



# Full wwPDB X-ray Structure Validation Report ⓘ

Nov 6, 2023 – 09:17 AM EST

PDB ID : 4Y4O  
Title : Crystal structure of the *Thermus thermophilus* 70S ribosome with rRNA modifications and bound to protein Y (YfiA) at 2.3Å resolution  
Authors : Polikanov, Y.S.; Melnikov, S.V.; Soll, D.; Steitz, T.A.  
Deposited on : 2015-02-10  
Resolution : 2.30 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.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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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 : 2.36  
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) : 2.36

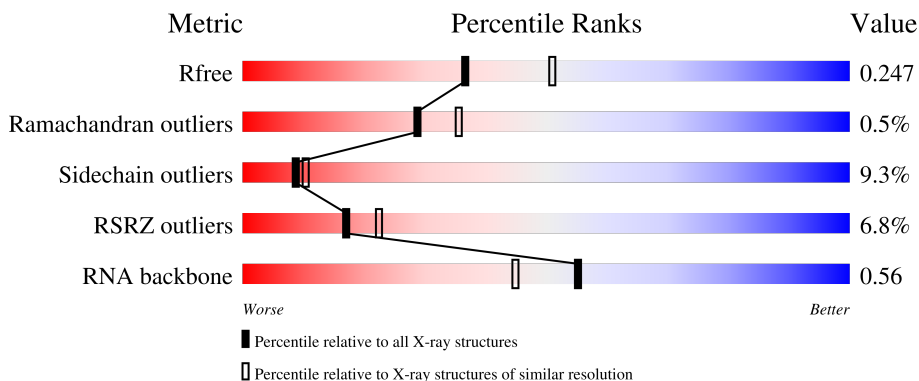
# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.30 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	5042 (2.30-2.30)
Ramachandran outliers	138981	5575 (2.30-2.30)
Sidechain outliers	138945	5575 (2.30-2.30)
RSRZ outliers	127900	4938 (2.30-2.30)
RNA backbone	3102	1090 (2.70-1.90)

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 of 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 style="display: flex; align-items: center;"> <div style="width: 3%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 80%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 16%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 1%; height: 10px; background-color: orange; margin-right: 5px;"></div> <div style="width: 1%; height: 10px; background-color: grey;"></div> </div> <p style="text-align: center;">3%      80%      16%      ..</p>
1	2A	2915	<div style="display: flex; align-items: center;"> <div style="width: 4%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 79%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 17%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 1%; height: 10px; background-color: orange; margin-right: 5px;"></div> <div style="width: 1%; height: 10px; background-color: grey;"></div> </div> <p style="text-align: center;">4%      79%      17%      ..</p>
2	1B	121	<div style="display: flex; align-items: center;"> <div style="width: 89%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 10%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 1%; height: 10px; background-color: orange; margin-right: 5px;"></div> <div style="width: 1%; height: 10px; background-color: grey;"></div> </div> <p style="text-align: center;">89%      10%      .</p>
2	2B	121	<div style="display: flex; align-items: center;"> <div style="width: 0%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 87%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 12%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 1%; height: 10px; background-color: orange; margin-right: 5px;"></div> <div style="width: 1%; height: 10px; background-color: grey;"></div> </div> <p style="text-align: center;">%      87%      12%      ..</p>
3	1D	276	<div style="display: flex; align-items: center;"> <div style="width: 2%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 94%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 5%; height: 10px; background-color: yellow; margin-right: 5px;"></div> </div> <p style="text-align: center;">2%      94%      5%</p>

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Mol	Chain	Length	Quality of chain
3	2D	276	95% 5%
4	1E	206	91% 8%
4	2E	206	90% 8%
5	1F	210	88% 8%
5	2F	210	89% 8%
6	1G	182	90% 9%
6	2G	182	88% 12%
7	1H	180	92%
7	2H	180	88% 7%
8	1I	148	86% 14%
8	2I	148	90% 8%
9	1N	140	91% 9%
9	2N	140	92% 8%
10	1O	122	98%
10	2O	122	98%
11	1P	150	93% 7%
11	2P	150	93% 6%
12	1Q	141	92% 8%
12	2Q	141	93% 6%
13	1R	118	88% 12%
13	2R	118	89% 11%
14	1S	112	88% 11%
14	2S	112	89% 9%
15	1T	146	84% 6% 10%
15	2T	146	85% 5% 10%

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Mol	Chain	Length	Quality of chain
16	1U	118	2% 90% 8% .
16	2U	118	92% 6% .
17	1V	101	2% 92% 8%
17	2V	101	% 92% 8%
18	1W	113	% 89% 9% ..
18	2W	113	91% 8% .
19	1X	96	3% 94% . . .
19	2X	96	8% 93% 5% ..
20	1Y	110	2% 94% . .
20	2Y	110	10% 90% 7% .
21	1Z	206	% 88% 10% .
21	2Z	206	9% 89% 9% .
22	10	85	% 85% 6% 9%
22	20	85	6% 86% 5% 9%
23	11	98	2% 89% 10% .
23	21	98	% 91% 8% .
24	12	72	93% . .
24	22	72	% 90% 7% .
25	13	60	2% 92% 7% .
25	23	60	10% 85% 13% .
26	14	71	20% 79% 15% . .
26	24	71	37% 79% 17% . .
27	15	60	3% 87% 12% .
27	25	60	2% 87% 12% .
28	16	54	87% 11% .

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Mol	Chain	Length	Quality of chain
28	26	54	2% 93% 6%
29	17	49	10% 92% 6%
29	27	49	8% 96% ..
30	18	65	92% 6%
30	28	65	92% 6%
31	19	37	3% 100%
31	29	37	5% 100%
32	1a	1521	3% 82% 16% ..
32	2a	1521	4% 81% 17% ..
33	1b	256	12% 77% 13% 10%
33	2b	256	29% 77% 13% 10%
34	1c	239	4% 81% 5% 14%
34	2c	239	30% 80% 6% 14%
35	1d	209	11% 91% 8%
35	2d	209	13% 93% 7%
36	1e	162	2% 88% 9%
36	2e	162	7% 86% 5% 9%
37	1f	101	5% 95% ..
37	2f	101	2% 95% ..
38	1g	156	4% 94% 5%
38	2g	156	19% 90% 10%
39	1h	138	6% 92% 7%
39	2h	138	6% 91% 8%
40	1i	128	15% 88% 11%
40	2i	128	59% 88% 10%

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Mol	Chain	Length	Quality of chain
41	1j	105	28% 85% 8% 8%
41	2j	105	38% 86% 6% 9%
42	1k	129	3% 82% 5% 12%
42	2k	129	13% 84% 5% 12%
43	1l	132	7% 89% 8%
43	2l	132	6% 89% 8%
44	1m	126	10% 83% 10% 8%
44	2m	126	42% 82% 9% 10%
45	1n	61	31% 90% 8%
45	2n	61	67% 90% 8%
46	1o	89	3% 91% 8%
46	2o	89	3% 89% 10%
47	1p	88	6% 85% 8% 7%
47	2p	88	13% 85% 8% 7%
48	1q	105	10% 91% 6%
48	2q	105	8% 90% 6%
49	1r	88	8% 70% 7% 23%
49	2r	88	2% 70% 7% 23%
50	1s	93	13% 82% 8% 11%
50	2s	93	65% 83% 6% 11%
51	1t	106	13% 84% 6% 9%
51	2t	106	4% 84% 8% 8%
52	1u	27	26% 74% 11% 15%
52	2u	27	52% 74% 7% 15%
53	1y	113	2% 82% 14%

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Mol	Chain	Length	Quality of chain
53	2y	113	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
54	MG	1A	3612	-	-	-	X
54	MG	1A	4003	-	-	-	X
54	MG	1a	1744	-	-	-	X
54	MG	2A	3081	-	-	-	X
54	MG	2A	3174	-	-	-	X
54	MG	2A	3187	-	-	-	X
54	MG	2A	3234	-	-	-	X
54	MG	2A	3408	-	-	-	X
54	MG	2A	3431	-	-	-	X
54	MG	2A	3478	-	-	-	X
54	MG	2A	3535	-	-	-	X
54	MG	2A	3633	-	-	-	X

## 2 Entry composition [i](#)

There are 59 unique types of molecules in this entry. The entry contains 298502 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
			Total	C	N	O	P			
1	1A	2872	Total	C	N	O	P	0	0	0
			61869	27540	11574	19884	2871			
1	2A	2867	Total	C	N	O	P	0	0	0
			61758	27491	11552	19850	2865			

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
22	10	77	Total	C	N	O	S	0	0	0
			608	375	129	103	1			
22	20	77	Total	C	N	O	S	0	0	0
			608	375	129	103	1			

- Molecule 23 is a protein called 50S ribosomal protein L28.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
23	11	97	Total	C	N	O	S	0	0	0
			754	475	148	130	1			
23	21	97	Total	C	N	O	S	0	0	0
			759	478	149	131	1			

- Molecule 24 is a protein called 50S ribosomal protein L29.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
24	12	70	Total	C	N	O	S	0	0	0
			588	365	118	103	2			
24	22	70	Total	C	N	O	S	0	0	0
			592	368	119	103	2			

- Molecule 25 is a protein called 50S ribosomal protein L30.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
25	13	59	Total	C	N	O	0	0	0
			469	298	90	81			
25	23	59	Total	C	N	O	0	0	0
			464	296	90	78			

- Molecule 26 is a protein called 50S ribosomal protein L31.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
26	14	69	Total	C	N	O	S	0	0	0
			546	346	96	99	5			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
26	24	69	Total	C	N	O	S	0	0	0
			536	342	98	91	5			

- Molecule 27 is a protein called 50S ribosomal protein L32.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
27	15	59	Total	C	N	O	S	0	0	0
			459	288	90	76	5			
27	25	59	Total	C	N	O	S	0	0	0
			455	285	89	76	5			

- Molecule 28 is a protein called 50S ribosomal protein L33.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
28	16	53	Total	C	N	O	S	0	0	0
			453	281	91	77	4			
28	26	53	Total	C	N	O	S	0	0	0
			449	279	91	75	4			

- Molecule 29 is a protein called 50S ribosomal protein L34.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
29	17	48	Total	C	N	O	S	0	0	0
			418	257	104	55	2			
29	27	48	Total	C	N	O	S	0	0	0
			418	257	104	55	2			

- Molecule 30 is a protein called 50S ribosomal protein L35.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
30	18	64	Total	C	N	O	S	0	0	0
			517	331	102	82	2			
30	28	64	Total	C	N	O	S	0	0	0
			517	331	102	82	2			

- Molecule 31 is a protein called 50S ribosomal protein L36.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
31	19	37	Total	C	N	O	S	0	0	0
			307	188	68	47	4			
31	29	37	Total	C	N	O	S	0	0	0
			307	188	68	47	4			

- Molecule 32 is a RNA chain called 16S Ribosomal RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
32	1a	1500	Total	C	N	O	P	0	0	0
			32246	14358	5975	10413	1500			
32	2a	1504	Total	C	N	O	P	0	0	0
			32331	14396	5990	10441	1504			

- Molecule 33 is a protein called 30S ribosomal protein S2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
33	1b	231	Total	C	N	O	S	0	0	0
			1842	1175	330	332	5			
33	2b	231	Total	C	N	O	S	0	0	0
			1825	1167	326	327	5			

- Molecule 34 is a protein called 30S ribosomal protein S3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
34	1c	206	Total	C	N	O	S	0	0	0
			1558	979	305	273	1			
34	2c	206	Total	C	N	O	S	0	0	0
			1542	968	300	273	1			

- Molecule 35 is a protein called 30S ribosomal protein S4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
35	1d	208	Total	C	N	O	S	0	0	0
			1665	1043	329	286	7			
35	2d	208	Total	C	N	O	S	0	0	0
			1668	1047	330	284	7			

- Molecule 36 is a protein called 30S ribosomal protein S5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
36	1e	148	Total	C	N	O	S	0	0	0
			1133	716	214	199	4			
36	2e	148	Total	C	N	O	S	0	0	0
			1133	716	214	199	4			

- Molecule 37 is a protein called 30S ribosomal protein S6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
37	1f	100	Total	C	N	O	S	0	0	0
			814	516	144	151	3			
37	2f	100	Total	C	N	O	S	0	0	0
			816	516	146	151	3			

- Molecule 38 is a protein called 30S ribosomal protein S7.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
38	1g	155	Total	C	N	O	S	0	0	0
			1235	769	244	216	6			
38	2g	155	Total	C	N	O	S	0	0	0
			1229	766	241	216	6			

- Molecule 39 is a protein called 30S ribosomal protein S8.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
39	1h	137	Total	C	N	O	S	0	0	0
			1098	694	210	192	2			
39	2h	137	Total	C	N	O	S	0	0	0
			1088	689	206	191	2			

- Molecule 40 is a protein called 30S ribosomal protein S9.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
40	1i	127	Total	C	N	O	0	0	0
			986	625	193	168			
40	2i	126	Total	C	N	O	0	0	0
			966	613	186	167			

- Molecule 41 is a protein called 30S ribosomal protein S10.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
41	1j	97	Total	C	N	O	0	0	0
			719	446	142	131			
41	2j	96	Total	C	N	O	0	0	0
			710	442	137	131			

- Molecule 42 is a protein called 30S ribosomal protein S11.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
42	1k	114	Total	C	N	O	S	0	0	0
			834	520	156	155	3			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
42	2k	114	833	519	156	155	3	0	0	0

- Molecule 43 is a protein called 30S ribosomal protein S12.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
43	1l	122	932	586	185	159	2	0	0	0
43	2l	122	932	586	185	159	2	0	0	0

- Molecule 44 is a protein called 30S ribosomal protein S13.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
44	1m	116	914	564	189	159	2	0	0	0
44	2m	114	895	550	186	157	2	0	0	0

- Molecule 45 is a protein called 30S ribosomal protein S14 type Z.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
45	1n	60	492	312	104	72	4	0	0	0
45	2n	60	492	312	104	72	4	0	0	0

- Molecule 46 is a protein called 30S ribosomal protein S15.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
46	1o	88	728	456	144	126	2	0	0	0
46	2o	88	728	456	144	126	2	0	0	0

- Molecule 47 is a protein called 30S ribosomal protein S16.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
47	1p	82	681	433	134	113	1	0	0	0
47	2p	82	677	430	133	113	1	0	0	0



- Molecule 48 is a protein called 30S ribosomal protein S17.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
48	1q	99	Total 823	C 528	N 151	O 142	S 2	0	0	0
48	2q	99	Total 823	C 528	N 151	O 142	S 2	0	0	0

- Molecule 49 is a protein called 30S ribosomal protein S18.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
49	1r	68	Total 555	C 355	N 108	O 92	0	0	0
49	2r	68	Total 555	C 355	N 108	O 92	0	0	0

- Molecule 50 is a protein called 30S ribosomal protein S19.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
50	1s	83	Total 648	C 415	N 120	O 111	S 2	0	0	0
50	2s	83	Total 645	C 410	N 118	O 115	S 2	0	0	0

- Molecule 51 is a protein called 30S ribosomal protein S20.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
51	1t	96	Total 732	C 449	N 157	O 124	S 2	0	0	0
51	2t	98	Total 733	C 451	N 154	O 126	S 2	0	0	0

- Molecule 52 is a protein called 30S ribosomal protein Thx.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
52	1u	23	Total 199	C 122	N 48	O 29	0	0	0
52	2u	23	Total 199	C 122	N 48	O 29	0	0	0

- Molecule 53 is a protein called Ribosome-associated inhibitor A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
53	1y	97	Total	C	N	O	S	0	0	0
			764	478	144	139	3			
53	2y	96	Total	C	N	O	S	0	0	0
			749	468	141	137	3			

- Molecule 54 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
54	1A	1075	Total	Mg	0	0
			1075	1075		
54	1B	30	Total	Mg	0	0
			30	30		
54	1D	14	Total	Mg	0	0
			14	14		
54	1E	6	Total	Mg	0	0
			6	6		
54	1F	10	Total	Mg	0	0
			10	10		
54	1G	4	Total	Mg	0	0
			4	4		
54	1H	2	Total	Mg	0	0
			2	2		
54	1N	3	Total	Mg	0	0
			3	3		
54	1O	1	Total	Mg	0	0
			1	1		
54	1P	2	Total	Mg	0	0
			2	2		
54	1Q	4	Total	Mg	0	0
			4	4		
54	1R	3	Total	Mg	0	0
			3	3		
54	1T	3	Total	Mg	0	0
			3	3		
54	1U	2	Total	Mg	0	0
			2	2		
54	1V	3	Total	Mg	0	0
			3	3		
54	1W	2	Total	Mg	0	0
			2	2		
54	1X	1	Total	Mg	0	0
			1	1		
54	1Z	1	Total	Mg	0	0
			1	1		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
54	10	5	Total 5	Mg 5	0	0
54	11	4	Total 4	Mg 4	0	0
54	13	2	Total 2	Mg 2	0	0
54	14	1	Total 1	Mg 1	0	0
54	15	2	Total 2	Mg 2	0	0
54	17	2	Total 2	Mg 2	0	0
54	18	1	Total 1	Mg 1	0	0
54	19	2	Total 2	Mg 2	0	0
54	1a	280	Total 280	Mg 280	0	0
54	1b	1	Total 1	Mg 1	0	0
54	1d	5	Total 5	Mg 5	0	0
54	1e	4	Total 4	Mg 4	0	0
54	1f	1	Total 1	Mg 1	0	0
54	1g	3	Total 3	Mg 3	0	0
54	1h	2	Total 2	Mg 2	0	0
54	1i	1	Total 1	Mg 1	0	0
54	1l	2	Total 2	Mg 2	0	0
54	1n	2	Total 2	Mg 2	0	0
54	1o	1	Total 1	Mg 1	0	0
54	1q	2	Total 2	Mg 2	0	0
54	1r	1	Total 1	Mg 1	0	0

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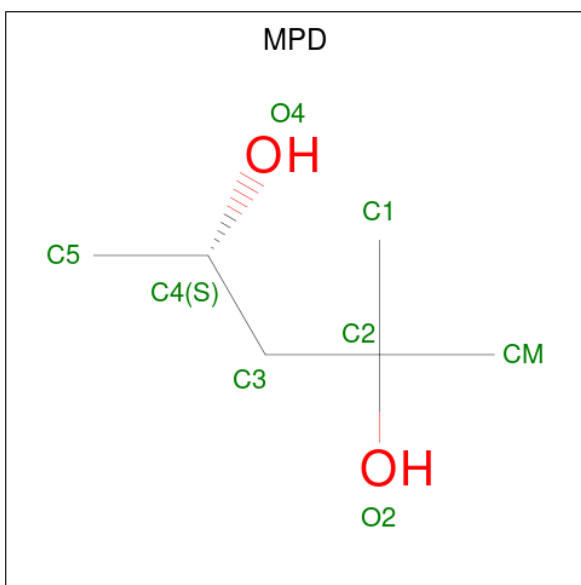
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
54	1t	1	Total Mg 1 1	0	0
54	1y	4	Total Mg 4 4	0	0
54	2A	761	Total Mg 761 761	0	0
54	2B	19	Total Mg 19 19	0	0
54	2D	9	Total Mg 9 9	0	0
54	2E	5	Total Mg 5 5	0	0
54	2F	3	Total Mg 3 3	0	0
54	2G	3	Total Mg 3 3	0	0
54	2I	1	Total Mg 1 1	0	0
54	2N	1	Total Mg 1 1	0	0
54	2O	2	Total Mg 2 2	0	0
54	2P	2	Total Mg 2 2	0	0
54	2Q	2	Total Mg 2 2	0	0
54	2R	1	Total Mg 1 1	0	0
54	2T	3	Total Mg 3 3	0	0
54	2V	1	Total Mg 1 1	0	0
54	2W	2	Total Mg 2 2	0	0
54	2X	1	Total Mg 1 1	0	0
54	20	2	Total Mg 2 2	0	0
54	21	1	Total Mg 1 1	0	0
54	26	1	Total Mg 1 1	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
54	27	1	Total Mg 1 1	0	0
54	28	2	Total Mg 2 2	0	0
54	2a	193	Total Mg 193 193	0	0
54	2e	1	Total Mg 1 1	0	0
54	2f	1	Total Mg 1 1	0	0
54	2j	1	Total Mg 1 1	0	0
54	2l	1	Total Mg 1 1	0	0
54	2r	1	Total Mg 1 1	0	0
54	2t	1	Total Mg 1 1	0	0

- Molecule 55 is (4S)-2-METHYL-2,4-PENTANEDIOL (three-letter code: MPD) (formula:  $C_6H_{14}O_2$ ).



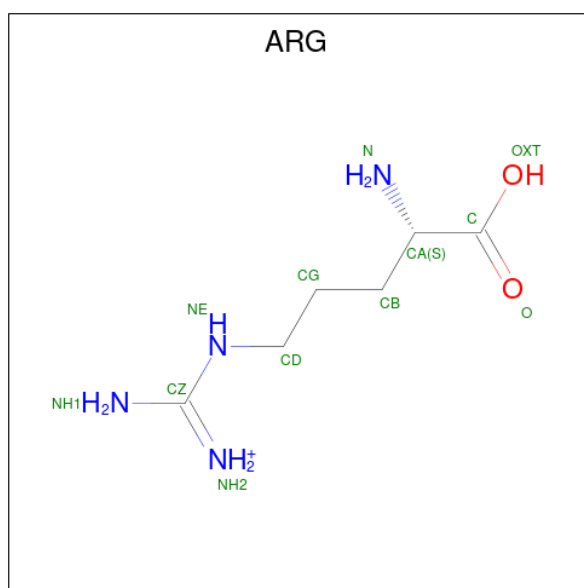
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
55	1A	1	Total C O 8 6 2	0	0
55	1T	1	Total C O 8 6 2	0	0

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
55	18	1	Total	C	O	0	0
			8	6	2		
55	1a	1	Total	C	O	0	0
			8	6	2		
55	2A	1	Total	C	O	0	0
			8	6	2		
55	2A	1	Total	C	O	0	0
			8	6	2		
55	2B	1	Total	C	O	0	0
			8	6	2		

- Molecule 56 is ARGinine (three-letter code: ARG) (formula:  $C_6H_{15}N_4O_2$ ).



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

- Molecule 57 is ZINC ION (three-letter code: ZN) (formula: Zn).

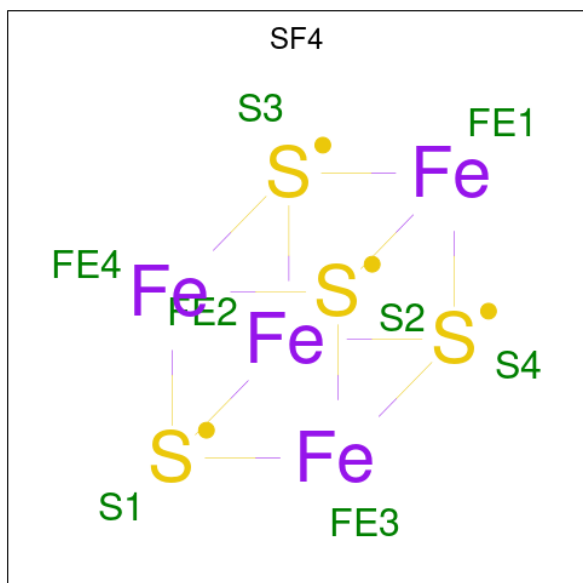
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
57	1Y	1	Total	Zn	0	0
			1	1		
57	14	1	Total	Zn	0	0
			1	1		

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
57	15	1	Total Zn 1 1	0	0
57	16	1	Total Zn 1 1	0	0
57	19	1	Total Zn 1 1	0	0
57	1n	1	Total Zn 1 1	0	0
57	2Y	1	Total Zn 1 1	0	0
57	24	1	Total Zn 1 1	0	0
57	25	1	Total Zn 1 1	0	0
57	26	1	Total Zn 1 1	0	0
57	29	1	Total Zn 1 1	0	0
57	2n	1	Total Zn 1 1	0	0

- 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 8 4 4	0	0

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

- Molecule 59 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
59	1A	4154	4154	4154	0	0
59	1B	109	109	109	0	0
59	1D	119	119	119	0	0
59	1E	81	81	81	0	0
59	1F	66	66	66	0	0
59	1G	20	20	20	0	0
59	1H	16	16	16	0	0
59	1I	9	9	9	0	0
59	1N	55	55	55	0	0
59	1O	29	29	29	0	0
59	1P	56	56	56	0	0
59	1Q	46	46	46	0	0
59	1R	37	37	37	0	0
59	1S	11	11	11	0	0
59	1T	39	39	39	0	0
59	1U	49	49	49	0	0
59	1V	34	34	34	0	0
59	1W	27	27	27	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
59	1X	27	Total 27	O 27	0	0
59	1Y	20	Total 20	O 20	0	0
59	1Z	13	Total 13	O 13	0	0
59	10	25	Total 25	O 25	0	0
59	11	25	Total 25	O 25	0	0
59	12	15	Total 15	O 15	0	0
59	13	25	Total 25	O 25	0	0
59	14	4	Total 4	O 4	0	0
59	15	25	Total 25	O 25	0	0
59	16	22	Total 22	O 22	0	0
59	17	19	Total 19	O 19	0	0
59	18	31	Total 31	O 31	0	0
59	19	9	Total 9	O 9	0	0
59	1a	599	Total 599	O 599	0	0
59	1b	1	Total 1	O 1	0	0
59	1c	1	Total 1	O 1	0	0
59	1d	8	Total 8	O 8	0	0
59	1e	5	Total 5	O 5	0	0
59	1f	3	Total 3	O 3	0	0
59	1h	1	Total 1	O 1	0	0
59	1i	1	Total 1	O 1	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
59	1j	1	Total O 1 1	0	0
59	1k	1	Total O 1 1	0	0
59	1l	5	Total O 5 5	0	0
59	1m	2	Total O 2 2	0	0
59	1o	7	Total O 7 7	0	0
59	1p	3	Total O 3 3	0	0
59	1t	1	Total O 1 1	0	0
59	1y	7	Total O 7 7	0	0
59	2A	2665	Total O 2665 2665	0	0
59	2B	69	Total O 69 69	0	0
59	2D	59	Total O 59 59	0	0
59	2E	33	Total O 33 33	0	0
59	2F	26	Total O 26 26	0	0
59	2G	9	Total O 9 9	0	0
59	2H	4	Total O 4 4	0	0
59	2I	4	Total O 4 4	0	0
59	2N	6	Total O 6 6	0	0
59	2O	23	Total O 23 23	0	0
59	2P	30	Total O 30 30	0	0
59	2Q	28	Total O 28 28	0	0
59	2R	21	Total O 21 21	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
59	2S	7	Total 7	O 7	0	0
59	2T	11	Total 11	O 11	0	0
59	2U	20	Total 20	O 20	0	0
59	2V	6	Total 6	O 6	0	0
59	2W	20	Total 20	O 20	0	0
59	2X	10	Total 10	O 10	0	0
59	2Y	4	Total 4	O 4	0	0
59	2Z	16	Total 16	O 16	0	0
59	20	13	Total 13	O 13	0	0
59	21	22	Total 22	O 22	0	0
59	22	4	Total 4	O 4	0	0
59	23	3	Total 3	O 3	0	0
59	24	2	Total 2	O 2	0	0
59	25	10	Total 10	O 10	0	0
59	26	5	Total 5	O 5	0	0
59	27	9	Total 9	O 9	0	0
59	28	16	Total 16	O 16	0	0
59	29	3	Total 3	O 3	0	0
59	2a	459	Total 459	O 459	0	0
59	2d	6	Total 6	O 6	0	0
59	2e	2	Total 2	O 2	0	0

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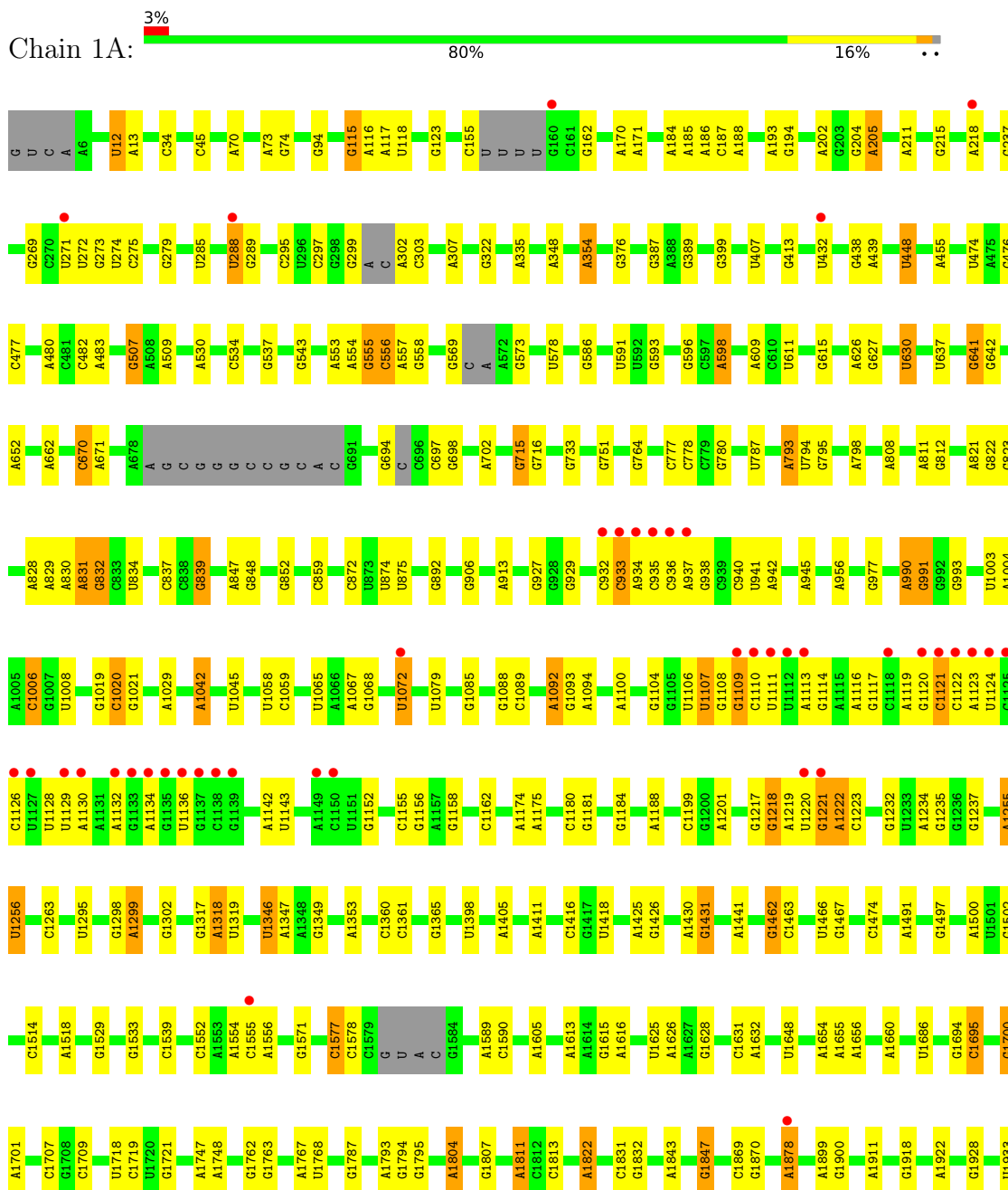
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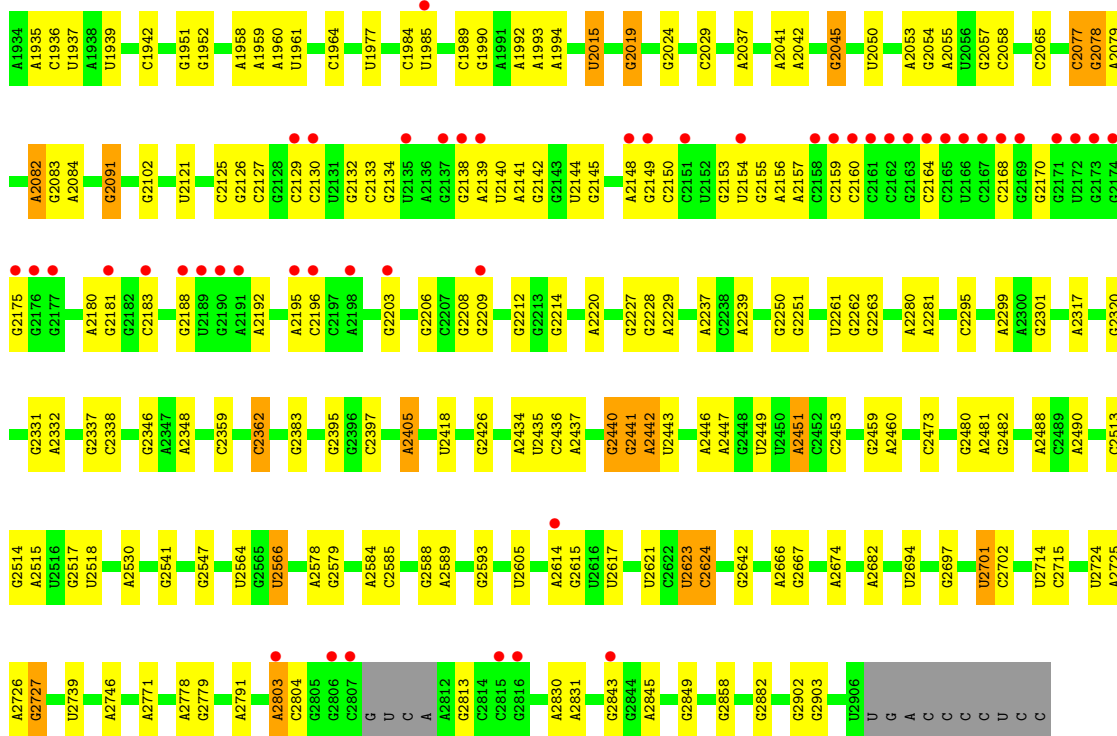
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59	2f	1	Total 1	O 1	0	0
59	2j	2	Total 2	O 2	0	0
59	2l	5	Total 5	O 5	0	0
59	2m	2	Total 2	O 2	0	0
59	2o	2	Total 2	O 2	0	0
59	2p	3	Total 3	O 3	0	0
59	2q	1	Total 1	O 1	0	0
59	2r	5	Total 5	O 5	0	0
59	2t	2	Total 2	O 2	0	0
59	2y	5	Total 5	O 5	0	0

### 3 Residue-property plots [i](#)

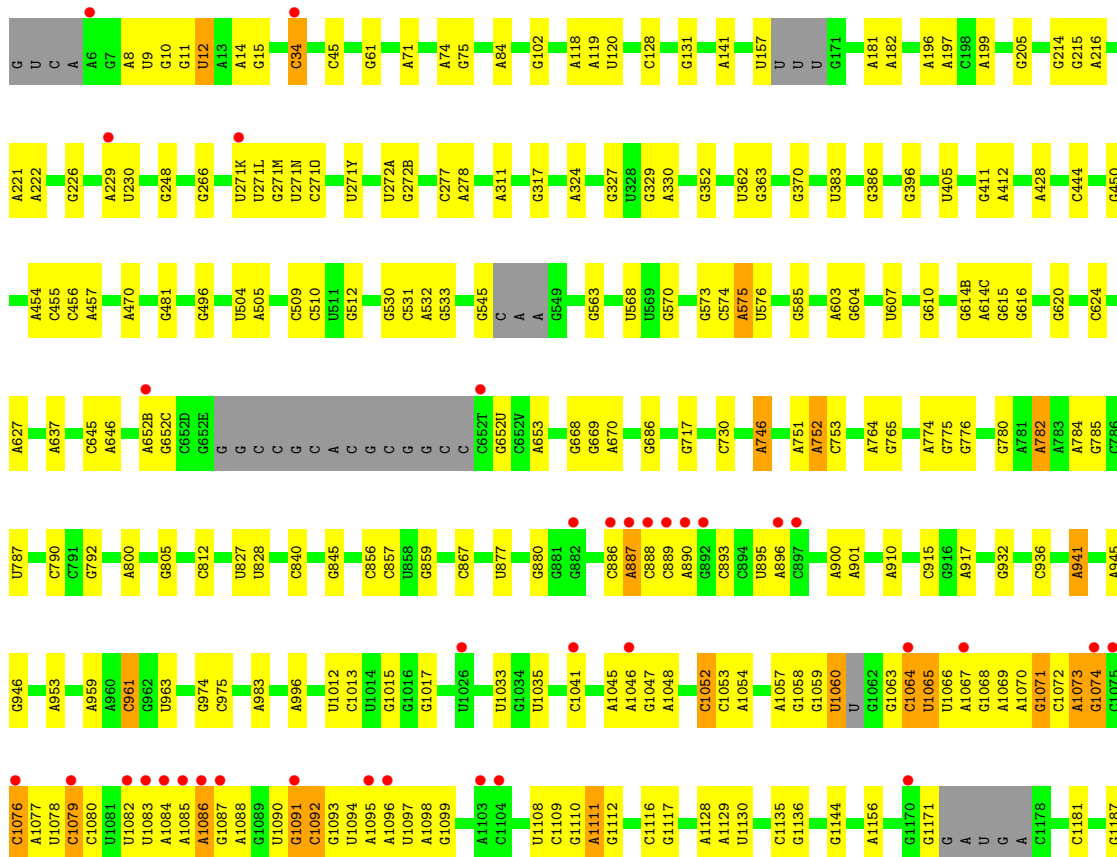
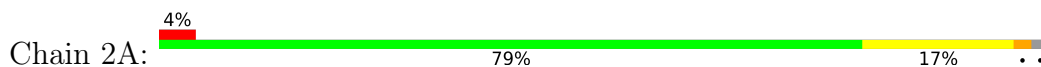
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

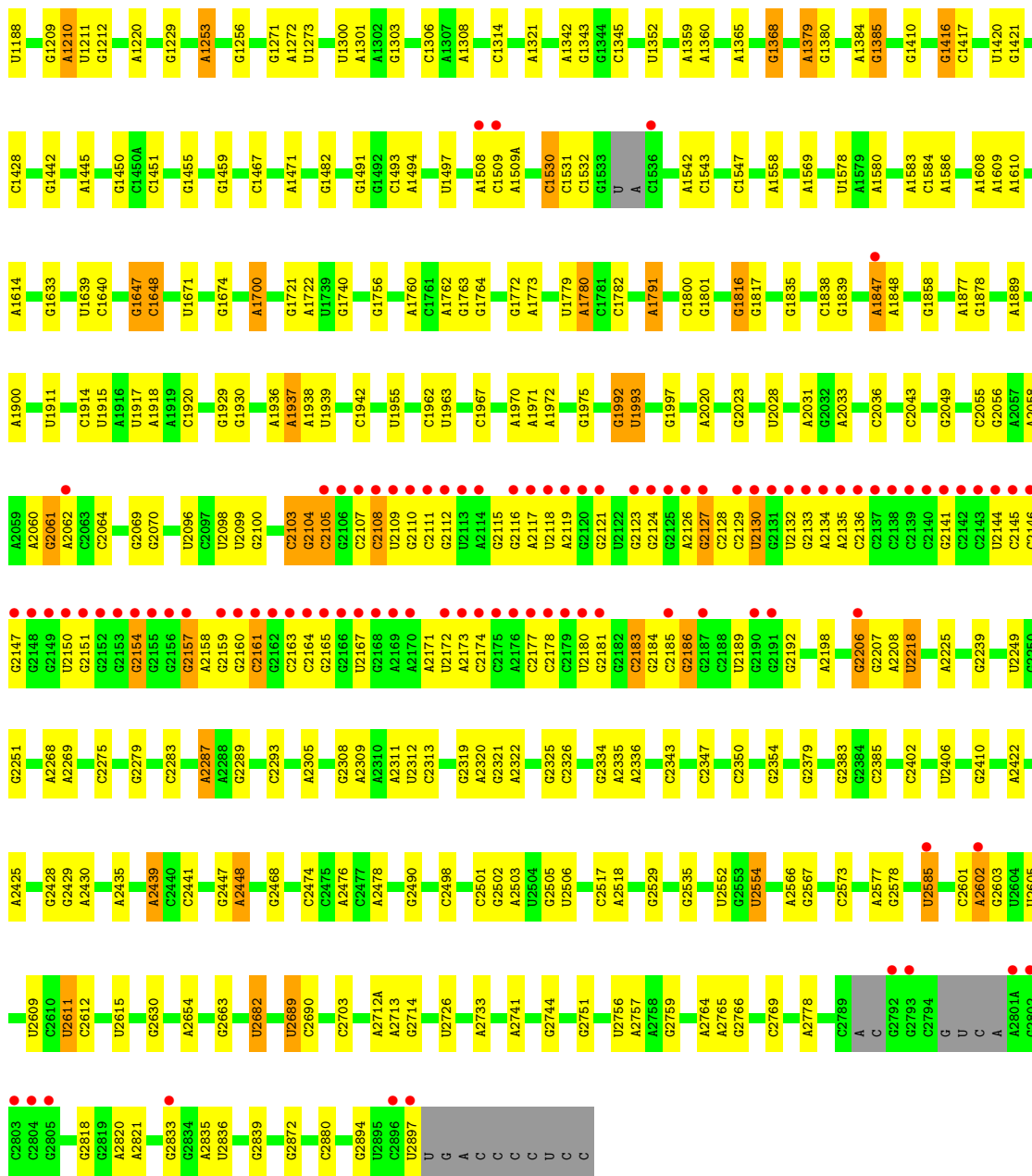
- Molecule 1: 23S Ribosomal RNA



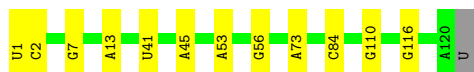


• Molecule 1: 23S Ribosomal RNA

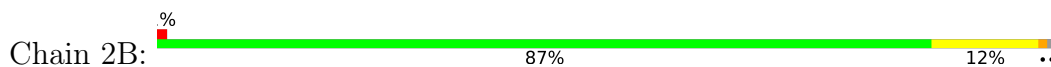




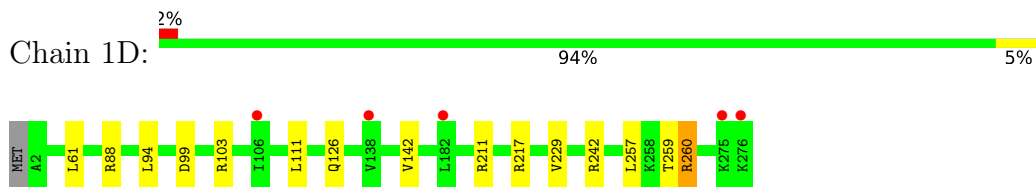
• Molecule 2: 5S Ribosomal RNA



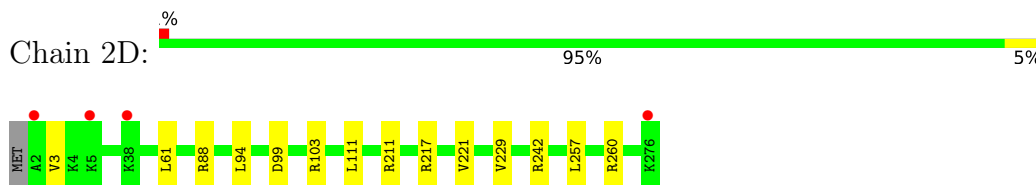
• Molecule 2: 5S Ribosomal RNA



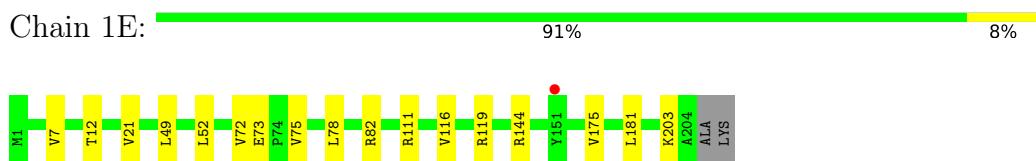
- Molecule 3: 50S ribosomal protein L2



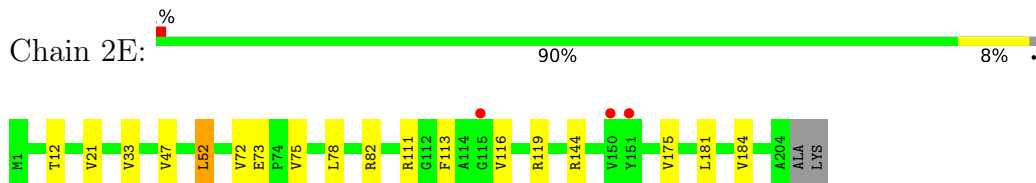
- Molecule 3: 50S ribosomal protein L2



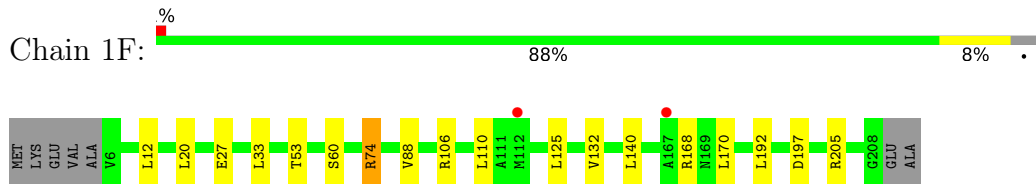
- Molecule 4: 50S ribosomal protein L3



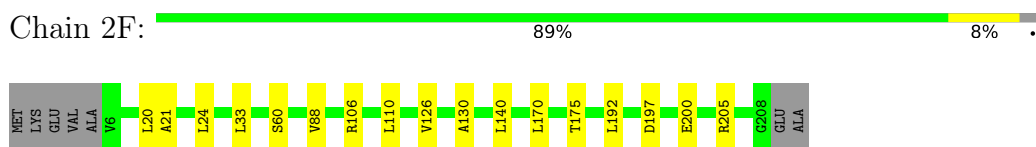
- Molecule 4: 50S ribosomal protein L3



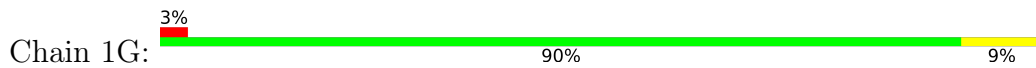
- Molecule 5: 50S ribosomal protein L4



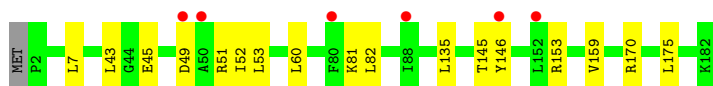
- Molecule 5: 50S ribosomal protein L4



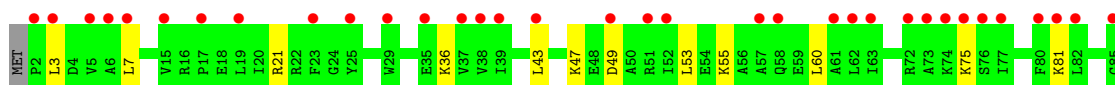
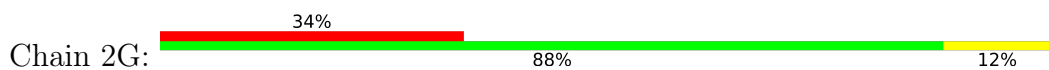
- Molecule 6: 50S ribosomal protein L5







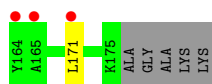
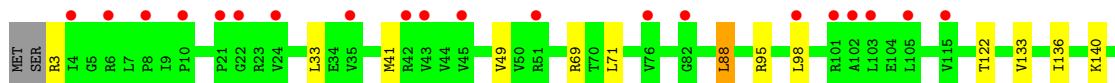
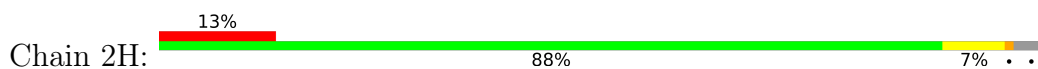
- Molecule 6: 50S ribosomal protein L5



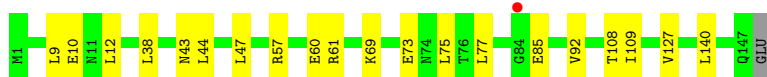
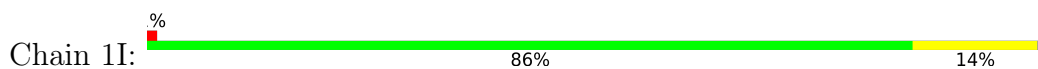
- Molecule 7: 50S ribosomal protein L6



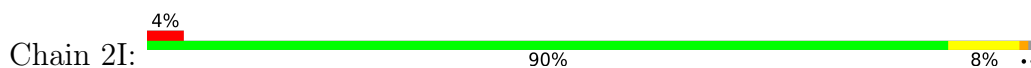
- Molecule 7: 50S ribosomal protein L6



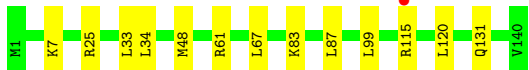
- Molecule 8: 50S ribosomal protein L9



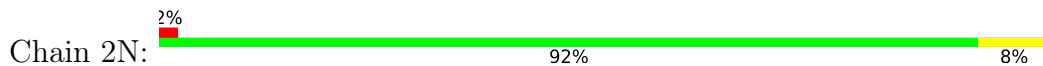
- Molecule 8: 50S ribosomal protein L9



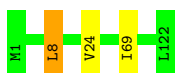
- Molecule 9: 50S ribosomal protein L13



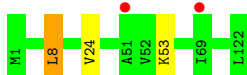
- Molecule 9: 50S ribosomal protein L13



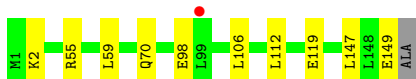
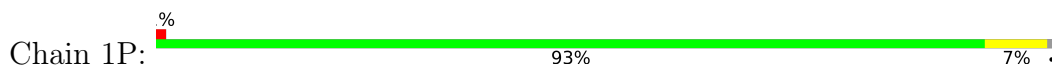
- Molecule 10: 50S ribosomal protein L14



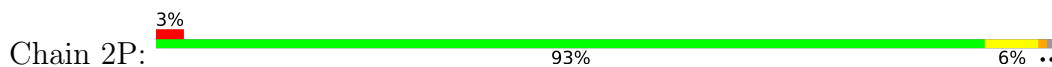
- Molecule 10: 50S ribosomal protein L14



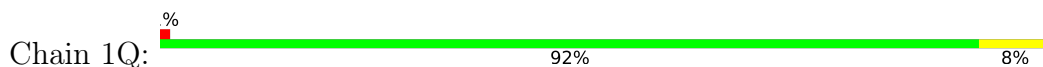
- Molecule 11: 50S ribosomal protein L15



- Molecule 11: 50S ribosomal protein L15



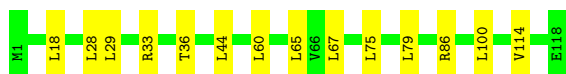
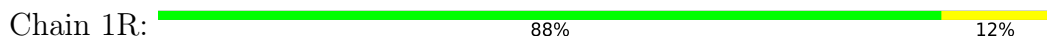
- Molecule 12: 50S ribosomal protein L16



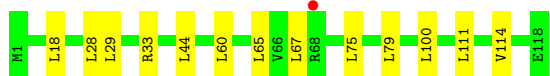
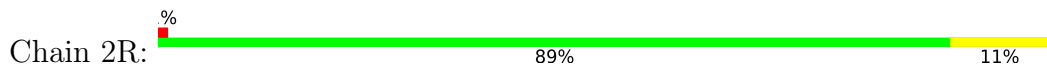
• Molecule 12: 50S ribosomal protein L16



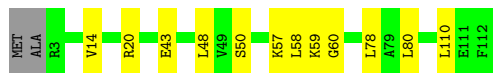
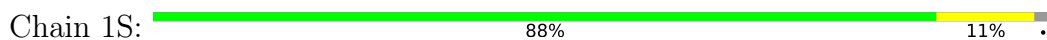
• Molecule 13: 50S ribosomal protein L17



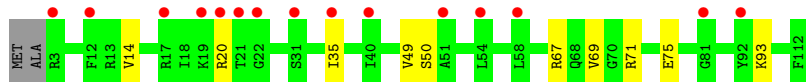
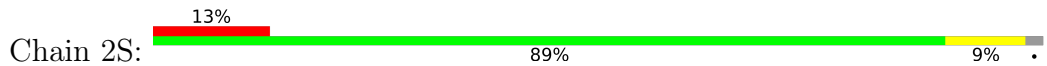
• Molecule 13: 50S ribosomal protein L17



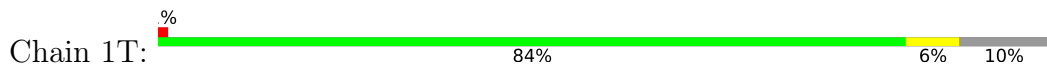
• Molecule 14: 50S ribosomal protein L18



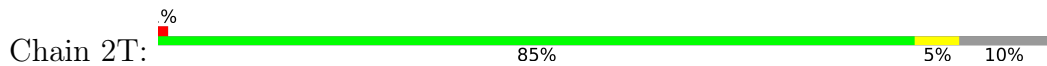
• Molecule 14: 50S ribosomal protein L18

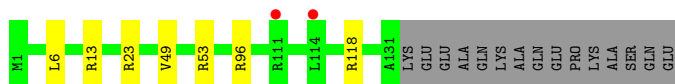


• Molecule 15: 50S ribosomal protein L19

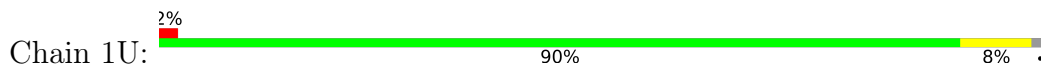


• Molecule 15: 50S ribosomal protein L19





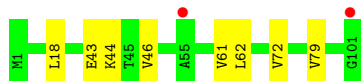
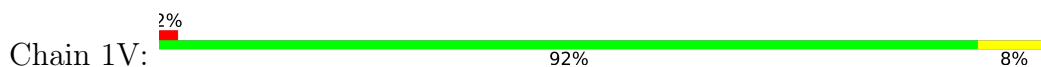
- Molecule 16: 50S ribosomal protein L20



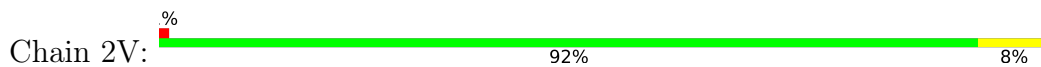
- Molecule 16: 50S ribosomal protein L20



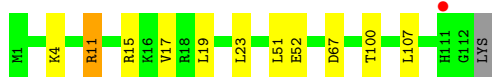
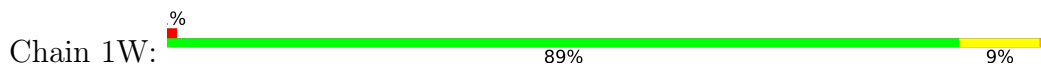
- Molecule 17: 50S ribosomal protein L21



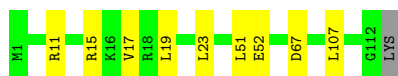
- Molecule 17: 50S ribosomal protein L21



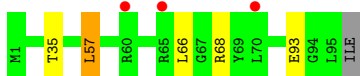
- Molecule 18: 50S ribosomal protein L22



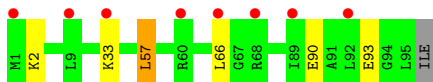
- Molecule 18: 50S ribosomal protein L22



- Molecule 19: 50S ribosomal protein L23



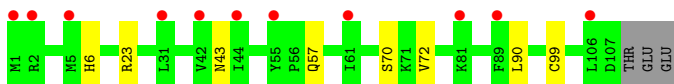
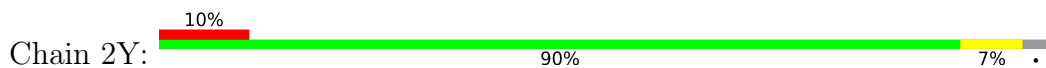
- Molecule 19: 50S ribosomal protein L23



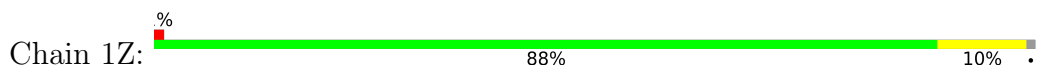
- Molecule 20: 50S ribosomal protein L24



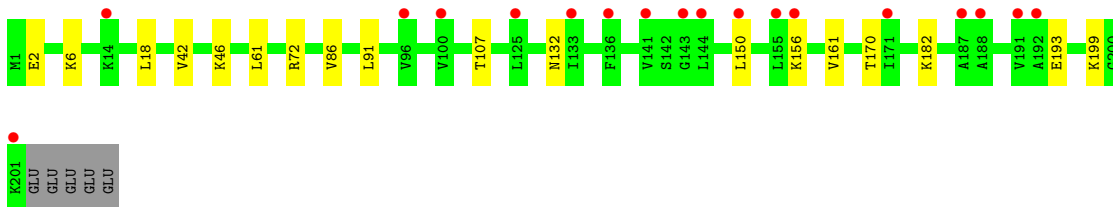
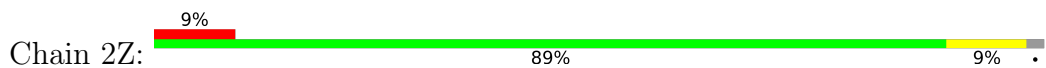
- Molecule 20: 50S ribosomal protein L24



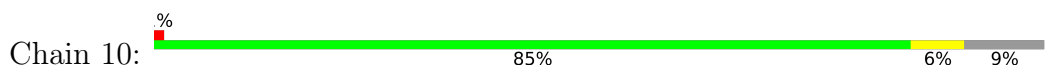
- Molecule 21: 50S ribosomal protein L25



- Molecule 21: 50S ribosomal protein L25

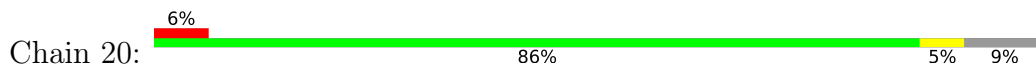


- Molecule 22: 50S ribosomal protein L27

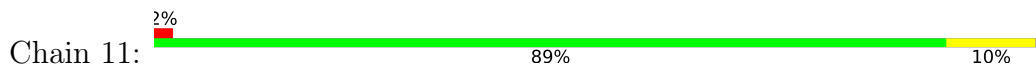




- Molecule 22: 50S ribosomal protein L27



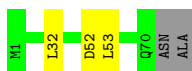
- Molecule 23: 50S ribosomal protein L28



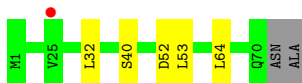
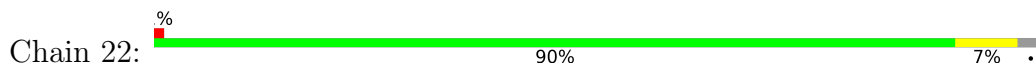
- Molecule 23: 50S ribosomal protein L28



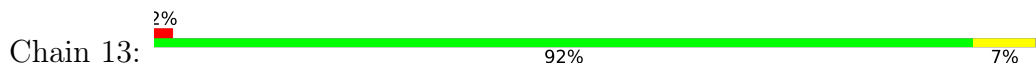
- Molecule 24: 50S ribosomal protein L29



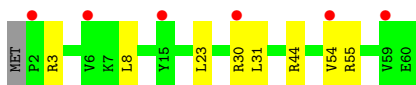
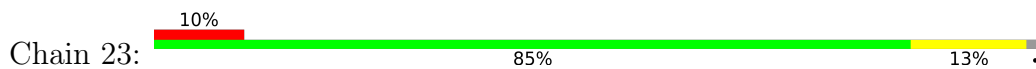
- Molecule 24: 50S ribosomal protein L29



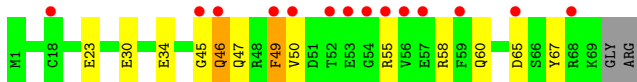
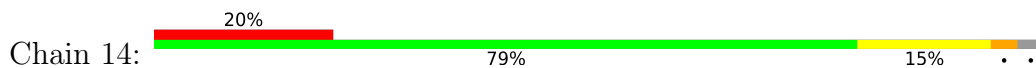
- Molecule 25: 50S ribosomal protein L30



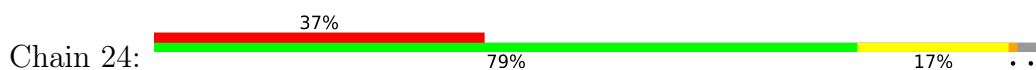
- Molecule 25: 50S ribosomal protein L30



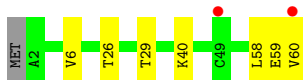
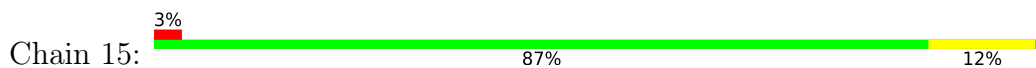
- Molecule 26: 50S ribosomal protein L31



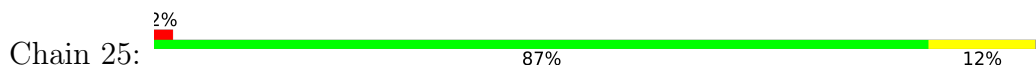
- Molecule 26: 50S ribosomal protein L31



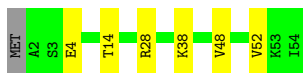
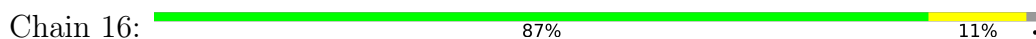
- Molecule 27: 50S ribosomal protein L32



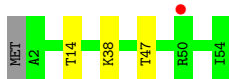
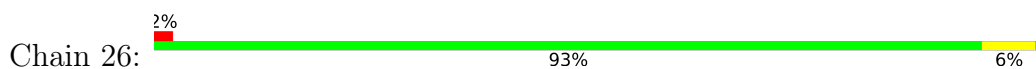
- Molecule 27: 50S ribosomal protein L32



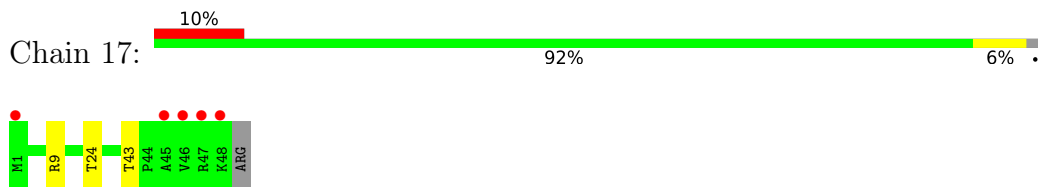
- Molecule 28: 50S ribosomal protein L33



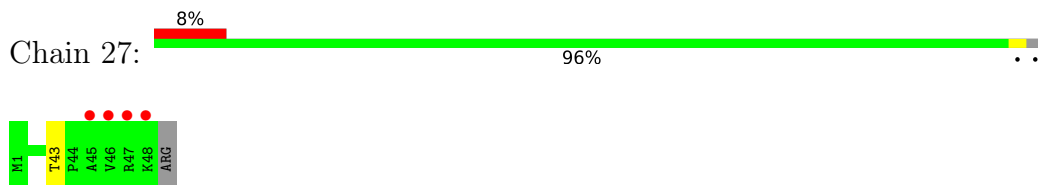
- Molecule 28: 50S ribosomal protein L33



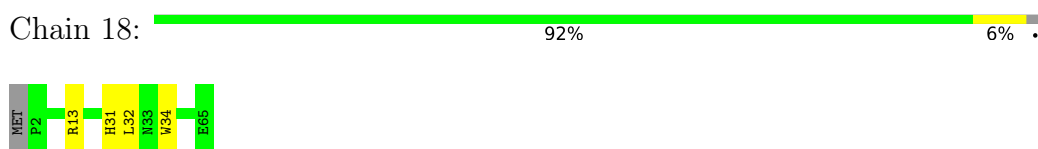
• Molecule 29: 50S ribosomal protein L34



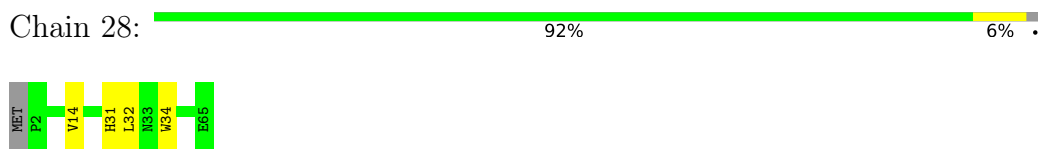
• Molecule 29: 50S ribosomal protein L34



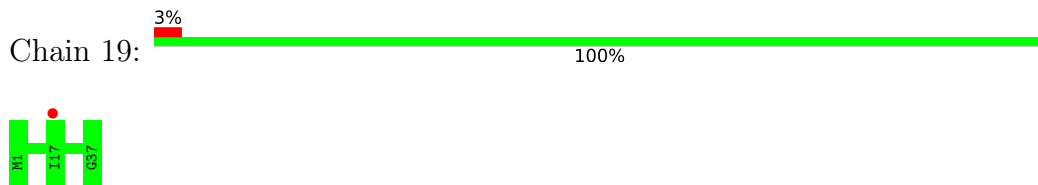
• Molecule 30: 50S ribosomal protein L35



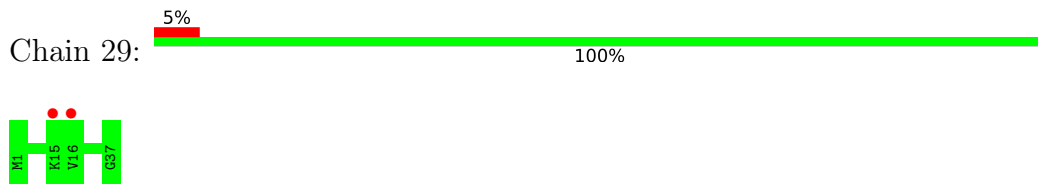
• Molecule 30: 50S ribosomal protein L35



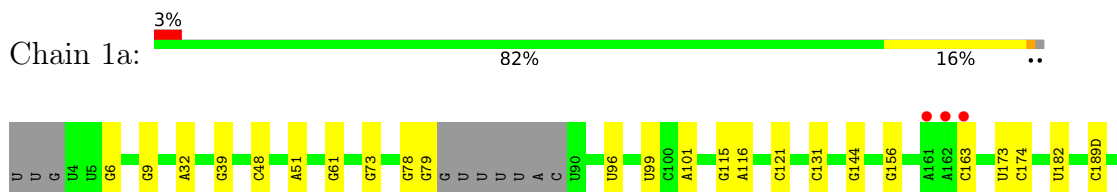
• Molecule 31: 50S ribosomal protein L36



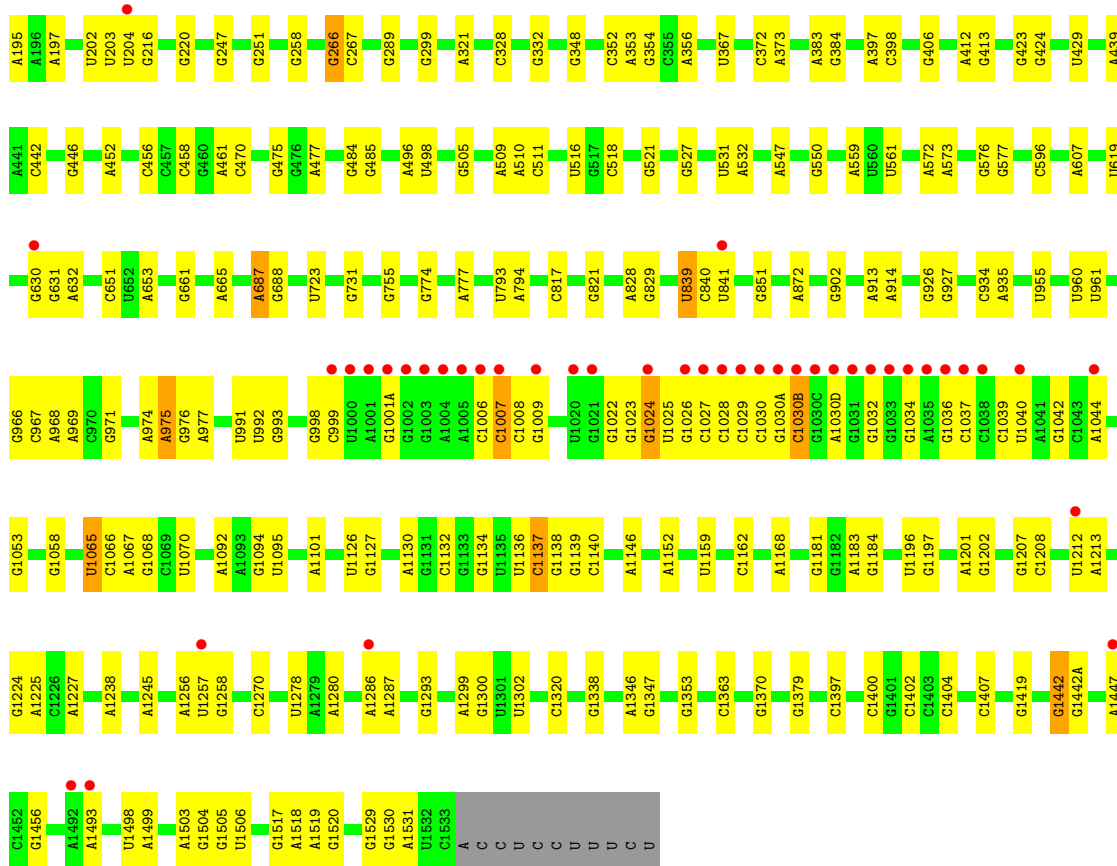
• Molecule 31: 50S ribosomal protein L36



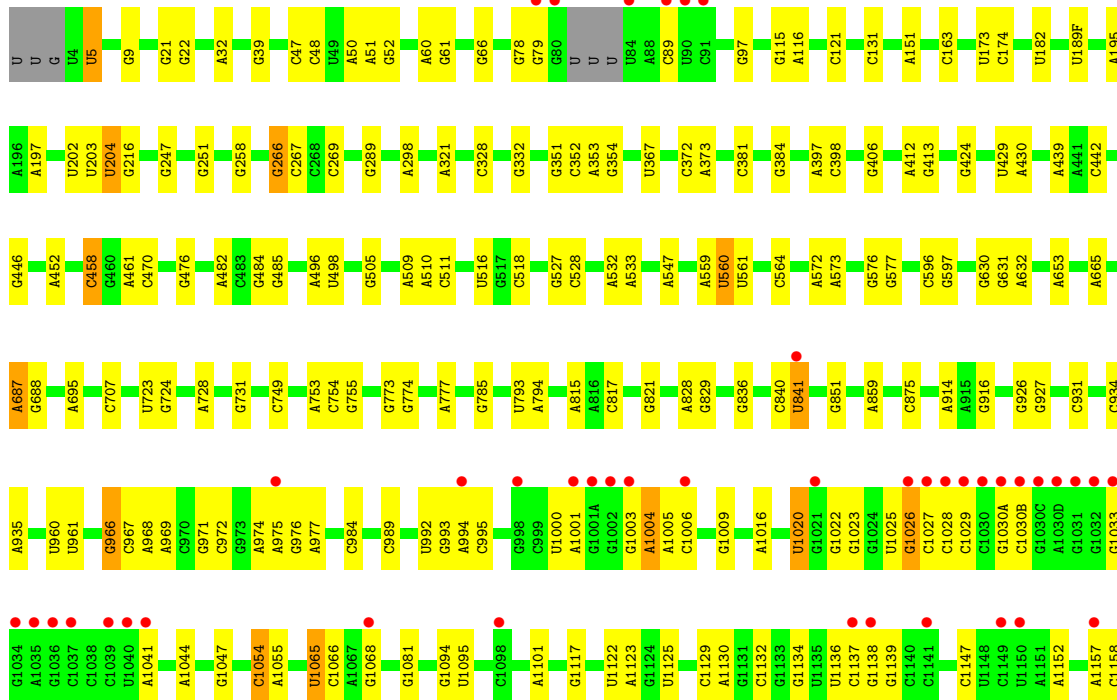
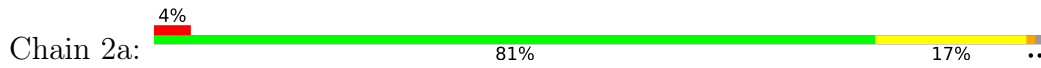
• Molecule 32: 16S Ribosomal RNA

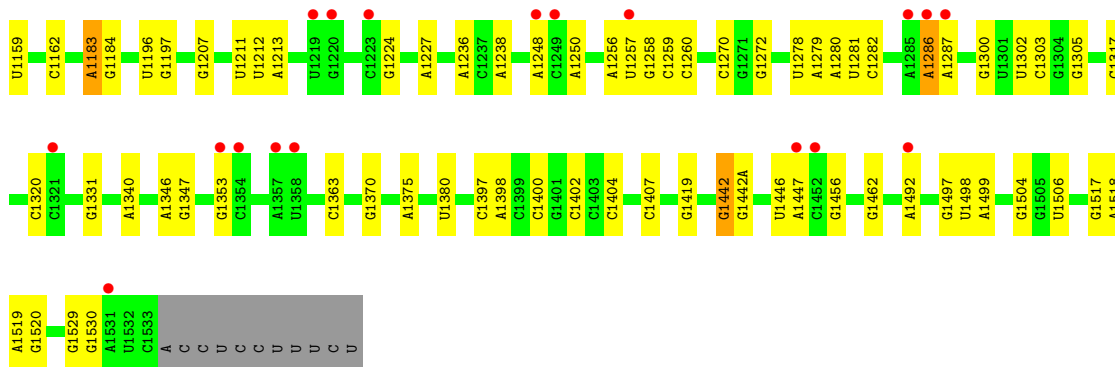




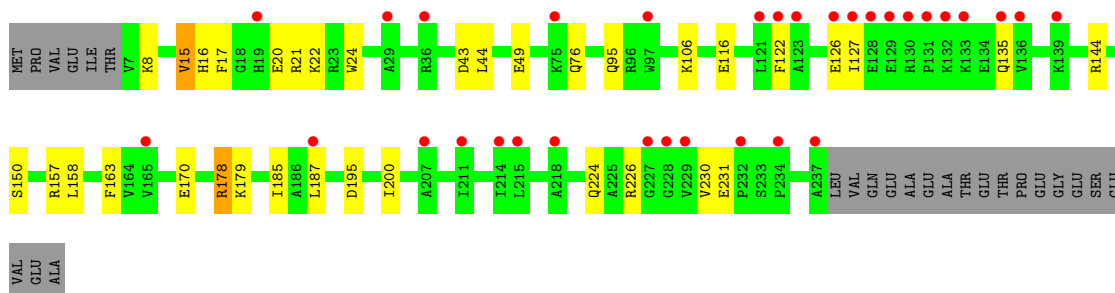
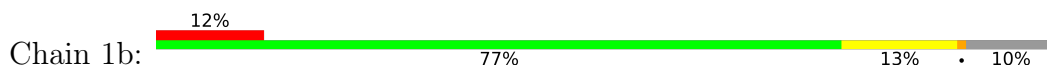


● Molecule 32: 16S Ribosomal RNA

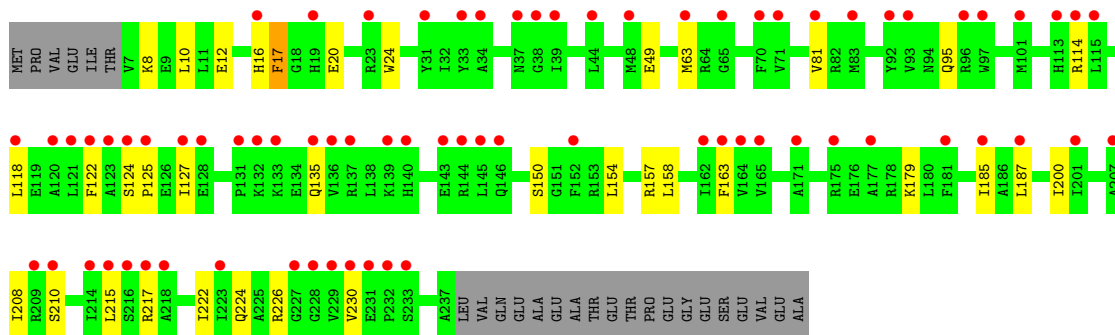
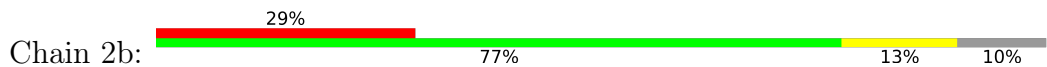




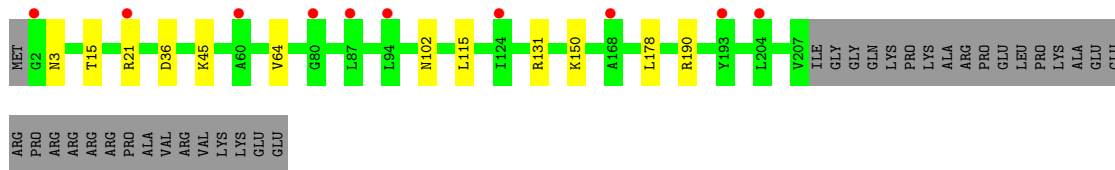
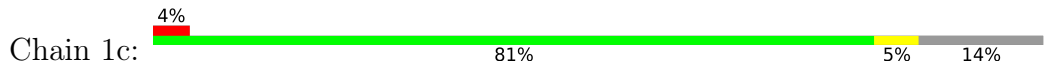
• Molecule 33: 30S ribosomal protein S2



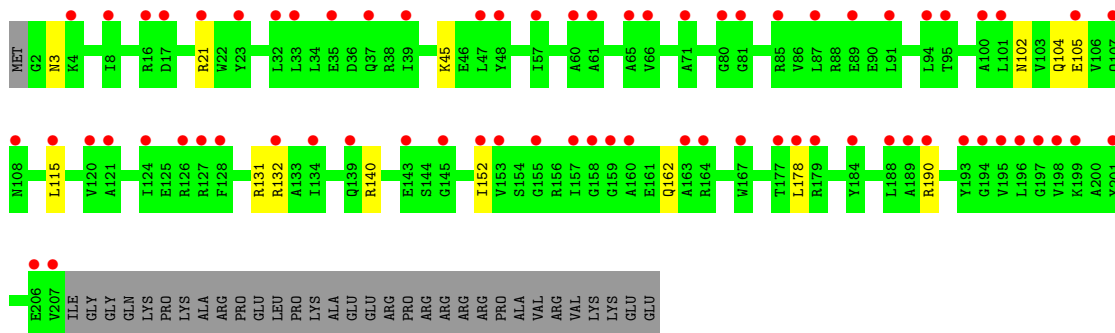
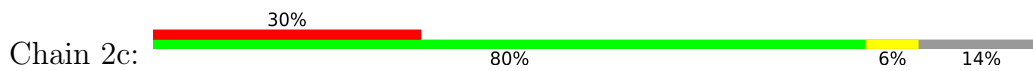
• Molecule 33: 30S ribosomal protein S2



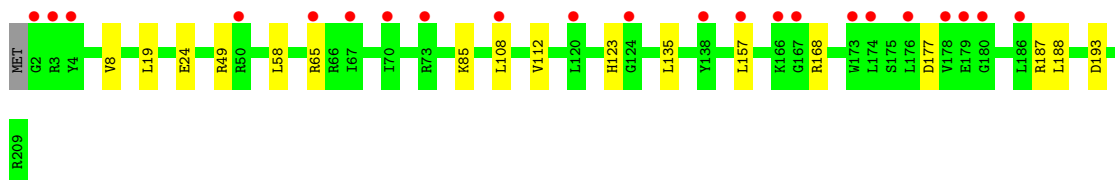
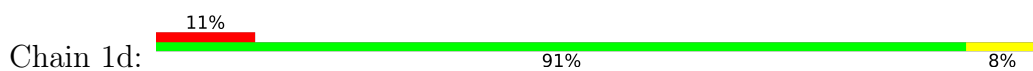
• Molecule 34: 30S ribosomal protein S3



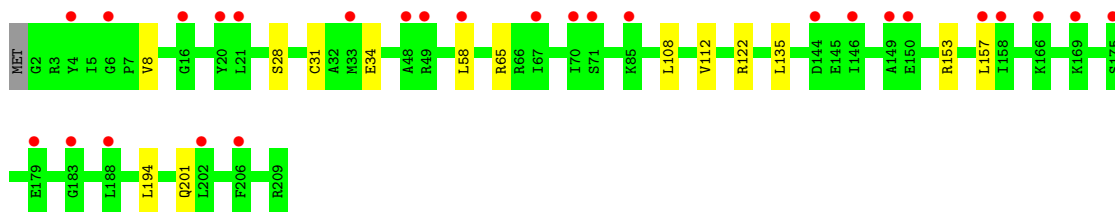
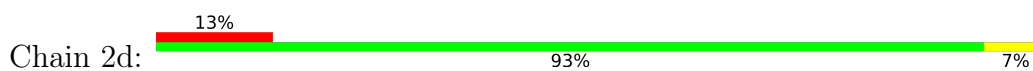
• Molecule 34: 30S ribosomal protein S3



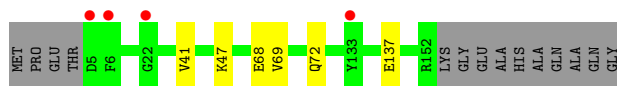
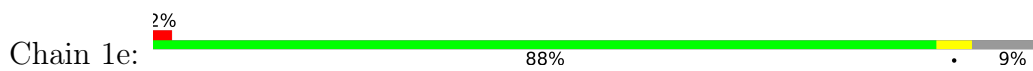
• Molecule 35: 30S ribosomal protein S4



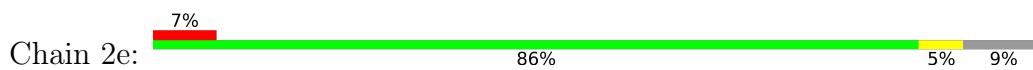
• Molecule 35: 30S ribosomal protein S4



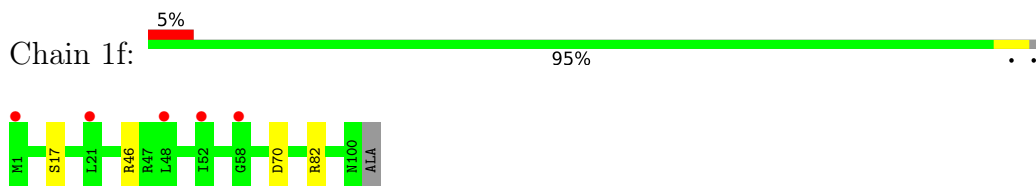
• Molecule 36: 30S ribosomal protein S5



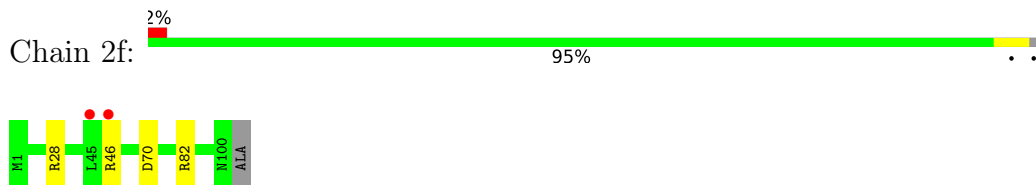
• Molecule 36: 30S ribosomal protein S5



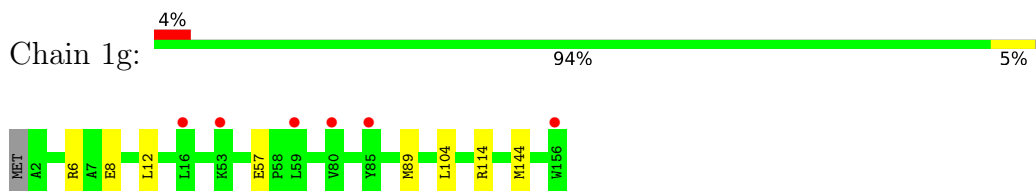
• Molecule 37: 30S ribosomal protein S6



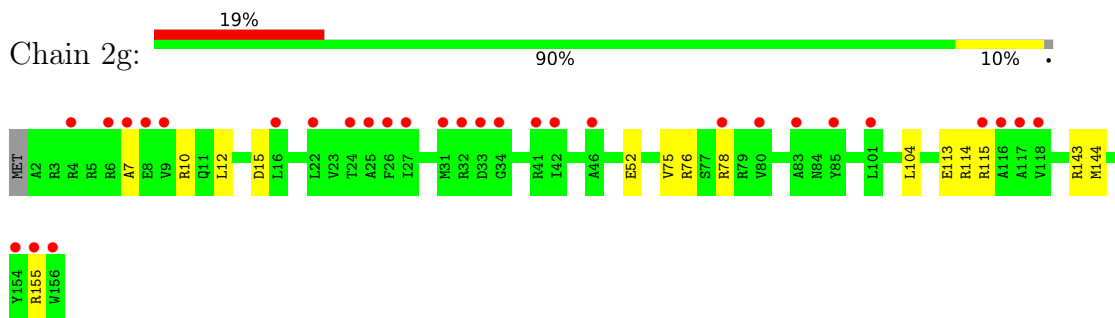
- Molecule 37: 30S ribosomal protein S6



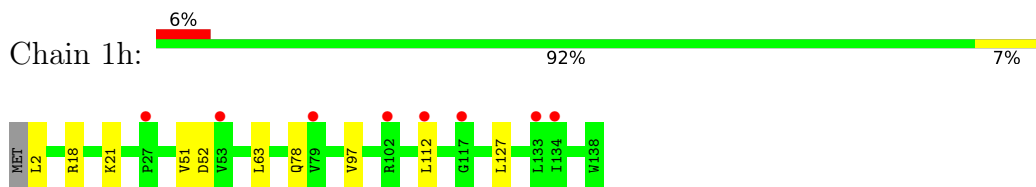
- Molecule 38: 30S ribosomal protein S7



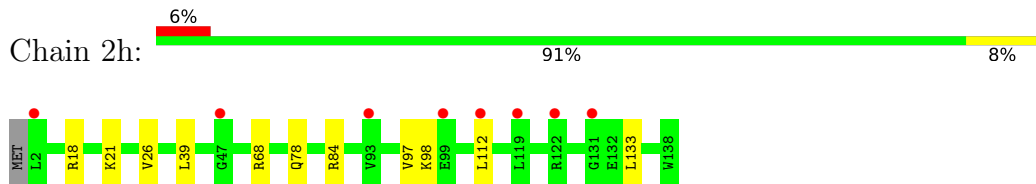
- Molecule 38: 30S ribosomal protein S7



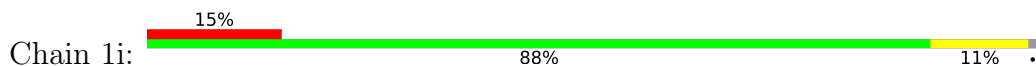
- Molecule 39: 30S ribosomal protein S8

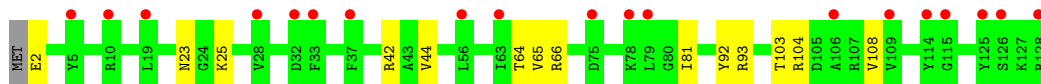


- Molecule 39: 30S ribosomal protein S8

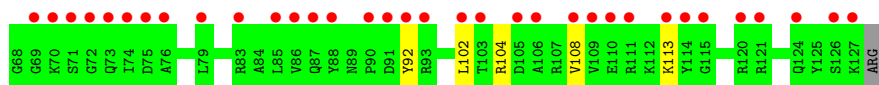
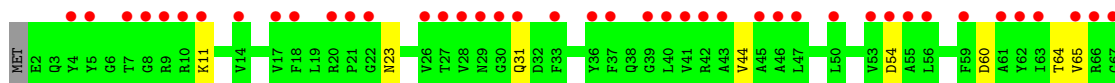
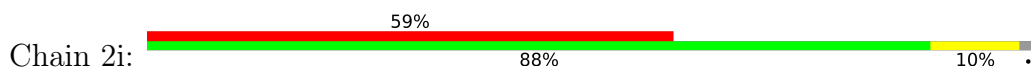


- Molecule 40: 30S ribosomal protein S9

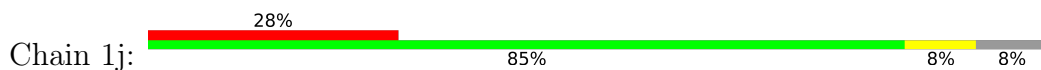




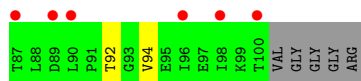
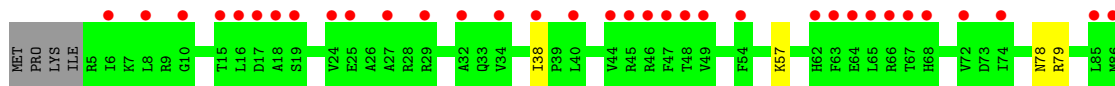
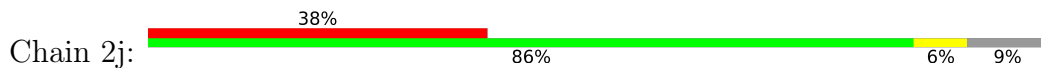
- Molecule 40: 30S ribosomal protein S9



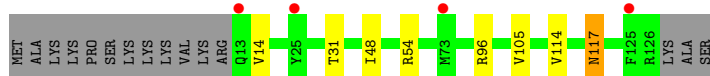
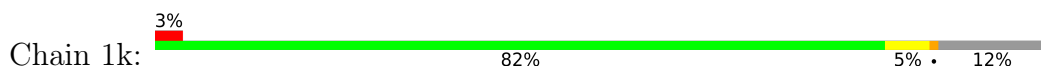
- Molecule 41: 30S ribosomal protein S10



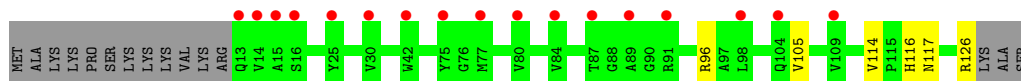
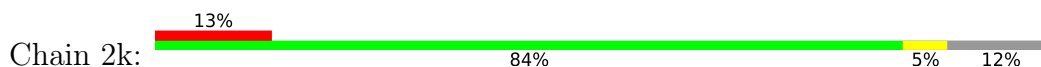
- Molecule 41: 30S ribosomal protein S10



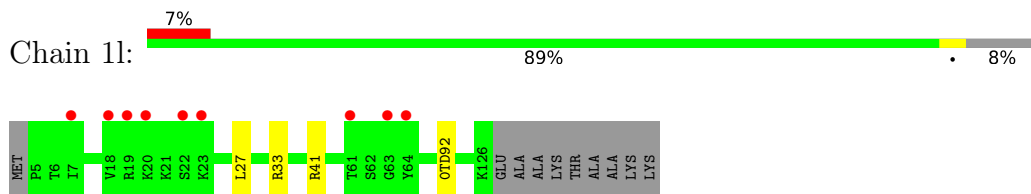
- Molecule 42: 30S ribosomal protein S11



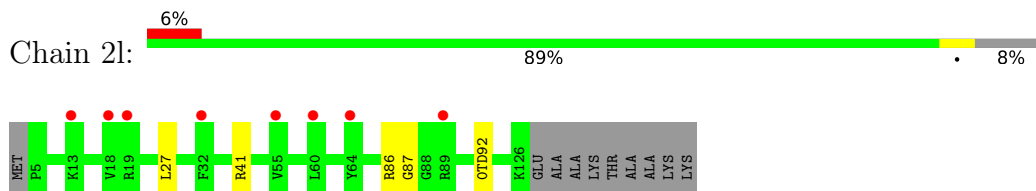
- Molecule 42: 30S ribosomal protein S11



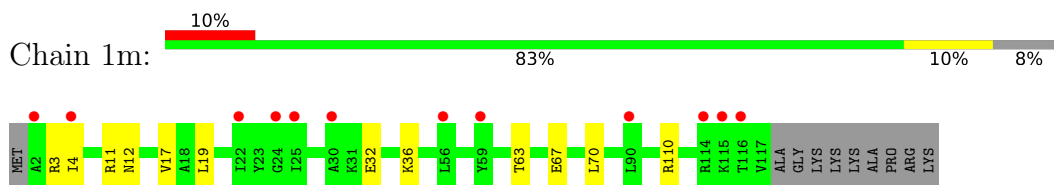
- Molecule 43: 30S ribosomal protein S12



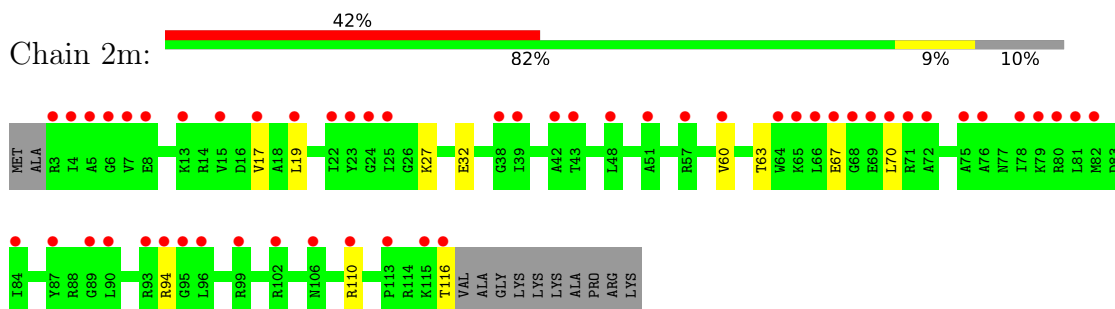
- Molecule 43: 30S ribosomal protein S12



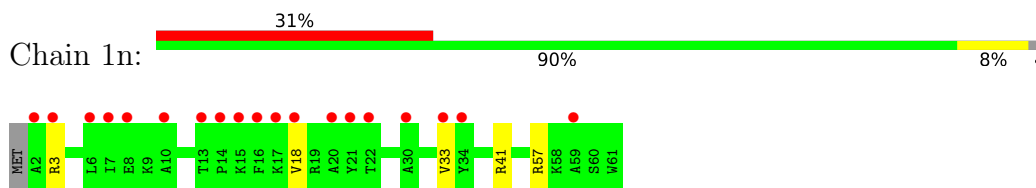
- Molecule 44: 30S ribosomal protein S13



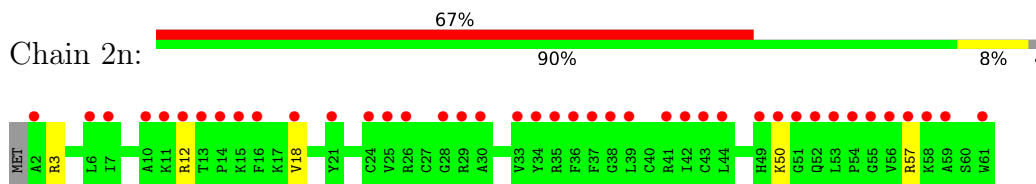
- Molecule 44: 30S ribosomal protein S13



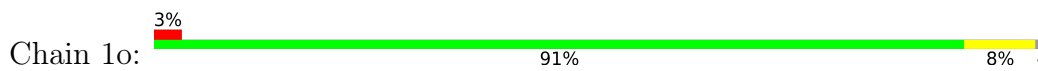
- Molecule 45: 30S ribosomal protein S14 type Z



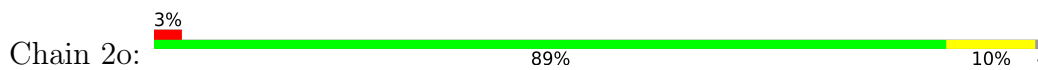
- Molecule 45: 30S ribosomal protein S14 type Z



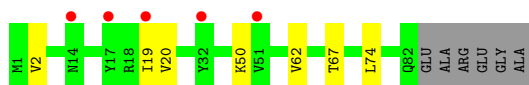
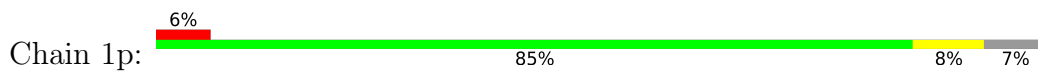
- Molecule 46: 30S ribosomal protein S15



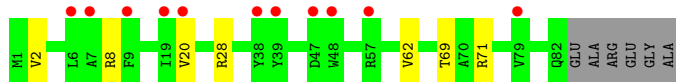
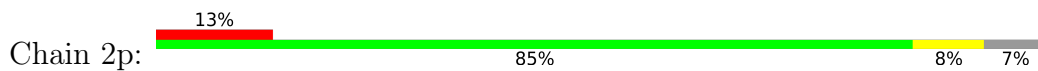
• Molecule 46: 30S ribosomal protein S15



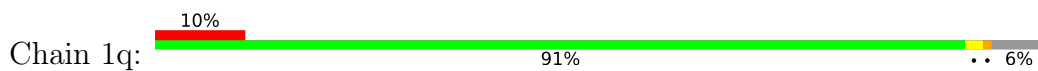
• Molecule 47: 30S ribosomal protein S16



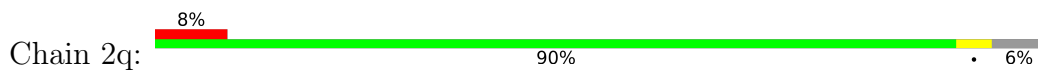
• Molecule 47: 30S ribosomal protein S16



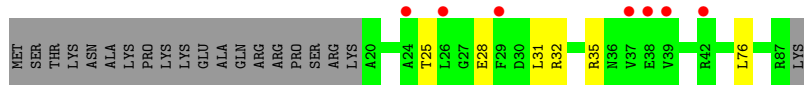
• Molecule 48: 30S ribosomal protein S17



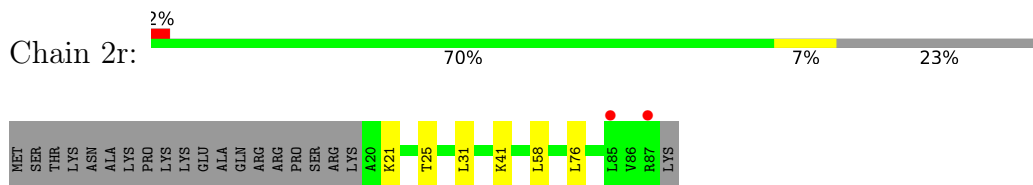
• Molecule 48: 30S ribosomal protein S17



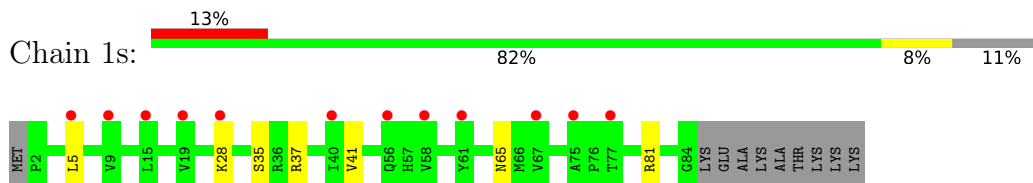
• Molecule 49: 30S ribosomal protein S18



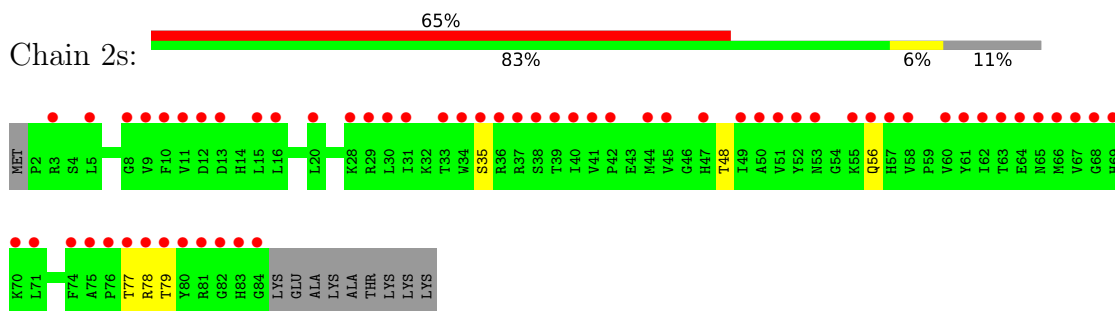
- Molecule 49: 30S ribosomal protein S18



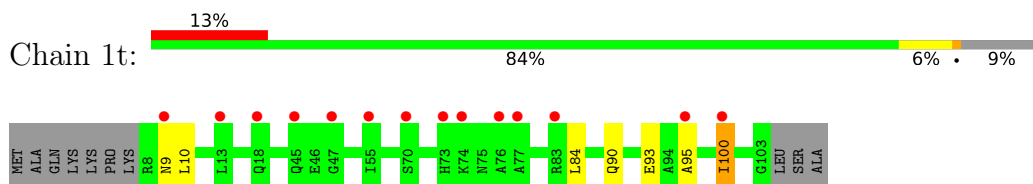
- Molecule 50: 30S ribosomal protein S19



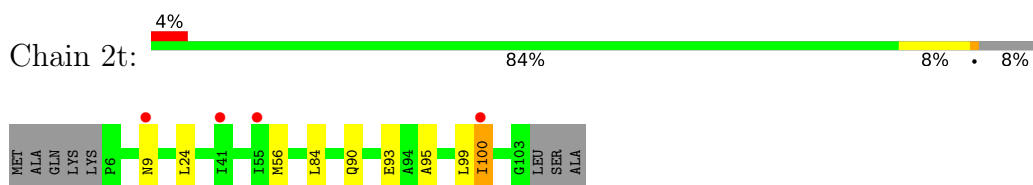
- Molecule 50: 30S ribosomal protein S19



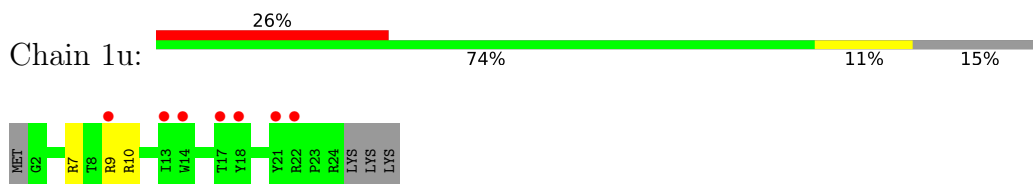
- Molecule 51: 30S ribosomal protein S20



- Molecule 51: 30S ribosomal protein S20

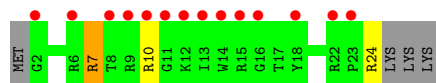
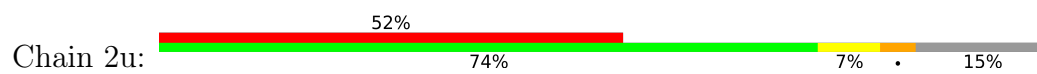


- Molecule 52: 30S ribosomal protein Thx

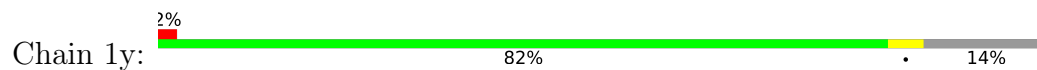


- Molecule 52: 30S ribosomal protein Thx

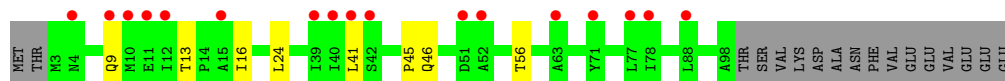
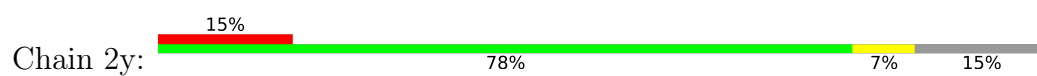




- Molecule 53: Ribosome-associated inhibitor A



- Molecule 53: Ribosome-associated inhibitor A



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	209.16Å 448.37Å 618.12Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	173.22 – 2.30 309.06 – 2.30	Depositor EDS
% Data completeness (in resolution range)	97.5 (173.22-2.30) 97.5 (309.06-2.30)	Depositor EDS
$R_{merge}$	0.15	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.18 (at 2.29Å)	Xtrriage
Refinement program	PHENIX (phenix.refine: 1.8.2_1309)	Depositor
R, $R_{free}$	0.207 , 0.247 0.207 , 0.247	Depositor DCC
$R_{free}$ test set	123763 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	48.4	Xtrriage
Anisotropy	0.173	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.29 , 49.8	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.44$ , $\langle L^2 \rangle = 0.26$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	298502	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	55.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.49% 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 i

### 5.1 Standard geometry i

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

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	0.70	4/69029 (0.0%)	1.14	238/107746 (0.2%)
1	2A	0.58	5/68901 (0.0%)	1.09	188/107544 (0.2%)
2	1B	0.54	0/2876	0.98	2/4486 (0.0%)
2	2B	0.58	0/2878	0.99	2/4490 (0.0%)
3	1D	0.47	0/2181	0.69	1/2940 (0.0%)
3	2D	0.41	0/2186	0.64	0/2944
4	1E	0.48	0/1592	0.64	0/2149
4	2E	0.41	0/1592	0.67	1/2149 (0.0%)
5	1F	0.44	0/1619	0.67	2/2193 (0.1%)
5	2F	0.39	0/1615	0.61	0/2188
6	1G	0.33	0/1451	0.56	0/1961
6	2G	0.38	0/1449	0.54	0/1957
7	1H	0.38	0/1356	0.55	0/1834
7	2H	0.37	0/1350	0.57	1/1826 (0.1%)
8	1I	0.34	0/1109	0.58	0/1512
8	2I	0.32	0/1091	0.59	1/1490 (0.1%)
9	1N	0.44	0/1148	0.64	1/1547 (0.1%)
9	2N	0.33	0/1144	0.55	0/1543
10	1O	0.47	0/943	0.66	1/1269 (0.1%)
10	2O	0.38	0/943	0.61	1/1269 (0.1%)
11	1P	0.47	0/1152	0.70	0/1533
11	2P	0.37	0/1152	0.59	1/1533 (0.1%)
12	1Q	0.48	0/1143	0.63	0/1527
12	2Q	0.41	0/1143	0.59	1/1527 (0.1%)
13	1R	0.47	0/982	0.68	0/1312
13	2R	0.39	0/982	0.63	0/1312
14	1S	0.40	0/887	0.59	0/1180
14	2S	0.40	0/880	0.61	0/1172
15	1T	0.43	0/1105	0.65	0/1477
15	2T	0.39	0/1097	0.61	0/1468
16	1U	0.47	0/977	0.66	0/1301

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
16	2U	0.42	0/977	0.62	0/1301
17	1V	0.44	0/786	0.61	0/1053
17	2V	0.42	0/782	0.62	0/1049
18	1W	0.48	0/897	0.65	1/1205 (0.1%)
18	2W	0.45	0/897	0.59	0/1205
19	1X	0.49	0/764	0.65	1/1025 (0.1%)
19	2X	0.44	0/764	0.62	1/1025 (0.1%)
20	1Y	0.43	0/823	0.65	0/1099
20	2Y	0.38	0/823	0.59	0/1100
21	1Z	0.36	0/1620	0.54	0/2200
21	2Z	0.37	0/1590	0.56	0/2162
22	10	0.48	0/616	0.67	1/821 (0.1%)
22	20	0.35	0/616	0.54	0/821
23	11	0.41	0/761	0.60	0/1013
23	21	0.40	0/766	0.59	0/1018
24	12	0.38	0/590	0.54	0/781
24	22	0.40	0/594	0.50	0/785
25	13	0.45	0/474	0.62	0/635
25	23	0.36	0/469	0.61	0/630
26	14	0.40	0/559	0.71	0/754
26	24	0.44	0/549	0.67	0/741
27	15	0.46	0/473	0.67	0/639
27	25	0.38	0/469	0.57	0/635
28	16	0.43	0/460	0.55	0/613
28	26	0.40	0/456	0.53	0/608
29	17	0.49	0/426	0.76	1/561 (0.2%)
29	27	0.42	0/426	0.66	0/561
30	18	0.47	0/525	0.65	1/691 (0.1%)
30	28	0.42	0/525	0.65	0/691
31	19	0.44	0/310	0.58	0/407
31	29	0.37	0/310	0.54	0/407
32	1a	0.46	0/35795	0.95	28/55864 (0.1%)
32	2a	0.43	0/35890	0.92	43/56012 (0.1%)
33	1b	0.35	0/1876	0.61	1/2533 (0.0%)
33	2b	0.37	0/1860	0.59	0/2518
34	1c	0.33	0/1582	0.53	0/2137
34	2c	0.36	0/1566	0.54	0/2119
35	1d	0.35	0/1695	0.55	0/2274
35	2d	0.33	0/1698	0.52	0/2277
36	1e	0.34	0/1149	0.57	0/1548
36	2e	0.35	0/1149	0.55	0/1548
37	1f	0.37	0/827	0.57	0/1120
37	2f	0.35	0/829	0.55	0/1123

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
38	1g	0.31	0/1254	0.48	0/1683
38	2g	0.33	0/1248	0.51	0/1676
39	1h	0.31	0/1118	0.53	0/1506
39	2h	0.30	0/1108	0.54	0/1494
40	1i	0.32	0/1005	0.56	0/1351
40	2i	0.37	0/985	0.57	0/1329
41	1j	0.31	0/732	0.57	0/993
41	2j	0.33	0/723	0.55	0/984
42	1k	0.34	0/849	0.54	0/1150
42	2k	0.34	0/848	0.58	0/1149
43	1l	0.35	0/937	0.54	0/1260
43	2l	0.35	0/937	0.62	1/1260 (0.1%)
44	1m	0.33	0/924	0.57	0/1242
44	2m	0.31	0/905	0.57	0/1217
45	1n	0.36	0/501	0.48	0/664
45	2n	0.35	0/501	0.50	0/664
46	1o	0.33	0/739	0.55	0/985
46	2o	0.32	0/739	0.53	0/985
47	1p	0.32	0/697	0.59	0/939
47	2p	0.34	0/693	0.55	0/935
48	1q	0.34	0/836	0.54	0/1117
48	2q	0.35	0/836	0.54	0/1117
49	1r	0.33	0/560	0.59	0/746
49	2r	0.34	0/560	0.53	0/746
50	1s	0.30	0/663	0.57	0/895
50	2s	0.35	0/660	0.56	0/893
51	1t	0.34	0/734	0.56	0/969
51	2t	0.30	0/736	0.49	0/976
52	1u	0.30	0/203	0.47	0/266
52	2u	0.35	0/203	0.54	0/266
53	1y	0.35	0/776	0.53	0/1048
53	2y	0.31	0/761	0.48	0/1030
All	All	0.53	9/309937 (0.0%)	0.95	520/463223 (0.1%)

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
14	1S	0	1
19	1X	0	1

*Continued on next page...*

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Mol	Chain	#Chirality outliers	#Planarity outliers
19	2X	0	1
33	1b	0	1
43	2l	0	1
All	All	0	5

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	1A	354	A	N9-C4	-7.97	1.33	1.37
1	2A	2104	G	N1-C2	-7.56	1.31	1.37
1	1A	2261	U	C4-O4	-6.50	1.18	1.23
1	2A	1086	A	N9-C4	6.07	1.41	1.37
1	2A	2104	G	C6-N1	-5.82	1.35	1.39
1	2A	2185	C	N3-C4	-5.82	1.29	1.33
1	2A	1059	G	N3-C4	5.59	1.39	1.35
1	1A	2050	U	C4-O4	-5.41	1.19	1.23
1	1A	2803	A	N9-C4	5.35	1.41	1.37

All (520) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	2A	2185	C	N1-C2-O2	19.49	130.60	118.90
1	2A	1079	C	N1-C2-O2	17.91	129.65	118.90
1	2A	2104	G	C5-C6-O6	17.73	139.24	128.60
1	2A	2104	G	N3-C2-N2	17.60	132.22	119.90
1	1A	991	G	O5'-P-OP1	-15.11	92.10	105.70
1	2A	2104	G	N1-C2-N2	-14.60	103.06	116.20
1	1A	1184	G	O5'-P-OP2	-14.56	92.60	105.70
1	2A	1079	C	N3-C2-O2	-13.77	112.26	121.90
1	1A	2566	U	O5'-P-OP1	-13.67	93.40	105.70
1	2A	1064	C	N1-C2-O2	13.36	126.91	118.90
1	2A	2185	C	C2-N3-C4	13.21	126.51	119.90
1	1A	593	G	C5-C6-O6	-12.59	121.05	128.60
1	1A	2019	G	O5'-P-OP2	-12.55	94.41	105.70
1	1A	354	A	C2-N3-C4	-12.16	104.52	110.60
1	2A	2104	G	C6-N1-C2	11.90	132.24	125.10
1	1A	537	G	O4'-C1'-N9	11.64	117.51	108.20
1	2A	1648	C	O5'-P-OP1	-11.55	95.31	105.70
1	1A	1132	A	N1-C6-N6	-11.03	111.98	118.60
1	1A	598	A	O5'-P-OP1	-10.68	96.09	105.70
1	1A	1686	U	O5'-P-OP2	-10.63	96.14	105.70
1	1A	1042	A	O5'-P-OP1	-10.58	96.17	105.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1A	2045	G	O5'-P-OP1	-10.57	96.18	105.70
1	1A	1822	A	O5'-P-OP1	-10.37	96.37	105.70
1	1A	354	A	N1-C2-N3	9.89	134.25	129.30
1	2A	2104	G	N1-C6-O6	-9.86	113.98	119.90
1	1A	2159	C	C6-N1-C2	-9.84	116.37	120.30
1	2A	1079	C	C2-N1-C1'	9.74	129.52	118.80
1	2A	2185	C	N3-C2-O2	-9.72	115.10	121.90
1	2A	1079	C	C6-N1-C2	-9.68	116.43	120.30
1	2A	2682	U	O5'-P-OP2	-9.61	97.05	105.70
1	2A	2185	C	N3-C4-N4	-9.60	111.28	118.00
1	2A	512	G	O4'-C1'-N9	9.58	115.87	108.20
1	2A	2185	C	C5-C6-N1	9.57	125.79	121.00
1	2A	2104	G	C5-C6-N1	-9.47	106.77	111.50
1	1A	630	U	O5'-P-OP1	-9.46	97.19	105.70
1	1A	1318	A	O5'-P-OP2	-9.46	97.19	105.70
1	1A	1811	A	O5'-P-OP2	-9.43	97.22	105.70
1	1A	2281	A	O5'-P-OP1	-9.42	97.22	105.70
1	1A	2442	A	O5'-P-OP2	-9.36	97.28	105.70
1	1A	593	G	C5-C6-N1	9.21	116.10	111.50
1	2A	1791	A	O5'-P-OP1	-9.15	97.46	105.70
1	1A	215	G	O4'-C1'-N9	9.13	115.50	108.20
1	2A	2185	C	C5-C4-N4	9.12	126.58	120.20
1	2A	1059	G	N3-C2-N2	9.06	126.25	119.90
1	1A	1418	U	C5-C4-O4	-9.05	120.47	125.90
1	1A	1110	C	N1-C2-O2	8.98	124.29	118.90
1	1A	798	A	O5'-P-OP1	-8.89	97.70	105.70
1	2A	746	A	O4'-C1'-N9	8.70	115.16	108.20
1	2A	2185	C	C4-C5-C6	-8.66	113.07	117.40
1	1A	1072	U	O5'-P-OP1	-8.64	97.92	105.70
1	2A	568	U	C5-C4-O4	-8.61	120.73	125.90
1	1A	1441	A	O5'-P-OP1	-8.57	97.99	105.70
32	2a	1003	G	C8-N9-C4	-8.57	102.97	106.40
1	1A	1418	U	N3-C4-O4	8.52	125.36	119.40
1	1A	2159	C	N3-C2-O2	-8.50	115.95	121.90
1	2A	1064	C	C2-N3-C4	8.40	124.10	119.90
1	2A	1368	G	O5'-P-OP2	-8.30	98.23	105.70
1	1A	2623	U	O5'-P-OP1	-8.27	98.25	105.70
1	1A	2159	C	C2-N1-C1'	8.19	127.80	118.80
1	1A	2589	A	O5'-P-OP1	-8.18	98.34	105.70
1	2A	1064	C	N3-C2-O2	-8.18	116.17	121.90
1	1A	2605	U	N3-C4-O4	-8.16	113.69	119.40
1	1A	1648	U	N3-C4-O4	-8.11	113.72	119.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	2a	1003	G	N3-C4-C5	-8.05	124.58	128.60
32	2a	1158	C	C2-N1-C1'	8.04	127.65	118.80
1	1A	1121	C	N1-C2-O2	8.00	123.70	118.90
1	1A	2261	U	N3-C4-C5	7.95	119.37	114.60
1	1A	593	G	N9-C4-C5	-7.90	102.24	105.40
1	2A	1092	C	C6-N1-C2	-7.83	117.17	120.30
32	2a	1054	C	N1-C2-O2	7.82	123.59	118.90
32	2a	1003	G	C4-N9-C1'	7.78	136.62	126.50
19	2X	57	LEU	CA-CB-CG	7.74	133.10	115.30
1	2A	780	G	C5-C6-O6	-7.73	123.96	128.60
1	2A	2105	C	C5-C6-N1	7.72	124.86	121.00
32	2a	1003	G	N7-C8-N9	7.71	116.96	113.10
1	2A	2554	U	O5'-P-OP1	-7.71	98.76	105.70
1	1A	2159	C	N3-C4-C5	-7.70	118.82	121.90
32	1a	1137	C	C5-C6-N1	7.69	124.84	121.00
1	2A	570	G	C4-C5-N7	7.69	113.88	110.80
1	2A	2036	C	O5'-P-OP1	-7.68	98.79	105.70
32	1a	1030(B)	C	N1-C2-O2	7.67	123.50	118.90
1	1A	2091	G	O5'-P-OP2	-7.66	98.81	105.70
1	1A	2697	G	N1-C6-O6	-7.62	115.33	119.90
1	1A	848	G	O5'-P-OP2	-7.56	98.90	105.70
32	1a	1137	C	C6-N1-C2	-7.55	117.28	120.30
1	1A	2694	U	O5'-P-OP2	-7.53	98.92	105.70
1	2A	12	U	N3-C2-O2	-7.52	116.93	122.20
1	2A	576	U	O5'-P-OP1	-7.47	98.97	105.70
1	2A	1671	U	O5'-P-OP2	-7.47	98.97	105.70
1	2A	1079	C	C5-C6-N1	7.44	124.72	121.00
1	2A	1097	U	C2-N1-C1'	7.39	126.57	117.70
1	2A	2439	A	O5'-P-OP2	-7.39	99.05	105.70
1	1A	2079	A	N1-C6-N6	-7.38	114.17	118.60
1	2A	585	G	O5'-P-OP2	-7.36	99.07	105.70
1	1A	2045	G	O5'-P-OP2	7.33	119.50	110.70
1	2A	2689	U	P-O3'-C3'	7.33	128.50	119.70
32	2a	1158	C	C6-N1-C2	-7.33	117.37	120.30
1	1A	1346	U	P-O3'-C3'	7.27	128.43	119.70
32	1a	1030(B)	C	C2-N1-C1'	7.25	126.77	118.80
1	2A	1074	G	N3-C2-N2	7.22	124.95	119.90
1	2A	2249	U	N3-C4-C5	7.18	118.91	114.60
32	2a	266	G	P-O3'-C3'	7.16	128.29	119.70
1	1A	2037	A	C8-N9-C4	7.16	108.66	105.80
1	1A	1700	G	C8-N9-C4	-7.15	103.54	106.40
1	1A	1660	A	O5'-P-OP1	-7.14	99.27	105.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1A	892	G	O4'-C1'-N9	7.12	113.90	108.20
1	2A	2104	G	C2-N3-C4	-7.11	108.34	111.90
1	2A	2517	C	O5'-P-OP2	-7.11	99.31	105.70
32	2a	1158	C	N1-C2-O2	7.10	123.16	118.90
1	1A	12	U	C2-N1-C1'	7.09	126.21	117.70
32	1a	1030(B)	C	C6-N1-C2	-7.09	117.47	120.30
1	1A	593	G	N3-C4-N9	7.06	130.24	126.00
1	2A	1614	A	O5'-P-OP1	-7.06	99.35	105.70
10	1O	8	LEU	CA-CB-CG	7.05	131.53	115.30
9	1N	25	ARG	NE-CZ-NH1	-7.05	116.78	120.30
1	1A	2050	U	N3-C4-C5	7.01	118.81	114.60
1	2A	1059	G	N1-C2-N3	-7.00	119.70	123.90
1	2A	2185	C	N1-C2-N3	-7.00	114.30	119.20
1	1A	1847	G	O5'-P-OP1	-6.98	99.42	105.70
1	2A	1059	G	N3-C4-N9	6.98	130.19	126.00
1	2A	570	G	C5-C6-N1	6.95	114.97	111.50
5	1F	74	ARG	NE-CZ-NH1	6.93	123.76	120.30
3	1D	260	ARG	NE-CZ-NH1	6.89	123.74	120.30
1	1A	637	U	N3-C2-O2	-6.88	117.38	122.20
1	1A	2513	C	C2-N1-C1'	-6.88	111.24	118.80
4	2E	52	LEU	CA-CB-CG	6.87	131.11	115.30
32	2a	1183	A	P-O3'-C3'	6.87	127.94	119.70
1	1A	593	G	C4-C5-N7	6.85	113.54	110.80
1	1A	2727	G	O5'-P-OP2	-6.84	99.55	105.70
1	1A	993	G	O5'-P-OP1	-6.83	99.55	105.70
1	1A	1008	U	O5'-P-OP2	-6.83	99.56	105.70
1	2A	941	A	O5'-P-OP1	-6.82	99.56	105.70
1	2A	2287	A	O4'-C1'-N9	6.81	113.65	108.20
1	1A	1072	U	N1-C2-O2	6.80	127.56	122.80
1	1A	2261	U	N1-C2-O2	6.79	127.56	122.80
1	2A	1092	C	C5-C6-N1	6.79	124.39	121.00
1	1A	1648	U	N1-C2-O2	6.78	127.55	122.80
1	2A	1092	C	N1-C2-O2	6.78	122.97	118.90
1	1A	593	G	C6-N1-C2	-6.75	121.05	125.10
19	1X	57	LEU	CA-CB-CG	6.75	130.82	115.30
1	2A	1082	U	C2-N1-C1'	6.74	125.79	117.70
32	2a	1158	C	N3-C2-O2	-6.74	117.18	121.90
1	1A	1695	C	O5'-P-OP1	-6.74	99.64	105.70
1	2A	1064	C	C5-C6-N1	6.70	124.35	121.00
1	1A	354	A	N3-C4-N9	-6.67	122.07	127.40
10	2O	8	LEU	CA-CB-CG	6.66	130.62	115.30
1	2A	624	C	O5'-P-OP1	-6.66	99.71	105.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	1a	872	A	O4'-C1'-N9	6.63	113.50	108.20
1	1A	1807	G	O5'-P-OP2	-6.62	99.74	105.70
32	1a	1067	A	P-O3'-C3'	6.62	127.64	119.70
32	1a	1030(B)	C	N3-C2-O2	-6.62	117.27	121.90
1	1A	448	U	O5'-P-OP2	-6.61	99.75	105.70
1	1A	399	G	O4'-C1'-N9	6.61	113.49	108.20
1	2A	751	A	O5'-P-OP1	-6.61	99.76	105.70
1	2A	570	G	C5-C6-O6	-6.60	124.64	128.60
1	1A	1222	A	O5'-P-OP1	-6.58	99.78	105.70
1	1A	832	G	O5'-P-OP2	-6.57	99.78	105.70
1	2A	1772	G	N1-C6-O6	-6.56	115.96	119.90
1	1A	2159	C	C4-C5-C6	6.55	120.67	117.40
1	1A	611	U	O5'-P-OP2	-6.54	99.81	105.70
1	1A	1021	G	O5'-P-OP2	-6.54	99.81	105.70
1	1A	1847	G	O5'-P-OP2	6.54	118.55	110.70
1	1A	1120	G	N3-C2-N2	6.53	124.47	119.90
1	1A	2239	A	O5'-P-OP2	-6.52	99.83	105.70
32	2a	1004	A	O4'-C1'-N9	6.52	113.41	108.20
1	1A	1255	A	P-O3'-C3'	6.51	127.51	119.70
32	2a	1054	C	N3-C2-O2	-6.51	117.34	121.90
1	2A	226	G	O4'-C1'-N9	6.50	113.40	108.20
1	2A	1936	A	O4'-C1'-N9	6.50	113.40	108.20
1	1A	990	A	C8-N9-C4	6.50	108.40	105.80
1	1A	1418	U	C5-C6-N1	6.48	125.94	122.70
1	1A	1132	A	C2-N3-C4	6.48	113.84	110.60
1	2A	1086	A	C6-N1-C2	-6.46	114.72	118.60
1	1A	1199	C	O5'-P-OP2	-6.43	99.91	105.70
5	1F	74	ARG	NE-CZ-NH2	-6.43	117.09	120.30
1	2A	1079	C	C2-N3-C4	6.42	123.11	119.90
1	2A	887	A	O4'-C1'-N9	6.40	113.32	108.20
1	1A	872	C	C6-N1-C2	6.39	122.86	120.30
1	1A	1318	A	O5'-P-OP1	6.39	118.36	110.70
1	1A	2459	G	C5-C6-O6	6.38	132.43	128.60
1	2A	845	G	O4'-C1'-N9	6.38	113.30	108.20
1	2A	1076	C	OP1-P-O3'	6.38	119.23	105.20
1	2A	1992	G	P-O3'-C3'	6.38	127.35	119.70
1	1A	2858	G	O4'-C1'-N9	6.37	113.30	108.20
1	1A	1121	C	C2-N1-C1'	6.37	125.80	118.80
1	1A	1462	G	O4'-C1'-N9	6.36	113.29	108.20
1	1A	1109	G	C5-C6-O6	6.34	132.41	128.60
1	2A	2028	U	N3-C4-O4	-6.33	114.97	119.40
1	1A	1718	U	N3-C4-O4	-6.31	114.98	119.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1A	2037	A	N7-C8-N9	-6.31	110.65	113.80
1	2A	1633	G	N1-C6-O6	-6.30	116.12	119.90
1	1A	2019	G	O5'-P-OP1	6.29	118.24	110.70
1	1A	2058	C	O5'-P-OP1	-6.27	100.05	105.70
29	17	9	ARG	NE-CZ-NH1	6.27	123.44	120.30
1	2A	782	A	O5'-P-OP1	-6.27	100.06	105.70
1	1A	1072	U	N3-C2-O2	-6.26	117.82	122.20
1	1A	2050	U	N3-C4-O4	-6.23	115.04	119.40
1	1A	184	A	P-O3'-C3'	6.22	127.16	119.70
1	1A	787	U	O5'-P-OP2	-6.21	100.11	105.70
1	2A	570	G	N9-C4-C5	-6.20	102.92	105.40
1	1A	2082	A	C8-N9-C4	6.20	108.28	105.80
1	2A	1074	G	C6-N1-C2	6.20	128.82	125.10
1	1A	751	G	O4'-C1'-N9	6.19	113.15	108.20
32	2a	79	G	C5-C6-O6	6.17	132.30	128.60
1	1A	2459	G	N1-C6-O6	-6.15	116.21	119.90
1	1A	2440	G	OP1-P-O3'	6.15	118.73	105.20
32	2a	1183	A	OP1-P-O3'	6.14	118.72	105.20
1	2A	1156	A	O5'-P-OP2	-6.13	100.19	105.70
1	1A	354	A	N3-C4-C5	6.12	131.09	126.80
1	2A	2103	C	C5-C4-N4	6.12	124.48	120.20
8	2I	75	LEU	CA-CB-CG	6.11	129.34	115.30
1	1A	1232	G	N1-C6-O6	-6.10	116.24	119.90
33	1b	178	ARG	NE-CZ-NH1	6.10	123.35	120.30
1	1A	641	G	O5'-P-OP2	-6.09	100.22	105.70
1	1A	830	A	OP1-P-OP2	-6.08	110.48	119.60
1	1A	2077	C	OP1-P-O3'	6.07	118.56	105.20
1	2A	12	U	N1-C2-O2	6.07	127.05	122.80
32	1a	266	G	P-O3'-C3'	6.06	126.98	119.70
1	1A	830	A	C2-N3-C4	6.06	113.63	110.60
1	1A	1958	A	O4'-C1'-N9	6.05	113.04	108.20
32	1a	299	G	C5-C6-O6	-6.04	124.98	128.60
1	1A	348	A	O5'-P-OP2	-6.04	100.27	105.70
32	2a	754	C	C2-N1-C1'	6.03	125.43	118.80
1	1A	2261	U	N3-C4-O4	-6.02	115.18	119.40
1	1A	1045	U	O5'-P-OP2	-6.02	100.28	105.70
1	2A	510	C	N1-C2-O2	6.02	122.51	118.90
1	1A	2593	G	O4'-C1'-N9	6.00	113.00	108.20
1	2A	1937	A	O4'-C1'-N9	5.99	113.00	108.20
1	2A	1780	A	O5'-P-OP2	-5.99	100.31	105.70
1	1A	834	U	O5'-P-OP1	-5.96	100.33	105.70
1	1A	1694	G	O4'-C1'-N9	-5.96	103.43	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1A	615	G	O5'-P-OP2	-5.96	100.34	105.70
32	1a	73	G	C5-C6-O6	5.95	132.17	128.60
1	2A	2130	U	C5-C6-N1	5.95	125.67	122.70
11	2P	147	LEU	CA-CB-CG	5.95	128.98	115.30
1	1A	193	A	N7-C8-N9	-5.94	110.83	113.80
1	1A	593	G	C8-N9-C4	5.94	108.78	106.40
32	1a	115	G	P-O3'-C3'	5.94	126.83	119.70
1	2A	1609	A	C8-N9-C4	5.94	108.18	105.80
1	2A	1779	U	O4'-C1'-N1	5.93	112.94	108.20
1	2A	1816	G	O5'-P-OP1	-5.92	100.37	105.70
1	1A	476	G	N1-C6-O6	-5.90	116.36	119.90
1	2A	2028	U	C5-C6-N1	-5.90	119.75	122.70
1	1A	2624	C	O5'-P-OP2	-5.90	100.39	105.70
1	1A	1418	U	C2-N1-C1'	5.89	124.77	117.70
1	1A	2261	U	C4-C5-C6	-5.89	116.17	119.70
32	2a	1442	G	N3-C4-C5	-5.89	125.65	128.60
1	1A	1113	A	C2-N3-C4	5.89	113.54	110.60
1	2A	752	A	P-O3'-C3'	5.88	126.75	119.70
1	2A	787	U	O5'-P-OP1	-5.88	100.41	105.70
1	2A	1343	G	O5'-P-OP1	-5.87	100.41	105.70
1	2A	2070	G	N1-C6-O6	-5.87	116.38	119.90
1	1A	847	A	O5'-P-OP1	-5.86	100.42	105.70
1	1A	2383	G	C5-C6-N1	5.86	114.43	111.50
1	1A	2459	G	C4-C5-N7	-5.86	108.46	110.80
1	2A	2061	G	O5'-P-OP2	-5.86	100.43	105.70
1	1A	1132	A	C5-C6-N6	5.86	128.38	123.70
1	1A	2697	G	C5-C6-N1	5.85	114.43	111.50
1	1A	1221	G	OP1-P-O3'	5.85	118.07	105.20
32	2a	1123	A	C5-C6-N6	5.85	128.38	123.70
1	2A	575	A	O5'-P-OP1	-5.83	100.45	105.70
32	2a	1286	A	C8-N9-C4	-5.83	103.47	105.80
32	2a	1442	G	N3-C4-N9	5.83	129.50	126.00
32	2a	687	A	P-O3'-C3'	5.83	126.69	119.70
1	2A	1064	C	C6-N1-C2	-5.83	117.97	120.30
1	2A	2154	G	C6-N1-C2	5.82	128.59	125.10
32	2a	1286	A	N7-C8-N9	5.82	116.71	113.80
1	1A	1234	A	O5'-P-OP2	-5.82	100.46	105.70
1	1A	2150	C	N1-C2-O2	5.81	122.39	118.90
1	1A	2331	G	O4'-C1'-N9	5.81	112.85	108.20
1	2A	1086	A	N3-C4-C5	-5.81	122.73	126.80
1	2A	271(Y)	U	O4'-C1'-N1	5.80	112.84	108.20
1	2A	2501	C	C2-N1-C1'	-5.80	112.42	118.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1A	1822	A	C5'-C4'-C3'	-5.80	106.72	116.00
1	1A	1237	G	N7-C8-N9	-5.79	110.20	113.10
1	1A	2724	U	O4'-C1'-N1	5.79	112.83	108.20
1	2A	2161	C	C5-C4-N4	5.79	124.25	120.20
1	1A	2584	A	C8-N9-C4	5.78	108.11	105.80
1	1A	1235	G	C5-N7-C8	5.78	107.19	104.30
1	1A	778	C	O5'-P-OP2	-5.78	100.50	105.70
1	2A	2326	C	C6-N1-C2	-5.78	117.99	120.30
32	2a	1003	G	N3-C4-N9	5.78	129.47	126.00
2	1B	1	U	C2-N1-C1'	5.77	124.62	117.70
1	1A	1615	G	C5-N7-C8	5.77	107.18	104.30
1	2A	961	C	C6-N1-C2	5.76	122.60	120.30
1	2A	1065	U	P-O3'-C3'	5.76	126.61	119.70
2	2B	1	U	C2-N1-C1'	5.76	124.61	117.70
1	2A	575	A	O5'-P-OP2	5.76	117.61	110.70
1	1A	1006	C	O5'-P-OP2	-5.75	100.52	105.70
1	2A	1092	C	C2-N1-C1'	5.75	125.12	118.80
32	1a	913	A	P-O3'-C3'	5.75	126.60	119.70
32	1a	955	U	C5-C4-O4	5.74	129.35	125.90
1	1A	1869	C	N1-C2-O2	-5.74	115.46	118.90
1	2A	2186	G	C5-C6-O6	5.74	132.04	128.60
1	1A	2079	A	N9-C4-C5	5.73	108.09	105.80
1	2A	1099	G	C5-C6-O6	5.73	132.04	128.60
1	2A	2108	C	C2-N3-C4	5.73	122.77	119.90
1	1A	2605	U	N3-C4-C5	5.73	118.04	114.60
1	2A	2218	U	N1-C2-O2	5.73	126.81	122.80
1	2A	2448	A	O5'-P-OP1	-5.72	100.55	105.70
1	1A	1232	G	C5-C6-N1	5.72	114.36	111.50
1	2A	1064	C	C2-N1-C1'	5.72	125.09	118.80
1	2A	800	A	O5'-P-OP1	-5.71	100.56	105.70
32	2a	115	G	P-O3'-C3'	5.71	126.56	119.70
1	1A	1218	G	O4'-C1'-N9	5.71	112.77	108.20
30	18	13	ARG	NE-CZ-NH2	-5.71	117.44	120.30
1	2A	2689	U	N3-C2-O2	-5.71	118.20	122.20
1	2A	1074	G	N9-C4-C5	-5.71	103.12	105.40
32	2a	1026	G	N3-C4-C5	-5.71	125.75	128.60
1	1A	1092	A	O4'-C1'-N9	5.70	112.76	108.20
1	1A	1695	C	O5'-P-OP2	5.70	117.53	110.70
1	1A	1120	G	N9-C4-C5	-5.69	103.12	105.40
1	1A	1709	C	C6-N1-C2	-5.68	118.03	120.30
1	2A	1385	G	O4'-C1'-N9	5.68	112.74	108.20
32	2a	1123	A	N1-C6-N6	-5.67	115.20	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	2A	2103	C	C2-N3-C4	5.67	122.73	119.90
32	2a	458	C	C2-N1-C1'	5.66	125.03	118.80
1	1A	808	A	C5-N7-C8	5.65	106.73	103.90
1	1A	2079	A	C5-C6-N6	5.65	128.22	123.70
1	1A	2057	G	O4'-C1'-N9	5.64	112.71	108.20
1	2A	1086	A	C4-N9-C1'	5.63	136.43	126.30
1	1A	1107	U	N1-C2-O2	5.62	126.74	122.80
1	2A	1079	C	C6-N1-C1'	-5.62	114.05	120.80
1	1A	12	U	N3-C2-O2	-5.62	118.27	122.20
1	1A	507	G	O5'-P-OP2	-5.62	100.64	105.70
32	1a	1442	G	N3-C4-C5	-5.61	125.79	128.60
1	2A	1700	A	O5'-P-OP2	5.60	117.42	110.70
2	2B	8	U	C5-C6-N1	5.59	125.49	122.70
1	2A	1187	G	N1-C6-O6	-5.58	116.55	119.90
1	2A	1647	G	O4'-C1'-N9	-5.58	103.73	108.20
1	1A	1256	U	O5'-P-OP1	-5.58	100.68	105.70
1	1A	2029	C	N3-C2-O2	-5.57	118.00	121.90
1	2A	2741	A	C8-N9-C4	5.57	108.03	105.80
1	2A	383	U	O4'-C1'-N1	5.57	112.66	108.20
1	2A	1416	G	O4'-C1'-N9	5.57	112.66	108.20
1	1A	1361	C	O5'-P-OP2	-5.56	100.70	105.70
1	2A	1847	A	O4'-C1'-N9	5.55	112.64	108.20
1	1A	2441	G	O5'-P-OP1	-5.54	100.71	105.70
2	1B	41	U	C5-C6-N1	-5.54	119.93	122.70
22	10	14	ARG	NE-CZ-NH2	-5.54	117.53	120.30
1	1A	670	C	C2-N1-C1'	5.54	124.89	118.80
1	2A	34	C	C6-N1-C2	-5.54	118.09	120.30
1	1A	205	A	O5'-P-OP1	-5.53	100.72	105.70
1	2A	1099	G	C6-N1-C2	5.53	128.42	125.10
1	2A	1111	A	O4'-C1'-N9	5.52	112.62	108.20
1	2A	2585	U	OP1-P-O3'	5.52	117.34	105.20
1	1A	543	G	O5'-P-OP2	-5.52	100.73	105.70
1	1A	1109	G	C6-N1-C2	5.51	128.41	125.10
1	2A	2490	G	C5-C6-N1	5.51	114.25	111.50
1	2A	1639	U	O5'-P-OP2	-5.51	100.74	105.70
1	1A	2405	A	O5'-P-OP1	-5.50	100.75	105.70
1	1A	1707	C	O5'-P-OP2	-5.50	100.75	105.70
1	1A	1042	A	O5'-P-OP2	5.50	117.30	110.70
1	1A	798	A	O5'-P-OP2	5.50	117.29	110.70
1	2A	2185	C	C2-N1-C1'	5.49	124.84	118.80
1	2A	1091	G	C8-N9-C4	-5.49	104.21	106.40
1	2A	1993	U	O5'-P-OP1	-5.48	100.77	105.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1A	1648	U	N3-C2-O2	-5.47	118.37	122.20
32	1a	1007	C	N1-C2-O2	5.47	122.18	118.90
32	1a	687	A	P-O3'-C3'	5.46	126.26	119.70
1	1A	2459	G	C5-N7-C8	5.46	107.03	104.30
1	2A	1816	G	O5'-P-OP2	5.46	117.25	110.70
1	2A	963	U	O5'-P-OP2	-5.45	100.79	105.70
1	2A	1052	C	C2-N1-C1'	5.45	124.79	118.80
1	2A	2185	C	C6-N1-C2	-5.45	118.12	120.30
1	1A	715	G	OP2-P-O3'	5.45	117.18	105.20
32	1a	1442	G	C2-N3-C4	5.45	114.62	111.90
1	1A	2079	A	C4-C5-N7	-5.44	107.98	110.70
1	1A	2513	C	C5-C6-N1	-5.44	118.28	121.00
1	2A	2108	C	N1-C2-O2	5.44	122.16	118.90
1	1A	780	G	C5-N7-C8	5.44	107.02	104.30
1	2A	1838	C	O4'-C1'-N1	5.43	112.55	108.20
1	1A	288	U	O4'-C1'-N1	5.43	112.54	108.20
1	1A	187	C	O5'-P-OP2	-5.42	100.82	105.70
1	2A	1647	G	C8-N9-C4	5.42	108.57	106.40
1	2A	2611	U	O5'-P-OP1	-5.42	100.82	105.70
1	1A	591	U	C5-C4-O4	-5.41	122.65	125.90
32	1a	902	G	O5'-P-OP2	-5.41	100.83	105.70
1	2A	570	G	N3-C4-N9	5.41	129.25	126.00
1	1A	2451	A	O5'-P-OP1	5.41	117.19	110.70
1	1A	2348	A	O4'-C1'-N9	-5.41	103.88	108.20
1	1A	354	A	C5-N7-C8	-5.40	101.20	103.90
32	1a	1201	A	P-O3'-C3'	5.40	126.18	119.70
1	1A	839	G	O4'-C1'-N9	-5.40	103.88	108.20
1	1A	2091	G	C8-N9-C4	5.39	108.56	106.40
32	1a	1024	G	N3-C4-C5	-5.39	125.91	128.60
1	1A	831	A	OP1-P-O3'	5.38	117.03	105.20
1	1A	990	A	O5'-P-OP1	5.37	117.15	110.70
1	2A	2602	A	O4'-C1'-N9	5.37	112.50	108.20
1	1A	991	G	OP1-P-OP2	5.37	127.65	119.60
1	1A	322	G	C5-N7-C8	5.36	106.98	104.30
1	1A	991	G	C8-N9-C4	5.36	108.54	106.40
1	1A	1878	A	O4'-C1'-N9	5.36	112.49	108.20
1	1A	2041	A	P-O3'-C3'	5.36	126.13	119.70
1	1A	1431	G	O4'-C1'-N9	5.35	112.48	108.20
32	1a	1065	U	P-O3'-C3'	5.35	126.12	119.70
1	2A	2144	U	C2-N1-C1'	5.35	124.12	117.70
1	2A	670	A	O4'-C1'-N9	-5.34	103.92	108.20
1	1A	1295	U	O5'-P-OP1	-5.34	100.89	105.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1A	1237	G	C5-N7-C8	5.33	106.97	104.30
1	2A	1092	C	N3-C2-O2	-5.32	118.17	121.90
1	1A	2050	U	C2-N3-C4	-5.32	123.81	127.00
1	1A	123	G	O4'-C1'-N9	-5.32	103.95	108.20
32	2a	841	U	C5-C6-N1	5.32	125.36	122.70
32	1a	975	A	O4'-C1'-N9	-5.31	103.95	108.20
1	2A	1210	A	P-O3'-C3'	5.31	126.07	119.70
32	1a	1181	G	N3-C4-C5	5.31	131.25	128.60
1	1A	2588	G	C2-N3-C4	5.31	114.55	111.90
1	2A	1060	U	C2-N1-C1'	5.30	124.06	117.70
1	1A	285	U	O4'-C1'-N1	5.30	112.44	108.20
32	2a	560	U	C2-N1-C1'	5.30	124.06	117.70
1	2A	450	G	C5-C6-N1	5.29	114.14	111.50
32	2a	1020	U	N1-C2-O2	5.29	126.50	122.80
1	2A	2105	C	C6-N1-C2	-5.28	118.19	120.30
1	2A	1772	G	C5-C6-O6	5.28	131.76	128.60
12	2Q	56	ARG	NE-CZ-NH1	5.27	122.94	120.30
1	2A	1530	C	P-O3'-C3'	5.27	126.03	119.70
1	2A	2058	A	C8-N9-C4	-5.27	103.69	105.80
32	2a	5	U	C2-N1-C1'	5.27	124.02	117.70
32	2a	841	U	C6-N1-C2	-5.26	117.84	121.00
32	2a	1158	C	C5-C6-N1	5.26	123.63	121.00
1	1A	831	A	C8-N9-C4	5.26	107.90	105.80
1	2A	1209	G	O5'-P-OP2	-5.26	100.97	105.70
1	1A	1020	C	O5'-P-OP1	-5.26	100.97	105.70
1	2A	1253	A	N1-C6-N6	5.25	121.75	118.60
1	2A	1059	G	C6-N1-C2	5.25	128.25	125.10
1	1A	1120	G	C4-C5-N7	5.25	112.90	110.80
1	2A	1772	G	C6-C5-N7	5.25	133.55	130.40
1	1A	115	G	C5-C6-O6	-5.24	125.46	128.60
1	2A	2064	C	C2-N1-C1'	-5.24	113.04	118.80
1	2A	1073	A	P-O3'-C3'	5.23	125.98	119.70
1	1A	2449	U	C2-N3-C4	-5.23	123.86	127.00
1	1A	1110	C	C2-N3-C4	5.23	122.51	119.90
1	1A	934	A	O4'-C1'-N9	5.22	112.38	108.20
1	1A	1360	C	C2-N1-C1'	5.22	124.54	118.80
32	2a	1065	U	P-O3'-C3'	5.22	125.96	119.70
1	1A	2513	C	C6-N1-C2	5.21	122.38	120.30
1	1A	1990	G	C5-C6-O6	-5.21	125.48	128.60
1	1A	202	A	OP2-P-O3'	5.20	116.65	105.20
1	2A	1059	G	N9-C4-C5	-5.20	103.32	105.40
1	1A	537	G	C5-N7-C8	5.20	106.90	104.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	2A	2447	G	N7-C8-N9	-5.20	110.50	113.10
1	2A	1097	U	N1-C2-O2	5.20	126.44	122.80
1	1A	2262	G	OP1-P-OP2	5.19	127.39	119.60
1	2A	574	C	O5'-P-OP1	-5.19	101.03	105.70
1	1A	2078	G	N9-C4-C5	-5.18	103.33	105.40
1	1A	795	G	O4'-C1'-N9	5.18	112.34	108.20
1	2A	1076	C	P-O3'-C3'	5.18	125.92	119.70
1	2A	2058	A	N9-C4-C5	5.18	107.87	105.80
1	1A	1121	C	C5-C6-N1	5.18	123.59	121.00
1	1A	1700	G	P-O3'-C3'	5.18	125.91	119.70
1	2A	2183	C	C2-N3-C4	5.16	122.48	119.90
1	1A	193	A	C8-N9-C4	5.16	107.86	105.80
1	2A	1087	G	N3-C4-N9	-5.16	122.90	126.00
43	2l	87	GLY	N-CA-C	5.16	126.00	113.10
1	2A	2127	G	C6-N1-C2	5.16	128.19	125.10
32	2a	266	G	OP2-P-O3'	5.16	116.55	105.20
1	2A	1086	A	N3-C4-N9	5.16	131.52	127.40
1	2A	1059	G	C2-N3-C4	5.15	114.48	111.90
1	2A	2206	G	C4-N9-C1'	-5.15	119.80	126.50
1	1A	1804	A	N9-C1'-C2'	-5.15	106.34	112.00
1	1A	2015	U	C5-C4-O4	5.14	128.99	125.90
1	1A	2024	G	C5-N7-C8	5.14	106.87	104.30
1	2A	128	C	C6-N1-C2	-5.14	118.25	120.30
1	1A	933	C	N1-C2-O2	5.14	121.98	118.90
1	1A	1577	C	P-O3'-C3'	5.14	125.86	119.70
1	2A	1071	G	C8-N9-C4	-5.13	104.35	106.40
32	2a	1331	G	O4'-C1'-N9	5.13	112.30	108.20
1	1A	2701	U	N3-C2-O2	-5.12	118.61	122.20
1	2A	2070	G	C4-C5-N7	-5.12	108.75	110.80
1	1A	2667	G	O4'-C1'-N9	5.11	112.29	108.20
1	2A	2157	G	C8-N9-C4	-5.11	104.36	106.40
32	2a	21	G	O5'-P-OP1	-5.11	101.10	105.70
1	1A	828	A	C2-N3-C4	5.11	113.15	110.60
1	2A	2447	G	C4-N9-C1'	-5.10	119.87	126.50
1	1A	2473	C	C6-N1-C2	-5.10	118.26	120.30
1	2A	1074	G	C4-C5-N7	5.10	112.84	110.80
1	2A	2577	A	O5'-P-OP1	-5.09	101.12	105.70
1	1A	2159	C	N1-C2-O2	5.09	121.95	118.90
1	1A	184	A	C5-N7-C8	5.09	106.44	103.90
1	2A	2147	G	N7-C8-N9	5.09	115.64	113.10
1	1A	1298	G	O4'-C1'-N9	-5.08	104.14	108.20
32	2a	204	U	C2-N1-C1'	5.08	123.80	117.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1A	2362	C	C6-N1-C2	-5.08	118.27	120.30
32	2a	1003	G	C8-N9-C1'	-5.07	120.40	127.00
1	2A	1992	G	C2'-C3'-O3'	5.07	121.81	113.70
1	1A	1128	U	N3-C4-O4	-5.06	115.86	119.40
1	1A	872	C	OP2-P-O3'	5.06	116.33	105.20
1	1A	1299	A	C5-N7-C8	5.06	106.43	103.90
1	1A	1353	A	C8-N9-C4	5.06	107.82	105.80
1	1A	556	C	O5'-P-OP2	-5.05	101.15	105.70
18	1W	11	ARG	NE-CZ-NH1	5.05	122.83	120.30
32	2a	1026	G	N3-C4-N9	5.05	129.03	126.00
1	1A	2203	G	N3-C4-N9	-5.05	122.97	126.00
32	1a	1058	G	C5-C6-O6	-5.05	125.57	128.60
1	2A	2402	C	N1-C2-O2	-5.05	115.87	118.90
1	2A	1379	A	N1-C6-N6	5.05	121.63	118.60
1	2A	2127	G	N3-C2-N2	5.05	123.43	119.90
32	1a	839	U	OP1-P-O3'	5.04	116.30	105.20
1	1A	808	A	N7-C8-N9	-5.04	111.28	113.80
1	2A	1087	G	C8-N9-C1'	5.04	133.56	127.00
1	1A	793	A	O4'-C1'-N9	5.04	112.23	108.20
1	2A	1760	A	C5-C6-N6	5.04	127.73	123.70
1	1A	578	U	O4'-C1'-N1	5.03	112.23	108.20
1	2A	2249	U	C2-N3-C4	-5.03	123.98	127.00
32	2a	560	U	C3'-C2'-C1'	5.03	105.52	101.50
1	1A	1648	U	N3-C4-C5	5.03	117.62	114.60
1	1A	555	G	OP1-P-O3'	5.02	116.25	105.20
1	1A	702	A	O4'-C1'-N9	5.02	112.22	108.20
32	1a	991	U	P-O3'-C3'	5.02	125.72	119.70
32	1a	1225	A	C6-N1-C2	5.02	121.61	118.60
1	2A	568	U	N3-C4-C5	5.02	117.61	114.60
1	2A	1835	G	O5'-P-OP1	-5.02	101.18	105.70
1	2A	2609	U	N3-C2-O2	-5.02	118.69	122.20
32	2a	1000	U	C5-C4-O4	5.02	128.91	125.90
32	2a	60	A	P-O3'-C3'	5.01	125.72	119.70
7	2H	88	LEU	CA-CB-CG	5.01	126.83	115.30
1	1A	1719	C	OP1-P-O3'	5.01	116.22	105.20
1	2A	1076	C	C6-N1-C2	-5.00	118.30	120.30
1	1A	2803	A	C2-N3-C4	5.00	113.10	110.60

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
14	1S	58	LEU	Peptide
19	1X	93	GLU	Peptide
33	1b	231	GLU	Peptide
19	2X	93	GLU	Peptide
43	2l	86	ARG	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%)	262 (96%)	11 (4%)	0	100	100
3	2D	273/276 (99%)	260 (95%)	13 (5%)	0	100	100
4	1E	202/206 (98%)	195 (96%)	6 (3%)	1 (0%)	29	35
4	2E	202/206 (98%)	196 (97%)	6 (3%)	0	100	100
5	1F	201/210 (96%)	197 (98%)	4 (2%)	0	100	100
5	2F	201/210 (96%)	196 (98%)	3 (2%)	2 (1%)	15	17
6	1G	179/182 (98%)	167 (93%)	11 (6%)	1 (1%)	25	31
6	2G	179/182 (98%)	170 (95%)	8 (4%)	1 (1%)	25	31
7	1H	172/180 (96%)	167 (97%)	5 (3%)	0	100	100
7	2H	171/180 (95%)	165 (96%)	6 (4%)	0	100	100
8	1I	145/148 (98%)	133 (92%)	11 (8%)	1 (1%)	22	26
8	2I	144/148 (97%)	135 (94%)	9 (6%)	0	100	100
9	1N	138/140 (99%)	136 (99%)	2 (1%)	0	100	100
9	2N	138/140 (99%)	136 (99%)	2 (1%)	0	100	100
10	1O	120/122 (98%)	114 (95%)	6 (5%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
10	2O	120/122 (98%)	115 (96%)	5 (4%)	0	100	100
11	1P	147/150 (98%)	141 (96%)	6 (4%)	0	100	100
11	2P	147/150 (98%)	141 (96%)	5 (3%)	1 (1%)	22	26
12	1Q	139/141 (99%)	134 (96%)	5 (4%)	0	100	100
12	2Q	139/141 (99%)	134 (96%)	5 (4%)	0	100	100
13	1R	116/118 (98%)	113 (97%)	3 (3%)	0	100	100
13	2R	116/118 (98%)	114 (98%)	2 (2%)	0	100	100
14	1S	108/112 (96%)	104 (96%)	3 (3%)	1 (1%)	17	20
14	2S	108/112 (96%)	105 (97%)	3 (3%)	0	100	100
15	1T	129/146 (88%)	124 (96%)	5 (4%)	0	100	100
15	2T	129/146 (88%)	125 (97%)	4 (3%)	0	100	100
16	1U	114/118 (97%)	114 (100%)	0	0	100	100
16	2U	114/118 (97%)	114 (100%)	0	0	100	100
17	1V	99/101 (98%)	97 (98%)	2 (2%)	0	100	100
17	2V	99/101 (98%)	96 (97%)	3 (3%)	0	100	100
18	1W	110/113 (97%)	109 (99%)	1 (1%)	0	100	100
18	2W	110/113 (97%)	110 (100%)	0	0	100	100
19	1X	93/96 (97%)	92 (99%)	1 (1%)	0	100	100
19	2X	93/96 (97%)	91 (98%)	2 (2%)	0	100	100
20	1Y	105/110 (96%)	99 (94%)	6 (6%)	0	100	100
20	2Y	105/110 (96%)	101 (96%)	4 (4%)	0	100	100
21	1Z	201/206 (98%)	196 (98%)	5 (2%)	0	100	100
21	2Z	199/206 (97%)	194 (98%)	5 (2%)	0	100	100
22	10	75/85 (88%)	73 (97%)	2 (3%)	0	100	100
22	20	75/85 (88%)	73 (97%)	2 (3%)	0	100	100
23	11	95/98 (97%)	94 (99%)	0	1 (1%)	14	15
23	21	95/98 (97%)	93 (98%)	1 (1%)	1 (1%)	14	15
24	12	68/72 (94%)	67 (98%)	1 (2%)	0	100	100
24	22	68/72 (94%)	67 (98%)	1 (2%)	0	100	100
25	13	57/60 (95%)	55 (96%)	2 (4%)	0	100	100
25	23	57/60 (95%)	55 (96%)	2 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
26	14	67/71 (94%)	56 (84%)	5 (8%)	6 (9%)	1	0
26	24	67/71 (94%)	53 (79%)	11 (16%)	3 (4%)	2	1
27	15	57/60 (95%)	55 (96%)	2 (4%)	0	100	100
27	25	57/60 (95%)	56 (98%)	1 (2%)	0	100	100
28	16	51/54 (94%)	49 (96%)	2 (4%)	0	100	100
28	26	51/54 (94%)	49 (96%)	2 (4%)	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%)	61 (98%)	1 (2%)	0	100	100
30	28	62/65 (95%)	61 (98%)	1 (2%)	0	100	100
31	19	35/37 (95%)	35 (100%)	0	0	100	100
31	29	35/37 (95%)	35 (100%)	0	0	100	100
33	1b	229/256 (90%)	202 (88%)	20 (9%)	7 (3%)	4	2
33	2b	229/256 (90%)	205 (90%)	19 (8%)	5 (2%)	6	5
34	1c	204/239 (85%)	190 (93%)	14 (7%)	0	100	100
34	2c	204/239 (85%)	187 (92%)	17 (8%)	0	100	100
35	1d	206/209 (99%)	197 (96%)	9 (4%)	0	100	100
35	2d	206/209 (99%)	199 (97%)	7 (3%)	0	100	100
36	1e	146/162 (90%)	144 (99%)	2 (1%)	0	100	100
36	2e	146/162 (90%)	145 (99%)	1 (1%)	0	100	100
37	1f	98/101 (97%)	96 (98%)	2 (2%)	0	100	100
37	2f	98/101 (97%)	96 (98%)	2 (2%)	0	100	100
38	1g	153/156 (98%)	148 (97%)	5 (3%)	0	100	100
38	2g	153/156 (98%)	148 (97%)	4 (3%)	1 (1%)	22	26
39	1h	135/138 (98%)	133 (98%)	2 (2%)	0	100	100
39	2h	135/138 (98%)	130 (96%)	5 (4%)	0	100	100
40	1i	125/128 (98%)	115 (92%)	9 (7%)	1 (1%)	19	23
40	2i	124/128 (97%)	113 (91%)	8 (6%)	3 (2%)	6	4
41	1j	95/105 (90%)	83 (87%)	8 (8%)	4 (4%)	3	1
41	2j	94/105 (90%)	85 (90%)	7 (7%)	2 (2%)	7	5
42	1k	112/129 (87%)	103 (92%)	7 (6%)	2 (2%)	8	7

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
42	2k	112/129 (87%)	106 (95%)	5 (4%)	1 (1%)	17	20
43	1l	119/132 (90%)	117 (98%)	2 (2%)	0	100	100
43	2l	119/132 (90%)	116 (98%)	3 (2%)	0	100	100
44	1m	114/126 (90%)	105 (92%)	7 (6%)	2 (2%)	8	7
44	2m	112/126 (89%)	105 (94%)	6 (5%)	1 (1%)	17	20
45	1n	58/61 (95%)	56 (97%)	2 (3%)	0	100	100
45	2n	58/61 (95%)	56 (97%)	2 (3%)	0	100	100
46	1o	86/89 (97%)	82 (95%)	4 (5%)	0	100	100
46	2o	86/89 (97%)	82 (95%)	4 (5%)	0	100	100
47	1p	80/88 (91%)	77 (96%)	3 (4%)	0	100	100
47	2p	80/88 (91%)	76 (95%)	4 (5%)	0	100	100
48	1q	97/105 (92%)	94 (97%)	2 (2%)	1 (1%)	15	17
48	2q	97/105 (92%)	95 (98%)	2 (2%)	0	100	100
49	1r	66/88 (75%)	65 (98%)	1 (2%)	0	100	100
49	2r	66/88 (75%)	65 (98%)	1 (2%)	0	100	100
50	1s	81/93 (87%)	78 (96%)	3 (4%)	0	100	100
50	2s	81/93 (87%)	79 (98%)	2 (2%)	0	100	100
51	1t	94/106 (89%)	86 (92%)	6 (6%)	2 (2%)	7	5
51	2t	96/106 (91%)	88 (92%)	6 (6%)	2 (2%)	7	5
52	1u	21/27 (78%)	19 (90%)	2 (10%)	0	100	100
52	2u	21/27 (78%)	19 (90%)	1 (5%)	1 (5%)	2	1
53	1y	95/113 (84%)	94 (99%)	1 (1%)	0	100	100
53	2y	94/113 (83%)	89 (95%)	4 (4%)	1 (1%)	14	15
All	All	11629/12354 (94%)	11139 (96%)	435 (4%)	55 (0%)	29	35

All (55) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
26	14	49	PHE
33	1b	16	HIS
33	1b	17	PHE
33	1b	22	LYS
51	1t	95	ALA
23	21	3	LYS

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
33	2b	17	PHE
33	2b	20	GLU
33	2b	124	SER
40	2i	44	VAL
40	2i	54	ASP
6	1G	51	ARG
14	1S	60	GLY
26	14	45	GLY
26	14	47	GLN
40	1i	44	VAL
41	1j	31	GLY
41	1j	78	ASN
41	1j	79	ARG
6	2G	81	LYS
26	24	60	GLN
33	2b	10	LEU
41	2j	79	ARG
44	2m	67	GLU
51	2t	95	ALA
4	1E	52	LEU
44	1m	12	ASN
5	2F	21	ALA
26	24	45	GLY
33	2b	125	PRO
41	2j	78	ASN
53	2y	45	PRO
26	14	46	GLN
26	14	55	ARG
33	1b	20	GLU
44	1m	67	GLU
38	2g	7	ALA
8	1I	73	GLU
23	11	3	LYS
26	14	60	GLN
33	1b	43	ASP
33	1b	127	ILE
42	1k	117	ASN
5	2F	130	ALA
26	24	55	ARG
51	2t	100	ILE
52	2u	7	ARG
48	1q	68	ARG

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Mol	Chain	Res	Type
51	1t	100	ILE
11	2P	29	LYS
40	2i	11	LYS
42	1k	105	VAL
42	2k	105	VAL
33	1b	15	VAL
41	1j	77	PRO

### 5.3.2 Protein sidechains [i](#)

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	214/218 (98%)	199 (93%)	15 (7%)	15	19
3	2D	215/218 (99%)	201 (94%)	14 (6%)	17	23
4	1E	164/166 (99%)	148 (90%)	16 (10%)	8	9
4	2E	164/166 (99%)	146 (89%)	18 (11%)	6	7
5	1F	160/166 (96%)	142 (89%)	18 (11%)	6	6
5	2F	159/166 (96%)	144 (91%)	15 (9%)	8	10
6	1G	144/156 (92%)	128 (89%)	16 (11%)	6	7
6	2G	142/156 (91%)	122 (86%)	20 (14%)	3	3
7	1H	144/148 (97%)	136 (94%)	8 (6%)	21	29
7	2H	143/148 (97%)	129 (90%)	14 (10%)	8	9
8	1I	111/124 (90%)	92 (83%)	19 (17%)	2	2
8	2I	108/124 (87%)	95 (88%)	13 (12%)	5	5
9	1N	119/119 (100%)	107 (90%)	12 (10%)	7	9
9	2N	118/119 (99%)	107 (91%)	11 (9%)	9	10
10	1O	100/100 (100%)	97 (97%)	3 (3%)	41	57
10	2O	100/100 (100%)	97 (97%)	3 (3%)	41	57
11	1P	115/116 (99%)	105 (91%)	10 (9%)	10	12
11	2P	115/116 (99%)	106 (92%)	9 (8%)	12	16

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
12	1Q	111/111 (100%)	100 (90%)	11 (10%)	8	9
12	2Q	111/111 (100%)	101 (91%)	10 (9%)	9	11
13	1R	101/101 (100%)	87 (86%)	14 (14%)	3	3
13	2R	101/101 (100%)	88 (87%)	13 (13%)	4	4
14	1S	87/88 (99%)	77 (88%)	10 (12%)	5	6
14	2S	85/88 (97%)	75 (88%)	10 (12%)	5	5
15	1T	115/127 (91%)	106 (92%)	9 (8%)	12	16
15	2T	113/127 (89%)	106 (94%)	7 (6%)	18	25
16	1U	93/94 (99%)	83 (89%)	10 (11%)	6	7
16	2U	93/94 (99%)	86 (92%)	7 (8%)	13	17
17	1V	81/82 (99%)	73 (90%)	8 (10%)	8	9
17	2V	80/82 (98%)	72 (90%)	8 (10%)	7	9
18	1W	90/92 (98%)	79 (88%)	11 (12%)	5	5
18	2W	90/92 (98%)	81 (90%)	9 (10%)	7	9
19	1X	77/78 (99%)	73 (95%)	4 (5%)	23	32
19	2X	77/78 (99%)	72 (94%)	5 (6%)	17	23
20	1Y	86/91 (94%)	82 (95%)	4 (5%)	26	37
20	2Y	86/91 (94%)	78 (91%)	8 (9%)	9	10
21	1Z	169/179 (94%)	148 (88%)	21 (12%)	4	5
21	2Z	165/179 (92%)	147 (89%)	18 (11%)	6	7
22	10	61/67 (91%)	57 (93%)	4 (7%)	16	22
22	20	61/67 (91%)	57 (93%)	4 (7%)	16	22
23	11	79/83 (95%)	70 (89%)	9 (11%)	5	6
23	21	81/83 (98%)	74 (91%)	7 (9%)	10	12
24	12	65/67 (97%)	62 (95%)	3 (5%)	27	38
24	22	66/67 (98%)	61 (92%)	5 (8%)	13	16
25	13	51/52 (98%)	47 (92%)	4 (8%)	12	16
25	23	50/52 (96%)	42 (84%)	8 (16%)	2	2
26	14	58/63 (92%)	49 (84%)	9 (16%)	2	2
26	24	54/63 (86%)	43 (80%)	11 (20%)	1	1
27	15	51/52 (98%)	44 (86%)	7 (14%)	3	3

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
27	25	50/52 (96%)	43 (86%)	7 (14%)	3	3
28	16	51/52 (98%)	45 (88%)	6 (12%)	5	5
28	26	50/52 (96%)	47 (94%)	3 (6%)	19	26
29	17	41/42 (98%)	39 (95%)	2 (5%)	25	35
29	27	41/42 (98%)	40 (98%)	1 (2%)	49	66
30	18	54/55 (98%)	51 (94%)	3 (6%)	21	29
30	28	54/55 (98%)	50 (93%)	4 (7%)	13	17
31	19	34/34 (100%)	34 (100%)	0	100	100
31	29	34/34 (100%)	34 (100%)	0	100	100
33	1b	191/220 (87%)	163 (85%)	28 (15%)	3	3
33	2b	187/220 (85%)	156 (83%)	31 (17%)	2	2
34	1c	144/188 (77%)	132 (92%)	12 (8%)	11	14
34	2c	140/188 (74%)	126 (90%)	14 (10%)	7	9
35	1d	171/181 (94%)	154 (90%)	17 (10%)	8	9
35	2d	172/181 (95%)	158 (92%)	14 (8%)	11	15
36	1e	114/123 (93%)	108 (95%)	6 (5%)	22	31
36	2e	114/123 (93%)	106 (93%)	8 (7%)	15	19
37	1f	85/90 (94%)	81 (95%)	4 (5%)	26	37
37	2f	85/90 (94%)	81 (95%)	4 (5%)	26	37
38	1g	120/127 (94%)	112 (93%)	8 (7%)	16	21
38	2g	119/127 (94%)	105 (88%)	14 (12%)	5	5
39	1h	116/119 (98%)	106 (91%)	10 (9%)	10	12
39	2h	114/119 (96%)	103 (90%)	11 (10%)	8	10
40	1i	91/99 (92%)	78 (86%)	13 (14%)	3	3
40	2i	88/99 (89%)	78 (89%)	10 (11%)	5	6
41	1j	68/92 (74%)	64 (94%)	4 (6%)	19	27
41	2j	68/92 (74%)	64 (94%)	4 (6%)	19	27
42	1k	83/99 (84%)	76 (92%)	7 (8%)	11	13
42	2k	83/99 (84%)	78 (94%)	5 (6%)	19	26
43	1l	96/108 (89%)	93 (97%)	3 (3%)	40	55
43	2l	96/108 (89%)	94 (98%)	2 (2%)	53	70

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
44	1m	90/101 (89%)	80 (89%)	10 (11%)	6	7
44	2m	87/101 (86%)	77 (88%)	10 (12%)	5	6
45	1n	49/50 (98%)	44 (90%)	5 (10%)	7	8
45	2n	49/50 (98%)	44 (90%)	5 (10%)	7	8
46	1o	78/80 (98%)	71 (91%)	7 (9%)	9	11
46	2o	78/80 (98%)	69 (88%)	9 (12%)	5	6
47	1p	69/74 (93%)	62 (90%)	7 (10%)	7	9
47	2p	68/74 (92%)	61 (90%)	7 (10%)	7	8
48	1q	94/97 (97%)	91 (97%)	3 (3%)	39	54
48	2q	94/97 (97%)	90 (96%)	4 (4%)	29	40
49	1r	59/77 (77%)	53 (90%)	6 (10%)	7	8
49	2r	59/77 (77%)	53 (90%)	6 (10%)	7	8
50	1s	68/80 (85%)	61 (90%)	7 (10%)	7	8
50	2s	67/80 (84%)	61 (91%)	6 (9%)	9	11
51	1t	71/82 (87%)	65 (92%)	6 (8%)	10	13
51	2t	70/82 (85%)	62 (89%)	8 (11%)	5	6
52	1u	18/22 (82%)	15 (83%)	3 (17%)	2	2
52	2u	18/22 (82%)	15 (83%)	3 (17%)	2	2
53	1y	82/98 (84%)	78 (95%)	4 (5%)	25	35
53	2y	79/98 (81%)	72 (91%)	7 (9%)	9	11
All	All	9524/10260 (93%)	8644 (91%)	880 (9%)	9	11

All (880) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	1D	61	LEU
3	1D	88	ARG
3	1D	94	LEU
3	1D	99	ASP
3	1D	103	ARG
3	1D	111	LEU
3	1D	126	GLN
3	1D	142	VAL
3	1D	211	ARG
3	1D	217	ARG

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
3	1D	229	VAL
3	1D	242	ARG
3	1D	257	LEU
3	1D	259	THR
3	1D	260	ARG
4	1E	7	VAL
4	1E	12	THR
4	1E	21	VAL
4	1E	49	LEU
4	1E	72	VAL
4	1E	73	GLU
4	1E	75	VAL
4	1E	78	LEU
4	1E	82	ARG
4	1E	111	ARG
4	1E	116	VAL
4	1E	119	ARG
4	1E	144	ARG
4	1E	175	VAL
4	1E	181	LEU
4	1E	203	LYS
5	1F	12	LEU
5	1F	20	LEU
5	1F	27	GLU
5	1F	33	LEU
5	1F	53	THR
5	1F	60	SER
5	1F	74	ARG
5	1F	88	VAL
5	1F	106	ARG
5	1F	110	LEU
5	1F	125	LEU
5	1F	132	VAL
5	1F	140	LEU
5	1F	168	ARG
5	1F	170	LEU
5	1F	192	LEU
5	1F	197	ASP
5	1F	205	ARG
6	1G	7	LEU
6	1G	43	LEU
6	1G	45	GLU

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
6	1G	49	ASP
6	1G	52	ILE
6	1G	53	LEU
6	1G	60	LEU
6	1G	81	LYS
6	1G	82	LEU
6	1G	135	LEU
6	1G	145	THR
6	1G	146	TYR
6	1G	153	ARG
6	1G	159	VAL
6	1G	170	ARG
6	1G	175	LEU
7	1H	6	ARG
7	1H	15	VAL
7	1H	23	ARG
7	1H	59	ARG
7	1H	69	ARG
7	1H	71	LEU
7	1H	116	GLU
7	1H	122	THR
8	1I	9	LEU
8	1I	10	GLU
8	1I	12	LEU
8	1I	38	LEU
8	1I	43	ASN
8	1I	44	LEU
8	1I	47	LEU
8	1I	57	ARG
8	1I	60	GLU
8	1I	61	ARG
8	1I	69	LYS
8	1I	75	LEU
8	1I	77	LEU
8	1I	85	GLU
8	1I	92	VAL
8	1I	108	THR
8	1I	109	ILE
8	1I	127	VAL
8	1I	140	LEU
9	1N	7	LYS
9	1N	33	LEU

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
9	1N	34	LEU
9	1N	48	MET
9	1N	61	ARG
9	1N	67	LEU
9	1N	83	LYS
9	1N	87	LEU
9	1N	99	LEU
9	1N	115	ARG
9	1N	120	LEU
9	1N	131	GLN
10	1O	8	LEU
10	1O	24	VAL
10	1O	69	ILE
11	1P	2	LYS
11	1P	55	ARG
11	1P	59	LEU
11	1P	70	GLN
11	1P	98	GLU
11	1P	106	LEU
11	1P	112	LEU
11	1P	119	GLU
11	1P	147	LEU
11	1P	149	GLU
12	1Q	6	ARG
12	1Q	7	MET
12	1Q	16	ARG
12	1Q	18	LYS
12	1Q	21	THR
12	1Q	45	GLN
12	1Q	55	VAL
12	1Q	56	ARG
12	1Q	60	ARG
12	1Q	75	THR
12	1Q	109	VAL
13	1R	18	LEU
13	1R	28	LEU
13	1R	29	LEU
13	1R	33	ARG
13	1R	36	THR
13	1R	44	LEU
13	1R	60	LEU
13	1R	65	LEU

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
13	1R	67	LEU
13	1R	75	LEU
13	1R	79	LEU
13	1R	86	ARG
13	1R	100	LEU
13	1R	114	VAL
14	1S	14	VAL
14	1S	20	ARG
14	1S	43	GLU
14	1S	48	LEU
14	1S	50	SER
14	1S	57	LYS
14	1S	59	LYS
14	1S	78	LEU
14	1S	80	LEU
14	1S	110	LEU
15	1T	6	LEU
15	1T	23	ARG
15	1T	35	LYS
15	1T	49	VAL
15	1T	53	ARG
15	1T	59	THR
15	1T	96	ARG
15	1T	118	ARG
15	1T	125	ARG
16	1U	5	LYS
16	1U	31	SER
16	1U	36	ARG
16	1U	59	ARG
16	1U	74	LEU
16	1U	83	LEU
16	1U	92	ARG
16	1U	95	LEU
16	1U	104	GLN
16	1U	108	GLU
17	1V	18	LEU
17	1V	43	GLU
17	1V	44	LYS
17	1V	46	VAL
17	1V	61	VAL
17	1V	62	LEU
17	1V	72	VAL

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
17	1V	79	VAL
18	1W	4	LYS
18	1W	11	ARG
18	1W	15	ARG
18	1W	17	VAL
18	1W	19	LEU
18	1W	23	LEU
18	1W	51	LEU
18	1W	52	GLU
18	1W	67	ASP
18	1W	100	THR
18	1W	107	LEU
19	1X	35	THR
19	1X	57	LEU
19	1X	66	LEU
19	1X	68	ARG
20	1Y	23	ARG
20	1Y	43	ASN
20	1Y	72	VAL
20	1Y	99	CYS
21	1Z	5	LEU
21	1Z	6	LYS
21	1Z	11	GLU
21	1Z	18	LEU
21	1Z	31	ARG
21	1Z	42	VAL
21	1Z	61	LEU
21	1Z	72	ARG
21	1Z	86	VAL
21	1Z	91	LEU
21	1Z	93	ASP
21	1Z	102	LEU
21	1Z	103	ARG
21	1Z	126	VAL
21	1Z	150	LEU
21	1Z	156	LYS
21	1Z	161	VAL
21	1Z	170	THR
21	1Z	185	GLU
21	1Z	191	VAL
21	1Z	199	LYS
22	10	11	ARG

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
22	10	20	ARG
22	10	55	ARG
22	10	59	LEU
23	11	21	ARG
23	11	30	VAL
23	11	40	ARG
23	11	52	ARG
23	11	57	GLU
23	11	80	LEU
23	11	83	GLU
23	11	89	GLU
23	11	95	LEU
24	12	32	LEU
24	12	52	ASP
24	12	53	LEU
25	13	8	LEU
25	13	23	LEU
25	13	31	LEU
25	13	54	VAL
26	14	23	GLU
26	14	30	GLU
26	14	34	GLU
26	14	46	GLN
26	14	49	PHE
26	14	50	VAL
26	14	58	ARG
26	14	65	ASP
26	14	67	TYR
27	15	6	VAL
27	15	26	THR
27	15	29	THR
27	15	40	LYS
27	15	58	LEU
27	15	59	GLU
27	15	60	VAL
28	16	4	GLU
28	16	14	THR
28	16	28	ARG
28	16	38	LYS
28	16	48	VAL
28	16	52	VAL
29	17	24	THR

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
29	17	43	THR
30	18	31	HIS
30	18	32	LEU
30	18	34	TRP
33	1b	8	LYS
33	1b	15	VAL
33	1b	21	ARG
33	1b	24	TRP
33	1b	44	LEU
33	1b	49	GLU
33	1b	76	GLN
33	1b	95	GLN
33	1b	106	LYS
33	1b	116	GLU
33	1b	122	PHE
33	1b	126	GLU
33	1b	135	GLN
33	1b	144	ARG
33	1b	150	SER
33	1b	157	ARG
33	1b	158	LEU
33	1b	163	PHE
33	1b	170	GLU
33	1b	178	ARG
33	1b	179	LYS
33	1b	185	ILE
33	1b	187	LEU
33	1b	195	ASP
33	1b	200	ILE
33	1b	224	GLN
33	1b	226	ARG
33	1b	230	VAL
34	1c	3	ASN
34	1c	15	THR
34	1c	21	ARG
34	1c	36	ASP
34	1c	45	LYS
34	1c	64	VAL
34	1c	102	ASN
34	1c	115	LEU
34	1c	131	ARG
34	1c	150	LYS

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
34	1c	178	LEU
34	1c	190	ARG
35	1d	8	VAL
35	1d	19	LEU
35	1d	24	GLU
35	1d	49	ARG
35	1d	58	LEU
35	1d	65	ARG
35	1d	85	LYS
35	1d	108	LEU
35	1d	112	VAL
35	1d	123	HIS
35	1d	135	LEU
35	1d	157	LEU
35	1d	168	ARG
35	1d	177	ASP
35	1d	187	ARG
35	1d	188	LEU
35	1d	193	ASP
36	1e	41	VAL
36	1e	47	LYS
36	1e	68	GLU
36	1e	69	VAL
36	1e	72	GLN
36	1e	137	GLU
37	1f	17	SER
37	1f	46	ARG
37	1f	70	ASP
37	1f	82	ARG
38	1g	6	ARG
38	1g	8	GLU
38	1g	12	LEU
38	1g	57	GLU
38	1g	89	MET
38	1g	104	LEU
38	1g	114	ARG
38	1g	144	MET
39	1h	2	LEU
39	1h	18	ARG
39	1h	21	LYS
39	1h	51	VAL
39	1h	52	ASP

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
39	1h	63	LEU
39	1h	78	GLN
39	1h	97	VAL
39	1h	112	LEU
39	1h	127	LEU
40	1i	2	GLU
40	1i	23	ASN
40	1i	25	LYS
40	1i	42	ARG
40	1i	64	THR
40	1i	65	VAL
40	1i	66	ARG
40	1i	81	ILE
40	1i	92	TYR
40	1i	93	ARG
40	1i	103	THR
40	1i	104	ARG
40	1i	108	VAL
41	1j	5	ARG
41	1j	38	ILE
41	1j	84	GLN
41	1j	92	THR
42	1k	14	VAL
42	1k	31	THR
42	1k	48	ILE
42	1k	54	ARG
42	1k	96	ARG
42	1k	114	VAL
42	1k	117	ASN
43	1l	27	LEU
43	1l	33	ARG
43	1l	41	ARG
44	1m	3	ARG
44	1m	4	ILE
44	1m	11	ARG
44	1m	17	VAL
44	1m	19	LEU
44	1m	32	GLU
44	1m	36	LYS
44	1m	63	THR
44	1m	70	LEU
44	1m	110	ARG

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
45	1n	3	ARG
45	1n	18	VAL
45	1n	33	VAL
45	1n	41	ARG
45	1n	57	ARG
46	1o	3	ILE
46	1o	26	GLU
46	1o	38	ARG
46	1o	39	LEU
46	1o	41	GLU
46	1o	48	LYS
46	1o	71	GLN
47	1p	2	VAL
47	1p	19	ILE
47	1p	20	VAL
47	1p	50	LYS
47	1p	62	VAL
47	1p	67	THR
47	1p	74	LEU
48	1q	68	ARG
48	1q	74	LEU
48	1q	85	VAL
49	1r	25	THR
49	1r	28	GLU
49	1r	31	LEU
49	1r	32	ARG
49	1r	35	ARG
49	1r	76	LEU
50	1s	5	LEU
50	1s	28	LYS
50	1s	35	SER
50	1s	37	ARG
50	1s	41	VAL
50	1s	65	ASN
50	1s	81	ARG
51	1t	9	ASN
51	1t	10	LEU
51	1t	84	LEU
51	1t	90	GLN
51	1t	93	GLU
51	1t	100	ILE
52	1u	7	ARG

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
52	1u	9	ARG
52	1u	10	ARG
53	1y	42	SER
53	1y	66	LYS
53	1y	77	LEU
53	1y	95	ARG
3	2D	3	VAL
3	2D	61	LEU
3	2D	88	ARG
3	2D	94	LEU
3	2D	99	ASP
3	2D	103	ARG
3	2D	111	LEU
3	2D	211	ARG
3	2D	217	ARG
3	2D	221	VAL
3	2D	229	VAL
3	2D	242	ARG
3	2D	257	LEU
3	2D	260	ARG
4	2E	12	THR
4	2E	21	VAL
4	2E	33	VAL
4	2E	47	VAL
4	2E	52	LEU
4	2E	72	VAL
4	2E	73	GLU
4	2E	75	VAL
4	2E	78	LEU
4	2E	82	ARG
4	2E	111	ARG
4	2E	113	PHE
4	2E	116	VAL
4	2E	119	ARG
4	2E	144	ARG
4	2E	175	VAL
4	2E	181	LEU
4	2E	184	VAL
5	2F	20	LEU
5	2F	24	LEU
5	2F	33	LEU
5	2F	60	SER

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
5	2F	88	VAL
5	2F	106	ARG
5	2F	110	LEU
5	2F	126	VAL
5	2F	140	LEU
5	2F	170	LEU
5	2F	175	THR
5	2F	192	LEU
5	2F	197	ASP
5	2F	200	GLU
5	2F	205	ARG
6	2G	3	LEU
6	2G	7	LEU
6	2G	21	ARG
6	2G	36	LYS
6	2G	43	LEU
6	2G	47	LYS
6	2G	49	ASP
6	2G	53	LEU
6	2G	55	LYS
6	2G	60	LEU
6	2G	75	LYS
6	2G	135	LEU
6	2G	136	ARG
6	2G	145	THR
6	2G	146	TYR
6	2G	153	ARG
6	2G	159	VAL
6	2G	164	GLU
6	2G	167	GLU
6	2G	170	ARG
7	2H	3	ARG
7	2H	33	LEU
7	2H	41	MET
7	2H	49	VAL
7	2H	69	ARG
7	2H	71	LEU
7	2H	88	LEU
7	2H	95	ARG
7	2H	98	LEU
7	2H	122	THR
7	2H	133	VAL

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
7	2H	136	ILE
7	2H	140	LYS
7	2H	171	LEU
8	2I	38	LEU
8	2I	44	LEU
8	2I	50	ARG
8	2I	54	GLN
8	2I	68	LEU
8	2I	75	LEU
8	2I	76	THR
8	2I	77	LEU
8	2I	92	VAL
8	2I	108	THR
8	2I	116	LEU
8	2I	127	VAL
8	2I	140	LEU
9	2N	28	THR
9	2N	34	LEU
9	2N	48	MET
9	2N	68	GLU
9	2N	83	LYS
9	2N	87	LEU
9	2N	90	MET
9	2N	99	LEU
9	2N	120	LEU
9	2N	131	GLN
9	2N	137	LYS
10	2O	8	LEU
10	2O	24	VAL
10	2O	53	LYS
11	2P	55	ARG
11	2P	59	LEU
11	2P	70	GLN
11	2P	86	LYS
11	2P	98	GLU
11	2P	99	LEU
11	2P	112	LEU
11	2P	147	LEU
11	2P	148	LEU
12	2Q	1	MET
12	2Q	7	MET
12	2Q	8	LYS

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
12	2Q	16	ARG
12	2Q	21	THR
12	2Q	45	GLN
12	2Q	48	GLU
12	2Q	55	VAL
12	2Q	56	ARG
12	2Q	60	ARG
13	2R	18	LEU
13	2R	28	LEU
13	2R	29	LEU
13	2R	33	ARG
13	2R	44	LEU
13	2R	60	LEU
13	2R	65	LEU
13	2R	67	LEU
13	2R	75	LEU
13	2R	79	LEU
13	2R	100	LEU
13	2R	111	LEU
13	2R	114	VAL
14	2S	14	VAL
14	2S	20	ARG
14	2S	35	ILE
14	2S	49	VAL
14	2S	50	SER
14	2S	67	ARG
14	2S	69	VAL
14	2S	71	ARG
14	2S	75	GLU
14	2S	93	LYS
15	2T	6	LEU
15	2T	13	ARG
15	2T	23	ARG
15	2T	49	VAL
15	2T	53	ARG
15	2T	96	ARG
15	2T	118	ARG
16	2U	31	SER
16	2U	36	ARG
16	2U	74	LEU
16	2U	83	LEU
16	2U	89	GLU

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
16	2U	92	ARG
16	2U	104	GLN
17	2V	18	LEU
17	2V	35	LEU
17	2V	38	LEU
17	2V	46	VAL
17	2V	62	LEU
17	2V	72	VAL
17	2V	79	VAL
17	2V	100	ARG
18	2W	11	ARG
18	2W	15	ARG
18	2W	17	VAL
18	2W	19	LEU
18	2W	23	LEU
18	2W	51	LEU
18	2W	52	GLU
18	2W	67	ASP
18	2W	107	LEU
19	2X	2	LYS
19	2X	33	LYS
19	2X	57	LEU
19	2X	66	LEU
19	2X	90	GLU
20	2Y	6	HIS
20	2Y	23	ARG
20	2Y	43	ASN
20	2Y	57	GLN
20	2Y	70	SER
20	2Y	72	VAL
20	2Y	90	LEU
20	2Y	99	CYS
21	2Z	2	GLU
21	2Z	6	LYS
21	2Z	18	LEU
21	2Z	42	VAL
21	2Z	46	LYS
21	2Z	61	LEU
21	2Z	72	ARG
21	2Z	86	VAL
21	2Z	91	LEU
21	2Z	107	THR

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
21	2Z	132	ASN
21	2Z	150	LEU
21	2Z	156	LYS
21	2Z	161	VAL
21	2Z	170	THR
21	2Z	182	LYS
21	2Z	193	GLU
21	2Z	199	LYS
22	20	19	LYS
22	20	20	ARG
22	20	55	ARG
22	20	70	GLN
23	21	4	VAL
23	21	21	ARG
23	21	40	ARG
23	21	52	ARG
23	21	80	LEU
23	21	85	LEU
23	21	95	LEU
24	22	32	LEU
24	22	40	SER
24	22	52	ASP
24	22	53	LEU
24	22	64	LEU
25	23	3	ARG
25	23	8	LEU
25	23	23	LEU
25	23	30	ARG
25	23	31	LEU
25	23	44	ARG
25	23	54	VAL
25	23	55	ARG
26	24	34	GLU
26	24	46	GLN
26	24	48	ARG
26	24	50	VAL
26	24	58	ARG
26	24	60	GLN
26	24	61	ARG
26	24	62	ARG
26	24	63	TYR
26	24	67	TYR

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
26	24	69	LYS
27	25	6	VAL
27	25	29	THR
27	25	35	GLU
27	25	40	LYS
27	25	48	GLU
27	25	58	LEU
27	25	59	GLU
28	26	14	THR
28	26	38	LYS
28	26	47	THR
29	27	43	THR
30	28	14	VAL
30	28	31	HIS
30	28	32	LEU
30	28	34	TRP
33	2b	8	LYS
33	2b	12	GLU
33	2b	16	HIS
33	2b	17	PHE
33	2b	24	TRP
33	2b	49	GLU
33	2b	63	MET
33	2b	81	VAL
33	2b	95	GLN
33	2b	114	ARG
33	2b	118	LEU
33	2b	122	PHE
33	2b	127	ILE
33	2b	135	GLN
33	2b	150	SER
33	2b	154	LEU
33	2b	157	ARG
33	2b	158	LEU
33	2b	163	PHE
33	2b	179	LYS
33	2b	185	ILE
33	2b	187	LEU
33	2b	200	ILE
33	2b	208	ILE
33	2b	210	SER
33	2b	215	LEU

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
33	2b	217	ARG
33	2b	222	ILE
33	2b	224	GLN
33	2b	226	ARG
33	2b	230	VAL
34	2c	3	ASN
34	2c	21	ARG
34	2c	45	LYS
34	2c	102	ASN
34	2c	104	GLN
34	2c	105	GLU
34	2c	115	LEU
34	2c	131	ARG
34	2c	132	ARG
34	2c	140	ARG
34	2c	152	ILE
34	2c	162	GLN
34	2c	178	LEU
34	2c	190	ARG
35	2d	8	VAL
35	2d	28	SER
35	2d	31	CYS
35	2d	34	GLU
35	2d	58	LEU
35	2d	65	ARG
35	2d	108	LEU
35	2d	112	VAL
35	2d	122	ARG
35	2d	135	LEU
35	2d	153	ARG
35	2d	157	LEU
35	2d	194	LEU
35	2d	201	GLN
36	2e	8	GLU
36	2e	31	LEU
36	2e	41	VAL
36	2e	47	LYS
36	2e	69	VAL
36	2e	72	GLN
36	2e	79	GLU
36	2e	150	ARG
37	2f	28	ARG

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
37	2f	46	ARG
37	2f	70	ASP
37	2f	82	ARG
38	2g	10	ARG
38	2g	12	LEU
38	2g	15	ASP
38	2g	52	GLU
38	2g	75	VAL
38	2g	76	ARG
38	2g	78	ARG
38	2g	104	LEU
38	2g	113	GLU
38	2g	114	ARG
38	2g	115	ARG
38	2g	143	ARG
38	2g	144	MET
38	2g	155	ARG
39	2h	18	ARG
39	2h	21	LYS
39	2h	26	VAL
39	2h	39	LEU
39	2h	68	ARG
39	2h	78	GLN
39	2h	84	ARG
39	2h	97	VAL
39	2h	98	LYS
39	2h	112	LEU
39	2h	133	LEU
40	2i	23	ASN
40	2i	31	GLN
40	2i	60	ASP
40	2i	64	THR
40	2i	65	VAL
40	2i	92	TYR
40	2i	102	LEU
40	2i	104	ARG
40	2i	108	VAL
40	2i	113	LYS
41	2j	38	ILE
41	2j	57	LYS
41	2j	92	THR
41	2j	94	VAL

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
42	2k	96	ARG
42	2k	114	VAL
42	2k	116	HIS
42	2k	117	ASN
42	2k	126	ARG
43	2l	27	LEU
43	2l	41	ARG
44	2m	17	VAL
44	2m	19	LEU
44	2m	27	LYS
44	2m	32	GLU
44	2m	60	VAL
44	2m	63	THR
44	2m	70	LEU
44	2m	94	ARG
44	2m	110	ARG
44	2m	116	THR
45	2n	3	ARG
45	2n	12	ARG
45	2n	18	VAL
45	2n	50	LYS
45	2n	57	ARG
46	2o	3	ILE
46	2o	26	GLU
46	2o	38	ARG
46	2o	39	LEU
46	2o	41	GLU
46	2o	54	ARG
46	2o	68	ARG
46	2o	71	GLN
46	2o	88	ARG
47	2p	2	VAL
47	2p	8	ARG
47	2p	20	VAL
47	2p	28	ARG
47	2p	62	VAL
47	2p	69	THR
47	2p	71	ARG
48	2q	6	LEU
48	2q	36	ILE
48	2q	68	ARG
48	2q	74	LEU

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
49	2r	21	LYS
49	2r	25	THR
49	2r	31	LEU
49	2r	41	LYS
49	2r	58	LEU
49	2r	76	LEU
50	2s	35	SER
50	2s	48	THR
50	2s	56	GLN
50	2s	77	THR
50	2s	78	ARG
50	2s	79	THR
51	2t	9	ASN
51	2t	24	LEU
51	2t	56	MET
51	2t	84	LEU
51	2t	90	GLN
51	2t	93	GLU
51	2t	99	LEU
51	2t	100	ILE
52	2u	7	ARG
52	2u	10	ARG
52	2u	24	ARG
53	2y	9	GLN
53	2y	13	THR
53	2y	16	ILE
53	2y	24	LEU
53	2y	41	LEU
53	2y	46	GLN
53	2y	56	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (142) such sidechains are listed below:

<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
3	1D	87	ASN
3	1D	164	GLN
3	1D	253	GLN
4	1E	85	ASN
5	1F	69	HIS
5	1F	169	ASN
5	1F	203	GLN
6	1G	26	GLN

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
8	1I	43	ASN
8	1I	54	GLN
8	1I	104	GLN
11	1P	38	GLN
15	1T	43	GLN
15	1T	58	ASN
15	1T	123	GLN
16	1U	117	GLN
19	1X	31	HIS
19	1X	82	GLN
20	1Y	43	ASN
20	1Y	92	ASN
21	1Z	118	GLN
22	10	35	ASN
25	13	32	GLN
31	19	36	GLN
33	1b	95	GLN
33	1b	224	GLN
34	1c	6	HIS
34	1c	28	GLN
34	1c	37	GLN
34	1c	102	ASN
34	1c	123	GLN
34	1c	136	GLN
35	1d	77	ASN
35	1d	123	HIS
35	1d	129	ASN
36	1e	20	GLN
36	1e	38	GLN
36	1e	56	GLN
36	1e	141	GLN
37	1f	73	ASN
37	1f	100	ASN
38	1g	13	GLN
38	1g	28	ASN
38	1g	56	GLN
38	1g	86	GLN
38	1g	110	GLN
40	1i	23	ASN
40	1i	34	ASN
40	1i	124	GLN
41	1j	56	HIS

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
42	1k	104	GLN
43	1l	99	HIS
44	1m	92	HIS
46	1o	28	GLN
47	1p	16	HIS
47	1p	76	GLN
48	1q	16	GLN
50	1s	57	HIS
50	1s	65	ASN
50	1s	69	HIS
50	1s	83	HIS
51	1t	90	GLN
53	1y	18	GLN
53	1y	38	HIS
3	2D	87	ASN
3	2D	126	GLN
3	2D	164	GLN
3	2D	253	GLN
4	2E	85	ASN
5	2F	69	HIS
5	2F	169	ASN
5	2F	203	GLN
6	2G	26	GLN
6	2G	40	ASN
7	2H	74	ASN
8	2I	43	ASN
8	2I	54	GLN
11	2P	27	HIS
11	2P	38	GLN
13	2R	91	GLN
15	2T	43	GLN
15	2T	58	ASN
15	2T	123	GLN
16	2U	104	GLN
17	2V	64	HIS
18	2W	60	ASN
19	2X	31	HIS
19	2X	82	GLN
21	2Z	50	GLN
21	2Z	151	HIS
22	20	35	ASN
25	23	32	GLN

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
31	29	36	GLN
33	2b	19	HIS
33	2b	76	GLN
33	2b	95	GLN
33	2b	212	GLN
34	2c	6	HIS
34	2c	28	GLN
34	2c	37	GLN
34	2c	104	GLN
34	2c	123	GLN
34	2c	136	GLN
34	2c	176	HIS
34	2c	181	ASN
35	2d	45	GLN
35	2d	77	ASN
35	2d	123	HIS
35	2d	125	HIS
35	2d	161	ASN
36	2e	56	GLN
36	2e	78	HIS
36	2e	141	GLN
37	2f	73	ASN
38	2g	28	ASN
38	2g	56	GLN
39	2h	78	GLN
40	2i	23	ASN
40	2i	31	GLN
40	2i	73	GLN
40	2i	124	GLN
41	2j	84	GLN
42	2k	93	GLN
43	2l	99	HIS
44	2m	77	ASN
46	2o	9	GLN
46	2o	28	GLN
46	2o	62	GLN
46	2o	71	GLN
47	2p	14	ASN
47	2p	16	HIS
48	2q	16	GLN
50	2s	14	HIS
50	2s	23	ASN

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Mol	Chain	Res	Type
50	2s	56	GLN
50	2s	69	HIS
50	2s	83	HIS
51	2t	9	ASN
53	2y	18	GLN
53	2y	31	GLN
53	2y	36	ASN
53	2y	46	GLN

### 5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	1A	2862/2915 (98%)	403 (14%)	41 (1%)
1	2A	2855/2915 (97%)	483 (16%)	41 (1%)
2	1B	119/121 (98%)	10 (8%)	0
2	2B	119/121 (98%)	14 (11%)	0
32	1a	1494/1521 (98%)	229 (15%)	0
32	2a	1498/1521 (98%)	251 (16%)	0
All	All	8947/9114 (98%)	1390 (15%)	82 (0%)

All (1390) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	1A	12	U
1	1A	13	A
1	1A	34	C
1	1A	45	C
1	1A	70	A
1	1A	73	A
1	1A	74	G
1	1A	94	G
1	1A	116	A
1	1A	117	A
1	1A	118	U
1	1A	155	C
1	1A	162	G
1	1A	170	A
1	1A	171	A
1	1A	185	A
1	1A	186	A
1	1A	194	G

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	1A	204	G
1	1A	205	A
1	1A	211	A
1	1A	218	A
1	1A	237	G
1	1A	269	G
1	1A	271	U
1	1A	272	U
1	1A	273	G
1	1A	274	U
1	1A	275	C
1	1A	279	G
1	1A	288	U
1	1A	289	G
1	1A	295	C
1	1A	297	C
1	1A	299	G
1	1A	303	C
1	1A	307	A
1	1A	335	A
1	1A	354	A
1	1A	376	G
1	1A	387	G
1	1A	389	G
1	1A	407	U
1	1A	413	G
1	1A	432	U
1	1A	438	G
1	1A	439	A
1	1A	448	U
1	1A	455	A
1	1A	474	U
1	1A	477	C
1	1A	480	A
1	1A	482	C
1	1A	483	A
1	1A	507	G
1	1A	530	A
1	1A	534	C
1	1A	553	A
1	1A	554	A
1	1A	555	G

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	1A	556	C
1	1A	557	A
1	1A	558	G
1	1A	569	G
1	1A	573	G
1	1A	586	G
1	1A	596	G
1	1A	598	A
1	1A	609	A
1	1A	626	A
1	1A	627	G
1	1A	630	U
1	1A	641	G
1	1A	642	G
1	1A	652	A
1	1A	662	A
1	1A	670	C
1	1A	671	A
1	1A	694	G
1	1A	697	C
1	1A	698	G
1	1A	715	G
1	1A	716	G
1	1A	733	G
1	1A	764	G
1	1A	777	C
1	1A	793	A
1	1A	794	U
1	1A	812	G
1	1A	822	G
1	1A	823	G
1	1A	829	A
1	1A	831	A
1	1A	832	G
1	1A	837	C
1	1A	839	G
1	1A	852	G
1	1A	859	C
1	1A	874	U
1	1A	875	U
1	1A	906	G
1	1A	913	A

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	1A	927	G
1	1A	929	G
1	1A	932	C
1	1A	933	C
1	1A	935	C
1	1A	936	C
1	1A	937	A
1	1A	938	G
1	1A	940	C
1	1A	942	A
1	1A	945	A
1	1A	956	A
1	1A	977	G
1	1A	990	A
1	1A	991	G
1	1A	1003	U
1	1A	1004	A
1	1A	1006	C
1	1A	1019	G
1	1A	1020	C
1	1A	1029	A
1	1A	1042	A
1	1A	1058	U
1	1A	1059	C
1	1A	1068	G
1	1A	1072	U
1	1A	1079	U
1	1A	1085	G
1	1A	1088	G
1	1A	1089	C
1	1A	1092	A
1	1A	1093	G
1	1A	1094	A
1	1A	1100	A
1	1A	1104	G
1	1A	1106	U
1	1A	1107	U
1	1A	1108	G
1	1A	1109	G
1	1A	1111	U
1	1A	1114	G
1	1A	1116	A

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	1A	1117	G
1	1A	1119	A
1	1A	1121	C
1	1A	1122	C
1	1A	1123	A
1	1A	1124	U
1	1A	1126	C
1	1A	1129	U
1	1A	1130	A
1	1A	1134	A
1	1A	1136	U
1	1A	1142	A
1	1A	1143	U
1	1A	1152	G
1	1A	1155	C
1	1A	1156	G
1	1A	1158	G
1	1A	1162	C
1	1A	1174	A
1	1A	1175	A
1	1A	1180	C
1	1A	1181	G
1	1A	1217	G
1	1A	1218	G
1	1A	1219	A
1	1A	1220	U
1	1A	1221	G
1	1A	1222	A
1	1A	1223	C
1	1A	1255	A
1	1A	1256	U
1	1A	1263	C
1	1A	1299	A
1	1A	1302	G
1	1A	1317	G
1	1A	1318	A
1	1A	1319	U
1	1A	1346	U
1	1A	1347	A
1	1A	1349	G
1	1A	1365	G
1	1A	1398	U

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	1A	1405	A
1	1A	1411	A
1	1A	1416	C
1	1A	1426	G
1	1A	1430	A
1	1A	1431	G
1	1A	1462	G
1	1A	1463	C
1	1A	1466	U
1	1A	1467	G
1	1A	1474	C
1	1A	1491	A
1	1A	1497	G
1	1A	1500	A
1	1A	1502	G
1	1A	1514	C
1	1A	1518	A
1	1A	1529	G
1	1A	1533	G
1	1A	1539	C
1	1A	1552	C
1	1A	1554	A
1	1A	1555	C
1	1A	1556	A
1	1A	1571	G
1	1A	1578	C
1	1A	1589	A
1	1A	1590	C
1	1A	1605	A
1	1A	1613	A
1	1A	1616	A
1	1A	1625	U
1	1A	1626	A
1	1A	1628	G
1	1A	1631	C
1	1A	1632	A
1	1A	1654	A
1	1A	1655	A
1	1A	1656	A
1	1A	1695	C
1	1A	1701	A
1	1A	1721	G

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	1A	1747	A
1	1A	1748	A
1	1A	1762	G
1	1A	1763	G
1	1A	1767	A
1	1A	1768	U
1	1A	1787	G
1	1A	1794	G
1	1A	1795	G
1	1A	1804	A
1	1A	1811	A
1	1A	1813	C
1	1A	1822	A
1	1A	1831	C
1	1A	1832	G
1	1A	1843	A
1	1A	1847	G
1	1A	1870	G
1	1A	1878	A
1	1A	1899	A
1	1A	1900	G
1	1A	1911	A
1	1A	1918	G
1	1A	1922	A
1	1A	1928	G
1	1A	1935	A
1	1A	1936	C
1	1A	1951	G
1	1A	1952	G
1	1A	1959	A
1	1A	1960	A
1	1A	1977	U
1	1A	1985	U
1	1A	1989	C
1	1A	1992	A
1	1A	1993	A
1	1A	1994	A
1	1A	2015	U
1	1A	2019	G
1	1A	2042	A
1	1A	2045	G
1	1A	2053	A

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	1A	2054	G
1	1A	2055	A
1	1A	2065	C
1	1A	2077	C
1	1A	2078	G
1	1A	2082	A
1	1A	2083	G
1	1A	2084	A
1	1A	2091	G
1	1A	2102	G
1	1A	2121	U
1	1A	2125	C
1	1A	2126	G
1	1A	2127	C
1	1A	2129	C
1	1A	2130	C
1	1A	2132	G
1	1A	2134	G
1	1A	2138	G
1	1A	2139	A
1	1A	2140	U
1	1A	2141	A
1	1A	2142	G
1	1A	2144	U
1	1A	2145	G
1	1A	2148	A
1	1A	2149	G
1	1A	2153	G
1	1A	2154	U
1	1A	2155	G
1	1A	2156	A
1	1A	2157	A
1	1A	2160	C
1	1A	2164	C
1	1A	2168	C
1	1A	2170	G
1	1A	2175	G
1	1A	2180	A
1	1A	2181	G
1	1A	2183	C
1	1A	2188	G
1	1A	2192	A

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	1A	2195	A
1	1A	2196	C
1	1A	2206	G
1	1A	2208	G
1	1A	2209	G
1	1A	2212	G
1	1A	2214	G
1	1A	2220	A
1	1A	2227	G
1	1A	2228	G
1	1A	2229	A
1	1A	2237	A
1	1A	2250	G
1	1A	2251	G
1	1A	2280	A
1	1A	2295	C
1	1A	2299	A
1	1A	2301	G
1	1A	2317	A
1	1A	2320	G
1	1A	2332	A
1	1A	2337	G
1	1A	2338	C
1	1A	2346	G
1	1A	2359	C
1	1A	2362	C
1	1A	2395	G
1	1A	2397	C
1	1A	2405	A
1	1A	2418	U
1	1A	2426	G
1	1A	2434	A
1	1A	2435	U
1	1A	2436	C
1	1A	2437	A
1	1A	2440	G
1	1A	2441	G
1	1A	2442	A
1	1A	2443	U
1	1A	2446	A
1	1A	2447	A
1	1A	2451	A

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	1A	2453	C
1	1A	2460	A
1	1A	2480	G
1	1A	2481	A
1	1A	2482	G
1	1A	2488	A
1	1A	2490	A
1	1A	2514	G
1	1A	2517	G
1	1A	2518	U
1	1A	2530	A
1	1A	2541	G
1	1A	2547	G
1	1A	2566	U
1	1A	2578	A
1	1A	2579	G
1	1A	2585	C
1	1A	2614	A
1	1A	2615	G
1	1A	2621	U
1	1A	2623	U
1	1A	2624	C
1	1A	2642	G
1	1A	2666	A
1	1A	2674	A
1	1A	2682	A
1	1A	2701	U
1	1A	2702	C
1	1A	2714	U
1	1A	2715	C
1	1A	2725	A
1	1A	2726	A
1	1A	2727	G
1	1A	2739	U
1	1A	2746	A
1	1A	2771	A
1	1A	2778	A
1	1A	2779	G
1	1A	2791	A
1	1A	2803	A
1	1A	2804	C
1	1A	2813	G

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	1A	2830	A
1	1A	2831	A
1	1A	2843	G
1	1A	2845	A
1	1A	2849	G
1	1A	2882	G
1	1A	2903	G
2	1B	2	C
2	1B	7	G
2	1B	13	A
2	1B	45	A
2	1B	53	A
2	1B	56	G
2	1B	73	A
2	1B	84	C
2	1B	110	G
2	1B	116	G
32	1a	6	G
32	1a	9	G
32	1a	32	A
32	1a	39	G
32	1a	48	C
32	1a	51	A
32	1a	61	G
32	1a	78	G
32	1a	79	G
32	1a	96	U
32	1a	99	U
32	1a	101	A
32	1a	116	A
32	1a	121	C
32	1a	131	C
32	1a	144	G
32	1a	156	G
32	1a	163	C
32	1a	173	U
32	1a	174	C
32	1a	182	U
32	1a	189(D)	C
32	1a	195	A
32	1a	197	A
32	1a	202	U

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
32	1a	203	U
32	1a	204	U
32	1a	216	G
32	1a	220	G
32	1a	247	G
32	1a	251	G
32	1a	258	G
32	1a	266	G
32	1a	267	C
32	1a	289	G
32	1a	321	A
32	1a	328	C
32	1a	332	G
32	1a	348	G
32	1a	352	C
32	1a	353	A
32	1a	354	G
32	1a	356	A
32	1a	367	U
32	1a	372	C
32	1a	373	A
32	1a	383	A
32	1a	384	G
32	1a	397	A
32	1a	398	C
32	1a	406	G
32	1a	412	A
32	1a	413	G
32	1a	423	G
32	1a	424	G
32	1a	429	U
32	1a	439	A
32	1a	442	C
32	1a	446	G
32	1a	452	A
32	1a	456	C
32	1a	458	C
32	1a	461	A
32	1a	470	C
32	1a	475	G
32	1a	477	A
32	1a	484	G

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
32	1a	485	G
32	1a	496	A
32	1a	498	U
32	1a	505	G
32	1a	509	A
32	1a	510	A
32	1a	511	C
32	1a	518	C
32	1a	521	G
32	1a	531	U
32	1a	532	A
32	1a	547	A
32	1a	550	G
32	1a	559	A
32	1a	561	U
32	1a	572	A
32	1a	573	A
32	1a	576	G
32	1a	577	G
32	1a	596	C
32	1a	607	A
32	1a	619	U
32	1a	630	G
32	1a	631	G
32	1a	632	A
32	1a	651	C
32	1a	653	A
32	1a	661	G
32	1a	665	A
32	1a	687	A
32	1a	688	G
32	1a	723	U
32	1a	731	G
32	1a	755	G
32	1a	774	G
32	1a	777	A
32	1a	793	U
32	1a	794	A
32	1a	817	C
32	1a	821	G
32	1a	828	A
32	1a	829	G

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
32	1a	839	U
32	1a	840	C
32	1a	841	U
32	1a	851	G
32	1a	914	A
32	1a	926	G
32	1a	927	G
32	1a	934	C
32	1a	935	A
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	992	U
32	1a	993	G
32	1a	998	G
32	1a	999	C
32	1a	1001(A)	G
32	1a	1006	C
32	1a	1007	C
32	1a	1008	C
32	1a	1009	G
32	1a	1022	G
32	1a	1023	G
32	1a	1024	G
32	1a	1025	U
32	1a	1026	G
32	1a	1027	C
32	1a	1028	C
32	1a	1029	C
32	1a	1030	C
32	1a	1030(A)	G
32	1a	1030(B)	C
32	1a	1030(D)	A
32	1a	1032	G
32	1a	1034	G
32	1a	1036	G

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
32	1a	1037	C
32	1a	1039	C
32	1a	1040	U
32	1a	1042	G
32	1a	1044	A
32	1a	1053	G
32	1a	1065	U
32	1a	1066	C
32	1a	1068	G
32	1a	1070	U
32	1a	1092	A
32	1a	1094	G
32	1a	1095	U
32	1a	1101	A
32	1a	1126	U
32	1a	1127	G
32	1a	1130	A
32	1a	1132	C
32	1a	1134	G
32	1a	1136	U
32	1a	1137	C
32	1a	1138	G
32	1a	1139	G
32	1a	1140	C
32	1a	1146	A
32	1a	1152	A
32	1a	1159	U
32	1a	1162	C
32	1a	1168	A
32	1a	1183	A
32	1a	1184	G
32	1a	1196	U
32	1a	1197	G
32	1a	1202	G
32	1a	1208	C
32	1a	1212	U
32	1a	1213	A
32	1a	1224	G
32	1a	1227	A
32	1a	1238	A
32	1a	1245	A
32	1a	1256	A

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
32	1a	1257	U
32	1a	1258	G
32	1a	1270	C
32	1a	1278	U
32	1a	1280	A
32	1a	1286	A
32	1a	1287	A
32	1a	1293	G
32	1a	1299	A
32	1a	1300	G
32	1a	1302	U
32	1a	1320	C
32	1a	1338	G
32	1a	1346	A
32	1a	1347	G
32	1a	1353	G
32	1a	1363	C
32	1a	1370	G
32	1a	1379	G
32	1a	1397	C
32	1a	1419	G
32	1a	1442	G
32	1a	1442(A)	G
32	1a	1447	A
32	1a	1456	G
32	1a	1493	A
32	1a	1499	A
32	1a	1503	A
32	1a	1504	G
32	1a	1505	G
32	1a	1506	U
32	1a	1517	G
32	1a	1520	G
32	1a	1529	G
32	1a	1530	G
32	1a	1531	A
1	2A	8	A
1	2A	10	G
1	2A	11	G
1	2A	12	U
1	2A	14	A
1	2A	15	G

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	2A	34	C
1	2A	45	C
1	2A	61	G
1	2A	71	A
1	2A	74	A
1	2A	75	G
1	2A	84	A
1	2A	102	G
1	2A	118	A
1	2A	119	A
1	2A	120	U
1	2A	131	G
1	2A	141	A
1	2A	157	U
1	2A	181	A
1	2A	182	A
1	2A	196	A
1	2A	197	A
1	2A	199	A
1	2A	205	G
1	2A	214	G
1	2A	215	G
1	2A	216	A
1	2A	221	A
1	2A	222	A
1	2A	229	A
1	2A	230	U
1	2A	248	G
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(A)	U
1	2A	272(B)	G
1	2A	277	C
1	2A	278	A
1	2A	311	A
1	2A	317	G
1	2A	324	A
1	2A	327	G
1	2A	329	G

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	2A	330	A
1	2A	352	G
1	2A	362	U
1	2A	363	G
1	2A	370	G
1	2A	386	G
1	2A	396	G
1	2A	405	U
1	2A	411	G
1	2A	412	A
1	2A	428	A
1	2A	444	C
1	2A	454	A
1	2A	455	C
1	2A	456	C
1	2A	457	A
1	2A	470	A
1	2A	481	G
1	2A	496	G
1	2A	504	U
1	2A	505	A
1	2A	509	C
1	2A	530	G
1	2A	531	C
1	2A	532	A
1	2A	533	G
1	2A	545	G
1	2A	563	G
1	2A	573	G
1	2A	575	A
1	2A	603	A
1	2A	604	G
1	2A	607	U
1	2A	610	G
1	2A	614(B)	G
1	2A	614(C)	A
1	2A	615	G
1	2A	616	G
1	2A	620	G
1	2A	627	A
1	2A	637	A
1	2A	645	C

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	2A	646	A
1	2A	652(B)	A
1	2A	652(C)	G
1	2A	652(U)	G
1	2A	653	A
1	2A	668	G
1	2A	669	G
1	2A	686	G
1	2A	717	G
1	2A	730	C
1	2A	752	A
1	2A	753	C
1	2A	764	A
1	2A	765	G
1	2A	774	A
1	2A	775	G
1	2A	776	G
1	2A	782	A
1	2A	784	A
1	2A	785	G
1	2A	790	C
1	2A	792	G
1	2A	805	G
1	2A	812	C
1	2A	827	U
1	2A	828	U
1	2A	857	C
1	2A	859	G
1	2A	867	C
1	2A	877	U
1	2A	880	G
1	2A	886	C
1	2A	887	A
1	2A	888	C
1	2A	889	C
1	2A	890	A
1	2A	893	C
1	2A	895	U
1	2A	896	A
1	2A	900	A
1	2A	901	A
1	2A	910	A

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	2A	915	C
1	2A	917	A
1	2A	932	G
1	2A	936	C
1	2A	941	A
1	2A	945	A
1	2A	946	G
1	2A	953	A
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	1012	U
1	2A	1013	C
1	2A	1015	G
1	2A	1017	G
1	2A	1033	U
1	2A	1035	U
1	2A	1041	C
1	2A	1045	A
1	2A	1046	A
1	2A	1047	G
1	2A	1048	A
1	2A	1052	C
1	2A	1053	C
1	2A	1054	A
1	2A	1058	G
1	2A	1060	U
1	2A	1063	G
1	2A	1064	C
1	2A	1065	U
1	2A	1066	U
1	2A	1067	A
1	2A	1068	G
1	2A	1069	A
1	2A	1070	A
1	2A	1071	G
1	2A	1072	C
1	2A	1073	A
1	2A	1074	G

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	2A	1076	C
1	2A	1077	A
1	2A	1078	U
1	2A	1079	C
1	2A	1080	C
1	2A	1083	U
1	2A	1084	A
1	2A	1085	A
1	2A	1086	A
1	2A	1088	A
1	2A	1090	U
1	2A	1091	G
1	2A	1092	C
1	2A	1093	G
1	2A	1094	U
1	2A	1095	A
1	2A	1096	A
1	2A	1098	A
1	2A	1108	U
1	2A	1109	C
1	2A	1110	G
1	2A	1112	G
1	2A	1116	C
1	2A	1117	G
1	2A	1128	A
1	2A	1129	A
1	2A	1130	U
1	2A	1135	C
1	2A	1136	G
1	2A	1144	G
1	2A	1171	G
1	2A	1181	C
1	2A	1188	U
1	2A	1210	A
1	2A	1211	U
1	2A	1212	G
1	2A	1220	A
1	2A	1229	G
1	2A	1253	A
1	2A	1256	G
1	2A	1271	G
1	2A	1272	A

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	2A	1273	U
1	2A	1300	U
1	2A	1301	A
1	2A	1303	G
1	2A	1306	C
1	2A	1308	A
1	2A	1314	C
1	2A	1321	A
1	2A	1342	A
1	2A	1345	C
1	2A	1352	U
1	2A	1359	A
1	2A	1360	A
1	2A	1365	A
1	2A	1368	G
1	2A	1380	G
1	2A	1384	A
1	2A	1385	G
1	2A	1410	G
1	2A	1416	G
1	2A	1417	C
1	2A	1420	U
1	2A	1421	G
1	2A	1428	C
1	2A	1445	A
1	2A	1450	G
1	2A	1451	C
1	2A	1455	G
1	2A	1459	G
1	2A	1467	C
1	2A	1471	A
1	2A	1482	G
1	2A	1493	C
1	2A	1494	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	1542	A
1	2A	1543	C

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	2A	1547	C
1	2A	1558	A
1	2A	1569	A
1	2A	1578	U
1	2A	1580	A
1	2A	1583	A
1	2A	1584	C
1	2A	1586	A
1	2A	1608	A
1	2A	1610	A
1	2A	1640	C
1	2A	1647	G
1	2A	1648	C
1	2A	1674	G
1	2A	1700	A
1	2A	1721	G
1	2A	1722	A
1	2A	1740	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	1791	A
1	2A	1800	C
1	2A	1801	G
1	2A	1816	G
1	2A	1817	G
1	2A	1839	G
1	2A	1847	A
1	2A	1848	A
1	2A	1858	G
1	2A	1877	A
1	2A	1878	G
1	2A	1889	A
1	2A	1900	A
1	2A	1914	C
1	2A	1918	A
1	2A	1929	G
1	2A	1930	G

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	2A	1937	A
1	2A	1938	A
1	2A	1955	U
1	2A	1963	U
1	2A	1967	C
1	2A	1970	A
1	2A	1971	A
1	2A	1972	A
1	2A	1975	G
1	2A	1992	G
1	2A	1993	U
1	2A	1997	G
1	2A	2020	A
1	2A	2023	G
1	2A	2031	A
1	2A	2033	A
1	2A	2043	C
1	2A	2049	G
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	2096	U
1	2A	2098	U
1	2A	2099	U
1	2A	2100	G
1	2A	2103	C
1	2A	2104	G
1	2A	2105	C
1	2A	2107	C
1	2A	2108	C
1	2A	2109	U
1	2A	2110	G
1	2A	2111	C
1	2A	2112	G
1	2A	2115	G
1	2A	2116	G
1	2A	2117	A
1	2A	2118	U
1	2A	2119	A

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	2A	2121	G
1	2A	2123	G
1	2A	2124	G
1	2A	2126	A
1	2A	2127	G
1	2A	2128	C
1	2A	2129	C
1	2A	2130	U
1	2A	2132	U
1	2A	2133	G
1	2A	2134	A
1	2A	2135	A
1	2A	2136	C
1	2A	2141	G
1	2A	2145	C
1	2A	2146	C
1	2A	2150	U
1	2A	2151	G
1	2A	2154	G
1	2A	2157	G
1	2A	2158	A
1	2A	2159	G
1	2A	2160	G
1	2A	2161	C
1	2A	2163	C
1	2A	2164	C
1	2A	2165	G
1	2A	2167	U
1	2A	2172	U
1	2A	2173	A
1	2A	2174	C
1	2A	2177	C
1	2A	2178	C
1	2A	2180	U
1	2A	2181	G
1	2A	2183	C
1	2A	2184	G
1	2A	2186	G
1	2A	2189	U
1	2A	2192	G
1	2A	2198	A
1	2A	2206	G

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	2A	2207	G
1	2A	2208	A
1	2A	2218	U
1	2A	2225	A
1	2A	2239	G
1	2A	2268	A
1	2A	2269	A
1	2A	2275	C
1	2A	2279	G
1	2A	2283	C
1	2A	2287	A
1	2A	2289	G
1	2A	2293	C
1	2A	2305	A
1	2A	2308	G
1	2A	2309	A
1	2A	2311	A
1	2A	2312	U
1	2A	2313	C
1	2A	2319	G
1	2A	2320	A
1	2A	2321	G
1	2A	2322	A
1	2A	2325	G
1	2A	2334	G
1	2A	2335	A
1	2A	2336	A
1	2A	2343	C
1	2A	2347	C
1	2A	2350	C
1	2A	2354	G
1	2A	2379	G
1	2A	2383	G
1	2A	2385	C
1	2A	2406	U
1	2A	2410	G
1	2A	2422	A
1	2A	2425	A
1	2A	2428	G
1	2A	2429	G
1	2A	2430	A
1	2A	2435	A

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	2A	2439	A
1	2A	2441	C
1	2A	2448	A
1	2A	2468	G
1	2A	2474	C
1	2A	2476	A
1	2A	2478	A
1	2A	2498	C
1	2A	2502	G
1	2A	2505	G
1	2A	2506	U
1	2A	2518	A
1	2A	2529	G
1	2A	2535	G
1	2A	2554	U
1	2A	2566	A
1	2A	2567	G
1	2A	2573	C
1	2A	2578	G
1	2A	2585	U
1	2A	2602	A
1	2A	2603	G
1	2A	2611	U
1	2A	2612	C
1	2A	2615	U
1	2A	2630	G
1	2A	2654	A
1	2A	2663	G
1	2A	2682	U
1	2A	2689	U
1	2A	2690	C
1	2A	2703	C
1	2A	2712(A)	A
1	2A	2713	A
1	2A	2714	G
1	2A	2726	U
1	2A	2733	A
1	2A	2744	G
1	2A	2751	G
1	2A	2757	A
1	2A	2759	G
1	2A	2764	A

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	2A	2765	A
1	2A	2766	G
1	2A	2769	C
1	2A	2778	A
1	2A	2818	G
1	2A	2820	A
1	2A	2821	A
1	2A	2833	G
1	2A	2835	A
1	2A	2836	U
1	2A	2839	G
1	2A	2872	G
1	2A	2880	C
1	2A	2894	G
1	2A	2897	U
2	2B	2	C
2	2B	7	G
2	2B	8	U
2	2B	12	C
2	2B	13	A
2	2B	23	G
2	2B	33	G
2	2B	51	G
2	2B	56	G
2	2B	73	A
2	2B	84	C
2	2B	108	U
2	2B	110	G
2	2B	116	G
32	2a	5	U
32	2a	9	G
32	2a	22	G
32	2a	32	A
32	2a	39	G
32	2a	47	C
32	2a	48	C
32	2a	50	A
32	2a	51	A
32	2a	52	G
32	2a	61	G
32	2a	66	G
32	2a	78	G

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
32	2a	89	C
32	2a	97	G
32	2a	116	A
32	2a	121	C
32	2a	131	C
32	2a	151	A
32	2a	163	C
32	2a	173	U
32	2a	174	C
32	2a	182	U
32	2a	189(F)	U
32	2a	195	A
32	2a	197	A
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	258	G
32	2a	266	G
32	2a	267	C
32	2a	269	C
32	2a	289	G
32	2a	298	A
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	373	A
32	2a	381	C
32	2a	384	G
32	2a	397	A
32	2a	398	C
32	2a	406	G
32	2a	412	A
32	2a	413	G

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
32	2a	424	G
32	2a	429	U
32	2a	430	A
32	2a	439	A
32	2a	442	C
32	2a	446	G
32	2a	452	A
32	2a	458	C
32	2a	461	A
32	2a	470	C
32	2a	476	G
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	528	C
32	2a	532	A
32	2a	533	A
32	2a	547	A
32	2a	559	A
32	2a	560	U
32	2a	561	U
32	2a	564	C
32	2a	572	A
32	2a	573	A
32	2a	576	G
32	2a	577	G
32	2a	596	C
32	2a	597	G
32	2a	630	G
32	2a	631	G
32	2a	632	A
32	2a	653	A
32	2a	665	A
32	2a	687	A
32	2a	688	G

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
32	2a	695	A
32	2a	707	C
32	2a	723	U
32	2a	724	G
32	2a	728	A
32	2a	731	G
32	2a	749	C
32	2a	753	A
32	2a	755	G
32	2a	773	G
32	2a	774	G
32	2a	777	A
32	2a	785	G
32	2a	793	U
32	2a	794	A
32	2a	815	A
32	2a	817	C
32	2a	821	G
32	2a	828	A
32	2a	829	G
32	2a	836	G
32	2a	840	C
32	2a	841	U
32	2a	851	G
32	2a	859	A
32	2a	875	C
32	2a	914	A
32	2a	916	G
32	2a	926	G
32	2a	927	G
32	2a	931	C
32	2a	934	C
32	2a	935	A
32	2a	960	U
32	2a	961	U
32	2a	966	M2G
32	2a	968	A
32	2a	969	A
32	2a	971	G
32	2a	972	C
32	2a	974	A
32	2a	975	A

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
32	2a	976	G
32	2a	977	A
32	2a	984	C
32	2a	989	C
32	2a	992	U
32	2a	993	G
32	2a	994	A
32	2a	995	C
32	2a	1001	A
32	2a	1004	A
32	2a	1005	A
32	2a	1006	C
32	2a	1009	G
32	2a	1016	A
32	2a	1020	U
32	2a	1022	G
32	2a	1023	G
32	2a	1025	U
32	2a	1026	G
32	2a	1027	C
32	2a	1028	C
32	2a	1029	C
32	2a	1030(A)	G
32	2a	1030(B)	C
32	2a	1033	G
32	2a	1041	A
32	2a	1044	A
32	2a	1047	G
32	2a	1054	C
32	2a	1055	A
32	2a	1065	U
32	2a	1066	C
32	2a	1068	G
32	2a	1081	G
32	2a	1094	G
32	2a	1095	U
32	2a	1101	A
32	2a	1117	G
32	2a	1122	U
32	2a	1125	U
32	2a	1129	C
32	2a	1130	A

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
32	2a	1132	C
32	2a	1134	G
32	2a	1136	U
32	2a	1137	C
32	2a	1138	G
32	2a	1139	G
32	2a	1147	C
32	2a	1152	A
32	2a	1157	A
32	2a	1159	U
32	2a	1162	C
32	2a	1183	A
32	2a	1184	G
32	2a	1196	U
32	2a	1197	G
32	2a	1211	U
32	2a	1212	U
32	2a	1213	A
32	2a	1224	G
32	2a	1227	A
32	2a	1236	A
32	2a	1238	A
32	2a	1248	A
32	2a	1250	A
32	2a	1256	A
32	2a	1257	U
32	2a	1258	G
32	2a	1259	C
32	2a	1260	C
32	2a	1270	C
32	2a	1272	G
32	2a	1278	U
32	2a	1279	A
32	2a	1280	A
32	2a	1281	U
32	2a	1282	C
32	2a	1286	A
32	2a	1287	A
32	2a	1300	G
32	2a	1302	U
32	2a	1303	C
32	2a	1305	G

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
32	2a	1317	C
32	2a	1320	C
32	2a	1340	A
32	2a	1346	A
32	2a	1347	G
32	2a	1353	G
32	2a	1363	C
32	2a	1370	G
32	2a	1375	A
32	2a	1380	U
32	2a	1397	C
32	2a	1398	A
32	2a	1419	G
32	2a	1442	G
32	2a	1442(A)	G
32	2a	1446	U
32	2a	1447	A
32	2a	1456	G
32	2a	1462	G
32	2a	1492	A
32	2a	1497	G
32	2a	1499	A
32	2a	1504	G
32	2a	1506	U
32	2a	1517	G
32	2a	1520	G
32	2a	1529	G
32	2a	1530	G

All (82) RNA pucker outliers are listed below:

<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	1A	34	C
1	1A	115	G
1	1A	185	A
1	1A	188	A
1	1A	302	A
1	1A	509	A
1	1A	596	G
1	1A	793	A
1	1A	811	A
1	1A	821	A

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	1A	874	U
1	1A	913	A
1	1A	935	C
1	1A	941	U
1	1A	1003	U
1	1A	1019	G
1	1A	1065	U
1	1A	1067	A
1	1A	1093	G
1	1A	1188	A
1	1A	1201	A
1	1A	1220	U
1	1A	1221	G
1	1A	1255	A
1	1A	1346	U
1	1A	1425	A
1	1A	1577	C
1	1A	1654	A
1	1A	1700	G
1	1A	1793	A
1	1A	2019	G
1	1A	2133	C
1	1A	2148	A
1	1A	2418	U
1	1A	2434	A
1	1A	2442	A
1	1A	2451	A
1	1A	2614	A
1	1A	2623	U
1	1A	2701	U
1	1A	2902	G
1	2A	9	U
1	2A	196	A
1	2A	266	G
1	2A	271(M)	G
1	2A	277	C
1	2A	746	A
1	2A	752	A
1	2A	764	A
1	2A	774	A
1	2A	827	U
1	2A	840	C

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Mol	Chain	Res	Type
1	2A	856	C
1	2A	900	A
1	2A	974	G
1	2A	1047	G
1	2A	1053	C
1	2A	1057	A
1	2A	1065	U
1	2A	1067	A
1	2A	1073	A
1	2A	1076	C
1	2A	1111	A
1	2A	1210	A
1	2A	1379	A
1	2A	1420	U
1	2A	1442	G
1	2A	1491	G
1	2A	1530	C
1	2A	1608	A
1	2A	1992	G
1	2A	2126	A
1	2A	2171	A
1	2A	2172	U
1	2A	2321	G
1	2A	2406	U
1	2A	2439	A
1	2A	2601	C
1	2A	2602	A
1	2A	2689	U
1	2A	2726	U
1	2A	2756	U

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
1	PSU	1A	2617	1	18,21,22	1.42	2 (11%)	22,30,33	1.81	3 (13%)
32	5MC	1a	1404	32	18,22,23	0.99	2 (11%)	26,32,35	1.21	3 (11%)
32	UR3	2a	1498	54,32	19,22,23	0.96	1 (5%)	26,32,35	1.42	2 (7%)
1	4OC	1A	1942	54,1	19,22,24	0.84	0	26,31,35	0.91	1 (3%)
32	5MC	1a	967	32	18,22,23	0.98	2 (11%)	26,32,35	1.17	3 (11%)
32	PSU	1a	516	54,32	18,21,22	1.37	2 (11%)	22,30,33	1.86	4 (18%)
1	5MC	2A	1942	1	18,22,23	0.98	2 (11%)	26,32,35	1.29	2 (7%)
1	2MU	2A	2552	54,1	19,22,24	1.30	3 (15%)	26,31,36	1.84	5 (19%)
32	M2G	2a	966	54,32	20,27,28	1.31	2 (10%)	22,40,43	1.31	3 (13%)
1	PSU	1A	1939	1	18,21,22	1.34	2 (11%)	22,30,33	1.74	4 (18%)
43	0TD	1l	92	43	7,9,10	6.73	5 (71%)	6,11,13	4.12	2 (33%)
1	PSU	1A	1933	1	18,21,22	1.33	2 (11%)	22,30,33	1.82	3 (13%)
1	5MC	1A	1964	54,1	18,22,23	1.04	2 (11%)	26,32,35	1.11	2 (7%)
32	5MC	1a	1407	32	18,22,23	1.03	2 (11%)	26,32,35	1.27	3 (11%)
1	PSU	2A	1917	1	18,21,22	1.33	2 (11%)	22,30,33	1.96	3 (13%)
1	5MC	2A	1962	54,1	18,22,23	0.96	2 (11%)	26,32,35	1.30	3 (11%)
32	MA6	2a	1518	32	19,26,27	0.99	1 (5%)	18,38,41	1.64	6 (33%)
32	M2G	1a	966	32	20,27,28	1.45	3 (15%)	22,40,43	1.03	2 (9%)
1	2MA	1A	2515	54,1	17,25,26	0.94	1 (5%)	17,37,40	1.08	2 (11%)
32	4OC	1a	1402	32	20,23,24	0.74	1 (5%)	26,32,35	0.94	1 (3%)
32	7MG	1a	527	54,32	22,26,27	1.33	3 (13%)	29,39,42	2.42	7 (24%)
1	5MC	1A	1984	54,1	18,22,23	0.96	1 (5%)	26,32,35	1.42	4 (15%)
1	5MU	2A	1939	54,1	19,22,23	1.36	4 (21%)	28,32,35	2.49	7 (25%)
1	2MA	2A	2503	54,1	17,25,26	1.09	1 (5%)	17,37,40	0.96	2 (11%)
1	PSU	2A	2605	1	18,21,22	1.33	3 (16%)	22,30,33	1.83	4 (18%)
32	5MC	2a	1404	32	18,22,23	1.01	2 (11%)	26,32,35	1.29	4 (15%)
32	7MG	2a	527	32	22,26,27	1.46	4 (18%)	29,39,42	2.44	5 (17%)
1	OMG	1A	2263	54,1	18,26,27	1.10	1 (5%)	19,38,41	1.07	2 (10%)
32	MA6	1a	1519	32	19,26,27	0.99	1 (5%)	18,38,41	1.59	4 (22%)
32	5MC	2a	967	32	18,22,23	0.98	2 (11%)	26,32,35	1.15	2 (7%)
32	UR3	1a	1498	32	19,22,23	0.97	0	26,32,35	1.50	2 (7%)
43	0TD	2l	92	43	7,9,10	4.88	1 (14%)	6,11,13	2.19	2 (33%)
32	4OC	2a	1402	32	20,23,24	0.74	0	26,32,35	0.94	1 (3%)
1	5MU	2A	1915	1	19,22,23	1.51	4 (21%)	28,32,35	2.13	8 (28%)
1	2MU	1A	2564	54,1	19,22,24	1.30	3 (15%)	26,31,36	1.77	6 (23%)



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
1	OMG	2A	2251	54,1	18,26,27	0.93	1 (5%)	19,38,41	1.17	2 (10%)
32	2MG	1a	1207	54,32	18,26,27	1.00	1 (5%)	16,38,41	1.57	5 (31%)
32	2MG	2a	1207	32	18,26,27	0.86	0	16,38,41	1.09	1 (6%)
1	PSU	2A	1911	1	18,21,22	1.42	2 (11%)	22,30,33	1.84	3 (13%)
1	5MU	1A	1937	54,1	19,22,23	1.46	4 (21%)	28,32,35	2.25	8 (28%)
32	5MC	2a	1407	32	18,22,23	0.97	2 (11%)	26,32,35	1.20	3 (11%)
1	4OC	2A	1920	1	19,22,24	0.84	0	26,31,35	0.96	1 (3%)
32	MA6	1a	1518	32	19,26,27	0.96	1 (5%)	18,38,41	1.65	4 (22%)
32	MA6	2a	1519	32	19,26,27	1.07	1 (5%)	18,38,41	1.81	4 (22%)
32	5MC	2a	1400	32	18,22,23	0.97	2 (11%)	26,32,35	1.15	3 (11%)
1	5MU	1A	1961	1	19,22,23	1.34	4 (21%)	28,32,35	2.27	7 (25%)
32	PSU	2a	516	54,32	18,21,22	1.28	2 (11%)	22,30,33	2.02	5 (22%)
32	5MC	1a	1400	32	18,22,23	1.08	2 (11%)	26,32,35	1.30	2 (7%)

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	PSU	1A	2617	1	-	0/7/25/26	0/2/2/2
32	5MC	1a	1404	32	-	0/7/25/26	0/2/2/2
32	UR3	2a	1498	54,32	-	0/7/25/26	0/2/2/2
1	4OC	1A	1942	54,1	-	1/9/27/30	0/2/2/2
32	5MC	1a	967	32	-	0/7/25/26	0/2/2/2
32	PSU	1a	516	54,32	-	0/7/25/26	0/2/2/2
1	5MC	2A	1942	1	-	0/7/25/26	0/2/2/2
1	2MU	2A	2552	54,1	-	0/9/27/28	0/2/2/2
32	M2G	2a	966	54,32	-	0/7/29/30	0/3/3/3
1	PSU	1A	1939	1	-	0/7/25/26	0/2/2/2
43	0TD	1l	92	43	-	2/7/12/14	-
1	PSU	1A	1933	1	-	0/7/25/26	0/2/2/2
1	5MC	1A	1964	54,1	-	0/7/25/26	0/2/2/2
32	5MC	1a	1407	32	-	0/7/25/26	0/2/2/2
1	PSU	2A	1917	1	-	0/7/25/26	0/2/2/2
1	5MC	2A	1962	54,1	-	0/7/25/26	0/2/2/2
32	MA6	2a	1518	32	-	1/7/29/30	0/3/3/3
32	M2G	1a	966	32	-	0/7/29/30	0/3/3/3
1	2MA	1A	2515	54,1	-	2/3/25/26	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
32	4OC	1a	1402	32	-	2/9/29/30	0/2/2/2
32	7MG	1a	527	54,32	-	2/7/37/38	0/3/3/3
1	5MC	1A	1984	54,1	-	0/7/25/26	0/2/2/2
1	5MU	2A	1939	54,1	-	0/7/25/26	0/2/2/2
1	2MA	2A	2503	54,1	-	1/3/25/26	0/3/3/3
1	PSU	2A	2605	1	-	0/7/25/26	0/2/2/2
32	5MC	2a	1404	32	-	0/7/25/26	0/2/2/2
32	7MG	2a	527	32	-	0/7/37/38	0/3/3/3
1	OMG	1A	2263	54,1	-	1/5/27/28	0/3/3/3
32	MA6	1a	1519	32	-	3/7/29/30	0/3/3/3
32	5MC	2a	967	32	-	0/7/25/26	0/2/2/2
32	UR3	1a	1498	32	-	0/7/25/26	0/2/2/2
43	0TD	2l	92	43	-	3/7/12/14	-
32	4OC	2a	1402	32	-	1/9/29/30	0/2/2/2
1	5MU	2A	1915	1	-	2/7/25/26	0/2/2/2
1	2MU	1A	2564	54,1	-	0/9/27/28	0/2/2/2
1	OMG	2A	2251	54,1	-	1/5/27/28	0/3/3/3
32	2MG	1a	1207	54,32	-	0/5/27/28	0/3/3/3
32	2MG	2a	1207	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	1937	54,1	-	2/7/25/26	0/2/2/2
32	5MC	2a	1407	32	-	0/7/25/26	0/2/2/2
1	4OC	2A	1920	1	-	0/9/27/30	0/2/2/2
32	MA6	1a	1518	32	-	3/7/29/30	0/3/3/3
32	MA6	2a	1519	32	-	5/7/29/30	0/3/3/3
32	5MC	2a	1400	32	-	0/7/25/26	0/2/2/2
1	5MU	1A	1961	1	-	0/7/25/26	0/2/2/2
32	PSU	2a	516	54,32	-	0/7/25/26	0/2/2/2
32	5MC	1a	1400	32	-	0/7/25/26	0/2/2/2

All (91) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
43	1l	92	0TD	CB-SB	-16.91	1.65	1.82
43	2l	92	0TD	CB-SB	-12.55	1.69	1.82
32	1a	966	M2G	C2-N3	4.47	1.36	1.30
32	2a	966	M2G	C2-N3	4.13	1.35	1.30
1	2A	1911	PSU	C6-C5	3.65	1.39	1.35
32	1a	516	PSU	C6-C5	3.49	1.39	1.35
32	1a	527	7MG	C4-N9	-3.47	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	1A	2617	PSU	C6-C5	3.33	1.39	1.35
1	1A	2617	PSU	C4-N3	-3.21	1.32	1.38
43	1l	92	0TD	CA-N	-3.18	1.37	1.47
1	1A	1939	PSU	C6-C5	3.14	1.39	1.35
32	1a	1407	5MC	C6-C5	3.11	1.39	1.34
32	1a	1400	5MC	C6-C5	3.10	1.39	1.34
1	2A	1915	5MU	C6-C5	3.10	1.39	1.34
32	2a	527	7MG	C4-N9	-3.07	1.34	1.37
1	1A	1933	PSU	C6-C5	3.06	1.38	1.35
1	1A	1984	5MC	C6-N1	-3.06	1.32	1.38
32	2a	527	7MG	C8-N9	3.01	1.47	1.46
32	2a	527	7MG	C5-C4	3.00	1.47	1.38
1	2A	1917	PSU	C6-C5	2.99	1.38	1.35
1	2A	2605	PSU	C4-N3	-2.98	1.33	1.38
1	1A	2263	OMG	C6-N1	-2.97	1.33	1.37
1	2A	1915	5MU	C2-N1	2.96	1.43	1.38
1	2A	1939	5MU	C4-N3	-2.93	1.33	1.38
1	1A	1964	5MC	C6-C5	2.92	1.39	1.34
1	1A	1937	5MU	C2-N1	2.92	1.43	1.38
32	1a	1404	5MC	C6-C5	2.91	1.39	1.34
32	2a	1404	5MC	C6-C5	2.90	1.39	1.34
1	1A	1937	5MU	C4-N3	-2.90	1.33	1.38
32	1a	527	7MG	C5-C4	2.88	1.47	1.38
32	2a	516	PSU	C6-C5	2.85	1.38	1.35
1	1A	1937	5MU	C6-C5	2.82	1.39	1.34
32	2a	1407	5MC	C6-C5	2.76	1.39	1.34
1	1A	2564	2MU	C4-N3	-2.76	1.33	1.38
1	2A	1915	5MU	C4-N3	-2.74	1.33	1.38
32	2a	967	5MC	C6-C5	2.71	1.39	1.34
1	2A	1942	5MC	C6-C5	2.71	1.39	1.34
43	1l	92	0TD	OD2-CG	-2.71	1.21	1.30
1	1A	1961	5MU	C6-C5	2.70	1.39	1.34
1	2A	1939	5MU	C6-C5	2.69	1.39	1.34
32	2a	1518	MA6	C5-C4	2.69	1.48	1.40
32	2a	1400	5MC	C6-C5	2.69	1.39	1.34
1	1A	1964	5MC	C6-N1	-2.67	1.33	1.38
43	1l	92	0TD	CB-CG	-2.67	1.47	1.52
1	2A	1911	PSU	C4-N3	-2.66	1.33	1.38
1	1A	2564	2MU	C5-C4	2.65	1.49	1.43
32	2a	1519	MA6	C5-C4	2.63	1.47	1.40
1	2A	1962	5MC	C6-C5	2.63	1.38	1.34
32	1a	966	M2G	C6-N1	-2.63	1.34	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	1a	967	5MC	C6-C5	2.62	1.38	1.34
1	2A	1917	PSU	C4-N3	-2.61	1.34	1.38
32	1a	966	M2G	C2-N2	2.60	1.40	1.35
32	2a	966	M2G	C2-N2	2.59	1.40	1.35
1	1A	1933	PSU	C4-N3	-2.59	1.34	1.38
1	2A	2605	PSU	C6-C5	2.58	1.38	1.35
1	2A	2552	2MU	C5-C4	2.56	1.49	1.43
32	1a	1518	MA6	C5-C4	2.54	1.47	1.40
32	2a	527	7MG	C6-N1	-2.53	1.34	1.38
43	1l	92	0TD	CSB-SB	-2.53	1.74	1.79
32	1a	1400	5MC	C6-N1	-2.49	1.33	1.38
32	1a	1519	MA6	C5-C4	2.48	1.47	1.40
1	1A	1961	5MU	C6-N1	-2.48	1.33	1.38
1	1A	1939	PSU	C4-N3	-2.48	1.34	1.38
1	2A	2552	2MU	C4-N3	-2.43	1.34	1.38
32	1a	1207	2MG	C6-N1	-2.41	1.34	1.37
1	2A	1915	5MU	C4-C5	2.41	1.48	1.44
1	2A	2503	2MA	C2-N3	2.39	1.36	1.31
32	1a	1404	5MC	C6-N1	-2.39	1.34	1.38
1	2A	2552	2MU	C2-N1	2.37	1.42	1.38
1	2A	2251	OMG	C6-N1	-2.37	1.34	1.37
32	2a	1400	5MC	C6-N1	-2.34	1.34	1.38
1	2A	1939	5MU	C4-C5	2.32	1.48	1.44
32	2a	967	5MC	C6-N1	-2.32	1.34	1.38
32	2a	516	PSU	C4-N3	-2.32	1.34	1.38
1	2A	1942	5MC	C6-N1	-2.30	1.34	1.38
32	2a	1404	5MC	C6-N1	-2.29	1.34	1.38
32	1a	516	PSU	C4-N3	-2.26	1.34	1.38
1	1A	1961	5MU	C4-C5	2.23	1.48	1.44
32	1a	527	7MG	C6-N1	-2.23	1.34	1.38
1	2A	1962	5MC	C6-N1	-2.23	1.34	1.38
1	2A	2605	PSU	C2-N3	-2.20	1.33	1.37
32	2a	1407	5MC	C6-N1	-2.20	1.34	1.38
1	2A	1939	5MU	C6-N1	-2.18	1.34	1.38
32	1a	967	5MC	C6-N1	-2.14	1.34	1.38
1	1A	2564	2MU	C2-N3	-2.14	1.34	1.38
32	2a	1498	UR3	C6-C5	2.13	1.40	1.35
1	1A	1937	5MU	C2-N3	-2.10	1.34	1.38
1	1A	2515	2MA	C2-N3	2.06	1.35	1.31
32	1a	1407	5MC	C6-N1	-2.03	1.34	1.38
32	1a	1402	4OC	C6-C5	2.03	1.39	1.35
1	1A	1961	5MU	C4-N3	-2.02	1.35	1.38

All (165) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	2a	527	7MG	N9-C4-N3	8.49	138.17	125.47
32	1a	527	7MG	N9-C4-N3	8.25	137.81	125.47
43	1l	92	0TD	CB-CA-N	-7.53	93.06	109.10
1	2A	1939	5MU	C4-N3-C2	-6.50	118.94	127.35
32	1a	1498	UR3	C4-N3-C2	-6.26	118.67	124.56
43	1l	92	0TD	CSB-SB-CB	6.20	113.66	102.44
1	2A	1911	PSU	N1-C2-N3	6.11	122.05	115.13
1	2A	1939	5MU	C5-C4-N3	6.08	120.50	115.31
32	2a	516	PSU	N1-C2-N3	6.06	122.00	115.13
32	2a	1498	UR3	C4-N3-C2	-6.00	118.92	124.56
1	1A	2617	PSU	N1-C2-N3	5.86	121.77	115.13
1	2A	1917	PSU	N1-C2-N3	5.85	121.75	115.13
1	2A	1939	5MU	N3-C2-N1	5.74	122.52	114.89
1	1A	1961	5MU	C4-N3-C2	-5.72	119.95	127.35
1	1A	1933	PSU	N1-C2-N3	5.46	121.31	115.13
32	1a	516	PSU	N1-C2-N3	5.34	121.18	115.13
1	2A	2605	PSU	N1-C2-N3	5.33	121.17	115.13
32	2a	527	7MG	C5-C4-N3	-5.31	118.00	128.13
1	2A	2552	2MU	N3-C2-N1	5.31	121.94	114.89
1	1A	1939	PSU	N1-C2-N3	5.25	121.08	115.13
32	2a	527	7MG	N9-C8-N7	-5.23	95.90	103.38
32	1a	527	7MG	C5-C4-N3	-5.21	118.20	128.13
1	1A	1961	5MU	C5-C4-N3	5.14	119.70	115.31
1	2A	1915	5MU	N3-C2-N1	5.11	121.67	114.89
1	1A	2564	2MU	N3-C2-N1	5.02	121.56	114.89
32	1a	1400	5MC	C5-C6-N1	-4.98	118.21	123.34
1	1A	1937	5MU	N3-C2-N1	4.93	121.44	114.89
1	2A	2552	2MU	C4-N3-C2	-4.89	120.14	126.58
1	1A	1961	5MU	O4-C4-C5	-4.85	119.27	124.90
1	1A	1937	5MU	C5-C4-N3	4.85	119.45	115.31
1	1A	1961	5MU	N3-C2-N1	4.81	121.28	114.89
1	1A	1937	5MU	C4-N3-C2	-4.80	121.14	127.35
32	1a	527	7MG	N9-C8-N7	-4.79	96.53	103.38
1	2A	1915	5MU	C4-N3-C2	-4.77	121.17	127.35
1	2A	1917	PSU	O2-C2-N1	-4.47	117.87	122.79
32	2a	516	PSU	C4-N3-C2	-4.33	120.11	126.34
1	2A	1942	5MC	C5-C6-N1	-4.22	118.99	123.34
32	2a	527	7MG	C2-N3-C4	4.21	119.80	112.30
1	1A	1984	5MC	C1 <sup>?</sup> -N1-C6	-4.18	114.16	121.12
43	2l	92	0TD	CSB-SB-CB	4.18	110.00	102.44
1	1A	2564	2MU	C4-N3-C2	-4.17	121.07	126.58
1	2A	1939	5MU	C5-C6-N1	-4.17	119.05	123.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1A	1937	5MU	O4-C4-C5	-4.16	120.08	124.90
32	1a	527	7MG	C2-N3-C4	4.15	119.70	112.30
1	2A	1915	5MU	C5-C4-N3	4.13	118.83	115.31
1	1A	1937	5MU	C1'-N1-C2	4.11	125.00	117.57
32	2a	516	PSU	O2-C2-N1	-4.09	118.28	122.79
32	1a	1404	5MC	C5-C6-N1	-4.06	119.16	123.34
32	1a	1407	5MC	C5-C6-N1	-4.06	119.16	123.34
32	2a	1519	MA6	C4-C5-N7	-4.05	105.18	109.40
1	2A	2605	PSU	C4-N3-C2	-4.01	120.57	126.34
32	2a	967	5MC	C5-C6-N1	-3.99	119.23	123.34
32	2a	1519	MA6	C10-N6-C6	-3.96	107.54	119.51
1	2A	1962	5MC	C5-C6-N1	-3.89	119.33	123.34
1	2A	1917	PSU	C4-N3-C2	-3.89	120.74	126.34
1	1A	1933	PSU	C4-N3-C2	-3.82	120.84	126.34
32	1a	1518	MA6	C4-C5-N7	-3.79	105.45	109.40
32	1a	516	PSU	C4-N3-C2	-3.79	120.88	126.34
1	2A	1939	5MU	O2-C2-N1	-3.76	117.78	122.79
1	1A	2564	2MU	O2-C2-N1	-3.74	117.81	122.79
1	2A	1939	5MU	O4-C4-C5	-3.74	120.57	124.90
32	1a	967	5MC	C5-C6-N1	-3.61	119.63	123.34
1	1A	1939	PSU	C4-N3-C2	-3.60	121.16	126.34
1	1A	1961	5MU	C5-C6-N1	-3.59	119.64	123.34
1	2A	1911	PSU	C4-N3-C2	-3.58	121.18	126.34
1	1A	2617	PSU	C4-N3-C2	-3.58	121.18	126.34
32	1a	1519	MA6	C4-C5-N7	-3.55	105.70	109.40
32	2a	1404	5MC	C5-C4-N3	-3.55	117.85	121.67
1	2A	1915	5MU	C1'-N1-C2	3.52	123.95	117.57
32	1a	516	PSU	O2-C2-N1	-3.52	118.92	122.79
32	2a	966	M2G	N1-C2-N2	3.50	121.02	118.04
1	1A	1933	PSU	O2-C2-N1	-3.50	118.94	122.79
32	2a	1400	5MC	C5-C6-N1	-3.49	119.74	123.34
1	1A	1961	5MU	O2-C2-N1	-3.48	118.16	122.79
32	2a	1404	5MC	C5-C6-N1	-3.40	119.84	123.34
1	1A	1964	5MC	C5-C6-N1	-3.38	119.86	123.34
32	2a	1407	5MC	C5-C6-N1	-3.34	119.90	123.34
32	2a	1519	MA6	N3-C2-N1	-3.31	123.50	128.68
1	1A	1937	5MU	C1'-N1-C6	-3.27	115.68	121.12
1	2A	1915	5MU	O4-C4-C5	-3.18	121.21	124.90
32	1a	1518	MA6	N3-C2-N1	-3.18	123.71	128.68
32	2a	1518	MA6	C4-C5-N7	-3.15	106.12	109.40
32	2a	1518	MA6	C9-N6-C6	-3.11	110.08	119.51
32	1a	1519	MA6	C9-N6-C6	-3.11	110.11	119.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	1a	1518	MA6	C9-N6-C6	-3.10	110.12	119.51
1	2A	2552	2MU	O2-C2-N1	-3.09	118.68	122.79
1	1A	1984	5MC	C5-C6-N1	-3.03	120.22	123.34
1	2A	1915	5MU	C5-C6-N1	-2.93	120.32	123.34
32	2a	1518	MA6	N3-C2-N1	-2.87	124.19	128.68
1	1A	1939	PSU	O2-C2-N1	-2.85	119.65	122.79
32	1a	516	PSU	C6-C5-C4	-2.80	116.24	118.20
32	2a	527	7MG	C5-C6-N1	2.77	115.87	110.99
32	2a	1518	MA6	N1-C6-N6	2.75	119.95	117.06
1	2A	2552	2MU	C5-C4-N3	2.74	118.94	114.84
1	2A	1920	4OC	O2-C2-N3	-2.73	117.89	122.33
1	2A	1915	5MU	C1'-N1-C6	-2.70	116.62	121.12
32	1a	1207	2MG	C8-N7-C5	2.69	108.12	102.99
1	1A	2564	2MU	C2'-C1'-N1	-2.69	109.00	114.22
1	1A	1964	5MC	C5-C4-N3	-2.69	118.77	121.67
1	1A	1937	5MU	O2-C2-N3	-2.68	116.50	121.50
32	1a	1519	MA6	N3-C2-N1	-2.67	124.50	128.68
1	1A	2263	OMG	C8-N7-C5	2.67	108.07	102.99
1	2A	1911	PSU	O2-C2-N1	-2.66	119.86	122.79
32	1a	1404	5MC	C5-C4-N3	-2.66	118.81	121.67
32	1a	527	7MG	C5-C6-N1	2.65	115.66	110.99
1	1A	1937	5MU	C5-C6-N1	-2.65	120.61	123.34
1	1A	1984	5MC	CM5-C5-C6	-2.64	119.32	122.85
32	2a	1519	MA6	C10-N6-C9	-2.61	107.70	116.12
32	1a	1407	5MC	O2-C2-N3	-2.60	118.10	122.33
32	2a	1407	5MC	O2-C2-N3	-2.60	118.11	122.33
32	2a	1407	5MC	C5-C4-N3	-2.58	118.89	121.67
1	2A	1942	5MC	C5-C4-N3	-2.55	118.92	121.67
1	1A	2515	2MA	C8-N7-C5	2.54	107.83	102.99
1	2A	1915	5MU	O2-C2-N3	-2.54	116.78	121.50
32	2a	1402	4OC	C6-C5-C4	2.52	120.04	116.96
32	1a	1402	4OC	C6-C5-C4	2.51	120.04	116.96
32	1a	1207	2MG	CM2-N2-C2	-2.50	118.34	123.86
32	1a	1407	5MC	C5-C4-N3	-2.49	118.98	121.67
32	2a	1404	5MC	O2-C2-N3	-2.49	118.29	122.33
1	1A	2263	OMG	C5-C6-N1	2.47	118.31	113.95
1	1A	2564	2MU	C5-C4-N3	2.47	118.53	114.84
1	2A	2552	2MU	O4-C4-C5	-2.46	120.83	125.16
32	2a	1207	2MG	C8-N7-C5	2.45	107.66	102.99
43	2l	92	0TD	OD2-CG-CB	2.41	118.35	113.15
32	1a	1518	MA6	C10-N6-C9	-2.40	108.38	116.12
32	2a	966	M2G	C5-C6-N1	2.39	118.17	113.95

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	1a	1519	MA6	N1-C6-N6	2.39	119.57	117.06
1	1A	2515	2MA	C5-C6-N1	2.38	118.13	114.02
32	1a	1400	5MC	C5-C4-N3	-2.38	119.11	121.67
1	2A	2503	2MA	C8-N7-C5	2.38	107.52	102.99
32	2a	966	M2G	C8-N7-C5	2.37	107.50	102.99
32	1a	1207	2MG	O3'-C3'-C2'	2.37	119.48	111.82
1	2A	1962	5MC	C1'-N1-C6	-2.36	117.20	121.12
32	2a	1518	MA6	C10-N6-C6	-2.35	112.41	119.51
32	2a	516	PSU	C5-C6-N1	-2.34	118.60	122.11
32	2a	967	5MC	CM5-C5-C6	-2.33	119.73	122.85
32	1a	966	M2G	C8-N7-C5	2.33	107.43	102.99
1	1A	1942	4OC	O2-C2-N3	-2.32	118.55	122.33
32	2a	1400	5MC	C5-C4-N3	-2.32	119.17	121.67
1	2A	2251	OMG	C5-C6-N1	2.31	118.03	113.95
32	1a	527	7MG	O6-C6-C5	-2.31	121.88	127.54
32	2a	516	PSU	O4'-C1'-C2'	2.30	108.39	105.14
32	1a	1207	2MG	C5-C6-N1	2.30	118.01	113.95
1	1A	1939	PSU	C6-C5-C4	-2.28	116.60	118.20
32	1a	1404	5MC	CM5-C5-C6	-2.26	119.82	122.85
1	2A	2251	OMG	C8-N7-C5	2.26	107.30	102.99
1	2A	2605	PSU	C6-C5-C4	-2.26	116.62	118.20
1	1A	1961	5MU	C5M-C5-C4	2.25	121.25	118.77
1	2A	2503	2MA	C5-C6-N1	2.24	117.89	114.02
32	2a	1400	5MC	CM5-C5-C6	-2.24	119.85	122.85
32	2a	1404	5MC	CM5-C5-C6	-2.23	119.87	122.85
1	1A	2617	PSU	O2-C2-N3	-2.23	117.62	121.82
32	1a	967	5MC	C5-C4-N3	-2.20	119.30	121.67
32	1a	966	M2G	C5-C6-N1	2.19	117.82	113.95
32	1a	1498	UR3	C3U-N3-C2	2.18	121.14	117.31
32	1a	527	7MG	CM7-N7-C5	2.17	132.00	126.40
1	1A	2564	2MU	O4-C4-C5	-2.17	121.34	125.16
1	2A	1939	5MU	C5M-C5-C4	2.16	121.15	118.77
1	1A	1984	5MC	C1'-N1-C2	2.14	123.21	118.42
1	2A	2605	PSU	O2-C2-N1	-2.13	120.45	122.79
1	2A	1962	5MC	C5-C4-N4	-2.08	118.36	121.48
32	2a	1498	UR3	C3U-N3-C4	2.04	120.81	117.89
32	1a	967	5MC	O2-C2-N3	-2.04	119.02	122.33
32	1a	1207	2MG	O3'-C3'-C4'	2.02	116.88	111.05
32	2a	1518	MA6	C10-N6-C9	-2.01	109.65	116.12

There are no chirality outliers.

All (32) torsion outliers are listed below:



Mol	Chain	Res	Type	Atoms
1	1A	1937	5MU	O4'-C1'-N1-C2
1	1A	1937	5MU	O4'-C1'-N1-C6
1	1A	2263	OMG	C1'-C2'-O2'-CM2
32	1a	1518	MA6	C5-C6-N6-C9
32	1a	1519	MA6	C5-C6-N6-C10
43	1l	92	0TD	SB-CB-CG-OD2
1	2A	1915	5MU	O4'-C1'-N1-C2
1	2A	1915	5MU	O4'-C1'-N1-C6
32	2a	1519	MA6	C5-C6-N6-C9
32	2a	1519	MA6	C5-C6-N6-C10
43	2l	92	0TD	O-C-CA-CB
32	2a	1519	MA6	O4'-C4'-C5'-O5'
32	1a	1518	MA6	N1-C6-N6-C9
32	2a	1519	MA6	N1-C6-N6-C10
32	1a	1518	MA6	C5-C6-N6-C10
32	1a	1402	4OC	O4'-C4'-C5'-O5'
32	2a	1519	MA6	C3'-C4'-C5'-O5'
43	1l	92	0TD	CG-CB-SB-CSB
43	2l	92	0TD	CG-CB-SB-CSB
32	1a	527	7MG	C3'-C4'-C5'-O5'
32	2a	1518	MA6	C5-C6-N6-C10
32	1a	1519	MA6	O4'-C4'-C5'-O5'
32	2a	1402	4OC	O4'-C4'-C5'-O5'
1	1A	2515	2MA	C4'-C5'-O5'-P
43	2l	92	0TD	CA-CB-SB-CSB
32	1a	1402	4OC	C3'-C4'-C5'-O5'
1	2A	2251	OMG	C1'-C2'-O2'-CM2
1	1A	1942	4OC	C2'-C1'-N1-C2
1	1A	2515	2MA	O4'-C4'-C5'-O5'
32	1a	1519	MA6	C3'-C4'-C5'-O5'
1	2A	2503	2MA	O4'-C4'-C5'-O5'
32	1a	527	7MG	C4'-C5'-O5'-P

There are no ring outliers.

No monomer is involved in short contacts.

## 5.5 Carbohydrates

There are no monosaccharides in this entry.

## 5.6 Ligand geometry

Of 2540 ligands modelled in this entry, 2529 are monoatomic - leaving 11 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
55	MPD	1T	8004	-	7,7,7	0.30	0	9,10,10	0.35	0
55	MPD	1A	4028	-	7,7,7	0.28	0	9,10,10	0.19	0
58	SF4	2d	501	35	0,12,12	-	-	-	-	-
55	MPD	2A	3747	-	7,7,7	0.38	0	9,10,10	0.48	0
58	SF4	1d	501	35	0,12,12	-	-	-	-	-
56	ARG	1B	230	54	10,11,11	0.79	1 (10%)	11,13,13	1.26	1 (9%)
55	MPD	18	102	-	7,7,7	0.24	0	9,10,10	0.57	0
55	MPD	1a	1880	-	7,7,7	0.59	0	9,10,10	0.65	0
55	MPD	2B	3020	-	7,7,7	0.32	0	9,10,10	0.34	0
56	ARG	1F	311	-	10,11,11	0.71	0	11,13,13	1.25	2 (18%)
55	MPD	2A	3748	-	7,7,7	0.31	0	9,10,10	0.26	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
55	MPD	1T	8004	-	-	2/5/5/5	-
55	MPD	1A	4028	-	-	0/5/5/5	-
58	SF4	2d	501	35	-	-	0/6/5/5
55	MPD	2A	3747	-	-	0/5/5/5	-
58	SF4	1d	501	35	-	-	0/6/5/5
56	ARG	1B	230	54	-	2/11/11/11	-
55	MPD	18	102	-	-	1/5/5/5	-
55	MPD	1a	1880	-	-	1/5/5/5	-
55	MPD	2B	3020	-	-	1/5/5/5	-
56	ARG	1F	311	-	-	2/11/11/11	-
55	MPD	2A	3748	-	-	5/5/5/5	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
56	1B	230	ARG	OXT-C	-2.38	1.22	1.30

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
56	1F	311	ARG	OXT-C-O	-3.05	117.16	124.09
56	1B	230	ARG	OXT-C-O	-2.82	117.69	124.09
56	1F	311	ARG	OXT-C-CA	2.55	122.08	113.38

There are no chirality outliers.

All (14) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
55	2A	3748	MPD	O2-C2-C3-C4
55	2A	3748	MPD	C2-C3-C4-O4
56	1F	311	ARG	C-CA-CB-CG
56	1B	230	ARG	NE-CD-CG-CB
56	1B	230	ARG	CA-CB-CG-CD
56	1F	311	ARG	CA-CB-CG-CD
55	1a	1880	MPD	C2-C3-C4-C5
55	2A	3748	MPD	C2-C3-C4-C5
55	18	102	MPD	C2-C3-C4-O4
55	2A	3748	MPD	C1-C2-C3-C4
55	2A	3748	MPD	CM-C2-C3-C4
55	1T	8004	MPD	C2-C3-C4-C5
55	1T	8004	MPD	C2-C3-C4-O4
55	2B	3020	MPD	C2-C3-C4-O4

There are no ring outliers.

No monomer is involved in short contacts.

## 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 i

### 6.1 Protein, DNA and RNA chains i

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	2861/2915 (98%)	0.88	90 (3%) 49 56	23, 40, 90, 100	0
1	2A	2856/2915 (97%)	0.35	130 (4%) 32 39	26, 44, 91, 104	0
2	1B	120/121 (99%)	0.57	0 100 100	34, 56, 71, 86	0
2	2B	120/121 (99%)	0.02	1 (0%) 86 89	41, 61, 74, 87	0
3	1D	275/276 (99%)	0.71	5 (1%) 68 74	23, 37, 53, 78	0
3	2D	275/276 (99%)	0.37	4 (1%) 73 79	25, 41, 55, 77	0
4	1E	204/206 (99%)	0.78	1 (0%) 91 94	22, 43, 63, 72	0
4	2E	204/206 (99%)	0.33	3 (1%) 73 79	26, 47, 65, 74	0
5	1F	203/210 (96%)	0.75	2 (0%) 82 86	20, 46, 72, 84	0
5	2F	203/210 (96%)	0.13	0 100 100	25, 52, 73, 85	0
6	1G	181/182 (99%)	0.44	6 (3%) 46 53	54, 70, 81, 90	0
6	2G	181/182 (99%)	1.65	62 (34%) 0 0	58, 73, 83, 91	0
7	1H	174/180 (96%)	0.75	4 (2%) 60 67	45, 62, 73, 78	0
7	2H	173/180 (96%)	0.82	23 (13%) 3 4	54, 67, 76, 80	0
8	1I	147/148 (99%)	0.26	1 (0%) 87 91	43, 71, 80, 84	0
8	2I	146/148 (98%)	0.37	6 (4%) 37 44	47, 71, 81, 84	0
9	1N	140/140 (100%)	0.57	1 (0%) 87 91	25, 36, 60, 81	0
9	2N	140/140 (100%)	0.49	3 (2%) 63 70	39, 58, 74, 81	0
10	1O	122/122 (100%)	0.52	0 100 100	25, 37, 57, 64	0
10	2O	122/122 (100%)	0.42	2 (1%) 72 77	38, 52, 66, 74	0
11	1P	149/150 (99%)	0.48	1 (0%) 87 91	19, 43, 67, 78	0
11	2P	149/150 (99%)	0.40	5 (3%) 45 52	32, 62, 79, 85	0
12	1Q	141/141 (100%)	0.75	1 (0%) 87 91	28, 44, 58, 72	0
12	2Q	141/141 (100%)	0.25	3 (2%) 63 70	33, 49, 61, 74	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
13	1R	118/118 (100%)	0.72	0 100 100	27, 38, 54, 63	0
13	2R	118/118 (100%)	0.36	1 (0%) 86 89	32, 42, 56, 64	0
14	1S	110/112 (98%)	0.58	0 100 100	42, 56, 67, 71	0
14	2S	110/112 (98%)	0.63	15 (13%) 3 4	48, 60, 70, 74	0
15	1T	131/146 (89%)	0.62	2 (1%) 73 79	34, 47, 72, 82	0
15	2T	131/146 (89%)	0.32	2 (1%) 73 79	39, 49, 74, 83	0
16	1U	116/118 (98%)	0.93	2 (1%) 70 76	25, 36, 53, 68	0
16	2U	116/118 (98%)	0.29	0 100 100	30, 43, 57, 70	0
17	1V	101/101 (100%)	0.82	2 (1%) 65 71	26, 48, 63, 73	0
17	2V	101/101 (100%)	0.16	1 (0%) 82 86	30, 54, 67, 74	0
18	1W	112/113 (99%)	0.74	1 (0%) 84 88	28, 34, 55, 87	0
18	2W	112/113 (99%)	0.29	0 100 100	32, 38, 58, 87	0
19	1X	95/96 (98%)	0.80	3 (3%) 47 54	32, 42, 63, 74	0
19	2X	95/96 (98%)	0.68	8 (8%) 11 15	37, 47, 67, 76	0
20	1Y	107/110 (97%)	0.72	2 (1%) 66 73	39, 54, 69, 78	0
20	2Y	107/110 (97%)	0.86	11 (10%) 6 9	43, 58, 72, 80	0
21	1Z	203/206 (98%)	0.59	3 (1%) 73 79	45, 63, 78, 83	0
21	2Z	201/206 (97%)	0.60	18 (8%) 9 12	50, 66, 78, 82	0
22	10	77/85 (90%)	0.46	1 (1%) 77 81	26, 35, 52, 63	0
22	20	77/85 (90%)	0.85	5 (6%) 18 24	41, 57, 68, 81	0
23	11	97/98 (98%)	0.56	2 (2%) 63 70	26, 41, 68, 76	0
23	21	97/98 (98%)	0.52	1 (1%) 82 86	35, 51, 72, 75	0
24	12	70/72 (97%)	0.64	0 100 100	40, 53, 65, 82	0
24	22	70/72 (97%)	0.42	1 (1%) 75 80	45, 59, 68, 81	0
25	13	59/60 (98%)	0.75	1 (1%) 70 76	28, 40, 67, 80	0
25	23	59/60 (98%)	0.88	6 (10%) 6 9	34, 45, 70, 80	0
26	14	69/71 (97%)	1.04	14 (20%) 1 1	67, 81, 90, 94	0
26	24	69/71 (97%)	2.18	26 (37%) 0 0	70, 82, 90, 94	0
27	15	59/60 (98%)	0.77	2 (3%) 45 52	22, 37, 59, 69	0
27	25	59/60 (98%)	0.14	1 (1%) 70 76	25, 40, 61, 70	0
28	16	53/54 (98%)	0.64	0 100 100	34, 45, 61, 64	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
28	26	53/54 (98%)	0.23	1 (1%) 66 73	39, 49, 61, 66	0
29	17	48/49 (97%)	1.02	5 (10%) 6 9	22, 30, 58, 68	0
29	27	48/49 (97%)	0.84	4 (8%) 11 15	26, 33, 60, 68	0
30	18	64/65 (98%)	0.70	0 100 100	30, 38, 45, 61	0
30	28	64/65 (98%)	0.37	0 100 100	33, 42, 49, 64	0
31	19	37/37 (100%)	0.47	1 (2%) 54 62	29, 39, 55, 56	0
31	29	37/37 (100%)	0.86	2 (5%) 25 32	45, 60, 72, 75	0
32	1a	1488/1521 (97%)	0.33	45 (3%) 50 57	34, 63, 89, 102	0
32	2a	1492/1521 (98%)	0.38	61 (4%) 37 44	44, 73, 92, 103	0
33	1b	231/256 (90%)	0.75	32 (13%) 2 4	65, 78, 86, 91	0
33	2b	231/256 (90%)	1.62	74 (32%) 0 0	67, 79, 87, 93	0
34	1c	206/239 (86%)	0.57	10 (4%) 29 36	63, 74, 83, 89	0
34	2c	206/239 (86%)	1.65	71 (34%) 0 0	65, 76, 84, 90	0
35	1d	208/209 (99%)	0.82	22 (10%) 6 8	55, 69, 79, 84	0
35	2d	208/209 (99%)	1.03	27 (12%) 3 4	57, 69, 78, 84	0
36	1e	148/162 (91%)	0.44	4 (2%) 54 62	46, 61, 72, 87	0
36	2e	148/162 (91%)	0.71	12 (8%) 12 16	56, 70, 79, 87	0
37	1f	100/101 (99%)	0.55	5 (5%) 28 35	53, 64, 74, 79	0
37	2f	100/101 (99%)	0.24	2 (2%) 65 71	53, 64, 74, 79	0
38	1g	155/156 (99%)	0.48	6 (3%) 39 46	62, 72, 81, 84	0
38	2g	155/156 (99%)	1.08	30 (19%) 1 1	66, 74, 81, 84	0
39	1h	137/138 (99%)	0.73	8 (5%) 23 29	54, 67, 74, 77	0
39	2h	137/138 (99%)	0.61	8 (5%) 23 29	56, 68, 75, 78	0
40	1i	127/128 (99%)	1.07	19 (14%) 2 3	60, 78, 85, 88	0
40	2i	126/128 (98%)	2.58	76 (60%) 0 0	64, 79, 86, 89	0
41	1j	97/105 (92%)	1.42	29 (29%) 0 0	59, 79, 88, 91	0
41	2j	96/105 (91%)	1.93	40 (41%) 0 0	65, 80, 88, 91	0
42	1k	114/129 (88%)	0.57	4 (3%) 44 51	46, 63, 77, 79	0
42	2k	114/129 (88%)	1.02	17 (14%) 2 3	48, 65, 77, 80	0
43	1l	121/132 (91%)	0.66	9 (7%) 14 19	48, 58, 70, 75	0
43	2l	121/132 (91%)	0.64	8 (6%) 18 23	51, 60, 70, 77	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
44	1m	116/126 (92%)	0.78	12 (10%) 6 9	54, 71, 79, 84	0
44	2m	114/126 (90%)	2.05	53 (46%) 0 0	73, 82, 87, 91	0
45	1n	60/61 (98%)	1.70	19 (31%) 0 0	64, 71, 78, 79	0
45	2n	60/61 (98%)	2.90	41 (68%) 0 0	67, 74, 80, 87	0
46	1o	88/89 (98%)	0.48	3 (3%) 45 52	46, 64, 77, 79	0
46	2o	88/89 (98%)	0.37	3 (3%) 45 52	50, 65, 78, 80	0
47	1p	82/88 (93%)	0.69	5 (6%) 21 27	58, 68, 78, 81	0
47	2p	82/88 (93%)	0.98	11 (13%) 3 4	59, 68, 77, 83	0
48	1q	99/105 (94%)	0.82	11 (11%) 5 7	53, 66, 75, 79	0
48	2q	99/105 (94%)	0.86	8 (8%) 12 16	53, 66, 76, 80	0
49	1r	68/88 (77%)	0.66	7 (10%) 6 9	55, 65, 77, 79	0
49	2r	68/88 (77%)	0.48	2 (2%) 51 58	55, 66, 77, 79	0
50	1s	83/93 (89%)	1.04	12 (14%) 2 3	67, 77, 83, 85	0
50	2s	83/93 (89%)	3.24	60 (72%) 0 0	70, 79, 84, 86	0
51	1t	96/106 (90%)	1.04	14 (14%) 2 3	57, 68, 79, 83	0
51	2t	98/106 (92%)	0.63	4 (4%) 37 44	57, 69, 81, 83	0
52	1u	23/27 (85%)	1.44	7 (30%) 0 0	69, 72, 76, 78	0
52	2u	23/27 (85%)	2.48	14 (60%) 0 0	71, 74, 77, 80	0
53	1y	97/113 (85%)	0.45	2 (2%) 63 70	44, 56, 70, 74	0
53	2y	96/113 (84%)	1.06	17 (17%) 1 1	57, 71, 79, 83	0
All	All	20766/21468 (96%)	0.67	1422 (6%) 17 22	19, 58, 85, 104	0

All (1422) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
26	24	50	VAL	10.3
1	2A	2142	C	10.0
1	1A	1122	C	10.0
33	2b	127	ILE	9.8
1	2A	2147	G	9.5
1	2A	2139	C	9.4
1	2A	2140	C	9.3
1	2A	2146	C	9.2
26	24	49	PHE	9.2
1	1A	1110	C	9.1

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	2A	2138	C	9.1
32	1a	1030(B)	C	8.7
1	2A	2602	A	8.7
35	2d	149	ALA	8.4
32	2a	1030(B)	C	8.2
32	1a	1001	A	8.2
1	2A	2141	G	8.1
6	2G	62	LEU	8.0
40	2i	109	VAL	8.0
33	2b	122	PHE	7.9
1	2A	2154	G	7.7
1	2A	2153	G	7.7
32	2a	1030(A)	G	7.7
50	2s	11	VAL	7.7
1	1A	2614	A	7.6
1	2A	2169	A	7.6
34	2c	196	LEU	7.6
40	2i	88	TYR	7.6
1	2A	229	A	7.5
44	2m	116	THR	7.5
43	2l	18	VAL	7.5
50	2s	49	ILE	7.4
1	2A	2155	G	7.4
50	2s	40	ILE	7.4
50	2s	41	VAL	7.3
1	2A	1046	A	7.2
50	2s	10	PHE	7.2
1	2A	2148	G	7.2
1	1A	1555	C	7.1
1	2A	2145	C	7.1
1	2A	888	C	6.9
1	2A	1509	C	6.9
50	2s	35	SER	6.9
23	11	2	SER	6.8
1	2A	1064	C	6.7
1	1A	2163	G	6.7
20	2Y	1	MET	6.6
35	2d	146	ILE	6.5
45	1n	2	ALA	6.5
38	2g	41	ARG	6.5
32	1a	1030(C)	G	6.4
32	2a	1028	C	6.4

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
33	2b	232	PRO	6.4
1	2A	2137	C	6.4
1	1A	2138	G	6.3
6	2G	152	LEU	6.3
26	24	45	GLY	6.3
34	2c	94	LEU	6.3
45	2n	44	LEU	6.3
50	2s	30	LEU	6.3
34	2c	81	GLY	6.2
26	14	49	PHE	6.2
26	14	45	GLY	6.2
1	1A	2162	C	6.2
40	2i	90	PRO	6.2
41	2j	67	THR	6.2
41	2j	47	PHE	6.1
52	2u	14	TRP	6.1
26	24	51	ASP	6.1
50	2s	15	LEU	6.1
1	2A	2110	G	6.1
33	2b	227	GLY	6.1
40	2i	72	GLY	6.1
45	2n	35	ARG	6.1
45	2n	34	TYR	6.0
42	2k	98	LEU	6.0
48	1q	99	SER	6.0
50	2s	31	ILE	6.0
32	1a	1028	C	6.0
40	2i	71	SER	5.9
1	2A	2174	C	5.9
26	24	54	GLY	5.9
32	1a	1031	G	5.9
26	24	56	VAL	5.9
44	2m	84	ILE	5.8
1	2A	2152	G	5.8
44	2m	102	ARG	5.8
33	2b	70	PHE	5.8
1	1A	1221	G	5.8
38	1g	156	TRP	5.7
26	24	66	SER	5.7
1	2A	1076	C	5.7
21	1Z	189	ALA	5.7
26	24	63	TYR	5.7

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
40	2i	108	VAL	5.6
27	15	60	VAL	5.6
32	2a	1036	G	5.6
1	2A	652(B)	A	5.6
34	2c	157	ILE	5.6
48	1q	98	LEU	5.6
32	1a	1030	C	5.5
44	2m	87	TYR	5.5
50	2s	63	THR	5.5
42	2k	13	GLN	5.5
32	2a	1030(C)	G	5.5
1	2A	2136	C	5.5
40	1i	128	ARG	5.5
52	2u	16	GLY	5.4
44	2m	6	GLY	5.4
34	2c	124	ILE	5.4
6	2G	39	ILE	5.4
1	1A	935	C	5.4
1	2A	2179	C	5.4
33	2b	165	VAL	5.4
50	2s	80	TYR	5.3
32	1a	1001(A)	G	5.3
32	1a	1257	U	5.3
6	2G	146	TYR	5.3
32	1a	1030(D)	A	5.2
23	2l	2	SER	5.2
1	1A	1120	G	5.2
1	2A	2106	G	5.2
47	2p	48	TRP	5.2
43	1l	20	LYS	5.2
1	1A	1113	A	5.2
50	2s	5	LEU	5.2
50	2s	75	ALA	5.2
33	2b	214	ILE	5.2
1	1A	1121	C	5.2
32	2a	1030	C	5.2
32	2a	1034	G	5.1
34	2c	87	LEU	5.1
1	2A	2143	C	5.1
26	14	50	VAL	5.1
44	2m	5	ALA	5.1
40	2i	69	GLY	5.1

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
45	2n	25	VAL	5.1
25	23	59	VAL	5.1
32	1a	1036	G	5.1
50	2s	82	GLY	5.0
1	1A	1109	G	5.0
50	2s	69	HIS	5.0
32	2a	1001	A	5.0
33	2b	97	TRP	5.0
1	1A	2169	G	5.0
50	2s	52	TYR	5.0
40	2i	63	ILE	5.0
6	2G	3	LEU	5.0
19	2X	92	LEU	5.0
45	2n	24	CYS	5.0
1	2A	2107	C	5.0
1	2A	2168	G	5.0
45	2n	33	VAL	4.9
1	2A	889	C	4.9
26	14	59	PHE	4.9
41	2j	96	ILE	4.9
35	1d	2	GLY	4.9
45	2n	38	GLY	4.9
50	2s	67	VAL	4.9
32	2a	1029	C	4.9
44	2m	15	VAL	4.9
6	2G	75	LYS	4.9
45	2n	56	VAL	4.9
50	2s	9	VAL	4.9
26	24	52	THR	4.9
1	2A	887	A	4.9
21	2Z	192	ALA	4.8
45	2n	2	ALA	4.8
40	2i	92	TYR	4.8
41	2j	68	HIS	4.8
1	2A	2135	A	4.8
32	2a	1286	A	4.8
40	2i	86	VAL	4.8
32	2a	1027	C	4.8
33	2b	207	ALA	4.8
50	2s	71	LEU	4.8
1	2A	2116	G	4.8
45	2n	13	THR	4.8

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	1A	1137	G	4.8
33	1b	133	LYS	4.8
26	24	44	THR	4.8
34	2c	190	ARG	4.8
34	2c	66	VAL	4.8
1	2A	2801(A)	A	4.8
40	2i	65	VAL	4.7
1	2A	2176	A	4.7
34	2c	188	LEU	4.7
1	1A	218	A	4.7
45	2n	59	ALA	4.7
1	2A	2151	G	4.7
32	1a	1029	C	4.7
33	2b	140	HIS	4.7
44	2m	75	ALA	4.7
35	1d	167	GLY	4.7
44	2m	4	ILE	4.7
32	2a	1001(A)	G	4.7
32	2a	1033	G	4.7
41	1j	27	ALA	4.7
1	2A	2125	G	4.7
7	2H	101	ARG	4.6
38	2g	32	ARG	4.6
50	2s	16	LEU	4.6
9	2N	140	VAL	4.6
45	2n	12	ARG	4.6
1	2A	6	A	4.6
20	2Y	42	VAL	4.6
42	1k	25	TYR	4.6
42	2k	75	TYR	4.6
34	2c	65	ALA	4.6
34	2c	159	GLY	4.6
1	1A	1133	G	4.6
1	2A	2124	G	4.6
41	2j	72	VAL	4.6
40	2i	7	THR	4.6
42	2k	25	TYR	4.6
32	2a	1257	U	4.6
44	2m	93	ARG	4.6
36	2e	12	LEU	4.6
26	14	52	THR	4.5
33	2b	124	SER	4.5

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Mol	Chain	Res	Type	RSRZ
38	2g	154	TYR	4.5
36	2e	13	ILE	4.5
50	2s	66	MET	4.5
1	2A	890	A	4.5
50	2s	51	VAL	4.5
38	2g	34	GLY	4.5
40	2i	4	TYR	4.5
1	2A	2793	G	4.5
41	2j	74	ILE	4.5
1	2A	2120	G	4.5
1	1A	1112	U	4.5
6	2G	135	LEU	4.5
40	2i	14	VAL	4.5
29	27	48	LYS	4.4
36	2e	22	GLY	4.4
38	2g	9	VAL	4.4
32	1a	1492	A	4.4
43	1l	64	TYR	4.4
45	1n	17	LYS	4.4
1	2A	2161	C	4.4
33	1b	127	ILE	4.4
40	2i	62	TYR	4.4
45	1n	34	TYR	4.4
40	2i	66	ARG	4.4
52	2u	6	ARG	4.4
29	17	46	VAL	4.4
14	2S	22	GLY	4.4
33	2b	81	VAL	4.4
40	2i	18	PHE	4.4
45	2n	61	TRP	4.4
1	2A	2111	C	4.4
1	2A	2175	C	4.4
29	17	47	ARG	4.3
1	2A	1067	A	4.3
34	1c	193	TYR	4.3
44	2m	72	ALA	4.3
26	24	19	GLY	4.3
34	2c	85	ARG	4.3
33	1b	136	VAL	4.3
44	2m	64	TRP	4.3
41	2j	19	SER	4.3
38	2g	42	ILE	4.2

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
50	2s	62	ILE	4.2
33	1b	121	LEU	4.2
33	1b	128	GLU	4.2
41	2j	62	HIS	4.2
32	2a	1026	G	4.2
32	2a	1035	A	4.2
1	1A	2165	C	4.2
33	2b	230	VAL	4.2
40	2i	21	PRO	4.2
40	1i	33	PHE	4.2
40	2i	102	LEU	4.2
52	2u	23	PRO	4.2
34	2c	8	ILE	4.2
1	2A	2144	U	4.2
32	2a	91	C	4.2
6	2G	87	PRO	4.2
1	1A	1123	A	4.2
1	1A	2164	C	4.2
1	2A	1075	C	4.2
6	2G	136	ARG	4.2
51	1t	9	ASN	4.2
38	2g	155	ARG	4.1
33	2b	123	ALA	4.1
3	2D	2	ALA	4.1
50	2s	70	LYS	4.1
7	2H	82	GLY	4.1
50	2s	84	GLY	4.1
1	2A	2802	G	4.1
26	14	56	VAL	4.1
40	2i	36	TYR	4.1
33	2b	133	LYS	4.1
26	24	68	ARG	4.1
1	2A	2159	G	4.1
34	2c	71	ALA	4.1
40	2i	76	ALA	4.1
45	2n	10	ALA	4.1
1	2A	2118	U	4.1
50	2s	65	ASN	4.1
40	2i	75	ASP	4.1
50	2s	79	THR	4.1
45	2n	39	LEU	4.1
1	2A	1079	C	4.1

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
44	2m	60	VAL	4.1
33	1b	129	GLU	4.1
38	1g	16	LEU	4.1
45	2n	37	PHE	4.1
49	1r	24	ALA	4.0
6	2G	52	ILE	4.0
32	1a	1030(A)	G	4.0
43	2l	19	ARG	4.0
33	1b	228	GLY	4.0
50	2s	20	LEU	4.0
26	14	53	GLU	4.0
51	1t	76	ALA	4.0
41	2j	44	VAL	4.0
26	24	27	THR	4.0
40	2i	105	ASP	4.0
33	2b	118	LEU	4.0
1	1A	2154	U	4.0
33	2b	121	LEU	4.0
34	2c	193	TYR	4.0
33	1b	232	PRO	4.0
34	2c	160	ALA	4.0
1	1A	936	C	4.0
45	1n	33	VAL	4.0
1	1A	2137	G	4.0
33	2b	136	VAL	4.0
41	2j	38	ILE	3.9
50	2s	81	ARG	3.9
40	2i	43	ALA	3.9
33	1b	130	ARG	3.9
33	1b	214	ILE	3.9
44	2m	113	PRO	3.9
1	2A	1083	U	3.9
48	2q	98	LEU	3.9
1	2A	2134	A	3.9
1	2A	2173	A	3.9
40	2i	114	TYR	3.9
51	1t	73	HIS	3.9
1	1A	1126	C	3.9
34	2c	33	LEU	3.9
44	2m	76	ALA	3.9
45	2n	6	LEU	3.9
26	24	67	TYR	3.9

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
34	2c	177	THR	3.9
41	2j	46	ARG	3.9
45	2n	55	GLY	3.8
1	2A	1085	A	3.8
1	2A	2119	A	3.8
34	2c	128	PHE	3.8
1	2A	2165	G	3.8
33	1b	122	PHE	3.8
19	2X	89	ILE	3.8
1	2A	2108	C	3.8
38	2g	22	LEU	3.8
50	1s	19	VAL	3.8
21	2Z	187	ALA	3.8
50	2s	29	ARG	3.8
6	2G	43	LEU	3.8
6	2G	133	LEU	3.8
41	2j	48	THR	3.8
40	2i	127	LYS	3.8
41	2j	63	PHE	3.8
29	27	46	VAL	3.8
40	2i	26	VAL	3.8
50	2s	45	VAL	3.8
32	1a	1002	G	3.8
33	2b	231	GLU	3.8
44	1m	115	LYS	3.8
41	2j	90	LEU	3.8
41	2j	100	THR	3.7
14	2S	3	ARG	3.7
21	2Z	125	LEU	3.7
32	1a	1033	G	3.7
40	2i	67	GLY	3.7
6	2G	61	ALA	3.7
7	2H	165	ALA	3.7
1	1A	1878	A	3.7
45	2n	42	ILE	3.7
47	2p	19	ILE	3.7
29	17	1	MET	3.7
40	2i	40	LEU	3.7
45	2n	28	GLY	3.7
6	2G	58	GLN	3.7
34	2c	39	ILE	3.7
32	2a	1030(D)	A	3.7

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
33	1b	131	PRO	3.7
39	2h	2	LEU	3.7
6	2G	51	ARG	3.7
1	1A	2181	G	3.7
32	1a	1003	G	3.7
40	2i	59	PHE	3.7
50	2s	60	VAL	3.7
41	2j	85	LEU	3.7
52	1u	14	TRP	3.7
29	17	45	ALA	3.7
33	2b	177	ALA	3.7
41	1j	85	LEU	3.7
1	1A	2168	C	3.7
40	2i	110	GLU	3.7
1	1A	1220	U	3.7
53	2y	52	ALA	3.7
49	1r	42	ARG	3.7
50	2s	39	THR	3.7
44	2m	7	VAL	3.7
44	2m	90	LEU	3.6
40	2i	27	THR	3.6
26	24	59	PHE	3.6
44	2m	23	TYR	3.6
33	2b	44	LEU	3.6
50	2s	38	SER	3.6
41	1j	32	ALA	3.6
6	2G	80	PHE	3.6
1	1A	2167	C	3.6
6	2G	82	LEU	3.6
35	2d	58	LEU	3.6
41	2j	16	LEU	3.6
41	2j	27	ALA	3.6
42	2k	87	THR	3.6
35	1d	3	ARG	3.6
6	2G	23	PHE	3.6
45	2n	36	PHE	3.6
32	2a	80	G	3.6
33	2b	215	LEU	3.6
41	2j	34	VAL	3.6
49	2r	85	LEU	3.6
34	2c	155	GLY	3.6
7	2H	6	ARG	3.6

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
32	1a	1000	U	3.6
34	2c	120	VAL	3.6
35	2d	158	ILE	3.5
39	2h	131	GLY	3.5
50	2s	12	ASP	3.5
21	2Z	191	VAL	3.5
35	2d	48	ALA	3.5
44	2m	8	GLU	3.5
40	2i	42	ARG	3.5
52	2u	9	ARG	3.5
35	1d	180	GLY	3.5
45	1n	18	VAL	3.5
50	2s	64	GLU	3.5
32	1a	1037	C	3.5
1	1A	1134	A	3.5
7	2H	103	LEU	3.5
1	2A	2181	G	3.5
41	2j	89	ASP	3.5
6	2G	74	LYS	3.5
50	2s	36	ARG	3.5
1	2A	2126	A	3.5
45	1n	16	PHE	3.5
50	2s	33	THR	3.5
44	2m	51	ALA	3.5
34	2c	126	ARG	3.5
1	2A	2162	G	3.5
38	2g	31	MET	3.4
35	1d	50	ARG	3.4
1	1A	1136	U	3.4
1	1A	2159	C	3.4
32	1a	1034	G	3.4
40	2i	70	LYS	3.4
41	2j	98	ILE	3.4
38	2g	118	VAL	3.4
1	1A	2166	U	3.4
1	2A	34	C	3.4
33	2b	144	ARG	3.4
39	2h	122	ARG	3.4
44	2m	110	ARG	3.4
45	2n	49	HIS	3.4
32	2a	1041	A	3.4
33	2b	201	ILE	3.4

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
35	2d	157	LEU	3.4
40	2i	126	SER	3.4
41	1j	44	VAL	3.4
14	2S	20	ARG	3.4
15	2T	111	ARG	3.4
33	2b	228	GLY	3.4
1	2A	1082	U	3.4
20	1Y	1	MET	3.4
32	2a	1031	G	3.4
1	2A	1095	A	3.4
45	2n	29	ARG	3.4
43	2l	13	LYS	3.4
44	2m	95	GLY	3.4
35	1d	70	ILE	3.4
48	2q	9	VAL	3.4
48	2q	91	ARG	3.4
34	2c	197	GLY	3.4
41	1j	93	GLY	3.4
45	2n	54	PRO	3.4
6	1G	146	TYR	3.4
6	2G	137	GLU	3.4
33	2b	187	LEU	3.4
38	2g	7	ALA	3.4
35	2d	70	ILE	3.4
40	2i	10	ARG	3.4
40	2i	56	LEU	3.4
50	2s	53	ASN	3.4
1	2A	2149	G	3.4
33	1b	165	VAL	3.3
1	1A	1132	A	3.3
50	2s	34	TRP	3.3
33	2b	92	TYR	3.3
49	2r	87	ARG	3.3
34	2c	101	LEU	3.3
39	1h	134	ILE	3.3
40	2i	37	PHE	3.3
41	1j	98	ILE	3.3
45	1n	14	PRO	3.3
33	2b	139	LYS	3.3
15	1T	38	ASN	3.3
33	2b	33	TYR	3.3
33	2b	218	ALA	3.3

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
38	2g	25	ALA	3.3
38	2g	6	ARG	3.3
34	2c	152	ILE	3.3
40	2i	33	PHE	3.3
42	2k	104	GLN	3.3
1	2A	2132	U	3.3
26	24	55	ARG	3.3
44	2m	19	LEU	3.3
33	2b	152	PHE	3.3
50	2s	56	GLN	3.3
6	2G	92	VAL	3.3
41	1j	34	VAL	3.3
1	2A	2160	G	3.3
34	2c	189	ALA	3.3
33	2b	146	GLN	3.3
44	2m	82	MET	3.3
8	2I	19	VAL	3.3
38	2g	80	VAL	3.3
45	2n	26	ARG	3.3
50	2s	77	THR	3.3
33	2b	135	GLN	3.2
40	1i	114	TYR	3.2
41	2j	65	LEU	3.2
50	1s	15	LEU	3.2
50	2s	61	TYR	3.2
21	2Z	96	VAL	3.2
1	2A	2109	U	3.2
32	1a	162	A	3.2
1	2A	2121	G	3.2
6	2G	149	VAL	3.2
8	2I	18	VAL	3.2
21	2Z	141	VAL	3.2
33	2b	71	VAL	3.2
33	2b	229	VAL	3.2
50	2s	8	GLY	3.2
40	1i	126	SER	3.2
1	1A	2177	G	3.2
33	2b	83	MET	3.2
32	2a	84	U	3.2
49	1r	29	PHE	3.2
34	2c	206	GLU	3.2
44	2m	24	GLY	3.2

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
40	2i	28	VAL	3.2
45	2n	30	ALA	3.2
51	1t	18	GLN	3.2
32	1a	999	C	3.2
36	2e	6	PHE	3.2
44	2m	115	LYS	3.2
1	1A	1124	U	3.2
1	1A	2129	C	3.2
1	2A	1104	C	3.2
1	2A	2131	G	3.2
1	2A	2803	C	3.2
6	2G	108	ASN	3.2
40	2i	8	GLY	3.2
33	2b	39	ILE	3.2
51	1t	55	ILE	3.2
35	1d	138	TYR	3.2
33	2b	164	VAL	3.2
33	1b	126	GLU	3.2
34	2c	163	ALA	3.2
41	1j	20	ALA	3.2
26	14	54	GLY	3.2
53	1y	95	ARG	3.2
1	1A	2139	A	3.2
35	1d	179	GLU	3.1
33	2b	163	PHE	3.1
44	1m	116	THR	3.1
33	2b	210	SER	3.1
34	2c	158	GLY	3.1
44	2m	48	LEU	3.1
1	2A	2804	C	3.1
32	1a	1024	G	3.1
6	2G	6	ALA	3.1
26	14	55	ARG	3.1
38	1g	80	VAL	3.1
40	1i	28	VAL	3.1
40	2i	113	LYS	3.1
52	2u	2	GLY	3.1
1	1A	2160	C	3.1
1	2A	2105	C	3.1
6	1G	80	PHE	3.1
33	2b	143	GLU	3.1
1	2A	2123	G	3.1

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	2A	2191	G	3.1
40	2i	29	ASN	3.1
6	2G	37	VAL	3.1
21	1Z	192	ALA	3.1
34	2c	23	TYR	3.1
35	1d	4	TYR	3.1
38	2g	8	GLU	3.1
6	2G	141	PHE	3.1
26	24	64	GLY	3.1
39	2h	47	GLY	3.1
40	2i	17	VAL	3.1
51	1t	47	GLY	3.1
1	1A	2806	G	3.1
20	2Y	55	TYR	3.1
33	2b	233	SER	3.1
44	2m	66	LEU	3.1
53	2y	88	LEU	3.1
6	2G	63	ILE	3.1
35	2d	67	ILE	3.1
50	1s	40	ILE	3.1
29	27	45	ALA	3.1
42	2k	30	VAL	3.1
35	2d	175	SER	3.1
39	1h	112	LEU	3.1
1	2A	2129	C	3.1
41	2j	45	ARG	3.1
48	1q	27	PHE	3.1
26	24	46	GLN	3.0
52	2u	18	TYR	3.0
7	1H	2	SER	3.0
40	2i	11	LYS	3.0
20	2Y	106	LEU	3.0
33	2b	185	ILE	3.0
1	2A	1536	C	3.0
50	2s	74	PHE	3.0
34	2c	207	VAL	3.0
32	2a	1220	G	3.0
6	2G	155	MET	3.0
7	2H	22	GLY	3.0
19	2X	68	ARG	3.0
41	1j	90	LEU	3.0
3	2D	276	LYS	3.0

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
20	2Y	44	ILE	3.0
33	2b	19	HIS	3.0
53	2y	39	ILE	3.0
32	2a	1039	C	3.0
33	2b	128	GLU	3.0
49	1r	38	GLU	3.0
51	2t	9	ASN	3.0
32	1a	161	A	3.0
32	1a	1286	A	3.0
32	2a	1492	A	3.0
6	2G	25	TYR	3.0
40	2i	5	TYR	3.0
22	20	46	LYS	3.0
34	2c	100	ALA	3.0
6	2G	142	PRO	3.0
40	1i	125	TYR	3.0
39	1h	133	LEU	3.0
43	2l	60	LEU	3.0
38	2g	117	ALA	3.0
45	2n	41	ARG	3.0
32	2a	1321	C	3.0
35	1d	166	LYS	3.0
34	2c	194	GLY	3.0
34	1c	87	LEU	3.0
40	2i	50	LEU	3.0
41	2j	8	LEU	3.0
51	1t	13	LEU	3.0
46	2o	68	ARG	3.0
32	1a	630	G	3.0
6	2G	164	GLU	3.0
41	1j	38	ILE	3.0
39	2h	112	LEU	2.9
45	1n	6	LEU	2.9
1	2A	2896	C	2.9
25	23	6	VAL	2.9
33	2b	37	ASN	2.9
1	2A	1847	A	2.9
34	2c	37	GLN	2.9
35	1d	157	LEU	2.9
40	1i	79	LEU	2.9
43	2l	64	TYR	2.9
52	1u	18	TYR	2.9

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
44	1m	24	GLY	2.9
6	2G	157	ILE	2.9
38	2g	27	ILE	2.9
44	2m	39	ILE	2.9
35	2d	150	GLU	2.9
41	2j	64	GLU	2.9
53	2y	11	GLU	2.9
3	1D	138	VAL	2.9
39	1h	53	VAL	2.9
47	2p	20	VAL	2.9
33	1b	75	LYS	2.9
35	2d	33	MET	2.9
40	1i	78	LYS	2.9
47	2p	7	ALA	2.9
53	2y	63	ALA	2.9
43	1l	61	THR	2.9
8	2I	3	VAL	2.9
42	2k	109	VAL	2.9
44	2m	17	VAL	2.9
19	1X	60	ARG	2.9
32	1a	1035	A	2.9
41	1j	36	GLY	2.9
45	1n	30	ALA	2.9
26	24	15	ILE	2.9
31	29	16	VAL	2.9
33	2b	93	VAL	2.9
35	2d	183	GLY	2.9
53	2y	77	LEU	2.9
32	2a	1447	A	2.9
29	17	48	LYS	2.9
40	2i	74	ILE	2.9
35	1d	73	ARG	2.9
44	2m	94	ARG	2.9
1	1A	1111	U	2.9
1	2A	2156	G	2.9
40	2i	73	GLN	2.9
6	2G	173	LEU	2.9
34	2c	121	ALA	2.9
45	2n	53	LEU	2.9
1	2A	1084	A	2.9
1	2A	1086	A	2.9
6	2G	49	ASP	2.9

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
29	27	47	ARG	2.9
48	2q	36	ILE	2.8
46	1o	89	GLY	2.8
1	2A	2833	G	2.8
7	2H	105	LEU	2.8
38	2g	33	ASP	2.8
1	2A	2062	A	2.8
1	2A	2130	U	2.8
32	1a	841	U	2.8
6	2G	182	LYS	2.8
35	2d	166	LYS	2.8
40	2i	53	VAL	2.8
47	1p	51	VAL	2.8
1	1A	1135	G	2.8
1	1A	2174	G	2.8
1	2A	892	G	2.8
1	2A	2166	G	2.8
32	1a	1040	U	2.8
50	2s	76	PRO	2.8
14	2S	40	ILE	2.8
47	2p	39	TYR	2.8
52	2u	13	ILE	2.8
43	1l	18	VAL	2.8
44	2m	65	LYS	2.8
45	1n	15	LYS	2.8
33	2b	48	MET	2.8
52	1u	17	THR	2.8
45	1n	21	TYR	2.8
50	2s	3	ARG	2.8
50	2s	78	ARG	2.8
1	2A	2150	U	2.8
1	1A	1138	C	2.8
32	1a	1007	C	2.8
42	2k	14	VAL	2.8
15	2T	114	LEU	2.8
1	2A	2805	G	2.8
34	2c	145	GLY	2.8
40	2i	30	GLY	2.8
33	1b	36	ARG	2.8
1	2A	2170	A	2.8
36	2e	133	TYR	2.8
1	1A	1125	C	2.8

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	2A	2164	C	2.8
6	2G	15	VAL	2.8
7	2H	10	PRO	2.8
22	10	8	GLY	2.8
50	1s	28	LYS	2.8
33	1b	29	ALA	2.7
1	2A	886	C	2.7
9	2N	46	VAL	2.7
33	1b	132	LYS	2.7
35	2d	169	LYS	2.7
45	1n	7	ILE	2.7
45	2n	15	LYS	2.7
32	2a	994	A	2.7
50	2s	13	ASP	2.7
48	1q	28	PRO	2.7
6	2G	5	VAL	2.7
40	2i	85	LEU	2.7
42	1k	13	GLN	2.7
40	2i	54	ASP	2.7
32	1a	1447	A	2.7
35	2d	4	TYR	2.7
35	2d	16	GLY	2.7
6	2G	57	ALA	2.7
43	1l	23	LYS	2.7
34	2c	115	LEU	2.7
44	2m	80	ARG	2.7
1	2A	2585	U	2.7
6	2G	77	ILE	2.7
32	1a	1026	G	2.7
35	2d	6	GLY	2.7
14	2S	92	TYR	2.7
53	2y	71	TYR	2.7
34	2c	179	ARG	2.7
21	2Z	155	LEU	2.7
53	2y	10	MET	2.7
33	1b	135	GLN	2.7
21	2Z	201	LYS	2.7
32	2a	1003	G	2.7
38	2g	78	ARG	2.7
33	2b	181	PHE	2.7
33	2b	16	HIS	2.7
39	2h	119	LEU	2.7

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
41	2j	40	LEU	2.7
45	1n	13	THR	2.7
19	2X	33	LYS	2.7
20	2Y	81	LYS	2.7
50	2s	28	LYS	2.7
33	2b	38	GLY	2.7
50	2s	68	GLY	2.7
40	1i	10	ARG	2.7
45	1n	3	ARG	2.7
45	2n	14	PRO	2.7
6	1G	49	ASP	2.7
1	2A	2127	G	2.7
45	2n	21	TYR	2.7
33	2b	113	HIS	2.7
52	2u	8	THR	2.7
1	1A	2807	C	2.7
6	2G	29	TRP	2.6
50	2s	42	PRO	2.6
33	2b	223	ILE	2.6
34	2c	108	ASN	2.6
44	1m	4	ILE	2.6
1	1A	160	G	2.6
12	2Q	59	ARG	2.6
32	2a	1248	A	2.6
34	1c	94	LEU	2.6
41	2j	87	THR	2.6
7	2H	8	PRO	2.6
34	2c	4	LYS	2.6
50	2s	55	LYS	2.6
26	14	46	GLN	2.6
38	2g	116	ALA	2.6
9	1N	115	ARG	2.6
1	1A	2173	G	2.6
1	1A	2176	G	2.6
1	1A	2816	G	2.6
32	2a	1138	G	2.6
38	1g	85	TYR	2.6
44	2m	70	LEU	2.6
39	1h	27	PRO	2.6
7	2H	102	ALA	2.6
20	2Y	61	ILE	2.6
26	14	68	ARG	2.6

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
38	2g	83	ALA	2.6
40	2i	45	ALA	2.6
40	2i	120	ARG	2.6
38	2g	24	THR	2.6
12	2Q	32	TYR	2.6
33	2b	101	MET	2.6
1	1A	2161	C	2.6
32	2a	1141	C	2.6
35	2d	49	ARG	2.6
6	1G	50	ALA	2.6
44	1m	30	ALA	2.6
44	2m	38	GLY	2.6
47	2p	47	ASP	2.6
48	1q	97	SER	2.6
7	2H	21	PRO	2.6
41	1j	8	LEU	2.6
44	2m	81	LEU	2.6
9	2N	9	VAL	2.6
34	2c	105	GLU	2.6
35	1d	124	GLY	2.6
44	2m	42	ALA	2.6
53	2y	40	ILE	2.6
43	1l	22	SER	2.6
44	2m	43	THR	2.6
26	24	30	GLU	2.6
41	2j	66	ARG	2.6
45	2n	57	ARG	2.6
34	2c	201	TYR	2.6
38	2g	85	TYR	2.6
1	1A	2195	A	2.6
1	2A	2112	G	2.6
1	2A	2133	G	2.6
32	2a	1002	G	2.6
33	1b	139	LYS	2.6
7	2H	42	ARG	2.5
25	23	30	ARG	2.5
33	2b	96	ARG	2.5
34	2c	21	ARG	2.5
38	2g	4	ARG	2.5
19	2X	66	LEU	2.5
35	1d	174	LEU	2.5
53	2y	41	LEU	2.5

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Mol	Chain	Res	Type	RSRZ
7	2H	115	VAL	2.5
41	2j	86	MET	2.5
48	2q	73	VAL	2.5
50	2s	57	HIS	2.5
40	2i	39	GLY	2.5
21	2Z	14	LYS	2.5
33	2b	132	LYS	2.5
35	2d	85	LYS	2.5
33	2b	34	ALA	2.5
47	2p	57	ARG	2.5
52	2u	15	ARG	2.5
8	2I	35	LEU	2.5
3	1D	275	LYS	2.5
26	24	40	HIS	2.5
25	23	54	VAL	2.5
35	1d	178	VAL	2.5
40	2i	41	VAL	2.5
42	2k	77	MET	2.5
51	1t	74	LYS	2.5
32	1a	1493	A	2.5
1	1A	2175	G	2.5
1	2A	1087	G	2.5
1	2A	2187	G	2.5
32	1a	1032	G	2.5
34	1c	124	ILE	2.5
1	2A	2167	U	2.5
6	2G	138	GLN	2.5
45	1n	8	GLU	2.5
31	29	15	LYS	2.5
40	1i	56	LEU	2.5
50	1s	5	LEU	2.5
39	2h	93	VAL	2.5
1	2A	2185	C	2.5
32	2a	1137	C	2.5
32	2a	1149	C	2.5
33	2b	31	TYR	2.5
44	1m	2	ALA	2.5
1	1A	1127	U	2.5
1	1A	2803	A	2.5
1	2A	1508	A	2.5
1	2A	1170	G	2.5
32	2a	1068	G	2.5

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
41	1j	100	THR	2.5
44	1m	22	ILE	2.5
46	2o	86	GLY	2.5
52	2u	11	GLY	2.5
6	2G	19	LEU	2.5
34	1c	204	LEU	2.5
38	1g	59	LEU	2.5
21	2Z	136	PHE	2.5
24	22	25	VAL	2.5
34	2c	195	VAL	2.5
34	2c	198	VAL	2.5
49	1r	37	VAL	2.5
53	2y	15	ALA	2.5
1	1A	2151	C	2.5
4	2E	151	TYR	2.5
6	2G	72	ARG	2.5
33	1b	234	PRO	2.5
34	2c	57	ILE	2.5
41	2j	6	ILE	2.5
32	2a	1032	G	2.5
6	2G	35	GLU	2.5
23	11	98	LEU	2.5
34	2c	47	LEU	2.5
34	2c	91	LEU	2.5
37	2f	45	LEU	2.5
40	2i	47	LEU	2.5
40	2i	31	GLN	2.5
1	2A	2180	U	2.5
50	2s	44	MET	2.5
6	2G	178	PHE	2.5
7	2H	35	VAL	2.5
38	2g	156	TRP	2.5
22	20	11	ARG	2.5
32	2a	1452	C	2.5
33	2b	23	ARG	2.5
41	2j	15	THR	2.5
32	2a	1357	A	2.5
32	2a	1531	A	2.5
32	1a	1020	U	2.5
35	2d	202	LEU	2.5
7	2H	45	VAL	2.4
41	1j	26	ALA	2.4

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Mol	Chain	Res	Type	RSRZ
47	2p	79	VAL	2.4
1	1A	2183	C	2.4
47	2p	38	TYR	2.4
7	2H	4	ILE	2.4
31	19	17	ILE	2.4
32	2a	1287	A	2.4
33	2b	162	ILE	2.4
40	1i	63	ILE	2.4
1	1A	2171	G	2.4
14	2S	54	LEU	2.4
34	1c	168	ALA	2.4
40	2i	61	ALA	2.4
41	2j	54	PHE	2.4
34	2c	80	GLY	2.4
48	1q	33	GLY	2.4
19	2X	60	ARG	2.4
1	1A	2148	A	2.4
45	2n	58	LYS	2.4
32	2a	998	G	2.4
33	1b	187	LEU	2.4
44	2m	96	LEU	2.4
34	1c	60	ALA	2.4
38	2g	46	ALA	2.4
51	1t	45	GLN	2.4
1	1A	271	U	2.4
21	2Z	143	GLY	2.4
1	2A	652(T)	C	2.4
13	2R	68	ARG	2.4
34	2c	143	GLU	2.4
32	1a	1027	C	2.4
44	2m	99	ARG	2.4
38	1g	53	LYS	2.4
44	1m	59	TYR	2.4
52	1u	21	TYR	2.4
1	2A	2117	A	2.4
11	2P	6	LEU	2.4
35	1d	108	LEU	2.4
49	1r	26	LEU	2.4
15	1T	37	GLY	2.4
33	1b	19	HIS	2.4
6	2G	147	ASP	2.4
6	2G	161	THR	2.4

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
26	14	65	ASP	2.4
1	1A	1150	C	2.4
1	1A	2130	C	2.4
1	2A	2163	C	2.4
26	24	32	TYR	2.4
44	2m	78	ILE	2.4
19	2X	9	LEU	2.4
33	2b	115	LEU	2.4
34	2c	178	LEU	2.4
35	2d	188	LEU	2.4
6	2G	151	ALA	2.4
8	2I	46	ALA	2.4
33	2b	137	ARG	2.4
34	2c	60	ALA	2.4
40	2i	9	ARG	2.4
40	2i	83	ARG	2.4
40	2i	106	ALA	2.4
43	1l	63	GLY	2.4
32	2a	1021	G	2.4
20	2Y	89	PHE	2.4
1	1A	1118	C	2.4
2	2B	88	C	2.4
40	2i	121	ARG	2.4
41	1j	5	ARG	2.4
44	2m	89	GLY	2.4
1	2A	1103	A	2.4
7	2H	171	LEU	2.4
35	1d	186	LEU	2.4
38	2g	101	LEU	2.4
44	1m	56	LEU	2.4
26	24	7	PRO	2.4
50	1s	75	ALA	2.4
40	2i	103	THR	2.4
7	2H	43	VAL	2.4
50	2s	58	VAL	2.4
1	1A	2209	G	2.4
53	2y	9	GLN	2.4
14	2S	31	SER	2.4
45	2n	50	LYS	2.3
21	1Z	80	ARG	2.3
52	1u	22	ARG	2.3
4	1E	151	TYR	2.3

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
22	20	76	GLY	2.3
33	1b	227	GLY	2.3
50	1s	61	TYR	2.3
17	2V	71	LEU	2.3
35	1d	120	LEU	2.3
35	1d	176	LEU	2.3
1	1A	1130	A	2.3
1	2A	1096	A	2.3
32	1a	1005	A	2.3
6	2G	117	PHE	2.3
7	1H	45	VAL	2.3
44	2m	3	ARG	2.3
41	1j	17	ASP	2.3
1	1A	933	C	2.3
6	2G	177	GLY	2.3
40	1i	115	GLY	2.3
6	2G	140	ILE	2.3
52	1u	13	ILE	2.3
34	2c	139	GLN	2.3
6	2G	73	ALA	2.3
20	2Y	5	MET	2.3
32	1a	1004	A	2.3
32	1a	1044	A	2.3
33	2b	216	SER	2.3
51	1t	70	SER	2.3
53	2y	42	SER	2.3
36	1e	6	PHE	2.3
50	1s	9	VAL	2.3
41	1j	97	GLU	2.3
1	1A	1139	G	2.3
1	2A	2190	G	2.3
32	1a	163	C	2.3
32	2a	89	C	2.3
21	2Z	133	ILE	2.3
33	1b	211	ILE	2.3
47	1p	19	ILE	2.3
1	1A	2189	U	2.3
32	1a	1212	U	2.3
6	1G	152	LEU	2.3
7	2H	51	ARG	2.3
11	2P	79	ARG	2.3
12	1Q	59	ARG	2.3

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
33	1b	218	ALA	2.3
41	2j	18	ALA	2.3
48	1q	91	ARG	2.3
53	1y	71	TYR	2.3
41	1j	73	ASP	2.3
1	1A	937	A	2.3
3	2D	5	LYS	2.3
25	13	54	VAL	2.3
41	2j	49	VAL	2.3
42	2k	84	VAL	2.3
11	2P	109	GLY	2.3
45	2n	16	PHE	2.3
50	1s	56	GLN	2.3
32	1a	204	U	2.3
33	2b	209	ARG	2.3
41	1j	29	ARG	2.3
41	1j	75	ILE	2.3
33	1b	237	ALA	2.3
40	2i	46	ALA	2.3
40	1i	19	LEU	2.3
47	2p	6	LEU	2.3
52	2u	12	LYS	2.3
14	2S	81	GLY	2.3
40	2i	22	GLY	2.3
7	2H	24	VAL	2.3
27	25	60	VAL	2.3
34	2c	153	VAL	2.3
1	1A	2135	U	2.3
32	2a	1358	U	2.3
44	1m	114	ARG	2.3
1	1A	2188	G	2.3
1	2A	2178	C	2.3
32	1a	1006	C	2.3
51	1t	100	ILE	2.3
10	2O	51	ALA	2.3
17	1V	55	ALA	2.3
40	2i	55	ALA	2.3
45	2n	43	CYS	2.3
8	1I	84	GLY	2.3
19	2X	1	MET	2.3
22	20	42	GLY	2.3
36	2e	10	MET	2.3

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	1A	1985	U	2.3
1	2A	271(K)	U	2.3
41	2j	29	ARG	2.3
50	1s	67	VAL	2.3
3	1D	276	LYS	2.3
33	2b	131	PRO	2.3
34	2c	199	LYS	2.3
44	2m	79	LYS	2.3
1	2A	882	G	2.3
6	2G	76	SER	2.3
7	1H	92	ILE	2.3
14	2S	51	ALA	2.3
45	1n	59	ALA	2.3
8	2I	38	LEU	2.2
1	1A	1072	U	2.2
1	2A	1026	U	2.2
32	2a	90	U	2.2
34	2c	164	ARG	2.2
36	1e	22	GLY	2.2
36	2e	50	GLU	2.2
44	2m	67	GLU	2.2
50	2s	83	HIS	2.2
12	2Q	65	PHE	2.2
14	2S	12	PHE	2.2
26	24	29	PRO	2.2
33	2b	125	PRO	2.2
42	2k	42	TRP	2.2
34	2c	127	ARG	2.2
44	1m	25	ILE	2.2
51	2t	100	ILE	2.2
1	1A	2190	G	2.2
21	2Z	156	LYS	2.2
33	1b	215	LEU	2.2
44	2m	68	GLY	2.2
47	1p	17	TYR	2.2
26	24	53	GLU	2.2
34	2c	35	GLU	2.2
34	2c	89	GLU	2.2
49	1r	39	VAL	2.2
35	2d	206	PHE	2.2
36	2e	84	PHE	2.2
41	1j	57	LYS	2.2

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
10	2O	69	ILE	2.2
35	1d	67	ILE	2.2
41	2j	32	ALA	2.2
42	2k	15	ALA	2.2
43	1l	7	ILE	2.2
44	2m	25	ILE	2.2
46	1o	87	ILE	2.2
44	1m	90	LEU	2.2
40	2i	20	ARG	2.2
40	2i	93	ARG	2.2
40	2i	111	ARG	2.2
52	2u	22	ARG	2.2
44	2m	13	LYS	2.2
22	20	52	GLY	2.2
41	1j	31	GLY	2.2
34	2c	95	THR	2.2
35	1d	173	TRP	2.2
45	1n	10	ALA	2.2
53	2y	51	ASP	2.2
18	1W	111	HIS	2.2
32	2a	1037	C	2.2
32	2a	1098	C	2.2
41	2j	25	GLU	2.2
1	2A	2206	G	2.2
6	2G	86	MET	2.2
32	1a	1009	G	2.2
34	1c	21	ARG	2.2
1	1A	288	U	2.2
32	2a	841	U	2.2
34	2c	48	TYR	2.2
4	2E	150	VAL	2.2
33	1b	229	VAL	2.2
6	2G	85	GLY	2.2
17	1V	101	GLY	2.2
33	2b	65	GLY	2.2
34	2c	17	ASP	2.2
35	2d	144	ASP	2.2
40	2i	115	GLY	2.2
41	1j	58	ASP	2.2
1	2A	2114	A	2.2
26	14	18	CYS	2.2
14	2S	21	THR	2.2

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
20	2Y	31	LEU	2.2
21	2Z	144	LEU	2.2
33	2b	114	ARG	2.2
1	1A	2149	G	2.2
1	2A	1091	G	2.2
1	2A	2157	G	2.2
40	1i	75	ASP	2.2
41	1j	83	GLU	2.2
6	2G	134	GLY	2.2
38	2g	26	PHE	2.2
45	2n	52	GLN	2.2
1	1A	1149	A	2.2
3	1D	106	ILE	2.2
21	2Z	150	LEU	2.2
46	1o	83	GLU	2.2
37	1f	1	MET	2.2
40	2i	91	ASP	2.2
47	1p	32	TYR	2.1
33	2b	175	ARG	2.1
38	2g	115	ARG	2.1
1	1A	2172	U	2.1
34	2c	61	ALA	2.1
45	1n	22	THR	2.1
50	2s	50	ALA	2.1
1	1A	2191	A	2.1
41	1j	96	ILE	2.1
3	1D	182	LEU	2.1
7	2H	98	LEU	2.1
32	1a	1038	C	2.1
32	2a	1223	C	2.1
3	2D	38	LYS	2.1
6	2G	2	PRO	2.1
33	2b	217	ARG	2.1
43	2l	89	ARG	2.1
50	2s	37	ARG	2.1
52	2u	10	ARG	2.1
1	1A	2843	G	2.1
1	2A	2792	G	2.1
25	23	15	TYR	2.1
7	2H	76	VAL	2.1
44	2m	69	GLU	2.1
45	2n	18	VAL	2.1

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
50	1s	58	VAL	2.1
33	1b	207	ALA	2.1
33	2b	120	ALA	2.1
36	2e	45	PHE	2.1
51	1t	77	ALA	2.1
14	2S	35	ILE	2.1
32	2a	1157	A	2.1
19	1X	70	LEU	2.1
25	23	2	PRO	2.1
16	1U	69	CYS	2.1
20	2Y	2	ARG	2.1
28	26	50	ARG	2.1
34	1c	2	GLY	2.1
34	1c	80	GLY	2.1
42	2k	91	ARG	2.1
44	2m	57	ARG	2.1
1	2A	2897	U	2.1
26	14	57	GLU	2.1
6	2G	38	VAL	2.1
11	2P	71	VAL	2.1
20	1Y	7	VAL	2.1
1	2A	1074	G	2.1
32	1a	1021	G	2.1
32	2a	79	G	2.1
40	1i	37	PHE	2.1
45	1n	20	ALA	2.1
41	2j	17	ASP	2.1
6	1G	88	ILE	2.1
11	2P	102	ARG	2.1
14	2S	17	ARG	2.1
21	2Z	171	ILE	2.1
34	2c	134	ILE	2.1
35	1d	65	ARG	2.1
35	2d	71	SER	2.1
42	2k	16	SER	2.1
44	2m	106	ASN	2.1
51	2t	41	ILE	2.1
51	2t	55	ILE	2.1
37	1f	48	LEU	2.1
48	2q	6	LEU	2.1
1	1A	932	C	2.1
1	2A	897	C	2.1

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	2A	2113	U	2.1
1	2A	2172	U	2.1
32	2a	1219	U	2.1
6	2G	81	LYS	2.1
34	2c	107	GLN	2.1
48	1q	23	VAL	2.1
51	1t	83	ARG	2.1
53	2y	4	ASN	2.1
4	2E	115	GLY	2.1
37	1f	52	ILE	2.1
53	2y	78	ILE	2.1
6	2G	7	LEU	2.1
33	2b	145	LEU	2.1
38	2g	16	LEU	2.1
40	2i	79	LEU	2.1
45	2n	11	LYS	2.1
32	2a	975	A	2.1
1	2A	2177	C	2.1
32	2a	1006	C	2.1
40	1i	32	ASP	2.1
27	15	49	CYS	2.1
34	2c	167	TRP	2.1
46	2o	17	ARG	2.1
50	1s	77	THR	2.1
52	1u	9	ARG	2.1
40	1i	106	ALA	2.1
47	1p	14	ASN	2.1
7	1H	49	VAL	2.1
32	2a	1150	U	2.1
39	1h	117	GLY	2.1
1	1A	2203	G	2.1
14	2S	58	LEU	2.1
37	1f	21	LEU	2.1
53	2y	12	ILE	2.1
40	2i	124	GLN	2.1
41	1j	89	ASP	2.1
1	1A	2158	C	2.1
1	1A	2196	C	2.1
1	1A	2198	A	2.1
33	2b	63	MET	2.1
34	2c	16	ARG	2.1
34	2c	132	ARG	2.1

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
44	2m	71	ARG	2.1
21	2Z	188	ALA	2.1
33	1b	123	ALA	2.1
42	2k	89	ALA	2.1
48	1q	100	LYS	2.1
39	1h	79	VAL	2.1
40	1i	109	VAL	2.1
7	2H	164	TYR	2.1
35	2d	20	TYR	2.1
36	1e	133	TYR	2.1
43	2l	32	PHE	2.1
6	2G	139	LEU	2.0
16	1U	65	ILE	2.0
36	2e	89	ILE	2.0
37	2f	46	ARG	2.0
1	2A	1041	C	2.0
5	1F	167	ALA	2.0
33	2b	171	ALA	2.0
41	1j	35	SER	2.0
41	2j	10	GLY	2.0
45	2n	51	GLY	2.0
51	1t	95	ALA	2.0
6	2G	17	PRO	2.0
43	2l	55	VAL	2.0
48	2q	77	VAL	2.0
19	1X	65	ARG	2.0
26	24	39	CYS	2.0
34	2c	184	TYR	2.0
41	1j	54	PHE	2.0
42	1k	125	PHE	2.0
43	1l	19	ARG	2.0
47	2p	9	PHE	2.0
11	1P	99	LEU	2.0
35	2d	21	LEU	2.0
45	2n	7	ILE	2.0
1	1A	432	U	2.0
1	1A	1129	U	2.0
32	2a	1040	U	2.0
1	1A	2815	C	2.0
32	2a	1249	C	2.0
1	1A	934	A	2.0
1	2A	896	A	2.0

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Mol	Chain	Res	Type	RSRZ
32	2a	1285	A	2.0
35	2d	179	GLU	2.0
36	2e	86	ALA	2.0
36	1e	5	ASP	2.0
39	1h	102	ARG	2.0
21	2Z	100	VAL	2.0
41	2j	24	VAL	2.0
42	2k	80	VAL	2.0
48	2q	5	VAL	2.0
50	2s	47	HIS	2.0
33	1b	97	TRP	2.0
40	1i	5	TYR	2.0
34	2c	32	LEU	2.0
36	2e	129	ILE	2.0
39	2h	99	GLU	2.0
44	2m	22	ILE	2.0
5	1F	112	MET	2.0
32	2a	1353	G	2.0
37	1f	58	GLY	2.0
40	2i	87	GLN	2.0
42	1k	73	MET	2.0
48	1q	26	GLN	2.0
32	2a	1354	C	2.0
14	2S	19	LYS	2.0
48	1q	38	ARG	2.0
41	1j	18	ALA	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( $\text{\AA}^2$ )	Q<0.9
1	5MU	1A	1937	21/22	0.90	0.17	65,79,86,95	0
1	5MU	2A	1915	21/22	0.90	0.13	70,82,87,103	0
32	2MG	2a	1207	24/25	0.90	0.19	75,83,90,94	0
32	M2G	2a	966	25/26	0.91	0.14	52,68,81,90	0
1	PSU	2A	1917	20/21	0.92	0.16	62,74,84,89	0
1	PSU	2A	1911	20/21	0.92	0.12	62,68,73,82	0
1	PSU	1A	1939	20/21	0.92	0.17	63,73,82,86	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
43	0TD	2l	92	10/11	0.93	0.11	57,63,66,74	0
32	PSU	2a	516	20/21	0.94	0.12	69,76,81,82	0
32	5MC	2a	1404	21/22	0.94	0.17	54,61,64,67	0
43	0TD	1l	92	10/11	0.94	0.18	54,59,68,68	0
32	2MG	1a	1207	24/25	0.95	0.14	60,68,71,74	0
32	5MC	2a	967	21/22	0.95	0.13	61,68,77,86	0
1	PSU	1A	1933	20/21	0.95	0.14	59,66,68,81	0
32	4OC	2a	1402	22/23	0.95	0.15	53,64,74,82	0
32	5MC	1a	967	21/22	0.95	0.16	51,61,73,83	0
32	7MG	2a	527	24/25	0.95	0.14	57,66,70,73	0
1	4OC	2A	1920	21/23	0.96	0.13	57,62,67,67	0
32	UR3	1a	1498	21/22	0.96	0.16	35,46,53,56	0
32	5MC	2a	1407	21/22	0.96	0.12	46,62,69,70	0
32	UR3	2a	1498	21/22	0.96	0.15	53,60,65,73	0
32	MA6	2a	1518	24/25	0.96	0.16	47,58,65,68	0
32	5MC	2a	1400	21/22	0.96	0.20	62,68,74,77	0
32	5MC	1a	1400	21/22	0.97	0.15	37,50,57,58	0
32	5MC	1a	1404	21/22	0.97	0.15	33,43,49,51	0
32	M2G	1a	966	25/26	0.97	0.15	48,53,59,65	0
1	5MC	2A	1942	21/22	0.97	0.15	36,45,52,53	0
32	MA6	1a	1518	24/25	0.97	0.18	37,44,51,56	0
32	MA6	1a	1519	24/25	0.97	0.18	40,45,52,52	0
1	4OC	1A	1942	21/23	0.97	0.16	52,60,63,65	0
32	MA6	2a	1519	24/25	0.97	0.19	51,61,64,69	0
32	PSU	1a	516	20/21	0.97	0.14	49,58,65,67	0
1	5MC	1A	1964	21/22	0.98	0.17	34,41,47,52	0
32	5MC	1a	1407	21/22	0.98	0.16	41,48,54,56	0
1	2MA	1A	2515	23/24	0.98	0.21	17,23,28,31	0
1	5MU	1A	1961	21/22	0.98	0.19	24,30,34,37	0
1	5MU	2A	1939	21/22	0.98	0.15	28,33,37,42	0
32	7MG	1a	527	24/25	0.98	0.16	40,48,55,55	0
1	5MC	2A	1962	21/22	0.98	0.15	32,38,44,54	0
1	OMG	2A	2251	24/25	0.98	0.15	27,31,35,37	0
1	2MA	2A	2503	23/24	0.98	0.17	21,28,32,37	0
1	2MU	2A	2552	21/23	0.98	0.17	27,33,38,38	0
1	PSU	2A	2605	20/21	0.98	0.17	27,31,39,41	0
32	4OC	1a	1402	22/23	0.98	0.16	41,47,51,56	0
1	5MC	1A	1984	21/22	0.99	0.17	29,36,41,47	0
1	2MU	1A	2564	21/23	0.99	0.19	24,29,33,36	0
1	PSU	1A	2617	20/21	0.99	0.18	23,29,35,38	0
1	OMG	1A	2263	24/25	0.99	0.21	22,28,29,33	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
54	MG	2A	3598	1/1	0.21	0.21	72,72,72,72	0
54	MG	2A	3659	1/1	0.22	0.12	76,76,76,76	0
54	MG	10	104	1/1	0.29	0.13	64,64,64,64	0
54	MG	2A	3509	1/1	0.32	0.28	75,75,75,75	0
54	MG	1A	3950	1/1	0.37	0.20	77,77,77,77	0
54	MG	1a	1817	1/1	0.38	0.07	98,98,98,98	0
54	MG	1A	3708	1/1	0.38	0.17	64,64,64,64	0
54	MG	2A	3697	1/1	0.39	0.08	67,67,67,67	0
54	MG	1a	1773	1/1	0.40	0.09	85,85,85,85	0
54	MG	1A	3836	1/1	0.41	0.12	57,57,57,57	0
54	MG	2A	3626	1/1	0.41	0.22	47,47,47,47	0
54	MG	2A	3663	1/1	0.43	0.16	74,74,74,74	0
54	MG	2B	3007	1/1	0.43	0.22	76,76,76,76	0
54	MG	1A	3889	1/1	0.44	0.23	47,47,47,47	0
54	MG	1B	221	1/1	0.45	0.13	48,48,48,48	0
54	MG	2A	3638	1/1	0.45	0.13	55,55,55,55	0
54	MG	1A	3990	1/1	0.45	0.13	83,83,83,83	0
54	MG	2Q	3002	1/1	0.46	0.11	63,63,63,63	0
54	MG	2A	3640	1/1	0.48	0.05	63,63,63,63	0
54	MG	2A	3488	1/1	0.48	0.09	58,58,58,58	0
54	MG	2A	3375	1/1	0.49	0.13	51,51,51,51	0
54	MG	1A	3496	1/1	0.49	0.10	56,56,56,56	0
54	MG	2a	1750	1/1	0.49	0.10	79,79,79,79	0
54	MG	1a	1744	1/1	0.50	0.71	88,88,88,88	0
54	MG	1A	3409	1/1	0.51	0.22	58,58,58,58	0
54	MG	1A	3377	1/1	0.52	0.15	67,67,67,67	0
54	MG	2A	3569	1/1	0.52	0.17	55,55,55,55	0
54	MG	1a	1870	1/1	0.52	0.13	93,93,93,93	0
54	MG	2a	1747	1/1	0.53	0.14	78,78,78,78	0
54	MG	2A	3681	1/1	0.53	0.08	70,70,70,70	0
54	MG	2A	3586	1/1	0.54	0.07	62,62,62,62	0
54	MG	2B	3012	1/1	0.55	0.13	77,77,77,77	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
54	MG	2a	1749	1/1	0.55	0.10	85,85,85,85	0
54	MG	2A	3593	1/1	0.55	0.14	48,48,48,48	0
54	MG	2A	3584	1/1	0.56	0.21	49,49,49,49	0
54	MG	1a	1676	1/1	0.56	0.26	75,75,75,75	0
54	MG	2A	3588	1/1	0.56	0.14	88,88,88,88	0
54	MG	2a	1789	1/1	0.56	0.19	80,80,80,80	0
54	MG	2A	3727	1/1	0.57	0.09	70,70,70,70	0
54	MG	2A	3495	1/1	0.57	0.10	54,54,54,54	0
54	MG	2A	3464	1/1	0.57	0.15	63,63,63,63	0
54	MG	1A	3513	1/1	0.57	0.19	58,58,58,58	0
54	MG	1A	3499	1/1	0.58	0.11	55,55,55,55	0
54	MG	10	101	1/1	0.58	0.07	52,52,52,52	0
54	MG	1a	1673	1/1	0.59	0.14	71,71,71,71	0
54	MG	2A	3642	1/1	0.59	0.23	77,77,77,77	0
54	MG	2A	3729	1/1	0.60	0.11	59,59,59,59	0
54	MG	2A	3478	1/1	0.60	0.45	64,64,64,64	0
54	MG	1A	3171	1/1	0.61	0.17	56,56,56,56	0
54	MG	1B	202	1/1	0.61	0.20	63,63,63,63	0
54	MG	1a	1875	1/1	0.62	0.10	77,77,77,77	0
54	MG	1A	3799	1/1	0.62	0.10	51,51,51,51	0
54	MG	1a	1783	1/1	0.62	0.23	87,87,87,87	0
54	MG	1A	3616	1/1	0.62	0.14	55,55,55,55	0
54	MG	1A	3612	1/1	0.62	0.70	66,66,66,66	0
54	MG	2a	1755	1/1	0.63	0.23	82,82,82,82	0
57	ZN	2Y	501	1/1	0.63	0.24	169,169,169,169	0
54	MG	2B	3015	1/1	0.64	0.23	87,87,87,87	0
54	MG	2A	3597	1/1	0.64	0.05	72,72,72,72	0
54	MG	2a	1649	1/1	0.64	0.10	75,75,75,75	0
54	MG	2a	1729	1/1	0.64	0.10	71,71,71,71	0
54	MG	1A	3450	1/1	0.64	0.15	57,57,57,57	0
54	MG	1A	3985	1/1	0.64	0.11	75,75,75,75	0
54	MG	1A	3374	1/1	0.64	0.10	57,57,57,57	0
54	MG	2A	3481	1/1	0.64	0.16	69,69,69,69	0
54	MG	1A	3580	1/1	0.64	0.07	59,59,59,59	0
54	MG	1A	3924	1/1	0.64	0.11	61,61,61,61	0
54	MG	1A	3431	1/1	0.65	0.12	61,61,61,61	0
54	MG	2A	3709	1/1	0.65	0.07	50,50,50,50	0
54	MG	2A	3431	1/1	0.65	0.44	57,57,57,57	0
54	MG	2A	3684	1/1	0.65	0.12	62,62,62,62	0
54	MG	2A	3171	1/1	0.66	0.18	56,56,56,56	0
54	MG	2A	3484	1/1	0.66	0.18	66,66,66,66	0
54	MG	2a	1788	1/1	0.66	0.10	102,102,102,102	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
54	MG	2A	3312	1/1	0.66	0.10	65,65,65,65	0
54	MG	1A	3936	1/1	0.66	0.17	55,55,55,55	0
54	MG	1A	3593	1/1	0.67	0.14	62,62,62,62	0
54	MG	1B	217	1/1	0.67	0.35	70,70,70,70	0
54	MG	1a	1872	1/1	0.67	0.21	83,83,83,83	0
54	MG	2A	3465	1/1	0.67	0.15	67,67,67,67	0
54	MG	2A	3665	1/1	0.67	0.10	53,53,53,53	0
54	MG	2A	3468	1/1	0.67	0.27	72,72,72,72	0
54	MG	1A	3615	1/1	0.67	0.10	60,60,60,60	0
54	MG	1A	3745	1/1	0.67	0.09	71,71,71,71	0
54	MG	2A	3288	1/1	0.67	0.14	51,51,51,51	0
54	MG	1A	3772	1/1	0.67	0.10	50,50,50,50	0
54	MG	2A	3633	1/1	0.67	0.74	68,68,68,68	0
54	MG	2A	3325	1/1	0.67	0.14	50,50,50,50	0
54	MG	1A	3786	1/1	0.68	0.12	64,64,64,64	0
54	MG	2A	3680	1/1	0.68	0.24	53,53,53,53	0
54	MG	1A	3621	1/1	0.68	0.18	65,65,65,65	0
54	MG	2A	3603	1/1	0.68	0.30	78,78,78,78	0
54	MG	2A	3685	1/1	0.68	0.08	60,60,60,60	0
54	MG	2D	306	1/1	0.68	0.18	60,60,60,60	0
54	MG	1A	3833	1/1	0.68	0.13	60,60,60,60	0
54	MG	1A	3295	1/1	0.68	0.13	84,84,84,84	0
54	MG	1a	1791	1/1	0.69	0.15	72,72,72,72	0
54	MG	1A	3788	1/1	0.69	0.25	66,66,66,66	0
54	MG	2A	3513	1/1	0.69	0.19	58,58,58,58	0
54	MG	1A	3485	1/1	0.69	0.09	72,72,72,72	0
54	MG	2A	3609	1/1	0.69	0.12	58,58,58,58	0
54	MG	2A	3622	1/1	0.69	0.08	69,69,69,69	0
54	MG	1F	309	1/1	0.69	0.08	69,69,69,69	0
54	MG	1A	4019	1/1	0.69	0.26	58,58,58,58	0
54	MG	1A	3805	1/1	0.69	0.09	63,63,63,63	0
54	MG	1A	3956	1/1	0.70	0.20	60,60,60,60	0
54	MG	1A	3553	1/1	0.70	0.15	68,68,68,68	0
54	MG	1a	1751	1/1	0.70	0.08	67,67,67,67	0
54	MG	1d	506	1/1	0.70	0.19	93,93,93,93	0
54	MG	2a	1629	1/1	0.70	0.11	61,61,61,61	0
54	MG	2A	3081	1/1	0.70	0.46	55,55,55,55	0
54	MG	2a	1681	1/1	0.70	0.08	74,74,74,74	0
54	MG	1A	3511	1/1	0.70	0.27	64,64,64,64	0
54	MG	2A	3223	1/1	0.70	0.22	58,58,58,58	0
54	MG	1A	3991	1/1	0.70	0.06	50,50,50,50	0
54	MG	1A	3528	1/1	0.70	0.25	61,61,61,61	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
54	MG	2A	3505	1/1	0.70	0.09	73,73,73,73	0
54	MG	2a	1778	1/1	0.70	0.24	79,79,79,79	0
54	MG	1A	3530	1/1	0.70	0.30	69,69,69,69	0
54	MG	1a	1868	1/1	0.70	0.07	71,71,71,71	0
54	MG	2A	3384	1/1	0.70	0.09	46,46,46,46	0
57	ZN	24	501	1/1	0.70	0.09	257,257,257,257	0
54	MG	2A	3561	1/1	0.71	0.14	50,50,50,50	0
54	MG	1R	203	1/1	0.71	0.23	48,48,48,48	0
54	MG	2A	3627	1/1	0.71	0.16	60,60,60,60	0
54	MG	2a	1707	1/1	0.71	0.11	65,65,65,65	0
54	MG	1A	3639	1/1	0.71	0.09	65,65,65,65	0
54	MG	2A	3367	1/1	0.71	0.12	66,66,66,66	0
54	MG	1A	3579	1/1	0.71	0.25	74,74,74,74	0
54	MG	1A	3858	1/1	0.71	0.17	68,68,68,68	0
54	MG	2A	3737	1/1	0.71	0.20	37,37,37,37	0
54	MG	2A	3658	1/1	0.71	0.09	52,52,52,52	0
54	MG	2A	3388	1/1	0.71	0.16	55,55,55,55	0
54	MG	1E	304	1/1	0.71	0.18	59,59,59,59	0
54	MG	1a	1694	1/1	0.71	0.13	67,67,67,67	0
54	MG	1A	3719	1/1	0.71	0.15	47,47,47,47	0
54	MG	1a	1793	1/1	0.72	0.13	67,67,67,67	0
54	MG	1A	3011	1/1	0.72	0.14	62,62,62,62	0
54	MG	1A	4017	1/1	0.72	0.11	62,62,62,62	0
54	MG	1G	3002	1/1	0.72	0.12	62,62,62,62	0
54	MG	1A	3294	1/1	0.72	0.09	74,74,74,74	0
54	MG	2A	3616	1/1	0.72	0.19	47,47,47,47	0
54	MG	2A	3349	1/1	0.72	0.17	46,46,46,46	0
54	MG	2A	3625	1/1	0.72	0.20	43,43,43,43	0
54	MG	2a	1771	1/1	0.72	0.33	86,86,86,86	0
54	MG	2D	301	1/1	0.72	0.30	55,55,55,55	0
54	MG	1A	3706	1/1	0.72	0.17	64,64,64,64	0
54	MG	1A	3759	1/1	0.72	0.20	45,45,45,45	0
54	MG	20	101	1/1	0.72	0.14	64,64,64,64	0
54	MG	1A	3763	1/1	0.72	0.19	53,53,53,53	0
54	MG	2A	3187	1/1	0.73	0.69	61,61,61,61	0
54	MG	1a	1841	1/1	0.73	0.20	61,61,61,61	0
54	MG	1a	1767	1/1	0.73	0.16	79,79,79,79	0
54	MG	1A	3927	1/1	0.73	0.09	63,63,63,63	0
54	MG	2A	3679	1/1	0.73	0.10	56,56,56,56	0
54	MG	2a	1752	1/1	0.73	0.19	67,67,67,67	0
54	MG	2A	3578	1/1	0.73	0.20	71,71,71,71	0
54	MG	1A	3888	1/1	0.73	0.10	58,58,58,58	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
54	MG	1A	3825	1/1	0.73	0.10	70,70,70,70	0
54	MG	2a	1786	1/1	0.73	0.15	67,67,67,67	0
54	MG	1b	3001	1/1	0.73	0.10	87,87,87,87	0
54	MG	1A	4006	1/1	0.73	0.17	55,55,55,55	0
54	MG	1A	3568	1/1	0.73	0.18	55,55,55,55	0
54	MG	1a	1836	1/1	0.73	0.15	83,83,83,83	0
54	MG	1A	3455	1/1	0.74	0.14	50,50,50,50	0
54	MG	1A	3597	1/1	0.74	0.09	62,62,62,62	0
54	MG	2a	1605	1/1	0.74	0.16	63,63,63,63	0
54	MG	2a	1610	1/1	0.74	0.16	61,61,61,61	0
54	MG	1A	3367	1/1	0.74	0.12	54,54,54,54	0
54	MG	2a	1645	1/1	0.74	0.17	67,67,67,67	0
54	MG	1A	3576	1/1	0.74	0.23	57,57,57,57	0
54	MG	2a	1656	1/1	0.74	0.13	69,69,69,69	0
54	MG	2a	1667	1/1	0.74	0.15	83,83,83,83	0
54	MG	1A	3084	1/1	0.74	0.15	58,58,58,58	0
54	MG	1A	3196	1/1	0.74	0.19	72,72,72,72	0
54	MG	2A	3360	1/1	0.74	0.11	72,72,72,72	0
54	MG	1A	3830	1/1	0.74	0.14	65,65,65,65	0
54	MG	1A	3634	1/1	0.74	0.37	43,43,43,43	0
54	MG	1a	1788	1/1	0.74	0.11	85,85,85,85	0
54	MG	2A	3720	1/1	0.74	0.24	55,55,55,55	0
54	MG	2A	3545	1/1	0.74	0.10	75,75,75,75	0
54	MG	2A	3556	1/1	0.74	0.09	62,62,62,62	0
54	MG	2A	3629	1/1	0.74	0.15	62,62,62,62	0
54	MG	14	502	1/1	0.74	0.12	83,83,83,83	0
54	MG	2A	3563	1/1	0.74	0.07	50,50,50,50	0
54	MG	1a	1664	1/1	0.74	0.12	58,58,58,58	0
54	MG	2A	3455	1/1	0.74	0.14	62,62,62,62	0
54	MG	2A	3174	1/1	0.74	0.62	61,61,61,61	0
54	MG	2a	1754	1/1	0.75	0.33	84,84,84,84	0
54	MG	1A	3902	1/1	0.75	0.06	69,69,69,69	0
54	MG	1A	3625	1/1	0.75	0.20	63,63,63,63	0
54	MG	2A	3512	1/1	0.75	0.09	54,54,54,54	0
54	MG	1A	4025	1/1	0.75	0.12	70,70,70,70	0
54	MG	2a	1635	1/1	0.75	0.14	67,67,67,67	0
54	MG	2A	3418	1/1	0.75	0.10	71,71,71,71	0
54	MG	2A	3426	1/1	0.75	0.12	58,58,58,58	0
54	MG	2A	3502	1/1	0.75	0.18	61,61,61,61	0
54	MG	2A	3576	1/1	0.76	0.10	49,49,49,49	0
54	MG	2a	1664	1/1	0.76	0.16	79,79,79,79	0
54	MG	1A	3766	1/1	0.76	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
54	MG	1A	4003	1/1	0.76	0.44	66,66,66,66	0
54	MG	2a	1692	1/1	0.76	0.10	77,77,77,77	0
54	MG	2B	3001	1/1	0.76	0.11	68,68,68,68	0
54	MG	2A	3162	1/1	0.76	0.28	57,57,57,57	0
54	MG	2A	3383	1/1	0.76	0.17	52,52,52,52	0
54	MG	1A	3866	1/1	0.76	0.11	64,64,64,64	0
54	MG	1a	1865	1/1	0.76	0.17	46,46,46,46	0
54	MG	1A	3312	1/1	0.76	0.15	72,72,72,72	0
54	MG	2A	3190	1/1	0.76	0.14	61,61,61,61	0
54	MG	1a	1869	1/1	0.76	0.11	74,74,74,74	0
54	MG	2a	1601	1/1	0.76	0.25	69,69,69,69	0
54	MG	2A	3244	1/1	0.76	0.20	56,56,56,56	0
54	MG	2A	3551	1/1	0.76	0.12	61,61,61,61	0
54	MG	1A	3655	1/1	0.76	0.11	40,40,40,40	0
54	MG	1A	3464	1/1	0.76	0.18	47,47,47,47	0
54	MG	2a	1792	1/1	0.76	0.14	67,67,67,67	0
55	MPD	1a	1880	8/8	0.76	0.20	48,59,72,72	0
54	MG	1A	3558	1/1	0.76	0.11	62,62,62,62	0
54	MG	1a	1801	1/1	0.76	0.25	80,80,80,80	0
54	MG	1A	3152	1/1	0.77	0.19	66,66,66,66	0
54	MG	2A	3129	1/1	0.77	0.11	63,63,63,63	0
54	MG	1A	3988	1/1	0.77	0.10	81,81,81,81	0
54	MG	2A	3688	1/1	0.77	0.11	67,67,67,67	0
54	MG	1A	3692	1/1	0.77	0.10	55,55,55,55	0
54	MG	1a	1718	1/1	0.77	0.17	58,58,58,58	0
54	MG	1A	3497	1/1	0.77	0.16	45,45,45,45	0
54	MG	1A	3600	1/1	0.77	0.10	57,57,57,57	0
54	MG	2A	3206	1/1	0.77	0.18	56,56,56,56	0
54	MG	2A	3438	1/1	0.77	0.20	56,56,56,56	0
54	MG	2a	1744	1/1	0.77	0.11	75,75,75,75	0
54	MG	1A	3443	1/1	0.77	0.07	48,48,48,48	0
54	MG	2A	3234	1/1	0.77	0.41	65,65,65,65	0
54	MG	2A	3575	1/1	0.77	0.09	43,43,43,43	0
54	MG	1A	3566	1/1	0.77	0.14	60,60,60,60	0
54	MG	2B	3018	1/1	0.77	0.11	76,76,76,76	0
54	MG	2A	3645	1/1	0.77	0.04	77,77,77,77	0
54	MG	2A	3251	1/1	0.77	0.16	53,53,53,53	0
54	MG	1A	3861	1/1	0.77	0.18	54,54,54,54	0
54	MG	1A	3758	1/1	0.77	0.10	66,66,66,66	0
54	MG	1a	1614	1/1	0.77	0.19	74,74,74,74	0
54	MG	2a	1604	1/1	0.77	0.17	66,66,66,66	0
54	MG	2A	3668	1/1	0.77	0.27	73,73,73,73	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
54	MG	1A	3959	1/1	0.77	0.07	70,70,70,70	0
54	MG	2a	1614	1/1	0.77	0.13	55,55,55,55	0
54	MG	2A	3023	1/1	0.77	0.14	54,54,54,54	0
54	MG	1F	307	1/1	0.78	0.21	49,49,49,49	0
54	MG	1A	3571	1/1	0.78	0.09	65,65,65,65	0
54	MG	2a	1721	1/1	0.78	0.11	71,71,71,71	0
54	MG	1a	1746	1/1	0.78	0.09	56,56,56,56	0
54	MG	1a	1631	1/1	0.78	0.25	70,70,70,70	0
54	MG	1A	3962	1/1	0.78	0.18	59,59,59,59	0
54	MG	1A	3375	1/1	0.78	0.14	49,49,49,49	0
54	MG	2A	3635	1/1	0.78	0.16	65,65,65,65	0
54	MG	1A	3685	1/1	0.78	0.08	70,70,70,70	0
54	MG	1A	3592	1/1	0.78	0.08	54,54,54,54	0
54	MG	2a	1626	1/1	0.78	0.20	70,70,70,70	0
54	MG	2A	3526	1/1	0.78	0.13	66,66,66,66	0
54	MG	2A	3530	1/1	0.78	0.10	50,50,50,50	0
54	MG	2A	3535	1/1	0.78	0.42	71,71,71,71	0
54	MG	2A	3231	1/1	0.78	0.13	61,61,61,61	0
54	MG	2A	3082	1/1	0.78	0.39	59,59,59,59	0
54	MG	2A	3553	1/1	0.78	0.26	76,76,76,76	0
54	MG	2A	3237	1/1	0.78	0.12	65,65,65,65	0
54	MG	2A	3671	1/1	0.78	0.14	36,36,36,36	0
54	MG	2a	1686	1/1	0.78	0.35	66,66,66,66	0
54	MG	2A	3323	1/1	0.79	0.16	59,59,59,59	0
54	MG	1A	3862	1/1	0.79	0.07	54,54,54,54	0
54	MG	1A	3507	1/1	0.79	0.21	32,32,32,32	0
54	MG	2A	3544	1/1	0.79	0.07	55,55,55,55	0
54	MG	1a	1670	1/1	0.79	0.25	68,68,68,68	0
54	MG	1A	3775	1/1	0.79	0.18	36,36,36,36	0
54	MG	1A	3534	1/1	0.79	0.18	67,67,67,67	0
54	MG	2a	1646	1/1	0.79	0.09	77,77,77,77	0
54	MG	1A	3590	1/1	0.79	0.19	72,72,72,72	0
54	MG	1a	1700	1/1	0.79	0.10	66,66,66,66	0
54	MG	2A	3387	1/1	0.79	0.23	55,55,55,55	0
54	MG	1A	3794	1/1	0.79	0.14	65,65,65,65	0
54	MG	2A	3570	1/1	0.79	0.10	57,57,57,57	0
54	MG	2A	3408	1/1	0.79	0.60	74,74,74,74	0
54	MG	2a	1689	1/1	0.79	0.12	70,70,70,70	0
54	MG	1A	3525	1/1	0.79	0.15	57,57,57,57	0
54	MG	1B	208	1/1	0.79	0.33	72,72,72,72	0
54	MG	2a	1715	1/1	0.79	0.09	71,71,71,71	0
54	MG	1a	1749	1/1	0.79	0.15	70,70,70,70	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
54	MG	1A	3641	1/1	0.79	0.14	62,62,62,62	0
54	MG	2a	1737	1/1	0.79	0.08	67,67,67,67	0
54	MG	1A	3810	1/1	0.79	0.12	80,80,80,80	0
54	MG	1A	3747	1/1	0.79	0.10	62,62,62,62	0
54	MG	1A	3649	1/1	0.79	0.12	59,59,59,59	0
54	MG	1a	1787	1/1	0.79	0.12	64,64,64,64	0
54	MG	2A	3473	1/1	0.79	0.06	51,51,51,51	0
54	MG	2B	3004	1/1	0.79	0.15	77,77,77,77	0
54	MG	1A	3066	1/1	0.79	0.10	64,64,64,64	0
54	MG	1A	3964	1/1	0.79	0.10	68,68,68,68	0
54	MG	2a	1774	1/1	0.79	0.12	66,66,66,66	0
54	MG	1A	3967	1/1	0.79	0.33	81,81,81,81	0
54	MG	1A	3975	1/1	0.79	0.17	52,52,52,52	0
54	MG	1A	3680	1/1	0.79	0.15	66,66,66,66	0
54	MG	1a	1818	1/1	0.79	0.04	69,69,69,69	0
54	MG	1A	3620	1/1	0.79	0.24	40,40,40,40	0
54	MG	1A	3770	1/1	0.79	0.22	34,34,34,34	0
57	ZN	14	501	1/1	0.79	0.25	225,225,225,225	0
54	MG	1a	1843	1/1	0.79	0.10	67,67,67,67	0
54	MG	1a	1859	1/1	0.79	0.13	72,72,72,72	0
54	MG	1a	1659	1/1	0.80	0.11	76,76,76,76	0
54	MG	2A	3463	1/1	0.80	0.15	55,55,55,55	0
54	MG	2A	3577	1/1	0.80	0.08	57,57,57,57	0
54	MG	1A	3891	1/1	0.80	0.17	73,73,73,73	0
54	MG	1A	3529	1/1	0.80	0.13	55,55,55,55	0
54	MG	1a	1832	1/1	0.80	0.11	72,72,72,72	0
54	MG	2A	3692	1/1	0.80	0.10	52,52,52,52	0
54	MG	1A	3577	1/1	0.80	0.31	41,41,41,41	0
54	MG	1a	1839	1/1	0.80	0.07	67,67,67,67	0
54	MG	2A	3712	1/1	0.80	0.18	67,67,67,67	0
54	MG	1A	3360	1/1	0.80	0.14	55,55,55,55	0
54	MG	1a	1685	1/1	0.80	0.11	75,75,75,75	0
54	MG	1A	3203	1/1	0.80	0.11	61,61,61,61	0
54	MG	1A	3583	1/1	0.80	0.19	43,43,43,43	0
54	MG	2a	1735	1/1	0.80	0.10	64,64,64,64	0
54	MG	1A	3589	1/1	0.80	0.14	57,57,57,57	0
54	MG	1A	3957	1/1	0.80	0.11	40,40,40,40	0
54	MG	1A	3416	1/1	0.80	0.27	33,33,33,33	0
54	MG	1A	3426	1/1	0.80	0.21	34,34,34,34	0
54	MG	2B	3013	1/1	0.80	0.07	76,76,76,76	0
54	MG	1A	3855	1/1	0.80	0.12	62,62,62,62	0
54	MG	1a	1764	1/1	0.80	0.13	65,65,65,65	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
54	MG	1A	3643	1/1	0.80	0.26	72,72,72,72	0
54	MG	2A	3380	1/1	0.80	0.15	35,35,35,35	0
54	MG	2A	3540	1/1	0.80	0.12	47,47,47,47	0
54	MG	2A	3001	1/1	0.80	0.11	57,57,57,57	0
54	MG	1A	3519	1/1	0.80	0.08	59,59,59,59	0
54	MG	2A	3068	1/1	0.80	0.10	61,61,61,61	0
54	MG	1A	3595	1/1	0.80	0.18	48,48,48,48	0
54	MG	1a	1785	1/1	0.80	0.15	76,76,76,76	0
54	MG	1A	3027	1/1	0.80	0.15	60,60,60,60	0
54	MG	1A	3882	1/1	0.80	0.23	74,74,74,74	0
54	MG	1A	3344	1/1	0.80	0.18	59,59,59,59	0
54	MG	1A	3573	1/1	0.80	0.22	59,59,59,59	0
54	MG	1A	4005	1/1	0.81	0.09	97,97,97,97	0
54	MG	2a	1675	1/1	0.81	0.20	69,69,69,69	0
54	MG	1q	202	1/1	0.81	0.16	73,73,73,73	0
54	MG	1a	1795	1/1	0.81	0.08	71,71,71,71	0
54	MG	1O	8001	1/1	0.81	0.11	62,62,62,62	0
54	MG	1a	1705	1/1	0.81	0.16	56,56,56,56	0
54	MG	2a	1693	1/1	0.81	0.14	88,88,88,88	0
54	MG	2a	1705	1/1	0.81	0.14	75,75,75,75	0
54	MG	1A	3418	1/1	0.81	0.19	55,55,55,55	0
54	MG	1A	3331	1/1	0.81	0.12	75,75,75,75	0
54	MG	2A	3582	1/1	0.81	0.33	70,70,70,70	0
54	MG	1a	1834	1/1	0.81	0.15	59,59,59,59	0
54	MG	2E	305	1/1	0.81	0.25	65,65,65,65	0
54	MG	2O	202	1/1	0.81	0.12	94,94,94,94	0
54	MG	1A	3067	1/1	0.81	0.13	60,60,60,60	0
54	MG	1A	3502	1/1	0.81	0.17	56,56,56,56	0
54	MG	1A	3903	1/1	0.81	0.13	67,67,67,67	0
54	MG	1A	3795	1/1	0.81	0.09	68,68,68,68	0
54	MG	1A	3697	1/1	0.81	0.21	53,53,53,53	0
54	MG	1a	1768	1/1	0.81	0.10	71,71,71,71	0
54	MG	2A	3534	1/1	0.81	0.63	78,78,78,78	0
54	MG	2a	1770	1/1	0.81	0.07	82,82,82,82	0
54	MG	2a	1618	1/1	0.81	0.09	75,75,75,75	0
54	MG	2A	3207	1/1	0.81	0.09	46,46,46,46	0
54	MG	2A	3214	1/1	0.81	0.27	49,49,49,49	0
54	MG	2a	1785	1/1	0.81	0.10	76,76,76,76	0
54	MG	2a	1631	1/1	0.81	0.11	77,77,77,77	0
54	MG	1A	3481	1/1	0.81	0.18	57,57,57,57	0
54	MG	1D	313	1/1	0.81	0.16	52,52,52,52	0
54	MG	1A	3942	1/1	0.81	0.09	59,59,59,59	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
54	MG	1A	3318	1/1	0.81	0.20	44,44,44,44	0
54	MG	1A	3492	1/1	0.81	0.10	60,60,60,60	0
54	MG	1a	1689	1/1	0.81	0.10	73,73,73,73	0
54	MG	2a	1666	1/1	0.81	0.09	78,78,78,78	0
54	MG	1A	3666	1/1	0.82	0.11	64,64,64,64	0
54	MG	1A	3998	1/1	0.82	0.19	51,51,51,51	0
54	MG	2A	3624	1/1	0.82	0.13	66,66,66,66	0
54	MG	1A	3383	1/1	0.82	0.19	34,34,34,34	0
54	MG	1G	3001	1/1	0.82	0.08	72,72,72,72	0
54	MG	2A	3209	1/1	0.82	0.18	63,63,63,63	0
54	MG	2a	1688	1/1	0.82	0.16	58,58,58,58	0
54	MG	1A	3400	1/1	0.82	0.22	61,61,61,61	0
54	MG	1a	1871	1/1	0.82	0.14	75,75,75,75	0
54	MG	1A	3638	1/1	0.82	0.13	35,35,35,35	0
54	MG	1A	3960	1/1	0.82	0.14	71,71,71,71	0
54	MG	2A	3639	1/1	0.82	0.09	59,59,59,59	0
54	MG	1W	3001	1/1	0.82	0.33	59,59,59,59	0
54	MG	1A	3531	1/1	0.82	0.15	66,66,66,66	0
54	MG	2D	302	1/1	0.82	0.20	52,52,52,52	0
54	MG	2a	1731	1/1	0.82	0.13	73,73,73,73	0
54	MG	2A	3644	1/1	0.82	0.08	58,58,58,58	0
54	MG	1g	203	1/1	0.82	0.19	78,78,78,78	0
54	MG	1a	1813	1/1	0.82	0.12	81,81,81,81	0
54	MG	1a	1815	1/1	0.82	0.12	75,75,75,75	0
54	MG	2A	3661	1/1	0.82	0.11	46,46,46,46	0
54	MG	1a	1732	1/1	0.82	0.10	92,92,92,92	0
54	MG	2a	1603	1/1	0.82	0.45	69,69,69,69	0
54	MG	2A	3058	1/1	0.82	0.21	58,58,58,58	0
54	MG	1A	3112	1/1	0.82	0.25	67,67,67,67	0
54	MG	1A	3549	1/1	0.82	0.11	63,63,63,63	0
54	MG	2A	3675	1/1	0.82	0.05	61,61,61,61	0
54	MG	1a	1603	1/1	0.82	0.14	77,77,77,77	0
54	MG	2a	1620	1/1	0.82	0.11	77,77,77,77	0
54	MG	2a	1783	1/1	0.82	0.06	62,62,62,62	0
54	MG	2a	1623	1/1	0.82	0.17	73,73,73,73	0
54	MG	1A	3415	1/1	0.82	0.17	63,63,63,63	0
54	MG	1A	3010	1/1	0.82	0.13	49,49,49,49	0
54	MG	2A	3163	1/1	0.82	0.46	62,62,62,62	0
54	MG	2A	3514	1/1	0.82	0.11	60,60,60,60	0
54	MG	1A	3657	1/1	0.82	0.26	55,55,55,55	0
54	MG	2A	3608	1/1	0.82	0.08	64,64,64,64	0
54	MG	1A	3756	1/1	0.82	0.17	47,47,47,47	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
54	MG	2A	3614	1/1	0.82	0.14	42,42,42,42	0
54	MG	2A	3363	1/1	0.83	0.10	64,64,64,64	0
54	MG	2A	3662	1/1	0.83	0.06	59,59,59,59	0
54	MG	2a	1691	1/1	0.83	0.14	71,71,71,71	0
54	MG	1A	3768	1/1	0.83	0.17	67,67,67,67	0
54	MG	2A	3508	1/1	0.83	0.18	59,59,59,59	0
54	MG	2A	3667	1/1	0.83	0.15	49,49,49,49	0
54	MG	1G	3003	1/1	0.83	0.11	63,63,63,63	0
54	MG	1A	3293	1/1	0.83	0.12	50,50,50,50	0
54	MG	1A	3690	1/1	0.83	0.18	51,51,51,51	0
54	MG	1A	3937	1/1	0.83	0.07	71,71,71,71	0
54	MG	1a	1797	1/1	0.83	0.07	74,74,74,74	0
54	MG	1a	1874	1/1	0.83	0.11	66,66,66,66	0
54	MG	1A	3987	1/1	0.83	0.14	44,44,44,44	0
54	MG	1a	1804	1/1	0.83	0.09	65,65,65,65	0
54	MG	1B	211	1/1	0.83	0.16	69,69,69,69	0
54	MG	1l	103	1/1	0.83	0.14	60,60,60,60	0
54	MG	1A	3870	1/1	0.83	0.21	71,71,71,71	0
54	MG	2A	3547	1/1	0.83	0.21	63,63,63,63	0
54	MG	1A	3348	1/1	0.83	0.13	44,44,44,44	0
54	MG	2A	3457	1/1	0.83	0.13	62,62,62,62	0
54	MG	1B	223	1/1	0.83	0.08	69,69,69,69	0
54	MG	2a	1644	1/1	0.83	0.18	75,75,75,75	0
54	MG	2A	3728	1/1	0.83	0.12	58,58,58,58	0
54	MG	2A	3247	1/1	0.83	0.19	55,55,55,55	0
54	MG	1B	224	1/1	0.83	0.12	44,44,44,44	0
54	MG	1A	3784	1/1	0.83	0.11	36,36,36,36	0
54	MG	2A	3310	1/1	0.83	0.27	62,62,62,62	0
54	MG	1A	3190	1/1	0.83	0.14	61,61,61,61	0
54	MG	1A	3672	1/1	0.83	0.07	68,68,68,68	0
54	MG	1A	3673	1/1	0.83	0.07	55,55,55,55	0
54	MG	2a	1678	1/1	0.83	0.21	66,66,66,66	0
54	MG	2A	3146	1/1	0.83	0.18	61,61,61,61	0
54	MG	2a	1685	1/1	0.83	0.34	64,64,64,64	0
54	MG	1A	3432	1/1	0.83	0.15	67,67,67,67	0
54	MG	2A	3714	1/1	0.84	0.08	56,56,56,56	0
54	MG	1A	3397	1/1	0.84	0.17	33,33,33,33	0
54	MG	1a	1822	1/1	0.84	0.13	68,68,68,68	0
54	MG	2A	3511	1/1	0.84	0.08	62,62,62,62	0
54	MG	1B	227	1/1	0.84	0.11	76,76,76,76	0
54	MG	1a	1613	1/1	0.84	0.17	71,71,71,71	0
54	MG	1A	3292	1/1	0.84	0.14	58,58,58,58	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
54	MG	2A	3519	1/1	0.84	0.22	60,60,60,60	0
54	MG	1a	1625	1/1	0.84	0.10	53,53,53,53	0
54	MG	2B	3008	1/1	0.84	0.08	66,66,66,66	0
54	MG	2B	3011	1/1	0.84	0.06	61,61,61,61	0
54	MG	2A	3371	1/1	0.84	0.12	70,70,70,70	0
54	MG	2A	3159	1/1	0.84	0.20	46,46,46,46	0
54	MG	1E	301	1/1	0.84	0.32	40,40,40,40	0
54	MG	1A	3912	1/1	0.84	0.12	39,39,39,39	0
54	MG	2a	1714	1/1	0.84	0.09	69,69,69,69	0
54	MG	1A	3601	1/1	0.84	0.25	38,38,38,38	0
54	MG	1a	1777	1/1	0.84	0.11	55,55,55,55	0
54	MG	2a	1724	1/1	0.84	0.14	82,82,82,82	0
54	MG	1A	3925	1/1	0.84	0.07	54,54,54,54	0
54	MG	1A	3261	1/1	0.84	0.13	64,64,64,64	0
54	MG	2A	3202	1/1	0.84	0.16	49,49,49,49	0
54	MG	1A	3969	1/1	0.84	0.24	61,61,61,61	0
54	MG	2A	3430	1/1	0.84	0.13	52,52,52,52	0
54	MG	2a	1745	1/1	0.84	0.08	46,46,46,46	0
54	MG	1A	3933	1/1	0.84	0.17	68,68,68,68	0
54	MG	1A	3319	1/1	0.84	0.15	65,65,65,65	0
54	MG	2A	3446	1/1	0.84	0.07	58,58,58,58	0
54	MG	2A	3212	1/1	0.84	0.12	70,70,70,70	0
54	MG	1A	3459	1/1	0.84	0.11	55,55,55,55	0
54	MG	1a	1696	1/1	0.84	0.20	68,68,68,68	0
54	MG	1B	215	1/1	0.84	0.12	59,59,59,59	0
54	MG	1a	1702	1/1	0.84	0.16	67,67,67,67	0
54	MG	2a	1622	1/1	0.84	0.15	74,74,74,74	0
54	MG	1e	201	1/1	0.84	0.16	65,65,65,65	0
54	MG	1A	3596	1/1	0.84	0.26	47,47,47,47	0
54	MG	1A	3849	1/1	0.84	0.11	53,53,53,53	0
54	MG	1y	204	1/1	0.84	0.29	93,93,93,93	0
54	MG	2A	3257	1/1	0.84	0.15	58,58,58,58	0
54	MG	2a	1636	1/1	0.84	0.11	64,64,64,64	0
54	MG	2A	3260	1/1	0.84	0.12	53,53,53,53	0
54	MG	2A	3696	1/1	0.84	0.08	56,56,56,56	0
55	MPD	2A	3747	8/8	0.84	0.23	37,47,59,61	0
54	MG	1a	1730	1/1	0.84	0.12	62,62,62,62	0
54	MG	1A	3721	1/1	0.84	0.11	64,64,64,64	0
54	MG	2A	3035	1/1	0.84	0.13	67,67,67,67	0
54	MG	1A	3022	1/1	0.85	0.17	46,46,46,46	0
54	MG	2A	3695	1/1	0.85	0.14	57,57,57,57	0
54	MG	2A	3213	1/1	0.85	0.14	60,60,60,60	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
54	MG	2a	1650	1/1	0.85	0.23	74,74,74,74	0
54	MG	2a	1654	1/1	0.85	0.15	60,60,60,60	0
54	MG	1A	3965	1/1	0.85	0.13	63,63,63,63	0
54	MG	2a	1661	1/1	0.85	0.15	74,74,74,74	0
54	MG	2a	1663	1/1	0.85	0.19	67,67,67,67	0
54	MG	1A	3904	1/1	0.85	0.08	51,51,51,51	0
54	MG	1A	3288	1/1	0.85	0.42	57,57,57,57	0
54	MG	1a	1642	1/1	0.85	0.15	70,70,70,70	0
54	MG	1A	3973	1/1	0.85	0.16	44,44,44,44	0
54	MG	2a	1676	1/1	0.85	0.23	62,62,62,62	0
54	MG	1A	3916	1/1	0.85	0.17	68,68,68,68	0
54	MG	1A	3843	1/1	0.85	0.19	53,53,53,53	0
54	MG	1B	229	1/1	0.85	0.12	60,60,60,60	0
54	MG	1A	3090	1/1	0.85	0.24	55,55,55,55	0
54	MG	2a	1687	1/1	0.85	0.08	82,82,82,82	0
54	MG	1A	3407	1/1	0.85	0.19	66,66,66,66	0
54	MG	2B	3003	1/1	0.85	0.21	71,71,71,71	0
54	MG	1A	3739	1/1	0.85	0.09	45,45,45,45	0
54	MG	2A	3302	1/1	0.85	0.15	57,57,57,57	0
54	MG	1A	3212	1/1	0.85	0.18	48,48,48,48	0
54	MG	2A	3034	1/1	0.85	0.16	49,49,49,49	0
54	MG	1a	1812	1/1	0.85	0.10	51,51,51,51	0
54	MG	1A	3439	1/1	0.85	0.14	49,49,49,49	0
54	MG	2A	3329	1/1	0.85	0.18	60,60,60,60	0
54	MG	2a	1719	1/1	0.85	0.10	76,76,76,76	0
54	MG	2a	1720	1/1	0.85	0.09	63,63,63,63	0
54	MG	1a	1814	1/1	0.85	0.06	67,67,67,67	0
54	MG	1A	3939	1/1	0.85	0.11	61,61,61,61	0
54	MG	2A	3529	1/1	0.85	0.10	54,54,54,54	0
54	MG	1A	3353	1/1	0.85	0.13	53,53,53,53	0
54	MG	2D	309	1/1	0.85	0.17	65,65,65,65	0
54	MG	2A	3118	1/1	0.85	0.22	45,45,45,45	0
54	MG	2F	301	1/1	0.85	0.13	44,44,44,44	0
54	MG	1A	3609	1/1	0.85	0.16	54,54,54,54	0
54	MG	2A	3142	1/1	0.85	0.09	47,47,47,47	0
54	MG	2a	1748	1/1	0.85	0.09	75,75,75,75	0
54	MG	1A	4016	1/1	0.85	0.10	62,62,62,62	0
54	MG	1A	3803	1/1	0.85	0.15	50,50,50,50	0
54	MG	1A	3688	1/1	0.85	0.09	80,80,80,80	0
54	MG	1A	3610	1/1	0.85	0.16	35,35,35,35	0
54	MG	2A	3166	1/1	0.85	0.16	61,61,61,61	0
54	MG	2a	1763	1/1	0.85	0.13	51,51,51,51	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
54	MG	2A	3389	1/1	0.85	0.11	56,56,56,56	0
54	MG	1A	4027	1/1	0.85	0.22	55,55,55,55	0
54	MG	1a	1840	1/1	0.85	0.17	58,58,58,58	0
54	MG	2A	3565	1/1	0.85	0.21	57,57,57,57	0
54	MG	1A	4051	1/1	0.85	0.24	52,52,52,52	0
54	MG	1A	3591	1/1	0.85	0.10	55,55,55,55	0
54	MG	2A	3571	1/1	0.85	0.14	44,44,44,44	0
54	MG	1a	1752	1/1	0.85	0.10	73,73,73,73	0
54	MG	1a	1759	1/1	0.85	0.08	65,65,65,65	0
54	MG	2a	1633	1/1	0.85	0.11	69,69,69,69	0
54	MG	1A	3644	1/1	0.85	0.18	48,48,48,48	0
54	MG	1a	1606	1/1	0.85	0.12	63,63,63,63	0
54	MG	2a	1637	1/1	0.85	0.10	92,92,92,92	0
54	MG	2a	1638	1/1	0.85	0.14	62,62,62,62	0
54	MG	2A	3690	1/1	0.85	0.06	63,63,63,63	0
54	MG	1A	3480	1/1	0.86	0.22	28,28,28,28	0
54	MG	1A	3765	1/1	0.86	0.10	71,71,71,71	0
54	MG	1a	1753	1/1	0.86	0.10	62,62,62,62	0
54	MG	1A	3089	1/1	0.86	0.22	47,47,47,47	0
54	MG	2A	3144	1/1	0.86	0.21	53,53,53,53	0
54	MG	1a	1667	1/1	0.86	0.14	63,63,63,63	0
54	MG	2A	3153	1/1	0.86	0.14	48,48,48,48	0
54	MG	1A	3611	1/1	0.86	0.13	54,54,54,54	0
54	MG	2A	3704	1/1	0.86	0.06	48,48,48,48	0
54	MG	2A	3572	1/1	0.86	0.15	52,52,52,52	0
54	MG	1A	3646	1/1	0.86	0.63	81,81,81,81	0
54	MG	1a	1675	1/1	0.86	0.19	70,70,70,70	0
54	MG	2a	1671	1/1	0.86	0.21	70,70,70,70	0
54	MG	1a	1850	1/1	0.86	0.11	94,94,94,94	0
54	MG	1A	3516	1/1	0.86	0.15	60,60,60,60	0
54	MG	1a	1863	1/1	0.86	0.08	64,64,64,64	0
54	MG	1a	1677	1/1	0.86	0.17	63,63,63,63	0
54	MG	2A	3189	1/1	0.86	0.22	57,57,57,57	0
54	MG	1a	1866	1/1	0.86	0.10	69,69,69,69	0
54	MG	2A	3191	1/1	0.86	0.10	53,53,53,53	0
54	MG	1a	1784	1/1	0.86	0.09	66,66,66,66	0
54	MG	2B	3005	1/1	0.86	0.22	60,60,60,60	0
54	MG	2B	3006	1/1	0.86	0.08	72,72,72,72	0
54	MG	2A	3204	1/1	0.86	0.19	66,66,66,66	0
54	MG	2A	3458	1/1	0.86	0.11	57,57,57,57	0
54	MG	2a	1702	1/1	0.86	0.10	65,65,65,65	0
54	MG	1a	1680	1/1	0.86	0.09	69,69,69,69	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
54	MG	1A	3841	1/1	0.86	0.17	49,49,49,49	0
54	MG	1A	3370	1/1	0.86	0.06	54,54,54,54	0
54	MG	2B	3014	1/1	0.86	0.12	65,65,65,65	0
54	MG	1a	1789	1/1	0.86	0.08	67,67,67,67	0
54	MG	1a	1790	1/1	0.86	0.14	52,52,52,52	0
54	MG	1A	3921	1/1	0.86	0.16	61,61,61,61	0
54	MG	1a	1878	1/1	0.86	0.13	66,66,66,66	0
54	MG	1A	3035	1/1	0.86	0.26	57,57,57,57	0
54	MG	1a	1794	1/1	0.86	0.10	58,58,58,58	0
54	MG	2A	3235	1/1	0.86	0.36	48,48,48,48	0
54	MG	1A	3527	1/1	0.86	0.15	32,32,32,32	0
54	MG	2a	1740	1/1	0.86	0.10	80,80,80,80	0
54	MG	2G	3001	1/1	0.86	0.07	76,76,76,76	0
54	MG	2G	3002	1/1	0.86	0.13	79,79,79,79	0
54	MG	1A	3414	1/1	0.86	0.15	33,33,33,33	0
54	MG	2P	201	1/1	0.86	0.11	55,55,55,55	0
54	MG	1n	502	1/1	0.86	0.10	46,46,46,46	0
54	MG	1A	3789	1/1	0.86	0.13	58,58,58,58	0
54	MG	2A	3252	1/1	0.86	0.17	54,54,54,54	0
54	MG	1a	1803	1/1	0.86	0.14	87,87,87,87	0
54	MG	1A	3002	1/1	0.86	0.12	54,54,54,54	0
54	MG	2A	3266	1/1	0.86	0.17	55,55,55,55	0
54	MG	2A	3650	1/1	0.86	0.06	61,61,61,61	0
54	MG	2A	3275	1/1	0.86	0.10	58,58,58,58	0
54	MG	2a	1617	1/1	0.86	0.12	65,65,65,65	0
54	MG	2A	3521	1/1	0.86	0.45	57,57,57,57	0
54	MG	1a	1719	1/1	0.86	0.11	94,94,94,94	0
54	MG	1A	3282	1/1	0.86	0.15	60,60,60,60	0
54	MG	1A	3284	1/1	0.86	0.12	59,59,59,59	0
54	MG	2A	3040	1/1	0.86	0.18	58,58,58,58	0
54	MG	2A	3055	1/1	0.86	0.25	54,54,54,54	0
54	MG	1A	3873	1/1	0.86	0.14	48,48,48,48	0
54	MG	2A	3060	1/1	0.86	0.13	42,42,42,42	0
54	MG	2A	3336	1/1	0.86	0.11	55,55,55,55	0
55	MPD	2B	3020	8/8	0.86	0.17	47,70,77,79	0
54	MG	1A	3949	1/1	0.86	0.14	69,69,69,69	0
54	MG	2A	3548	1/1	0.86	0.08	55,55,55,55	0
54	MG	1A	3142	1/1	0.86	0.15	51,51,51,51	0
54	MG	11	102	1/1	0.87	0.08	49,49,49,49	0
54	MG	2A	3306	1/1	0.87	0.12	56,56,56,56	0
54	MG	1A	4076	1/1	0.87	0.20	57,57,57,57	0
54	MG	2A	3114	1/1	0.87	0.10	47,47,47,47	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
54	MG	2A	3524	1/1	0.87	0.12	64,64,64,64	0
54	MG	2A	3320	1/1	0.87	0.13	47,47,47,47	0
54	MG	1A	3230	1/1	0.87	0.18	44,44,44,44	0
54	MG	1a	1837	1/1	0.87	0.07	74,74,74,74	0
54	MG	2A	3136	1/1	0.87	0.10	64,64,64,64	0
54	MG	2a	1658	1/1	0.87	0.14	60,60,60,60	0
54	MG	2a	1660	1/1	0.87	0.12	72,72,72,72	0
54	MG	2A	3333	1/1	0.87	0.15	38,38,38,38	0
54	MG	2A	3537	1/1	0.87	0.11	55,55,55,55	0
54	MG	2A	3538	1/1	0.87	0.12	49,49,49,49	0
54	MG	1A	3581	1/1	0.87	0.10	67,67,67,67	0
54	MG	2A	3340	1/1	0.87	0.10	54,54,54,54	0
54	MG	2A	3345	1/1	0.87	0.13	35,35,35,35	0
54	MG	2A	3346	1/1	0.87	0.14	55,55,55,55	0
54	MG	1a	1605	1/1	0.87	0.13	61,61,61,61	0
54	MG	1A	3451	1/1	0.87	0.10	48,48,48,48	0
54	MG	2A	3152	1/1	0.87	0.20	61,61,61,61	0
54	MG	2A	3366	1/1	0.87	0.07	53,53,53,53	0
54	MG	1A	3454	1/1	0.87	0.23	31,31,31,31	0
54	MG	1B	216	1/1	0.87	0.35	58,58,58,58	0
54	MG	2A	3372	1/1	0.87	0.17	51,51,51,51	0
54	MG	1a	1856	1/1	0.87	0.06	58,58,58,58	0
54	MG	2A	3751	1/1	0.87	0.22	48,48,48,48	0
54	MG	1a	1621	1/1	0.87	0.16	48,48,48,48	0
54	MG	2A	3164	1/1	0.87	0.37	58,58,58,58	0
54	MG	1a	1622	1/1	0.87	0.07	47,47,47,47	0
54	MG	1A	3752	1/1	0.87	0.25	57,57,57,57	0
54	MG	1A	3814	1/1	0.87	0.12	60,60,60,60	0
54	MG	1A	3335	1/1	0.87	0.16	37,37,37,37	0
54	MG	1A	3339	1/1	0.87	0.11	54,54,54,54	0
54	MG	2A	3416	1/1	0.87	0.18	61,61,61,61	0
54	MG	1A	3134	1/1	0.87	0.20	45,45,45,45	0
54	MG	2A	3422	1/1	0.87	0.09	56,56,56,56	0
54	MG	2A	3587	1/1	0.87	0.10	52,52,52,52	0
54	MG	1A	3678	1/1	0.87	0.06	62,62,62,62	0
54	MG	2A	3428	1/1	0.87	0.09	57,57,57,57	0
54	MG	2A	3197	1/1	0.87	0.14	47,47,47,47	0
54	MG	1A	3679	1/1	0.87	0.04	69,69,69,69	0
54	MG	2A	3434	1/1	0.87	0.09	56,56,56,56	0
54	MG	1a	1671	1/1	0.87	0.28	63,63,63,63	0
54	MG	1A	3926	1/1	0.87	0.12	65,65,65,65	0
54	MG	1A	3150	1/1	0.87	0.15	58,58,58,58	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
54	MG	1F	305	1/1	0.87	0.30	66,66,66,66	0
54	MG	1A	3846	1/1	0.87	0.13	47,47,47,47	0
54	MG	1A	3219	1/1	0.87	0.14	65,65,65,65	0
54	MG	1a	1684	1/1	0.87	0.34	73,73,73,73	0
54	MG	1A	3627	1/1	0.87	0.23	42,42,42,42	0
54	MG	1A	3321	1/1	0.87	0.12	50,50,50,50	0
54	MG	2a	1757	1/1	0.87	0.09	49,49,49,49	0
54	MG	2A	3469	1/1	0.87	0.22	62,62,62,62	0
54	MG	1A	3434	1/1	0.87	0.14	72,72,72,72	0
54	MG	2A	3475	1/1	0.87	0.09	62,62,62,62	0
54	MG	1A	3598	1/1	0.87	0.14	35,35,35,35	0
54	MG	1A	3703	1/1	0.87	0.10	41,41,41,41	0
54	MG	2A	3483	1/1	0.87	0.17	37,37,37,37	0
54	MG	1V	203	1/1	0.87	0.12	63,63,63,63	0
54	MG	2A	3486	1/1	0.87	0.04	63,63,63,63	0
54	MG	1A	3365	1/1	0.87	0.14	69,69,69,69	0
54	MG	1a	1712	1/1	0.87	0.06	50,50,50,50	0
54	MG	2a	1791	1/1	0.87	0.07	61,61,61,61	0
54	MG	2A	3050	1/1	0.87	0.13	54,54,54,54	0
54	MG	1W	3002	1/1	0.87	0.16	52,52,52,52	0
54	MG	1A	3324	1/1	0.87	0.19	61,61,61,61	0
54	MG	2A	3059	1/1	0.87	0.15	45,45,45,45	0
54	MG	1a	1820	1/1	0.87	0.10	76,76,76,76	0
54	MG	2A	3664	1/1	0.87	0.05	61,61,61,61	0
54	MG	1A	3607	1/1	0.87	0.23	52,52,52,52	0
54	MG	1A	3192	1/1	0.88	0.15	68,68,68,68	0
54	MG	1A	3835	1/1	0.88	0.13	47,47,47,47	0
54	MG	1A	3958	1/1	0.88	0.08	63,63,63,63	0
54	MG	2a	1606	1/1	0.88	0.19	57,57,57,57	0
54	MG	2a	1608	1/1	0.88	0.17	69,69,69,69	0
54	MG	2A	3618	1/1	0.88	0.18	37,37,37,37	0
54	MG	2A	3444	1/1	0.88	0.09	61,61,61,61	0
54	MG	1a	1849	1/1	0.88	0.13	66,66,66,66	0
54	MG	1A	3441	1/1	0.88	0.18	64,64,64,64	0
54	MG	1A	3285	1/1	0.88	0.17	53,53,53,53	0
54	MG	1A	3632	1/1	0.88	0.14	56,56,56,56	0
54	MG	1A	3584	1/1	0.88	0.14	47,47,47,47	0
54	MG	2A	3630	1/1	0.88	0.10	52,52,52,52	0
54	MG	1A	3737	1/1	0.88	0.12	57,57,57,57	0
54	MG	1A	3399	1/1	0.88	0.15	54,54,54,54	0
54	MG	2A	3467	1/1	0.88	0.15	67,67,67,67	0
54	MG	1A	3033	1/1	0.88	0.23	44,44,44,44	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
54	MG	1A	3402	1/1	0.88	0.15	73,73,73,73	0
54	MG	1A	3642	1/1	0.88	0.27	39,39,39,39	0
54	MG	2A	3474	1/1	0.88	0.15	65,65,65,65	0
54	MG	2A	3218	1/1	0.88	0.19	60,60,60,60	0
54	MG	2A	3476	1/1	0.88	0.08	55,55,55,55	0
54	MG	1A	3405	1/1	0.88	0.25	65,65,65,65	0
54	MG	2A	3226	1/1	0.88	0.20	69,69,69,69	0
54	MG	1a	1758	1/1	0.88	0.23	73,73,73,73	0
54	MG	1A	3458	1/1	0.88	0.14	48,48,48,48	0
54	MG	2a	1655	1/1	0.88	0.16	69,69,69,69	0
54	MG	1A	3199	1/1	0.88	0.19	70,70,70,70	0
54	MG	2A	3487	1/1	0.88	0.15	73,73,73,73	0
54	MG	2A	3236	1/1	0.88	0.11	49,49,49,49	0
54	MG	1A	3761	1/1	0.88	0.14	58,58,58,58	0
54	MG	2A	3501	1/1	0.88	0.17	72,72,72,72	0
54	MG	1A	3883	1/1	0.88	0.17	38,38,38,38	0
54	MG	2A	3245	1/1	0.88	0.13	56,56,56,56	0
54	MG	1a	1772	1/1	0.88	0.12	77,77,77,77	0
54	MG	2a	1670	1/1	0.88	0.14	65,65,65,65	0
54	MG	1A	3051	1/1	0.88	0.39	48,48,48,48	0
54	MG	18	101	1/1	0.88	0.05	60,60,60,60	0
54	MG	1a	1602	1/1	0.88	0.09	73,73,73,73	0
54	MG	1q	201	1/1	0.88	0.24	55,55,55,55	0
54	MG	2A	3687	1/1	0.88	0.12	39,39,39,39	0
54	MG	1A	3479	1/1	0.88	0.21	42,42,42,42	0
54	MG	2A	3515	1/1	0.88	0.22	34,34,34,34	0
54	MG	2A	3267	1/1	0.88	0.07	60,60,60,60	0
54	MG	2A	3693	1/1	0.88	0.11	57,57,57,57	0
54	MG	1A	3109	1/1	0.88	0.18	45,45,45,45	0
54	MG	1A	3900	1/1	0.88	0.14	29,29,29,29	0
54	MG	1A	3662	1/1	0.88	0.07	48,48,48,48	0
54	MG	1A	3060	1/1	0.88	0.16	49,49,49,49	0
54	MG	2a	1696	1/1	0.88	0.11	73,73,73,73	0
54	MG	2A	3707	1/1	0.88	0.10	39,39,39,39	0
54	MG	1A	3669	1/1	0.88	0.06	46,46,46,46	0
54	MG	1A	4023	1/1	0.88	0.09	60,60,60,60	0
54	MG	2a	1711	1/1	0.88	0.08	79,79,79,79	0
54	MG	2A	3042	1/1	0.88	0.19	47,47,47,47	0
54	MG	2A	3719	1/1	0.88	0.11	56,56,56,56	0
54	MG	2a	1717	1/1	0.88	0.06	77,77,77,77	0
54	MG	1A	3304	1/1	0.88	0.26	62,62,62,62	0
54	MG	2A	3722	1/1	0.88	0.17	57,57,57,57	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
54	MG	2A	3723	1/1	0.88	0.30	44,44,44,44	0
54	MG	1A	3560	1/1	0.88	0.12	57,57,57,57	0
54	MG	1A	3674	1/1	0.88	0.19	58,58,58,58	0
54	MG	1A	3608	1/1	0.88	0.17	37,37,37,37	0
54	MG	2A	3730	1/1	0.88	0.17	56,56,56,56	0
54	MG	1a	1800	1/1	0.88	0.19	70,70,70,70	0
54	MG	2A	3062	1/1	0.88	0.17	53,53,53,53	0
54	MG	2A	3066	1/1	0.88	0.08	45,45,45,45	0
54	MG	1A	3490	1/1	0.88	0.14	66,66,66,66	0
54	MG	2A	3347	1/1	0.88	0.13	34,34,34,34	0
54	MG	1a	1665	1/1	0.88	0.08	67,67,67,67	0
54	MG	2A	3358	1/1	0.88	0.11	69,69,69,69	0
54	MG	1B	203	1/1	0.88	0.09	70,70,70,70	0
54	MG	1A	3225	1/1	0.88	0.13	49,49,49,49	0
54	MG	2A	3568	1/1	0.88	0.20	42,42,42,42	0
54	MG	1A	3683	1/1	0.88	0.09	57,57,57,57	0
54	MG	1A	3930	1/1	0.88	0.16	60,60,60,60	0
54	MG	2a	1759	1/1	0.88	0.09	75,75,75,75	0
54	MG	1A	3166	1/1	0.88	0.24	61,61,61,61	0
54	MG	1A	3935	1/1	0.88	0.12	53,53,53,53	0
54	MG	1B	219	1/1	0.88	0.18	44,44,44,44	0
54	MG	2a	1772	1/1	0.88	0.12	58,58,58,58	0
54	MG	1A	3428	1/1	0.88	0.11	48,48,48,48	0
54	MG	1a	1821	1/1	0.88	0.12	72,72,72,72	0
54	MG	2a	1779	1/1	0.88	0.08	78,78,78,78	0
54	MG	1A	3689	1/1	0.88	0.09	71,71,71,71	0
54	MG	2D	308	1/1	0.88	0.12	31,31,31,31	0
54	MG	2A	3157	1/1	0.88	0.74	68,68,68,68	0
54	MG	1a	1823	1/1	0.88	0.11	75,75,75,75	0
54	MG	1a	1830	1/1	0.88	0.28	84,84,84,84	0
54	MG	1A	3115	1/1	0.88	0.13	46,46,46,46	0
54	MG	1B	225	1/1	0.88	0.21	68,68,68,68	0
55	MPD	1T	8004	8/8	0.88	0.16	56,61,69,80	0
54	MG	1A	3273	1/1	0.88	0.12	55,55,55,55	0
54	MG	1A	3695	1/1	0.88	0.11	51,51,51,51	0
54	MG	2A	3172	1/1	0.88	0.12	61,61,61,61	0
54	MG	1A	3129	1/1	0.88	0.14	49,49,49,49	0
54	MG	28	8001	1/1	0.88	0.12	66,66,66,66	0
54	MG	2A	3182	1/1	0.88	0.13	49,49,49,49	0
57	ZN	29	501	1/1	0.88	0.22	131,131,131,131	0
54	MG	2A	3073	1/1	0.89	0.18	49,49,49,49	0
54	MG	2A	3678	1/1	0.89	0.07	54,54,54,54	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
54	MG	1A	3974	1/1	0.89	0.16	75,75,75,75	0
54	MG	2A	3314	1/1	0.89	0.09	38,38,38,38	0
54	MG	1A	3548	1/1	0.89	0.11	57,57,57,57	0
54	MG	2A	3083	1/1	0.89	0.08	69,69,69,69	0
54	MG	2A	3094	1/1	0.89	0.20	40,40,40,40	0
54	MG	1A	3684	1/1	0.89	0.19	39,39,39,39	0
54	MG	1A	3102	1/1	0.89	0.14	48,48,48,48	0
54	MG	1A	3213	1/1	0.89	0.25	63,63,63,63	0
54	MG	2A	3527	1/1	0.89	0.07	66,66,66,66	0
54	MG	2A	3132	1/1	0.89	0.09	60,60,60,60	0
54	MG	1A	3635	1/1	0.89	0.08	59,59,59,59	0
54	MG	1T	8003	1/1	0.89	0.10	72,72,72,72	0
54	MG	2A	3143	1/1	0.89	0.09	40,40,40,40	0
54	MG	2A	3700	1/1	0.89	0.10	49,49,49,49	0
54	MG	2A	3348	1/1	0.89	0.10	62,62,62,62	0
54	MG	1a	1725	1/1	0.89	0.10	67,67,67,67	0
54	MG	2a	1672	1/1	0.89	0.12	73,73,73,73	0
54	MG	2a	1673	1/1	0.89	0.11	68,68,68,68	0
54	MG	1A	3555	1/1	0.89	0.14	53,53,53,53	0
54	MG	1a	1731	1/1	0.89	0.11	54,54,54,54	0
54	MG	1A	3995	1/1	0.89	0.16	44,44,44,44	0
54	MG	1A	3997	1/1	0.89	0.19	58,58,58,58	0
54	MG	1A	3557	1/1	0.89	0.08	61,61,61,61	0
54	MG	1A	3694	1/1	0.89	0.22	69,69,69,69	0
54	MG	1A	3905	1/1	0.89	0.13	55,55,55,55	0
54	MG	2A	3725	1/1	0.89	0.14	61,61,61,61	0
54	MG	1A	3083	1/1	0.89	0.13	38,38,38,38	0
54	MG	1A	3224	1/1	0.89	0.09	69,69,69,69	0
54	MG	2A	3381	1/1	0.89	0.12	39,39,39,39	0
54	MG	1a	1756	1/1	0.89	0.15	57,57,57,57	0
54	MG	1A	3563	1/1	0.89	0.23	53,53,53,53	0
54	MG	1A	3565	1/1	0.89	0.15	50,50,50,50	0
54	MG	1a	1762	1/1	0.89	0.09	80,80,80,80	0
54	MG	1A	3012	1/1	0.89	0.14	38,38,38,38	0
54	MG	2A	3395	1/1	0.89	0.06	51,51,51,51	0
54	MG	1A	3716	1/1	0.89	0.28	48,48,48,48	0
54	MG	2A	3412	1/1	0.89	0.05	60,60,60,60	0
54	MG	2A	3413	1/1	0.89	0.21	59,59,59,59	0
54	MG	1A	4026	1/1	0.89	0.11	46,46,46,46	0
54	MG	1A	3718	1/1	0.89	0.19	47,47,47,47	0
54	MG	1A	3929	1/1	0.89	0.08	52,52,52,52	0
54	MG	1A	3647	1/1	0.89	0.08	49,49,49,49	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
54	MG	2a	1725	1/1	0.89	0.06	64,64,64,64	0
54	MG	2A	3427	1/1	0.89	0.07	51,51,51,51	0
54	MG	1a	1778	1/1	0.89	0.10	67,67,67,67	0
54	MG	2a	1733	1/1	0.89	0.19	83,83,83,83	0
54	MG	1a	1780	1/1	0.89	0.14	53,53,53,53	0
54	MG	1a	1782	1/1	0.89	0.12	75,75,75,75	0
54	MG	2A	3433	1/1	0.89	0.11	32,32,32,32	0
54	MG	1A	3603	1/1	0.89	0.04	53,53,53,53	0
54	MG	1A	3725	1/1	0.89	0.14	51,51,51,51	0
54	MG	1A	3731	1/1	0.89	0.16	38,38,38,38	0
54	MG	1A	3653	1/1	0.89	0.11	40,40,40,40	0
54	MG	1a	1644	1/1	0.89	0.08	57,57,57,57	0
54	MG	1a	1645	1/1	0.89	0.27	61,61,61,61	0
54	MG	1r	3001	1/1	0.89	0.14	65,65,65,65	0
54	MG	2A	3230	1/1	0.89	0.14	62,62,62,62	0
54	MG	1A	3195	1/1	0.89	0.15	47,47,47,47	0
54	MG	2P	202	1/1	0.89	0.10	55,55,55,55	0
54	MG	1A	3305	1/1	0.89	0.17	54,54,54,54	0
54	MG	2A	3014	1/1	0.89	0.14	53,53,53,53	0
54	MG	1A	3014	1/1	0.89	0.14	58,58,58,58	0
54	MG	1A	3847	1/1	0.89	0.13	59,59,59,59	0
54	MG	2A	3241	1/1	0.89	0.09	48,48,48,48	0
54	MG	1A	3314	1/1	0.89	0.14	73,73,73,73	0
54	MG	2A	3037	1/1	0.89	0.29	52,52,52,52	0
54	MG	1A	3753	1/1	0.89	0.13	57,57,57,57	0
54	MG	1A	3465	1/1	0.89	0.08	59,59,59,59	0
54	MG	1A	3315	1/1	0.89	0.17	34,34,34,34	0
54	MG	1A	3154	1/1	0.89	0.12	67,67,67,67	0
54	MG	1A	3863	1/1	0.89	0.08	51,51,51,51	0
54	MG	1A	3278	1/1	0.89	0.13	56,56,56,56	0
54	MG	1A	3073	1/1	0.89	0.12	38,38,38,38	0
54	MG	2A	3273	1/1	0.89	0.06	44,44,44,44	0
54	MG	2j	8001	1/1	0.89	0.11	82,82,82,82	0
54	MG	2l	3001	1/1	0.89	0.24	64,64,64,64	0
54	MG	2A	3492	1/1	0.89	0.18	57,57,57,57	0
54	MG	2A	3061	1/1	0.89	0.16	50,50,50,50	0
54	MG	2A	3497	1/1	0.89	0.09	47,47,47,47	0
54	MG	2A	3277	1/1	0.89	0.14	58,58,58,58	0
54	MG	1A	3205	1/1	0.89	0.30	57,57,57,57	0
54	MG	2A	3296	1/1	0.89	0.14	42,42,42,42	0
54	MG	1A	3877	1/1	0.89	0.20	40,40,40,40	0
54	MG	1A	3206	1/1	0.89	0.32	65,65,65,65	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
54	MG	2a	1616	1/1	0.90	0.10	48,48,48,48	0
54	MG	1a	1653	1/1	0.90	0.15	64,64,64,64	0
54	MG	2A	3637	1/1	0.90	0.12	49,49,49,49	0
54	MG	1A	3961	1/1	0.90	0.09	45,45,45,45	0
54	MG	1A	3279	1/1	0.90	0.31	69,69,69,69	0
54	MG	2A	3026	1/1	0.90	0.14	45,45,45,45	0
54	MG	1A	3963	1/1	0.90	0.14	67,67,67,67	0
54	MG	1a	1666	1/1	0.90	0.08	53,53,53,53	0
54	MG	1A	3670	1/1	0.90	0.05	64,64,64,64	0
54	MG	2A	3038	1/1	0.90	0.11	53,53,53,53	0
54	MG	2A	3651	1/1	0.90	0.06	66,66,66,66	0
54	MG	1A	3501	1/1	0.90	0.09	69,69,69,69	0
54	MG	2A	3041	1/1	0.90	0.13	50,50,50,50	0
54	MG	1A	3419	1/1	0.90	0.25	49,49,49,49	0
54	MG	2A	3256	1/1	0.90	0.19	61,61,61,61	0
54	MG	2A	3049	1/1	0.90	0.11	50,50,50,50	0
54	MG	2A	3258	1/1	0.90	0.28	44,44,44,44	0
54	MG	1A	3724	1/1	0.90	0.06	66,66,66,66	0
54	MG	2A	3490	1/1	0.90	0.16	66,66,66,66	0
54	MG	1D	312	1/1	0.90	0.11	54,54,54,54	0
54	MG	1A	3898	1/1	0.90	0.17	50,50,50,50	0
54	MG	2A	3674	1/1	0.90	0.18	25,25,25,25	0
54	MG	1A	3346	1/1	0.90	0.14	35,35,35,35	0
54	MG	2A	3498	1/1	0.90	0.15	58,58,58,58	0
54	MG	1A	3802	1/1	0.90	0.09	47,47,47,47	0
54	MG	1a	1807	1/1	0.90	0.06	73,73,73,73	0
54	MG	1a	1681	1/1	0.90	0.15	61,61,61,61	0
54	MG	2a	1665	1/1	0.90	0.17	66,66,66,66	0
54	MG	1A	3983	1/1	0.90	0.15	74,74,74,74	0
54	MG	2A	3300	1/1	0.90	0.11	55,55,55,55	0
54	MG	1A	3561	1/1	0.90	0.08	62,62,62,62	0
54	MG	1A	3058	1/1	0.90	0.21	49,49,49,49	0
54	MG	2A	3689	1/1	0.90	0.05	45,45,45,45	0
54	MG	2A	3080	1/1	0.90	0.07	50,50,50,50	0
54	MG	1A	3429	1/1	0.90	0.20	57,57,57,57	0
54	MG	1A	3320	1/1	0.90	0.22	33,33,33,33	0
54	MG	2A	3317	1/1	0.90	0.10	37,37,37,37	0
54	MG	1A	3471	1/1	0.90	0.19	29,29,29,29	0
54	MG	1H	8001	1/1	0.90	0.19	62,62,62,62	0
54	MG	2A	3097	1/1	0.90	0.09	57,57,57,57	0
54	MG	2A	3702	1/1	0.90	0.16	55,55,55,55	0
54	MG	2A	3328	1/1	0.90	0.25	36,36,36,36	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
54	MG	2A	3706	1/1	0.90	0.13	51,51,51,51	0
54	MG	2A	3105	1/1	0.90	0.19	55,55,55,55	0
54	MG	2A	3113	1/1	0.90	0.26	57,57,57,57	0
54	MG	1A	3750	1/1	0.90	0.25	33,33,33,33	0
54	MG	2A	3116	1/1	0.90	0.11	65,65,65,65	0
54	MG	2A	3718	1/1	0.90	0.18	67,67,67,67	0
54	MG	1P	202	1/1	0.90	0.10	73,73,73,73	0
54	MG	2A	3124	1/1	0.90	0.16	66,66,66,66	0
54	MG	1A	3922	1/1	0.90	0.20	30,30,30,30	0
54	MG	2a	1713	1/1	0.90	0.09	61,61,61,61	0
54	MG	1T	8002	1/1	0.90	0.10	61,61,61,61	0
54	MG	2A	3133	1/1	0.90	0.45	57,57,57,57	0
54	MG	2A	3350	1/1	0.90	0.11	43,43,43,43	0
54	MG	1a	1720	1/1	0.90	0.10	65,65,65,65	0
54	MG	1A	3139	1/1	0.90	0.11	45,45,45,45	0
54	MG	1A	3254	1/1	0.90	0.17	53,53,53,53	0
54	MG	1A	3437	1/1	0.90	0.12	41,41,41,41	0
54	MG	2A	3745	1/1	0.90	0.27	67,67,67,67	0
54	MG	2A	3557	1/1	0.90	0.06	52,52,52,52	0
54	MG	2A	3758	1/1	0.90	0.11	52,52,52,52	0
54	MG	1A	3484	1/1	0.90	0.14	41,41,41,41	0
54	MG	1a	1738	1/1	0.90	0.12	64,64,64,64	0
54	MG	1A	3328	1/1	0.90	0.28	19,19,19,19	0
54	MG	10	102	1/1	0.90	0.13	51,51,51,51	0
54	MG	1A	3062	1/1	0.90	0.27	46,46,46,46	0
54	MG	1a	1851	1/1	0.90	0.06	68,68,68,68	0
54	MG	1A	3932	1/1	0.90	0.07	55,55,55,55	0
54	MG	2B	3010	1/1	0.90	0.17	80,80,80,80	0
54	MG	1A	3124	1/1	0.90	0.14	45,45,45,45	0
54	MG	1A	3494	1/1	0.90	0.18	41,41,41,41	0
54	MG	2A	3170	1/1	0.90	0.10	59,59,59,59	0
54	MG	1A	3850	1/1	0.90	0.13	33,33,33,33	0
54	MG	1A	3699	1/1	0.90	0.14	41,41,41,41	0
54	MG	2a	1756	1/1	0.90	0.07	57,57,57,57	0
54	MG	2A	3400	1/1	0.90	0.18	40,40,40,40	0
54	MG	1A	3065	1/1	0.90	0.09	39,39,39,39	0
54	MG	2A	3180	1/1	0.90	0.16	49,49,49,49	0
54	MG	2a	1767	1/1	0.90	0.07	70,70,70,70	0
54	MG	2D	304	1/1	0.90	0.16	36,36,36,36	0
54	MG	1a	1760	1/1	0.90	0.10	63,63,63,63	0
54	MG	1a	1761	1/1	0.90	0.16	64,64,64,64	0
54	MG	1A	3704	1/1	0.90	0.16	58,58,58,58	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
54	MG	1A	3771	1/1	0.90	0.13	44,44,44,44	0
54	MG	1A	3705	1/1	0.90	0.19	67,67,67,67	0
54	MG	1B	206	1/1	0.90	0.10	51,51,51,51	0
54	MG	2A	3607	1/1	0.90	0.10	67,67,67,67	0
54	MG	1A	3585	1/1	0.90	0.15	54,54,54,54	0
54	MG	2a	1787	1/1	0.90	0.18	82,82,82,82	0
54	MG	1a	1881	1/1	0.90	0.07	68,68,68,68	0
54	MG	1A	3779	1/1	0.90	0.20	29,29,29,29	0
54	MG	1a	1775	1/1	0.90	0.15	59,59,59,59	0
54	MG	2R	8001	1/1	0.90	0.19	52,52,52,52	0
54	MG	2f	3001	1/1	0.90	0.12	53,53,53,53	0
54	MG	1B	214	1/1	0.90	0.15	42,42,42,42	0
54	MG	1A	3781	1/1	0.90	0.08	48,48,48,48	0
54	MG	1h	3002	1/1	0.90	0.18	58,58,58,58	0
54	MG	1a	1637	1/1	0.90	0.26	68,68,68,68	0
54	MG	1A	3875	1/1	0.90	0.08	50,50,50,50	0
54	MG	2A	3219	1/1	0.90	0.29	62,62,62,62	0
54	MG	1A	3341	1/1	0.90	0.12	46,46,46,46	0
54	MG	1B	218	1/1	0.90	0.09	48,48,48,48	0
54	MG	2A	3631	1/1	0.90	0.04	64,64,64,64	0
54	MG	1a	1649	1/1	0.90	0.19	58,58,58,58	0
54	MG	1A	4030	1/1	0.91	0.41	53,53,53,53	0
54	MG	2A	3183	1/1	0.91	0.23	66,66,66,66	0
54	MG	2A	3419	1/1	0.91	0.12	54,54,54,54	0
54	MG	2A	3186	1/1	0.91	0.19	53,53,53,53	0
54	MG	1A	3408	1/1	0.91	0.19	38,38,38,38	0
54	MG	1A	3191	1/1	0.91	0.20	55,55,55,55	0
54	MG	1A	3110	1/1	0.91	0.23	43,43,43,43	0
54	MG	1a	1607	1/1	0.91	0.19	54,54,54,54	0
54	MG	2A	3192	1/1	0.91	0.10	44,44,44,44	0
54	MG	1a	1609	1/1	0.91	0.11	57,57,57,57	0
54	MG	1f	8001	1/1	0.91	0.14	52,52,52,52	0
54	MG	1A	3938	1/1	0.91	0.15	56,56,56,56	0
54	MG	1A	3537	1/1	0.91	0.17	31,31,31,31	0
54	MG	1a	1617	1/1	0.91	0.10	50,50,50,50	0
54	MG	2A	3454	1/1	0.91	0.05	58,58,58,58	0
54	MG	2A	3208	1/1	0.91	0.24	48,48,48,48	0
54	MG	1a	1620	1/1	0.91	0.13	48,48,48,48	0
54	MG	1A	3631	1/1	0.91	0.18	74,74,74,74	0
54	MG	1A	3944	1/1	0.91	0.14	24,24,24,24	0
54	MG	1y	202	1/1	0.91	0.08	59,59,59,59	0
54	MG	2A	3216	1/1	0.91	0.06	64,64,64,64	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
54	MG	1B	213	1/1	0.91	0.15	55,55,55,55	0
54	MG	1A	3542	1/1	0.91	0.19	49,49,49,49	0
54	MG	2a	1648	1/1	0.91	0.29	76,76,76,76	0
54	MG	2A	3002	1/1	0.91	0.19	38,38,38,38	0
54	MG	2A	3470	1/1	0.91	0.12	50,50,50,50	0
54	MG	1A	3079	1/1	0.91	0.19	40,40,40,40	0
54	MG	2A	3019	1/1	0.91	0.33	46,46,46,46	0
54	MG	2A	3666	1/1	0.91	0.15	54,54,54,54	0
54	MG	1A	3687	1/1	0.91	0.11	61,61,61,61	0
54	MG	2a	1659	1/1	0.91	0.24	75,75,75,75	0
54	MG	2A	3024	1/1	0.91	0.23	49,49,49,49	0
54	MG	1A	3081	1/1	0.91	0.30	46,46,46,46	0
54	MG	1A	3636	1/1	0.91	0.13	37,37,37,37	0
54	MG	1A	3495	1/1	0.91	0.21	45,45,45,45	0
54	MG	1A	3869	1/1	0.91	0.08	50,50,50,50	0
54	MG	1A	3251	1/1	0.91	0.12	52,52,52,52	0
54	MG	2A	3039	1/1	0.91	0.18	55,55,55,55	0
54	MG	1a	1660	1/1	0.91	0.11	69,69,69,69	0
54	MG	1a	1663	1/1	0.91	0.20	58,58,58,58	0
54	MG	1A	3594	1/1	0.91	0.17	58,58,58,58	0
54	MG	2A	3045	1/1	0.91	0.18	41,41,41,41	0
54	MG	1A	3101	1/1	0.91	0.19	47,47,47,47	0
54	MG	1A	3456	1/1	0.91	0.18	62,62,62,62	0
54	MG	1A	3698	1/1	0.91	0.15	51,51,51,51	0
54	MG	2A	3263	1/1	0.91	0.12	41,41,41,41	0
54	MG	2A	3264	1/1	0.91	0.17	59,59,59,59	0
54	MG	2A	3265	1/1	0.91	0.17	55,55,55,55	0
54	MG	1A	3126	1/1	0.91	0.17	44,44,44,44	0
54	MG	1A	3887	1/1	0.91	0.16	56,56,56,56	0
54	MG	1A	3263	1/1	0.91	0.23	49,49,49,49	0
54	MG	2A	3701	1/1	0.91	0.10	63,63,63,63	0
54	MG	1A	3460	1/1	0.91	0.25	55,55,55,55	0
54	MG	2A	3703	1/1	0.91	0.08	59,59,59,59	0
54	MG	1a	1808	1/1	0.91	0.12	67,67,67,67	0
54	MG	2a	1699	1/1	0.91	0.10	53,53,53,53	0
54	MG	2a	1701	1/1	0.91	0.08	70,70,70,70	0
54	MG	2A	3282	1/1	0.91	0.07	52,52,52,52	0
54	MG	2A	3286	1/1	0.91	0.07	31,31,31,31	0
54	MG	1E	305	1/1	0.91	0.17	38,38,38,38	0
54	MG	1A	3462	1/1	0.91	0.12	60,60,60,60	0
54	MG	1A	3651	1/1	0.91	0.16	58,58,58,58	0
54	MG	1A	3034	1/1	0.91	0.13	53,53,53,53	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
54	MG	2A	3528	1/1	0.91	0.42	67,67,67,67	0
54	MG	1F	310	1/1	0.91	0.16	53,53,53,53	0
54	MG	1A	3712	1/1	0.91	0.10	36,36,36,36	0
54	MG	1A	3567	1/1	0.91	0.15	49,49,49,49	0
54	MG	2A	3085	1/1	0.91	0.11	46,46,46,46	0
54	MG	2a	1722	1/1	0.91	0.16	64,64,64,64	0
54	MG	1a	1690	1/1	0.91	0.14	71,71,71,71	0
54	MG	1a	1693	1/1	0.91	0.15	40,40,40,40	0
54	MG	2a	1728	1/1	0.91	0.23	77,77,77,77	0
54	MG	2A	3099	1/1	0.91	0.14	53,53,53,53	0
54	MG	2A	3100	1/1	0.91	0.07	54,54,54,54	0
54	MG	2A	3732	1/1	0.91	0.25	47,47,47,47	0
54	MG	1A	3170	1/1	0.91	0.14	38,38,38,38	0
54	MG	2a	1736	1/1	0.91	0.10	67,67,67,67	0
54	MG	2A	3740	1/1	0.91	0.13	54,54,54,54	0
54	MG	1a	1824	1/1	0.91	0.14	73,73,73,73	0
54	MG	1A	3518	1/1	0.91	0.16	65,65,65,65	0
54	MG	1H	8002	1/1	0.91	0.27	58,58,58,58	0
54	MG	2A	3339	1/1	0.91	0.13	36,36,36,36	0
54	MG	1A	3663	1/1	0.91	0.26	37,37,37,37	0
54	MG	1A	3664	1/1	0.91	0.07	60,60,60,60	0
54	MG	1Q	203	1/1	0.91	0.17	50,50,50,50	0
54	MG	2A	3562	1/1	0.91	0.06	50,50,50,50	0
54	MG	1A	3210	1/1	0.91	0.29	58,58,58,58	0
54	MG	1A	3726	1/1	0.91	0.09	50,50,50,50	0
54	MG	2B	3009	1/1	0.91	0.17	64,64,64,64	0
54	MG	2A	3134	1/1	0.91	0.17	49,49,49,49	0
54	MG	1A	4004	1/1	0.91	0.08	56,56,56,56	0
54	MG	2A	3138	1/1	0.91	0.10	61,61,61,61	0
54	MG	1A	3815	1/1	0.91	0.11	47,47,47,47	0
54	MG	1a	1846	1/1	0.91	0.13	74,74,74,74	0
54	MG	1A	3819	1/1	0.91	0.09	76,76,76,76	0
54	MG	1A	4015	1/1	0.91	0.18	41,41,41,41	0
54	MG	2B	3019	1/1	0.91	0.15	51,51,51,51	0
54	MG	2a	1776	1/1	0.91	0.07	76,76,76,76	0
54	MG	2A	3151	1/1	0.91	0.07	48,48,48,48	0
54	MG	1A	3727	1/1	0.91	0.18	42,42,42,42	0
54	MG	1a	1854	1/1	0.91	0.05	52,52,52,52	0
54	MG	1A	3477	1/1	0.91	0.21	39,39,39,39	0
54	MG	2A	3585	1/1	0.91	0.15	38,38,38,38	0
54	MG	1a	1743	1/1	0.91	0.09	53,53,53,53	0
54	MG	2E	303	1/1	0.91	0.11	72,72,72,72	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
54	MG	2A	3161	1/1	0.91	0.11	51,51,51,51	0
54	MG	1A	3928	1/1	0.91	0.17	58,58,58,58	0
54	MG	1A	3037	1/1	0.91	0.21	39,39,39,39	0
54	MG	1a	1748	1/1	0.91	0.07	58,58,58,58	0
54	MG	1A	3436	1/1	0.91	0.15	43,43,43,43	0
54	MG	2A	3599	1/1	0.91	0.09	57,57,57,57	0
54	MG	13	101	1/1	0.91	0.13	62,62,62,62	0
54	MG	1A	3744	1/1	0.91	0.22	51,51,51,51	0
54	MG	2A	3406	1/1	0.91	0.14	42,42,42,42	0
55	MPD	2A	3748	8/8	0.91	0.13	54,65,67,73	0
54	MG	15	103	1/1	0.91	0.15	71,71,71,71	0
54	MG	2I	101	1/1	0.91	0.06	69,69,69,69	0
54	MG	2A	3610	1/1	0.91	0.13	44,44,44,44	0
54	MG	17	101	1/1	0.91	0.19	64,64,64,64	0
54	MG	1A	3138	1/1	0.91	0.13	60,60,60,60	0
57	ZN	2n	501	1/1	0.91	0.08	84,84,84,84	0
54	MG	1A	3216	1/1	0.92	0.14	44,44,44,44	0
54	MG	1a	1698	1/1	0.92	0.20	60,60,60,60	0
54	MG	1A	3918	1/1	0.92	0.07	52,52,52,52	0
54	MG	1U	202	1/1	0.92	0.13	47,47,47,47	0
54	MG	1A	3559	1/1	0.92	0.11	46,46,46,46	0
54	MG	2A	3135	1/1	0.92	0.24	61,61,61,61	0
54	MG	2A	3573	1/1	0.92	0.06	50,50,50,50	0
54	MG	1A	3813	1/1	0.92	0.15	31,31,31,31	0
54	MG	1a	1714	1/1	0.92	0.20	62,62,62,62	0
54	MG	2I	3001	1/1	0.92	0.09	52,52,52,52	0
54	MG	1A	4014	1/1	0.92	0.07	33,33,33,33	0
54	MG	2A	3351	1/1	0.92	0.10	35,35,35,35	0
54	MG	2A	3579	1/1	0.92	0.12	56,56,56,56	0
54	MG	1a	1848	1/1	0.92	0.09	64,64,64,64	0
54	MG	1Z	8001	1/1	0.92	0.17	64,64,64,64	0
54	MG	1A	3119	1/1	0.92	0.37	47,47,47,47	0
54	MG	1A	3283	1/1	0.92	0.17	60,60,60,60	0
54	MG	1a	1729	1/1	0.92	0.05	56,56,56,56	0
54	MG	1A	3668	1/1	0.92	0.26	52,52,52,52	0
54	MG	2A	3592	1/1	0.92	0.15	47,47,47,47	0
54	MG	2A	3154	1/1	0.92	0.15	45,45,45,45	0
54	MG	2A	3594	1/1	0.92	0.17	46,46,46,46	0
54	MG	11	101	1/1	0.92	0.34	66,66,66,66	0
54	MG	2a	1607	1/1	0.92	0.14	72,72,72,72	0
54	MG	1A	3736	1/1	0.92	0.12	54,54,54,54	0
54	MG	1a	1736	1/1	0.92	0.20	66,66,66,66	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
54	MG	2a	1613	1/1	0.92	0.25	68,68,68,68	0
54	MG	1A	3827	1/1	0.92	0.20	27,27,27,27	0
54	MG	2A	3606	1/1	0.92	0.08	48,48,48,48	0
54	MG	1a	1741	1/1	0.92	0.24	65,65,65,65	0
54	MG	2A	3385	1/1	0.92	0.24	43,43,43,43	0
54	MG	1A	3562	1/1	0.92	0.16	54,54,54,54	0
54	MG	1A	3500	1/1	0.92	0.20	19,19,19,19	0
54	MG	1A	3931	1/1	0.92	0.08	35,35,35,35	0
54	MG	1A	3352	1/1	0.92	0.16	53,53,53,53	0
54	MG	1A	4033	1/1	0.92	0.36	47,47,47,47	0
54	MG	2A	3619	1/1	0.92	0.09	53,53,53,53	0
54	MG	2A	3620	1/1	0.92	0.15	42,42,42,42	0
54	MG	19	101	1/1	0.92	0.27	62,62,62,62	0
54	MG	2A	3176	1/1	0.92	0.16	45,45,45,45	0
54	MG	2A	3411	1/1	0.92	0.10	62,62,62,62	0
54	MG	2A	3178	1/1	0.92	0.13	59,59,59,59	0
54	MG	1A	4043	1/1	0.92	0.14	32,32,32,32	0
54	MG	1a	1879	1/1	0.92	0.18	72,72,72,72	0
54	MG	1A	3032	1/1	0.92	0.15	56,56,56,56	0
54	MG	2a	1647	1/1	0.92	0.31	67,67,67,67	0
54	MG	1A	3837	1/1	0.92	0.17	29,29,29,29	0
54	MG	1d	502	1/1	0.92	0.16	77,77,77,77	0
54	MG	2A	3634	1/1	0.92	0.13	50,50,50,50	0
54	MG	2a	1652	1/1	0.92	0.24	57,57,57,57	0
54	MG	1A	3506	1/1	0.92	0.23	36,36,36,36	0
54	MG	1A	3748	1/1	0.92	0.25	54,54,54,54	0
54	MG	1A	3413	1/1	0.92	0.17	68,68,68,68	0
54	MG	1A	3570	1/1	0.92	0.17	71,71,71,71	0
54	MG	2A	3194	1/1	0.92	0.13	53,53,53,53	0
54	MG	1h	3001	1/1	0.92	0.18	65,65,65,65	0
54	MG	2A	3643	1/1	0.92	0.06	63,63,63,63	0
54	MG	2A	3201	1/1	0.92	0.09	53,53,53,53	0
54	MG	2A	3436	1/1	0.92	0.18	49,49,49,49	0
54	MG	2A	3648	1/1	0.92	0.09	48,48,48,48	0
54	MG	2A	3649	1/1	0.92	0.08	56,56,56,56	0
54	MG	1A	3357	1/1	0.92	0.18	51,51,51,51	0
54	MG	2A	3203	1/1	0.92	0.17	58,58,58,58	0
54	MG	1A	3622	1/1	0.92	0.23	53,53,53,53	0
54	MG	2A	3448	1/1	0.92	0.12	66,66,66,66	0
54	MG	1n	503	1/1	0.92	0.15	59,59,59,59	0
54	MG	1a	1766	1/1	0.92	0.11	71,71,71,71	0
54	MG	1A	3948	1/1	0.92	0.10	49,49,49,49	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
54	MG	1A	3198	1/1	0.92	0.27	56,56,56,56	0
54	MG	1a	1771	1/1	0.92	0.07	79,79,79,79	0
54	MG	2a	1682	1/1	0.92	0.12	51,51,51,51	0
54	MG	2a	1684	1/1	0.92	0.32	59,59,59,59	0
54	MG	1A	3093	1/1	0.92	0.14	54,54,54,54	0
54	MG	1a	1624	1/1	0.92	0.14	52,52,52,52	0
54	MG	2A	3466	1/1	0.92	0.12	51,51,51,51	0
54	MG	1A	3629	1/1	0.92	0.11	68,68,68,68	0
54	MG	1a	1776	1/1	0.92	0.22	80,80,80,80	0
54	MG	1A	3762	1/1	0.92	0.14	52,52,52,52	0
54	MG	2A	3220	1/1	0.92	0.10	58,58,58,58	0
54	MG	1a	1632	1/1	0.92	0.15	36,36,36,36	0
54	MG	2A	3224	1/1	0.92	0.23	49,49,49,49	0
54	MG	1A	3173	1/1	0.92	0.25	52,52,52,52	0
54	MG	1a	1638	1/1	0.92	0.16	61,61,61,61	0
54	MG	2A	3032	1/1	0.92	0.06	46,46,46,46	0
54	MG	2A	3480	1/1	0.92	0.18	53,53,53,53	0
54	MG	2a	1706	1/1	0.92	0.06	74,74,74,74	0
54	MG	1A	3174	1/1	0.92	0.15	57,57,57,57	0
54	MG	1A	3424	1/1	0.92	0.09	46,46,46,46	0
54	MG	2A	3036	1/1	0.92	0.12	64,64,64,64	0
54	MG	2A	3691	1/1	0.92	0.05	54,54,54,54	0
54	MG	1A	3425	1/1	0.92	0.20	57,57,57,57	0
54	MG	1a	1647	1/1	0.92	0.23	57,57,57,57	0
54	MG	1A	3475	1/1	0.92	0.27	40,40,40,40	0
54	MG	2A	3489	1/1	0.92	0.15	33,33,33,33	0
54	MG	1A	3371	1/1	0.92	0.16	65,65,65,65	0
54	MG	1a	1654	1/1	0.92	0.12	64,64,64,64	0
54	MG	2a	1723	1/1	0.92	0.17	68,68,68,68	0
54	MG	2A	3250	1/1	0.92	0.15	62,62,62,62	0
54	MG	1A	3177	1/1	0.92	0.29	52,52,52,52	0
54	MG	1A	3128	1/1	0.92	0.33	65,65,65,65	0
54	MG	2A	3499	1/1	0.92	0.10	47,47,47,47	0
54	MG	2A	3705	1/1	0.92	0.17	57,57,57,57	0
54	MG	2A	3500	1/1	0.92	0.10	62,62,62,62	0
54	MG	1a	1662	1/1	0.92	0.26	64,64,64,64	0
54	MG	2A	3708	1/1	0.92	0.22	51,51,51,51	0
54	MG	1A	3298	1/1	0.92	0.10	62,62,62,62	0
54	MG	2a	1739	1/1	0.92	0.06	79,79,79,79	0
54	MG	1A	3884	1/1	0.92	0.18	27,27,27,27	0
54	MG	2A	3057	1/1	0.92	0.21	63,63,63,63	0
54	MG	1a	1799	1/1	0.92	0.06	65,65,65,65	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
54	MG	1A	3970	1/1	0.92	0.18	62,62,62,62	0
54	MG	1A	3382	1/1	0.92	0.15	32,32,32,32	0
54	MG	1E	306	1/1	0.92	0.17	68,68,68,68	0
54	MG	1A	3538	1/1	0.92	0.14	36,36,36,36	0
54	MG	2a	1751	1/1	0.92	0.10	65,65,65,65	0
54	MG	2A	3724	1/1	0.92	0.06	66,66,66,66	0
54	MG	2A	3063	1/1	0.92	0.08	61,61,61,61	0
54	MG	2A	3726	1/1	0.92	0.14	58,58,58,58	0
54	MG	1F	306	1/1	0.92	0.30	48,48,48,48	0
54	MG	1A	3336	1/1	0.92	0.19	45,45,45,45	0
54	MG	2A	3522	1/1	0.92	0.10	55,55,55,55	0
54	MG	2A	3280	1/1	0.92	0.11	48,48,48,48	0
54	MG	2a	1764	1/1	0.92	0.08	64,64,64,64	0
54	MG	2a	1765	1/1	0.92	0.23	68,68,68,68	0
54	MG	2A	3070	1/1	0.92	0.18	46,46,46,46	0
54	MG	2A	3735	1/1	0.92	0.14	38,38,38,38	0
54	MG	1a	1809	1/1	0.92	0.19	62,62,62,62	0
54	MG	1A	3979	1/1	0.92	0.19	62,62,62,62	0
54	MG	2A	3289	1/1	0.92	0.11	69,69,69,69	0
54	MG	2A	3746	1/1	0.92	0.23	55,55,55,55	0
54	MG	2A	3750	1/1	0.92	0.28	48,48,48,48	0
54	MG	2A	3295	1/1	0.92	0.09	33,33,33,33	0
54	MG	2A	3755	1/1	0.92	0.43	52,52,52,52	0
54	MG	1A	3544	1/1	0.92	0.12	58,58,58,58	0
54	MG	2A	3763	1/1	0.92	0.09	40,40,40,40	0
54	MG	1A	3893	1/1	0.92	0.21	40,40,40,40	0
54	MG	2A	3301	1/1	0.92	0.12	48,48,48,48	0
54	MG	1a	1679	1/1	0.92	0.23	55,55,55,55	0
54	MG	1A	3388	1/1	0.92	0.24	31,31,31,31	0
54	MG	1A	3650	1/1	0.92	0.29	61,61,61,61	0
54	MG	1a	1683	1/1	0.92	0.19	58,58,58,58	0
54	MG	1A	3158	1/1	0.92	0.10	49,49,49,49	0
54	MG	1A	3797	1/1	0.92	0.11	65,65,65,65	0
54	MG	1A	3493	1/1	0.92	0.19	53,53,53,53	0
54	MG	2A	3552	1/1	0.92	0.09	57,57,57,57	0
54	MG	1A	3996	1/1	0.92	0.17	59,59,59,59	0
54	MG	2A	3555	1/1	0.92	0.11	52,52,52,52	0
54	MG	1A	3164	1/1	0.92	0.12	45,45,45,45	0
54	MG	1a	1831	1/1	0.92	0.13	67,67,67,67	0
54	MG	2A	3559	1/1	0.92	0.08	55,55,55,55	0
54	MG	1A	3343	1/1	0.92	0.15	31,31,31,31	0
54	MG	2A	3332	1/1	0.92	0.16	50,50,50,50	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
54	MG	2A	3119	1/1	0.92	0.10	49,49,49,49	0
54	MG	1a	1658	1/1	0.93	0.25	61,61,61,61	0
54	MG	1D	302	1/1	0.93	0.15	60,60,60,60	0
54	MG	2A	3546	1/1	0.93	0.09	58,58,58,58	0
54	MG	1D	304	1/1	0.93	0.16	61,61,61,61	0
54	MG	1D	311	1/1	0.93	0.08	69,69,69,69	0
54	MG	2A	3549	1/1	0.93	0.13	51,51,51,51	0
54	MG	2A	3550	1/1	0.93	0.08	53,53,53,53	0
54	MG	2D	303	1/1	0.93	0.42	44,44,44,44	0
54	MG	2A	3294	1/1	0.93	0.19	56,56,56,56	0
54	MG	1A	3390	1/1	0.93	0.17	42,42,42,42	0
54	MG	1A	3890	1/1	0.93	0.12	62,62,62,62	0
54	MG	1a	1802	1/1	0.93	0.06	63,63,63,63	0
54	MG	2A	3071	1/1	0.93	0.17	52,52,52,52	0
54	MG	1A	3395	1/1	0.93	0.21	32,32,32,32	0
54	MG	1E	302	1/1	0.93	0.10	42,42,42,42	0
54	MG	1E	303	1/1	0.93	0.21	31,31,31,31	0
54	MG	1A	3675	1/1	0.93	0.14	60,60,60,60	0
54	MG	2G	3003	1/1	0.93	0.09	65,65,65,65	0
54	MG	2A	3313	1/1	0.93	0.17	52,52,52,52	0
54	MG	1A	3677	1/1	0.93	0.10	54,54,54,54	0
54	MG	2A	3566	1/1	0.93	0.16	63,63,63,63	0
54	MG	1A	3812	1/1	0.93	0.14	46,46,46,46	0
54	MG	2A	3086	1/1	0.93	0.10	57,57,57,57	0
54	MG	2A	3087	1/1	0.93	0.20	47,47,47,47	0
54	MG	2X	8001	1/1	0.93	0.09	47,47,47,47	0
54	MG	1a	1674	1/1	0.93	0.15	63,63,63,63	0
54	MG	20	102	1/1	0.93	0.10	60,60,60,60	0
54	MG	2A	3096	1/1	0.93	0.18	63,63,63,63	0
54	MG	1A	3982	1/1	0.93	0.17	62,62,62,62	0
54	MG	1A	3901	1/1	0.93	0.13	46,46,46,46	0
54	MG	1A	3435	1/1	0.93	0.14	52,52,52,52	0
54	MG	1A	3540	1/1	0.93	0.12	52,52,52,52	0
54	MG	1a	1819	1/1	0.93	0.23	64,64,64,64	0
54	MG	1A	3221	1/1	0.93	0.15	54,54,54,54	0
54	MG	2A	3342	1/1	0.93	0.13	45,45,45,45	0
54	MG	1A	3201	1/1	0.93	0.12	47,47,47,47	0
54	MG	1a	1682	1/1	0.93	0.19	47,47,47,47	0
54	MG	1A	3908	1/1	0.93	0.20	27,27,27,27	0
54	MG	1A	3821	1/1	0.93	0.19	36,36,36,36	0
54	MG	2A	3127	1/1	0.93	0.13	44,44,44,44	0
54	MG	2A	3591	1/1	0.93	0.13	43,43,43,43	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
54	MG	1a	1829	1/1	0.93	0.18	70,70,70,70	0
54	MG	1A	3187	1/1	0.93	0.19	56,56,56,56	0
54	MG	2A	3352	1/1	0.93	0.12	25,25,25,25	0
54	MG	1A	3204	1/1	0.93	0.16	60,60,60,60	0
54	MG	2a	1624	1/1	0.93	0.17	73,73,73,73	0
54	MG	1N	202	1/1	0.93	0.14	61,61,61,61	0
54	MG	1A	3920	1/1	0.93	0.08	47,47,47,47	0
54	MG	2A	3601	1/1	0.93	0.07	50,50,50,50	0
54	MG	2A	3365	1/1	0.93	0.08	68,68,68,68	0
54	MG	1A	3999	1/1	0.93	0.18	39,39,39,39	0
54	MG	1a	1695	1/1	0.93	0.28	67,67,67,67	0
54	MG	2A	3368	1/1	0.93	0.07	64,64,64,64	0
54	MG	2A	3369	1/1	0.93	0.15	51,51,51,51	0
54	MG	2a	1641	1/1	0.93	0.30	70,70,70,70	0
54	MG	2A	3140	1/1	0.93	0.12	54,54,54,54	0
54	MG	1a	1838	1/1	0.93	0.09	66,66,66,66	0
54	MG	2A	3373	1/1	0.93	0.13	50,50,50,50	0
54	MG	1A	4001	1/1	0.93	0.06	68,68,68,68	0
54	MG	2A	3377	1/1	0.93	0.10	57,57,57,57	0
54	MG	1A	3828	1/1	0.93	0.16	27,27,27,27	0
54	MG	1a	1699	1/1	0.93	0.23	73,73,73,73	0
54	MG	2A	3148	1/1	0.93	0.25	51,51,51,51	0
54	MG	1A	3247	1/1	0.93	0.25	61,61,61,61	0
54	MG	1A	3358	1/1	0.93	0.20	27,27,27,27	0
54	MG	1A	3099	1/1	0.93	0.09	59,59,59,59	0
54	MG	1a	1706	1/1	0.93	0.12	47,47,47,47	0
54	MG	2A	3156	1/1	0.93	0.14	36,36,36,36	0
54	MG	2A	3391	1/1	0.93	0.17	71,71,71,71	0
54	MG	2A	3394	1/1	0.93	0.17	33,33,33,33	0
54	MG	1a	1707	1/1	0.93	0.10	74,74,74,74	0
54	MG	1A	4009	1/1	0.93	0.16	41,41,41,41	0
54	MG	2A	3636	1/1	0.93	0.06	66,66,66,66	0
54	MG	1a	1852	1/1	0.93	0.08	52,52,52,52	0
54	MG	1a	1853	1/1	0.93	0.11	54,54,54,54	0
54	MG	2a	1668	1/1	0.93	0.16	77,77,77,77	0
54	MG	2A	3410	1/1	0.93	0.11	57,57,57,57	0
54	MG	1A	3363	1/1	0.93	0.18	33,33,33,33	0
54	MG	1a	1855	1/1	0.93	0.04	59,59,59,59	0
54	MG	1a	1717	1/1	0.93	0.06	64,64,64,64	0
54	MG	2a	1674	1/1	0.93	0.11	74,74,74,74	0
54	MG	2A	3414	1/1	0.93	0.12	65,65,65,65	0
54	MG	1A	3411	1/1	0.93	0.23	35,35,35,35	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
54	MG	2A	3646	1/1	0.93	0.09	71,71,71,71	0
54	MG	2a	1680	1/1	0.93	0.14	75,75,75,75	0
54	MG	1a	1861	1/1	0.93	0.12	52,52,52,52	0
54	MG	1A	3838	1/1	0.93	0.10	55,55,55,55	0
54	MG	1A	3167	1/1	0.93	0.20	53,53,53,53	0
54	MG	2A	3425	1/1	0.93	0.18	55,55,55,55	0
54	MG	2A	3656	1/1	0.93	0.17	61,61,61,61	0
54	MG	2A	3657	1/1	0.93	0.10	40,40,40,40	0
54	MG	1a	1721	1/1	0.93	0.09	71,71,71,71	0
54	MG	1A	3457	1/1	0.93	0.17	51,51,51,51	0
54	MG	10	103	1/1	0.93	0.11	53,53,53,53	0
54	MG	1A	4022	1/1	0.93	0.09	55,55,55,55	0
54	MG	10	105	1/1	0.93	0.11	65,65,65,65	0
54	MG	2A	3185	1/1	0.93	0.20	50,50,50,50	0
54	MG	1A	3327	1/1	0.93	0.16	32,32,32,32	0
54	MG	1a	1873	1/1	0.93	0.09	65,65,65,65	0
54	MG	1A	3153	1/1	0.93	0.23	46,46,46,46	0
54	MG	2A	3442	1/1	0.93	0.13	51,51,51,51	0
54	MG	1A	3848	1/1	0.93	0.08	41,41,41,41	0
54	MG	1A	3604	1/1	0.93	0.19	59,59,59,59	0
54	MG	2a	1709	1/1	0.93	0.07	66,66,66,66	0
54	MG	2a	1710	1/1	0.93	0.06	71,71,71,71	0
54	MG	1A	3038	1/1	0.93	0.31	60,60,60,60	0
54	MG	2a	1712	1/1	0.93	0.15	62,62,62,62	0
54	MG	15	102	1/1	0.93	0.08	55,55,55,55	0
54	MG	2A	3196	1/1	0.93	0.11	49,49,49,49	0
54	MG	1a	1745	1/1	0.93	0.14	73,73,73,73	0
54	MG	1A	3372	1/1	0.93	0.20	39,39,39,39	0
54	MG	2a	1718	1/1	0.93	0.09	82,82,82,82	0
54	MG	2A	3683	1/1	0.93	0.11	51,51,51,51	0
54	MG	1d	503	1/1	0.93	0.16	69,69,69,69	0
54	MG	1d	505	1/1	0.93	0.14	60,60,60,60	0
54	MG	1a	1747	1/1	0.93	0.18	54,54,54,54	0
54	MG	1A	3297	1/1	0.93	0.10	71,71,71,71	0
54	MG	1e	204	1/1	0.93	0.08	62,62,62,62	0
54	MG	1A	4044	1/1	0.93	0.42	52,52,52,52	0
54	MG	1g	202	1/1	0.93	0.27	66,66,66,66	0
54	MG	1A	4047	1/1	0.93	0.12	59,59,59,59	0
54	MG	1A	4048	1/1	0.93	0.15	35,35,35,35	0
54	MG	2a	1732	1/1	0.93	0.07	62,62,62,62	0
54	MG	1A	4049	1/1	0.93	0.15	41,41,41,41	0
54	MG	1i	3001	1/1	0.93	0.13	62,62,62,62	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
54	MG	1A	3272	1/1	0.93	0.15	30,30,30,30	0
54	MG	2A	3477	1/1	0.93	0.10	49,49,49,49	0
54	MG	1A	4057	1/1	0.93	0.12	38,38,38,38	0
54	MG	2A	3479	1/1	0.93	0.13	38,38,38,38	0
54	MG	2a	1743	1/1	0.93	0.13	61,61,61,61	0
54	MG	1A	3940	1/1	0.93	0.07	43,43,43,43	0
54	MG	1a	1608	1/1	0.93	0.14	54,54,54,54	0
54	MG	1A	3466	1/1	0.93	0.16	53,53,53,53	0
54	MG	2A	3225	1/1	0.93	0.12	54,54,54,54	0
54	MG	2A	3485	1/1	0.93	0.09	54,54,54,54	0
54	MG	1A	3943	1/1	0.93	0.18	38,38,38,38	0
54	MG	2A	3227	1/1	0.93	0.10	51,51,51,51	0
54	MG	2A	3228	1/1	0.93	0.13	64,64,64,64	0
54	MG	2A	3229	1/1	0.93	0.15	51,51,51,51	0
54	MG	2A	3717	1/1	0.93	0.10	60,60,60,60	0
54	MG	1A	3709	1/1	0.93	0.07	53,53,53,53	0
54	MG	1A	3864	1/1	0.93	0.21	48,48,48,48	0
54	MG	1A	3711	1/1	0.93	0.09	40,40,40,40	0
54	MG	2a	1761	1/1	0.93	0.14	65,65,65,65	0
54	MG	1B	212	1/1	0.93	0.11	59,59,59,59	0
54	MG	1A	3868	1/1	0.93	0.09	39,39,39,39	0
54	MG	1A	3955	1/1	0.93	0.11	60,60,60,60	0
54	MG	1A	3467	1/1	0.93	0.24	43,43,43,43	0
54	MG	1a	1774	1/1	0.93	0.10	68,68,68,68	0
54	MG	1a	1629	1/1	0.93	0.20	65,65,65,65	0
54	MG	2A	3504	1/1	0.93	0.20	63,63,63,63	0
54	MG	2A	3246	1/1	0.93	0.09	51,51,51,51	0
54	MG	2A	3033	1/1	0.93	0.35	54,54,54,54	0
54	MG	2a	1777	1/1	0.93	0.09	72,72,72,72	0
54	MG	1A	3120	1/1	0.93	0.12	37,37,37,37	0
54	MG	1A	3665	1/1	0.93	0.16	60,60,60,60	0
54	MG	1A	3151	1/1	0.93	0.22	41,41,41,41	0
54	MG	2A	3253	1/1	0.93	0.09	50,50,50,50	0
54	MG	2A	3744	1/1	0.93	0.14	40,40,40,40	0
54	MG	1A	3791	1/1	0.93	0.16	60,60,60,60	0
54	MG	1a	1781	1/1	0.93	0.14	62,62,62,62	0
54	MG	1a	1639	1/1	0.93	0.13	47,47,47,47	0
54	MG	1a	1641	1/1	0.93	0.19	75,75,75,75	0
54	MG	2A	3262	1/1	0.93	0.06	58,58,58,58	0
54	MG	2A	3523	1/1	0.93	0.07	51,51,51,51	0
54	MG	1A	3165	1/1	0.93	0.15	37,37,37,37	0
54	MG	1A	3313	1/1	0.93	0.39	70,70,70,70	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
54	MG	1a	1786	1/1	0.93	0.15	70,70,70,70	0
54	MG	1A	3389	1/1	0.93	0.24	35,35,35,35	0
54	MG	1A	3885	1/1	0.93	0.09	67,67,67,67	0
54	MG	1B	226	1/1	0.93	0.15	37,37,37,37	0
54	MG	1a	1650	1/1	0.93	0.27	65,65,65,65	0
54	MG	2A	3276	1/1	0.93	0.13	40,40,40,40	0
57	ZN	1n	501	1/1	0.93	0.13	65,65,65,65	0
54	MG	1A	3623	1/1	0.93	0.22	29,29,29,29	0
54	MG	2A	3279	1/1	0.93	0.22	37,37,37,37	0
54	MG	2A	3539	1/1	0.93	0.14	38,38,38,38	0
54	MG	1A	3801	1/1	0.93	0.08	45,45,45,45	0
54	MG	1A	3361	1/1	0.94	0.16	47,47,47,47	0
54	MG	1A	3578	1/1	0.94	0.30	58,58,58,58	0
54	MG	1A	3512	1/1	0.94	0.06	61,61,61,61	0
54	MG	2A	3541	1/1	0.94	0.14	43,43,43,43	0
54	MG	1Q	202	1/1	0.94	0.16	55,55,55,55	0
54	MG	2A	3093	1/1	0.94	0.09	61,61,61,61	0
54	MG	1A	3186	1/1	0.94	0.31	43,43,43,43	0
54	MG	1A	3159	1/1	0.94	0.19	53,53,53,53	0
54	MG	1a	1691	1/1	0.94	0.14	56,56,56,56	0
54	MG	1A	3189	1/1	0.94	0.23	44,44,44,44	0
54	MG	1A	3463	1/1	0.94	0.12	53,53,53,53	0
54	MG	2A	3103	1/1	0.94	0.17	37,37,37,37	0
54	MG	2A	3319	1/1	0.94	0.13	42,42,42,42	0
54	MG	2A	3104	1/1	0.94	0.22	46,46,46,46	0
54	MG	2A	3554	1/1	0.94	0.20	43,43,43,43	0
54	MG	1U	201	1/1	0.94	0.35	61,61,61,61	0
54	MG	2A	3108	1/1	0.94	0.12	60,60,60,60	0
54	MG	2A	3327	1/1	0.94	0.18	34,34,34,34	0
54	MG	1A	3369	1/1	0.94	0.10	39,39,39,39	0
54	MG	2N	8001	1/1	0.94	0.07	78,78,78,78	0
54	MG	1a	1697	1/1	0.94	0.25	60,60,60,60	0
54	MG	1V	202	1/1	0.94	0.10	64,64,64,64	0
54	MG	1A	3587	1/1	0.94	0.17	50,50,50,50	0
54	MG	2A	3334	1/1	0.94	0.19	31,31,31,31	0
54	MG	2A	3335	1/1	0.94	0.21	63,63,63,63	0
54	MG	2T	3001	1/1	0.94	0.12	65,65,65,65	0
54	MG	2W	8001	1/1	0.94	0.14	50,50,50,50	0
54	MG	1A	3818	1/1	0.94	0.15	47,47,47,47	0
54	MG	2A	3120	1/1	0.94	0.19	55,55,55,55	0
54	MG	2A	3122	1/1	0.94	0.11	44,44,44,44	0
54	MG	1A	3648	1/1	0.94	0.16	29,29,29,29	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
54	MG	2A	3125	1/1	0.94	0.17	44,44,44,44	0
54	MG	28	8002	1/1	0.94	0.20	51,51,51,51	0
54	MG	1a	1703	1/1	0.94	0.20	66,66,66,66	0
54	MG	1a	1704	1/1	0.94	0.18	68,68,68,68	0
54	MG	1A	3161	1/1	0.94	0.09	49,49,49,49	0
54	MG	1A	3822	1/1	0.94	0.16	34,34,34,34	0
54	MG	1A	3059	1/1	0.94	0.26	26,26,26,26	0
54	MG	1A	3723	1/1	0.94	0.12	44,44,44,44	0
54	MG	2A	3580	1/1	0.94	0.16	39,39,39,39	0
54	MG	2a	1609	1/1	0.94	0.11	74,74,74,74	0
54	MG	1A	3145	1/1	0.94	0.12	43,43,43,43	0
54	MG	2a	1612	1/1	0.94	0.26	63,63,63,63	0
54	MG	2A	3353	1/1	0.94	0.15	44,44,44,44	0
54	MG	2A	3355	1/1	0.94	0.13	49,49,49,49	0
54	MG	2a	1615	1/1	0.94	0.13	63,63,63,63	0
54	MG	1A	3652	1/1	0.94	0.05	56,56,56,56	0
54	MG	1A	3468	1/1	0.94	0.17	64,64,64,64	0
54	MG	2A	3141	1/1	0.94	0.12	59,59,59,59	0
54	MG	1A	3654	1/1	0.94	0.12	34,34,34,34	0
54	MG	1A	3728	1/1	0.94	0.12	68,68,68,68	0
54	MG	1A	3470	1/1	0.94	0.19	49,49,49,49	0
54	MG	2A	3145	1/1	0.94	0.14	49,49,49,49	0
54	MG	2a	1625	1/1	0.94	0.12	73,73,73,73	0
54	MG	2A	3596	1/1	0.94	0.08	58,58,58,58	0
54	MG	2a	1627	1/1	0.94	0.15	49,49,49,49	0
54	MG	1A	3096	1/1	0.94	0.15	40,40,40,40	0
54	MG	2a	1630	1/1	0.94	0.13	71,71,71,71	0
54	MG	2A	3370	1/1	0.94	0.13	33,33,33,33	0
54	MG	1a	1857	1/1	0.94	0.11	68,68,68,68	0
54	MG	2A	3600	1/1	0.94	0.11	67,67,67,67	0
54	MG	2A	3150	1/1	0.94	0.21	46,46,46,46	0
54	MG	1a	1858	1/1	0.94	0.13	54,54,54,54	0
54	MG	1a	1727	1/1	0.94	0.12	54,54,54,54	0
54	MG	2a	1640	1/1	0.94	0.20	66,66,66,66	0
54	MG	1a	1860	1/1	0.94	0.07	66,66,66,66	0
54	MG	2a	1643	1/1	0.94	0.07	76,76,76,76	0
54	MG	1A	4050	1/1	0.94	0.21	29,29,29,29	0
54	MG	1A	3659	1/1	0.94	0.08	54,54,54,54	0
54	MG	1a	1864	1/1	0.94	0.11	70,70,70,70	0
54	MG	2A	3612	1/1	0.94	0.18	33,33,33,33	0
54	MG	1A	3661	1/1	0.94	0.07	46,46,46,46	0
54	MG	17	102	1/1	0.94	0.14	63,63,63,63	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
54	MG	2A	3386	1/1	0.94	0.18	45,45,45,45	0
54	MG	1a	1735	1/1	0.94	0.07	68,68,68,68	0
54	MG	2a	1653	1/1	0.94	0.18	62,62,62,62	0
54	MG	1A	4064	1/1	0.94	0.26	40,40,40,40	0
54	MG	1a	1737	1/1	0.94	0.16	54,54,54,54	0
54	MG	2A	3623	1/1	0.94	0.18	61,61,61,61	0
54	MG	1A	4070	1/1	0.94	0.12	32,32,32,32	0
54	MG	1A	4074	1/1	0.94	0.12	43,43,43,43	0
54	MG	1A	3742	1/1	0.94	0.21	47,47,47,47	0
54	MG	1a	1604	1/1	0.94	0.20	54,54,54,54	0
54	MG	2a	1662	1/1	0.94	0.04	79,79,79,79	0
54	MG	2A	3628	1/1	0.94	0.12	56,56,56,56	0
54	MG	2A	3402	1/1	0.94	0.11	52,52,52,52	0
54	MG	2A	3404	1/1	0.94	0.08	70,70,70,70	0
54	MG	1A	3472	1/1	0.94	0.17	36,36,36,36	0
54	MG	2A	3632	1/1	0.94	0.04	72,72,72,72	0
54	MG	2A	3407	1/1	0.94	0.12	41,41,41,41	0
54	MG	1A	3474	1/1	0.94	0.20	35,35,35,35	0
54	MG	1A	3945	1/1	0.94	0.12	37,37,37,37	0
54	MG	2A	3179	1/1	0.94	0.17	56,56,56,56	0
54	MG	1B	207	1/1	0.94	0.18	68,68,68,68	0
54	MG	1A	3036	1/1	0.94	0.20	41,41,41,41	0
54	MG	1B	210	1/1	0.94	0.21	56,56,56,56	0
54	MG	1A	3057	1/1	0.94	0.22	53,53,53,53	0
54	MG	1a	1615	1/1	0.94	0.21	28,28,28,28	0
54	MG	1a	1754	1/1	0.94	0.12	66,66,66,66	0
54	MG	2A	3420	1/1	0.94	0.09	54,54,54,54	0
54	MG	1A	3543	1/1	0.94	0.26	46,46,46,46	0
54	MG	1e	203	1/1	0.94	0.25	58,58,58,58	0
54	MG	2A	3647	1/1	0.94	0.18	58,58,58,58	0
54	MG	1a	1757	1/1	0.94	0.10	71,71,71,71	0
54	MG	1a	1619	1/1	0.94	0.09	65,65,65,65	0
54	MG	2A	3193	1/1	0.94	0.18	41,41,41,41	0
54	MG	1A	3751	1/1	0.94	0.22	27,27,27,27	0
54	MG	1A	3135	1/1	0.94	0.28	41,41,41,41	0
54	MG	1A	3545	1/1	0.94	0.30	64,64,64,64	0
54	MG	2A	3198	1/1	0.94	0.24	56,56,56,56	0
54	MG	2a	1694	1/1	0.94	0.14	50,50,50,50	0
54	MG	2A	3200	1/1	0.94	0.28	57,57,57,57	0
54	MG	2a	1697	1/1	0.94	0.09	66,66,66,66	0
54	MG	2a	1698	1/1	0.94	0.18	69,69,69,69	0
54	MG	1A	3546	1/1	0.94	0.10	42,42,42,42	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
54	MG	2A	3440	1/1	0.94	0.09	45,45,45,45	0
54	MG	1A	3200	1/1	0.94	0.32	63,63,63,63	0
54	MG	2A	3443	1/1	0.94	0.11	41,41,41,41	0
54	MG	1l	3002	1/1	0.94	0.10	72,72,72,72	0
54	MG	2A	3445	1/1	0.94	0.12	66,66,66,66	0
54	MG	1a	1765	1/1	0.94	0.18	48,48,48,48	0
54	MG	1a	1627	1/1	0.94	0.16	54,54,54,54	0
54	MG	2A	3670	1/1	0.94	0.19	38,38,38,38	0
54	MG	2A	3449	1/1	0.94	0.05	60,60,60,60	0
54	MG	1A	3385	1/1	0.94	0.24	40,40,40,40	0
54	MG	1a	1630	1/1	0.94	0.11	64,64,64,64	0
54	MG	2A	3677	1/1	0.94	0.21	52,52,52,52	0
54	MG	1a	1770	1/1	0.94	0.12	58,58,58,58	0
54	MG	2A	3210	1/1	0.94	0.15	53,53,53,53	0
54	MG	2A	3462	1/1	0.94	0.10	53,53,53,53	0
54	MG	1A	3237	1/1	0.94	0.18	36,36,36,36	0
54	MG	1y	203	1/1	0.94	0.12	61,61,61,61	0
54	MG	1B	220	1/1	0.94	0.15	34,34,34,34	0
54	MG	1A	3245	1/1	0.94	0.15	35,35,35,35	0
54	MG	1B	222	1/1	0.94	0.12	65,65,65,65	0
54	MG	2A	3009	1/1	0.94	0.18	44,44,44,44	0
54	MG	1A	3676	1/1	0.94	0.09	71,71,71,71	0
54	MG	2A	3017	1/1	0.94	0.07	54,54,54,54	0
54	MG	2A	3471	1/1	0.94	0.19	30,30,30,30	0
54	MG	1A	3488	1/1	0.94	0.10	45,45,45,45	0
54	MG	1A	3489	1/1	0.94	0.13	61,61,61,61	0
54	MG	1a	1643	1/1	0.94	0.12	62,62,62,62	0
54	MG	2A	3025	1/1	0.94	0.14	44,44,44,44	0
54	MG	1A	3045	1/1	0.94	0.17	33,33,33,33	0
54	MG	2A	3029	1/1	0.94	0.10	47,47,47,47	0
54	MG	1A	3878	1/1	0.94	0.29	65,65,65,65	0
54	MG	1a	1646	1/1	0.94	0.16	39,39,39,39	0
54	MG	1A	3880	1/1	0.94	0.21	39,39,39,39	0
54	MG	2A	3482	1/1	0.94	0.18	36,36,36,36	0
54	MG	2a	1746	1/1	0.94	0.09	56,56,56,56	0
54	MG	1B	231	1/1	0.94	0.07	59,59,59,59	0
54	MG	1A	3881	1/1	0.94	0.22	28,28,28,28	0
54	MG	1A	3394	1/1	0.94	0.20	26,26,26,26	0
54	MG	2A	3239	1/1	0.94	0.32	49,49,49,49	0
54	MG	1A	3681	1/1	0.94	0.17	29,29,29,29	0
54	MG	1a	1655	1/1	0.94	0.21	69,69,69,69	0
54	MG	1a	1656	1/1	0.94	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
54	MG	2A	3715	1/1	0.94	0.08	50,50,50,50	0
54	MG	2A	3716	1/1	0.94	0.06	54,54,54,54	0
54	MG	1A	3618	1/1	0.94	0.23	32,32,32,32	0
54	MG	2A	3491	1/1	0.94	0.19	51,51,51,51	0
54	MG	1A	3980	1/1	0.94	0.15	58,58,58,58	0
54	MG	2a	1762	1/1	0.94	0.07	54,54,54,54	0
54	MG	1A	3619	1/1	0.94	0.22	37,37,37,37	0
54	MG	2A	3048	1/1	0.94	0.06	66,66,66,66	0
54	MG	1A	3250	1/1	0.94	0.14	39,39,39,39	0
54	MG	1A	3984	1/1	0.94	0.14	59,59,59,59	0
54	MG	2A	3051	1/1	0.94	0.19	57,57,57,57	0
54	MG	2A	3052	1/1	0.94	0.17	43,43,43,43	0
54	MG	1A	3440	1/1	0.94	0.11	42,42,42,42	0
54	MG	2A	3259	1/1	0.94	0.11	51,51,51,51	0
54	MG	2A	3056	1/1	0.94	0.16	62,62,62,62	0
54	MG	2A	3507	1/1	0.94	0.09	52,52,52,52	0
54	MG	2A	3261	1/1	0.94	0.17	47,47,47,47	0
54	MG	1A	3202	1/1	0.94	0.27	49,49,49,49	0
54	MG	2a	1781	1/1	0.94	0.07	60,60,60,60	0
54	MG	1A	3252	1/1	0.94	0.21	59,59,59,59	0
54	MG	1F	301	1/1	0.94	0.16	36,36,36,36	0
54	MG	1a	1668	1/1	0.94	0.10	59,59,59,59	0
54	MG	1A	3989	1/1	0.94	0.11	48,48,48,48	0
54	MG	1A	3787	1/1	0.94	0.13	25,25,25,25	0
54	MG	2A	3516	1/1	0.94	0.05	58,58,58,58	0
54	MG	2A	3517	1/1	0.94	0.07	57,57,57,57	0
54	MG	1A	3155	1/1	0.94	0.11	54,54,54,54	0
54	MG	2A	3520	1/1	0.94	0.27	38,38,38,38	0
54	MG	2A	3759	1/1	0.94	0.24	46,46,46,46	0
54	MG	2A	3065	1/1	0.94	0.59	47,47,47,47	0
54	MG	1A	3310	1/1	0.94	0.15	45,45,45,45	0
54	MG	1A	3453	1/1	0.94	0.14	40,40,40,40	0
54	MG	1A	3355	1/1	0.94	0.23	43,43,43,43	0
54	MG	1A	3256	1/1	0.94	0.15	35,35,35,35	0
54	MG	2A	3072	1/1	0.94	0.31	36,36,36,36	0
56	ARG	1B	230	12/12	0.94	0.17	29,41,51,51	0
56	ARG	1F	311	12/12	0.94	0.15	44,63,72,77	0
54	MG	1A	3080	1/1	0.94	0.22	52,52,52,52	0
54	MG	1A	4000	1/1	0.94	0.16	78,78,78,78	0
54	MG	1a	1816	1/1	0.94	0.08	73,73,73,73	0
54	MG	2A	3290	1/1	0.94	0.17	33,33,33,33	0
54	MG	2A	3292	1/1	0.94	0.10	55,55,55,55	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
54	MG	1A	3262	1/1	0.94	0.18	60,60,60,60	0
54	MG	26	502	1/1	0.95	0.16	68,68,68,68	0
54	MG	1A	3183	1/1	0.95	0.25	41,41,41,41	0
54	MG	1A	3130	1/1	0.95	0.24	55,55,55,55	0
54	MG	1A	3131	1/1	0.95	0.09	46,46,46,46	0
54	MG	2A	3398	1/1	0.95	0.19	56,56,56,56	0
54	MG	2A	3399	1/1	0.95	0.15	61,61,61,61	0
54	MG	1a	1633	1/1	0.95	0.24	67,67,67,67	0
54	MG	2A	3005	1/1	0.95	0.19	45,45,45,45	0
54	MG	2A	3403	1/1	0.95	0.19	36,36,36,36	0
54	MG	1a	1635	1/1	0.95	0.14	37,37,37,37	0
54	MG	2A	3405	1/1	0.95	0.15	53,53,53,53	0
54	MG	2A	3012	1/1	0.95	0.15	39,39,39,39	0
54	MG	1a	1636	1/1	0.95	0.09	47,47,47,47	0
54	MG	2A	3016	1/1	0.95	0.15	59,59,59,59	0
54	MG	1A	3384	1/1	0.95	0.19	43,43,43,43	0
54	MG	1A	3188	1/1	0.95	0.14	40,40,40,40	0
54	MG	1A	3714	1/1	0.95	0.14	45,45,45,45	0
54	MG	1a	1640	1/1	0.95	0.15	61,61,61,61	0
54	MG	1A	3820	1/1	0.95	0.20	31,31,31,31	0
54	MG	1A	3447	1/1	0.95	0.10	53,53,53,53	0
54	MG	2a	1621	1/1	0.95	0.30	56,56,56,56	0
54	MG	1A	3215	1/1	0.95	0.15	50,50,50,50	0
54	MG	1A	3503	1/1	0.95	0.12	52,52,52,52	0
54	MG	1A	3504	1/1	0.95	0.28	26,26,26,26	0
54	MG	1A	3274	1/1	0.95	0.12	74,74,74,74	0
54	MG	2A	3424	1/1	0.95	0.16	61,61,61,61	0
54	MG	1A	3116	1/1	0.95	0.28	49,49,49,49	0
54	MG	2a	1628	1/1	0.95	0.09	66,66,66,66	0
54	MG	1A	3954	1/1	0.95	0.16	24,24,24,24	0
54	MG	1A	3160	1/1	0.95	0.34	44,44,44,44	0
54	MG	1a	1652	1/1	0.95	0.18	44,44,44,44	0
54	MG	1A	3338	1/1	0.95	0.18	46,46,46,46	0
54	MG	1A	3117	1/1	0.95	0.14	39,39,39,39	0
54	MG	1A	3586	1/1	0.95	0.19	55,55,55,55	0
54	MG	1A	3118	1/1	0.95	0.17	43,43,43,43	0
54	MG	2A	3435	1/1	0.95	0.06	43,43,43,43	0
54	MG	2a	1639	1/1	0.95	0.10	73,73,73,73	0
54	MG	1a	1657	1/1	0.95	0.19	53,53,53,53	0
54	MG	1A	3839	1/1	0.95	0.29	60,60,60,60	0
54	MG	1D	308	1/1	0.95	0.09	45,45,45,45	0
54	MG	1A	3840	1/1	0.95	0.10	39,39,39,39	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
54	MG	1A	3734	1/1	0.95	0.07	41,41,41,41	0
54	MG	2A	3232	1/1	0.95	0.11	52,52,52,52	0
54	MG	1A	3842	1/1	0.95	0.17	41,41,41,41	0
54	MG	1A	3735	1/1	0.95	0.09	39,39,39,39	0
54	MG	1A	3064	1/1	0.95	0.19	44,44,44,44	0
54	MG	1A	3656	1/1	0.95	0.18	26,26,26,26	0
54	MG	2a	1651	1/1	0.95	0.29	67,67,67,67	0
54	MG	1A	3738	1/1	0.95	0.17	34,34,34,34	0
54	MG	1A	3401	1/1	0.95	0.14	32,32,32,32	0
54	MG	2A	3243	1/1	0.95	0.38	46,46,46,46	0
54	MG	1a	1811	1/1	0.95	0.10	78,78,78,78	0
54	MG	2A	3655	1/1	0.95	0.10	54,54,54,54	0
54	MG	2A	3461	1/1	0.95	0.18	52,52,52,52	0
54	MG	1A	3520	1/1	0.95	0.17	32,32,32,32	0
54	MG	1A	3851	1/1	0.95	0.12	44,44,44,44	0
54	MG	1a	1672	1/1	0.95	0.18	58,58,58,58	0
54	MG	1F	302	1/1	0.95	0.23	40,40,40,40	0
54	MG	1A	3743	1/1	0.95	0.19	45,45,45,45	0
54	MG	2A	3067	1/1	0.95	0.12	49,49,49,49	0
54	MG	1A	3522	1/1	0.95	0.12	61,61,61,61	0
54	MG	1A	3229	1/1	0.95	0.09	47,47,47,47	0
54	MG	1A	3981	1/1	0.95	0.14	58,58,58,58	0
54	MG	1A	3746	1/1	0.95	0.14	59,59,59,59	0
54	MG	2a	1669	1/1	0.95	0.17	77,77,77,77	0
54	MG	2A	3472	1/1	0.95	0.07	65,65,65,65	0
54	MG	1A	3404	1/1	0.95	0.10	33,33,33,33	0
54	MG	2A	3075	1/1	0.95	0.37	46,46,46,46	0
54	MG	2A	3672	1/1	0.95	0.13	39,39,39,39	0
54	MG	1A	3345	1/1	0.95	0.13	61,61,61,61	0
54	MG	1A	3030	1/1	0.95	0.11	33,33,33,33	0
54	MG	1A	3867	1/1	0.95	0.27	32,32,32,32	0
54	MG	2a	1677	1/1	0.95	0.07	66,66,66,66	0
54	MG	1A	3231	1/1	0.95	0.13	44,44,44,44	0
54	MG	2a	1679	1/1	0.95	0.13	67,67,67,67	0
54	MG	1N	201	1/1	0.95	0.11	44,44,44,44	0
54	MG	1A	3350	1/1	0.95	0.23	37,37,37,37	0
54	MG	1N	203	1/1	0.95	0.12	53,53,53,53	0
54	MG	2a	1683	1/1	0.95	0.15	69,69,69,69	0
54	MG	2A	3682	1/1	0.95	0.06	40,40,40,40	0
54	MG	2A	3269	1/1	0.95	0.19	38,38,38,38	0
54	MG	2A	3272	1/1	0.95	0.13	46,46,46,46	0
54	MG	2A	3089	1/1	0.95	0.12	33,33,33,33	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
54	MG	2A	3090	1/1	0.95	0.11	63,63,63,63	0
54	MG	2A	3092	1/1	0.95	0.11	59,59,59,59	0
54	MG	1A	3232	1/1	0.95	0.16	42,42,42,42	0
54	MG	2A	3278	1/1	0.95	0.12	50,50,50,50	0
54	MG	1A	3754	1/1	0.95	0.28	59,59,59,59	0
54	MG	1A	3236	1/1	0.95	0.14	59,59,59,59	0
54	MG	2a	1695	1/1	0.95	0.15	67,67,67,67	0
54	MG	2A	3281	1/1	0.95	0.12	33,33,33,33	0
54	MG	1A	3876	1/1	0.95	0.16	37,37,37,37	0
54	MG	2A	3284	1/1	0.95	0.12	41,41,41,41	0
54	MG	2A	3496	1/1	0.95	0.10	41,41,41,41	0
54	MG	2A	3098	1/1	0.95	0.14	53,53,53,53	0
54	MG	2A	3287	1/1	0.95	0.11	48,48,48,48	0
54	MG	2a	1704	1/1	0.95	0.18	67,67,67,67	0
54	MG	1Q	204	1/1	0.95	0.21	55,55,55,55	0
54	MG	1A	3757	1/1	0.95	0.15	50,50,50,50	0
54	MG	1A	3602	1/1	0.95	0.25	32,32,32,32	0
54	MG	2A	3291	1/1	0.95	0.16	54,54,54,54	0
54	MG	1a	1842	1/1	0.95	0.12	64,64,64,64	0
54	MG	2A	3293	1/1	0.95	0.10	42,42,42,42	0
54	MG	1A	3354	1/1	0.95	0.08	63,63,63,63	0
54	MG	2A	3106	1/1	0.95	0.25	56,56,56,56	0
54	MG	1A	3048	1/1	0.95	0.14	28,28,28,28	0
54	MG	2A	3297	1/1	0.95	0.10	43,43,43,43	0
54	MG	2A	3112	1/1	0.95	0.17	50,50,50,50	0
54	MG	1A	3242	1/1	0.95	0.15	40,40,40,40	0
54	MG	1A	3417	1/1	0.95	0.27	40,40,40,40	0
54	MG	1A	3125	1/1	0.95	0.17	49,49,49,49	0
54	MG	2A	3307	1/1	0.95	0.12	53,53,53,53	0
54	MG	2A	3308	1/1	0.95	0.16	56,56,56,56	0
54	MG	1A	3476	1/1	0.95	0.21	39,39,39,39	0
54	MG	1A	3767	1/1	0.95	0.12	43,43,43,43	0
54	MG	1X	8001	1/1	0.95	0.18	43,43,43,43	0
54	MG	1a	1708	1/1	0.95	0.12	55,55,55,55	0
54	MG	2A	3315	1/1	0.95	0.10	57,57,57,57	0
54	MG	1A	3015	1/1	0.95	0.14	38,38,38,38	0
54	MG	1A	4011	1/1	0.95	0.11	58,58,58,58	0
54	MG	1A	3547	1/1	0.95	0.15	41,41,41,41	0
54	MG	2a	1734	1/1	0.95	0.06	64,64,64,64	0
54	MG	1A	3614	1/1	0.95	0.12	38,38,38,38	0
54	MG	1A	3478	1/1	0.95	0.21	36,36,36,36	0
54	MG	2A	3326	1/1	0.95	0.21	30,30,30,30	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
54	MG	2A	3531	1/1	0.95	0.07	62,62,62,62	0
54	MG	2A	3532	1/1	0.95	0.18	47,47,47,47	0
54	MG	2a	1741	1/1	0.95	0.10	82,82,82,82	0
54	MG	2a	1742	1/1	0.95	0.06	69,69,69,69	0
54	MG	1A	3421	1/1	0.95	0.24	24,24,24,24	0
54	MG	1A	3897	1/1	0.95	0.25	44,44,44,44	0
54	MG	2A	3536	1/1	0.95	0.06	63,63,63,63	0
54	MG	1a	1723	1/1	0.95	0.12	64,64,64,64	0
54	MG	2A	3331	1/1	0.95	0.08	47,47,47,47	0
54	MG	2A	3753	1/1	0.95	0.29	39,39,39,39	0
54	MG	1A	4020	1/1	0.95	0.22	63,63,63,63	0
54	MG	2A	3137	1/1	0.95	0.09	57,57,57,57	0
54	MG	1A	3777	1/1	0.95	0.16	40,40,40,40	0
54	MG	1a	1728	1/1	0.95	0.15	56,56,56,56	0
54	MG	2a	1753	1/1	0.95	0.08	74,74,74,74	0
54	MG	1a	1867	1/1	0.95	0.11	47,47,47,47	0
54	MG	2B	3002	1/1	0.95	0.13	72,72,72,72	0
54	MG	1l	104	1/1	0.95	0.10	41,41,41,41	0
54	MG	1A	3778	1/1	0.95	0.14	34,34,34,34	0
54	MG	1A	3552	1/1	0.95	0.21	45,45,45,45	0
54	MG	2a	1760	1/1	0.95	0.08	63,63,63,63	0
54	MG	2A	3344	1/1	0.95	0.14	42,42,42,42	0
54	MG	1A	3127	1/1	0.95	0.32	57,57,57,57	0
54	MG	1A	3782	1/1	0.95	0.14	35,35,35,35	0
54	MG	1A	3783	1/1	0.95	0.18	37,37,37,37	0
54	MG	1A	3554	1/1	0.95	0.12	58,58,58,58	0
54	MG	2a	1766	1/1	0.95	0.04	63,63,63,63	0
54	MG	1A	4035	1/1	0.95	0.20	27,27,27,27	0
54	MG	2a	1768	1/1	0.95	0.09	52,52,52,52	0
54	MG	2a	1769	1/1	0.95	0.13	50,50,50,50	0
54	MG	1a	1877	1/1	0.95	0.08	55,55,55,55	0
54	MG	1A	3785	1/1	0.95	0.12	58,58,58,58	0
54	MG	1A	3910	1/1	0.95	0.10	42,42,42,42	0
54	MG	2A	3558	1/1	0.95	0.07	32,32,32,32	0
54	MG	1A	3307	1/1	0.95	0.13	46,46,46,46	0
54	MG	2A	3354	1/1	0.95	0.09	56,56,56,56	0
54	MG	1A	3040	1/1	0.95	0.19	39,39,39,39	0
54	MG	1A	3691	1/1	0.95	0.12	54,54,54,54	0
54	MG	2A	3359	1/1	0.95	0.16	40,40,40,40	0
54	MG	1A	3311	1/1	0.95	0.12	46,46,46,46	0
54	MG	2a	1784	1/1	0.95	0.09	64,64,64,64	0
54	MG	1d	504	1/1	0.95	0.21	67,67,67,67	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
54	MG	1A	3624	1/1	0.95	0.15	60,60,60,60	0
54	MG	1A	3486	1/1	0.95	0.16	31,31,31,31	0
54	MG	2E	302	1/1	0.95	0.10	41,41,41,41	0
54	MG	1A	3696	1/1	0.95	0.23	38,38,38,38	0
54	MG	2A	3168	1/1	0.95	0.36	46,46,46,46	0
54	MG	1a	1610	1/1	0.95	0.20	45,45,45,45	0
54	MG	2e	201	1/1	0.95	0.15	71,71,71,71	0
54	MG	1a	1611	1/1	0.95	0.13	38,38,38,38	0
54	MG	1A	4067	1/1	0.95	0.18	42,42,42,42	0
54	MG	1a	1755	1/1	0.95	0.17	58,58,58,58	0
54	MG	2t	3001	1/1	0.95	0.17	52,52,52,52	0
55	MPD	1A	4028	8/8	0.95	0.15	39,59,65,70	0
54	MG	1A	3796	1/1	0.95	0.14	60,60,60,60	0
54	MG	2A	3374	1/1	0.95	0.11	57,57,57,57	0
54	MG	1A	3176	1/1	0.95	0.26	46,46,46,46	0
54	MG	1A	3100	1/1	0.95	0.23	50,50,50,50	0
54	MG	1A	3255	1/1	0.95	0.25	45,45,45,45	0
54	MG	1l	3001	1/1	0.95	0.33	62,62,62,62	0
54	MG	1A	3701	1/1	0.95	0.27	68,68,68,68	0
54	MG	1B	204	1/1	0.95	0.37	65,65,65,65	0
54	MG	1A	3180	1/1	0.95	0.18	48,48,48,48	0
54	MG	1A	3257	1/1	0.95	0.37	51,51,51,51	0
54	MG	1A	3806	1/1	0.95	0.15	62,62,62,62	0
57	ZN	25	101	1/1	0.95	0.15	64,64,64,64	0
54	MG	1A	3258	1/1	0.95	0.21	40,40,40,40	0
54	MG	1A	3934	1/1	0.95	0.12	35,35,35,35	0
54	MG	1A	3780	1/1	0.96	0.12	48,48,48,48	0
54	MG	1A	3483	1/1	0.96	0.21	31,31,31,31	0
54	MG	2a	1602	1/1	0.96	0.08	58,58,58,58	0
54	MG	2A	3215	1/1	0.96	0.11	54,54,54,54	0
54	MG	2A	3409	1/1	0.96	0.16	44,44,44,44	0
54	MG	2A	3605	1/1	0.96	0.11	36,36,36,36	0
54	MG	1A	3362	1/1	0.96	0.17	39,39,39,39	0
54	MG	2A	3217	1/1	0.96	0.16	61,61,61,61	0
54	MG	1A	3309	1/1	0.96	0.10	47,47,47,47	0
54	MG	1A	3993	1/1	0.96	0.41	54,54,54,54	0
54	MG	1A	3994	1/1	0.96	0.20	38,38,38,38	0
54	MG	2A	3611	1/1	0.96	0.12	34,34,34,34	0
54	MG	2A	3415	1/1	0.96	0.21	49,49,49,49	0
54	MG	2A	3613	1/1	0.96	0.13	49,49,49,49	0
54	MG	1A	3049	1/1	0.96	0.24	55,55,55,55	0
54	MG	2A	3046	1/1	0.96	0.13	48,48,48,48	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
54	MG	2A	3047	1/1	0.96	0.08	46,46,46,46	0
54	MG	1a	1805	1/1	0.96	0.11	68,68,68,68	0
54	MG	2A	3421	1/1	0.96	0.14	69,69,69,69	0
54	MG	1a	1806	1/1	0.96	0.11	52,52,52,52	0
54	MG	1A	3001	1/1	0.96	0.21	33,33,33,33	0
54	MG	1A	3427	1/1	0.96	0.18	39,39,39,39	0
54	MG	1A	3368	1/1	0.96	0.13	24,24,24,24	0
54	MG	1a	1810	1/1	0.96	0.15	60,60,60,60	0
54	MG	1A	3637	1/1	0.96	0.13	49,49,49,49	0
54	MG	2A	3233	1/1	0.96	0.14	58,58,58,58	0
54	MG	1A	3491	1/1	0.96	0.23	24,24,24,24	0
54	MG	1A	3172	1/1	0.96	0.13	48,48,48,48	0
54	MG	1A	4002	1/1	0.96	0.16	68,68,68,68	0
54	MG	1a	1678	1/1	0.96	0.16	64,64,64,64	0
54	MG	2a	1632	1/1	0.96	0.23	59,59,59,59	0
54	MG	1A	3793	1/1	0.96	0.13	55,55,55,55	0
54	MG	2a	1634	1/1	0.96	0.17	37,37,37,37	0
54	MG	2A	3437	1/1	0.96	0.18	52,52,52,52	0
54	MG	1A	3640	1/1	0.96	0.23	71,71,71,71	0
54	MG	2A	3439	1/1	0.96	0.05	46,46,46,46	0
54	MG	1A	3894	1/1	0.96	0.13	62,62,62,62	0
54	MG	1A	3430	1/1	0.96	0.17	56,56,56,56	0
54	MG	1A	3143	1/1	0.96	0.15	44,44,44,44	0
54	MG	1R	202	1/1	0.96	0.10	50,50,50,50	0
54	MG	2A	3641	1/1	0.96	0.13	49,49,49,49	0
54	MG	1A	4010	1/1	0.96	0.18	34,34,34,34	0
54	MG	2A	3249	1/1	0.96	0.15	49,49,49,49	0
54	MG	2A	3447	1/1	0.96	0.20	48,48,48,48	0
54	MG	1a	1688	1/1	0.96	0.16	70,70,70,70	0
54	MG	1A	3715	1/1	0.96	0.20	48,48,48,48	0
54	MG	1a	1825	1/1	0.96	0.08	77,77,77,77	0
54	MG	1a	1827	1/1	0.96	0.15	73,73,73,73	0
54	MG	1a	1828	1/1	0.96	0.07	55,55,55,55	0
54	MG	1A	4013	1/1	0.96	0.11	43,43,43,43	0
54	MG	2A	3460	1/1	0.96	0.20	54,54,54,54	0
54	MG	2A	3654	1/1	0.96	0.04	56,56,56,56	0
54	MG	1A	3798	1/1	0.96	0.07	71,71,71,71	0
54	MG	1A	3207	1/1	0.96	0.07	60,60,60,60	0
54	MG	1V	201	1/1	0.96	0.17	55,55,55,55	0
54	MG	2A	3084	1/1	0.96	0.11	49,49,49,49	0
54	MG	1a	1833	1/1	0.96	0.15	48,48,48,48	0
54	MG	1A	3800	1/1	0.96	0.17	38,38,38,38	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
54	MG	1A	3054	1/1	0.96	0.21	34,34,34,34	0
54	MG	1A	3317	1/1	0.96	0.27	45,45,45,45	0
54	MG	1A	3147	1/1	0.96	0.21	46,46,46,46	0
54	MG	1A	4021	1/1	0.96	0.14	34,34,34,34	0
54	MG	1A	3804	1/1	0.96	0.18	37,37,37,37	0
54	MG	2A	3271	1/1	0.96	0.34	47,47,47,47	0
54	MG	1A	3055	1/1	0.96	0.29	42,42,42,42	0
54	MG	1A	3914	1/1	0.96	0.11	49,49,49,49	0
54	MG	1A	3380	1/1	0.96	0.19	26,26,26,26	0
54	MG	1a	1844	1/1	0.96	0.12	54,54,54,54	0
54	MG	2A	3673	1/1	0.96	0.15	38,38,38,38	0
54	MG	1a	1845	1/1	0.96	0.20	68,68,68,68	0
54	MG	1A	3809	1/1	0.96	0.18	46,46,46,46	0
54	MG	2A	3102	1/1	0.96	0.17	49,49,49,49	0
54	MG	1A	3381	1/1	0.96	0.21	24,24,24,24	0
54	MG	1A	3811	1/1	0.96	0.17	32,32,32,32	0
54	MG	1A	3265	1/1	0.96	0.12	40,40,40,40	0
54	MG	1A	3270	1/1	0.96	0.21	32,32,32,32	0
54	MG	2A	3107	1/1	0.96	0.10	53,53,53,53	0
54	MG	1A	3505	1/1	0.96	0.21	28,28,28,28	0
54	MG	2A	3109	1/1	0.96	0.10	47,47,47,47	0
54	MG	1a	1715	1/1	0.96	0.08	65,65,65,65	0
54	MG	2A	3686	1/1	0.96	0.14	43,43,43,43	0
54	MG	1a	1716	1/1	0.96	0.27	74,74,74,74	0
54	MG	1A	4046	1/1	0.96	0.21	29,29,29,29	0
54	MG	2A	3115	1/1	0.96	0.07	50,50,50,50	0
54	MG	1A	3444	1/1	0.96	0.18	61,61,61,61	0
54	MG	1A	3816	1/1	0.96	0.09	32,32,32,32	0
54	MG	2a	1690	1/1	0.96	0.06	71,71,71,71	0
54	MG	2A	3493	1/1	0.96	0.06	53,53,53,53	0
54	MG	1A	3733	1/1	0.96	0.11	55,55,55,55	0
54	MG	2A	3694	1/1	0.96	0.13	41,41,41,41	0
54	MG	1A	3446	1/1	0.96	0.21	30,30,30,30	0
54	MG	2A	3121	1/1	0.96	0.09	58,58,58,58	0
54	MG	1A	3322	1/1	0.96	0.20	30,30,30,30	0
54	MG	1a	1724	1/1	0.96	0.15	36,36,36,36	0
54	MG	1a	1862	1/1	0.96	0.07	64,64,64,64	0
54	MG	2A	3126	1/1	0.96	0.17	28,28,28,28	0
54	MG	2a	1700	1/1	0.96	0.23	47,47,47,47	0
54	MG	1A	4053	1/1	0.96	0.18	45,45,45,45	0
54	MG	1A	3056	1/1	0.96	0.11	47,47,47,47	0
54	MG	2A	3309	1/1	0.96	0.15	39,39,39,39	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
54	MG	2A	3506	1/1	0.96	0.09	59,59,59,59	0
54	MG	1A	3386	1/1	0.96	0.16	41,41,41,41	0
54	MG	1A	3823	1/1	0.96	0.21	36,36,36,36	0
54	MG	2a	1708	1/1	0.96	0.10	55,55,55,55	0
54	MG	1A	4068	1/1	0.96	0.32	43,43,43,43	0
54	MG	2A	3711	1/1	0.96	0.07	50,50,50,50	0
54	MG	1A	4069	1/1	0.96	0.23	40,40,40,40	0
54	MG	2A	3713	1/1	0.96	0.10	57,57,57,57	0
54	MG	1A	3660	1/1	0.96	0.21	23,23,23,23	0
54	MG	1A	4071	1/1	0.96	0.14	39,39,39,39	0
54	MG	1A	3515	1/1	0.96	0.18	34,34,34,34	0
54	MG	2a	1716	1/1	0.96	0.05	64,64,64,64	0
54	MG	1A	3740	1/1	0.96	0.19	22,22,22,22	0
54	MG	2A	3321	1/1	0.96	0.15	33,33,33,33	0
54	MG	2A	3322	1/1	0.96	0.13	40,40,40,40	0
54	MG	1A	3387	1/1	0.96	0.21	25,25,25,25	0
54	MG	1A	3182	1/1	0.96	0.16	61,61,61,61	0
54	MG	1a	1742	1/1	0.96	0.20	55,55,55,55	0
54	MG	1a	1612	1/1	0.96	0.22	62,62,62,62	0
54	MG	1A	3075	1/1	0.96	0.12	41,41,41,41	0
54	MG	1A	3076	1/1	0.96	0.12	44,44,44,44	0
54	MG	2a	1727	1/1	0.96	0.09	69,69,69,69	0
54	MG	2A	3525	1/1	0.96	0.11	51,51,51,51	0
54	MG	2A	3147	1/1	0.96	0.09	47,47,47,47	0
54	MG	2a	1730	1/1	0.96	0.14	55,55,55,55	0
54	MG	1A	3392	1/1	0.96	0.22	27,27,27,27	0
54	MG	1A	3039	1/1	0.96	0.12	48,48,48,48	0
54	MG	1a	1618	1/1	0.96	0.17	65,65,65,65	0
54	MG	1B	209	1/1	0.96	0.15	39,39,39,39	0
54	MG	2A	3736	1/1	0.96	0.18	50,50,50,50	0
54	MG	1A	3281	1/1	0.96	0.12	39,39,39,39	0
54	MG	2A	3738	1/1	0.96	0.10	46,46,46,46	0
54	MG	2a	1738	1/1	0.96	0.10	71,71,71,71	0
54	MG	2A	3338	1/1	0.96	0.15	33,33,33,33	0
54	MG	2A	3741	1/1	0.96	0.28	50,50,50,50	0
54	MG	2A	3743	1/1	0.96	0.12	63,63,63,63	0
54	MG	2A	3533	1/1	0.96	0.14	58,58,58,58	0
54	MG	1A	3103	1/1	0.96	0.20	44,44,44,44	0
54	MG	1A	3946	1/1	0.96	0.20	56,56,56,56	0
54	MG	1A	3157	1/1	0.96	0.22	39,39,39,39	0
54	MG	2A	3158	1/1	0.96	0.10	44,44,44,44	0
54	MG	2A	3752	1/1	0.96	0.18	46,46,46,46	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
54	MG	1A	3107	1/1	0.96	0.19	38,38,38,38	0
54	MG	2A	3160	1/1	0.96	0.23	44,44,44,44	0
54	MG	1a	1626	1/1	0.96	0.10	43,43,43,43	0
54	MG	1A	3108	1/1	0.96	0.15	41,41,41,41	0
54	MG	2A	3761	1/1	0.96	0.19	37,37,37,37	0
54	MG	2A	3762	1/1	0.96	0.16	53,53,53,53	0
54	MG	1A	3844	1/1	0.96	0.14	58,58,58,58	0
54	MG	1A	3845	1/1	0.96	0.21	22,22,22,22	0
54	MG	2A	3165	1/1	0.96	0.12	64,64,64,64	0
54	MG	1A	3004	1/1	0.96	0.16	44,44,44,44	0
54	MG	1A	3755	1/1	0.96	0.14	47,47,47,47	0
54	MG	1A	3403	1/1	0.96	0.18	25,25,25,25	0
54	MG	1a	1634	1/1	0.96	0.12	61,61,61,61	0
54	MG	2A	3357	1/1	0.96	0.14	41,41,41,41	0
54	MG	1A	3291	1/1	0.96	0.18	43,43,43,43	0
54	MG	1A	3235	1/1	0.96	0.23	41,41,41,41	0
54	MG	2A	3175	1/1	0.96	0.09	52,52,52,52	0
54	MG	1A	3347	1/1	0.96	0.20	24,24,24,24	0
54	MG	1A	3853	1/1	0.96	0.10	40,40,40,40	0
54	MG	1A	3854	1/1	0.96	0.10	42,42,42,42	0
54	MG	1A	3008	1/1	0.96	0.17	40,40,40,40	0
54	MG	2A	3181	1/1	0.96	0.08	46,46,46,46	0
54	MG	2B	3017	1/1	0.96	0.09	68,68,68,68	0
54	MG	1t	3001	1/1	0.96	0.07	49,49,49,49	0
54	MG	1y	201	1/1	0.96	0.10	72,72,72,72	0
54	MG	1A	3111	1/1	0.96	0.12	38,38,38,38	0
54	MG	1A	3859	1/1	0.96	0.12	33,33,33,33	0
54	MG	1A	3613	1/1	0.96	0.25	42,42,42,42	0
54	MG	1A	3473	1/1	0.96	0.17	33,33,33,33	0
54	MG	1D	303	1/1	0.96	0.23	36,36,36,36	0
54	MG	2a	1782	1/1	0.96	0.10	65,65,65,65	0
54	MG	2D	307	1/1	0.96	0.12	37,37,37,37	0
54	MG	2A	3376	1/1	0.96	0.07	58,58,58,58	0
54	MG	1A	3197	1/1	0.96	0.12	52,52,52,52	0
54	MG	1A	3047	1/1	0.96	0.35	63,63,63,63	0
54	MG	2A	3010	1/1	0.96	0.20	60,60,60,60	0
54	MG	2E	304	1/1	0.96	0.12	35,35,35,35	0
54	MG	2A	3382	1/1	0.96	0.10	58,58,58,58	0
54	MG	2a	1790	1/1	0.96	0.08	61,61,61,61	0
54	MG	1a	1648	1/1	0.96	0.23	56,56,56,56	0
54	MG	2A	3195	1/1	0.96	0.14	66,66,66,66	0
54	MG	2a	1793	1/1	0.96	0.18	51,51,51,51	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
54	MG	1D	309	1/1	0.96	0.12	40,40,40,40	0
54	MG	1D	310	1/1	0.96	0.20	52,52,52,52	0
54	MG	1a	1651	1/1	0.96	0.17	38,38,38,38	0
54	MG	2A	3199	1/1	0.96	0.18	56,56,56,56	0
54	MG	2A	3583	1/1	0.96	0.07	34,34,34,34	0
54	MG	1A	3136	1/1	0.96	0.17	39,39,39,39	0
54	MG	1A	3976	1/1	0.96	0.13	50,50,50,50	0
55	MPD	18	102	8/8	0.96	0.23	30,34,40,47	0
54	MG	2Q	3001	1/1	0.96	0.12	44,44,44,44	0
54	MG	1A	3301	1/1	0.96	0.27	48,48,48,48	0
54	MG	1A	3551	1/1	0.96	0.19	50,50,50,50	0
54	MG	2A	3396	1/1	0.96	0.13	50,50,50,50	0
54	MG	2T	3002	1/1	0.96	0.08	69,69,69,69	0
54	MG	2T	3003	1/1	0.96	0.09	68,68,68,68	0
54	MG	1A	3302	1/1	0.96	0.19	34,34,34,34	0
54	MG	1A	3773	1/1	0.96	0.12	31,31,31,31	0
54	MG	1A	3024	1/1	0.96	0.27	18,18,18,18	0
54	MG	1A	3168	1/1	0.96	0.15	32,32,32,32	0
54	MG	1A	3169	1/1	0.96	0.11	53,53,53,53	0
54	MG	1a	1661	1/1	0.96	0.30	44,44,44,44	0
54	MG	1A	3482	1/1	0.96	0.19	30,30,30,30	0
58	SF4	1d	501	8/8	0.96	0.14	64,70,74,95	0
54	MG	1A	3829	1/1	0.97	0.10	25,25,25,25	0
54	MG	2A	3031	1/1	0.97	0.19	27,27,27,27	0
54	MG	1A	3246	1/1	0.97	0.18	54,54,54,54	0
54	MG	1A	3831	1/1	0.97	0.11	53,53,53,53	0
54	MG	1A	3074	1/1	0.97	0.20	36,36,36,36	0
54	MG	2A	3211	1/1	0.97	0.09	56,56,56,56	0
54	MG	1A	3175	1/1	0.97	0.15	43,43,43,43	0
54	MG	1A	3564	1/1	0.97	0.22	26,26,26,26	0
54	MG	2A	3617	1/1	0.97	0.10	23,23,23,23	0
54	MG	2a	1611	1/1	0.97	0.10	41,41,41,41	0
54	MG	1A	3303	1/1	0.97	0.13	31,31,31,31	0
54	MG	1A	3952	1/1	0.97	0.13	33,33,33,33	0
54	MG	1A	3063	1/1	0.97	0.18	31,31,31,31	0
54	MG	2A	3621	1/1	0.97	0.15	56,56,56,56	0
54	MG	1a	1792	1/1	0.97	0.11	62,62,62,62	0
54	MG	1A	3364	1/1	0.97	0.17	33,33,33,33	0
54	MG	1A	3741	1/1	0.97	0.17	56,56,56,56	0
54	MG	2A	3044	1/1	0.97	0.09	44,44,44,44	0
54	MG	2A	3221	1/1	0.97	0.25	45,45,45,45	0
54	MG	2A	3222	1/1	0.97	0.23	53,53,53,53	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
54	MG	1A	3007	1/1	0.97	0.24	35,35,35,35	0
54	MG	1A	3569	1/1	0.97	0.09	37,37,37,37	0
54	MG	1A	3253	1/1	0.97	0.26	34,34,34,34	0
54	MG	1A	3178	1/1	0.97	0.15	38,38,38,38	0
54	MG	1A	3572	1/1	0.97	0.20	30,30,30,30	0
54	MG	1A	3094	1/1	0.97	0.16	37,37,37,37	0
54	MG	1D	306	1/1	0.97	0.20	46,46,46,46	0
54	MG	1A	3095	1/1	0.97	0.34	45,45,45,45	0
54	MG	1A	3026	1/1	0.97	0.28	34,34,34,34	0
54	MG	2A	3432	1/1	0.97	0.11	35,35,35,35	0
54	MG	1A	3133	1/1	0.97	0.15	42,42,42,42	0
54	MG	1A	3373	1/1	0.97	0.12	52,52,52,52	0
54	MG	1A	3260	1/1	0.97	0.17	44,44,44,44	0
54	MG	1A	3852	1/1	0.97	0.09	46,46,46,46	0
54	MG	1A	3214	1/1	0.97	0.22	42,42,42,42	0
54	MG	1A	3438	1/1	0.97	0.16	27,27,27,27	0
54	MG	1A	3114	1/1	0.97	0.17	33,33,33,33	0
54	MG	1A	3856	1/1	0.97	0.11	33,33,33,33	0
54	MG	1a	1669	1/1	0.97	0.08	70,70,70,70	0
54	MG	2a	1642	1/1	0.97	0.10	80,80,80,80	0
54	MG	1A	3977	1/1	0.97	0.18	24,24,24,24	0
54	MG	1A	3857	1/1	0.97	0.16	23,23,23,23	0
54	MG	1A	3378	1/1	0.97	0.25	36,36,36,36	0
54	MG	1A	3097	1/1	0.97	0.18	42,42,42,42	0
54	MG	2A	3248	1/1	0.97	0.26	43,43,43,43	0
54	MG	2A	3652	1/1	0.97	0.16	38,38,38,38	0
54	MG	2A	3653	1/1	0.97	0.12	38,38,38,38	0
54	MG	1A	3860	1/1	0.97	0.10	48,48,48,48	0
54	MG	1A	3442	1/1	0.97	0.15	61,61,61,61	0
54	MG	2A	3450	1/1	0.97	0.10	58,58,58,58	0
54	MG	2A	3453	1/1	0.97	0.17	52,52,52,52	0
54	MG	1A	3217	1/1	0.97	0.34	49,49,49,49	0
54	MG	1A	3267	1/1	0.97	0.10	82,82,82,82	0
54	MG	2A	3077	1/1	0.97	0.23	48,48,48,48	0
54	MG	2a	1657	1/1	0.97	0.11	52,52,52,52	0
54	MG	2A	3255	1/1	0.97	0.24	45,45,45,45	0
54	MG	2A	3078	1/1	0.97	0.14	56,56,56,56	0
54	MG	2A	3079	1/1	0.97	0.19	44,44,44,44	0
54	MG	1A	3986	1/1	0.97	0.15	19,19,19,19	0
54	MG	1A	3509	1/1	0.97	0.11	62,62,62,62	0
54	MG	1A	3865	1/1	0.97	0.15	35,35,35,35	0
54	MG	1a	1826	1/1	0.97	0.06	70,70,70,70	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
54	MG	2A	3669	1/1	0.97	0.12	38,38,38,38	0
54	MG	1A	3445	1/1	0.97	0.20	31,31,31,31	0
54	MG	1G	3004	1/1	0.97	0.12	45,45,45,45	0
54	MG	1A	3269	1/1	0.97	0.14	53,53,53,53	0
54	MG	1A	3218	1/1	0.97	0.37	48,48,48,48	0
54	MG	2A	3088	1/1	0.97	0.39	47,47,47,47	0
54	MG	1A	3992	1/1	0.97	0.17	19,19,19,19	0
54	MG	2A	3676	1/1	0.97	0.09	48,48,48,48	0
54	MG	2A	3268	1/1	0.97	0.06	57,57,57,57	0
54	MG	1A	3448	1/1	0.97	0.12	67,67,67,67	0
54	MG	2A	3270	1/1	0.97	0.13	41,41,41,41	0
54	MG	1A	3769	1/1	0.97	0.20	57,57,57,57	0
54	MG	1A	3449	1/1	0.97	0.13	54,54,54,54	0
54	MG	1a	1835	1/1	0.97	0.17	60,60,60,60	0
54	MG	2A	3274	1/1	0.97	0.06	53,53,53,53	0
54	MG	1A	3517	1/1	0.97	0.24	22,22,22,22	0
54	MG	1a	1692	1/1	0.97	0.13	44,44,44,44	0
54	MG	1A	3162	1/1	0.97	0.21	40,40,40,40	0
54	MG	1A	3599	1/1	0.97	0.10	50,50,50,50	0
54	MG	1A	3326	1/1	0.97	0.20	33,33,33,33	0
54	MG	2A	3101	1/1	0.97	0.11	34,34,34,34	0
54	MG	1R	201	1/1	0.97	0.22	53,53,53,53	0
54	MG	1A	3879	1/1	0.97	0.13	38,38,38,38	0
54	MG	1A	3776	1/1	0.97	0.22	21,21,21,21	0
54	MG	2A	3285	1/1	0.97	0.15	32,32,32,32	0
54	MG	1T	8001	1/1	0.97	0.18	60,60,60,60	0
54	MG	1A	3682	1/1	0.97	0.14	59,59,59,59	0
54	MG	1A	3006	1/1	0.97	0.16	30,30,30,30	0
54	MG	1a	1847	1/1	0.97	0.10	42,42,42,42	0
54	MG	1A	3061	1/1	0.97	0.17	49,49,49,49	0
54	MG	2A	3110	1/1	0.97	0.19	28,28,28,28	0
54	MG	1A	3523	1/1	0.97	0.17	49,49,49,49	0
54	MG	1A	3329	1/1	0.97	0.23	39,39,39,39	0
54	MG	1A	3276	1/1	0.97	0.14	29,29,29,29	0
54	MG	1A	3391	1/1	0.97	0.20	49,49,49,49	0
54	MG	1A	3082	1/1	0.97	0.34	53,53,53,53	0
54	MG	2A	3117	1/1	0.97	0.14	52,52,52,52	0
54	MG	1a	1711	1/1	0.97	0.09	69,69,69,69	0
54	MG	2a	1703	1/1	0.97	0.14	69,69,69,69	0
54	MG	1A	3226	1/1	0.97	0.30	42,42,42,42	0
54	MG	2A	3710	1/1	0.97	0.09	45,45,45,45	0
54	MG	1a	1713	1/1	0.97	0.10	44,44,44,44	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
54	MG	2A	3303	1/1	0.97	0.21	61,61,61,61	0
54	MG	2A	3304	1/1	0.97	0.22	37,37,37,37	0
54	MG	1A	3337	1/1	0.97	0.17	35,35,35,35	0
54	MG	1A	3532	1/1	0.97	0.11	61,61,61,61	0
54	MG	1A	3227	1/1	0.97	0.31	37,37,37,37	0
54	MG	1A	3535	1/1	0.97	0.16	26,26,26,26	0
54	MG	1A	3536	1/1	0.97	0.18	33,33,33,33	0
54	MG	1A	3899	1/1	0.97	0.15	47,47,47,47	0
54	MG	2A	3128	1/1	0.97	0.20	45,45,45,45	0
54	MG	2A	3721	1/1	0.97	0.28	59,59,59,59	0
54	MG	1A	3228	1/1	0.97	0.31	41,41,41,41	0
54	MG	2A	3131	1/1	0.97	0.19	39,39,39,39	0
54	MG	1A	3617	1/1	0.97	0.19	24,24,24,24	0
54	MG	2A	3318	1/1	0.97	0.17	37,37,37,37	0
54	MG	1A	3700	1/1	0.97	0.17	41,41,41,41	0
54	MG	1A	3193	1/1	0.97	0.12	46,46,46,46	0
54	MG	1A	3702	1/1	0.97	0.13	43,43,43,43	0
54	MG	1a	1726	1/1	0.97	0.14	65,65,65,65	0
54	MG	1A	3342	1/1	0.97	0.12	57,57,57,57	0
54	MG	2A	3324	1/1	0.97	0.10	44,44,44,44	0
54	MG	2A	3734	1/1	0.97	0.19	41,41,41,41	0
54	MG	13	102	1/1	0.97	0.08	49,49,49,49	0
54	MG	1A	3906	1/1	0.97	0.23	38,38,38,38	0
54	MG	1A	4032	1/1	0.97	0.21	35,35,35,35	0
54	MG	1A	3907	1/1	0.97	0.13	13,13,13,13	0
54	MG	2A	3739	1/1	0.97	0.05	52,52,52,52	0
54	MG	1A	3194	1/1	0.97	0.29	42,42,42,42	0
54	MG	2A	3330	1/1	0.97	0.18	31,31,31,31	0
54	MG	2A	3742	1/1	0.97	0.19	56,56,56,56	0
54	MG	1a	1734	1/1	0.97	0.15	47,47,47,47	0
54	MG	1a	1876	1/1	0.97	0.24	41,41,41,41	0
54	MG	1A	3909	1/1	0.97	0.20	28,28,28,28	0
54	MG	1A	3068	1/1	0.97	0.26	49,49,49,49	0
54	MG	1A	3911	1/1	0.97	0.16	28,28,28,28	0
54	MG	2A	3149	1/1	0.97	0.15	28,28,28,28	0
54	MG	19	103	1/1	0.97	0.15	66,66,66,66	0
54	MG	1a	1740	1/1	0.97	0.24	69,69,69,69	0
54	MG	1A	3287	1/1	0.97	0.18	39,39,39,39	0
54	MG	2A	3756	1/1	0.97	0.52	52,52,52,52	0
54	MG	2A	3757	1/1	0.97	0.18	64,64,64,64	0
54	MG	1A	3913	1/1	0.97	0.16	22,22,22,22	0
54	MG	2A	3343	1/1	0.97	0.07	56,56,56,56	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
54	MG	2A	3760	1/1	0.97	0.41	40,40,40,40	0
54	MG	1A	3707	1/1	0.97	0.12	43,43,43,43	0
54	MG	1A	3915	1/1	0.97	0.20	34,34,34,34	0
54	MG	1A	3469	1/1	0.97	0.23	25,25,25,25	0
54	MG	1A	3052	1/1	0.97	0.28	44,44,44,44	0
54	MG	1e	202	1/1	0.97	0.27	58,58,58,58	0
54	MG	1A	4056	1/1	0.97	0.28	41,41,41,41	0
54	MG	1A	3406	1/1	0.97	0.17	30,30,30,30	0
54	MG	1A	4058	1/1	0.97	0.15	37,37,37,37	0
54	MG	1a	1750	1/1	0.97	0.08	69,69,69,69	0
54	MG	1A	4060	1/1	0.97	0.30	32,32,32,32	0
54	MG	1A	4062	1/1	0.97	0.14	37,37,37,37	0
54	MG	1A	4063	1/1	0.97	0.15	41,41,41,41	0
54	MG	2A	3356	1/1	0.97	0.07	48,48,48,48	0
54	MG	2A	3167	1/1	0.97	0.18	41,41,41,41	0
54	MG	1A	3289	1/1	0.97	0.16	31,31,31,31	0
54	MG	1A	4065	1/1	0.97	0.21	49,49,49,49	0
54	MG	1A	3807	1/1	0.97	0.12	52,52,52,52	0
54	MG	2A	3362	1/1	0.97	0.13	34,34,34,34	0
54	MG	2B	3016	1/1	0.97	0.13	67,67,67,67	0
54	MG	1A	3808	1/1	0.97	0.23	55,55,55,55	0
54	MG	2A	3567	1/1	0.97	0.07	46,46,46,46	0
54	MG	2a	1773	1/1	0.97	0.18	59,59,59,59	0
54	MG	2A	3173	1/1	0.97	0.10	55,55,55,55	0
54	MG	1A	3713	1/1	0.97	0.13	33,33,33,33	0
54	MG	1o	3001	1/1	0.97	0.26	65,65,65,65	0
54	MG	1A	3628	1/1	0.97	0.23	20,20,20,20	0
54	MG	2A	3177	1/1	0.97	0.25	39,39,39,39	0
54	MG	1A	3234	1/1	0.97	0.15	37,37,37,37	0
54	MG	1A	4072	1/1	0.97	0.17	36,36,36,36	0
54	MG	1a	1623	1/1	0.97	0.10	43,43,43,43	0
54	MG	1a	1763	1/1	0.97	0.15	59,59,59,59	0
54	MG	1A	3630	1/1	0.97	0.12	41,41,41,41	0
54	MG	1A	4075	1/1	0.97	0.15	39,39,39,39	0
54	MG	1A	3550	1/1	0.97	0.16	57,57,57,57	0
54	MG	2A	3581	1/1	0.97	0.14	48,48,48,48	0
54	MG	1A	3349	1/1	0.97	0.19	30,30,30,30	0
54	MG	2F	302	1/1	0.97	0.18	41,41,41,41	0
54	MG	2A	3378	1/1	0.97	0.08	47,47,47,47	0
54	MG	1a	1628	1/1	0.97	0.12	37,37,37,37	0
54	MG	2A	3188	1/1	0.97	0.08	57,57,57,57	0
54	MG	2A	3003	1/1	0.97	0.09	51,51,51,51	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
54	MG	1A	3720	1/1	0.97	0.20	33,33,33,33	0
54	MG	2O	201	1/1	0.97	0.16	58,58,58,58	0
54	MG	1A	3633	1/1	0.97	0.23	46,46,46,46	0
54	MG	2r	101	1/1	0.97	0.08	68,68,68,68	0
54	MG	2A	3589	1/1	0.97	0.06	54,54,54,54	0
54	MG	2A	3590	1/1	0.97	0.05	49,49,49,49	0
54	MG	1A	3410	1/1	0.97	0.14	36,36,36,36	0
54	MG	1A	3121	1/1	0.97	0.17	35,35,35,35	0
54	MG	1A	3412	1/1	0.97	0.24	27,27,27,27	0
54	MG	1A	3146	1/1	0.97	0.22	28,28,28,28	0
54	MG	1A	3122	1/1	0.97	0.13	37,37,37,37	0
54	MG	1A	3104	1/1	0.97	0.32	41,41,41,41	0
54	MG	2A	3021	1/1	0.97	0.13	31,31,31,31	0
54	MG	2W	8002	1/1	0.97	0.12	60,60,60,60	0
57	ZN	1Y	501	1/1	0.97	0.22	56,56,56,56	0
54	MG	2A	3022	1/1	0.97	0.35	44,44,44,44	0
54	MG	1A	3730	1/1	0.97	0.15	53,53,53,53	0
54	MG	1A	3296	1/1	0.97	0.16	31,31,31,31	0
54	MG	1A	3941	1/1	0.97	0.12	66,66,66,66	0
54	MG	2A	3604	1/1	0.97	0.18	35,35,35,35	0
54	MG	1A	3105	1/1	0.97	0.09	57,57,57,57	0
54	MG	2A	3401	1/1	0.97	0.10	43,43,43,43	0
54	MG	2A	3028	1/1	0.97	0.12	33,33,33,33	0
54	MG	1A	4059	1/1	0.98	0.22	28,28,28,28	0
54	MG	1A	3021	1/1	0.98	0.19	34,34,34,34	0
54	MG	1A	4061	1/1	0.98	0.23	37,37,37,37	0
54	MG	1A	3832	1/1	0.98	0.14	50,50,50,50	0
54	MG	1A	3575	1/1	0.98	0.18	33,33,33,33	0
54	MG	2A	3660	1/1	0.98	0.16	47,47,47,47	0
54	MG	1A	3046	1/1	0.98	0.28	13,13,13,13	0
54	MG	2A	3298	1/1	0.98	0.11	33,33,33,33	0
54	MG	2A	3299	1/1	0.98	0.08	35,35,35,35	0
54	MG	2A	3139	1/1	0.98	0.21	28,28,28,28	0
54	MG	1A	3306	1/1	0.98	0.18	29,29,29,29	0
54	MG	1A	4066	1/1	0.98	0.16	38,38,38,38	0
54	MG	1A	3140	1/1	0.98	0.22	31,31,31,31	0
54	MG	1A	3658	1/1	0.98	0.18	19,19,19,19	0
54	MG	1A	3211	1/1	0.98	0.14	40,40,40,40	0
54	MG	1A	3013	1/1	0.98	0.22	17,17,17,17	0
54	MG	1A	3003	1/1	0.98	0.27	24,24,24,24	0
54	MG	1A	3582	1/1	0.98	0.15	50,50,50,50	0
54	MG	1A	3749	1/1	0.98	0.13	27,27,27,27	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
54	MG	2A	3311	1/1	0.98	0.14	49,49,49,49	0
54	MG	1A	3113	1/1	0.98	0.14	34,34,34,34	0
54	MG	1A	3259	1/1	0.98	0.16	40,40,40,40	0
54	MG	1A	3947	1/1	0.98	0.14	50,50,50,50	0
54	MG	1A	3085	1/1	0.98	0.30	38,38,38,38	0
54	MG	2A	3316	1/1	0.98	0.12	40,40,40,40	0
54	MG	1A	3508	1/1	0.98	0.14	46,46,46,46	0
54	MG	1B	205	1/1	0.98	0.25	39,39,39,39	0
54	MG	2A	3155	1/1	0.98	0.20	52,52,52,52	0
54	MG	1A	3667	1/1	0.98	0.21	47,47,47,47	0
54	MG	1A	3951	1/1	0.98	0.14	31,31,31,31	0
54	MG	1A	3181	1/1	0.98	0.12	36,36,36,36	0
54	MG	1A	3953	1/1	0.98	0.21	19,19,19,19	0
54	MG	1a	1769	1/1	0.98	0.06	58,58,58,58	0
54	MG	1A	3588	1/1	0.98	0.20	21,21,21,21	0
54	MG	1A	3510	1/1	0.98	0.19	31,31,31,31	0
54	MG	1A	3316	1/1	0.98	0.17	39,39,39,39	0
54	MG	1A	3379	1/1	0.98	0.15	27,27,27,27	0
54	MG	1A	3760	1/1	0.98	0.12	34,34,34,34	0
54	MG	2A	3004	1/1	0.98	0.17	26,26,26,26	0
54	MG	2A	3510	1/1	0.98	0.16	47,47,47,47	0
54	MG	1A	3086	1/1	0.98	0.34	45,45,45,45	0
54	MG	2A	3006	1/1	0.98	0.10	46,46,46,46	0
54	MG	2A	3169	1/1	0.98	0.10	41,41,41,41	0
54	MG	2A	3698	1/1	0.98	0.15	39,39,39,39	0
54	MG	2A	3699	1/1	0.98	0.16	44,44,44,44	0
54	MG	2A	3007	1/1	0.98	0.16	36,36,36,36	0
54	MG	2A	3008	1/1	0.98	0.11	30,30,30,30	0
54	MG	1A	3088	1/1	0.98	0.14	47,47,47,47	0
54	MG	2A	3337	1/1	0.98	0.12	32,32,32,32	0
54	MG	1A	3264	1/1	0.98	0.23	29,29,29,29	0
54	MG	1A	3764	1/1	0.98	0.20	29,29,29,29	0
54	MG	1a	1779	1/1	0.98	0.13	56,56,56,56	0
54	MG	2A	3341	1/1	0.98	0.13	36,36,36,36	0
54	MG	2A	3015	1/1	0.98	0.25	36,36,36,36	0
54	MG	1A	3184	1/1	0.98	0.13	35,35,35,35	0
54	MG	1A	3266	1/1	0.98	0.15	28,28,28,28	0
54	MG	1A	3220	1/1	0.98	0.17	39,39,39,39	0
54	MG	1A	3966	1/1	0.98	0.10	48,48,48,48	0
54	MG	1A	3323	1/1	0.98	0.20	28,28,28,28	0
54	MG	1A	3968	1/1	0.98	0.11	44,44,44,44	0
54	MG	1A	3521	1/1	0.98	0.15	31,31,31,31	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
54	MG	2A	3184	1/1	0.98	0.15	45,45,45,45	0
54	MG	1A	3452	1/1	0.98	0.16	56,56,56,56	0
54	MG	1A	3268	1/1	0.98	0.17	45,45,45,45	0
54	MG	2A	3027	1/1	0.98	0.15	45,45,45,45	0
54	MG	1B	228	1/1	0.98	0.13	65,65,65,65	0
54	MG	1A	3524	1/1	0.98	0.17	29,29,29,29	0
54	MG	1A	3005	1/1	0.98	0.26	24,24,24,24	0
54	MG	1D	301	1/1	0.98	0.17	37,37,37,37	0
54	MG	1A	3774	1/1	0.98	0.14	43,43,43,43	0
54	MG	1A	3686	1/1	0.98	0.09	50,50,50,50	0
54	MG	1A	3978	1/1	0.98	0.19	29,29,29,29	0
54	MG	2A	3543	1/1	0.98	0.09	42,42,42,42	0
54	MG	2A	3361	1/1	0.98	0.13	34,34,34,34	0
54	MG	1A	3526	1/1	0.98	0.09	48,48,48,48	0
54	MG	1a	1798	1/1	0.98	0.10	48,48,48,48	0
54	MG	2A	3364	1/1	0.98	0.14	49,49,49,49	0
54	MG	2A	3733	1/1	0.98	0.19	33,33,33,33	0
54	MG	1D	307	1/1	0.98	0.24	17,17,17,17	0
54	MG	1A	3605	1/1	0.98	0.18	40,40,40,40	0
54	MG	1A	3222	1/1	0.98	0.17	36,36,36,36	0
54	MG	1A	3271	1/1	0.98	0.19	37,37,37,37	0
54	MG	1A	3223	1/1	0.98	0.15	32,32,32,32	0
54	MG	2A	3043	1/1	0.98	0.14	23,23,23,23	0
54	MG	1A	3330	1/1	0.98	0.20	33,33,33,33	0
54	MG	1A	3393	1/1	0.98	0.24	26,26,26,26	0
54	MG	2A	3205	1/1	0.98	0.15	66,66,66,66	0
54	MG	1D	314	1/1	0.98	0.19	72,72,72,72	0
54	MG	1A	3050	1/1	0.98	0.24	44,44,44,44	0
54	MG	1A	3533	1/1	0.98	0.11	27,27,27,27	0
54	MG	1A	3461	1/1	0.98	0.16	44,44,44,44	0
54	MG	2A	3749	1/1	0.98	0.23	39,39,39,39	0
54	MG	1A	3333	1/1	0.98	0.16	47,47,47,47	0
54	MG	2A	3379	1/1	0.98	0.16	30,30,30,30	0
54	MG	2A	3564	1/1	0.98	0.08	57,57,57,57	0
54	MG	1A	3396	1/1	0.98	0.17	26,26,26,26	0
54	MG	2A	3754	1/1	0.98	0.34	46,46,46,46	0
54	MG	1A	3334	1/1	0.98	0.20	37,37,37,37	0
54	MG	2A	3054	1/1	0.98	0.11	44,44,44,44	0
54	MG	1A	3886	1/1	0.98	0.12	29,29,29,29	0
54	MG	1A	3398	1/1	0.98	0.20	22,22,22,22	0
54	MG	1F	303	1/1	0.98	0.11	34,34,34,34	0
54	MG	2a	1726	1/1	0.98	0.18	57,57,57,57	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
54	MG	1A	3790	1/1	0.98	0.13	21,21,21,21	0
54	MG	1A	3091	1/1	0.98	0.17	42,42,42,42	0
54	MG	1A	3541	1/1	0.98	0.18	27,27,27,27	0
54	MG	1F	308	1/1	0.98	0.17	41,41,41,41	0
54	MG	2A	3390	1/1	0.98	0.11	31,31,31,31	0
54	MG	1A	3016	1/1	0.98	0.26	42,42,42,42	0
54	MG	2A	3392	1/1	0.98	0.12	65,65,65,65	0
54	MG	2A	3393	1/1	0.98	0.14	43,43,43,43	0
54	MG	1A	3892	1/1	0.98	0.14	38,38,38,38	0
54	MG	2A	3064	1/1	0.98	0.14	38,38,38,38	0
54	MG	1A	3028	1/1	0.98	0.19	28,28,28,28	0
54	MG	2A	3397	1/1	0.98	0.16	36,36,36,36	0
54	MG	1A	3053	1/1	0.98	0.13	36,36,36,36	0
54	MG	1A	3895	1/1	0.98	0.15	35,35,35,35	0
54	MG	1A	3896	1/1	0.98	0.10	49,49,49,49	0
54	MG	2A	3069	1/1	0.98	0.21	44,44,44,44	0
54	MG	1a	1686	1/1	0.98	0.29	64,64,64,64	0
54	MG	1a	1687	1/1	0.98	0.11	52,52,52,52	0
54	MG	1A	3280	1/1	0.98	0.20	48,48,48,48	0
54	MG	1A	3340	1/1	0.98	0.19	25,25,25,25	0
54	MG	1A	3123	1/1	0.98	0.25	23,23,23,23	0
54	MG	2A	3076	1/1	0.98	0.20	51,51,51,51	0
54	MG	1A	3710	1/1	0.98	0.15	55,55,55,55	0
54	MG	2A	3595	1/1	0.98	0.16	33,33,33,33	0
54	MG	1A	4008	1/1	0.98	0.24	33,33,33,33	0
54	MG	1A	3069	1/1	0.98	0.12	37,37,37,37	0
54	MG	2A	3238	1/1	0.98	0.27	47,47,47,47	0
54	MG	2D	305	1/1	0.98	0.24	49,49,49,49	0
54	MG	1A	3070	1/1	0.98	0.23	43,43,43,43	0
54	MG	1A	3071	1/1	0.98	0.15	32,32,32,32	0
54	MG	2A	3242	1/1	0.98	0.26	48,48,48,48	0
54	MG	2a	1758	1/1	0.98	0.15	50,50,50,50	0
54	MG	2A	3602	1/1	0.98	0.13	32,32,32,32	0
54	MG	2E	301	1/1	0.98	0.06	50,50,50,50	0
54	MG	1A	3072	1/1	0.98	0.20	37,37,37,37	0
54	MG	1A	3029	1/1	0.98	0.18	40,40,40,40	0
54	MG	2A	3417	1/1	0.98	0.20	52,52,52,52	0
54	MG	1A	3017	1/1	0.98	0.20	37,37,37,37	0
54	MG	1A	3717	1/1	0.98	0.26	39,39,39,39	0
54	MG	1A	3031	1/1	0.98	0.20	24,24,24,24	0
54	MG	2F	303	1/1	0.98	0.26	43,43,43,43	0
54	MG	1a	1701	1/1	0.98	0.20	64,64,64,64	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
54	MG	1A	4018	1/1	0.98	0.11	44,44,44,44	0
54	MG	2A	3423	1/1	0.98	0.08	33,33,33,33	0
54	MG	1A	3290	1/1	0.98	0.22	36,36,36,36	0
54	MG	1A	3239	1/1	0.98	0.27	43,43,43,43	0
54	MG	2A	3091	1/1	0.98	0.15	34,34,34,34	0
54	MG	2A	3615	1/1	0.98	0.12	34,34,34,34	0
54	MG	2a	1775	1/1	0.98	0.12	57,57,57,57	0
54	MG	1A	3241	1/1	0.98	0.17	37,37,37,37	0
54	MG	1A	3722	1/1	0.98	0.14	32,32,32,32	0
54	MG	1A	3041	1/1	0.98	0.19	54,54,54,54	0
54	MG	1A	3243	1/1	0.98	0.16	33,33,33,33	0
54	MG	2a	1780	1/1	0.98	0.13	66,66,66,66	0
54	MG	1a	1709	1/1	0.98	0.14	39,39,39,39	0
54	MG	1a	1710	1/1	0.98	0.20	38,38,38,38	0
54	MG	1A	3244	1/1	0.98	0.34	36,36,36,36	0
54	MG	1A	3356	1/1	0.98	0.18	11,11,11,11	0
54	MG	2V	201	1/1	0.98	0.21	60,60,60,60	0
54	MG	1A	4029	1/1	0.98	0.15	49,49,49,49	0
54	MG	1A	3917	1/1	0.98	0.16	15,15,15,15	0
54	MG	1A	4031	1/1	0.98	0.32	38,38,38,38	0
54	MG	1A	3817	1/1	0.98	0.10	45,45,45,45	0
54	MG	1A	3919	1/1	0.98	0.24	35,35,35,35	0
54	MG	2A	3441	1/1	0.98	0.10	70,70,70,70	0
54	MG	1A	4034	1/1	0.98	0.12	31,31,31,31	0
54	MG	1A	3487	1/1	0.98	0.14	25,25,25,25	0
54	MG	1A	4036	1/1	0.98	0.20	35,35,35,35	0
54	MG	1A	4038	1/1	0.98	0.17	37,37,37,37	0
54	MG	1A	4039	1/1	0.98	0.24	41,41,41,41	0
54	MG	1A	4040	1/1	0.98	0.11	37,37,37,37	0
54	MG	1A	4042	1/1	0.98	0.16	36,36,36,36	0
54	MG	1A	3132	1/1	0.98	0.16	39,39,39,39	0
54	MG	1A	3729	1/1	0.98	0.21	27,27,27,27	0
54	MG	1A	4045	1/1	0.98	0.17	36,36,36,36	0
54	MG	1A	3923	1/1	0.98	0.06	43,43,43,43	0
54	MG	1A	3422	1/1	0.98	0.20	32,32,32,32	0
54	MG	1A	3078	1/1	0.98	0.23	38,38,38,38	0
54	MG	1A	3359	1/1	0.98	0.27	11,11,11,11	0
54	MG	2A	3459	1/1	0.98	0.16	49,49,49,49	0
54	MG	1A	3824	1/1	0.98	0.19	33,33,33,33	0
54	MG	1A	3106	1/1	0.98	0.18	30,30,30,30	0
54	MG	1A	4052	1/1	0.98	0.19	45,45,45,45	0
54	MG	1a	1601	1/1	0.98	0.12	57,57,57,57	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
54	MG	1A	3300	1/1	0.98	0.21	12,12,12,12	0
54	MG	1a	1739	1/1	0.98	0.16	60,60,60,60	0
54	MG	2a	1619	1/1	0.98	0.13	48,48,48,48	0
54	MG	1A	4054	1/1	0.98	0.13	44,44,44,44	0
57	ZN	26	501	1/1	0.98	0.18	60,60,60,60	0
54	MG	1A	3248	1/1	0.98	0.35	58,58,58,58	0
54	MG	1A	3042	1/1	0.98	0.22	24,24,24,24	0
54	MG	1A	3043	1/1	0.98	0.24	17,17,17,17	0
58	SF4	2d	501	8/8	0.98	0.12	61,78,84,104	0
54	MG	2A	3456	1/1	0.99	0.18	24,24,24,24	0
54	MG	2A	3111	1/1	0.99	0.11	54,54,54,54	0
54	MG	1A	3023	1/1	0.99	0.16	34,34,34,34	0
54	MG	1A	3874	1/1	0.99	0.17	24,24,24,24	0
54	MG	1A	3277	1/1	0.99	0.20	29,29,29,29	0
54	MG	2A	3283	1/1	0.99	0.21	19,19,19,19	0
54	MG	1a	1796	1/1	0.99	0.06	68,68,68,68	0
54	MG	1A	3514	1/1	0.99	0.20	23,23,23,23	0
54	MG	1A	3208	1/1	0.99	0.21	42,42,42,42	0
54	MG	2A	3560	1/1	0.99	0.17	23,23,23,23	0
54	MG	1A	3209	1/1	0.99	0.14	44,44,44,44	0
54	MG	1D	305	1/1	0.99	0.26	38,38,38,38	0
54	MG	1A	3826	1/1	0.99	0.16	8,8,8,8	0
54	MG	1A	3556	1/1	0.99	0.19	39,39,39,39	0
54	MG	1A	3732	1/1	0.99	0.18	32,32,32,32	0
54	MG	2A	3123	1/1	0.99	0.44	48,48,48,48	0
54	MG	1a	1733	1/1	0.99	0.15	34,34,34,34	0
54	MG	1A	3308	1/1	0.99	0.22	46,46,46,46	0
54	MG	1A	3156	1/1	0.99	0.26	30,30,30,30	0
54	MG	1A	3077	1/1	0.99	0.26	53,53,53,53	0
54	MG	1A	3019	1/1	0.99	0.20	30,30,30,30	0
54	MG	1A	4055	1/1	0.99	0.15	42,42,42,42	0
54	MG	2A	3130	1/1	0.99	0.24	42,42,42,42	0
54	MG	2A	3574	1/1	0.99	0.13	30,30,30,30	0
54	MG	1A	3645	1/1	0.99	0.20	30,30,30,30	0
54	MG	1A	3834	1/1	0.99	0.12	45,45,45,45	0
54	MG	1A	3376	1/1	0.99	0.15	45,45,45,45	0
54	MG	1A	3233	1/1	0.99	0.16	37,37,37,37	0
54	MG	1A	3693	1/1	0.99	0.36	54,54,54,54	0
54	MG	2A	3305	1/1	0.99	0.19	19,19,19,19	0
54	MG	2A	3053	1/1	0.99	0.13	39,39,39,39	0
54	MG	1A	3087	1/1	0.99	0.28	34,34,34,34	0
54	MG	1A	3144	1/1	0.99	0.17	41,41,41,41	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
54	MG	1A	3606	1/1	0.99	0.19	32,32,32,32	0
54	MG	1A	3286	1/1	0.99	0.12	41,41,41,41	0
54	MG	1A	3792	1/1	0.99	0.18	26,26,26,26	0
54	MG	1F	304	1/1	0.99	0.16	33,33,33,33	0
54	MG	1g	201	1/1	0.99	0.12	62,62,62,62	0
54	MG	1A	3098	1/1	0.99	0.24	12,12,12,12	0
54	MG	1A	3025	1/1	0.99	0.21	40,40,40,40	0
54	MG	2A	3494	1/1	0.99	0.17	27,27,27,27	0
54	MG	1A	3238	1/1	0.99	0.20	38,38,38,38	0
54	MG	1A	4007	1/1	0.99	0.25	17,17,17,17	0
54	MG	1a	1616	1/1	0.99	0.18	48,48,48,48	0
54	MG	1A	3179	1/1	0.99	0.15	34,34,34,34	0
54	MG	1A	3351	1/1	0.99	0.17	24,24,24,24	0
54	MG	1A	3420	1/1	0.99	0.25	24,24,24,24	0
54	MG	1A	4073	1/1	0.99	0.19	40,40,40,40	0
54	MG	1A	3240	1/1	0.99	0.27	38,38,38,38	0
54	MG	2A	3503	1/1	0.99	0.21	35,35,35,35	0
54	MG	1A	4012	1/1	0.99	0.21	23,23,23,23	0
54	MG	1A	3163	1/1	0.99	0.28	34,34,34,34	0
54	MG	1B	201	1/1	0.99	0.17	44,44,44,44	0
54	MG	2A	3240	1/1	0.99	0.14	34,34,34,34	0
54	MG	2A	3074	1/1	0.99	0.17	23,23,23,23	0
54	MG	1A	3574	1/1	0.99	0.22	31,31,31,31	0
54	MG	1A	3423	1/1	0.99	0.18	16,16,16,16	0
54	MG	1A	3044	1/1	0.99	0.20	32,32,32,32	0
54	MG	1A	3498	1/1	0.99	0.12	50,50,50,50	0
54	MG	1P	201	1/1	0.99	0.10	26,26,26,26	0
54	MG	1A	3148	1/1	0.99	0.17	33,33,33,33	0
54	MG	1Q	201	1/1	0.99	0.22	33,33,33,33	0
54	MG	1A	3020	1/1	0.99	0.20	39,39,39,39	0
54	MG	1A	3539	1/1	0.99	0.17	36,36,36,36	0
54	MG	2A	3518	1/1	0.99	0.15	35,35,35,35	0
54	MG	1A	3325	1/1	0.99	0.21	21,21,21,21	0
54	MG	1A	3009	1/1	0.99	0.18	26,26,26,26	0
54	MG	1A	3185	1/1	0.99	0.18	37,37,37,37	0
54	MG	2A	3254	1/1	0.99	0.33	39,39,39,39	0
54	MG	2A	3429	1/1	0.99	0.13	36,36,36,36	0
54	MG	1A	4024	1/1	0.99	0.34	36,36,36,36	0
54	MG	1A	3626	1/1	0.99	0.18	30,30,30,30	0
54	MG	1A	3671	1/1	0.99	0.18	36,36,36,36	0
54	MG	2A	3011	1/1	0.99	0.14	28,28,28,28	0
54	MG	1A	3092	1/1	0.99	0.15	35,35,35,35	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
54	MG	27	3001	1/1	0.99	0.18	43,43,43,43	0
54	MG	2A	3013	1/1	0.99	0.21	24,24,24,24	0
54	MG	1A	3299	1/1	0.99	0.23	22,22,22,22	0
54	MG	1A	3971	1/1	0.99	0.19	31,31,31,31	0
54	MG	2A	3095	1/1	0.99	0.20	38,38,38,38	0
54	MG	1A	3972	1/1	0.99	0.18	26,26,26,26	0
54	MG	1A	3137	1/1	0.99	0.24	42,42,42,42	0
54	MG	2A	3018	1/1	0.99	0.27	35,35,35,35	0
54	MG	1A	3249	1/1	0.99	0.18	35,35,35,35	0
54	MG	2A	3731	1/1	0.99	0.24	23,23,23,23	0
54	MG	2A	3020	1/1	0.99	0.20	44,44,44,44	0
54	MG	1A	3332	1/1	0.99	0.22	28,28,28,28	0
54	MG	1A	3018	1/1	0.99	0.20	33,33,33,33	0
54	MG	1A	3366	1/1	0.99	0.11	46,46,46,46	0
54	MG	1A	4037	1/1	0.99	0.19	32,32,32,32	0
57	ZN	15	101	1/1	0.99	0.16	50,50,50,50	0
57	ZN	16	501	1/1	0.99	0.22	39,39,39,39	0
57	ZN	19	102	1/1	0.99	0.19	37,37,37,37	0
54	MG	2A	3542	1/1	0.99	0.18	34,34,34,34	0
54	MG	1A	3275	1/1	0.99	0.21	41,41,41,41	0
54	MG	1A	3871	1/1	0.99	0.08	45,45,45,45	0
54	MG	1A	3872	1/1	0.99	0.12	42,42,42,42	0
54	MG	2A	3451	1/1	0.99	0.20	39,39,39,39	0
54	MG	2A	3452	1/1	0.99	0.13	48,48,48,48	0
54	MG	1A	4041	1/1	0.99	0.22	37,37,37,37	0
54	MG	1a	1722	1/1	0.99	0.14	40,40,40,40	0
54	MG	2A	3030	1/1	0.99	0.23	39,39,39,39	0
54	MG	1A	3141	1/1	1.00	0.31	36,36,36,36	0
54	MG	1A	3433	1/1	1.00	0.23	10,10,10,10	0
54	MG	1A	3149	1/1	1.00	0.21	28,28,28,28	0

## 6.5 Other polymers [\(i\)](#)

There are no such residues in this entry.