7
45	2n	57	ARG	2.7
46	1o	72	ARG	2.7
1	2A	2177	C	2.7
45	2n	47	LEU	2.7
1	2A	2154	G	2.7
2	2B	90	A	2.7
16	2U	14	HIS	2.7
36	1e	84	PHE	2.7
45	2n	26	ARG	2.7
8	2I	68	LEU	2.7
25	23	48	GLU	2.7
34	2c	206	GLU	2.7
51	1t	75	ASN	2.7
47	1p	23	ASP	2.7
6	2G	33	ARG	2.7
8	2I	72	LEU	2.6
11	2P	29	LYS	2.6
36	1e	119	LEU	2.6
20	2Y	42	VAL	2.6
38	2g	109	ASN	2.6
50	1s	33	THR	2.6

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Mol	Chain	Res	Type	RSRZ
41	2j	36	GLY	2.6
5	2F	72	ARG	2.6
48	2q	29	HIS	2.6
13	1R	14	SER	2.6
30	28	59	LYS	2.6
32	2a	1355	G	2.6
40	1i	11	LYS	2.6
43	2l	7	ILE	2.6
39	2h	63	LEU	2.6
53	1v	14	A	2.6
8	2l	144	VAL	2.6
26	14	45	GLY	2.6
3	2D	52	ARG	2.6
45	1n	3	ARG	2.6
36	1e	95	ALA	2.6
11	2P	34	GLY	2.6
52	1u	7	ARG	2.6
45	2n	24	CYS	2.6
38	1g	27	ILE	2.6
1	2A	2189	U	2.6
35	1d	78	LEU	2.6
35	2d	209	ARG	2.6
45	2n	12	ARG	2.6
47	2p	39	TYR	2.6
7	2H	133	VAL	2.6
32	1a	1368	G	2.6
21	2Z	83	PRO	2.6
41	2j	39	PRO	2.6
34	1c	166	GLU	2.6
35	1d	115	ARG	2.6
35	2d	114	ARG	2.6
13	2R	70	LEU	2.6
45	2n	53	LEU	2.6
19	2X	69	TYR	2.6
40	1i	75	ASP	2.6
47	2p	12	LYS	2.6
48	1q	42	TYR	2.6
7	2H	128	PRO	2.6
30	18	10	ALA	2.6
39	1h	5	PRO	2.6
32	1a	105	G	2.6
32	1a	388	G	2.6

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Mol	Chain	Res	Type	RSRZ
6	2G	39	ILE	2.6
32	1a	110	C	2.6
1	1A	2506	U	2.6
21	2Z	76	LEU	2.6
32	1a	375	U	2.6
51	2t	34	LYS	2.6
4	2E	127	ASP	2.6
38	2g	154	TYR	2.6
3	2D	53	PHE	2.6
5	2F	49	ALA	2.6
7	2H	123	PHE	2.6
34	2c	163	ALA	2.6
9	2N	69	GLN	2.6
17	2V	80	GLN	2.6
32	1a	1233	G	2.6
32	2a	108	G	2.6
39	1h	86	ILE	2.6
34	1c	175	LEU	2.6
47	2p	1	MET	2.6
51	2t	16	HIS	2.6
40	1i	17	VAL	2.6
20	2Y	46	LYS	2.6
44	1m	94	ARG	2.6
47	2p	7	ALA	2.6
34	1c	87	LEU	2.6
41	2j	52	GLY	2.6
32	1a	310	G	2.6
3	2D	18	VAL	2.6
6	2G	37	VAL	2.6
40	2i	75	ASP	2.6
30	28	21	LYS	2.6
15	1T	104	ASN	2.6
43	1l	85	ILE	2.5
50	2s	49	ILE	2.5
6	2G	139	LEU	2.5
11	2P	30	THR	2.5
11	2P	59	LEU	2.5
32	1a	974	A	2.5
32	2a	969	A	2.5
32	1a	371	G	2.5
48	1q	39	SER	2.5
39	2h	138	TRP	2.5

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Mol	Chain	Res	Type	RSRZ
14	2S	40	ILE	2.5
5	1F	53	THR	2.5
14	2S	56	LEU	2.5
22	20	68	GLU	2.5
35	2d	202	LEU	2.5
42	2k	98	LEU	2.5
50	2s	71	LEU	2.5
7	2H	130	ARG	2.5
11	2P	16	ARG	2.5
39	1h	9	MET	2.5
1	2A	1379	A	2.5
16	2U	32	PHE	2.5
26	24	66	SER	2.5
32	2a	104	G	2.5
6	2G	137	GLU	2.5
30	28	26	LYS	2.5
44	1m	110	ARG	2.5
1	1A	2130	U	2.5
1	2A	2172	U	2.5
31	29	3	VAL	2.5
33	2b	163	PHE	2.5
1	1A	1762	A	2.5
32	2a	977	A	2.5
47	1p	58	TYR	2.5
44	2m	13	LYS	2.5
3	2D	60	ARG	2.5
32	1a	102	G	2.5
32	1a	324	G	2.5
32	2a	976	G	2.5
35	2d	47	ARG	2.5
45	2n	19	ARG	2.5
32	1a	1030	C	2.5
32	2a	970	C	2.5
2	2B	52	A	2.5
32	1a	1001	A	2.5
32	2a	965	A	2.5
35	1d	73	ARG	2.5
35	2d	122	ARG	2.5
45	1n	26	ARG	2.5
1	2A	1125	G	2.5
32	1a	1365	G	2.5
12	1Q	85	LYS	2.5

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Mol	Chain	Res	Type	RSRZ
48	2q	24	GLU	2.5
22	20	72	ARG	2.5
27	25	19	ARG	2.5
35	2d	20	TYR	2.5
39	2h	85	ARG	2.5
13	1R	18	LEU	2.5
37	2f	45	LEU	2.5
5	1F	89	VAL	2.5
32	2a	1235	U	2.5
50	1s	55	LYS	2.5
6	2G	35	GLU	2.5
22	20	39	ARG	2.5
34	1c	177	THR	2.5
3	2D	235	GLY	2.5
43	1l	95	GLY	2.5
45	2n	21	TYR	2.5
32	1a	1287	A	2.5
8	2I	21	VAL	2.5
1	1A	2123	G	2.5
12	2Q	114	ALA	2.5
31	29	5	ALA	2.5
31	29	34	GLN	2.5
32	2a	951	G	2.5
47	2p	10	GLY	2.5
7	2H	85	LYS	2.5
35	2d	54	TYR	2.5
32	1a	390	C	2.5
51	2t	62	LEU	2.5
30	28	65	GLU	2.5
31	29	7	VAL	2.5
23	21	28	GLY	2.5
3	1D	92	ILE	2.5
6	2G	94	LEU	2.5
12	2Q	32	TYR	2.5
22	20	59	LEU	2.5
7	2H	69	ARG	2.4
16	2U	28	ARG	2.4
43	2l	5	PRO	2.4
32	1a	1363	C	2.4
20	2Y	24	VAL	2.4
48	1q	9	VAL	2.4
50	1s	41	VAL	2.4

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Mol	Chain	Res	Type	RSRZ
23	21	29	GLY	2.4
34	1c	15	THR	2.4
3	2D	54	ARG	2.4
9	2N	91	LEU	2.4
48	1q	24	GLU	2.4
48	1q	32	TYR	2.4
40	2i	21	PRO	2.4
32	2a	1190	G	2.4
1	2A	34	C	2.4
25	23	54	VAL	2.4
32	2a	950	U	2.4
10	1O	81	ASP	2.4
50	1s	12	ASP	2.4
7	2H	142	GLY	2.4
38	2g	39	ALA	2.4
32	2a	978	A	2.4
8	2I	82	ARG	2.4
23	21	11	ARG	2.4
13	2R	20	LEU	2.4
35	1d	11	LEU	2.4
36	2e	101	ILE	2.4
39	1h	21	LYS	2.4
7	2H	43	VAL	2.4
44	1m	98	VAL	2.4
47	2p	79	VAL	2.4
50	1s	35	SER	2.4
29	27	1	MET	2.4
32	1a	108	G	2.4
34	1c	179	ARG	2.4
25	23	53	LEU	2.4
35	2d	11	LEU	2.4
13	2R	110	PRO	2.4
23	21	12	PRO	2.4
38	1g	156	TRP	2.4
47	1p	46	PRO	2.4
30	28	49	VAL	2.4
43	1l	32	PHE	2.4
50	2s	38	SER	2.4
51	2t	70	SER	2.4
3	2D	87	ASN	2.4
5	2F	61	GLY	2.4
35	2d	102	ASP	2.4

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Mol	Chain	Res	Type	RSRZ
7	2H	145	ALA	2.4
32	1a	376	G	2.4
32	1a	1186	G	2.4
32	1a	1224	G	2.4
34	1c	206	GLU	2.4
45	2n	46	GLU	2.4
47	2p	31	LYS	2.4
14	2S	54	LEU	2.4
48	1q	30	PRO	2.4
1	1A	1094	U	2.4
22	20	25	ARG	2.4
48	1q	91	ARG	2.4
7	2H	150	ALA	2.4
32	1a	1113	C	2.4
32	2a	1369	C	2.4
36	2e	104	ALA	2.4
1	2A	1816	G	2.4
36	2e	110	LEU	2.4
39	2h	38	ILE	2.4
46	1o	32	LEU	2.4
50	1s	69	HIS	2.4
3	2D	62	TYR	2.4
11	2P	72	PRO	2.4
14	2S	87	PHE	2.4
48	2q	35	VAL	2.4
51	1t	8	ARG	2.4
44	2m	64	TRP	2.4
36	2e	83	GLU	2.4
3	2D	217	ARG	2.4
22	20	57	PHE	2.4
32	1a	333	G	2.4
32	2a	107	G	2.4
35	2d	198	VAL	2.4
43	1l	98	TYR	2.4
48	2q	37	LYS	2.4
45	2n	8	GLU	2.4
36	1e	86	ALA	2.4
51	2t	12	ALA	2.4
1	1A	2175	C	2.4
6	2G	90	LEU	2.4
23	21	37	ILE	2.4
32	2a	1234	C	2.4

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
39	1h	10	LEU	2.4
46	1o	66	LEU	2.4
47	2p	19	ILE	2.4
48	2q	98	LEU	2.4
6	2G	25	TYR	2.4
27	15	60	VAL	2.4
35	1d	7	PRO	2.4
32	2a	111	G	2.4
3	1D	225	ALA	2.4
50	1s	53	ASN	2.4
7	2H	162	ILE	2.4
8	2I	103	ARG	2.4
9	2N	23	LEU	2.4
9	2N	84	LYS	2.4
39	1h	109	ILE	2.4
35	2d	206	PHE	2.3
4	2E	150	VAL	2.3
1	2A	2106	G	2.3
36	2e	127	ASN	2.3
45	1n	60	SER	2.3
46	1o	56	LEU	2.3
6	1G	35	GLU	2.3
1	1A	1064	C	2.3
32	1a	136	C	2.3
32	1a	1354	C	2.3
50	1s	57	HIS	2.3
11	2P	19	VAL	2.3
34	1c	151	VAL	2.3
47	1p	76	GLN	2.3
20	2Y	55	TYR	2.3
32	1a	1532	U	2.3
36	1e	133	TYR	2.3
11	2P	18	ARG	2.3
15	2T	108	ARG	2.3
16	2U	33	ARG	2.3
35	1d	76	ARG	2.3
39	2h	4	ASP	2.3
34	2c	189	ALA	2.3
42	2k	31	THR	2.3
1	2A	2181	G	2.3
5	2F	56	GLU	2.3
20	2Y	29	GLU	2.3

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Mol	Chain	Res	Type	RSRZ
32	1a	971	G	2.3
36	2e	11	ILE	2.3
51	1t	41	ILE	2.3
32	2a	1447	A	2.3
1	1A	2142	C	2.3
4	2E	7	VAL	2.3
25	23	10	LYS	2.3
41	2j	68	HIS	2.3
35	2d	118	ARG	2.3
44	1m	99	ARG	2.3
9	2N	78	TYR	2.3
30	18	64	TYR	2.3
44	2m	23	TYR	2.3
11	2P	31	ALA	2.3
14	2S	6	ALA	2.3
16	2U	35	ALA	2.3
3	2D	204	ILE	2.3
43	1l	10	LEU	2.3
9	2N	104	LYS	2.3
35	1d	110	PHE	2.3
40	2i	78	LYS	2.3
1	2A	2176	A	2.3
3	2D	205	VAL	2.3
23	21	41	ARG	2.3
36	1e	18	ARG	2.3
38	2g	41	ARG	2.3
40	1i	10	ARG	2.3
48	2q	10	VAL	2.3
41	1j	53	PRO	2.3
45	1n	10	ALA	2.3
14	2S	11	LYS	2.3
39	2h	111	ILE	2.3
36	1e	90	VAL	2.3
47	2p	2	VAL	2.3
50	1s	9	VAL	2.3
1	1A	2132	U	2.3
32	2a	1358	U	2.3
6	2G	146	TYR	2.3
43	1l	16	GLU	2.3
51	1t	64	ASP	2.3
8	2I	26	ALA	2.3
19	2X	1	MET	2.3

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Mol	Chain	Res	Type	RSRZ
34	1c	193	TYR	2.3
14	2S	5	THR	2.3
15	2T	60	THR	2.3
19	2X	24	GLY	2.3
47	2p	5	ARG	2.3
52	1u	10	ARG	2.3
7	2H	24	VAL	2.3
23	2I	70	VAL	2.3
43	1I	11	VAL	2.3
38	2g	153	HIS	2.3
1	1A	2169	A	2.3
1	2A	2173	A	2.3
16	2U	2	PRO	2.3
16	2U	30	LYS	2.3
16	2U	37	GLU	2.3
29	27	32	LYS	2.3
30	28	44	LYS	2.3
31	29	8	LYS	2.3
32	1a	622	A	2.3
32	1a	1362	C	2.3
32	2a	322	C	2.3
36	2e	92	LYS	2.3
12	2Q	17	LEU	2.3
22	10	75	LEU	2.3
22	20	73	GLY	2.3
36	1e	22	GLY	2.3
38	2g	42	ILE	2.3
47	1p	60	LEU	2.3
6	2G	15	VAL	2.3
11	2P	101	VAL	2.3
22	10	16	SER	2.3
36	2e	125	SER	2.3
47	2p	65	GLN	2.3
39	2h	129	VAL	2.3
41	1j	56	HIS	2.3
1	2A	2163	C	2.3
13	1R	19	ALA	2.3
14	1S	13	ARG	2.3
41	1j	40	LEU	2.3
42	2k	50	TYR	2.3
1	1A	1058	G	2.3
6	2G	23	PHE	2.3

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Mol	Chain	Res	Type	RSRZ
16	2U	34	LYS	2.3
40	1i	31	GLN	2.3
45	2n	50	LYS	2.3
47	2p	3	LYS	2.3
35	2d	115	ARG	2.3
36	2e	123	LEU	2.3
38	2g	16	LEU	2.3
47	1p	49	LEU	2.3
51	1t	84	LEU	2.3
1	1A	2138	C	2.3
12	2Q	103	MET	2.3
20	2Y	61	ILE	2.3
32	2a	1254	C	2.3
44	1m	23	TYR	2.3
3	2D	68	LYS	2.3
32	2a	325	A	2.3
22	20	40	GLN	2.3
32	1a	391	G	2.3
32	2a	1233	G	2.3
36	1e	122	GLU	2.3
8	2I	92	VAL	2.2
12	2Q	129	THR	2.2
40	2i	86	VAL	2.2
43	2l	6	THR	2.2
9	2N	92	ALA	2.2
36	1e	121	LYS	2.2
39	1h	63	LEU	2.2
40	2i	102	LEU	2.2
50	1s	76	PRO	2.2
51	2t	10	LEU	2.2
8	2I	104	GLN	2.2
1	2A	1847	A	2.2
32	1a	60	A	2.2
38	1g	17	VAL	2.2
53	1v	12	A	2.2
53	2v	14	A	2.2
44	2m	77	ASN	2.2
8	2I	128	LEU	2.2
52	1u	23	PRO	2.2
32	1a	454	C	2.2
15	2T	93	ARG	2.2
32	1a	977	A	2.2

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Mol	Chain	Res	Type	RSRZ
48	1q	17	LYS	2.2
52	2u	8	THR	2.2
32	2a	953	G	2.2
39	2h	28	ALA	2.2
43	1l	94	PRO	2.2
47	2p	74	LEU	2.2
39	2h	99	GLU	2.2
26	24	68	ARG	2.2
40	2i	42	ARG	2.2
43	2l	89	ARG	2.2
3	1D	51	VAL	2.2
5	2F	57	VAL	2.2
6	1G	15	VAL	2.2
14	2S	14	VAL	2.2
17	2V	78	LYS	2.2
17	2V	85	LYS	2.2
20	2Y	4	LYS	2.2
27	25	10	LYS	2.2
47	1p	3	LYS	2.2
22	20	54	GLY	2.2
32	2a	1252	A	2.2
34	1c	33	LEU	2.2
44	1m	95	GLY	2.2
7	2H	111	HIS	2.2
12	2Q	39	PRO	2.2
19	2X	28	PHE	2.2
35	1d	70	ILE	2.2
40	2i	61	ALA	2.2
26	24	58	ARG	2.2
32	1a	1030(A)	G	2.2
32	2a	331	G	2.2
33	2b	101	MET	2.2
36	2e	24	ARG	2.2
39	1h	85	ARG	2.2
40	2i	73	GLN	2.2
47	2p	8	ARG	2.2
8	2I	126	TYR	2.2
50	2s	34	TRP	2.2
1	2A	580	C	2.2
36	2e	29	GLY	2.2
3	2D	40	THR	2.2
14	2S	4	LEU	2.2

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Mol	Chain	Res	Type	RSRZ
13	2R	47	PHE	2.2
36	2e	118	ILE	2.2
41	1j	51	ARG	2.2
10	2O	1	MET	2.2
32	1a	610	G	2.2
32	1a	951	G	2.2
12	2Q	102	VAL	2.2
22	20	51	VAL	2.2
30	28	23	VAL	2.2
36	2e	105	VAL	2.2
47	1p	51	VAL	2.2
1	2A	531	C	2.2
32	1a	1037	C	2.2
12	2Q	34	LEU	2.2
35	2d	100	ARG	2.2
4	2E	114	ALA	2.2
6	1G	80	PHE	2.2
34	2c	14	ILE	2.2
36	2e	89	ILE	2.2
39	1h	6	ILE	2.2
41	2j	96	ILE	2.2
51	1t	11	SER	2.2
6	2G	138	GLN	2.2
32	1a	389	A	2.2
32	2a	109	A	2.2
12	2Q	97	VAL	2.2
29	17	41	ARG	2.2
35	1d	122	ARG	2.2
43	1l	97	ARG	2.2
51	2t	17	ARG	2.2
8	2I	97	ILE	2.2
18	2W	95	ILE	2.2
40	2i	33	PHE	2.2
42	1k	117	ASN	2.2
48	2q	60	ILE	2.2
32	1a	134	A	2.2
12	2Q	130	LYS	2.2
38	2g	85	TYR	2.2
3	2D	256	GLY	2.2
12	2Q	33	GLY	2.2
46	1o	68	ARG	2.2
51	1t	74	LYS	2.2

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Mol	Chain	Res	Type	RSRZ
51	2t	83	ARG	2.2
8	2I	47	LEU	2.2
22	20	21	LEU	2.2
32	2a	106	C	2.2
32	2a	1308	U	2.2
34	1c	168	ALA	2.2
38	1g	26	PHE	2.2
22	20	24	LYS	2.2
38	2g	35	LYS	2.2
46	1o	65	ARG	2.2
1	2A	2320	A	2.2
2	2B	25	A	2.2
4	2E	160	TYR	2.2
32	2a	1349	A	2.2
11	2P	51	PHE	2.1
13	2R	65	LEU	2.1
34	2c	157	ILE	2.1
39	2h	109	ILE	2.1
44	2m	76	ALA	2.1
50	2s	50	ALA	2.1
4	1E	147	PRO	2.1
32	2a	1371	G	2.1
32	2a	1523	G	2.1
35	1d	165	MET	2.1
42	2k	35	PRO	2.1
5	2F	51	THR	2.1
41	2j	56	HIS	2.1
1	2A	255	A	2.1
32	1a	313	A	2.1
3	2D	67	PHE	2.1
35	2d	75	PHE	2.1
50	1s	30	LEU	2.1
14	1S	6	ALA	2.1
28	26	42	TRP	2.1
34	2c	199	LYS	2.1
35	2d	5	ILE	2.1
8	2I	10	GLU	2.1
32	1a	322	C	2.1
35	1d	132	ARG	2.1
36	1e	25	ARG	2.1
48	1q	68	ARG	2.1
32	1a	326	G	2.1

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Mol	Chain	Res	Type	RSRZ
32	1a	855	G	2.1
32	2a	941	G	2.1
39	2h	113	SER	2.1
7	2H	82	GLY	2.1
46	1o	60	VAL	2.1
7	2H	153	LYS	2.1
40	2i	59	PHE	2.1
7	2H	146	ALA	2.1
8	2I	17	GLN	2.1
50	1s	50	ALA	2.1
52	2u	7	ARG	2.1
20	2Y	43	ASN	2.1
38	2g	84	ASN	2.1
32	1a	311	C	2.1
35	1d	33	MET	2.1
4	1E	116	VAL	2.1
5	2F	76	GLY	2.1
35	1d	8	VAL	2.1
39	2h	131	GLY	2.1
41	1j	68	HIS	2.1
1	1A	1099	G	2.1
27	25	29	THR	2.1
30	18	3	LYS	2.1
32	1a	309	G	2.1
32	1a	1370	G	2.1
6	1G	25	TYR	2.1
44	2m	96	LEU	2.1
14	2S	13	ARG	2.1
40	1i	105	ASP	2.1
1	1A	1070	A	2.1
32	1a	59	A	2.1
32	2a	134	A	2.1
4	2E	196	VAL	2.1
5	2F	183	VAL	2.1
11	2P	64	LYS	2.1
51	1t	38	LYS	2.1
12	2Q	37	LEU	2.1
35	2d	139	ARG	2.1
44	2m	94	ARG	2.1
30	18	65	GLU	2.1
32	1a	104	G	2.1
32	2a	947	G	2.1

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Mol	Chain	Res	Type	RSRZ
43	2l	16	GLU	2.1
50	1s	10	PHE	2.1
50	2s	78	ARG	2.1
36	2e	79	GLU	2.1
1	2A	2150	U	2.1
3	2D	49	ILE	2.1
45	2n	10	ALA	2.1
6	2G	89	GLY	2.1
32	2a	974	A	2.1
35	2d	203	VAL	2.1
43	2l	11	VAL	2.1
47	2p	59	TRP	2.1
7	2H	6	ARG	2.1
50	2s	35	SER	2.1
51	1t	83	ARG	2.1
3	2D	147	LEU	2.1
3	2D	257	LEU	2.1
4	1E	195	LEU	2.1
8	2I	30	LEU	2.1
14	1S	92	TYR	2.1
36	2e	16	THR	2.1
40	2i	40	LEU	2.1
50	2s	39	THR	2.1
7	2H	165	ALA	2.1
32	1a	723	U	2.1
36	2e	109	ILE	2.1
38	2g	27	ILE	2.1
1	2A	2152	G	2.1
36	1e	92	LYS	2.1
40	1i	78	LYS	2.1
9	2N	45	ASN	2.1
3	1D	229	VAL	2.1
11	2P	77	ARG	2.1
25	23	29	ARG	2.1
32	1a	969	A	2.1
36	2e	82	VAL	2.1
36	2e	106	PRO	2.1
45	1n	56	VAL	2.1
1	2A	2128	C	2.1
9	2N	76	SER	2.1
33	1b	163	PHE	2.1
35	2d	120	LEU	2.1

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Mol	Chain	Res	Type	RSRZ
39	2h	10	LEU	2.1
6	2G	49	ASP	2.1
18	2W	38	TYR	2.1
47	1p	45	THR	2.1
1	2A	2506	U	2.1
28	26	7	ILE	2.1
29	27	45	ALA	2.1
34	1c	169	ALA	2.1
35	1d	23	GLY	2.1
1	2A	1678	G	2.1
1	2A	2018	G	2.1
2	2B	51	G	2.1
3	2D	51	VAL	2.1
7	2H	114	VAL	2.1
19	2X	83	VAL	2.1
32	1a	107	G	2.1
32	2a	326	G	2.1
32	2a	971	G	2.1
30	28	54	GLU	2.1
35	2d	56	VAL	2.1
39	1h	137	VAL	2.1
1	1A	2108	C	2.1
1	1A	2114	A	2.1
1	1A	2164	C	2.1
1	1A	2188	C	2.1
3	1D	275	LYS	2.1
32	2a	315	A	2.1
32	2a	1374	A	2.1
16	2U	31	SER	2.1
46	1o	31	LEU	2.1
45	1n	24	CYS	2.1
3	1D	93	ALA	2.1
47	1p	38	TYR	2.1
47	2p	4	ILE	2.1
47	2p	33	ILE	2.1
32	1a	223	U	2.1
39	2h	90	GLY	2.1
10	2O	31	LYS	2.1
11	2P	36	LYS	2.1
16	2U	15	LYS	2.1
35	1d	136	PRO	2.1
36	2e	100	VAL	2.1

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
32	1a	1356	G	2.1
3	2D	46	GLN	2.0
46	1o	70	LEU	2.0
32	1a	379	C	2.0
32	1a	1041	A	2.0
32	1a	1349	A	2.0
32	2a	1352	C	2.0
43	1l	22	SER	2.0
3	2D	263	ARG	2.0
5	2F	64	ILE	2.0
16	2U	36	ARG	2.0
36	1e	21	ALA	2.0
43	1l	68	ALA	2.0
44	1m	91	ARG	2.0
3	2D	4	LYS	2.0
14	2S	62	LYS	2.0
35	2d	61	LYS	2.0
34	1c	195	VAL	2.0
6	2G	178	PHE	2.0
8	2I	58	LEU	2.0
39	1h	133	LEU	2.0
39	2h	81	HIS	2.0
1	1A	2148	G	2.0
32	1a	306	G	2.0
1	2A	256	A	2.0
1	2A	2136	C	2.0
32	1a	312	C	2.0
32	1a	1355	G	2.0
32	1a	1350	A	2.0
32	1a	1492	A	2.0
32	2a	1362	C	2.0
34	2c	60	ALA	2.0
39	1h	111	ILE	2.0
21	2Z	156	LYS	2.0
27	25	9	LYS	2.0
44	1m	109	THR	2.0
10	1O	1	MET	2.0
41	2j	53	PRO	2.0
13	2R	111	LEU	2.0
31	29	4	ARG	2.0
34	1c	164	ARG	2.0
45	2n	9	LYS	2.0

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Mol	Chain	Res	Type	RSRZ
4	2E	157	ALA	2.0
7	1H	2	SER	2.0
32	1a	202	U	2.0
32	1a	1348	U	2.0
32	1a	1527	C	2.0
32	2a	948	C	2.0
32	2a	1019	C	2.0
40	2i	13	ALA	2.0
32	2a	815	A	2.0
32	2a	1036	G	2.0
32	2a	1311	G	2.0
35	1d	27	TYR	2.0
27	25	11	THR	2.0
7	2H	76	VAL	2.0
9	2N	9	VAL	2.0
15	1T	108	ARG	2.0
20	2Y	106	LEU	2.0
15	2T	94	ALA	2.0
38	2g	34	GLY	2.0
40	1i	46	ALA	2.0
44	2m	75	ALA	2.0
44	2m	107	ALA	2.0
1	1A	1065	U	2.0
1	1A	2140	C	2.0
1	1A	2177	C	2.0
32	1a	314	C	2.0
48	1q	88	TYR	2.0
32	1a	332	G	2.0
14	2S	30	ARG	2.0
40	2i	20	ARG	2.0
44	1m	93	ARG	2.0
44	2m	88	ARG	2.0
45	2n	45	ARG	2.0
47	2p	21	VAL	2.0
7	2H	71	LEU	2.0
13	1R	20	LEU	2.0
16	2U	16	LYS	2.0
18	2W	82	LEU	2.0
30	28	35	GLN	2.0
36	1e	49	PRO	2.0
42	1k	98	LEU	2.0
51	1t	53	LEU	2.0

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Mol	Chain	Res	Type	RSRZ
8	2I	43	ASN	2.0

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

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 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
1	5MU	2A	1915	21/22	0.88	0.16	74,81,86,91	0
54	PSU	2x	55	20/21	0.89	0.16	72,78,85,91	0
54	4SU	2x	8	20/21	0.89	0.13	72,83,87,87	0
1	5MU	1A	1915	21/22	0.90	0.16	58,70,76,89	0
54	5MC	2x	32	21/22	0.91	0.24	61,79,80,82	0
43	0TD	2I	92	10/11	0.91	0.25	57,66,71,84	0
32	PSU	2a	516	20/21	0.92	0.17	70,76,79,84	0
32	2MG	2a	1207	24/25	0.92	0.16	77,83,89,92	0
32	2MG	1a	1207	24/25	0.92	0.17	60,76,82,87	0
32	5MC	2a	1400	21/22	0.92	0.22	65,72,79,81	0
54	4SU	1x	8	20/21	0.93	0.16	58,68,74,78	0
54	PSU	1x	55	20/21	0.93	0.18	61,67,75,78	0
32	5MC	2a	967	21/22	0.93	0.30	67,72,79,80	0
32	M2G	2a	966	25/26	0.93	0.26	63,69,81,83	0
32	PSU	1a	516	20/21	0.94	0.12	65,70,76,78	0
1	PSU	2A	1917	20/21	0.94	0.16	60,70,75,77	0
32	7MG	2a	527	24/25	0.94	0.18	59,66,71,72	0
1	PSU	2A	1911	20/21	0.94	0.15	57,65,72,79	0
43	0TD	1I	92	10/11	0.94	0.15	52,57,60,75	0
54	5MU	1x	54	21/22	0.95	0.19	64,69,77,83	0
54	5MU	2x	54	21/22	0.95	0.14	72,79,82,87	0
1	PSU	1A	1917	20/21	0.95	0.16	50,59,68,74	0
32	4OC	2a	1402	22/23	0.95	0.19	55,63,68,75	0
54	5MC	1x	32	21/22	0.95	0.26	52,64,68,76	0
32	MA6	2a	1519	24/25	0.96	0.27	56,60,65,67	0
1	4OC	2A	1920	21/23	0.96	0.18	53,65,68,71	0
32	5MC	1a	967	21/22	0.96	0.28	54,62,71,74	0
32	5MC	2a	1404	21/22	0.96	0.21	45,57,67,68	0
1	5MU	2A	1939	21/22	0.96	0.19	39,43,47,50	0
32	4OC	1a	1402	22/23	0.96	0.21	49,53,59,62	0
1	5MC	2A	1942	21/22	0.96	0.16	47,55,60,63	0
1	PSU	2A	2605	20/21	0.96	0.20	28,38,44,46	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
32	MA6	2a	1518	24/25	0.96	0.24	55,62,66,67	0
32	5MC	1a	1404	21/22	0.96	0.20	34,46,49,51	0
32	UR3	2a	1498	21/22	0.96	0.23	52,59,63,70	0
32	7MG	1a	527	24/25	0.96	0.20	51,57,63,66	0
32	M2G	1a	966	25/26	0.96	0.22	51,59,65,73	0
1	5MC	2A	1962	21/22	0.96	0.18	40,53,61,65	0
1	2MA	2A	2503	23/24	0.97	0.24	30,34,39,42	0
1	2MU	2A	2552	21/23	0.97	0.18	34,38,44,47	0
32	MA6	1a	1519	24/25	0.97	0.22	38,43,48,51	0
1	PSU	1A	2605	20/21	0.97	0.20	20,27,29,31	0
1	4OC	1A	1920	21/23	0.97	0.19	34,46,49,54	0
32	5MC	1a	1407	21/22	0.97	0.18	41,43,48,52	0
1	OMG	2A	2251	24/25	0.97	0.22	30,40,46,46	0
32	5MC	1a	1400	21/22	0.97	0.21	36,57,61,62	0
32	MA6	1a	1518	24/25	0.97	0.24	35,43,48,52	0
1	PSU	1A	1911	20/21	0.97	0.16	42,49,56,58	0
1	5MC	1A	1942	21/22	0.97	0.19	28,34,40,43	0
32	5MC	2a	1407	21/22	0.97	0.21	51,57,62,64	0
32	UR3	1a	1498	21/22	0.98	0.18	39,46,49,52	0
1	2MA	1A	2503	23/24	0.98	0.22	14,21,24,25	0
1	OMG	1A	2251	24/25	0.98	0.23	23,29,33,35	0
1	5MU	1A	1939	21/22	0.98	0.23	22,27,32,34	0
1	2MU	1A	2552	21/23	0.98	0.21	26,29,34,37	0
1	5MC	1A	1962	21/22	0.98	0.18	28,37,44,54	0

## 6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 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
55	MG	1a	1765	1/1	0.32	0.13	90,90,90,90	0
55	MG	1B	229	1/1	0.36	1.61	72,72,72,72	0
55	MG	2a	3150	1/1	0.40	0.21	71,71,71,71	0
55	MG	18	105	1/1	0.47	0.41	75,75,75,75	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
55	MG	2a	3173	1/1	0.48	0.20	76,76,76,76	0
55	MG	1A	3879	1/1	0.50	0.19	64,64,64,64	0
55	MG	1A	3895	1/1	0.56	0.12	41,41,41,41	0
55	MG	2a	3128	1/1	0.60	0.37	90,90,90,90	0
55	MG	1a	1749	1/1	0.60	0.20	56,56,56,56	0
55	MG	1A	3723	1/1	0.62	0.20	14,14,14,14	0
55	MG	1A	4088	1/1	0.63	0.15	28,28,28,28	0
55	MG	2A	3270	1/1	0.63	0.11	70,70,70,70	0
55	MG	1a	1819	1/1	0.64	0.13	71,71,71,71	0
55	MG	1a	1612	1/1	0.64	0.33	57,57,57,57	0
55	MG	2A	3199	1/1	0.64	0.41	52,52,52,52	0
55	MG	2a	3160	1/1	0.66	0.30	81,81,81,81	0
55	MG	2a	3082	1/1	0.66	0.22	75,75,75,75	0
55	MG	2A	3222	1/1	0.66	0.88	68,68,68,68	0
55	MG	2A	3252	1/1	0.66	0.15	50,50,50,50	0
55	MG	1A	3983	1/1	0.66	0.21	56,56,56,56	0
55	MG	2A	3189	1/1	0.66	0.37	55,55,55,55	0
55	MG	1a	1618	1/1	0.66	0.33	51,51,51,51	0
55	MG	2A	3166	1/1	0.67	0.19	71,71,71,71	0
55	MG	2A	3653	1/1	0.67	0.61	72,72,72,72	0
55	MG	1a	1770	1/1	0.67	0.14	65,65,65,65	0
55	MG	2A	3191	1/1	0.67	0.60	62,62,62,62	0
55	MG	1A	4098	1/1	0.67	0.16	57,57,57,57	0
55	MG	1A	3810	1/1	0.67	0.15	52,52,52,52	0
55	MG	1A	3131	1/1	0.68	0.10	73,73,73,73	0
55	MG	2a	3091	1/1	0.68	0.14	71,71,71,71	0
55	MG	1A	3940	1/1	0.68	0.15	52,52,52,52	0
55	MG	2A	3375	1/1	0.69	0.20	65,65,65,65	0
55	MG	2A	3295	1/1	0.69	0.19	52,52,52,52	0
55	MG	2A	3741	1/1	0.69	0.47	72,72,72,72	0
55	MG	2a	3013	1/1	0.69	0.34	56,56,56,56	0
55	MG	1A	3347	1/1	0.70	1.67	60,60,60,60	0
55	MG	2A	3853	1/1	0.70	0.17	64,64,64,64	0
55	MG	2A	3740	1/1	0.70	0.40	68,68,68,68	0
55	MG	2a	3044	1/1	0.70	0.15	78,78,78,78	0
55	MG	1A	3329	1/1	0.71	0.25	58,58,58,58	0
55	MG	1A	4107	1/1	0.71	0.20	63,63,63,63	0
55	MG	2A	3505	1/1	0.71	0.21	48,48,48,48	0
55	MG	1a	1828	1/1	0.71	0.11	50,50,50,50	0
55	MG	2A	3858	1/1	0.71	0.14	68,68,68,68	0
55	MG	2a	3201	1/1	0.71	0.08	55,55,55,55	0
55	MG	1A	3165	1/1	0.72	0.22	51,51,51,51	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
55	MG	2a	3111	1/1	0.72	0.18	47,47,47,47	0
55	MG	2A	3676	1/1	0.72	0.09	69,69,69,69	0
55	MG	2A	3371	1/1	0.72	2.13	68,68,68,68	0
55	MG	2A	3484	1/1	0.72	0.15	58,58,58,58	0
55	MG	2A	3076	1/1	0.72	0.25	75,75,75,75	0
55	MG	2a	3206	1/1	0.72	0.38	78,78,78,78	0
55	MG	1A	3223	1/1	0.72	0.26	55,55,55,55	0
55	MG	1A	3624	1/1	0.72	0.18	81,81,81,81	0
55	MG	2A	3200	1/1	0.73	0.62	66,66,66,66	0
55	MG	2A	3771	1/1	0.73	0.08	56,56,56,56	0
55	MG	2a	3162	1/1	0.73	0.11	61,61,61,61	0
55	MG	2A	3192	1/1	0.73	0.42	70,70,70,70	0
55	MG	1A	3419	1/1	0.73	0.27	46,46,46,46	0
55	MG	2A	3266	1/1	0.73	0.16	59,59,59,59	0
55	MG	2B	210	1/1	0.73	0.23	59,59,59,59	0
55	MG	1A	3369	1/1	0.74	0.50	49,49,49,49	0
55	MG	1a	1643	1/1	0.74	0.56	65,65,65,65	0
55	MG	1a	1662	1/1	0.74	0.12	69,69,69,69	0
55	MG	2A	3558	1/1	0.74	0.15	36,36,36,36	0
55	MG	2x	101	1/1	0.74	0.52	84,84,84,84	0
55	MG	1A	4066	1/1	0.74	0.23	29,29,29,29	0
55	MG	1a	1792	1/1	0.74	0.36	84,84,84,84	0
55	MG	2x	104	1/1	0.74	0.17	70,70,70,70	0
55	MG	2A	3836	1/1	0.74	0.12	49,49,49,49	0
55	MG	2A	3232	1/1	0.75	0.41	58,58,58,58	0
55	MG	2A	3498	1/1	0.75	1.02	74,74,74,74	0
55	MG	1A	4032	1/1	0.75	0.11	39,39,39,39	0
55	MG	1B	232	1/1	0.75	0.27	65,65,65,65	0
55	MG	2A	3369	1/1	0.75	0.54	78,78,78,78	0
55	MG	1A	3394	1/1	0.75	0.26	65,65,65,65	0
55	MG	1A	3346	1/1	0.75	0.25	55,55,55,55	0
55	MG	2A	3457	1/1	0.75	0.98	62,62,62,62	0
55	MG	1A	4102	1/1	0.75	0.16	38,38,38,38	0
55	MG	2A	3086	1/1	0.75	0.32	66,66,66,66	0
55	MG	1A	3445	1/1	0.76	0.18	51,51,51,51	0
55	MG	2B	216	1/1	0.76	0.14	65,65,65,65	0
55	MG	2A	3441	1/1	0.76	0.13	63,63,63,63	0
55	MG	2T	201	1/1	0.76	0.61	65,65,65,65	0
55	MG	2a	3035	1/1	0.77	0.24	63,63,63,63	0
55	MG	1A	3537	1/1	0.77	0.24	44,44,44,44	0
55	MG	1A	3708	1/1	0.77	0.18	25,25,25,25	0
55	MG	2a	3090	1/1	0.77	0.28	72,72,72,72	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
55	MG	1a	1602	1/1	0.77	0.20	64,64,64,64	0
55	MG	1a	1636	1/1	0.77	0.22	63,63,63,63	0
55	MG	1A	3947	1/1	0.78	0.17	23,23,23,23	0
55	MG	1a	1803	1/1	0.78	0.18	66,66,66,66	0
55	MG	2U	201	1/1	0.78	0.85	58,58,58,58	0
55	MG	1a	1820	1/1	0.78	0.29	66,66,66,66	0
55	MG	1A	3524	1/1	0.78	0.22	59,59,59,59	0
55	MG	1A	4109	1/1	0.78	0.29	50,50,50,50	0
55	MG	2A	3089	1/1	0.78	0.31	72,72,72,72	0
55	MG	2A	3475	1/1	0.78	0.17	67,67,67,67	0
55	MG	2A	3201	1/1	0.78	0.56	66,66,66,66	0
55	MG	1A	3904	1/1	0.78	0.24	20,20,20,20	0
55	MG	1a	1775	1/1	0.78	0.11	59,59,59,59	0
55	MG	2a	3021	1/1	0.78	0.66	55,55,55,55	0
55	MG	2A	3090	1/1	0.78	0.12	57,57,57,57	0
55	MG	1a	1703	1/1	0.78	0.21	66,66,66,66	0
55	MG	1a	1810	1/1	0.78	0.15	58,58,58,58	0
55	MG	2A	3258	1/1	0.78	0.35	64,64,64,64	0
55	MG	1x	103	1/1	0.79	0.25	67,67,67,67	0
55	MG	1A	3358	1/1	0.79	0.36	56,56,56,56	0
55	MG	1a	1671	1/1	0.79	0.11	63,63,63,63	0
55	MG	2A	3230	1/1	0.79	0.29	78,78,78,78	0
55	MG	1n	102	1/1	0.79	0.65	66,66,66,66	0
55	MG	28	103	1/1	0.79	0.25	67,67,67,67	0
55	MG	2A	3341	1/1	0.79	0.32	56,56,56,56	0
55	MG	2A	3044	1/1	0.79	0.20	66,66,66,66	0
55	MG	2A	3499	1/1	0.79	0.10	59,59,59,59	0
55	MG	2a	3004	1/1	0.79	0.18	65,65,65,65	0
55	MG	2A	3323	1/1	0.79	0.68	67,67,67,67	0
55	MG	1a	1763	1/1	0.79	0.29	59,59,59,59	0
55	MG	1a	1718	1/1	0.79	0.25	68,68,68,68	0
55	MG	1A	3505	1/1	0.79	0.28	65,65,65,65	0
55	MG	1A	4061	1/1	0.79	0.51	62,62,62,62	0
55	MG	1a	1642	1/1	0.79	0.08	67,67,67,67	0
55	MG	1A	3992	1/1	0.79	0.17	58,58,58,58	0
55	MG	2A	3778	1/1	0.79	0.20	63,63,63,63	0
55	MG	2A	3380	1/1	0.79	0.21	74,74,74,74	0
55	MG	1A	4116	1/1	0.79	0.30	61,61,61,61	0
55	MG	1O	202	1/1	0.79	0.18	56,56,56,56	0
55	MG	1A	3851	1/1	0.79	0.17	49,49,49,49	0
55	MG	2A	3234	1/1	0.79	0.29	61,61,61,61	0
55	MG	1A	3450	1/1	0.79	1.15	74,74,74,74	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
55	MG	2A	3289	1/1	0.79	0.50	75,75,75,75	0
55	MG	1A	3348	1/1	0.79	0.18	55,55,55,55	0
55	MG	2A	3378	1/1	0.79	0.21	67,67,67,67	0
55	MG	2A	3280	1/1	0.79	0.11	70,70,70,70	0
55	MG	2A	3506	1/1	0.80	0.18	60,60,60,60	0
55	MG	1A	3264	1/1	0.80	0.30	41,41,41,41	0
55	MG	2A	3294	1/1	0.80	0.14	61,61,61,61	0
55	MG	2A	3543	1/1	0.80	0.11	35,35,35,35	0
55	MG	1A	4047	1/1	0.80	0.22	56,56,56,56	0
55	MG	1A	3662	1/1	0.80	0.10	42,42,42,42	0
55	MG	1v	102	1/1	0.80	0.09	74,74,74,74	0
55	MG	2A	3260	1/1	0.80	0.19	60,60,60,60	0
55	MG	1A	3326	1/1	0.80	0.24	40,40,40,40	0
55	MG	1A	3601	1/1	0.80	0.32	56,56,56,56	0
55	MG	2A	3551	1/1	0.80	0.16	42,42,42,42	0
55	MG	17	104	1/1	0.80	0.21	45,45,45,45	0
55	MG	1a	1818	1/1	0.80	0.20	73,73,73,73	0
55	MG	2F	302	1/1	0.80	0.40	43,43,43,43	0
55	MG	1A	3248	1/1	0.80	0.33	66,66,66,66	0
55	MG	1A	3303	1/1	0.80	0.84	62,62,62,62	0
55	MG	1A	3592	1/1	0.80	0.16	50,50,50,50	0
55	MG	2A	3472	1/1	0.80	0.09	60,60,60,60	0
55	MG	2A	3454	1/1	0.80	0.47	47,47,47,47	0
55	MG	1A	3120	1/1	0.80	0.67	49,49,49,49	0
55	MG	1a	1808	1/1	0.80	0.07	67,67,67,67	0
55	MG	2A	3361	1/1	0.80	0.12	64,64,64,64	0
55	MG	1B	230	1/1	0.80	0.51	82,82,82,82	0
55	MG	1a	1831	1/1	0.80	0.18	70,70,70,70	0
55	MG	1a	1717	1/1	0.80	0.32	62,62,62,62	0
55	MG	1a	1621	1/1	0.81	0.74	72,72,72,72	0
55	MG	1a	1719	1/1	0.81	0.10	61,61,61,61	0
55	MG	1a	1829	1/1	0.81	0.17	79,79,79,79	0
55	MG	2A	3050	1/1	0.81	0.23	56,56,56,56	0
55	MG	2a	3046	1/1	0.81	0.28	56,56,56,56	0
55	MG	2A	3461	1/1	0.81	0.71	60,60,60,60	0
55	MG	2A	3318	1/1	0.81	0.22	81,81,81,81	0
55	MG	1A	3945	1/1	0.81	0.12	56,56,56,56	0
55	MG	2r	101	1/1	0.81	0.13	66,66,66,66	0
55	MG	2V	201	1/1	0.81	2.31	62,62,62,62	0
55	MG	2A	3765	1/1	0.81	0.36	72,72,72,72	0
55	MG	1A	3737	1/1	0.81	0.16	23,23,23,23	0
55	MG	2A	3350	1/1	0.81	0.14	55,55,55,55	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
55	MG	1F	304	1/1	0.81	0.73	46,46,46,46	0
55	MG	2A	3832	1/1	0.81	0.38	65,65,65,65	0
55	MG	1a	1824	1/1	0.81	0.12	64,64,64,64	0
55	MG	18	101	1/1	0.81	0.21	44,44,44,44	0
55	MG	2A	3365	1/1	0.81	0.85	66,66,66,66	0
55	MG	2a	3208	1/1	0.81	0.22	58,58,58,58	0
55	MG	2A	3496	1/1	0.81	0.33	53,53,53,53	0
55	MG	2A	3424	1/1	0.81	0.17	48,48,48,48	0
55	MG	1B	231	1/1	0.81	0.23	30,30,30,30	0
55	MG	2A	3605	1/1	0.81	0.15	34,34,34,34	0
55	MG	1A	3775	1/1	0.81	0.16	19,19,19,19	0
55	MG	2a	3137	1/1	0.81	0.27	58,58,58,58	0
55	MG	1a	1804	1/1	0.81	0.11	49,49,49,49	0
55	MG	1A	3915	1/1	0.81	0.23	25,25,25,25	0
56	ZN	24	501	1/1	0.81	0.04	132,132,132,132	0
55	MG	2A	3293	1/1	0.81	0.45	68,68,68,68	0
55	MG	2A	3165	1/1	0.82	0.42	60,60,60,60	0
55	MG	2B	214	1/1	0.82	0.54	82,82,82,82	0
55	MG	2a	3209	1/1	0.82	0.16	63,63,63,63	0
55	MG	2A	3286	1/1	0.82	0.48	60,60,60,60	0
55	MG	1A	3777	1/1	0.82	0.13	51,51,51,51	0
55	MG	2a	3063	1/1	0.82	0.15	69,69,69,69	0
55	MG	2A	3095	1/1	0.82	0.14	65,65,65,65	0
55	MG	23	101	1/1	0.82	1.09	58,58,58,58	0
55	MG	2A	3587	1/1	0.82	0.17	39,39,39,39	0
55	MG	2A	3335	1/1	0.82	0.78	57,57,57,57	0
55	MG	2A	3001	1/1	0.82	0.22	48,48,48,48	0
55	MG	1a	1709	1/1	0.82	0.59	59,59,59,59	0
55	MG	2A	3645	1/1	0.82	0.31	54,54,54,54	0
55	MG	1A	3270	1/1	0.82	0.21	43,43,43,43	0
55	MG	1A	3395	1/1	0.82	0.11	58,58,58,58	0
55	MG	1Y	203	1/1	0.82	0.11	68,68,68,68	0
55	MG	2A	3108	1/1	0.82	0.60	61,61,61,61	0
55	MG	1a	1707	1/1	0.82	0.11	62,62,62,62	0
55	MG	1A	3717	1/1	0.82	0.23	41,41,41,41	0
55	MG	1a	1806	1/1	0.82	0.20	43,43,43,43	0
55	MG	1A	3376	1/1	0.82	0.25	39,39,39,39	0
55	MG	1a	1801	1/1	0.82	0.10	62,62,62,62	0
55	MG	1A	3988	1/1	0.82	0.24	50,50,50,50	0
55	MG	1a	1758	1/1	0.82	0.08	51,51,51,51	0
55	MG	2Q	202	1/1	0.82	0.20	56,56,56,56	0
55	MG	2a	3159	1/1	0.82	0.15	53,53,53,53	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
55	MG	2A	3123	1/1	0.82	0.15	39,39,39,39	0
55	MG	2A	3161	1/1	0.82	0.16	50,50,50,50	0
55	MG	2A	3339	1/1	0.82	0.26	60,60,60,60	0
55	MG	2A	3432	1/1	0.82	1.02	50,50,50,50	0
55	MG	1A	3982	1/1	0.82	0.15	26,26,26,26	0
55	MG	1B	226	1/1	0.82	0.14	68,68,68,68	0
55	MG	1A	3943	1/1	0.83	0.07	39,39,39,39	0
55	MG	2A	3813	1/1	0.83	0.11	52,52,52,52	0
55	MG	2A	3255	1/1	0.83	0.49	61,61,61,61	0
55	MG	1a	1607	1/1	0.83	0.08	75,75,75,75	0
55	MG	2a	3047	1/1	0.83	0.28	67,67,67,67	0
55	MG	2B	213	1/1	0.83	0.26	76,76,76,76	0
55	MG	2A	3292	1/1	0.83	0.40	45,45,45,45	0
55	MG	2A	3442	1/1	0.83	0.42	51,51,51,51	0
55	MG	2a	3105	1/1	0.83	0.53	80,80,80,80	0
55	MG	1A	3911	1/1	0.83	0.18	17,17,17,17	0
55	MG	1A	3025	1/1	0.83	0.14	44,44,44,44	0
55	MG	1a	1704	1/1	0.83	0.18	59,59,59,59	0
55	MG	2A	3831	1/1	0.83	0.09	51,51,51,51	0
55	MG	1A	3027	1/1	0.83	0.46	55,55,55,55	0
55	MG	1a	1608	1/1	0.83	0.11	57,57,57,57	0
55	MG	2A	3782	1/1	0.83	0.50	77,77,77,77	0
55	MG	2A	3172	1/1	0.83	0.14	41,41,41,41	0
55	MG	2A	3383	1/1	0.83	0.14	52,52,52,52	0
55	MG	1A	4011	1/1	0.83	0.41	57,57,57,57	0
55	MG	2a	3098	1/1	0.83	0.17	62,62,62,62	0
55	MG	2a	3130	1/1	0.83	0.25	69,69,69,69	0
55	MG	2a	3081	1/1	0.83	0.13	75,75,75,75	0
55	MG	1l	202	1/1	0.83	0.07	61,61,61,61	0
55	MG	2a	3040	1/1	0.83	0.24	55,55,55,55	0
55	MG	2A	3601	1/1	0.83	0.08	57,57,57,57	0
55	MG	1A	4042	1/1	0.83	0.09	57,57,57,57	0
55	MG	1A	3408	1/1	0.83	0.76	45,45,45,45	0
55	MG	2A	3586	1/1	0.83	0.56	66,66,66,66	0
55	MG	2A	3355	1/1	0.83	0.23	61,61,61,61	0
55	MG	1A	3298	1/1	0.83	0.11	42,42,42,42	0
55	MG	1A	3297	1/1	0.84	0.16	36,36,36,36	0
55	MG	2a	3085	1/1	0.84	0.13	64,64,64,64	0
55	MG	1U	207	1/1	0.84	0.68	54,54,54,54	0
55	MG	2A	3253	1/1	0.84	0.33	64,64,64,64	0
55	MG	1A	3741	1/1	0.84	0.38	56,56,56,56	0
55	MG	2a	3092	1/1	0.84	0.13	68,68,68,68	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
55	MG	2A	3377	1/1	0.84	0.28	65,65,65,65	0
55	MG	2A	3374	1/1	0.84	0.23	65,65,65,65	0
55	MG	2A	3071	1/1	0.84	0.18	55,55,55,55	0
55	MG	2a	3034	1/1	0.84	0.10	56,56,56,56	0
55	MG	2a	3129	1/1	0.84	0.28	64,64,64,64	0
55	MG	1A	4086	1/1	0.84	0.08	27,27,27,27	0
55	MG	1F	308	1/1	0.84	0.30	34,34,34,34	0
55	MG	1a	1676	1/1	0.84	0.29	59,59,59,59	0
55	MG	1A	3944	1/1	0.84	0.14	56,56,56,56	0
55	MG	1A	3590	1/1	0.84	0.17	31,31,31,31	0
55	MG	2A	3152	1/1	0.84	0.75	59,59,59,59	0
55	MG	1A	3291	1/1	0.84	0.34	43,43,43,43	0
55	MG	2A	3847	1/1	0.84	0.12	72,72,72,72	0
55	MG	2A	3717	1/1	0.84	0.24	65,65,65,65	0
55	MG	1A	3998	1/1	0.84	0.24	57,57,57,57	0
55	MG	1N	204	1/1	0.84	0.32	47,47,47,47	0
55	MG	1a	1639	1/1	0.84	0.15	73,73,73,73	0
55	MG	2W	201	1/1	0.84	0.17	36,36,36,36	0
55	MG	2A	3665	1/1	0.84	0.17	55,55,55,55	0
55	MG	2A	3356	1/1	0.84	0.28	37,37,37,37	0
55	MG	1A	3950	1/1	0.84	0.11	51,51,51,51	0
55	MG	2A	3113	1/1	0.84	0.19	40,40,40,40	0
55	MG	1G	202	1/1	0.84	0.54	57,57,57,57	0
55	MG	2F	301	1/1	0.84	0.14	49,49,49,49	0
55	MG	1a	1832	1/1	0.84	0.06	61,61,61,61	0
55	MG	2a	3134	1/1	0.84	0.14	47,47,47,47	0
55	MG	2j	201	1/1	0.84	0.15	71,71,71,71	0
55	MG	1a	1726	1/1	0.84	0.16	54,54,54,54	0
55	MG	2A	3373	1/1	0.84	0.13	64,64,64,64	0
55	MG	2A	3613	1/1	0.84	0.15	40,40,40,40	0
55	MG	2A	3419	1/1	0.84	0.15	53,53,53,53	0
55	MG	2A	3647	1/1	0.84	0.12	74,74,74,74	0
55	MG	1A	3212	1/1	0.84	0.17	53,53,53,53	0
55	MG	1A	3077	1/1	0.84	0.14	30,30,30,30	0
55	MG	2a	3038	1/1	0.84	0.12	45,45,45,45	0
55	MG	1A	3288	1/1	0.84	0.39	40,40,40,40	0
55	MG	1A	3913	1/1	0.84	0.11	22,22,22,22	0
55	MG	1A	3634	1/1	0.84	0.28	55,55,55,55	0
55	MG	2A	3624	1/1	0.84	0.16	47,47,47,47	0
55	MG	1A	3266	1/1	0.84	0.34	50,50,50,50	0
55	MG	1A	3576	1/1	0.84	0.13	54,54,54,54	0
55	MG	1A	3095	1/1	0.84	0.22	51,51,51,51	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
55	MG	1a	1641	1/1	0.84	0.18	60,60,60,60	0
55	MG	1B	207	1/1	0.85	0.17	49,49,49,49	0
55	MG	1A	3873	1/1	0.85	0.19	75,75,75,75	0
55	MG	1A	3620	1/1	0.85	0.50	38,38,38,38	0
55	MG	2B	204	1/1	0.85	0.14	75,75,75,75	0
55	MG	1a	1677	1/1	0.85	0.14	75,75,75,75	0
55	MG	1A	4082	1/1	0.85	0.10	42,42,42,42	0
55	MG	1A	3255	1/1	0.85	0.14	53,53,53,53	0
55	MG	2A	3043	1/1	0.85	0.17	49,49,49,49	0
55	MG	1A	3496	1/1	0.85	0.18	59,59,59,59	0
55	MG	2A	3563	1/1	0.85	0.18	41,41,41,41	0
55	MG	1a	1812	1/1	0.85	0.13	71,71,71,71	0
55	MG	1A	3969	1/1	0.85	0.23	45,45,45,45	0
55	MG	2A	3162	1/1	0.85	0.26	66,66,66,66	0
55	MG	1A	4089	1/1	0.85	0.69	39,39,39,39	0
55	MG	2A	3193	1/1	0.85	1.44	54,54,54,54	0
55	MG	2A	3333	1/1	0.85	0.34	58,58,58,58	0
55	MG	1A	4022	1/1	0.85	0.12	57,57,57,57	0
55	MG	1a	1825	1/1	0.85	0.10	58,58,58,58	0
55	MG	1A	3602	1/1	0.85	0.15	39,39,39,39	0
55	MG	1A	3219	1/1	0.85	0.17	68,68,68,68	0
55	MG	2a	3136	1/1	0.85	0.13	59,59,59,59	0
55	MG	1A	3244	1/1	0.85	0.83	38,38,38,38	0
55	MG	2A	3423	1/1	0.85	0.11	48,48,48,48	0
55	MG	1A	4041	1/1	0.85	0.10	74,74,74,74	0
55	MG	2A	3084	1/1	0.85	0.17	48,48,48,48	0
55	MG	1A	3486	1/1	0.85	0.38	56,56,56,56	0
55	MG	1A	3499	1/1	0.85	0.24	65,65,65,65	0
55	MG	1Q	204	1/1	0.85	0.29	51,51,51,51	0
55	MG	2A	3274	1/1	0.85	0.40	54,54,54,54	0
55	MG	1A	3857	1/1	0.85	0.24	42,42,42,42	0
55	MG	1A	3901	1/1	0.85	0.15	48,48,48,48	0
55	MG	2a	3177	1/1	0.85	0.52	64,64,64,64	0
55	MG	1a	1644	1/1	0.85	0.34	72,72,72,72	0
55	MG	1A	3541	1/1	0.85	0.33	67,67,67,67	0
55	MG	1A	3284	1/1	0.85	0.11	37,37,37,37	0
55	MG	1A	4103	1/1	0.85	0.12	57,57,57,57	0
55	MG	1D	306	1/1	0.85	0.14	45,45,45,45	0
55	MG	1x	113	1/1	0.85	0.12	68,68,68,68	0
55	MG	2a	3147	1/1	0.85	0.32	56,56,56,56	0
55	MG	1A	4004	1/1	0.85	0.22	14,14,14,14	0
55	MG	2A	3265	1/1	0.85	0.38	56,56,56,56	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
55	MG	1a	1748	1/1	0.85	0.17	63,63,63,63	0
55	MG	1A	3262	1/1	0.85	0.13	54,54,54,54	0
55	MG	2A	3229	1/1	0.85	0.18	59,59,59,59	0
55	MG	1A	3362	1/1	0.85	1.35	52,52,52,52	0
55	MG	1N	203	1/1	0.85	0.23	47,47,47,47	0
55	MG	2A	3174	1/1	0.85	0.24	58,58,58,58	0
55	MG	1A	3318	1/1	0.85	0.17	51,51,51,51	0
55	MG	1E	301	1/1	0.85	0.27	45,45,45,45	0
55	MG	2A	3185	1/1	0.85	0.13	55,55,55,55	0
55	MG	1a	1795	1/1	0.85	0.52	79,79,79,79	0
55	MG	1A	3920	1/1	0.85	0.09	56,56,56,56	0
55	MG	1A	3488	1/1	0.85	0.92	58,58,58,58	0
55	MG	2A	3735	1/1	0.85	0.16	60,60,60,60	0
55	MG	1n	101	1/1	0.85	0.17	78,78,78,78	0
55	MG	1a	1815	1/1	0.85	0.15	63,63,63,63	0
55	MG	1A	4050	1/1	0.85	0.79	70,70,70,70	0
55	MG	2A	3231	1/1	0.85	0.29	65,65,65,65	0
55	MG	2A	3793	1/1	0.86	0.14	49,49,49,49	0
55	MG	1A	4038	1/1	0.86	0.09	73,73,73,73	0
55	MG	1A	3170	1/1	0.86	0.35	47,47,47,47	0
55	MG	2A	3173	1/1	0.86	0.50	44,44,44,44	0
55	MG	1a	1701	1/1	0.86	0.35	54,54,54,54	0
55	MG	2A	3492	1/1	0.86	0.12	49,49,49,49	0
55	MG	1A	3410	1/1	0.86	0.22	40,40,40,40	0
55	MG	2A	3652	1/1	0.86	0.10	50,50,50,50	0
55	MG	2A	3098	1/1	0.86	0.28	44,44,44,44	0
55	MG	1A	3626	1/1	0.86	0.13	53,53,53,53	0
55	MG	1B	208	1/1	0.86	0.18	54,54,54,54	0
55	MG	2A	3133	1/1	0.86	0.36	62,62,62,62	0
55	MG	1A	3502	1/1	0.86	0.26	45,45,45,45	0
55	MG	1a	1653	1/1	0.86	0.16	69,69,69,69	0
55	MG	2A	3785	1/1	0.86	0.18	60,60,60,60	0
55	MG	2A	3795	1/1	0.86	0.12	42,42,42,42	0
55	MG	2A	3238	1/1	0.86	0.44	56,56,56,56	0
55	MG	1A	3319	1/1	0.86	0.19	54,54,54,54	0
55	MG	2T	202	1/1	0.86	0.30	59,59,59,59	0
55	MG	1A	3147	1/1	0.86	0.29	32,32,32,32	0
55	MG	1a	1638	1/1	0.86	0.11	55,55,55,55	0
55	MG	1A	3350	1/1	0.86	0.65	62,62,62,62	0
55	MG	2A	3111	1/1	0.86	0.32	65,65,65,65	0
55	MG	2a	3188	1/1	0.86	0.28	60,60,60,60	0
55	MG	2A	3806	1/1	0.86	0.16	37,37,37,37	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
55	MG	1A	3242	1/1	0.86	0.75	36,36,36,36	0
55	MG	2A	3685	1/1	0.86	0.30	68,68,68,68	0
55	MG	1A	3937	1/1	0.86	0.20	33,33,33,33	0
55	MG	1A	4023	1/1	0.86	0.15	73,73,73,73	0
55	MG	1A	3610	1/1	0.86	0.15	44,44,44,44	0
55	MG	1A	3989	1/1	0.86	0.34	36,36,36,36	0
55	MG	2a	3093	1/1	0.86	0.12	51,51,51,51	0
55	MG	2A	3690	1/1	0.86	0.13	64,64,64,64	0
55	MG	2A	3711	1/1	0.86	0.10	39,39,39,39	0
55	MG	2A	3011	1/1	0.86	0.27	50,50,50,50	0
55	MG	2A	3176	1/1	0.86	0.48	56,56,56,56	0
55	MG	2a	3024	1/1	0.86	0.16	77,77,77,77	0
55	MG	1A	3540	1/1	0.86	0.72	41,41,41,41	0
55	MG	1A	4077	1/1	0.86	0.16	34,34,34,34	0
55	MG	1A	3381	1/1	0.86	0.12	38,38,38,38	0
55	MG	2A	3716	1/1	0.86	0.08	64,64,64,64	0
55	MG	1A	4072	1/1	0.86	0.17	47,47,47,47	0
55	MG	1a	1659	1/1	0.86	0.45	67,67,67,67	0
55	MG	1A	3522	1/1	0.86	0.98	43,43,43,43	0
55	MG	1a	1743	1/1	0.86	0.20	62,62,62,62	0
55	MG	2A	3094	1/1	0.86	0.19	67,67,67,67	0
55	MG	1A	4117	1/1	0.86	0.26	49,49,49,49	0
55	MG	2a	3028	1/1	0.86	0.25	70,70,70,70	0
55	MG	2A	3236	1/1	0.86	0.19	51,51,51,51	0
55	MG	2A	3730	1/1	0.86	0.16	60,60,60,60	0
55	MG	2A	3157	1/1	0.86	0.15	60,60,60,60	0
55	MG	2A	3310	1/1	0.86	0.58	66,66,66,66	0
55	MG	1A	4113	1/1	0.86	0.15	57,57,57,57	0
55	MG	2A	3005	1/1	0.86	0.14	38,38,38,38	0
55	MG	2A	3077	1/1	0.86	0.19	64,64,64,64	0
55	MG	2A	3141	1/1	0.86	0.18	69,69,69,69	0
55	MG	2A	3285	1/1	0.86	0.86	52,52,52,52	0
55	MG	1A	3929	1/1	0.86	0.17	37,37,37,37	0
55	MG	1A	3221	1/1	0.86	1.08	54,54,54,54	0
55	MG	1A	3186	1/1	0.86	0.32	37,37,37,37	0
55	MG	1A	3539	1/1	0.86	0.17	48,48,48,48	0
55	MG	1X	105	1/1	0.86	0.13	34,34,34,34	0
55	MG	1a	1711	1/1	0.86	0.27	57,57,57,57	0
55	MG	1v	101	1/1	0.86	0.15	71,71,71,71	0
55	MG	2A	3312	1/1	0.86	0.39	51,51,51,51	0
55	MG	1A	3878	1/1	0.86	0.19	57,57,57,57	0
55	MG	2A	3240	1/1	0.86	0.22	54,54,54,54	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
55	MG	1A	3824	1/1	0.86	0.25	47,47,47,47	0
55	MG	2A	3547	1/1	0.86	0.16	59,59,59,59	0
55	MG	1A	3400	1/1	0.87	0.37	40,40,40,40	0
55	MG	1V	204	1/1	0.87	0.23	65,65,65,65	0
55	MG	2a	3094	1/1	0.87	0.09	63,63,63,63	0
55	MG	2A	3182	1/1	0.87	0.23	63,63,63,63	0
55	MG	1A	3361	1/1	0.87	0.47	56,56,56,56	0
55	MG	1A	3926	1/1	0.87	0.20	45,45,45,45	0
55	MG	1e	201	1/1	0.87	0.08	71,71,71,71	0
55	MG	2a	3086	1/1	0.87	0.54	56,56,56,56	0
55	MG	1a	1646	1/1	0.87	0.13	37,37,37,37	0
55	MG	1a	1614	1/1	0.87	0.21	69,69,69,69	0
55	MG	1A	3644	1/1	0.87	0.17	21,21,21,21	0
55	MG	2A	3760	1/1	0.87	0.20	76,76,76,76	0
55	MG	1A	3320	1/1	0.87	0.30	45,45,45,45	0
55	MG	1x	105	1/1	0.87	0.18	65,65,65,65	0
55	MG	1A	4049	1/1	0.87	0.24	53,53,53,53	0
55	MG	2A	3080	1/1	0.87	0.10	67,67,67,67	0
55	MG	2a	3175	1/1	0.87	0.20	70,70,70,70	0
55	MG	1A	3383	1/1	0.87	0.23	35,35,35,35	0
55	MG	1A	3016	1/1	0.87	0.10	55,55,55,55	0
55	MG	1B	214	1/1	0.87	0.38	51,51,51,51	0
55	MG	2A	3698	1/1	0.87	0.25	64,64,64,64	0
55	MG	2A	3013	1/1	0.87	0.16	51,51,51,51	0
55	MG	1A	3184	1/1	0.87	0.36	40,40,40,40	0
55	MG	1A	3182	1/1	0.87	0.16	38,38,38,38	0
55	MG	2B	206	1/1	0.87	0.20	57,57,57,57	0
55	MG	2N	201	1/1	0.87	0.24	62,62,62,62	0
55	MG	2A	3208	1/1	0.87	0.17	57,57,57,57	0
55	MG	1A	3336	1/1	0.87	0.20	53,53,53,53	0
55	MG	2A	3348	1/1	0.87	0.24	64,64,64,64	0
55	MG	1A	3382	1/1	0.87	0.20	43,43,43,43	0
55	MG	2A	3092	1/1	0.87	0.17	62,62,62,62	0
55	MG	2D	303	1/1	0.87	0.15	62,62,62,62	0
55	MG	2A	3103	1/1	0.87	0.16	30,30,30,30	0
55	MG	1A	3370	1/1	0.87	0.16	42,42,42,42	0
55	MG	2A	3710	1/1	0.87	0.11	50,50,50,50	0
55	MG	1A	3991	1/1	0.87	0.11	53,53,53,53	0
55	MG	1A	3213	1/1	0.87	0.12	50,50,50,50	0
55	MG	1A	3134	1/1	0.87	0.42	45,45,45,45	0
55	MG	1x	109	1/1	0.87	0.11	73,73,73,73	0
55	MG	2A	3248	1/1	0.87	0.21	58,58,58,58	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
55	MG	1A	3054	1/1	0.87	0.20	37,37,37,37	0
55	MG	1a	1782	1/1	0.87	0.36	57,57,57,57	0
55	MG	1A	4000	1/1	0.87	0.21	60,60,60,60	0
55	MG	1A	3268	1/1	0.87	0.19	46,46,46,46	0
55	MG	2A	3669	1/1	0.87	0.17	52,52,52,52	0
55	MG	1A	3794	1/1	0.87	0.14	29,29,29,29	0
55	MG	2A	3456	1/1	0.87	0.34	54,54,54,54	0
55	MG	2A	3316	1/1	0.87	0.13	48,48,48,48	0
55	MG	2a	3030	1/1	0.87	0.15	60,60,60,60	0
55	MG	2A	3241	1/1	0.87	0.33	58,58,58,58	0
55	MG	2A	3796	1/1	0.87	0.53	61,61,61,61	0
55	MG	1a	1675	1/1	0.87	0.21	57,57,57,57	0
55	MG	2A	3678	1/1	0.87	0.13	79,79,79,79	0
55	MG	2A	3520	1/1	0.87	0.47	44,44,44,44	0
55	MG	2A	3552	1/1	0.87	0.17	38,38,38,38	0
55	MG	2a	3071	1/1	0.87	0.10	51,51,51,51	0
55	MG	2l	202	1/1	0.87	0.20	67,67,67,67	0
55	MG	1A	3591	1/1	0.87	0.16	48,48,48,48	0
55	MG	2A	3859	1/1	0.87	0.17	53,53,53,53	0
55	MG	1A	3683	1/1	0.88	0.12	53,53,53,53	0
55	MG	2a	3073	1/1	0.88	0.18	61,61,61,61	0
55	MG	1A	3109	1/1	0.88	0.99	50,50,50,50	0
55	MG	1A	3501	1/1	0.88	0.28	46,46,46,46	0
55	MG	28	102	1/1	0.88	0.13	59,59,59,59	0
55	MG	1F	310	1/1	0.88	0.62	46,46,46,46	0
55	MG	2B	203	1/1	0.88	0.12	40,40,40,40	0
55	MG	1x	107	1/1	0.88	0.15	66,66,66,66	0
55	MG	1a	1649	1/1	0.88	0.10	61,61,61,61	0
55	MG	1Q	202	1/1	0.88	0.19	35,35,35,35	0
55	MG	1A	3703	1/1	0.88	0.21	41,41,41,41	0
55	MG	1A	3997	1/1	0.88	0.15	56,56,56,56	0
55	MG	1A	3310	1/1	0.88	0.15	60,60,60,60	0
55	MG	2A	3545	1/1	0.88	0.14	45,45,45,45	0
55	MG	2A	3188	1/1	0.88	0.14	48,48,48,48	0
55	MG	1P	202	1/1	0.88	0.67	59,59,59,59	0
55	MG	2A	3131	1/1	0.88	0.10	64,64,64,64	0
55	MG	1a	1800	1/1	0.88	0.14	72,72,72,72	0
55	MG	2a	3057	1/1	0.88	0.12	45,45,45,45	0
55	MG	2A	3297	1/1	0.88	0.25	47,47,47,47	0
55	MG	2A	3568	1/1	0.88	0.14	38,38,38,38	0
55	MG	2A	3570	1/1	0.88	0.09	65,65,65,65	0
55	MG	1A	4029	1/1	0.88	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
55	MG	2A	3725	1/1	0.88	0.13	68,68,68,68	0
55	MG	1A	3198	1/1	0.88	0.22	38,38,38,38	0
55	MG	1A	3356	1/1	0.88	0.71	62,62,62,62	0
55	MG	1a	1772	1/1	0.88	0.09	64,64,64,64	0
55	MG	1A	4057	1/1	0.88	0.16	47,47,47,47	0
55	MG	1A	3476	1/1	0.88	0.36	45,45,45,45	0
55	MG	1T	203	1/1	0.88	0.15	56,56,56,56	0
55	MG	1a	1665	1/1	0.88	0.25	49,49,49,49	0
55	MG	2A	3654	1/1	0.88	0.22	63,63,63,63	0
55	MG	1A	3126	1/1	0.88	0.92	37,37,37,37	0
55	MG	2A	3146	1/1	0.88	0.10	42,42,42,42	0
55	MG	2a	3142	1/1	0.88	0.18	54,54,54,54	0
55	MG	2A	3153	1/1	0.88	0.18	47,47,47,47	0
55	MG	2a	3070	1/1	0.88	0.14	63,63,63,63	0
55	MG	1A	3470	1/1	0.88	0.21	46,46,46,46	0
55	MG	2A	3321	1/1	0.88	0.22	70,70,70,70	0
55	MG	1A	3870	1/1	0.88	0.16	46,46,46,46	0
55	MG	1a	1764	1/1	0.88	0.15	39,39,39,39	0
55	MG	1A	4076	1/1	0.88	0.19	61,61,61,61	0
55	MG	1a	1606	1/1	0.88	0.32	49,49,49,49	0
55	MG	2a	3174	1/1	0.88	0.26	75,75,75,75	0
55	MG	2B	211	1/1	0.88	0.23	63,63,63,63	0
55	MG	2A	3758	1/1	0.88	0.12	53,53,53,53	0
55	MG	2a	3041	1/1	0.88	0.20	55,55,55,55	0
55	MG	2A	3666	1/1	0.88	0.11	72,72,72,72	0
55	MG	2A	3211	1/1	0.88	0.41	38,38,38,38	0
55	MG	1A	3208	1/1	0.88	0.29	64,64,64,64	0
55	MG	2a	3020	1/1	0.88	0.20	67,67,67,67	0
55	MG	1A	3282	1/1	0.88	0.16	58,58,58,58	0
55	MG	1A	3084	1/1	0.88	0.36	33,33,33,33	0
55	MG	2A	3170	1/1	0.88	1.04	65,65,65,65	0
55	MG	1a	1686	1/1	0.88	0.07	67,67,67,67	0
55	MG	2a	3096	1/1	0.88	0.36	44,44,44,44	0
55	MG	1a	1773	1/1	0.88	0.07	70,70,70,70	0
55	MG	1Q	203	1/1	0.88	0.11	55,55,55,55	0
55	MG	2A	3675	1/1	0.88	0.11	58,58,58,58	0
55	MG	2a	3143	1/1	0.88	0.10	56,56,56,56	0
55	MG	1V	203	1/1	0.88	0.99	47,47,47,47	0
55	MG	2a	3022	1/1	0.88	0.17	47,47,47,47	0
55	MG	1A	3331	1/1	0.88	0.12	41,41,41,41	0
55	MG	2a	3048	1/1	0.88	0.16	68,68,68,68	0
55	MG	1F	306	1/1	0.88	0.46	20,20,20,20	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
55	MG	2Q	203	1/1	0.88	0.17	43,43,43,43	0
55	MG	1a	1727	1/1	0.88	1.09	67,67,67,67	0
55	MG	2a	3158	1/1	0.88	0.15	70,70,70,70	0
55	MG	1a	1650	1/1	0.88	0.10	69,69,69,69	0
55	MG	2A	3501	1/1	0.89	0.15	58,58,58,58	0
55	MG	1B	212	1/1	0.89	0.26	52,52,52,52	0
55	MG	2a	3005	1/1	0.89	0.09	53,53,53,53	0
55	MG	2a	3172	1/1	0.89	0.11	56,56,56,56	0
55	MG	1A	3252	1/1	0.89	0.19	33,33,33,33	0
55	MG	2a	3161	1/1	0.89	0.13	51,51,51,51	0
55	MG	2A	3254	1/1	0.89	0.65	49,49,49,49	0
55	MG	2A	3403	1/1	0.89	0.14	55,55,55,55	0
55	MG	1A	3086	1/1	0.89	0.34	39,39,39,39	0
55	MG	1a	1771	1/1	0.89	0.09	64,64,64,64	0
55	MG	1B	215	1/1	0.89	0.18	43,43,43,43	0
55	MG	2A	3367	1/1	0.89	0.70	41,41,41,41	0
55	MG	1A	3912	1/1	0.89	0.16	27,27,27,27	0
55	MG	1A	4005	1/1	0.89	0.13	34,34,34,34	0
55	MG	2A	3422	1/1	0.89	0.17	51,51,51,51	0
55	MG	2A	3404	1/1	0.89	0.45	61,61,61,61	0
55	MG	2E	303	1/1	0.89	0.28	50,50,50,50	0
55	MG	1A	3431	1/1	0.89	0.10	36,36,36,36	0
55	MG	1a	1670	1/1	0.89	0.61	67,67,67,67	0
55	MG	2A	3163	1/1	0.89	0.16	64,64,64,64	0
55	MG	1A	3137	1/1	0.89	0.82	35,35,35,35	0
55	MG	1A	3464	1/1	0.89	0.15	40,40,40,40	0
55	MG	1A	3049	1/1	0.89	0.32	27,27,27,27	0
55	MG	1A	3625	1/1	0.89	0.35	50,50,50,50	0
55	MG	1a	1729	1/1	0.89	0.10	54,54,54,54	0
55	MG	1A	3645	1/1	0.89	0.17	50,50,50,50	0
55	MG	2A	3467	1/1	0.89	0.29	64,64,64,64	0
55	MG	1a	1640	1/1	0.89	0.27	48,48,48,48	0
55	MG	2A	3708	1/1	0.89	0.19	36,36,36,36	0
55	MG	1A	3388	1/1	0.89	0.42	28,28,28,28	0
55	MG	1A	3526	1/1	0.89	0.09	43,43,43,43	0
55	MG	2A	3227	1/1	0.89	0.95	69,69,69,69	0
55	MG	1A	3002	1/1	0.89	0.15	49,49,49,49	0
55	MG	1A	3140	1/1	0.89	0.40	36,36,36,36	0
55	MG	2A	3276	1/1	0.89	0.16	60,60,60,60	0
55	MG	1A	3766	1/1	0.89	0.62	64,64,64,64	0
55	MG	2A	3179	1/1	0.89	0.27	56,56,56,56	0
55	MG	1a	1668	1/1	0.89	0.38	62,62,62,62	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
55	MG	1A	3190	1/1	0.89	1.30	34,34,34,34	0
55	MG	1A	3111	1/1	0.89	0.40	30,30,30,30	0
55	MG	1A	3418	1/1	0.89	0.17	58,58,58,58	0
55	MG	1P	203	1/1	0.89	0.24	49,49,49,49	0
55	MG	2A	3861	1/1	0.89	0.19	50,50,50,50	0
55	MG	2E	302	1/1	0.89	0.56	47,47,47,47	0
55	MG	1a	1601	1/1	0.89	0.20	63,63,63,63	0
55	MG	2A	3600	1/1	0.89	0.09	50,50,50,50	0
55	MG	1a	1789	1/1	0.89	0.10	79,79,79,79	0
55	MG	1A	4044	1/1	0.89	0.12	57,57,57,57	0
55	MG	2A	3087	1/1	0.89	0.12	45,45,45,45	0
55	MG	2A	3562	1/1	0.89	0.18	57,57,57,57	0
55	MG	2A	3753	1/1	0.89	0.07	58,58,58,58	0
55	MG	2A	3142	1/1	0.89	0.27	54,54,54,54	0
55	MG	1D	301	1/1	0.89	1.02	36,36,36,36	0
55	MG	1A	3482	1/1	0.89	0.25	50,50,50,50	0
55	MG	2A	3273	1/1	0.89	0.21	50,50,50,50	0
55	MG	2A	3322	1/1	0.89	0.11	57,57,57,57	0
55	MG	1A	3467	1/1	0.89	0.69	46,46,46,46	0
55	MG	2A	3259	1/1	0.89	0.21	61,61,61,61	0
55	MG	2A	3130	1/1	0.89	0.21	57,57,57,57	0
55	MG	2A	3268	1/1	0.89	0.43	68,68,68,68	0
55	MG	2A	3311	1/1	0.89	0.37	41,41,41,41	0
55	MG	2A	3773	1/1	0.89	0.10	62,62,62,62	0
55	MG	2a	3061	1/1	0.89	0.14	68,68,68,68	0
55	MG	2A	3151	1/1	0.89	0.15	68,68,68,68	0
55	MG	2a	3103	1/1	0.89	0.11	54,54,54,54	0
55	MG	1A	3981	1/1	0.89	0.17	59,59,59,59	0
55	MG	1A	4045	1/1	0.89	0.08	49,49,49,49	0
55	MG	1A	3421	1/1	0.89	0.17	52,52,52,52	0
55	MG	1A	3523	1/1	0.89	0.49	47,47,47,47	0
55	MG	1a	1663	1/1	0.89	0.12	65,65,65,65	0
55	MG	2A	3202	1/1	0.89	0.17	55,55,55,55	0
55	MG	2a	3108	1/1	0.89	0.16	72,72,72,72	0
55	MG	1A	3680	1/1	0.89	0.29	33,33,33,33	0
55	MG	2G	201	1/1	0.89	0.09	68,68,68,68	0
55	MG	2A	3849	1/1	0.89	0.31	48,48,48,48	0
55	MG	1A	3820	1/1	0.89	0.20	22,22,22,22	0
55	MG	1A	3850	1/1	0.89	0.37	56,56,56,56	0
55	MG	2A	3416	1/1	0.89	0.23	44,44,44,44	0
55	MG	2A	3494	1/1	0.89	0.14	64,64,64,64	0
55	MG	2A	3317	1/1	0.89	0.09	78,78,78,78	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
55	MG	1A	3932	1/1	0.89	0.92	38,38,38,38	0
55	MG	1A	3837	1/1	0.89	0.18	51,51,51,51	0
55	MG	2a	3139	1/1	0.89	0.10	69,69,69,69	0
55	MG	2A	3224	1/1	0.89	0.15	45,45,45,45	0
57	V7A	2a	3210	35/35	0.89	0.37	68,82,90,91	0
55	MG	2A	3330	1/1	0.89	1.11	63,63,63,63	0
55	MG	1A	3302	1/1	0.89	0.12	45,45,45,45	0
55	MG	2A	3482	1/1	0.89	0.15	51,51,51,51	0
55	MG	2A	3519	1/1	0.89	0.20	39,39,39,39	0
55	MG	1A	3764	1/1	0.89	0.16	45,45,45,45	0
55	MG	1A	3509	1/1	0.89	0.59	32,32,32,32	0
55	MG	2a	3165	1/1	0.89	0.18	77,77,77,77	0
55	MG	1l	104	1/1	0.89	0.12	62,62,62,62	0
55	MG	2A	3344	1/1	0.89	0.75	45,45,45,45	0
55	MG	1A	3987	1/1	0.89	0.21	32,32,32,32	0
55	MG	2A	3290	1/1	0.89	0.13	68,68,68,68	0
55	MG	2A	3287	1/1	0.89	0.10	46,46,46,46	0
55	MG	2A	3362	1/1	0.89	0.14	57,57,57,57	0
55	MG	2A	3604	1/1	0.89	0.15	31,31,31,31	0
55	MG	1A	3239	1/1	0.89	0.09	35,35,35,35	0
55	MG	2g	201	1/1	0.89	0.09	73,73,73,73	0
55	MG	2A	3429	1/1	0.89	0.23	63,63,63,63	0
55	MG	1A	3455	1/1	0.89	0.12	48,48,48,48	0
55	MG	2A	3082	1/1	0.89	0.10	57,57,57,57	0
55	MG	1a	1609	1/1	0.89	0.18	62,62,62,62	0
55	MG	2A	3833	1/1	0.89	0.23	57,57,57,57	0
55	MG	1b	301	1/1	0.89	0.16	74,74,74,74	0
55	MG	2A	3630	1/1	0.89	0.28	54,54,54,54	0
55	MG	2A	3250	1/1	0.89	0.57	56,56,56,56	0
55	MG	1a	1619	1/1	0.90	0.21	70,70,70,70	0
55	MG	2A	3852	1/1	0.90	0.21	61,61,61,61	0
55	MG	1A	3603	1/1	0.90	0.14	53,53,53,53	0
55	MG	1a	1681	1/1	0.90	0.07	76,76,76,76	0
55	MG	1a	1783	1/1	0.90	0.23	61,61,61,61	0
55	MG	2A	3384	1/1	0.90	0.21	68,68,68,68	0
55	MG	2A	3143	1/1	0.90	0.08	44,44,44,44	0
55	MG	1A	3088	1/1	0.90	0.21	35,35,35,35	0
55	MG	2A	3343	1/1	0.90	0.09	50,50,50,50	0
55	MG	1A	3409	1/1	0.90	0.46	54,54,54,54	0
55	MG	2A	3283	1/1	0.90	0.22	54,54,54,54	0
55	MG	2A	3854	1/1	0.90	0.48	68,68,68,68	0
55	MG	1A	3949	1/1	0.90	0.24	56,56,56,56	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
55	MG	2a	3149	1/1	0.90	0.07	59,59,59,59	0
57	V7A	1a	1835	35/35	0.90	0.26	65,73,81,85	0
55	MG	1A	3977	1/1	0.90	0.11	40,40,40,40	0
55	MG	2a	3001	1/1	0.90	0.62	57,57,57,57	0
55	MG	1A	3307	1/1	0.90	0.15	43,43,43,43	0
55	MG	2A	3821	1/1	0.90	0.15	54,54,54,54	0
55	MG	1B	205	1/1	0.90	0.16	39,39,39,39	0
55	MG	1A	3914	1/1	0.90	0.32	35,35,35,35	0
55	MG	2A	3068	1/1	0.90	0.30	69,69,69,69	0
55	MG	1A	3858	1/1	0.90	0.47	69,69,69,69	0
55	MG	1A	3055	1/1	0.90	0.23	47,47,47,47	0
55	MG	1A	3241	1/1	0.90	0.09	42,42,42,42	0
55	MG	1A	3776	1/1	0.90	0.15	60,60,60,60	0
55	MG	1a	1805	1/1	0.90	0.08	74,74,74,74	0
55	MG	25	102	1/1	0.90	0.32	43,43,43,43	0
55	MG	1A	3748	1/1	0.90	0.44	45,45,45,45	0
55	MG	1A	3442	1/1	0.90	0.30	51,51,51,51	0
55	MG	2j	202	1/1	0.90	0.10	74,74,74,74	0
55	MG	1A	3452	1/1	0.90	0.40	45,45,45,45	0
55	MG	1A	3216	1/1	0.90	0.40	37,37,37,37	0
55	MG	1x	111	1/1	0.90	0.13	65,65,65,65	0
55	MG	2A	3437	1/1	0.90	0.54	36,36,36,36	0
55	MG	1W	202	1/1	0.90	0.13	44,44,44,44	0
55	MG	2A	3325	1/1	0.90	0.22	44,44,44,44	0
55	MG	1A	3156	1/1	0.90	0.56	36,36,36,36	0
55	MG	2A	3830	1/1	0.90	0.08	76,76,76,76	0
55	MG	2a	3198	1/1	0.90	0.13	66,66,66,66	0
55	MG	2A	3331	1/1	0.90	1.23	64,64,64,64	0
55	MG	2A	3026	1/1	0.90	0.13	42,42,42,42	0
55	MG	2a	3197	1/1	0.90	0.12	57,57,57,57	0
55	MG	1A	3655	1/1	0.90	0.14	30,30,30,30	0
55	MG	1A	3874	1/1	0.90	0.17	50,50,50,50	0
55	MG	2a	3126	1/1	0.90	0.25	62,62,62,62	0
55	MG	2A	3360	1/1	0.90	0.21	56,56,56,56	0
55	MG	1A	3852	1/1	0.90	0.12	39,39,39,39	0
55	MG	1A	3948	1/1	0.90	0.15	30,30,30,30	0
55	MG	2E	308	1/1	0.90	0.11	26,26,26,26	0
55	MG	2A	3453	1/1	0.90	0.19	66,66,66,66	0
55	MG	2A	3247	1/1	0.90	0.17	54,54,54,54	0
55	MG	2A	3528	1/1	0.90	0.07	32,32,32,32	0
55	MG	1A	3227	1/1	0.90	0.25	41,41,41,41	0
55	MG	1a	1645	1/1	0.90	0.08	70,70,70,70	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
55	MG	2A	3768	1/1	0.90	0.14	58,58,58,58	0
55	MG	2A	3109	1/1	0.90	0.12	52,52,52,52	0
55	MG	2A	3025	1/1	0.90	0.29	56,56,56,56	0
55	MG	1a	1817	1/1	0.90	0.07	68,68,68,68	0
55	MG	2a	3190	1/1	0.90	0.34	66,66,66,66	0
55	MG	2a	3069	1/1	0.90	0.14	57,57,57,57	0
55	MG	1a	1751	1/1	0.90	0.15	54,54,54,54	0
55	MG	2A	3618	1/1	0.90	0.16	28,28,28,28	0
55	MG	2A	3468	1/1	0.90	0.33	51,51,51,51	0
55	MG	2A	3673	1/1	0.90	0.09	52,52,52,52	0
55	MG	2a	3027	1/1	0.90	0.18	50,50,50,50	0
55	MG	1A	3964	1/1	0.90	0.23	18,18,18,18	0
55	MG	1x	101	1/1	0.90	0.12	59,59,59,59	0
55	MG	2A	3069	1/1	0.90	0.62	41,41,41,41	0
55	MG	2Q	201	1/1	0.90	0.10	57,57,57,57	0
55	MG	2A	3449	1/1	0.90	0.47	66,66,66,66	0
55	MG	2E	304	1/1	0.90	0.19	60,60,60,60	0
55	MG	15	102	1/1	0.90	0.16	47,47,47,47	0
55	MG	2a	3191	1/1	0.90	0.17	55,55,55,55	0
55	MG	2A	3489	1/1	0.90	0.23	49,49,49,49	0
55	MG	18	104	1/1	0.90	0.12	40,40,40,40	0
55	MG	1A	3254	1/1	0.90	0.15	58,58,58,58	0
55	MG	1t	201	1/1	0.90	0.34	59,59,59,59	0
55	MG	2A	3363	1/1	0.90	0.14	44,44,44,44	0
55	MG	2a	3067	1/1	0.90	0.15	58,58,58,58	0
55	MG	1a	1723	1/1	0.90	0.11	49,49,49,49	0
55	MG	1A	3744	1/1	0.90	0.11	53,53,53,53	0
55	MG	2A	3521	1/1	0.90	0.17	55,55,55,55	0
55	MG	1a	1725	1/1	0.90	0.15	48,48,48,48	0
55	MG	1A	3493	1/1	0.90	0.58	45,45,45,45	0
55	MG	1A	3435	1/1	0.90	0.22	47,47,47,47	0
55	MG	1A	3230	1/1	0.90	0.54	44,44,44,44	0
55	MG	2A	3610	1/1	0.90	0.17	59,59,59,59	0
55	MG	2A	3228	1/1	0.90	0.20	58,58,58,58	0
55	MG	1A	4033	1/1	0.90	0.09	36,36,36,36	0
55	MG	2a	3064	1/1	0.90	0.23	46,46,46,46	0
55	MG	1A	3070	1/1	0.90	0.13	49,49,49,49	0
55	MG	2A	3414	1/1	0.90	0.10	52,52,52,52	0
55	MG	1A	3160	1/1	0.90	0.39	29,29,29,29	0
55	MG	1a	1630	1/1	0.90	0.18	44,44,44,44	0
55	MG	1A	3504	1/1	0.90	0.18	41,41,41,41	0
55	MG	1a	1656	1/1	0.90	0.42	59,59,59,59	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
55	MG	1A	3357	1/1	0.90	0.24	36,36,36,36	0
55	MG	2A	3346	1/1	0.90	0.35	67,67,67,67	0
55	MG	1A	3518	1/1	0.90	0.27	50,50,50,50	0
55	MG	2A	3448	1/1	0.90	0.61	49,49,49,49	0
55	MG	2A	3789	1/1	0.90	0.14	47,47,47,47	0
55	MG	1f	201	1/1	0.90	0.16	64,64,64,64	0
55	MG	17	101	1/1	0.90	0.21	54,54,54,54	0
55	MG	1a	1731	1/1	0.90	0.20	63,63,63,63	0
55	MG	1A	3976	1/1	0.90	0.10	46,46,46,46	0
55	MG	1A	3423	1/1	0.90	0.74	43,43,43,43	0
55	MG	2A	3648	1/1	0.90	0.12	55,55,55,55	0
55	MG	2a	3023	1/1	0.90	0.12	60,60,60,60	0
55	MG	2A	3512	1/1	0.90	0.23	53,53,53,53	0
55	MG	2A	3755	1/1	0.90	0.08	52,52,52,52	0
55	MG	1A	3803	1/1	0.90	0.11	45,45,45,45	0
55	MG	2A	3632	1/1	0.90	0.26	53,53,53,53	0
55	MG	2A	3272	1/1	0.90	0.10	57,57,57,57	0
55	MG	2A	3462	1/1	0.90	0.93	60,60,60,60	0
55	MG	1a	1741	1/1	0.90	0.10	58,58,58,58	0
55	MG	2A	3679	1/1	0.90	0.13	43,43,43,43	0
55	MG	1A	3481	1/1	0.90	0.26	56,56,56,56	0
55	MG	2a	3097	1/1	0.90	0.10	75,75,75,75	0
55	MG	2A	3617	1/1	0.90	0.28	23,23,23,23	0
55	MG	2a	3019	1/1	0.90	0.19	60,60,60,60	0
55	MG	2d	302	1/1	0.90	0.15	73,73,73,73	0
55	MG	2A	3320	1/1	0.90	0.15	64,64,64,64	0
55	MG	2A	3566	1/1	0.90	0.25	48,48,48,48	0
55	MG	1A	3092	1/1	0.90	0.12	32,32,32,32	0
55	MG	2A	3299	1/1	0.91	0.26	53,53,53,53	0
55	MG	1A	3430	1/1	0.91	0.92	41,41,41,41	0
55	MG	1A	3888	1/1	0.91	0.14	29,29,29,29	0
55	MG	1A	3328	1/1	0.91	0.32	40,40,40,40	0
55	MG	1O	201	1/1	0.91	0.62	45,45,45,45	0
55	MG	1A	3796	1/1	0.91	0.17	34,34,34,34	0
55	MG	1A	3503	1/1	0.91	0.16	49,49,49,49	0
55	MG	1A	3316	1/1	0.91	0.32	42,42,42,42	0
55	MG	1A	3399	1/1	0.91	0.53	32,32,32,32	0
55	MG	1A	3196	1/1	0.91	0.14	41,41,41,41	0
55	MG	1x	102	1/1	0.91	0.10	59,59,59,59	0
55	MG	1A	3039	1/1	0.91	0.13	57,57,57,57	0
55	MG	1A	3036	1/1	0.91	0.13	34,34,34,34	0
55	MG	2A	3096	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
55	MG	1A	3332	1/1	0.91	0.20	44,44,44,44	0
55	MG	1A	3427	1/1	0.91	0.29	55,55,55,55	0
55	MG	1A	3067	1/1	0.91	0.17	49,49,49,49	0
55	MG	1a	1713	1/1	0.91	0.16	49,49,49,49	0
55	MG	1A	3385	1/1	0.91	0.64	48,48,48,48	0
55	MG	2A	3599	1/1	0.91	0.18	60,60,60,60	0
55	MG	1B	220	1/1	0.91	0.12	40,40,40,40	0
55	MG	1A	3972	1/1	0.91	0.17	43,43,43,43	0
55	MG	1A	3808	1/1	0.91	0.13	40,40,40,40	0
55	MG	2a	3039	1/1	0.91	0.12	43,43,43,43	0
55	MG	2a	3179	1/1	0.91	0.12	54,54,54,54	0
55	MG	2A	3431	1/1	0.91	0.23	46,46,46,46	0
55	MG	1A	3585	1/1	0.91	0.39	44,44,44,44	0
55	MG	1V	202	1/1	0.91	0.22	45,45,45,45	0
55	MG	2A	3649	1/1	0.91	0.20	40,40,40,40	0
55	MG	2A	3036	1/1	0.91	0.11	49,49,49,49	0
55	MG	1A	3877	1/1	0.91	0.13	40,40,40,40	0
55	MG	1A	3564	1/1	0.91	0.33	31,31,31,31	0
55	MG	1A	3742	1/1	0.91	0.17	51,51,51,51	0
55	MG	1A	3087	1/1	0.91	0.58	29,29,29,29	0
55	MG	2A	3334	1/1	0.91	0.32	64,64,64,64	0
55	MG	28	101	1/1	0.91	0.41	63,63,63,63	0
55	MG	2a	3176	1/1	0.91	0.07	67,67,67,67	0
55	MG	1a	1702	1/1	0.91	0.08	60,60,60,60	0
55	MG	2A	3856	1/1	0.91	0.15	63,63,63,63	0
55	MG	1B	201	1/1	0.91	0.20	50,50,50,50	0
55	MG	2A	3425	1/1	0.91	0.13	43,43,43,43	0
55	MG	2A	3169	1/1	0.91	0.15	48,48,48,48	0
55	MG	1A	3875	1/1	0.91	0.17	32,32,32,32	0
55	MG	2d	301	1/1	0.91	0.15	50,50,50,50	0
55	MG	10	103	1/1	0.91	0.19	55,55,55,55	0
55	MG	2a	3088	1/1	0.91	0.71	61,61,61,61	0
55	MG	1x	106	1/1	0.91	0.12	55,55,55,55	0
55	MG	15	105	1/1	0.91	0.18	43,43,43,43	0
55	MG	1A	4081	1/1	0.91	0.27	43,43,43,43	0
55	MG	2A	3465	1/1	0.91	0.14	54,54,54,54	0
55	MG	1A	4111	1/1	0.91	0.13	51,51,51,51	0
55	MG	1A	3814	1/1	0.91	0.14	41,41,41,41	0
55	MG	2A	3342	1/1	0.91	0.30	47,47,47,47	0
55	MG	2A	3671	1/1	0.91	0.15	60,60,60,60	0
55	MG	1A	3900	1/1	0.91	0.11	50,50,50,50	0
55	MG	2A	3184	1/1	0.91	0.11	39,39,39,39	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
55	MG	2A	3781	1/1	0.91	0.18	62,62,62,62	0
55	MG	1A	4018	1/1	0.91	0.73	57,57,57,57	0
55	MG	1A	3098	1/1	0.91	0.17	36,36,36,36	0
55	MG	1A	3695	1/1	0.91	0.20	20,20,20,20	0
55	MG	1A	3919	1/1	0.91	0.15	33,33,33,33	0
55	MG	1A	3203	1/1	0.91	0.18	29,29,29,29	0
55	MG	1A	3679	1/1	0.91	0.15	24,24,24,24	0
55	MG	2A	3357	1/1	0.91	0.20	44,44,44,44	0
55	MG	1A	3250	1/1	0.91	0.17	40,40,40,40	0
55	MG	2A	3622	1/1	0.91	0.13	61,61,61,61	0
55	MG	2A	3517	1/1	0.91	0.12	65,65,65,65	0
55	MG	1A	3705	1/1	0.91	0.17	23,23,23,23	0
55	MG	2A	3288	1/1	0.91	0.17	72,72,72,72	0
55	MG	1A	3515	1/1	0.91	0.10	55,55,55,55	0
55	MG	1A	3429	1/1	0.91	0.36	48,48,48,48	0
55	MG	1B	210	1/1	0.91	0.14	50,50,50,50	0
55	MG	1a	1793	1/1	0.91	0.11	63,63,63,63	0
55	MG	2A	3691	1/1	0.91	0.19	57,57,57,57	0
55	MG	1A	3772	1/1	0.91	0.16	16,16,16,16	0
55	MG	1A	4030	1/1	0.91	0.10	21,21,21,21	0
55	MG	2A	3447	1/1	0.91	0.16	71,71,71,71	0
55	MG	1A	3767	1/1	0.91	0.16	43,43,43,43	0
55	MG	2a	3032	1/1	0.91	0.21	58,58,58,58	0
55	MG	1l	204	1/1	0.91	0.08	64,64,64,64	0
55	MG	1A	3930	1/1	0.91	0.09	53,53,53,53	0
55	MG	2A	3860	1/1	0.91	0.38	43,43,43,43	0
55	MG	1A	3520	1/1	0.91	0.22	58,58,58,58	0
55	MG	2A	3663	1/1	0.91	0.22	52,52,52,52	0
55	MG	2A	3392	1/1	0.91	0.21	31,31,31,31	0
55	MG	1A	3081	1/1	0.91	0.24	57,57,57,57	0
55	MG	2A	3703	1/1	0.91	0.08	55,55,55,55	0
55	MG	1A	3612	1/1	0.91	0.29	61,61,61,61	0
55	MG	2A	3459	1/1	0.91	1.49	52,52,52,52	0
55	MG	2A	3749	1/1	0.91	0.14	45,45,45,45	0
55	MG	2A	3487	1/1	0.91	1.44	49,49,49,49	0
55	MG	1A	3595	1/1	0.91	0.15	36,36,36,36	0
55	MG	1A	3188	1/1	0.91	0.63	46,46,46,46	0
55	MG	2A	3303	1/1	0.91	0.49	60,60,60,60	0
55	MG	2A	3410	1/1	0.91	0.13	35,35,35,35	0
55	MG	1A	3731	1/1	0.91	0.12	31,31,31,31	0
55	MG	1A	4026	1/1	0.91	0.19	29,29,29,29	0
55	MG	1A	3030	1/1	0.91	0.17	39,39,39,39	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
55	MG	1A	3205	1/1	0.91	0.10	39,39,39,39	0
55	MG	2A	3264	1/1	0.91	0.46	55,55,55,55	0
55	MG	2A	3446	1/1	0.91	0.28	48,48,48,48	0
55	MG	1A	3533	1/1	0.91	0.14	24,24,24,24	0
55	MG	2A	3237	1/1	0.91	0.24	50,50,50,50	0
55	MG	1A	4083	1/1	0.91	0.10	26,26,26,26	0
55	MG	2A	3337	1/1	0.91	0.12	51,51,51,51	0
55	MG	2A	3834	1/1	0.91	0.11	29,29,29,29	0
55	MG	2A	3158	1/1	0.91	0.08	51,51,51,51	0
55	MG	1A	3260	1/1	0.91	0.15	38,38,38,38	0
55	MG	2A	3197	1/1	0.91	0.23	54,54,54,54	0
55	MG	2A	3181	1/1	0.91	0.87	59,59,59,59	0
55	MG	2A	3625	1/1	0.91	0.14	41,41,41,41	0
55	MG	2i	201	1/1	0.91	0.22	82,82,82,82	0
55	MG	2A	3088	1/1	0.91	0.10	32,32,32,32	0
55	MG	2a	3138	1/1	0.91	0.13	67,67,67,67	0
55	MG	1A	3946	1/1	0.91	0.26	50,50,50,50	0
55	MG	1A	3492	1/1	0.91	0.16	47,47,47,47	0
55	MG	1A	3411	1/1	0.91	0.28	43,43,43,43	0
55	MG	1A	3340	1/1	0.91	0.16	35,35,35,35	0
55	MG	2A	3516	1/1	0.91	0.08	60,60,60,60	0
55	MG	1A	3414	1/1	0.91	0.24	47,47,47,47	0
55	MG	2q	201	1/1	0.91	0.18	67,67,67,67	0
55	MG	1A	3177	1/1	0.91	0.64	41,41,41,41	0
55	MG	2a	3152	1/1	0.91	0.11	45,45,45,45	0
55	MG	2A	3732	1/1	0.91	0.17	44,44,44,44	0
55	MG	2A	3846	1/1	0.91	0.19	51,51,51,51	0
55	MG	2A	3308	1/1	0.91	0.41	54,54,54,54	0
55	MG	2A	3291	1/1	0.91	0.94	47,47,47,47	0
55	MG	1A	3287	1/1	0.91	0.16	51,51,51,51	0
55	MG	2A	3114	1/1	0.91	0.48	46,46,46,46	0
55	MG	1A	3185	1/1	0.91	0.18	50,50,50,50	0
55	MG	1A	3364	1/1	0.91	0.38	29,29,29,29	0
55	MG	2A	3118	1/1	0.91	0.56	59,59,59,59	0
55	MG	2A	3729	1/1	0.91	0.20	51,51,51,51	0
55	MG	2A	3257	1/1	0.91	0.14	52,52,52,52	0
55	MG	1a	1672	1/1	0.91	0.16	47,47,47,47	0
55	MG	1A	4019	1/1	0.91	0.20	28,28,28,28	0
55	MG	1A	3527	1/1	0.91	0.31	53,53,53,53	0
55	MG	2A	3784	1/1	0.91	0.15	39,39,39,39	0
55	MG	1A	3513	1/1	0.91	0.39	39,39,39,39	0
55	MG	2A	3015	1/1	0.91	0.11	63,63,63,63	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
55	MG	1a	1626	1/1	0.91	0.49	48,48,48,48	0
55	MG	1A	3465	1/1	0.91	0.23	57,57,57,57	0
55	MG	1A	3286	1/1	0.91	0.14	40,40,40,40	0
55	MG	1A	3633	1/1	0.92	0.11	54,54,54,54	0
55	MG	2A	3477	1/1	0.92	0.22	34,34,34,34	0
55	MG	2A	3571	1/1	0.92	0.11	69,69,69,69	0
55	MG	1a	1632	1/1	0.92	0.14	50,50,50,50	0
55	MG	2A	3751	1/1	0.92	0.17	50,50,50,50	0
55	MG	1A	3706	1/1	0.92	0.18	15,15,15,15	0
55	MG	1A	3716	1/1	0.92	0.18	30,30,30,30	0
55	MG	1F	311	1/1	0.92	0.51	27,27,27,27	0
55	MG	1a	1715	1/1	0.92	0.39	53,53,53,53	0
55	MG	1A	3700	1/1	0.92	0.13	23,23,23,23	0
55	MG	1A	3354	1/1	0.92	0.14	48,48,48,48	0
55	MG	1A	3671	1/1	0.92	0.08	36,36,36,36	0
55	MG	1a	1661	1/1	0.92	0.68	62,62,62,62	0
55	MG	1B	203	1/1	0.92	0.21	39,39,39,39	0
55	MG	2A	3598	1/1	0.92	0.16	59,59,59,59	0
55	MG	1A	3355	1/1	0.92	0.48	45,45,45,45	0
55	MG	2A	3488	1/1	0.92	0.20	73,73,73,73	0
55	MG	1E	310	1/1	0.92	0.74	43,43,43,43	0
55	MG	2A	3327	1/1	0.92	0.34	53,53,53,53	0
55	MG	2a	3018	1/1	0.92	0.13	60,60,60,60	0
55	MG	2A	3702	1/1	0.92	0.13	45,45,45,45	0
55	MG	1A	3313	1/1	0.92	0.18	44,44,44,44	0
55	MG	1A	3217	1/1	0.92	0.28	40,40,40,40	0
55	MG	1A	4043	1/1	0.92	0.08	49,49,49,49	0
55	MG	1a	1682	1/1	0.92	0.29	45,45,45,45	0
55	MG	2A	3070	1/1	0.92	0.13	60,60,60,60	0
55	MG	1A	3885	1/1	0.92	0.08	50,50,50,50	0
55	MG	2A	3177	1/1	0.92	0.24	56,56,56,56	0
55	MG	1X	101	1/1	0.92	0.20	35,35,35,35	0
55	MG	2A	3745	1/1	0.92	0.16	27,27,27,27	0
55	MG	1A	3229	1/1	0.92	0.19	51,51,51,51	0
55	MG	1a	1834	1/1	0.92	0.10	68,68,68,68	0
55	MG	1a	1660	1/1	0.92	1.06	77,77,77,77	0
55	MG	1a	1710	1/1	0.92	0.31	53,53,53,53	0
55	MG	2A	3575	1/1	0.92	0.13	49,49,49,49	0
55	MG	1A	3519	1/1	0.92	0.19	48,48,48,48	0
55	MG	1a	1708	1/1	0.92	0.35	58,58,58,58	0
55	MG	1A	3475	1/1	0.92	0.50	40,40,40,40	0
55	MG	1A	3333	1/1	0.92	0.32	41,41,41,41	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
55	MG	1a	1694	1/1	0.92	0.34	53,53,53,53	0
55	MG	1A	3237	1/1	0.92	0.69	33,33,33,33	0
55	MG	2x	102	1/1	0.92	0.18	73,73,73,73	0
55	MG	2A	3042	1/1	0.92	0.17	54,54,54,54	0
55	MG	1A	3508	1/1	0.92	0.56	35,35,35,35	0
55	MG	2a	3089	1/1	0.92	0.10	59,59,59,59	0
55	MG	1A	3434	1/1	0.92	0.11	51,51,51,51	0
55	MG	1A	3293	1/1	0.92	0.25	31,31,31,31	0
55	MG	1A	3047	1/1	0.92	0.19	43,43,43,43	0
55	MG	1A	3338	1/1	0.92	0.35	46,46,46,46	0
55	MG	1A	3115	1/1	0.92	0.21	47,47,47,47	0
55	MG	2A	3714	1/1	0.92	0.11	55,55,55,55	0
55	MG	2a	3050	1/1	0.92	0.11	79,79,79,79	0
55	MG	2A	3035	1/1	0.92	0.12	58,58,58,58	0
55	MG	2A	3464	1/1	0.92	0.24	77,77,77,77	0
55	MG	1A	3487	1/1	0.92	0.52	44,44,44,44	0
55	MG	2A	3376	1/1	0.92	0.21	60,60,60,60	0
55	MG	2a	3033	1/1	0.92	0.13	60,60,60,60	0
55	MG	2B	207	1/1	0.92	0.12	57,57,57,57	0
55	MG	1A	3745	1/1	0.92	0.24	48,48,48,48	0
55	MG	2a	3003	1/1	0.92	0.20	49,49,49,49	0
55	MG	1A	3629	1/1	0.92	0.15	32,32,32,32	0
55	MG	2A	3190	1/1	0.92	0.10	65,65,65,65	0
55	MG	2A	3842	1/1	0.92	0.12	48,48,48,48	0
55	MG	2A	3704	1/1	0.92	0.15	53,53,53,53	0
55	MG	1A	3669	1/1	0.92	0.15	21,21,21,21	0
55	MG	1A	3892	1/1	0.92	0.21	36,36,36,36	0
55	MG	1A	3698	1/1	0.92	0.14	39,39,39,39	0
55	MG	1a	1814	1/1	0.92	0.13	71,71,71,71	0
55	MG	1A	3334	1/1	0.92	0.34	33,33,33,33	0
55	MG	2A	3486	1/1	0.92	0.12	50,50,50,50	0
55	MG	2A	3405	1/1	0.92	0.21	57,57,57,57	0
55	MG	2A	3364	1/1	0.92	0.14	56,56,56,56	0
55	MG	1A	3593	1/1	0.92	0.11	53,53,53,53	0
55	MG	15	103	1/1	0.92	0.44	41,41,41,41	0
55	MG	1A	3060	1/1	0.92	0.35	46,46,46,46	0
55	MG	1a	1791	1/1	0.92	0.11	54,54,54,54	0
55	MG	1E	309	1/1	0.92	0.10	43,43,43,43	0
55	MG	1A	3285	1/1	0.92	0.12	38,38,38,38	0
55	MG	2A	3209	1/1	0.92	0.62	45,45,45,45	0
55	MG	2a	3055	1/1	0.92	0.11	59,59,59,59	0
55	MG	1A	3688	1/1	0.92	0.11	52,52,52,52	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
55	MG	2A	3761	1/1	0.92	0.14	49,49,49,49	0
55	MG	1A	3951	1/1	0.92	0.17	34,34,34,34	0
55	MG	2A	3156	1/1	0.92	0.14	58,58,58,58	0
55	MG	2a	3171	1/1	0.92	0.13	53,53,53,53	0
55	MG	2A	3712	1/1	0.92	0.17	61,61,61,61	0
55	MG	2A	3750	1/1	0.92	0.12	40,40,40,40	0
55	MG	1a	1746	1/1	0.92	0.17	52,52,52,52	0
55	MG	2A	3786	1/1	0.92	0.10	72,72,72,72	0
55	MG	2A	3056	1/1	0.92	0.24	42,42,42,42	0
55	MG	1A	3004	1/1	0.92	0.12	23,23,23,23	0
55	MG	1A	3299	1/1	0.92	0.12	42,42,42,42	0
55	MG	2A	3221	1/1	0.92	0.36	47,47,47,47	0
55	MG	1A	3654	1/1	0.92	0.15	36,36,36,36	0
55	MG	1A	3485	1/1	0.92	0.33	50,50,50,50	0
55	MG	2A	3282	1/1	0.92	0.28	72,72,72,72	0
55	MG	1A	3869	1/1	0.92	0.05	60,60,60,60	0
55	MG	1A	3100	1/1	0.92	0.11	40,40,40,40	0
55	MG	1A	3872	1/1	0.92	0.20	52,52,52,52	0
55	MG	2A	3548	1/1	0.92	0.16	39,39,39,39	0
55	MG	1A	3454	1/1	0.92	0.29	46,46,46,46	0
55	MG	1A	3353	1/1	0.92	0.26	50,50,50,50	0
55	MG	20	101	1/1	0.92	0.32	65,65,65,65	0
55	MG	2A	3635	1/1	0.92	0.21	42,42,42,42	0
55	MG	12	102	1/1	0.92	0.45	43,43,43,43	0
55	MG	2A	3417	1/1	0.92	0.14	50,50,50,50	0
55	MG	1A	3506	1/1	0.92	0.34	21,21,21,21	0
55	MG	1A	3292	1/1	0.92	0.39	29,29,29,29	0
55	MG	1A	3730	1/1	0.92	0.16	16,16,16,16	0
55	MG	2E	309	1/1	0.92	0.11	38,38,38,38	0
55	MG	1A	3844	1/1	0.92	0.14	45,45,45,45	0
55	MG	2A	3640	1/1	0.92	0.18	55,55,55,55	0
55	MG	2a	3194	1/1	0.92	0.17	61,61,61,61	0
55	MG	2A	3102	1/1	0.92	0.62	63,63,63,63	0
55	MG	2a	3025	1/1	0.92	0.10	55,55,55,55	0
55	MG	1a	1706	1/1	0.92	0.12	54,54,54,54	0
55	MG	2A	3407	1/1	0.92	0.14	53,53,53,53	0
55	MG	2A	3738	1/1	0.92	0.11	50,50,50,50	0
55	MG	1A	3204	1/1	0.92	0.15	24,24,24,24	0
55	MG	1A	3735	1/1	0.92	0.39	58,58,58,58	0
55	MG	1A	3159	1/1	0.92	0.09	47,47,47,47	0
55	MG	1a	1615	1/1	0.92	0.08	73,73,73,73	0
55	MG	2A	3418	1/1	0.92	0.66	56,56,56,56	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
55	MG	1a	1750	1/1	0.92	0.07	77,77,77,77	0
55	MG	2A	3596	1/1	0.92	0.14	48,48,48,48	0
55	MG	2A	3646	1/1	0.92	0.11	70,70,70,70	0
55	MG	2A	3155	1/1	0.92	0.16	47,47,47,47	0
55	MG	1B	209	1/1	0.92	0.11	53,53,53,53	0
55	MG	1A	3897	1/1	0.92	0.41	28,28,28,28	0
55	MG	2A	3351	1/1	0.92	0.16	38,38,38,38	0
55	MG	1A	3936	1/1	0.92	0.12	39,39,39,39	0
55	MG	1A	3390	1/1	0.92	0.50	34,34,34,34	0
55	MG	2E	305	1/1	0.92	0.11	38,38,38,38	0
55	MG	2A	3689	1/1	0.92	0.26	71,71,71,71	0
55	MG	1A	3278	1/1	0.92	0.20	40,40,40,40	0
55	MG	1A	4001	1/1	0.92	0.11	43,43,43,43	0
55	MG	2A	3115	1/1	0.92	0.14	42,42,42,42	0
55	MG	2E	301	1/1	0.92	0.40	55,55,55,55	0
55	MG	1A	3305	1/1	0.92	0.16	51,51,51,51	0
55	MG	1A	4069	1/1	0.92	0.21	34,34,34,34	0
55	MG	1A	3024	1/1	0.92	0.31	23,23,23,23	0
55	MG	1A	4010	1/1	0.92	0.10	54,54,54,54	0
55	MG	1A	3984	1/1	0.92	0.20	53,53,53,53	0
55	MG	1A	3812	1/1	0.92	0.14	24,24,24,24	0
55	MG	1A	4008	1/1	0.92	0.24	25,25,25,25	0
55	MG	2A	3226	1/1	0.92	0.11	61,61,61,61	0
55	MG	2A	3213	1/1	0.92	0.57	57,57,57,57	0
55	MG	2A	3399	1/1	0.92	0.33	47,47,47,47	0
55	MG	15	101	1/1	0.92	0.33	34,34,34,34	0
55	MG	2a	3109	1/1	0.92	0.11	75,75,75,75	0
55	MG	2A	3550	1/1	0.92	0.17	37,37,37,37	0
55	MG	2B	201	1/1	0.92	0.24	68,68,68,68	0
55	MG	2A	3660	1/1	0.92	0.11	54,54,54,54	0
55	MG	1A	3963	1/1	0.92	0.22	42,42,42,42	0
55	MG	2A	3615	1/1	0.92	0.13	67,67,67,67	0
55	MG	2A	3696	1/1	0.92	0.12	36,36,36,36	0
55	MG	1A	3902	1/1	0.92	0.09	58,58,58,58	0
55	MG	2A	3658	1/1	0.92	0.48	58,58,58,58	0
55	MG	1A	3234	1/1	0.92	0.25	29,29,29,29	0
55	MG	2A	3212	1/1	0.92	0.65	42,42,42,42	0
55	MG	2A	3695	1/1	0.92	0.20	29,29,29,29	0
55	MG	1A	3256	1/1	0.92	0.20	37,37,37,37	0
55	MG	2A	3742	1/1	0.92	0.18	59,59,59,59	0
55	MG	2A	3802	1/1	0.92	0.10	40,40,40,40	0
55	MG	2A	3800	1/1	0.92	0.18	52,52,52,52	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
55	MG	1A	3687	1/1	0.92	0.15	35,35,35,35	0
55	MG	2a	3140	1/1	0.92	0.18	59,59,59,59	0
55	MG	1A	3883	1/1	0.92	0.55	30,30,30,30	0
55	MG	1B	217	1/1	0.92	0.07	38,38,38,38	0
55	MG	1A	3710	1/1	0.92	0.09	21,21,21,21	0
55	MG	1a	1654	1/1	0.92	0.10	42,42,42,42	0
55	MG	2A	3225	1/1	0.92	0.27	54,54,54,54	0
55	MG	1A	3420	1/1	0.92	0.16	45,45,45,45	0
55	MG	2A	3609	1/1	0.92	0.21	33,33,33,33	0
55	MG	2a	3060	1/1	0.92	0.21	63,63,63,63	0
55	MG	1A	3622	1/1	0.92	0.08	37,37,37,37	0
55	MG	1A	3466	1/1	0.92	0.27	50,50,50,50	0
55	MG	2A	3196	1/1	0.92	0.17	50,50,50,50	0
55	MG	1A	3378	1/1	0.92	0.16	41,41,41,41	0
55	MG	2a	3148	1/1	0.92	0.14	69,69,69,69	0
55	MG	1a	1730	1/1	0.92	0.33	60,60,60,60	0
55	MG	2a	3120	1/1	0.92	0.08	57,57,57,57	0
55	MG	1A	3512	1/1	0.92	0.35	56,56,56,56	0
55	MG	2A	3798	1/1	0.92	0.10	57,57,57,57	0
55	MG	2A	3705	1/1	0.92	0.05	55,55,55,55	0
55	MG	1A	3834	1/1	0.92	0.15	33,33,33,33	0
55	MG	1A	3130	1/1	0.92	0.23	27,27,27,27	0
55	MG	1A	3195	1/1	0.92	0.12	40,40,40,40	0
55	MG	2a	3078	1/1	0.92	0.17	53,53,53,53	0
55	MG	1A	4055	1/1	0.92	0.08	38,38,38,38	0
55	MG	1A	3552	1/1	0.92	0.27	33,33,33,33	0
55	MG	1a	1744	1/1	0.92	0.12	50,50,50,50	0
55	MG	1U	202	1/1	0.93	0.71	49,49,49,49	0
55	MG	2A	3128	1/1	0.93	0.14	35,35,35,35	0
55	MG	1A	3646	1/1	0.93	0.12	30,30,30,30	0
55	MG	2A	3581	1/1	0.93	0.08	55,55,55,55	0
55	MG	2X	101	1/1	0.93	0.69	63,63,63,63	0
55	MG	2A	3743	1/1	0.93	0.10	69,69,69,69	0
55	MG	1A	3337	1/1	0.93	0.17	45,45,45,45	0
55	MG	1A	3628	1/1	0.93	0.18	54,54,54,54	0
55	MG	1A	4110	1/1	0.93	0.19	53,53,53,53	0
55	MG	1A	3468	1/1	0.93	0.41	46,46,46,46	0
55	MG	2a	3056	1/1	0.93	0.13	47,47,47,47	0
55	MG	1a	1611	1/1	0.93	0.28	43,43,43,43	0
55	MG	1A	3189	1/1	0.93	0.14	43,43,43,43	0
55	MG	2A	3017	1/1	0.93	0.74	46,46,46,46	0
55	MG	2R	202	1/1	0.93	0.12	52,52,52,52	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
55	MG	2A	3479	1/1	0.93	0.26	51,51,51,51	0
55	MG	1a	1673	1/1	0.93	0.20	59,59,59,59	0
55	MG	2A	3641	1/1	0.93	0.14	55,55,55,55	0
55	MG	1A	3599	1/1	0.93	0.19	39,39,39,39	0
55	MG	2A	3332	1/1	0.93	0.51	61,61,61,61	0
55	MG	1A	3993	1/1	0.93	0.10	54,54,54,54	0
55	MG	2A	3777	1/1	0.93	0.41	52,52,52,52	0
55	MG	2A	3707	1/1	0.93	0.15	56,56,56,56	0
55	MG	1A	3876	1/1	0.93	0.19	19,19,19,19	0
55	MG	2A	3132	1/1	0.93	0.24	52,52,52,52	0
55	MG	2A	3497	1/1	0.93	0.22	41,41,41,41	0
55	MG	2B	208	1/1	0.93	0.19	57,57,57,57	0
55	MG	2a	3181	1/1	0.93	0.13	56,56,56,56	0
55	MG	2A	3402	1/1	0.93	0.18	47,47,47,47	0
55	MG	1A	3962	1/1	0.93	0.48	51,51,51,51	0
55	MG	2A	3269	1/1	0.93	0.23	55,55,55,55	0
55	MG	1A	4065	1/1	0.93	0.24	26,26,26,26	0
55	MG	2A	3244	1/1	0.93	0.09	51,51,51,51	0
55	MG	1A	3132	1/1	0.93	0.61	40,40,40,40	0
55	MG	2a	3075	1/1	0.93	0.14	59,59,59,59	0
55	MG	1A	3231	1/1	0.93	0.22	55,55,55,55	0
55	MG	1a	1811	1/1	0.93	0.15	73,73,73,73	0
55	MG	2A	3835	1/1	0.93	0.14	59,59,59,59	0
55	MG	1A	3853	1/1	0.93	0.11	30,30,30,30	0
55	MG	2V	203	1/1	0.93	0.13	47,47,47,47	0
55	MG	2a	3076	1/1	0.93	0.09	50,50,50,50	0
55	MG	2a	3037	1/1	0.93	0.08	80,80,80,80	0
55	MG	2A	3541	1/1	0.93	0.17	40,40,40,40	0
55	MG	1A	3549	1/1	0.93	0.25	45,45,45,45	0
55	MG	1A	3367	1/1	0.93	0.30	34,34,34,34	0
55	MG	2a	3167	1/1	0.93	0.11	50,50,50,50	0
55	MG	1A	3210	1/1	0.93	0.53	43,43,43,43	0
55	MG	1A	3363	1/1	0.93	0.73	36,36,36,36	0
55	MG	2A	3443	1/1	0.93	0.70	41,41,41,41	0
55	MG	1A	3880	1/1	0.93	0.16	21,21,21,21	0
55	MG	1A	3566	1/1	0.93	0.22	32,32,32,32	0
55	MG	1R	201	1/1	0.93	0.80	44,44,44,44	0
55	MG	1A	3886	1/1	0.93	0.07	28,28,28,28	0
55	MG	2a	3012	1/1	0.93	0.24	63,63,63,63	0
55	MG	2A	3681	1/1	0.93	0.24	37,37,37,37	0
55	MG	2A	3401	1/1	0.93	0.21	43,43,43,43	0
55	MG	2a	3095	1/1	0.93	0.22	46,46,46,46	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
55	MG	2A	3827	1/1	0.93	0.14	64,64,64,64	0
55	MG	18	106	1/1	0.93	0.09	55,55,55,55	0
55	MG	1D	307	1/1	0.93	1.10	38,38,38,38	0
55	MG	1A	3606	1/1	0.93	0.16	37,37,37,37	0
55	MG	1A	3494	1/1	0.93	0.19	35,35,35,35	0
55	MG	1A	3438	1/1	0.93	0.50	41,41,41,41	0
55	MG	1N	202	1/1	0.93	0.29	33,33,33,33	0
55	MG	2A	3657	1/1	0.93	0.28	44,44,44,44	0
55	MG	2f	202	1/1	0.93	0.11	56,56,56,56	0
55	MG	2A	3554	1/1	0.93	0.16	67,67,67,67	0
55	MG	1A	3555	1/1	0.93	0.57	32,32,32,32	0
55	MG	1A	3417	1/1	0.93	0.26	44,44,44,44	0
55	MG	2A	3597	1/1	0.93	0.18	49,49,49,49	0
55	MG	1A	3154	1/1	0.93	0.10	34,34,34,34	0
55	MG	1A	3863	1/1	0.93	0.19	45,45,45,45	0
55	MG	2A	3345	1/1	0.93	0.37	49,49,49,49	0
55	MG	2B	212	1/1	0.93	0.21	52,52,52,52	0
55	MG	1a	1667	1/1	0.93	0.15	61,61,61,61	0
55	MG	1A	3928	1/1	0.93	0.22	44,44,44,44	0
55	MG	2A	3296	1/1	0.93	0.35	47,47,47,47	0
55	MG	2a	3087	1/1	0.93	0.21	61,61,61,61	0
55	MG	1A	3743	1/1	0.93	0.12	49,49,49,49	0
55	MG	1A	3965	1/1	0.93	0.19	27,27,27,27	0
55	MG	2A	3382	1/1	0.93	0.09	66,66,66,66	0
55	MG	1A	3387	1/1	0.93	0.63	34,34,34,34	0
55	MG	2A	3607	1/1	0.93	0.22	49,49,49,49	0
55	MG	1A	3510	1/1	0.93	0.15	33,33,33,33	0
55	MG	2A	3012	1/1	0.93	0.10	36,36,36,36	0
55	MG	1A	3704	1/1	0.93	0.10	42,42,42,42	0
55	MG	2A	3697	1/1	0.93	0.29	57,57,57,57	0
55	MG	1A	3532	1/1	0.93	0.14	33,33,33,33	0
55	MG	2x	105	1/1	0.93	0.13	67,67,67,67	0
55	MG	1P	201	1/1	0.93	0.48	27,27,27,27	0
55	MG	1A	3934	1/1	0.93	0.11	28,28,28,28	0
55	MG	1a	1629	1/1	0.93	0.10	51,51,51,51	0
55	MG	1A	3854	1/1	0.93	0.13	33,33,33,33	0
55	MG	1A	3480	1/1	0.93	0.12	42,42,42,42	0
55	MG	2A	3460	1/1	0.93	1.04	48,48,48,48	0
55	MG	1a	1722	1/1	0.93	0.11	66,66,66,66	0
55	MG	2A	3522	1/1	0.93	0.12	31,31,31,31	0
55	MG	1A	3267	1/1	0.93	0.47	33,33,33,33	0
55	MG	1a	1802	1/1	0.93	0.15	66,66,66,66	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
55	MG	2B	217	1/1	0.93	0.08	57,57,57,57	0
55	MG	1a	1624	1/1	0.93	0.11	59,59,59,59	0
55	MG	1A	3786	1/1	0.93	0.17	38,38,38,38	0
55	MG	2A	3659	1/1	0.93	0.73	44,44,44,44	0
55	MG	1a	1714	1/1	0.93	0.16	51,51,51,51	0
55	MG	2A	3284	1/1	0.93	0.11	50,50,50,50	0
55	MG	2A	3066	1/1	0.93	0.27	43,43,43,43	0
55	MG	1A	3542	1/1	0.93	0.79	35,35,35,35	0
55	MG	2A	3314	1/1	0.93	0.13	50,50,50,50	0
55	MG	1A	3458	1/1	0.93	0.21	47,47,47,47	0
55	MG	1A	3755	1/1	0.93	0.10	55,55,55,55	0
55	MG	1A	3073	1/1	0.93	0.60	37,37,37,37	0
55	MG	2A	3763	1/1	0.93	0.38	49,49,49,49	0
55	MG	1a	1674	1/1	0.93	0.13	56,56,56,56	0
55	MG	2A	3352	1/1	0.93	0.19	43,43,43,43	0
55	MG	1A	3065	1/1	0.93	0.14	50,50,50,50	0
55	MG	1A	3460	1/1	0.93	0.12	38,38,38,38	0
55	MG	1A	3959	1/1	0.93	0.16	40,40,40,40	0
55	MG	19	101	1/1	0.93	0.11	43,43,43,43	0
55	MG	2A	3175	1/1	0.93	0.21	52,52,52,52	0
55	MG	2A	3328	1/1	0.93	0.30	43,43,43,43	0
55	MG	1A	3896	1/1	0.93	0.43	32,32,32,32	0
55	MG	2A	3826	1/1	0.93	0.30	72,72,72,72	0
55	MG	1a	1691	1/1	0.93	0.17	46,46,46,46	0
55	MG	1A	3005	1/1	0.93	0.11	34,34,34,34	0
55	MG	2A	3529	1/1	0.93	0.24	49,49,49,49	0
55	MG	1A	3443	1/1	0.93	0.29	33,33,33,33	0
55	MG	2A	3081	1/1	0.93	0.08	69,69,69,69	0
55	MG	1N	201	1/1	0.93	0.27	43,43,43,43	0
55	MG	2A	3828	1/1	0.93	0.11	48,48,48,48	0
55	MG	1A	3279	1/1	0.93	0.49	47,47,47,47	0
55	MG	1A	3192	1/1	0.93	0.34	32,32,32,32	0
55	MG	1A	3117	1/1	0.93	0.36	31,31,31,31	0
55	MG	1a	1740	1/1	0.93	0.15	42,42,42,42	0
55	MG	2A	3734	1/1	0.93	0.68	42,42,42,42	0
55	MG	2A	3524	1/1	0.93	0.09	37,37,37,37	0
55	MG	2a	3164	1/1	0.93	0.07	66,66,66,66	0
55	MG	2A	3029	1/1	0.93	0.11	27,27,27,27	0
55	MG	2a	3125	1/1	0.93	0.09	61,61,61,61	0
55	MG	1A	3760	1/1	0.93	0.19	24,24,24,24	0
55	MG	1a	1755	1/1	0.93	0.22	60,60,60,60	0
55	MG	2a	3168	1/1	0.93	0.15	40,40,40,40	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
55	MG	1A	3477	1/1	0.93	0.19	49,49,49,49	0
55	MG	1A	3124	1/1	0.93	0.21	47,47,47,47	0
55	MG	1A	3312	1/1	0.93	0.50	38,38,38,38	0
55	MG	1A	3426	1/1	0.93	0.21	50,50,50,50	0
55	MG	1G	204	1/1	0.93	0.06	50,50,50,50	0
55	MG	1A	3413	1/1	0.93	0.41	55,55,55,55	0
55	MG	2A	3715	1/1	0.93	0.17	66,66,66,66	0
55	MG	2F	306	1/1	0.93	0.20	62,62,62,62	0
55	MG	1A	3818	1/1	0.93	0.18	40,40,40,40	0
55	MG	2D	302	1/1	0.93	0.66	42,42,42,42	0
55	MG	1A	3046	1/1	0.93	0.18	33,33,33,33	0
55	MG	1a	1827	1/1	0.93	0.09	48,48,48,48	0
55	MG	1A	3692	1/1	0.93	0.06	36,36,36,36	0
55	MG	1A	4015	1/1	0.93	0.18	39,39,39,39	0
55	MG	1O	204	1/1	0.93	0.12	60,60,60,60	0
55	MG	2A	3518	1/1	0.93	0.10	68,68,68,68	0
55	MG	1A	4037	1/1	0.93	0.14	58,58,58,58	0
55	MG	1A	3428	1/1	0.93	0.26	41,41,41,41	0
55	MG	1A	3393	1/1	0.93	0.12	43,43,43,43	0
55	MG	1A	3905	1/1	0.93	0.16	23,23,23,23	0
55	MG	1A	3632	1/1	0.93	0.18	35,35,35,35	0
55	MG	2A	3085	1/1	0.93	0.12	60,60,60,60	0
55	MG	1A	4034	1/1	0.93	0.62	57,57,57,57	0
55	MG	1A	3220	1/1	0.93	0.20	44,44,44,44	0
55	MG	1A	3600	1/1	0.93	0.26	40,40,40,40	0
55	MG	2A	3116	1/1	0.93	0.08	43,43,43,43	0
55	MG	2t	201	1/1	0.93	0.15	62,62,62,62	0
55	MG	2A	3121	1/1	0.93	0.15	39,39,39,39	0
55	MG	1a	1724	1/1	0.93	0.08	49,49,49,49	0
55	MG	2B	205	1/1	0.93	0.12	64,64,64,64	0
55	MG	2a	3029	1/1	0.93	0.16	78,78,78,78	0
55	MG	2A	3595	1/1	0.93	0.24	51,51,51,51	0
55	MG	1A	3372	1/1	0.93	0.62	38,38,38,38	0
55	MG	1a	1698	1/1	0.93	0.20	51,51,51,51	0
55	MG	1A	3432	1/1	0.93	0.29	32,32,32,32	0
55	MG	2A	3614	1/1	0.93	0.18	44,44,44,44	0
55	MG	1A	3924	1/1	0.93	0.36	38,38,38,38	0
55	MG	2l	201	1/1	0.93	0.09	76,76,76,76	0
55	MG	1Q	207	1/1	0.93	0.23	39,39,39,39	0
55	MG	1A	3635	1/1	0.93	0.82	49,49,49,49	0
55	MG	2A	3769	1/1	0.93	0.21	48,48,48,48	0
55	MG	1a	1669	1/1	0.93	0.10	54,54,54,54	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
55	MG	10	105	1/1	0.93	0.10	44,44,44,44	0
55	MG	1A	3935	1/1	0.93	0.11	21,21,21,21	0
55	MG	1A	4105	1/1	0.93	0.31	53,53,53,53	0
55	MG	1A	3436	1/1	0.93	0.78	45,45,45,45	0
55	MG	2a	3010	1/1	0.93	0.12	55,55,55,55	0
55	MG	1A	3103	1/1	0.93	0.17	58,58,58,58	0
55	MG	2A	3650	1/1	0.93	0.48	56,56,56,56	0
55	MG	1A	3449	1/1	0.93	0.13	58,58,58,58	0
55	MG	2A	3540	1/1	0.93	0.23	40,40,40,40	0
55	MG	1A	3749	1/1	0.93	0.16	37,37,37,37	0
55	MG	1A	3720	1/1	0.93	0.12	31,31,31,31	0
55	MG	2A	3723	1/1	0.93	0.11	29,29,29,29	0
55	MG	1a	1752	1/1	0.93	0.14	58,58,58,58	0
55	MG	1A	3918	1/1	0.93	0.19	38,38,38,38	0
55	MG	1A	3096	1/1	0.93	0.15	60,60,60,60	0
55	MG	1A	3483	1/1	0.93	0.13	53,53,53,53	0
55	MG	1A	3567	1/1	0.93	0.39	31,31,31,31	0
55	MG	2A	3527	1/1	0.93	0.21	54,54,54,54	0
55	MG	1a	1699	1/1	0.93	0.11	48,48,48,48	0
55	MG	1A	3015	1/1	0.93	0.25	33,33,33,33	0
55	MG	1B	233	1/1	0.93	0.17	53,53,53,53	0
55	MG	13	102	1/1	0.93	0.40	41,41,41,41	0
55	MG	2p	101	1/1	0.93	0.15	51,51,51,51	0
55	MG	1a	1688	1/1	0.93	0.73	53,53,53,53	0
55	MG	1A	3392	1/1	0.93	0.32	53,53,53,53	0
55	MG	2A	3780	1/1	0.93	0.28	53,53,53,53	0
55	MG	2A	3148	1/1	0.93	0.29	48,48,48,48	0
55	MG	1F	309	1/1	0.93	0.14	41,41,41,41	0
55	MG	1A	4101	1/1	0.93	0.68	61,61,61,61	0
55	MG	1a	1747	1/1	0.93	0.23	50,50,50,50	0
55	MG	1A	3265	1/1	0.93	0.54	37,37,37,37	0
55	MG	2A	3003	1/1	0.93	0.10	50,50,50,50	0
55	MG	2A	3439	1/1	0.93	0.13	64,64,64,64	0
55	MG	2A	3023	1/1	0.93	0.47	49,49,49,49	0
55	MG	1A	3979	1/1	0.93	0.12	52,52,52,52	0
55	MG	1A	3805	1/1	0.94	0.19	33,33,33,33	0
55	MG	1A	3056	1/1	0.94	0.11	39,39,39,39	0
55	MG	2A	3584	1/1	0.94	0.14	35,35,35,35	0
55	MG	2A	3406	1/1	0.94	0.12	45,45,45,45	0
55	MG	1A	4048	1/1	0.94	0.15	40,40,40,40	0
55	MG	1A	3495	1/1	0.94	0.15	60,60,60,60	0
55	MG	1A	4084	1/1	0.94	0.12	43,43,43,43	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
55	MG	1A	3040	1/1	0.94	0.76	35,35,35,35	0
55	MG	1A	4073	1/1	0.94	0.15	61,61,61,61	0
55	MG	1A	3686	1/1	0.94	0.16	33,33,33,33	0
55	MG	2A	3219	1/1	0.94	0.29	50,50,50,50	0
55	MG	2A	3589	1/1	0.94	0.14	44,44,44,44	0
55	MG	1A	3560	1/1	0.94	0.14	41,41,41,41	0
55	MG	2O	201	1/1	0.94	0.20	56,56,56,56	0
55	MG	1A	3179	1/1	0.94	0.15	42,42,42,42	0
55	MG	2A	3218	1/1	0.94	0.58	49,49,49,49	0
55	MG	2B	215	1/1	0.94	0.20	47,47,47,47	0
55	MG	2A	3349	1/1	0.94	0.25	45,45,45,45	0
55	MG	1A	3373	1/1	0.94	0.81	47,47,47,47	0
55	MG	2A	3435	1/1	0.94	0.72	41,41,41,41	0
55	MG	1A	4114	1/1	0.94	0.33	53,53,53,53	0
55	MG	1A	3006	1/1	0.94	0.47	50,50,50,50	0
55	MG	1A	4106	1/1	0.94	0.19	52,52,52,52	0
55	MG	1A	4007	1/1	0.94	0.12	25,25,25,25	0
55	MG	1A	3638	1/1	0.94	0.21	43,43,43,43	0
55	MG	2A	3567	1/1	0.94	0.11	38,38,38,38	0
55	MG	1A	3973	1/1	0.94	0.13	67,67,67,67	0
55	MG	2A	3718	1/1	0.94	0.11	57,57,57,57	0
55	MG	1A	3762	1/1	0.94	0.12	54,54,54,54	0
55	MG	2A	3839	1/1	0.94	0.28	40,40,40,40	0
55	MG	1A	3162	1/1	0.94	0.60	43,43,43,43	0
55	MG	1A	3548	1/1	0.94	0.72	42,42,42,42	0
55	MG	2A	3014	1/1	0.94	0.22	38,38,38,38	0
55	MG	1A	3588	1/1	0.94	0.10	58,58,58,58	0
55	MG	1A	3402	1/1	0.94	0.41	35,35,35,35	0
55	MG	2A	3389	1/1	0.94	0.17	47,47,47,47	0
55	MG	1A	3538	1/1	0.94	0.29	44,44,44,44	0
55	MG	2A	3159	1/1	0.94	0.07	48,48,48,48	0
55	MG	2a	3121	1/1	0.94	0.34	51,51,51,51	0
55	MG	2A	3774	1/1	0.94	0.19	42,42,42,42	0
55	MG	2a	3101	1/1	0.94	0.08	73,73,73,73	0
55	MG	1A	3665	1/1	0.94	0.16	25,25,25,25	0
55	MG	1A	3102	1/1	0.94	0.41	47,47,47,47	0
55	MG	2A	3727	1/1	0.94	0.59	66,66,66,66	0
55	MG	2a	3051	1/1	0.94	0.17	45,45,45,45	0
55	MG	1A	3999	1/1	0.94	0.46	64,64,64,64	0
55	MG	2A	3573	1/1	0.94	0.16	34,34,34,34	0
55	MG	2A	3807	1/1	0.94	0.16	36,36,36,36	0
55	MG	2A	3107	1/1	0.94	0.08	74,74,74,74	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
55	MG	2A	3643	1/1	0.94	0.28	64,64,64,64	0
55	MG	2A	3677	1/1	0.94	0.15	37,37,37,37	0
55	MG	2a	3100	1/1	0.94	0.05	57,57,57,57	0
55	MG	2A	3611	1/1	0.94	0.09	47,47,47,47	0
55	MG	1A	3975	1/1	0.94	0.12	53,53,53,53	0
55	MG	2A	3421	1/1	0.94	0.11	48,48,48,48	0
55	MG	1A	3859	1/1	0.94	0.88	59,59,59,59	0
55	MG	2a	3066	1/1	0.94	0.18	61,61,61,61	0
55	MG	2A	3217	1/1	0.94	0.18	35,35,35,35	0
55	MG	1a	1821	1/1	0.94	0.13	53,53,53,53	0
55	MG	1f	202	1/1	0.94	0.20	48,48,48,48	0
55	MG	2a	3045	1/1	0.94	0.27	92,92,92,92	0
55	MG	2B	202	1/1	0.94	0.10	43,43,43,43	0
55	MG	1A	3401	1/1	0.94	0.18	37,37,37,37	0
55	MG	2A	3198	1/1	0.94	0.17	47,47,47,47	0
55	MG	1A	4003	1/1	0.94	0.07	48,48,48,48	0
55	MG	1A	3069	1/1	0.94	0.15	36,36,36,36	0
55	MG	1A	3647	1/1	0.94	0.13	42,42,42,42	0
55	MG	1T	202	1/1	0.94	0.23	44,44,44,44	0
55	MG	1A	3349	1/1	0.94	0.17	42,42,42,42	0
55	MG	1A	3080	1/1	0.94	0.24	34,34,34,34	0
55	MG	2A	3850	1/1	0.94	0.23	51,51,51,51	0
55	MG	1A	3397	1/1	0.94	0.14	38,38,38,38	0
55	MG	1A	3800	1/1	0.94	0.15	22,22,22,22	0
55	MG	1A	3839	1/1	0.94	0.20	64,64,64,64	0
55	MG	1B	223	1/1	0.94	0.16	56,56,56,56	0
55	MG	1A	4090	1/1	0.94	0.10	42,42,42,42	0
55	MG	1A	3018	1/1	0.94	0.13	43,43,43,43	0
55	MG	2A	3603	1/1	0.94	0.13	34,34,34,34	0
55	MG	1a	1754	1/1	0.94	0.12	61,61,61,61	0
55	MG	1A	3569	1/1	0.94	1.07	40,40,40,40	0
55	MG	2A	3041	1/1	0.94	0.15	55,55,55,55	0
55	MG	2A	3390	1/1	0.94	0.16	53,53,53,53	0
55	MG	1A	3123	1/1	0.94	0.26	35,35,35,35	0
55	MG	1A	3500	1/1	0.94	0.15	37,37,37,37	0
55	MG	1A	3127	1/1	0.94	0.57	34,34,34,34	0
55	MG	1A	3558	1/1	0.94	0.93	30,30,30,30	0
55	MG	1B	206	1/1	0.94	0.23	40,40,40,40	0
55	MG	2A	3388	1/1	0.94	0.11	42,42,42,42	0
55	MG	1A	3311	1/1	0.94	0.29	28,28,28,28	0
55	MG	2A	3724	1/1	0.94	0.14	61,61,61,61	0
55	MG	1A	3579	1/1	0.94	0.34	45,45,45,45	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
55	MG	1a	1693	1/1	0.94	0.11	59,59,59,59	0
55	MG	1A	3547	1/1	0.94	0.50	30,30,30,30	0
55	MG	2A	3091	1/1	0.94	0.16	37,37,37,37	0
55	MG	1A	3797	1/1	0.94	0.23	26,26,26,26	0
55	MG	1A	3158	1/1	0.94	0.42	34,34,34,34	0
55	MG	2A	3427	1/1	0.94	0.11	54,54,54,54	0
55	MG	1E	306	1/1	0.94	0.19	22,22,22,22	0
55	MG	1A	3726	1/1	0.94	0.07	64,64,64,64	0
55	MG	1A	4074	1/1	0.94	0.18	14,14,14,14	0
55	MG	1B	204	1/1	0.94	0.16	52,52,52,52	0
55	MG	1A	3283	1/1	0.94	0.24	26,26,26,26	0
55	MG	1A	3849	1/1	0.94	0.23	39,39,39,39	0
55	MG	1A	3489	1/1	0.94	0.62	40,40,40,40	0
55	MG	2a	3145	1/1	0.94	0.29	67,67,67,67	0
55	MG	1A	4060	1/1	0.94	0.20	37,37,37,37	0
55	MG	1A	3246	1/1	0.94	0.20	43,43,43,43	0
55	MG	1I	102	1/1	0.94	0.15	28,28,28,28	0
55	MG	1A	3778	1/1	0.94	0.15	29,29,29,29	0
55	MG	2A	3791	1/1	0.94	0.11	46,46,46,46	0
55	MG	2A	3530	1/1	0.94	0.17	41,41,41,41	0
55	MG	1A	4056	1/1	0.94	0.21	56,56,56,56	0
55	MG	2A	3150	1/1	0.94	0.05	66,66,66,66	0
55	MG	2A	3706	1/1	0.94	0.12	39,39,39,39	0
55	MG	2a	3185	1/1	0.94	0.23	58,58,58,58	0
55	MG	1A	3461	1/1	0.94	0.82	48,48,48,48	0
55	MG	1a	1786	1/1	0.94	0.08	74,74,74,74	0
55	MG	2a	3062	1/1	0.94	0.12	50,50,50,50	0
55	MG	2A	3683	1/1	0.94	0.09	79,79,79,79	0
55	MG	2A	3737	1/1	0.94	0.07	50,50,50,50	0
55	MG	1A	3044	1/1	0.94	0.38	27,27,27,27	0
55	MG	2A	3062	1/1	0.94	0.38	45,45,45,45	0
55	MG	1A	3933	1/1	0.94	0.15	24,24,24,24	0
55	MG	2R	201	1/1	0.94	0.10	48,48,48,48	0
55	MG	2A	3779	1/1	0.94	0.20	73,73,73,73	0
55	MG	1A	3587	1/1	0.94	0.17	57,57,57,57	0
55	MG	1A	3453	1/1	0.94	1.01	46,46,46,46	0
55	MG	2A	3701	1/1	0.94	0.15	49,49,49,49	0
55	MG	1D	309	1/1	0.94	0.70	53,53,53,53	0
55	MG	1A	3478	1/1	0.94	0.17	44,44,44,44	0
55	MG	1A	3384	1/1	0.94	0.31	37,37,37,37	0
55	MG	1A	3240	1/1	0.94	0.21	61,61,61,61	0
55	MG	2A	3722	1/1	0.94	0.29	72,72,72,72	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
55	MG	1A	3108	1/1	0.94	0.10	29,29,29,29	0
55	MG	1A	3990	1/1	0.94	0.22	56,56,56,56	0
55	MG	1A	3659	1/1	0.94	0.10	52,52,52,52	0
55	MG	2A	3408	1/1	0.94	0.37	60,60,60,60	0
55	MG	2f	201	1/1	0.94	0.12	55,55,55,55	0
55	MG	2A	3513	1/1	0.94	0.12	43,43,43,43	0
55	MG	2A	3817	1/1	0.94	0.21	40,40,40,40	0
55	MG	2A	3556	1/1	0.94	0.12	35,35,35,35	0
55	MG	2A	3412	1/1	0.94	0.12	55,55,55,55	0
55	MG	2a	3083	1/1	0.94	0.38	64,64,64,64	0
55	MG	1A	3725	1/1	0.94	0.13	25,25,25,25	0
55	MG	1A	3891	1/1	0.94	0.23	39,39,39,39	0
55	MG	2a	3052	1/1	0.94	0.19	62,62,62,62	0
55	MG	2A	3020	1/1	0.94	0.19	54,54,54,54	0
55	MG	2X	102	1/1	0.94	0.12	52,52,52,52	0
55	MG	2a	3166	1/1	0.94	0.24	54,54,54,54	0
55	MG	1a	1692	1/1	0.94	0.10	55,55,55,55	0
55	MG	1A	3785	1/1	0.94	0.23	46,46,46,46	0
55	MG	1A	3226	1/1	0.94	0.68	32,32,32,32	0
55	MG	2A	3242	1/1	0.94	0.28	49,49,49,49	0
55	MG	1A	3848	1/1	0.94	0.14	37,37,37,37	0
55	MG	2a	3180	1/1	0.94	0.22	63,63,63,63	0
55	MG	1A	3658	1/1	0.94	0.17	43,43,43,43	0
55	MG	2a	3184	1/1	0.94	0.12	72,72,72,72	0
55	MG	1A	3642	1/1	0.94	0.16	26,26,26,26	0
55	MG	1A	3676	1/1	0.94	0.19	55,55,55,55	0
55	MG	1A	3341	1/1	0.94	0.19	33,33,33,33	0
55	MG	1A	3833	1/1	0.94	0.17	52,52,52,52	0
55	MG	1a	1712	1/1	0.94	0.21	65,65,65,65	0
55	MG	1A	3497	1/1	0.94	0.40	31,31,31,31	0
55	MG	1A	4062	1/1	0.94	0.13	37,37,37,37	0
55	MG	1A	4096	1/1	0.94	0.08	47,47,47,47	0
55	MG	1a	1794	1/1	0.94	0.31	50,50,50,50	0
55	MG	1A	3082	1/1	0.94	0.36	29,29,29,29	0
55	MG	1A	3551	1/1	0.94	0.26	31,31,31,31	0
55	MG	1a	1822	1/1	0.94	0.12	54,54,54,54	0
55	MG	26	101	1/1	0.94	0.13	52,52,52,52	0
55	MG	2A	3154	1/1	0.94	0.14	38,38,38,38	0
55	MG	2A	3539	1/1	0.94	0.13	57,57,57,57	0
55	MG	2A	3168	1/1	0.94	0.26	51,51,51,51	0
55	MG	1A	3206	1/1	0.94	0.72	36,36,36,36	0
55	MG	2a	3107	1/1	0.94	0.08	65,65,65,65	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
55	MG	1A	3249	1/1	0.94	0.41	37,37,37,37	0
55	MG	1A	3893	1/1	0.94	0.27	35,35,35,35	0
55	MG	1a	1761	1/1	0.94	0.10	49,49,49,49	0
55	MG	1a	1788	1/1	0.94	0.17	66,66,66,66	0
55	MG	2A	3748	1/1	0.94	0.12	50,50,50,50	0
55	MG	2A	3129	1/1	0.94	0.13	57,57,57,57	0
55	MG	2A	3559	1/1	0.94	0.10	50,50,50,50	0
55	MG	1A	3554	1/1	0.94	0.16	49,49,49,49	0
55	MG	1A	3784	1/1	0.94	0.12	49,49,49,49	0
55	MG	1a	1790	1/1	0.94	0.52	48,48,48,48	0
55	MG	1a	1678	1/1	0.94	0.20	85,85,85,85	0
55	MG	2A	3055	1/1	0.94	0.11	34,34,34,34	0
55	MG	1A	3031	1/1	0.94	0.54	32,32,32,32	0
55	MG	1A	3010	1/1	0.94	0.15	24,24,24,24	0
55	MG	2A	3415	1/1	0.94	0.36	57,57,57,57	0
55	MG	1a	1807	1/1	0.94	0.12	63,63,63,63	0
55	MG	1A	3804	1/1	0.94	0.12	24,24,24,24	0
55	MG	2A	3426	1/1	0.94	0.09	56,56,56,56	0
55	MG	1A	3473	1/1	0.94	0.68	36,36,36,36	0
55	MG	2D	301	1/1	0.94	0.17	31,31,31,31	0
55	MG	1A	3359	1/1	0.94	0.19	44,44,44,44	0
55	MG	2a	3207	1/1	0.94	0.11	53,53,53,53	0
55	MG	2a	3169	1/1	0.94	0.14	59,59,59,59	0
55	MG	2A	3117	1/1	0.94	0.55	38,38,38,38	0
55	MG	1A	3138	1/1	0.94	0.18	20,20,20,20	0
55	MG	2A	3368	1/1	0.94	0.33	54,54,54,54	0
55	MG	1A	3780	1/1	0.94	0.13	57,57,57,57	0
55	MG	2A	3205	1/1	0.94	0.19	51,51,51,51	0
55	MG	1A	4104	1/1	0.94	0.19	46,46,46,46	0
55	MG	1A	3469	1/1	0.94	0.14	49,49,49,49	0
55	MG	1A	3831	1/1	0.94	0.16	31,31,31,31	0
55	MG	1a	1784	1/1	0.94	0.13	58,58,58,58	0
55	MG	2A	3844	1/1	0.94	0.12	73,73,73,73	0
55	MG	1a	1769	1/1	0.94	0.07	71,71,71,71	0
55	MG	2V	202	1/1	0.94	1.88	53,53,53,53	0
55	MG	2a	3131	1/1	0.94	0.16	37,37,37,37	0
55	MG	1A	3627	1/1	0.94	0.16	41,41,41,41	0
55	MG	2A	3720	1/1	0.94	0.10	53,53,53,53	0
55	MG	2a	3053	1/1	0.94	0.06	42,42,42,42	0
55	MG	1A	3161	1/1	0.94	0.54	37,37,37,37	0
55	MG	1a	1728	1/1	0.94	0.16	50,50,50,50	0
55	MG	1A	3862	1/1	0.94	0.10	52,52,52,52	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
55	MG	2a	3058	1/1	0.94	0.68	52,52,52,52	0
55	MG	2A	3099	1/1	0.94	0.18	54,54,54,54	0
55	MG	2A	3047	1/1	0.94	0.52	53,53,53,53	0
55	MG	1A	3007	1/1	0.94	0.28	39,39,39,39	0
55	MG	1A	3277	1/1	0.94	0.11	38,38,38,38	0
55	MG	17	102	1/1	0.94	0.13	39,39,39,39	0
55	MG	2a	3132	1/1	0.94	0.15	45,45,45,45	0
55	MG	2a	3014	1/1	0.94	0.40	71,71,71,71	0
55	MG	1A	3721	1/1	0.94	0.15	27,27,27,27	0
55	MG	1A	3714	1/1	0.94	0.10	30,30,30,30	0
55	MG	2A	3440	1/1	0.94	0.68	50,50,50,50	0
55	MG	2F	304	1/1	0.94	0.20	51,51,51,51	0
55	MG	1A	3042	1/1	0.94	0.11	25,25,25,25	0
55	MG	1A	3444	1/1	0.94	0.07	43,43,43,43	0
55	MG	1A	3152	1/1	0.94	0.07	26,26,26,26	0
55	MG	2A	3207	1/1	0.94	0.59	50,50,50,50	0
55	MG	2A	3271	1/1	0.94	0.11	61,61,61,61	0
55	MG	1A	3020	1/1	0.94	0.11	22,22,22,22	0
55	MG	2A	3124	1/1	0.94	0.27	55,55,55,55	0
55	MG	1A	4027	1/1	0.94	0.16	21,21,21,21	0
55	MG	2A	3298	1/1	0.94	0.30	43,43,43,43	0
55	MG	1A	3674	1/1	0.94	0.15	14,14,14,14	0
55	MG	1A	3062	1/1	0.94	0.13	43,43,43,43	0
55	MG	2A	3301	1/1	0.94	0.22	62,62,62,62	0
55	MG	1A	3416	1/1	0.94	0.30	49,49,49,49	0
55	MG	1A	3995	1/1	0.94	0.14	53,53,53,53	0
55	MG	1A	4046	1/1	0.94	0.10	66,66,66,66	0
55	MG	1A	3546	1/1	0.94	0.26	31,31,31,31	0
55	MG	1A	3215	1/1	0.94	0.35	36,36,36,36	0
55	MG	2A	3315	1/1	0.94	0.46	69,69,69,69	0
55	MG	2A	3627	1/1	0.94	0.13	39,39,39,39	0
55	MG	2A	3235	1/1	0.94	0.32	53,53,53,53	0
55	MG	1A	3343	1/1	0.94	0.15	33,33,33,33	0
55	MG	1A	3274	1/1	0.94	0.25	37,37,37,37	0
55	MG	2A	3511	1/1	0.94	0.16	51,51,51,51	0
55	MG	1A	3290	1/1	0.94	0.23	48,48,48,48	0
55	MG	2A	3104	1/1	0.94	0.18	51,51,51,51	0
55	MG	1A	3517	1/1	0.94	0.34	50,50,50,50	0
55	MG	1A	3958	1/1	0.94	0.14	31,31,31,31	0
55	MG	1A	3144	1/1	0.94	0.28	39,39,39,39	0
55	MG	1A	3169	1/1	0.94	0.35	26,26,26,26	0
55	MG	1A	3516	1/1	0.94	0.10	69,69,69,69	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
55	MG	1A	3697	1/1	0.94	0.11	48,48,48,48	0
55	MG	1a	1623	1/1	0.94	0.10	50,50,50,50	0
55	MG	1A	3967	1/1	0.94	0.18	49,49,49,49	0
55	MG	1a	1799	1/1	0.94	0.14	68,68,68,68	0
55	MG	2a	3007	1/1	0.94	0.11	59,59,59,59	0
55	MG	2a	3002	1/1	0.95	0.06	60,60,60,60	0
55	MG	1a	1657	1/1	0.95	0.14	56,56,56,56	0
55	MG	2a	3049	1/1	0.95	0.14	67,67,67,67	0
55	MG	1A	3051	1/1	0.95	0.15	23,23,23,23	0
55	MG	1A	3345	1/1	0.95	0.59	25,25,25,25	0
55	MG	1A	3922	1/1	0.95	0.23	38,38,38,38	0
55	MG	1A	3011	1/1	0.95	0.12	39,39,39,39	0
55	MG	1A	3577	1/1	0.95	0.66	37,37,37,37	0
55	MG	2A	3733	1/1	0.95	0.24	49,49,49,49	0
55	MG	1A	3105	1/1	0.95	0.57	31,31,31,31	0
55	MG	2a	3015	1/1	0.95	0.29	55,55,55,55	0
55	MG	1a	1797	1/1	0.95	0.06	58,58,58,58	0
55	MG	2A	3628	1/1	0.95	0.10	33,33,33,33	0
55	MG	1A	3041	1/1	0.95	0.16	45,45,45,45	0
55	MG	1A	3582	1/1	0.95	0.20	32,32,32,32	0
55	MG	1A	3424	1/1	0.95	0.12	29,29,29,29	0
55	MG	1A	4012	1/1	0.95	0.15	47,47,47,47	0
55	MG	1A	3304	1/1	0.95	0.21	34,34,34,34	0
55	MG	1A	3079	1/1	0.95	0.49	34,34,34,34	0
55	MG	2A	3731	1/1	0.95	0.36	59,59,59,59	0
55	MG	2a	3006	1/1	0.95	0.13	57,57,57,57	0
55	MG	1A	3089	1/1	0.95	0.10	42,42,42,42	0
55	MG	2A	3759	1/1	0.95	0.16	46,46,46,46	0
55	MG	1A	3404	1/1	0.95	0.66	55,55,55,55	0
55	MG	1A	3701	1/1	0.95	0.13	18,18,18,18	0
55	MG	1A	3580	1/1	0.95	0.12	35,35,35,35	0
55	MG	1A	3822	1/1	0.95	0.19	21,21,21,21	0
55	MG	1A	3407	1/1	0.95	0.16	49,49,49,49	0
55	MG	2A	3565	1/1	0.95	0.14	44,44,44,44	0
55	MG	2a	3008	1/1	0.95	0.10	62,62,62,62	0
55	MG	1A	3167	1/1	0.95	0.32	37,37,37,37	0
55	MG	1A	3639	1/1	0.95	0.13	21,21,21,21	0
55	MG	1A	3571	1/1	0.95	0.09	32,32,32,32	0
55	MG	2A	3509	1/1	0.95	0.21	57,57,57,57	0
55	MG	1A	3091	1/1	0.95	0.25	49,49,49,49	0
55	MG	2A	3216	1/1	0.95	0.25	50,50,50,50	0
55	MG	1A	3827	1/1	0.95	0.05	42,42,42,42	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
55	MG	2Q	204	1/1	0.95	0.19	43,43,43,43	0
55	MG	1A	3861	1/1	0.95	0.25	48,48,48,48	0
55	MG	2A	3428	1/1	0.95	0.13	32,32,32,32	0
55	MG	1A	3722	1/1	0.95	0.13	33,33,33,33	0
55	MG	2A	3030	1/1	0.95	0.13	56,56,56,56	0
55	MG	2A	3812	1/1	0.95	0.09	55,55,55,55	0
55	MG	13	101	1/1	0.95	0.22	50,50,50,50	0
55	MG	2A	3358	1/1	0.95	0.12	37,37,37,37	0
55	MG	1a	1816	1/1	0.95	0.09	48,48,48,48	0
55	MG	1A	3157	1/1	0.95	0.49	26,26,26,26	0
55	MG	1A	3771	1/1	0.95	0.12	33,33,33,33	0
55	MG	1A	3058	1/1	0.95	0.09	35,35,35,35	0
55	MG	1A	3439	1/1	0.95	0.38	37,37,37,37	0
55	MG	2A	3249	1/1	0.95	0.11	59,59,59,59	0
55	MG	27	101	1/1	0.95	0.16	44,44,44,44	0
55	MG	1T	201	1/1	0.95	0.12	50,50,50,50	0
55	MG	2a	3204	1/1	0.95	0.17	55,55,55,55	0
55	MG	2a	3116	1/1	0.95	0.14	54,54,54,54	0
55	MG	1A	4071	1/1	0.95	0.15	20,20,20,20	0
55	MG	2A	3049	1/1	0.95	0.12	68,68,68,68	0
55	MG	1A	3360	1/1	0.95	0.14	41,41,41,41	0
55	MG	2A	3542	1/1	0.95	0.20	45,45,45,45	0
55	MG	2A	3686	1/1	0.95	0.09	49,49,49,49	0
55	MG	1A	3351	1/1	0.95	0.10	38,38,38,38	0
55	MG	2A	3480	1/1	0.95	0.22	37,37,37,37	0
55	MG	2A	3359	1/1	0.95	0.10	63,63,63,63	0
55	MG	2A	3538	1/1	0.95	0.18	32,32,32,32	0
55	MG	1A	3035	1/1	0.95	0.89	36,36,36,36	0
55	MG	1A	3380	1/1	0.95	0.71	38,38,38,38	0
55	MG	1A	3168	1/1	0.95	0.23	38,38,38,38	0
55	MG	1A	3440	1/1	0.95	0.61	39,39,39,39	0
55	MG	1a	1680	1/1	0.95	0.55	61,61,61,61	0
55	MG	1a	1753	1/1	0.95	0.07	67,67,67,67	0
55	MG	2a	3031	1/1	0.95	0.14	51,51,51,51	0
55	MG	1A	3398	1/1	0.95	0.57	29,29,29,29	0
55	MG	1A	3379	1/1	0.95	0.23	16,16,16,16	0
55	MG	1A	3916	1/1	0.95	0.13	68,68,68,68	0
55	MG	2A	3262	1/1	0.95	0.69	41,41,41,41	0
55	MG	2A	3277	1/1	0.95	0.17	50,50,50,50	0
55	MG	18	102	1/1	0.95	1.16	46,46,46,46	0
55	MG	2A	3579	1/1	0.95	0.09	55,55,55,55	0
55	MG	1a	1683	1/1	0.95	0.15	46,46,46,46	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
55	MG	2A	3851	1/1	0.95	0.09	49,49,49,49	0
55	MG	2A	3580	1/1	0.95	0.13	45,45,45,45	0
55	MG	1A	3589	1/1	0.95	0.34	28,28,28,28	0
55	MG	2A	3794	1/1	0.95	0.17	57,57,57,57	0
55	MG	2A	3436	1/1	0.95	0.15	55,55,55,55	0
55	MG	1A	3110	1/1	0.95	0.96	35,35,35,35	0
55	MG	2A	3510	1/1	0.95	0.11	36,36,36,36	0
55	MG	2A	3752	1/1	0.95	0.13	51,51,51,51	0
55	MG	1x	110	1/1	0.95	0.13	63,63,63,63	0
55	MG	1A	3281	1/1	0.95	0.13	36,36,36,36	0
55	MG	2a	3065	1/1	0.95	0.14	60,60,60,60	0
55	MG	2A	3394	1/1	0.95	0.15	37,37,37,37	0
55	MG	2a	3193	1/1	0.95	0.14	47,47,47,47	0
55	MG	2A	3420	1/1	0.95	0.10	38,38,38,38	0
55	MG	1A	3759	1/1	0.95	0.12	39,39,39,39	0
55	MG	1A	4100	1/1	0.95	0.19	37,37,37,37	0
55	MG	2a	3135	1/1	0.95	0.12	64,64,64,64	0
55	MG	1A	3769	1/1	0.95	0.10	42,42,42,42	0
55	MG	2A	3336	1/1	0.95	0.11	48,48,48,48	0
55	MG	2A	3010	1/1	0.95	0.11	30,30,30,30	0
55	MG	1A	3978	1/1	0.95	0.13	40,40,40,40	0
55	MG	2A	3787	1/1	0.95	0.85	66,66,66,66	0
55	MG	1A	3871	1/1	0.95	0.09	32,32,32,32	0
55	MG	1a	1684	1/1	0.95	0.19	49,49,49,49	0
55	MG	2A	3106	1/1	0.95	0.07	62,62,62,62	0
55	MG	1A	3938	1/1	0.95	0.56	28,28,28,28	0
55	MG	1A	3172	1/1	0.95	0.25	28,28,28,28	0
55	MG	1F	301	1/1	0.95	0.15	49,49,49,49	0
55	MG	2A	3491	1/1	0.95	0.22	49,49,49,49	0
55	MG	2A	3366	1/1	0.95	0.96	49,49,49,49	0
55	MG	2A	3313	1/1	0.95	0.18	68,68,68,68	0
55	MG	1A	3233	1/1	0.95	0.16	38,38,38,38	0
55	MG	2A	3736	1/1	0.95	0.26	58,58,58,58	0
55	MG	1A	4040	1/1	0.95	0.17	57,57,57,57	0
55	MG	1a	1666	1/1	0.95	0.25	69,69,69,69	0
55	MG	2T	203	1/1	0.95	0.11	35,35,35,35	0
55	MG	1A	3864	1/1	0.95	0.13	43,43,43,43	0
55	MG	1D	310	1/1	0.95	0.47	40,40,40,40	0
55	MG	1A	3806	1/1	0.95	0.09	28,28,28,28	0
55	MG	2B	218	1/1	0.95	0.28	59,59,59,59	0
55	MG	1A	3321	1/1	0.95	0.18	47,47,47,47	0
55	MG	1U	205	1/1	0.95	0.57	32,32,32,32	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
55	MG	1A	3191	1/1	0.95	0.49	29,29,29,29	0
55	MG	2A	3136	1/1	0.95	0.93	59,59,59,59	0
55	MG	2A	3776	1/1	0.95	0.43	59,59,59,59	0
55	MG	2A	3183	1/1	0.95	0.08	53,53,53,53	0
55	MG	2A	3393	1/1	0.95	0.16	40,40,40,40	0
55	MG	1A	4079	1/1	0.95	0.34	61,61,61,61	0
55	MG	2A	3037	1/1	0.95	0.12	35,35,35,35	0
55	MG	1A	3657	1/1	0.95	0.12	36,36,36,36	0
55	MG	1A	3789	1/1	0.95	0.23	37,37,37,37	0
55	MG	1A	3616	1/1	0.95	0.24	38,38,38,38	0
55	MG	2a	3200	1/1	0.95	0.14	47,47,47,47	0
55	MG	1A	3621	1/1	0.95	0.31	26,26,26,26	0
55	MG	2A	3078	1/1	0.95	0.09	43,43,43,43	0
55	MG	1A	4108	1/1	0.95	0.23	53,53,53,53	0
55	MG	2A	3549	1/1	0.95	0.14	35,35,35,35	0
55	MG	2A	3251	1/1	0.95	0.37	50,50,50,50	0
55	MG	2a	3202	1/1	0.95	0.78	76,76,76,76	0
55	MG	2A	3400	1/1	0.95	0.24	48,48,48,48	0
55	MG	1A	3608	1/1	0.95	0.27	23,23,23,23	0
55	MG	2a	3133	1/1	0.95	0.19	46,46,46,46	0
55	MG	2A	3326	1/1	0.95	0.67	46,46,46,46	0
55	MG	2A	3053	1/1	0.95	0.26	41,41,41,41	0
55	MG	2A	3031	1/1	0.95	0.13	45,45,45,45	0
55	MG	1R	202	1/1	0.95	0.20	35,35,35,35	0
55	MG	1A	3269	1/1	0.95	0.56	52,52,52,52	0
55	MG	1A	3474	1/1	0.95	0.35	39,39,39,39	0
55	MG	1A	3553	1/1	0.95	0.22	33,33,33,33	0
55	MG	1A	3057	1/1	0.95	0.11	21,21,21,21	0
55	MG	1A	3145	1/1	0.95	0.39	25,25,25,25	0
55	MG	1A	3550	1/1	0.95	0.22	41,41,41,41	0
55	MG	2A	3093	1/1	0.95	0.17	48,48,48,48	0
55	MG	1a	1697	1/1	0.95	0.13	35,35,35,35	0
55	MG	1A	3462	1/1	0.95	0.56	57,57,57,57	0
55	MG	1A	3238	1/1	0.95	0.40	31,31,31,31	0
55	MG	2A	3324	1/1	0.95	0.12	45,45,45,45	0
55	MG	1A	3908	1/1	0.95	0.19	40,40,40,40	0
55	MG	1A	3251	1/1	0.95	0.25	28,28,28,28	0
55	MG	1A	3339	1/1	0.95	0.71	42,42,42,42	0
55	MG	1a	1679	1/1	0.95	1.04	64,64,64,64	0
55	MG	1A	3511	1/1	0.95	0.53	48,48,48,48	0
55	MG	1A	3306	1/1	0.95	0.16	47,47,47,47	0
55	MG	1A	3245	1/1	0.95	0.10	57,57,57,57	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
55	MG	2A	3203	1/1	0.95	0.78	45,45,45,45	0
55	MG	2A	3079	1/1	0.95	0.13	35,35,35,35	0
55	MG	2A	3493	1/1	0.95	0.08	55,55,55,55	0
55	MG	2A	3682	1/1	0.95	0.14	59,59,59,59	0
55	MG	2A	3474	1/1	0.95	0.09	38,38,38,38	0
55	MG	1A	3125	1/1	0.95	0.87	30,30,30,30	0
55	MG	1A	3180	1/1	0.95	0.25	49,49,49,49	0
55	MG	1A	3187	1/1	0.95	0.37	29,29,29,29	0
55	MG	1A	3045	1/1	0.95	0.17	37,37,37,37	0
55	MG	1a	1739	1/1	0.95	0.29	47,47,47,47	0
55	MG	2A	3523	1/1	0.95	0.09	42,42,42,42	0
55	MG	2A	3537	1/1	0.95	0.24	54,54,54,54	0
55	MG	1G	203	1/1	0.95	0.10	50,50,50,50	0
55	MG	2a	3117	1/1	0.95	0.21	49,49,49,49	0
55	MG	2a	3123	1/1	0.95	0.12	46,46,46,46	0
55	MG	1A	3903	1/1	0.95	0.12	54,54,54,54	0
55	MG	2A	3073	1/1	0.95	0.49	43,43,43,43	0
55	MG	2A	3485	1/1	0.95	0.10	60,60,60,60	0
55	MG	1D	312	1/1	0.95	0.12	41,41,41,41	0
55	MG	1a	1774	1/1	0.95	0.08	34,34,34,34	0
55	MG	2A	3767	1/1	0.95	0.12	51,51,51,51	0
55	MG	1A	4031	1/1	0.95	0.14	33,33,33,33	0
55	MG	1A	3412	1/1	0.95	0.45	33,33,33,33	0
55	MG	1A	3171	1/1	0.95	0.26	31,31,31,31	0
55	MG	2a	3113	1/1	0.95	0.17	50,50,50,50	0
55	MG	2a	3112	1/1	0.95	0.15	58,58,58,58	0
55	MG	2A	3438	1/1	0.95	0.12	51,51,51,51	0
55	MG	2A	3739	1/1	0.95	0.22	43,43,43,43	0
55	MG	2A	3097	1/1	0.95	0.16	43,43,43,43	0
55	MG	1A	3668	1/1	0.95	0.20	49,49,49,49	0
55	MG	1A	3253	1/1	0.95	0.11	55,55,55,55	0
55	MG	2A	3140	1/1	0.95	0.30	40,40,40,40	0
55	MG	2a	3157	1/1	0.95	0.16	61,61,61,61	0
55	MG	1A	3718	1/1	0.95	0.09	19,19,19,19	0
55	MG	2a	3124	1/1	0.95	0.16	49,49,49,49	0
55	MG	2a	3196	1/1	0.95	0.12	52,52,52,52	0
55	MG	1A	3289	1/1	0.95	0.31	33,33,33,33	0
55	MG	1A	3584	1/1	0.95	0.57	33,33,33,33	0
55	MG	1A	3405	1/1	0.95	0.18	40,40,40,40	0
55	MG	1A	4039	1/1	0.95	0.12	38,38,38,38	0
55	MG	2a	3059	1/1	0.95	0.09	50,50,50,50	0
55	MG	1A	3666	1/1	0.95	0.16	22,22,22,22	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
55	MG	2A	3616	1/1	0.95	0.09	45,45,45,45	0
55	MG	2A	3801	1/1	0.95	0.16	51,51,51,51	0
55	MG	1A	3788	1/1	0.95	0.17	51,51,51,51	0
55	MG	1A	3942	1/1	0.95	0.11	34,34,34,34	0
55	MG	2A	3700	1/1	0.95	0.14	51,51,51,51	0
55	MG	1A	3619	1/1	0.95	0.10	32,32,32,32	0
55	MG	2A	3825	1/1	0.95	0.07	42,42,42,42	0
55	MG	1A	3197	1/1	0.95	0.53	42,42,42,42	0
55	MG	1O	203	1/1	0.95	0.17	35,35,35,35	0
55	MG	1A	4002	1/1	0.95	0.11	60,60,60,60	0
55	MG	1A	3422	1/1	0.95	0.29	41,41,41,41	0
55	MG	1X	106	1/1	0.95	0.24	47,47,47,47	0
55	MG	2A	3067	1/1	0.95	0.57	53,53,53,53	0
55	MG	2A	3065	1/1	0.95	0.18	48,48,48,48	0
55	MG	1A	3802	1/1	0.95	0.08	32,32,32,32	0
55	MG	2A	3398	1/1	0.95	0.11	33,33,33,33	0
55	MG	1A	3798	1/1	0.95	0.22	29,29,29,29	0
55	MG	1A	3365	1/1	0.95	0.09	48,48,48,48	0
55	MG	1A	3129	1/1	0.95	0.17	39,39,39,39	0
55	MG	1A	4112	1/1	0.95	0.11	56,56,56,56	0
55	MG	1A	3724	1/1	0.95	0.16	12,12,12,12	0
55	MG	2A	3508	1/1	0.95	0.24	50,50,50,50	0
55	MG	2A	3783	1/1	0.95	0.15	72,72,72,72	0
55	MG	2A	3590	1/1	0.95	0.18	53,53,53,53	0
55	MG	2A	3022	1/1	0.95	0.32	54,54,54,54	0
55	MG	1A	3921	1/1	0.95	0.16	45,45,45,45	0
55	MG	2A	3469	1/1	0.95	0.23	48,48,48,48	0
55	MG	2a	3077	1/1	0.95	0.09	39,39,39,39	0
55	MG	25	101	1/1	0.95	0.18	44,44,44,44	0
55	MG	1A	3247	1/1	0.95	0.16	57,57,57,57	0
55	MG	2A	3051	1/1	0.95	0.10	53,53,53,53	0
55	MG	2a	3189	1/1	0.95	0.11	62,62,62,62	0
55	MG	1A	3860	1/1	0.95	0.10	38,38,38,38	0
55	MG	1a	1613	1/1	0.95	0.15	37,37,37,37	0
55	MG	1A	3322	1/1	0.95	0.28	43,43,43,43	0
55	MG	1E	311	1/1	0.95	0.15	43,43,43,43	0
55	MG	1a	1685	1/1	0.95	0.21	58,58,58,58	0
55	MG	1A	3565	1/1	0.95	0.67	40,40,40,40	0
55	MG	1A	3832	1/1	0.95	0.45	32,32,32,32	0
55	MG	1A	3366	1/1	0.95	0.28	39,39,39,39	0
55	MG	1A	3389	1/1	0.95	0.53	48,48,48,48	0
55	MG	2a	3079	1/1	0.95	0.11	61,61,61,61	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
55	MG	2a	3141	1/1	0.95	0.24	66,66,66,66	0
55	MG	2A	3002	1/1	0.95	0.08	53,53,53,53	0
55	MG	2a	3183	1/1	0.95	0.15	53,53,53,53	0
55	MG	1A	3479	1/1	0.95	0.23	33,33,33,33	0
55	MG	1A	3330	1/1	0.95	0.17	34,34,34,34	0
55	MG	2A	3602	1/1	0.95	0.09	65,65,65,65	0
55	MG	2A	3451	1/1	0.95	1.38	51,51,51,51	0
55	MG	1A	3150	1/1	0.95	0.34	25,25,25,25	0
55	MG	2W	202	1/1	0.95	0.10	52,52,52,52	0
55	MG	1A	3053	1/1	0.95	0.24	33,33,33,33	0
55	MG	1A	3790	1/1	0.95	0.18	16,16,16,16	0
55	MG	2a	3151	1/1	0.95	0.12	69,69,69,69	0
55	MG	1a	1766	1/1	0.95	0.23	49,49,49,49	0
55	MG	1E	305	1/1	0.95	0.12	30,30,30,30	0
55	MG	2A	3560	1/1	0.95	0.12	30,30,30,30	0
55	MG	2A	3445	1/1	0.95	0.15	52,52,52,52	0
55	MG	1A	3050	1/1	0.95	0.21	36,36,36,36	0
55	MG	2a	3127	1/1	0.95	0.19	60,60,60,60	0
55	MG	2A	3009	1/1	0.95	0.23	40,40,40,40	0
55	MG	1A	3617	1/1	0.95	0.14	29,29,29,29	0
55	MG	1a	1779	1/1	0.95	0.11	49,49,49,49	0
55	MG	1a	1633	1/1	0.96	0.10	48,48,48,48	0
55	MG	1x	104	1/1	0.96	0.21	41,41,41,41	0
55	MG	1A	3325	1/1	0.96	0.27	48,48,48,48	0
55	MG	1x	108	1/1	0.96	0.12	55,55,55,55	0
55	MG	2a	3068	1/1	0.96	0.08	50,50,50,50	0
55	MG	1A	3243	1/1	0.96	0.14	41,41,41,41	0
55	MG	1A	3583	1/1	0.96	0.46	36,36,36,36	0
55	MG	2A	3526	1/1	0.96	0.32	60,60,60,60	0
55	MG	2a	3009	1/1	0.96	0.52	59,59,59,59	0
55	MG	2A	3820	1/1	0.96	0.12	33,33,33,33	0
55	MG	1A	3094	1/1	0.96	0.14	16,16,16,16	0
55	MG	1a	1634	1/1	0.96	0.09	58,58,58,58	0
55	MG	1W	204	1/1	0.96	0.35	38,38,38,38	0
55	MG	1A	3770	1/1	0.96	0.14	37,37,37,37	0
55	MG	1A	3889	1/1	0.96	0.10	43,43,43,43	0
55	MG	1F	305	1/1	0.96	0.22	41,41,41,41	0
55	MG	1A	3273	1/1	0.96	0.33	36,36,36,36	0
55	MG	2A	3338	1/1	0.96	0.12	52,52,52,52	0
55	MG	2A	3164	1/1	0.96	0.22	57,57,57,57	0
55	MG	2A	3372	1/1	0.96	1.16	59,59,59,59	0
55	MG	2A	3039	1/1	0.96	0.12	49,49,49,49	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
55	MG	1A	3437	1/1	0.96	0.20	36,36,36,36	0
55	MG	2a	3144	1/1	0.96	0.09	57,57,57,57	0
55	MG	2A	3515	1/1	0.96	0.28	57,57,57,57	0
55	MG	1A	3952	1/1	0.96	0.15	45,45,45,45	0
55	MG	1A	3868	1/1	0.96	0.10	57,57,57,57	0
55	MG	1A	3155	1/1	0.96	0.47	32,32,32,32	0
55	MG	1E	303	1/1	0.96	0.62	27,27,27,27	0
55	MG	2A	3721	1/1	0.96	0.15	48,48,48,48	0
55	MG	1A	3545	1/1	0.96	0.48	31,31,31,31	0
55	MG	1A	3773	1/1	0.96	0.40	29,29,29,29	0
55	MG	1a	1604	1/1	0.96	0.08	65,65,65,65	0
55	MG	2A	3766	1/1	0.96	0.12	47,47,47,47	0
55	MG	1A	3314	1/1	0.96	0.13	27,27,27,27	0
55	MG	2A	3754	1/1	0.96	0.24	48,48,48,48	0
55	MG	2A	3281	1/1	0.96	0.28	42,42,42,42	0
55	MG	1A	4051	1/1	0.96	0.05	41,41,41,41	0
55	MG	1a	1778	1/1	0.96	0.08	43,43,43,43	0
55	MG	2A	3797	1/1	0.96	0.11	35,35,35,35	0
55	MG	1A	3578	1/1	0.96	0.11	33,33,33,33	0
55	MG	2A	3243	1/1	0.96	0.20	39,39,39,39	0
55	MG	1A	4006	1/1	0.96	0.09	30,30,30,30	0
55	MG	1A	4017	1/1	0.96	0.10	20,20,20,20	0
55	MG	1A	3607	1/1	0.96	0.22	33,33,33,33	0
55	MG	1A	3597	1/1	0.96	0.15	45,45,45,45	0
55	MG	1a	1796	1/1	0.96	0.21	69,69,69,69	0
55	MG	1Z	302	1/1	0.96	0.13	43,43,43,43	0
55	MG	1A	3175	1/1	0.96	0.15	20,20,20,20	0
55	MG	1A	3609	1/1	0.96	0.29	27,27,27,27	0
55	MG	1A	3064	1/1	0.96	0.13	40,40,40,40	0
55	MG	1B	224	1/1	0.96	0.13	53,53,53,53	0
55	MG	2A	3588	1/1	0.96	0.14	49,49,49,49	0
55	MG	1A	3327	1/1	0.96	0.30	41,41,41,41	0
55	MG	2A	3855	1/1	0.96	0.19	52,52,52,52	0
55	MG	2A	3059	1/1	0.96	0.17	42,42,42,42	0
55	MG	1A	4075	1/1	0.96	0.11	58,58,58,58	0
55	MG	2A	3171	1/1	0.96	0.41	45,45,45,45	0
55	MG	1A	3641	1/1	0.96	0.16	23,23,23,23	0
55	MG	1a	1734	1/1	0.96	0.09	43,43,43,43	0
55	MG	1A	3425	1/1	0.96	0.72	53,53,53,53	0
55	MG	1A	3618	1/1	0.96	0.23	23,23,23,23	0
55	MG	1A	3842	1/1	0.96	0.62	35,35,35,35	0
55	MG	1Y	202	1/1	0.96	0.27	45,45,45,45	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
55	MG	1a	1767	1/1	0.96	0.07	32,32,32,32	0
55	MG	1A	3200	1/1	0.96	0.15	22,22,22,22	0
55	MG	2A	3816	1/1	0.96	0.16	54,54,54,54	0
55	MG	1A	3715	1/1	0.96	0.25	40,40,40,40	0
55	MG	2A	3409	1/1	0.96	0.24	45,45,45,45	0
55	MG	2A	3215	1/1	0.96	0.09	69,69,69,69	0
55	MG	2A	3347	1/1	0.96	0.37	46,46,46,46	0
55	MG	1A	3651	1/1	0.96	0.23	29,29,29,29	0
55	MG	1A	3448	1/1	0.96	0.75	40,40,40,40	0
56	ZN	2n	501	1/1	0.96	0.08	100,100,100,100	0
55	MG	2A	3772	1/1	0.96	0.11	80,80,80,80	0
55	MG	2A	3245	1/1	0.96	0.10	64,64,64,64	0
55	MG	1A	3787	1/1	0.96	0.16	13,13,13,13	0
55	MG	2A	3305	1/1	0.96	0.18	53,53,53,53	0
55	MG	1A	3740	1/1	0.96	0.15	34,34,34,34	0
55	MG	1A	3613	1/1	0.96	0.57	32,32,32,32	0
55	MG	2A	3841	1/1	0.96	0.07	57,57,57,57	0
55	MG	1A	3968	1/1	0.96	0.10	40,40,40,40	0
55	MG	1A	3228	1/1	0.96	0.16	44,44,44,44	0
55	MG	2A	3719	1/1	0.96	0.21	70,70,70,70	0
55	MG	1A	3907	1/1	0.96	0.16	28,28,28,28	0
55	MG	1A	3377	1/1	0.96	0.16	37,37,37,37	0
55	MG	1A	3681	1/1	0.96	0.12	34,34,34,34	0
55	MG	2A	3757	1/1	0.96	0.30	50,50,50,50	0
55	MG	2a	3074	1/1	0.96	0.14	47,47,47,47	0
55	MG	1A	3660	1/1	0.96	0.20	22,22,22,22	0
55	MG	2A	3502	1/1	0.96	0.12	48,48,48,48	0
55	MG	1A	4025	1/1	0.96	0.13	25,25,25,25	0
55	MG	1G	201	1/1	0.96	0.20	39,39,39,39	0
55	MG	2a	3084	1/1	0.96	0.18	69,69,69,69	0
55	MG	1a	1762	1/1	0.96	0.10	54,54,54,54	0
55	MG	1A	3719	1/1	0.96	0.09	60,60,60,60	0
55	MG	2A	3007	1/1	0.96	0.19	43,43,43,43	0
55	MG	1A	4070	1/1	0.96	0.15	19,19,19,19	0
55	MG	1U	206	1/1	0.96	0.40	28,28,28,28	0
55	MG	1A	3415	1/1	0.96	0.35	44,44,44,44	0
55	MG	1A	3052	1/1	0.96	0.23	21,21,21,21	0
55	MG	1a	1695	1/1	0.96	0.10	39,39,39,39	0
55	MG	1a	1830	1/1	0.96	0.10	59,59,59,59	0
55	MG	2A	3040	1/1	0.96	0.12	59,59,59,59	0
55	MG	1A	3232	1/1	0.96	0.36	23,23,23,23	0
55	MG	2A	3149	1/1	0.96	0.08	61,61,61,61	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
55	MG	2A	3636	1/1	0.96	0.11	57,57,57,57	0
55	MG	2a	3016	1/1	0.96	0.34	46,46,46,46	0
55	MG	1A	3559	1/1	0.96	0.45	31,31,31,31	0
55	MG	2A	3662	1/1	0.96	0.47	63,63,63,63	0
55	MG	2l	203	1/1	0.96	0.11	47,47,47,47	0
55	MG	2A	3667	1/1	0.96	0.11	46,46,46,46	0
55	MG	2A	3837	1/1	0.96	0.17	48,48,48,48	0
55	MG	1A	3261	1/1	0.96	0.12	33,33,33,33	0
55	MG	1A	3664	1/1	0.96	0.12	18,18,18,18	0
55	MG	2a	3102	1/1	0.96	0.13	67,67,67,67	0
55	MG	1a	1760	1/1	0.96	0.15	39,39,39,39	0
55	MG	1A	3649	1/1	0.96	0.16	21,21,21,21	0
55	MG	1A	3104	1/1	0.96	0.49	31,31,31,31	0
55	MG	1a	1720	1/1	0.96	0.29	41,41,41,41	0
55	MG	1A	3843	1/1	0.96	0.11	44,44,44,44	0
55	MG	2F	303	1/1	0.96	0.18	45,45,45,45	0
55	MG	1A	3368	1/1	0.96	0.22	40,40,40,40	0
55	MG	2A	3638	1/1	0.96	0.20	53,53,53,53	0
55	MG	1A	3037	1/1	0.96	0.30	28,28,28,28	0
55	MG	1A	3459	1/1	0.96	0.94	37,37,37,37	0
55	MG	2x	103	1/1	0.96	0.19	63,63,63,63	0
55	MG	2A	3395	1/1	0.96	0.15	35,35,35,35	0
55	MG	1a	1687	1/1	0.96	0.23	52,52,52,52	0
55	MG	2A	3060	1/1	0.96	0.18	38,38,38,38	0
55	MG	1A	3747	1/1	0.96	0.09	34,34,34,34	0
55	MG	2a	3199	1/1	0.96	0.26	69,69,69,69	0
55	MG	1A	3061	1/1	0.96	0.15	31,31,31,31	0
55	MG	2A	3815	1/1	0.96	0.07	40,40,40,40	0
55	MG	1A	3917	1/1	0.96	0.13	43,43,43,43	0
55	MG	1A	3702	1/1	0.96	0.17	14,14,14,14	0
55	MG	1A	3670	1/1	0.96	0.09	46,46,46,46	0
55	MG	1A	3675	1/1	0.96	0.10	14,14,14,14	0
55	MG	2A	3555	1/1	0.96	0.09	44,44,44,44	0
55	MG	2A	3206	1/1	0.96	0.42	38,38,38,38	0
55	MG	1A	3342	1/1	0.96	0.44	28,28,28,28	0
55	MG	2A	3674	1/1	0.96	0.16	57,57,57,57	0
55	MG	2A	3354	1/1	0.96	0.17	28,28,28,28	0
55	MG	2A	3606	1/1	0.96	0.17	39,39,39,39	0
55	MG	1A	3149	1/1	0.96	0.75	30,30,30,30	0
55	MG	2A	3019	1/1	0.96	0.37	53,53,53,53	0
55	MG	2A	3160	1/1	0.96	0.17	30,30,30,30	0
55	MG	1A	3028	1/1	0.96	0.10	65,65,65,65	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
55	MG	2e	201	1/1	0.96	0.09	80,80,80,80	0
55	MG	1x	112	1/1	0.96	0.08	64,64,64,64	0
55	MG	1A	4080	1/1	0.96	0.17	40,40,40,40	0
55	MG	1A	3451	1/1	0.96	0.33	36,36,36,36	0
55	MG	2A	3810	1/1	0.96	0.14	38,38,38,38	0
55	MG	2a	3054	1/1	0.96	0.14	46,46,46,46	0
55	MG	1a	1787	1/1	0.96	0.34	73,73,73,73	0
55	MG	2A	3100	1/1	0.96	0.08	27,27,27,27	0
55	MG	2a	3192	1/1	0.96	0.12	55,55,55,55	0
55	MG	1F	307	1/1	0.96	0.15	33,33,33,33	0
55	MG	1a	1742	1/1	0.96	0.18	35,35,35,35	0
55	MG	1A	3019	1/1	0.96	0.10	28,28,28,28	0
55	MG	1D	311	1/1	0.96	0.70	30,30,30,30	0
55	MG	2N	202	1/1	0.96	0.14	48,48,48,48	0
55	MG	2A	3304	1/1	0.96	1.10	51,51,51,51	0
55	MG	1A	3034	1/1	0.96	0.29	24,24,24,24	0
55	MG	1A	3119	1/1	0.96	0.33	30,30,30,30	0
55	MG	1A	3151	1/1	0.96	0.60	38,38,38,38	0
55	MG	1A	3563	1/1	0.96	0.34	36,36,36,36	0
55	MG	1A	4092	1/1	0.96	0.11	41,41,41,41	0
55	MG	1A	4087	1/1	0.96	0.13	37,37,37,37	0
55	MG	2A	3692	1/1	0.96	0.13	54,54,54,54	0
55	MG	1a	1605	1/1	0.96	0.14	60,60,60,60	0
55	MG	2a	3187	1/1	0.96	0.11	75,75,75,75	0
55	MG	2A	3370	1/1	0.96	0.20	63,63,63,63	0
55	MG	1A	3954	1/1	0.96	0.17	52,52,52,52	0
55	MG	1a	1736	1/1	0.96	0.22	39,39,39,39	0
55	MG	1A	3074	1/1	0.96	0.36	24,24,24,24	0
55	MG	1A	3696	1/1	0.96	0.14	39,39,39,39	0
55	MG	1A	3072	1/1	0.96	0.12	17,17,17,17	0
55	MG	1A	3960	1/1	0.96	0.16	36,36,36,36	0
55	MG	15	104	1/1	0.96	0.16	36,36,36,36	0
55	MG	1A	3939	1/1	0.96	0.13	49,49,49,49	0
55	MG	1A	3141	1/1	0.96	0.26	32,32,32,32	0
55	MG	1A	3280	1/1	0.96	0.13	45,45,45,45	0
55	MG	1a	1622	1/1	0.96	0.11	44,44,44,44	0
55	MG	1A	3008	1/1	0.96	0.11	25,25,25,25	0
55	MG	2O	202	1/1	0.96	0.11	46,46,46,46	0
55	MG	1A	3782	1/1	0.96	0.23	38,38,38,38	0
55	MG	1X	103	1/1	0.96	0.34	37,37,37,37	0
55	MG	2A	3574	1/1	0.96	0.19	48,48,48,48	0
55	MG	1A	3068	1/1	0.96	0.11	34,34,34,34	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
55	MG	1V	201	1/1	0.96	0.54	26,26,26,26	0
55	MG	2B	209	1/1	0.96	0.12	57,57,57,57	0
55	MG	2A	3054	1/1	0.96	0.18	47,47,47,47	0
55	MG	1A	3225	1/1	0.96	0.15	26,26,26,26	0
55	MG	1A	3953	1/1	0.96	0.17	19,19,19,19	0
55	MG	2A	3634	1/1	0.96	0.40	52,52,52,52	0
55	MG	1A	3433	1/1	0.96	0.15	44,44,44,44	0
55	MG	2A	3223	1/1	0.96	0.33	52,52,52,52	0
55	MG	1A	4097	1/1	0.96	0.14	35,35,35,35	0
55	MG	1A	3845	1/1	0.96	0.19	29,29,29,29	0
55	MG	1A	3009	1/1	0.96	0.13	28,28,28,28	0
55	MG	1A	3836	1/1	0.96	0.14	40,40,40,40	0
55	MG	1A	3925	1/1	0.96	0.15	49,49,49,49	0
55	MG	2A	3386	1/1	0.96	0.21	53,53,53,53	0
55	MG	2A	3818	1/1	0.96	0.41	41,41,41,41	0
55	MG	1a	1833	1/1	0.96	0.15	61,61,61,61	0
55	MG	1A	3840	1/1	0.96	0.20	28,28,28,28	0
55	MG	1Y	204	1/1	0.96	0.31	49,49,49,49	0
55	MG	1A	3498	1/1	0.96	0.24	24,24,24,24	0
55	MG	2A	3385	1/1	0.96	0.20	37,37,37,37	0
55	MG	2a	3163	1/1	0.96	0.14	60,60,60,60	0
56	ZN	16	102	1/1	0.96	0.23	41,41,41,41	0
55	MG	2a	3119	1/1	0.96	0.09	62,62,62,62	0
55	MG	2A	3122	1/1	0.96	0.18	32,32,32,32	0
55	MG	1A	3941	1/1	0.96	0.10	54,54,54,54	0
55	MG	2A	3848	1/1	0.96	0.17	55,55,55,55	0
55	MG	2A	3829	1/1	0.96	0.21	40,40,40,40	0
55	MG	1A	3214	1/1	0.96	0.45	36,36,36,36	0
55	MG	1A	3746	1/1	0.96	0.15	39,39,39,39	0
55	MG	11	103	1/1	0.96	0.18	35,35,35,35	0
55	MG	1A	3819	1/1	0.96	0.11	52,52,52,52	0
55	MG	2A	3804	1/1	0.96	0.21	46,46,46,46	0
55	MG	13	103	1/1	0.96	0.15	41,41,41,41	0
56	ZN	14	501	1/1	0.96	0.05	109,109,109,109	0
55	MG	2A	3684	1/1	0.96	0.20	54,54,54,54	0
55	MG	2A	3195	1/1	0.96	0.12	39,39,39,39	0
55	MG	1A	3112	1/1	0.96	0.45	38,38,38,38	0
55	MG	1Q	205	1/1	0.96	0.22	36,36,36,36	0
55	MG	2A	3483	1/1	0.96	0.20	34,34,34,34	0
55	MG	1A	3300	1/1	0.96	0.10	28,28,28,28	0
55	MG	1A	3573	1/1	0.96	0.22	28,28,28,28	0
55	MG	1A	3699	1/1	0.96	0.17	21,21,21,21	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
55	MG	2A	3728	1/1	0.96	0.25	53,53,53,53	0
55	MG	2A	3612	1/1	0.96	0.29	53,53,53,53	0
55	MG	1a	1637	1/1	0.96	0.11	59,59,59,59	0
55	MG	2A	3256	1/1	0.96	0.11	47,47,47,47	0
55	MG	1A	3970	1/1	0.96	0.34	71,71,71,71	0
55	MG	1A	3093	1/1	0.96	0.10	41,41,41,41	0
55	MG	1A	3971	1/1	0.96	0.22	42,42,42,42	0
55	MG	1a	1658	1/1	0.96	0.06	76,76,76,76	0
55	MG	2A	3275	1/1	0.96	0.34	64,64,64,64	0
55	MG	2A	3263	1/1	0.96	0.77	50,50,50,50	0
55	MG	1A	4064	1/1	0.96	0.13	39,39,39,39	0
55	MG	2A	3300	1/1	0.96	0.09	53,53,53,53	0
55	MG	1A	3830	1/1	0.96	0.11	31,31,31,31	0
55	MG	1A	4035	1/1	0.96	0.13	57,57,57,57	0
55	MG	2a	3154	1/1	0.96	0.19	47,47,47,47	0
55	MG	2A	3046	1/1	0.96	0.11	55,55,55,55	0
55	MG	1A	3529	1/1	0.96	0.16	42,42,42,42	0
55	MG	2A	3444	1/1	0.96	0.11	18,18,18,18	0
55	MG	1A	3543	1/1	0.96	0.81	48,48,48,48	0
55	MG	1W	203	1/1	0.96	0.20	29,29,29,29	0
55	MG	1A	3463	1/1	0.96	0.65	48,48,48,48	0
55	MG	2A	3668	1/1	0.96	0.10	36,36,36,36	0
55	MG	1A	3447	1/1	0.96	0.45	42,42,42,42	0
55	MG	2A	3534	1/1	0.96	0.33	40,40,40,40	0
55	MG	1A	3955	1/1	0.96	0.12	50,50,50,50	0
55	MG	1A	3653	1/1	0.96	0.09	40,40,40,40	0
55	MG	2A	3633	1/1	0.96	0.06	50,50,50,50	0
55	MG	2a	3195	1/1	0.96	0.08	62,62,62,62	0
55	MG	2A	3623	1/1	0.96	0.18	26,26,26,26	0
55	MG	1A	3890	1/1	0.96	0.16	52,52,52,52	0
55	MG	2A	3531	1/1	0.96	0.16	31,31,31,31	0
55	MG	1A	4058	1/1	0.96	0.15	38,38,38,38	0
55	MG	2A	3713	1/1	0.96	0.27	52,52,52,52	0
55	MG	2A	3008	1/1	0.96	0.56	46,46,46,46	0
55	MG	2A	3134	1/1	0.96	0.31	45,45,45,45	0
55	MG	2A	3396	1/1	0.96	0.23	47,47,47,47	0
55	MG	1A	3966	1/1	0.96	0.06	57,57,57,57	0
55	MG	1A	3894	1/1	0.96	0.21	26,26,26,26	0
55	MG	1A	3980	1/1	0.96	0.12	34,34,34,34	0
55	MG	2A	3083	1/1	0.96	0.22	35,35,35,35	0
55	MG	1D	308	1/1	0.96	0.95	35,35,35,35	0
55	MG	2A	3670	1/1	0.96	0.14	49,49,49,49	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
55	MG	1A	3756	1/1	0.96	0.14	49,49,49,49	0
55	MG	1A	3793	1/1	0.96	0.15	42,42,42,42	0
55	MG	1A	3561	1/1	0.96	0.53	38,38,38,38	0
55	MG	1A	3672	1/1	0.96	0.18	37,37,37,37	0
55	MG	2A	3233	1/1	0.96	0.22	54,54,54,54	0
55	MG	2A	3744	1/1	0.96	0.09	61,61,61,61	0
55	MG	1a	1690	1/1	0.96	0.08	28,28,28,28	0
55	MG	2a	3104	1/1	0.96	0.11	64,64,64,64	0
55	MG	2A	3194	1/1	0.96	0.07	28,28,28,28	0
55	MG	1A	3823	1/1	0.96	0.18	17,17,17,17	0
55	MG	1A	3712	1/1	0.96	0.14	41,41,41,41	0
55	MG	1A	3637	1/1	0.96	0.08	39,39,39,39	0
55	MG	1E	304	1/1	0.96	0.48	37,37,37,37	0
55	MG	1A	3456	1/1	0.96	0.17	32,32,32,32	0
55	MG	2A	3619	1/1	0.96	0.17	48,48,48,48	0
55	MG	1A	3957	1/1	0.96	0.15	28,28,28,28	0
55	MG	2a	3080	1/1	0.96	0.18	51,51,51,51	0
55	MG	1A	4115	1/1	0.96	0.10	59,59,59,59	0
55	MG	2a	3114	1/1	0.96	0.17	56,56,56,56	0
55	MG	2A	3594	1/1	0.96	0.21	49,49,49,49	0
55	MG	1Y	201	1/1	0.96	0.14	48,48,48,48	0
55	MG	2A	3629	1/1	0.96	0.15	36,36,36,36	0
55	MG	1A	3001	1/1	0.96	0.16	33,33,33,33	0
55	MG	2A	3582	1/1	0.96	0.05	56,56,56,56	0
55	MG	1A	3562	1/1	0.96	0.12	17,17,17,17	0
55	MG	2A	3126	1/1	0.96	0.18	34,34,34,34	0
55	MG	1A	4009	1/1	0.96	0.22	30,30,30,30	0
55	MG	1A	3598	1/1	0.96	0.15	47,47,47,47	0
55	MG	10	101	1/1	0.96	0.23	31,31,31,31	0
55	MG	2A	3620	1/1	0.96	0.14	38,38,38,38	0
55	MG	2a	3110	1/1	0.96	0.13	61,61,61,61	0
55	MG	1A	3678	1/1	0.96	0.23	20,20,20,20	0
55	MG	2A	3379	1/1	0.96	0.06	45,45,45,45	0
55	MG	10	102	1/1	0.96	0.26	37,37,37,37	0
55	MG	1A	4016	1/1	0.96	0.19	22,22,22,22	0
55	MG	1a	1696	1/1	0.96	0.20	55,55,55,55	0
55	MG	2A	3503	1/1	0.96	0.10	39,39,39,39	0
55	MG	1A	3865	1/1	0.96	0.09	45,45,45,45	0
55	MG	1a	1777	1/1	0.96	0.08	45,45,45,45	0
55	MG	1A	4053	1/1	0.96	0.10	29,29,29,29	0
55	MG	2a	3042	1/1	0.96	0.07	54,54,54,54	0
55	MG	2a	3186	1/1	0.96	0.18	50,50,50,50	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
55	MG	1B	227	1/1	0.96	0.15	57,57,57,57	0
55	MG	2A	3664	1/1	0.96	0.07	58,58,58,58	0
55	MG	2A	3180	1/1	0.96	0.19	44,44,44,44	0
55	MG	1A	3572	1/1	0.96	0.14	32,32,32,32	0
55	MG	2A	3651	1/1	0.96	0.29	50,50,50,50	0
55	MG	2a	3036	1/1	0.97	0.59	43,43,43,43	0
55	MG	1a	1756	1/1	0.97	0.14	41,41,41,41	0
55	MG	2A	3246	1/1	0.97	0.32	51,51,51,51	0
55	MG	1A	3222	1/1	0.97	0.40	28,28,28,28	0
55	MG	2A	3139	1/1	0.97	0.23	59,59,59,59	0
55	MG	2a	3178	1/1	0.97	0.12	43,43,43,43	0
55	MG	1a	1627	1/1	0.97	0.07	52,52,52,52	0
55	MG	1A	3910	1/1	0.97	0.17	41,41,41,41	0
55	MG	1A	3146	1/1	0.97	0.36	21,21,21,21	0
55	MG	1A	3581	1/1	0.97	0.58	41,41,41,41	0
55	MG	2A	3006	1/1	0.97	0.15	56,56,56,56	0
55	MG	1A	3838	1/1	0.97	0.14	40,40,40,40	0
55	MG	2A	3319	1/1	0.97	0.26	62,62,62,62	0
55	MG	1W	205	1/1	0.97	0.21	35,35,35,35	0
55	MG	2A	3186	1/1	0.97	0.09	40,40,40,40	0
55	MG	1A	3085	1/1	0.97	0.12	24,24,24,24	0
55	MG	2a	3072	1/1	0.97	0.11	62,62,62,62	0
55	MG	1A	3026	1/1	0.97	0.34	32,32,32,32	0
55	MG	2A	3167	1/1	0.97	0.42	68,68,68,68	0
55	MG	1A	3139	1/1	0.97	0.25	37,37,37,37	0
55	MG	2a	3146	1/1	0.97	0.26	38,38,38,38	0
55	MG	2A	3593	1/1	0.97	0.12	68,68,68,68	0
55	MG	1a	1648	1/1	0.97	0.11	36,36,36,36	0
55	MG	1a	1620	1/1	0.97	0.05	46,46,46,46	0
55	MG	1A	3071	1/1	0.97	0.14	28,28,28,28	0
55	MG	1A	3765	1/1	0.97	0.18	34,34,34,34	0
55	MG	1A	3728	1/1	0.97	0.15	31,31,31,31	0
55	MG	2A	3127	1/1	0.97	0.20	44,44,44,44	0
55	MG	1A	3821	1/1	0.97	0.18	21,21,21,21	0
55	MG	1A	3884	1/1	0.97	0.41	28,28,28,28	0
55	MG	2A	3471	1/1	0.97	0.10	21,21,21,21	0
55	MG	1A	3673	1/1	0.97	0.26	40,40,40,40	0
55	MG	2A	3214	1/1	0.97	0.11	43,43,43,43	0
55	MG	1A	3826	1/1	0.97	0.09	35,35,35,35	0
55	MG	1A	3317	1/1	0.97	0.17	36,36,36,36	0
55	MG	2A	3553	1/1	0.97	0.18	42,42,42,42	0
55	MG	2a	3099	1/1	0.97	0.10	66,66,66,66	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
55	MG	2A	3585	1/1	0.97	0.13	34,34,34,34	0
55	MG	1A	4094	1/1	0.97	0.12	14,14,14,14	0
55	MG	1X	104	1/1	0.97	0.17	40,40,40,40	0
55	MG	2A	3838	1/1	0.97	0.09	46,46,46,46	0
55	MG	1A	3121	1/1	0.97	0.41	29,29,29,29	0
55	MG	2A	3788	1/1	0.97	0.12	73,73,73,73	0
55	MG	2A	3063	1/1	0.97	0.20	50,50,50,50	0
55	MG	1A	3076	1/1	0.97	0.16	40,40,40,40	0
55	MG	1A	3003	1/1	0.97	0.13	22,22,22,22	0
55	MG	2A	3544	1/1	0.97	0.23	41,41,41,41	0
55	MG	1A	3396	1/1	0.97	0.58	31,31,31,31	0
55	MG	2A	3770	1/1	0.97	0.31	69,69,69,69	0
55	MG	1A	3758	1/1	0.97	0.09	34,34,34,34	0
55	MG	1A	3136	1/1	0.97	0.07	44,44,44,44	0
55	MG	1a	1631	1/1	0.97	0.12	57,57,57,57	0
55	MG	16	101	1/1	0.97	0.13	42,42,42,42	0
55	MG	1A	3738	1/1	0.97	0.18	34,34,34,34	0
55	MG	2A	3680	1/1	0.97	0.09	47,47,47,47	0
55	MG	1A	3296	1/1	0.97	0.11	27,27,27,27	0
55	MG	2A	3525	1/1	0.97	0.10	42,42,42,42	0
55	MG	2A	3840	1/1	0.97	0.22	43,43,43,43	0
55	MG	2A	3655	1/1	0.97	0.15	39,39,39,39	0
55	MG	1A	3801	1/1	0.97	0.18	18,18,18,18	0
55	MG	1A	3713	1/1	0.97	0.13	42,42,42,42	0
55	MG	1A	3557	1/1	0.97	0.12	21,21,21,21	0
55	MG	2A	3709	1/1	0.97	0.09	39,39,39,39	0
55	MG	1B	234	1/1	0.97	0.16	44,44,44,44	0
55	MG	1A	3623	1/1	0.97	0.16	38,38,38,38	0
55	MG	2a	3122	1/1	0.97	0.17	34,34,34,34	0
55	MG	1A	4014	1/1	0.97	0.14	39,39,39,39	0
55	MG	1a	1689	1/1	0.97	0.08	42,42,42,42	0
55	MG	1A	3308	1/1	0.97	0.15	36,36,36,36	0
55	MG	1A	3178	1/1	0.97	0.12	31,31,31,31	0
55	MG	1A	3615	1/1	0.97	0.24	48,48,48,48	0
55	MG	1A	3048	1/1	0.97	0.21	32,32,32,32	0
55	MG	2a	3156	1/1	0.97	0.14	48,48,48,48	0
55	MG	1A	3792	1/1	0.97	0.17	20,20,20,20	0
55	MG	1A	3586	1/1	0.97	0.43	44,44,44,44	0
55	MG	2a	3203	1/1	0.97	0.09	72,72,72,72	0
55	MG	1A	3114	1/1	0.97	0.72	38,38,38,38	0
55	MG	1A	3795	1/1	0.97	0.21	21,21,21,21	0
55	MG	1a	1700	1/1	0.97	0.17	42,42,42,42	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
55	MG	1A	3753	1/1	0.97	0.09	48,48,48,48	0
55	MG	2A	3764	1/1	0.97	0.08	65,65,65,65	0
55	MG	1A	4063	1/1	0.97	0.14	36,36,36,36	0
55	MG	1A	3224	1/1	0.97	0.34	35,35,35,35	0
55	MG	1a	1716	1/1	0.97	0.11	56,56,56,56	0
55	MG	2A	3843	1/1	0.97	0.18	37,37,37,37	0
55	MG	1A	3689	1/1	0.97	0.13	28,28,28,28	0
55	MG	10	104	1/1	0.97	0.09	51,51,51,51	0
55	MG	1a	1610	1/1	0.97	0.62	63,63,63,63	0
55	MG	1A	3927	1/1	0.97	0.21	34,34,34,34	0
55	MG	1A	3636	1/1	0.97	0.18	15,15,15,15	0
55	MG	1A	3043	1/1	0.97	0.29	25,25,25,25	0
55	MG	2A	3329	1/1	0.97	0.65	45,45,45,45	0
55	MG	1A	3391	1/1	0.97	0.56	52,52,52,52	0
55	MG	1A	3656	1/1	0.97	0.13	20,20,20,20	0
55	MG	1A	3021	1/1	0.97	0.17	24,24,24,24	0
55	MG	2A	3639	1/1	0.97	0.19	67,67,67,67	0
55	MG	2A	3458	1/1	0.97	0.73	52,52,52,52	0
55	MG	2A	3145	1/1	0.97	0.18	51,51,51,51	0
55	MG	1A	3898	1/1	0.97	0.32	22,22,22,22	0
55	MG	1a	1745	1/1	0.97	0.13	62,62,62,62	0
55	MG	1E	307	1/1	0.97	0.28	44,44,44,44	0
55	MG	2A	3621	1/1	0.97	0.15	46,46,46,46	0
55	MG	1A	3535	1/1	0.97	0.09	41,41,41,41	0
55	MG	2A	3577	1/1	0.97	0.10	44,44,44,44	0
55	MG	1A	3202	1/1	0.97	0.11	38,38,38,38	0
55	MG	1A	4091	1/1	0.97	0.16	24,24,24,24	0
55	MG	1A	3652	1/1	0.97	0.25	26,26,26,26	0
55	MG	1A	3575	1/1	0.97	0.31	32,32,32,32	0
55	MG	1a	1757	1/1	0.97	0.12	47,47,47,47	0
55	MG	2A	3790	1/1	0.97	0.10	59,59,59,59	0
55	MG	2a	3155	1/1	0.97	0.17	58,58,58,58	0
55	MG	2A	3353	1/1	0.97	0.13	61,61,61,61	0
55	MG	2A	3466	1/1	0.97	1.09	42,42,42,42	0
55	MG	1A	3899	1/1	0.97	0.57	41,41,41,41	0
55	MG	1A	3781	1/1	0.97	0.12	37,37,37,37	0
55	MG	1E	302	1/1	0.97	0.58	26,26,26,26	0
55	MG	1A	3484	1/1	0.97	0.24	35,35,35,35	0
55	MG	1A	3013	1/1	0.97	0.54	27,27,27,27	0
55	MG	1A	3017	1/1	0.97	0.09	25,25,25,25	0
55	MG	1a	1768	1/1	0.97	0.09	40,40,40,40	0
55	MG	1e	202	1/1	0.97	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
55	MG	2a	3043	1/1	0.97	0.14	60,60,60,60	0
55	MG	12	101	1/1	0.97	0.17	42,42,42,42	0
55	MG	2A	3809	1/1	0.97	0.09	43,43,43,43	0
55	MG	1A	3817	1/1	0.97	0.18	50,50,50,50	0
55	MG	1A	3556	1/1	0.97	0.64	31,31,31,31	0
55	MG	1a	1617	1/1	0.97	0.19	63,63,63,63	0
55	MG	2A	3822	1/1	0.97	0.17	26,26,26,26	0
55	MG	1B	211	1/1	0.97	0.12	33,33,33,33	0
55	MG	1E	308	1/1	0.97	0.17	16,16,16,16	0
55	MG	1A	3128	1/1	0.97	0.63	37,37,37,37	0
55	MG	1A	3856	1/1	0.97	0.14	40,40,40,40	0
55	MG	1A	3751	1/1	0.97	0.12	50,50,50,50	0
55	MG	1A	3033	1/1	0.97	0.32	24,24,24,24	0
55	MG	1A	3472	1/1	0.97	1.25	54,54,54,54	0
55	MG	1A	3199	1/1	0.97	0.17	18,18,18,18	0
55	MG	1A	3825	1/1	0.97	0.11	27,27,27,27	0
55	MG	2A	3557	1/1	0.97	0.18	40,40,40,40	0
55	MG	1A	3604	1/1	0.97	0.20	31,31,31,31	0
55	MG	2a	3170	1/1	0.97	0.14	36,36,36,36	0
55	MG	1A	3083	1/1	0.97	0.44	41,41,41,41	0
55	MG	2A	3473	1/1	0.97	0.23	23,23,23,23	0
55	MG	2A	3661	1/1	0.97	0.13	52,52,52,52	0
55	MG	2A	3434	1/1	0.97	0.16	69,69,69,69	0
55	MG	2A	3135	1/1	0.97	0.27	36,36,36,36	0
55	MG	1A	3324	1/1	0.97	0.11	43,43,43,43	0
55	MG	1W	201	1/1	0.97	0.33	34,34,34,34	0
55	MG	1D	313	1/1	0.97	0.31	30,30,30,30	0
55	MG	2A	3072	1/1	0.97	0.39	29,29,29,29	0
55	MG	1A	3528	1/1	0.97	0.23	29,29,29,29	0
55	MG	1a	1823	1/1	0.97	0.10	51,51,51,51	0
55	MG	1A	3294	1/1	0.97	0.29	40,40,40,40	0
55	MG	1a	1738	1/1	0.97	0.30	52,52,52,52	0
55	MG	1A	3022	1/1	0.97	0.11	29,29,29,29	0
55	MG	1a	1603	1/1	0.97	0.11	55,55,55,55	0
55	MG	1A	4067	1/1	0.97	0.19	26,26,26,26	0
55	MG	2A	3762	1/1	0.97	0.31	74,74,74,74	0
55	MG	1A	3846	1/1	0.97	0.10	28,28,28,28	0
55	MG	1A	3371	1/1	0.97	0.19	40,40,40,40	0
55	MG	1A	3757	1/1	0.97	0.11	55,55,55,55	0
55	MG	2A	3138	1/1	0.97	0.62	52,52,52,52	0
55	MG	2A	3450	1/1	0.97	0.84	61,61,61,61	0
55	MG	2A	3137	1/1	0.97	0.18	51,51,51,51	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
55	MG	1A	3295	1/1	0.97	0.31	31,31,31,31	0
55	MG	1A	3063	1/1	0.97	0.08	44,44,44,44	0
55	MG	2A	3340	1/1	0.97	0.29	61,61,61,61	0
55	MG	2A	3481	1/1	0.97	0.10	38,38,38,38	0
55	MG	2A	3204	1/1	0.97	0.42	49,49,49,49	0
55	MG	1B	235	1/1	0.97	0.17	23,23,23,23	0
55	MG	1A	3750	1/1	0.97	0.12	41,41,41,41	0
55	MG	1A	3536	1/1	0.97	0.13	56,56,56,56	0
55	MG	2A	3756	1/1	0.97	0.17	53,53,53,53	0
55	MG	1A	3835	1/1	0.97	0.10	39,39,39,39	0
55	MG	2a	3026	1/1	0.97	0.11	49,49,49,49	0
55	MG	1A	3682	1/1	0.97	0.16	33,33,33,33	0
55	MG	2A	3381	1/1	0.97	0.06	49,49,49,49	0
55	MG	1A	3258	1/1	0.97	0.13	47,47,47,47	0
55	MG	1S	201	1/1	0.97	0.13	47,47,47,47	0
55	MG	1A	3736	1/1	0.97	0.15	17,17,17,17	0
55	MG	1a	1616	1/1	0.97	0.19	51,51,51,51	0
55	MG	1A	3783	1/1	0.97	0.10	26,26,26,26	0
55	MG	1A	3507	1/1	0.97	0.47	27,27,27,27	0
55	MG	1A	3521	1/1	0.97	0.18	40,40,40,40	0
55	MG	2E	307	1/1	0.97	0.45	56,56,56,56	0
55	MG	2A	3021	1/1	0.97	0.08	40,40,40,40	0
55	MG	2A	3699	1/1	0.97	0.51	43,43,43,43	0
55	MG	1A	3685	1/1	0.97	0.18	34,34,34,34	0
55	MG	1A	3847	1/1	0.97	0.25	35,35,35,35	0
55	MG	1A	3097	1/1	0.97	0.19	30,30,30,30	0
55	MG	1A	4054	1/1	0.97	0.09	37,37,37,37	0
55	MG	1A	3594	1/1	0.97	0.17	23,23,23,23	0
55	MG	1Q	206	1/1	0.97	0.09	35,35,35,35	0
55	MG	2A	3387	1/1	0.97	0.18	29,29,29,29	0
55	MG	1A	3867	1/1	0.97	0.18	37,37,37,37	0
55	MG	1A	3352	1/1	0.97	0.34	40,40,40,40	0
55	MG	1a	1628	1/1	0.97	0.13	61,61,61,61	0
55	MG	1a	1780	1/1	0.97	0.09	42,42,42,42	0
55	MG	2A	3239	1/1	0.97	0.41	49,49,49,49	0
55	MG	2A	3857	1/1	0.97	0.21	36,36,36,36	0
55	MG	1A	3263	1/1	0.97	0.14	38,38,38,38	0
55	MG	2A	3862	1/1	0.97	0.34	56,56,56,56	0
55	MG	2A	3038	1/1	0.97	0.84	44,44,44,44	0
55	MG	1A	3107	1/1	0.97	0.46	31,31,31,31	0
55	MG	1A	4024	1/1	0.97	0.19	39,39,39,39	0
55	MG	1A	3531	1/1	0.97	0.30	49,49,49,49	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
55	MG	1A	4095	1/1	0.97	0.14	31,31,31,31	0
55	MG	2A	3592	1/1	0.97	0.25	36,36,36,36	0
55	MG	1A	3648	1/1	0.97	0.14	41,41,41,41	0
55	MG	1A	3323	1/1	0.97	0.16	52,52,52,52	0
55	MG	2A	3455	1/1	0.97	0.16	56,56,56,56	0
55	MG	1A	3534	1/1	0.97	0.27	31,31,31,31	0
55	MG	1A	3596	1/1	0.97	0.08	43,43,43,43	0
55	MG	1A	3931	1/1	0.97	0.43	35,35,35,35	0
55	MG	2A	3452	1/1	0.97	1.36	46,46,46,46	0
55	MG	1A	3335	1/1	0.97	0.20	36,36,36,36	0
55	MG	1A	3791	1/1	0.97	0.17	24,24,24,24	0
55	MG	1A	3309	1/1	0.97	0.14	40,40,40,40	0
55	MG	1A	4059	1/1	0.97	0.15	34,34,34,34	0
55	MG	1A	3807	1/1	0.97	0.19	36,36,36,36	0
55	MG	2A	3112	1/1	0.97	0.17	89,89,89,89	0
55	MG	1B	216	1/1	0.97	0.10	48,48,48,48	0
55	MG	2A	3306	1/1	0.97	0.33	55,55,55,55	0
55	MG	1A	3663	1/1	0.97	0.11	23,23,23,23	0
55	MG	1A	3809	1/1	0.97	0.19	28,28,28,28	0
55	MG	1A	3961	1/1	0.97	0.15	41,41,41,41	0
55	MG	1A	3974	1/1	0.97	0.14	44,44,44,44	0
55	MG	1I	203	1/1	0.97	0.06	54,54,54,54	0
55	MG	2A	3101	1/1	0.97	0.40	44,44,44,44	0
55	MG	2A	3578	1/1	0.97	0.20	28,28,28,28	0
55	MG	1A	3815	1/1	0.97	0.16	16,16,16,16	0
55	MG	1A	4099	1/1	0.97	0.14	37,37,37,37	0
55	MG	2U	202	1/1	0.97	0.19	30,30,30,30	0
55	MG	1A	3194	1/1	0.97	0.37	35,35,35,35	0
55	MG	2A	3267	1/1	0.97	0.58	66,66,66,66	0
55	MG	2A	3672	1/1	0.97	0.14	59,59,59,59	0
55	MG	1a	1759	1/1	0.97	0.07	40,40,40,40	0
55	MG	1a	1776	1/1	0.97	0.12	40,40,40,40	0
55	MG	17	103	1/1	0.97	0.30	32,32,32,32	0
55	MG	2A	3302	1/1	0.97	0.18	42,42,42,42	0
55	MG	1X	102	1/1	0.97	0.18	31,31,31,31	0
55	MG	2A	3626	1/1	0.97	0.26	44,44,44,44	0
55	MG	1Q	201	1/1	0.97	0.17	28,28,28,28	0
55	MG	1a	1625	1/1	0.97	0.98	58,58,58,58	0
55	MG	1A	3630	1/1	0.97	0.26	30,30,30,30	0
55	MG	1a	1798	1/1	0.97	0.10	73,73,73,73	0
55	MG	1A	3677	1/1	0.97	0.14	57,57,57,57	0
55	MG	1A	3259	1/1	0.97	0.73	36,36,36,36	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
55	MG	2a	3205	1/1	0.97	0.07	59,59,59,59	0
55	MG	2A	3147	1/1	0.97	0.12	60,60,60,60	0
55	MG	1A	3828	1/1	0.97	0.09	25,25,25,25	0
55	MG	1A	3090	1/1	0.97	0.25	29,29,29,29	0
55	MG	1A	3386	1/1	0.97	0.58	23,23,23,23	0
55	MG	1A	4020	1/1	0.97	0.08	26,26,26,26	0
55	MG	2A	3411	1/1	0.97	0.25	51,51,51,51	0
55	MG	1A	3811	1/1	0.97	0.19	43,43,43,43	0
55	MG	2A	3576	1/1	0.97	0.10	50,50,50,50	0
55	MG	2A	3463	1/1	0.97	0.25	25,25,25,25	0
55	MG	2A	3536	1/1	0.97	0.23	58,58,58,58	0
55	MG	2A	3478	1/1	0.97	0.24	30,30,30,30	0
55	MG	2A	3125	1/1	0.97	0.11	58,58,58,58	0
55	MG	1A	3207	1/1	0.97	0.16	41,41,41,41	0
55	MG	2A	3058	1/1	0.97	0.80	41,41,41,41	0
55	MG	2A	3061	1/1	0.97	0.10	51,51,51,51	0
55	MG	1A	3457	1/1	0.97	0.13	21,21,21,21	0
55	MG	2A	3642	1/1	0.97	0.18	69,69,69,69	0
55	MG	1A	3882	1/1	0.97	0.18	47,47,47,47	0
55	MG	1A	3643	1/1	0.97	0.18	43,43,43,43	0
55	MG	2A	3533	1/1	0.97	0.22	50,50,50,50	0
55	MG	2A	3819	1/1	0.97	0.16	33,33,33,33	0
55	MG	1A	3133	1/1	0.97	0.49	31,31,31,31	0
55	MG	2A	3561	1/1	0.97	0.18	46,46,46,46	0
55	MG	2A	3656	1/1	0.97	0.28	53,53,53,53	0
55	MG	1A	3236	1/1	0.97	0.45	23,23,23,23	0
55	MG	1A	3574	1/1	0.97	0.16	41,41,41,41	0
55	MG	1A	3153	1/1	0.98	0.29	49,49,49,49	0
55	MG	1A	3631	1/1	0.98	0.27	16,16,16,16	0
55	MG	2B	219	1/1	0.98	0.26	60,60,60,60	0
55	MG	1A	3272	1/1	0.98	0.32	22,22,22,22	0
55	MG	1A	3078	1/1	0.98	0.13	30,30,30,30	0
55	MG	1A	3012	1/1	0.98	0.12	28,28,28,28	0
55	MG	2A	3413	1/1	0.98	0.28	42,42,42,42	0
55	MG	1A	3142	1/1	0.98	0.17	15,15,15,15	0
55	MG	1A	4093	1/1	0.98	0.17	41,41,41,41	0
55	MG	2A	3845	1/1	0.98	0.23	42,42,42,42	0
55	MG	1A	3661	1/1	0.98	0.12	46,46,46,46	0
55	MG	1A	3173	1/1	0.98	0.20	24,24,24,24	0
55	MG	2A	3391	1/1	0.98	0.23	45,45,45,45	0
55	MG	11	101	1/1	0.98	0.44	34,34,34,34	0
55	MG	2A	3799	1/1	0.98	0.20	56,56,56,56	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
55	MG	1A	3211	1/1	0.98	0.71	33,33,33,33	0
55	MG	1A	3611	1/1	0.98	0.16	12,12,12,12	0
55	MG	1A	3693	1/1	0.98	0.14	26,26,26,26	0
55	MG	2A	3490	1/1	0.98	0.23	46,46,46,46	0
55	MG	1A	3829	1/1	0.98	0.10	24,24,24,24	0
55	MG	1A	3101	1/1	0.98	0.17	39,39,39,39	0
55	MG	2A	3687	1/1	0.98	0.10	53,53,53,53	0
55	MG	2A	3583	1/1	0.98	0.10	53,53,53,53	0
55	MG	2A	3279	1/1	0.98	0.17	40,40,40,40	0
55	MG	2a	3017	1/1	0.98	0.50	49,49,49,49	0
55	MG	1A	3201	1/1	0.98	0.11	32,32,32,32	0
55	MG	2a	3182	1/1	0.98	0.08	51,51,51,51	0
55	MG	2A	3824	1/1	0.98	0.12	54,54,54,54	0
55	MG	1a	1733	1/1	0.98	0.08	50,50,50,50	0
55	MG	1a	1826	1/1	0.98	0.14	45,45,45,45	0
55	MG	1D	302	1/1	0.98	0.11	23,23,23,23	0
55	MG	1A	3183	1/1	0.98	0.54	46,46,46,46	0
55	MG	2A	3307	1/1	0.98	0.21	47,47,47,47	0
55	MG	1A	3163	1/1	0.98	0.73	23,23,23,23	0
55	MG	1A	3994	1/1	0.98	0.16	36,36,36,36	0
55	MG	2A	3823	1/1	0.98	0.09	60,60,60,60	0
55	MG	2A	3504	1/1	0.98	0.08	35,35,35,35	0
55	MG	1A	3887	1/1	0.98	0.14	31,31,31,31	0
55	MG	1A	4021	1/1	0.98	0.20	64,64,64,64	0
55	MG	2A	3470	1/1	0.98	0.13	49,49,49,49	0
55	MG	2A	3507	1/1	0.98	0.16	30,30,30,30	0
55	MG	2A	3500	1/1	0.98	0.09	38,38,38,38	0
55	MG	2A	3546	1/1	0.98	0.21	33,33,33,33	0
55	MG	2a	3115	1/1	0.98	0.13	57,57,57,57	0
55	MG	1A	3374	1/1	0.98	0.21	31,31,31,31	0
55	MG	2A	3048	1/1	0.98	0.12	52,52,52,52	0
55	MG	2a	3118	1/1	0.98	0.19	45,45,45,45	0
55	MG	1A	3166	1/1	0.98	0.18	28,28,28,28	0
55	MG	1A	3235	1/1	0.98	0.12	35,35,35,35	0
55	MG	2A	3564	1/1	0.98	0.07	40,40,40,40	0
55	MG	1A	3135	1/1	0.98	0.18	25,25,25,25	0
55	MG	1a	1732	1/1	0.98	0.21	42,42,42,42	0
55	MG	1a	1664	1/1	0.98	0.12	68,68,68,68	0
55	MG	1A	4052	1/1	0.98	0.08	24,24,24,24	0
55	MG	1A	3164	1/1	0.98	0.18	42,42,42,42	0
55	MG	1A	3709	1/1	0.98	0.12	23,23,23,23	0
55	MG	1B	222	1/1	0.98	0.15	28,28,28,28	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
55	MG	1a	1785	1/1	0.98	0.07	51,51,51,51	0
55	MG	1A	3711	1/1	0.98	0.17	31,31,31,31	0
55	MG	2A	3027	1/1	0.98	0.11	31,31,31,31	0
55	MG	1A	3813	1/1	0.98	0.10	41,41,41,41	0
55	MG	1A	3544	1/1	0.98	0.33	30,30,30,30	0
55	MG	2A	3637	1/1	0.98	0.13	38,38,38,38	0
55	MG	1F	302	1/1	0.98	0.08	33,33,33,33	0
55	MG	2A	3430	1/1	0.98	0.24	31,31,31,31	0
55	MG	1A	3106	1/1	0.98	0.14	35,35,35,35	0
55	MG	1A	3301	1/1	0.98	0.20	32,32,32,32	0
55	MG	1A	3684	1/1	0.98	0.15	44,44,44,44	0
55	MG	1A	3118	1/1	0.98	0.21	26,26,26,26	0
55	MG	1A	3881	1/1	0.98	0.21	34,34,34,34	0
55	MG	1l	201	1/1	0.98	0.19	38,38,38,38	0
55	MG	1A	4078	1/1	0.98	0.21	61,61,61,61	0
55	MG	1D	305	1/1	0.98	0.21	33,33,33,33	0
55	MG	2E	306	1/1	0.98	0.15	42,42,42,42	0
55	MG	2A	3075	1/1	0.98	0.25	29,29,29,29	0
55	MG	1A	3490	1/1	0.98	0.29	28,28,28,28	0
55	MG	2A	3119	1/1	0.98	0.21	32,32,32,32	0
55	MG	2A	3746	1/1	0.98	0.22	37,37,37,37	0
56	ZN	26	102	1/1	0.98	0.21	54,54,54,54	0
55	MG	1A	3909	1/1	0.98	0.24	37,37,37,37	0
55	MG	1A	3768	1/1	0.98	0.14	36,36,36,36	0
55	MG	1A	3996	1/1	0.98	0.17	50,50,50,50	0
55	MG	1A	3729	1/1	0.98	0.13	23,23,23,23	0
55	MG	1B	213	1/1	0.98	0.43	44,44,44,44	0
55	MG	1A	3032	1/1	0.98	0.22	20,20,20,20	0
55	MG	2a	3011	1/1	0.98	0.05	55,55,55,55	0
55	MG	1A	3446	1/1	0.98	0.24	31,31,31,31	0
55	MG	2A	3278	1/1	0.98	0.55	76,76,76,76	0
55	MG	1A	3694	1/1	0.98	0.13	19,19,19,19	0
55	MG	1A	3956	1/1	0.98	0.10	24,24,24,24	0
55	MG	1A	3605	1/1	0.98	0.10	33,33,33,33	0
56	ZN	1n	103	1/1	0.98	0.12	69,69,69,69	0
55	MG	1A	3122	1/1	0.98	0.47	34,34,34,34	0
55	MG	1A	3023	1/1	0.98	0.28	35,35,35,35	0
55	MG	1A	3855	1/1	0.98	0.11	50,50,50,50	0
55	MG	1a	1647	1/1	0.98	0.18	53,53,53,53	0
55	MG	2A	3057	1/1	0.98	0.20	40,40,40,40	0
55	MG	1A	3375	1/1	0.98	0.13	26,26,26,26	0
55	MG	1A	3441	1/1	0.98	0.48	32,32,32,32	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
55	MG	1B	228	1/1	0.98	0.26	37,37,37,37	0
55	MG	1a	1635	1/1	0.98	0.09	30,30,30,30	0
55	MG	1A	3727	1/1	0.98	0.18	31,31,31,31	0
55	MG	2A	3032	1/1	0.98	0.15	42,42,42,42	0
55	MG	1B	225	1/1	0.98	0.23	46,46,46,46	0
55	MG	2a	3106	1/1	0.98	0.17	46,46,46,46	0
55	MG	1A	3209	1/1	0.98	0.11	27,27,27,27	0
55	MG	2A	3694	1/1	0.98	0.11	24,24,24,24	0
55	MG	2A	3775	1/1	0.98	0.07	74,74,74,74	0
55	MG	2A	3220	1/1	0.98	0.12	62,62,62,62	0
55	MG	2A	3805	1/1	0.98	0.20	54,54,54,54	0
58	SF4	1d	501	8/8	0.98	0.18	57,70,76,77	0
55	MG	1A	3525	1/1	0.98	0.17	35,35,35,35	0
55	MG	1A	3218	1/1	0.98	0.10	39,39,39,39	0
55	MG	1A	3739	1/1	0.98	0.15	27,27,27,27	0
55	MG	1U	203	1/1	0.98	0.21	22,22,22,22	0
55	MG	1A	3075	1/1	0.98	0.14	11,11,11,11	0
55	MG	1a	1813	1/1	0.98	0.12	40,40,40,40	0
55	MG	1A	3841	1/1	0.98	0.12	38,38,38,38	0
55	MG	1A	3640	1/1	0.98	0.13	28,28,28,28	0
55	MG	2A	3018	1/1	0.98	0.12	32,32,32,32	0
55	MG	2A	3803	1/1	0.98	0.09	29,29,29,29	0
55	MG	2P	202	1/1	0.98	0.13	48,48,48,48	0
55	MG	2A	3572	1/1	0.98	0.14	27,27,27,27	0
55	MG	2A	3644	1/1	0.98	0.15	68,68,68,68	0
55	MG	2A	3726	1/1	0.98	0.27	51,51,51,51	0
55	MG	1A	3667	1/1	0.98	0.22	49,49,49,49	0
55	MG	1A	3568	1/1	0.98	0.23	25,25,25,25	0
55	MG	2A	3178	1/1	0.98	0.07	37,37,37,37	0
55	MG	1A	4036	1/1	0.98	0.18	45,45,45,45	0
55	MG	1A	3733	1/1	0.98	0.21	20,20,20,20	0
55	MG	2A	3397	1/1	0.98	0.10	25,25,25,25	0
55	MG	2A	3074	1/1	0.98	0.08	43,43,43,43	0
55	MG	1a	1781	1/1	0.98	0.13	56,56,56,56	0
55	MG	1U	204	1/1	0.98	0.45	25,25,25,25	0
55	MG	2A	3110	1/1	0.98	0.42	56,56,56,56	0
55	MG	1A	3116	1/1	0.98	0.17	30,30,30,30	0
55	MG	1D	303	1/1	0.98	0.61	43,43,43,43	0
55	MG	2A	3045	1/1	0.98	0.17	57,57,57,57	0
55	MG	2A	3024	1/1	0.98	0.19	40,40,40,40	0
55	MG	2A	3004	1/1	0.98	0.12	43,43,43,43	0
55	MG	2a	3153	1/1	0.98	0.10	36,36,36,36	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
55	MG	1a	1655	1/1	0.98	0.06	39,39,39,39	0
55	MG	1A	3471	1/1	0.98	0.19	27,27,27,27	0
55	MG	2A	3569	1/1	0.98	0.08	38,38,38,38	0
55	MG	1A	3029	1/1	0.98	0.42	30,30,30,30	0
55	MG	1D	304	1/1	0.98	0.39	32,32,32,32	0
55	MG	1a	1721	1/1	0.98	0.19	28,28,28,28	0
55	MG	2A	3064	1/1	0.98	0.77	47,47,47,47	0
55	MG	2A	3028	1/1	0.98	0.26	41,41,41,41	0
55	MG	1A	3530	1/1	0.98	0.15	19,19,19,19	0
55	MG	1A	3038	1/1	0.98	0.16	18,18,18,18	0
55	MG	1A	3257	1/1	0.98	0.21	40,40,40,40	0
55	MG	1F	303	1/1	0.98	0.40	30,30,30,30	0
55	MG	2A	3608	1/1	0.98	0.20	38,38,38,38	0
55	MG	2A	3033	1/1	0.98	0.10	59,59,59,59	0
55	MG	1A	3752	1/1	0.98	0.16	23,23,23,23	0
55	MG	1B	221	1/1	0.98	0.16	34,34,34,34	0
55	MG	2A	3814	1/1	0.98	0.18	48,48,48,48	0
55	MG	1A	3193	1/1	0.98	0.76	33,33,33,33	0
55	MG	1A	3344	1/1	0.98	0.29	37,37,37,37	0
55	MG	2A	3187	1/1	0.98	0.27	53,53,53,53	0
55	MG	1U	201	1/1	0.98	0.65	33,33,33,33	0
55	MG	1A	4028	1/1	0.98	0.09	44,44,44,44	0
55	MG	1A	3113	1/1	0.98	0.24	34,34,34,34	0
55	MG	1a	1809	1/1	0.98	0.10	49,49,49,49	0
55	MG	2A	3144	1/1	0.98	0.23	45,45,45,45	0
55	MG	1A	3734	1/1	0.98	0.14	16,16,16,16	0
55	MG	1A	3181	1/1	0.98	0.21	58,58,58,58	0
55	MG	2A	3433	1/1	0.98	0.33	47,47,47,47	0
55	MG	2A	3631	1/1	0.98	0.12	35,35,35,35	0
55	MG	1A	3986	1/1	0.98	0.08	24,24,24,24	0
55	MG	1A	3906	1/1	0.98	0.17	17,17,17,17	0
55	MG	1A	3732	1/1	0.98	0.19	27,27,27,27	0
55	MG	1A	3754	1/1	0.99	0.17	30,30,30,30	0
56	ZN	2Y	501	1/1	0.99	0.17	77,77,77,77	0
55	MG	1A	3650	1/1	0.99	0.13	12,12,12,12	0
58	SF4	2d	303	8/8	0.99	0.18	58,77,87,92	0
55	MG	1A	3514	1/1	0.99	0.18	59,59,59,59	0
55	MG	1a	1737	1/1	0.99	0.09	42,42,42,42	0
55	MG	1A	3403	1/1	0.99	0.18	38,38,38,38	0
55	MG	2Z	301	1/1	0.99	0.19	67,67,67,67	0
55	MG	1A	3690	1/1	0.99	0.11	35,35,35,35	0
55	MG	1A	3761	1/1	0.99	0.17	14,14,14,14	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
55	MG	2A	3811	1/1	0.99	0.17	35,35,35,35	0
55	MG	1A	3059	1/1	0.99	0.16	28,28,28,28	0
55	MG	1A	3066	1/1	0.99	0.12	26,26,26,26	0
55	MG	1A	3315	1/1	0.99	0.33	51,51,51,51	0
55	MG	1A	3691	1/1	0.99	0.11	24,24,24,24	0
55	MG	1A	3614	1/1	0.99	0.21	15,15,15,15	0
55	MG	2A	3034	1/1	0.99	0.15	36,36,36,36	0
55	MG	1A	3174	1/1	0.99	0.23	25,25,25,25	0
55	MG	2A	3476	1/1	0.99	0.32	37,37,37,37	0
55	MG	1A	3176	1/1	0.99	0.11	24,24,24,24	0
55	MG	2A	3210	1/1	0.99	0.41	35,35,35,35	0
55	MG	2A	3016	1/1	0.99	0.21	40,40,40,40	0
55	MG	2A	3105	1/1	0.99	0.29	30,30,30,30	0
55	MG	1A	3099	1/1	0.99	0.14	14,14,14,14	0
55	MG	2A	3052	1/1	0.99	0.18	30,30,30,30	0
55	MG	2A	3747	1/1	0.99	0.09	56,56,56,56	0
55	MG	1A	3275	1/1	0.99	0.58	28,28,28,28	0
56	ZN	1Y	205	1/1	0.99	0.21	57,57,57,57	0
55	MG	1B	218	1/1	0.99	0.20	20,20,20,20	0
55	MG	1A	4013	1/1	0.99	0.18	35,35,35,35	0
55	MG	2A	3495	1/1	0.99	0.07	43,43,43,43	0
55	MG	2A	3535	1/1	0.99	0.15	39,39,39,39	0
55	MG	1A	3276	1/1	0.99	0.20	38,38,38,38	0
55	MG	1A	3014	1/1	0.99	0.12	18,18,18,18	0
55	MG	2A	3514	1/1	0.99	0.13	26,26,26,26	0
55	MG	1Z	301	1/1	0.99	0.15	36,36,36,36	0
55	MG	1B	202	1/1	0.99	0.21	35,35,35,35	0
55	MG	1a	1652	1/1	0.99	0.11	51,51,51,51	0
55	MG	1a	1651	1/1	0.99	0.09	41,41,41,41	0
55	MG	18	103	1/1	0.99	0.11	38,38,38,38	0
55	MG	1A	3816	1/1	0.99	0.15	42,42,42,42	0
55	MG	2A	3591	1/1	0.99	0.12	56,56,56,56	0
55	MG	2F	305	1/1	0.99	0.58	49,49,49,49	0
55	MG	1a	1705	1/1	0.99	0.19	57,57,57,57	0
55	MG	2A	3532	1/1	0.99	0.12	42,42,42,42	0
56	ZN	15	106	1/1	0.99	0.22	46,46,46,46	0
55	MG	1A	3923	1/1	0.99	0.26	29,29,29,29	0
55	MG	1A	3866	1/1	0.99	0.12	45,45,45,45	0
55	MG	1A	3799	1/1	0.99	0.11	41,41,41,41	0
55	MG	1A	3779	1/1	0.99	0.19	28,28,28,28	0
55	MG	1A	4085	1/1	0.99	0.11	39,39,39,39	0
56	ZN	29	501	1/1	0.99	0.09	61,61,61,61	0

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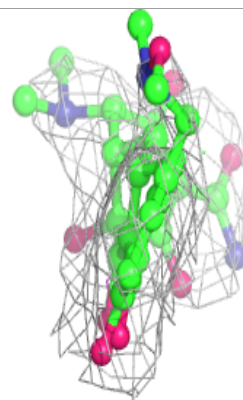
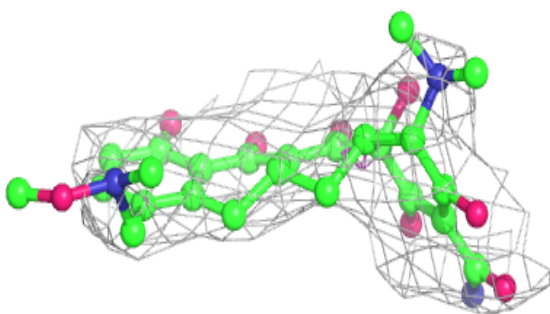
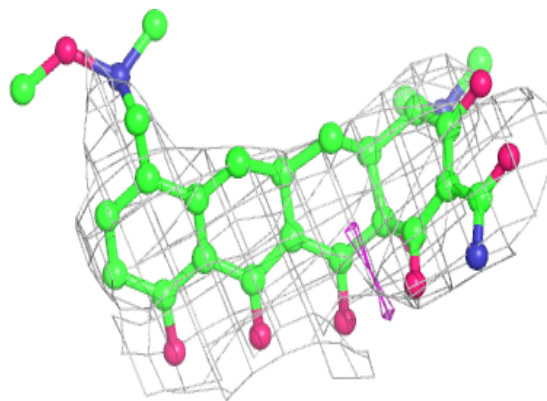
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
55	MG	1A	3707	1/1	0.99	0.20	18,18,18,18	0
55	MG	2A	3693	1/1	0.99	0.22	44,44,44,44	0
55	MG	2A	3309	1/1	0.99	0.14	63,63,63,63	0
55	MG	1A	3570	1/1	0.99	0.50	31,31,31,31	0
55	MG	1A	3271	1/1	0.99	0.33	26,26,26,26	0
55	MG	1A	3763	1/1	0.99	0.13	46,46,46,46	0
55	MG	1a	1735	1/1	0.99	0.11	50,50,50,50	0
55	MG	1A	4068	1/1	0.99	0.14	23,23,23,23	0
55	MG	1A	3148	1/1	0.99	0.13	31,31,31,31	0
55	MG	1A	3406	1/1	0.99	0.25	37,37,37,37	0
55	MG	2A	3120	1/1	0.99	0.09	55,55,55,55	0
55	MG	2A	3688	1/1	0.99	0.14	32,32,32,32	0
55	MG	2A	3808	1/1	0.99	0.14	45,45,45,45	0
55	MG	2P	201	1/1	0.99	0.17	40,40,40,40	0
55	MG	1A	3985	1/1	0.99	0.16	24,24,24,24	0
55	MG	1B	219	1/1	0.99	0.19	38,38,38,38	0
55	MG	1A	3491	1/1	0.99	0.36	29,29,29,29	0
55	MG	2A	3792	1/1	0.99	0.30	60,60,60,60	0
55	MG	1A	3143	1/1	0.99	0.09	28,28,28,28	0
55	MG	2A	3261	1/1	0.99	0.31	43,43,43,43	0
56	ZN	19	102	1/1	1.00	0.20	41,41,41,41	0
55	MG	1A	3774	1/1	1.00	0.12	37,37,37,37	0
56	ZN	25	103	1/1	1.00	0.20	52,52,52,52	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.

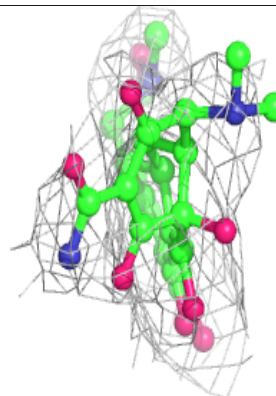
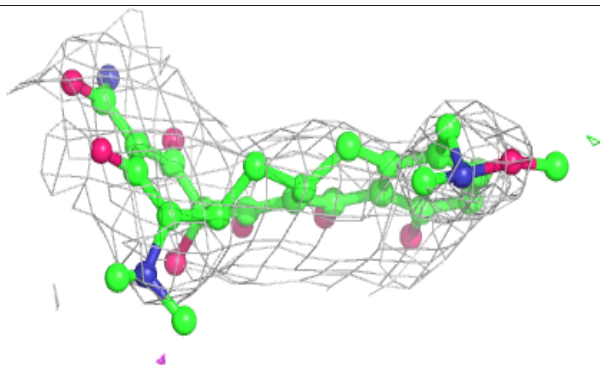
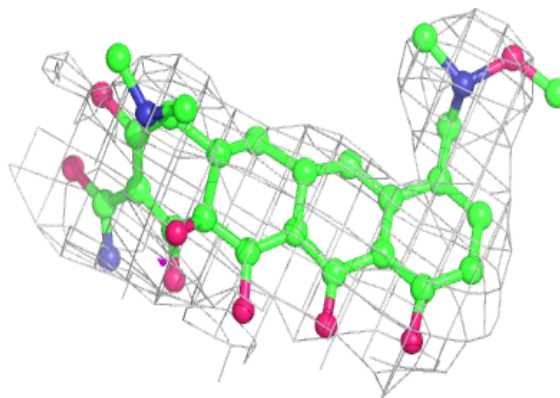


**Electron density around V7A 2a 3210:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

**Electron density around V7A 1a 1835:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



## 6.5 Other polymers

There are no such residues in this entry.