



Full wwPDB X-ray Structure Validation Report ⓘ

Oct 11, 2023 – 03:13 AM EDT

PDB ID : 4Y4P
Title : Crystal structure of the *Thermus thermophilus* 70S ribosome with rRNA modifications and bound to mRNA and A-, P- and E-site tRNAs at 2.5Å resolution
Authors : Polikanov, Y.S.; Melnikov, S.V.; Soll, D.; Steitz, T.A.
Deposited on : 2015-02-10
Resolution : 2.50 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.35.1
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) : 2.35.1

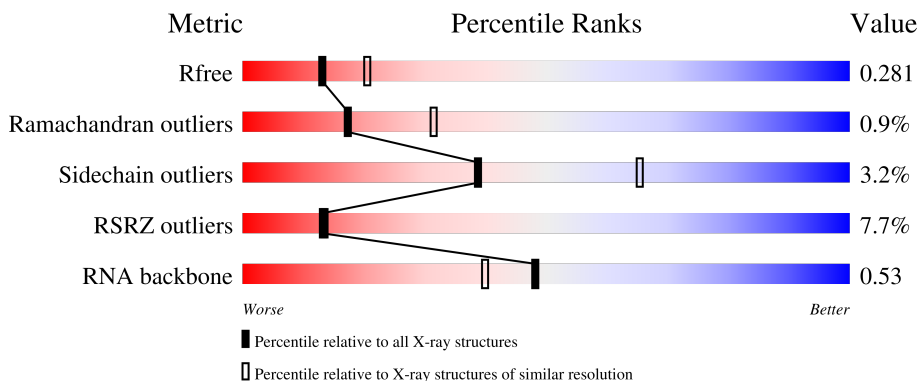
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 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.



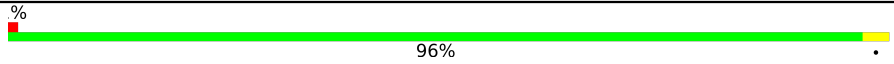
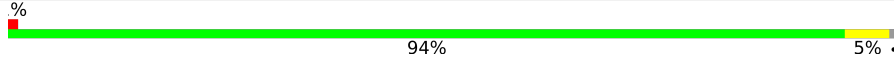
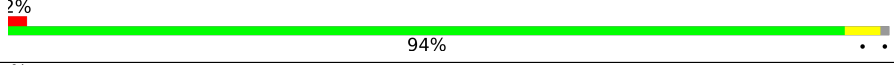
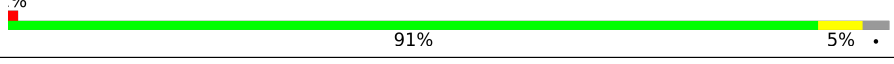
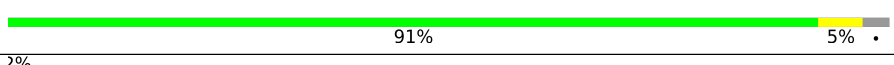
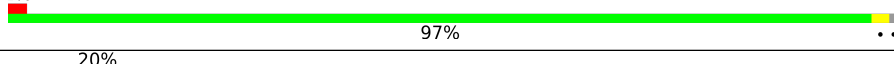
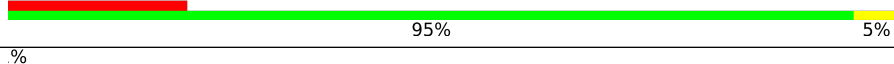
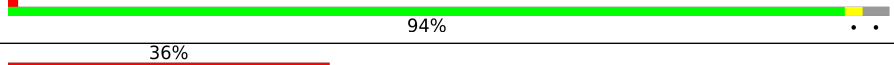
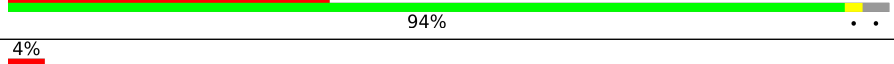
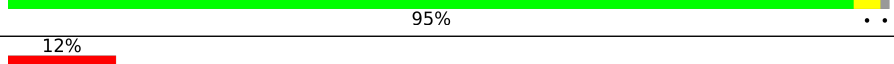
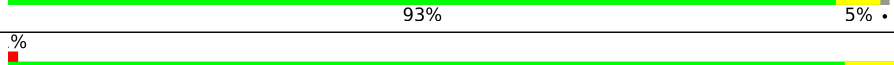
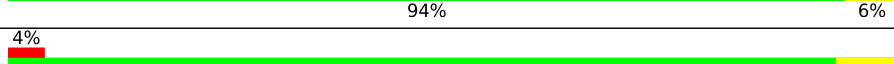
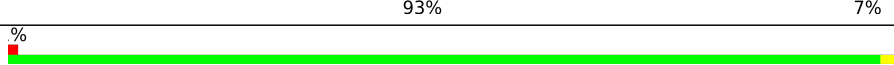
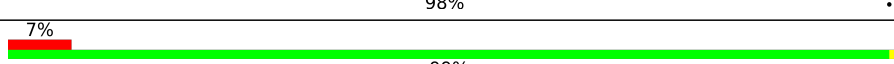
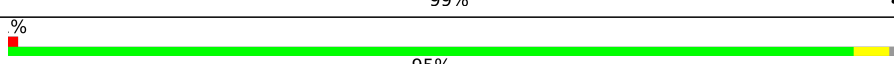
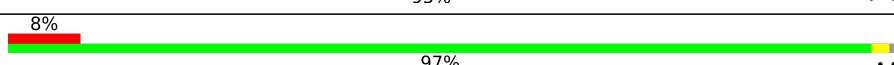
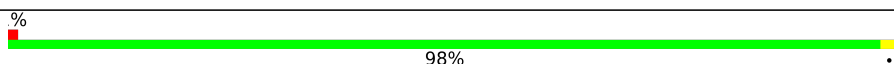
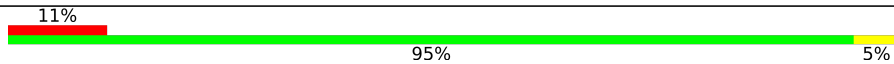
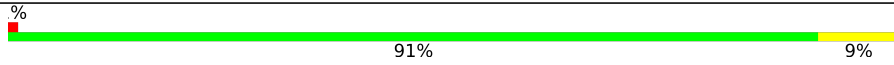
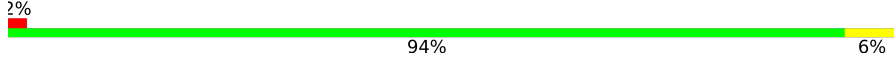
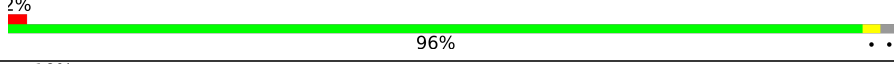
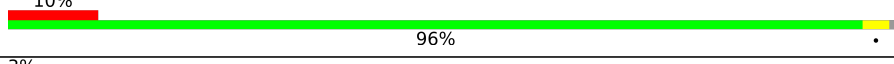
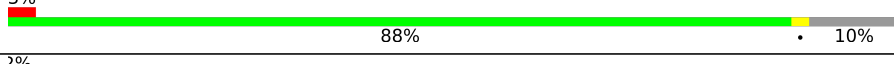
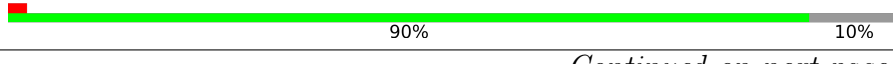

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	4661 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (2.50-2.50)
RSRZ outliers	127900	4559 (2.50-2.50)
RNA backbone	3102	1008 (2.84-2.16)

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 ≥ 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: 81%; 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;">81% 16% ..</p>
1	2A	2915	<div style="display: flex; align-items: center;"> <div style="width: 3%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 77%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 18%; 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;">77% 18% ..</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: 9%; 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% 9% ..</p>
2	2B	121	<div style="display: flex; align-items: center;"> <div style="width: 2%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 68%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 31%; 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;">68% 31% ..</p>
3	1D	276	<div style="display: flex; align-items: center;"> <div style="width: 0%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 97%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 1%; 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;">97% .</p>

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Mol	Chain	Length	Quality of chain
3	2D	276	 96% .
4	1E	206	 94% 5% .
4	2E	206	 94% ..
5	1F	210	 91% 5% .
5	2F	210	 91% 5% .
6	1G	182	 97% ..
6	2G	182	 20% 95% 5% .
7	1H	180	 94% ..
7	2H	180	 36% 94% ..
8	1I	148	 4% 95% ..
8	2I	148	 12% 93% 5% .
9	1N	140	 94% 6% .
9	2N	140	 4% 93% 7% .
10	1O	122	 98% .
10	2O	122	 7% 99% .
11	1P	150	 95% ..
11	2P	150	 8% 97% ..
12	1Q	141	 98% .
12	2Q	141	 11% 95% 5% .
13	1R	118	 91% 9% .
13	2R	118	 2% 94% 6% .
14	1S	112	 2% 96% ..
14	2S	112	 10% 96% ..
15	1T	146	 3% 88% . 10%
15	2T	146	 2% 90% 10%

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Mol	Chain	Length	Quality of chain
16	1U	118	3% 97% ..
16	2U	118	% 97% ..
17	1V	101	% 94% 5% .
17	2V	101	3% 94% 5% .
18	1W	113	% 95% ..
18	2W	113	% 95% ..
19	1X	96	% 97% ..
19	2X	96	2% 97% ...
20	1Y	110	2% 93% 5% .
20	2Y	110	14% 93% 5% .
21	1Z	206	4% 71% 25%
21	2Z	206	21% 77% 22%
22	10	85	4% 94% ...
22	20	85	7% 95% ..
23	11	98	2% 98% ..
23	21	98	6% 97% ..
24	12	72	% 96% ..
24	22	72	% 97% .
25	13	60	% 95% ..
25	23	60	2% 93% 5% .
26	14	71	10% 87% 10% .
26	24	71	20% 86% 11% .
27	15	60	2% 93% 5% .
27	25	60	% 92% 7% .
28	16	54	% 94% ..

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Mol	Chain	Length	Quality of chain
28	26	54	7% 96%
29	17	49	6% 96%
29	27	49	8% 94%
30	18	65	3% 95%
30	28	65	6% 95%
31	19	37	100%
31	29	37	24% 97%
32	1a	1521	3% 82% 16%
32	2a	1521	5% 81% 17%
33	1b	256	5% 86% 10%
33	2b	256	23% 86% 5% 10%
34	1c	239	9% 85% 14%
34	2c	239	33% 84% 14%
35	1d	209	12% 96%
35	2d	209	15% 96%
36	1e	162	9% 88% 9%
36	2e	162	27% 88% 9%
37	1f	101	% 99%
37	2f	101	% 97%
38	1g	156	11% 97%
38	2g	156	15% 96%
39	1h	138	5% 98%
39	2h	138	20% 99%
40	1i	128	18% 96%
40	2i	128	53% 95%

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Mol	Chain	Length	Quality of chain
41	1j	105	13% 88% 5% 8%
41	2j	105	44% 86% 5% 9%
42	1k	129	3% 85% 12%
42	2k	129	4% 87% 12%
43	1l	132	2% 89% 8%
43	2l	132	23% 89% 8%
44	1m	126	6% 97% ..
44	2m	126	30% 95% ..
45	1n	61	16% 90% 8% .
45	2n	61	75% 95% ..
46	1o	89	6% 97% ..
46	2o	89	6% 97% ..
47	1p	88	35% 88% 6% 7%
47	2p	88	10% 89% 5% 7%
48	1q	105	7% 93% 6%
48	2q	105	24% 91% 6%
49	1r	88	6% 76% 23%
49	2r	88	6% 77% 23%
50	1s	93	4% 87% 11%
50	2s	93	40% 84% 5% 11%
51	1t	106	28% 83% 8% 9%
51	2t	106	15% 87% 9%
52	1u	27	26% 85% 15%
52	2u	27	30% 85% 15%
53	1v	24	29% 38% 17% 46%

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Mol	Chain	Length	Quality of chain
53	2v	24	
54	1w	76	
54	1y	76	
54	2w	76	
54	2y	76	
55	1x	77	
55	2x	77	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
56	MG	1U	202	-	-	-	X
56	MG	2A	3716	-	-	-	X
56	MG	2a	3179	-	-	-	X
56	MG	2a	3204	-	-	-	X

2 Entry composition [i](#)

There are 60 unique types of molecules in this entry. The entry contains 300910 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	2871	Total	C	N	O	P	0	0	0
			61852	27531	11572	19878	2871			
1	2A	2800	Total	C	N	O	P	0	0	0
			60322	26848	11284	19390	2800			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
2	1B	120	Total	C	N	O	P	0	0	0
			2577	1146	476	835	120			
2	2B	120	Total	C	N	O	P	0	0	0
			2575	1146	476	833	120			

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			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 1423	C 913	N 253	O 253	S 4	0	0	0
6	2G	181	Total 1428	C 913	N 258	O 253	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	174	Total 1330	C 845	N 248	O 236	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	146	Total 1097	C 701	N 191	O 204	S 1	0	0	0
8	2I	146	Total 1064	C 681	N 186	O 196	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 1117	C 719	N 207	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
			873	550	174	149			
14	2S	110	Total	C	N	O	0	0	0
			870	549	173	148			

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

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

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

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
20	1Y	107	Total	C	N	O	S	0	0	0
			806	517	152	131	6			
20	2Y	107	Total	C	N	O	S	0	0	0
			806	517	152	131	6			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
21	1Z	154	Total	C	N	O	S	0	0	0
			1240	795	222	220	3			
21	2Z	160	Total	C	N	O	S	0	0	0
			1271	814	228	227	2			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
22	10	83	Total	C	N	O	S	0	0	0
			653	404	139	109	1			
22	20	83	Total	C	N	O	S	0	0	0
			653	404	139	109	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
23	11	97	Total	C	N	O	S	0	0	0
			755	475	148	131	1			
23	21	97	Total	C	N	O	S	0	0	0
			755	475	148	131	1			

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
26	14	69	Total	C	N	O	S	0	0	0
			552	349	99	99	5			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
26	24	69	Total	C	N	O	S	0	0	0
			532	339	97	91	5			

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

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

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

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
32	1a	1500	Total	C	N	O	P	0	0	0
			32246	14358	5975	10413	1500			
32	2a	1503	Total	C	N	O	P	0	0	0
			32327	14396	5990	10438	1503			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
33	1b	231	Total	C	N	O	S	0	0	0
			1846	1179	331	331	5			
33	2b	231	Total	C	N	O	S	0	0	0
			1825	1167	326	327	5			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
34	1c	206	Total	C	N	O	S	0	0	0
			1548	973	301	273	1			
34	2c	206	Total	C	N	O	S	0	0	0
			1542	968	300	273	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
35	1d	208	Total	C	N	O	S	0	0	0
			1655	1038	326	284	7			
35	2d	208	Total	C	N	O	S	0	0	0
			1674	1050	333	284	7			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
36	1e	148	Total	C	N	O	S	0	0	0
			1129	714	213	198	4			
36	2e	148	Total	C	N	O	S	0	0	0
			1133	716	214	199	4			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
37	1f	100	Total	C	N	O	S	0	0	0
			810	514	144	149	3			
37	2f	100	Total	C	N	O	S	0	0	0
			816	516	146	151	3			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
38	1g	155	Total	C	N	O	S	0	0	0
			1231	766	243	216	6			
38	2g	155	Total	C	N	O	S	0	0	0
			1235	769	244	216	6			

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

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

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
40	1i	127	Total	C	N	O	0	0	0
			983	623	193	167			
40	2i	127	Total	C	N	O	0	0	0
			978	619	190	169			

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
41	1j	97	Total	C	N	O	0	0	0
			709	440	138	131			
41	2j	96	Total	C	N	O	0	0	0
			714	445	138	131			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
42	1k	114	Total	C	N	O	S	0	0	0
			829	516	155	155	3			

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
44	1m	123	Total	C	N	O	S	0	0	0
			958	592	198	166	2			
44	2m	122	Total	C	N	O	S	0	0	0
			950	586	197	165	2			

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			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	S			
49	1r	68	Total 555	C 355	N 108	O 92	S	0	0	0
49	2r	68	Total 555	C 355	N 108	O 92	S	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 652	C 417	N 120	O 113	S 2	0	0	0
50	2s	83	Total 646	C 412	N 119	O 113	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 728	C 446	N 156	O 124	S 2	0	0	0
51	2t	96	Total 727	C 446	N 155	O 124	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 RNA chain called mRNA.

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

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

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
54	1w	74	Total	C	N	O	P	S	0	0	0
			1592	713	285	518	74	2			
54	1y	74	Total	C	N	O	P	S	0	0	0
			1585	707	285	518	74	1			
54	2w	72	Total	C	N	O	P	S	0	0	0
			1544	690	278	502	72	2			
54	2y	73	Total	C	N	O	P	S	0	0	0
			1565	698	283	510	73	1			

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

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

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
56	1A	1141	Total	Mg	0	0
			1141	1141		
56	1B	37	Total	Mg	0	0
			37	37		
56	1D	12	Total	Mg	0	0
			12	12		
56	1E	11	Total	Mg	0	0
			11	11		
56	1F	8	Total	Mg	0	0
			8	8		
56	1G	5	Total	Mg	0	0
			5	5		
56	1I	1	Total	Mg	0	0
			1	1		
56	1N	6	Total	Mg	0	0
			6	6		

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
56	1O	7	Total Mg 7 7	0	0
56	1P	4	Total Mg 4 4	0	0
56	1Q	6	Total Mg 6 6	0	0
56	1R	3	Total Mg 3 3	0	0
56	1S	3	Total Mg 3 3	0	0
56	1T	2	Total Mg 2 2	0	0
56	1U	8	Total Mg 8 8	0	0
56	1V	3	Total Mg 3 3	0	0
56	1W	5	Total Mg 5 5	0	0
56	1X	6	Total Mg 6 6	0	0
56	1Y	3	Total Mg 3 3	0	0
56	1Z	3	Total Mg 3 3	0	0
56	10	6	Total Mg 6 6	0	0
56	11	3	Total Mg 3 3	0	0
56	12	1	Total Mg 1 1	0	0
56	13	3	Total Mg 3 3	0	0
56	15	2	Total Mg 2 2	0	0
56	16	3	Total Mg 3 3	0	0
56	17	1	Total Mg 1 1	0	0
56	18	3	Total Mg 3 3	0	0
56	19	2	Total Mg 2 2	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
56	1a	229	Total Mg 229 229	0	0
56	1b	2	Total Mg 2 2	0	0
56	1d	1	Total Mg 1 1	0	0
56	1e	1	Total Mg 1 1	0	0
56	1f	2	Total Mg 2 2	0	0
56	1l	3	Total Mg 3 3	0	0
56	1n	2	Total Mg 2 2	0	0
56	1s	1	Total Mg 1 1	0	0
56	1t	1	Total Mg 1 1	0	0
56	1v	1	Total Mg 1 1	0	0
56	1w	11	Total Mg 11 11	0	0
56	1x	16	Total Mg 16 16	0	0
56	1y	4	Total Mg 4 4	0	0
56	2A	909	Total Mg 909 909	0	0
56	2B	21	Total Mg 21 21	0	0
56	2D	5	Total Mg 5 5	0	0
56	2E	9	Total Mg 9 9	0	0
56	2F	4	Total Mg 4 4	0	0
56	2G	1	Total Mg 1 1	0	0
56	2N	1	Total Mg 1 1	0	0
56	2O	1	Total Mg 1 1	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
56	2P	1	Total Mg 1 1	0	0
56	2Q	3	Total Mg 3 3	0	0
56	2R	1	Total Mg 1 1	0	0
56	2T	3	Total Mg 3 3	0	0
56	2U	4	Total Mg 4 4	0	0
56	2V	1	Total Mg 1 1	0	0
56	2W	3	Total Mg 3 3	0	0
56	2X	3	Total Mg 3 3	0	0
56	2Y	1	Total Mg 1 1	0	0
56	2Z	1	Total Mg 1 1	0	0
56	20	3	Total Mg 3 3	0	0
56	23	2	Total Mg 2 2	0	0
56	25	4	Total Mg 4 4	0	0
56	27	1	Total Mg 1 1	0	0
56	28	2	Total Mg 2 2	0	0
56	2a	244	Total Mg 244 244	0	0
56	2d	1	Total Mg 1 1	0	0
56	2e	1	Total Mg 1 1	0	0
56	2f	1	Total Mg 1 1	0	0
56	2g	1	Total Mg 1 1	0	0
56	2i	1	Total Mg 1 1	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
56	2j	2	Total Mg 2 2	0	0
56	2l	2	Total Mg 2 2	0	0
56	2n	1	Total Mg 1 1	0	0
56	2q	2	Total Mg 2 2	0	0
56	2r	2	Total Mg 2 2	0	0
56	2t	1	Total Mg 1 1	0	0
56	2v	2	Total Mg 2 2	0	0
56	2w	8	Total Mg 8 8	0	0
56	2x	5	Total Mg 5 5	0	0
56	2y	7	Total Mg 7 7	0	0

- Molecule 57 is POTASSIUM ION (three-letter code: K) (formula: K).

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

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

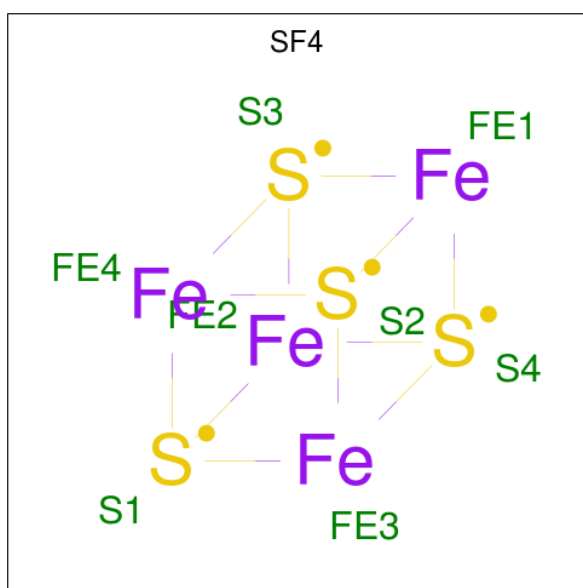
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
58	1Y	1	Total Zn 1 1	0	0
58	14	1	Total Zn 1 1	0	0
58	15	1	Total Zn 1 1	0	0
58	16	1	Total Zn 1 1	0	0
58	19	1	Total Zn 1 1	0	0

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

- Molecule 59 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe₄S₄).



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

- Molecule 60 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
60	1A	2238	Total O 2238 2238	0	0
60	1B	68	Total O 68 68	0	0
60	1D	28	Total O 28 28	0	0
60	1E	28	Total O 28 28	0	0
60	1F	13	Total O 13 13	0	0
60	1G	7	Total O 7 7	0	0
60	1H	2	Total O 2 2	0	0
60	1I	3	Total O 3 3	0	0
60	1N	7	Total O 7 7	0	0
60	1O	8	Total O 8 8	0	0
60	1P	23	Total O 23 23	0	0
60	1Q	14	Total O 14 14	0	0
60	1R	14	Total O 14 14	0	0
60	1S	5	Total O 5 5	0	0
60	1T	8	Total O 8 8	0	0
60	1U	11	Total O 11 11	0	0
60	1V	9	Total O 9 9	0	0
60	1W	6	Total O 6 6	0	0
60	1X	8	Total O 8 8	0	0
60	1Y	4	Total O 4 4	0	0
60	1Z	1	Total O 1 1	0	0
60	10	12	Total O 12 12	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
60	11	10	Total O 10 10	0	0
60	12	4	Total O 4 4	0	0
60	13	6	Total O 6 6	0	0
60	14	1	Total O 1 1	0	0
60	15	6	Total O 6 6	0	0
60	16	3	Total O 3 3	0	0
60	17	9	Total O 9 9	0	0
60	18	13	Total O 13 13	0	0
60	1a	438	Total O 438 438	0	0
60	1b	1	Total O 1 1	0	0
60	1d	1	Total O 1 1	0	0
60	1e	1	Total O 1 1	0	0
60	1f	1	Total O 1 1	0	0
60	1g	1	Total O 1 1	0	0
60	1i	1	Total O 1 1	0	0
60	1l	8	Total O 8 8	0	0
60	1m	2	Total O 2 2	0	0
60	1o	1	Total O 1 1	0	0
60	1p	1	Total O 1 1	0	0
60	1q	4	Total O 4 4	0	0
60	1u	1	Total O 1 1	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
60	1v	5	Total O 5 5	0	0
60	1w	21	Total O 21 21	0	0
60	1x	15	Total O 15 15	0	0
60	1y	1	Total O 1 1	0	0
60	2A	1389	Total O 1389 1389	0	0
60	2B	26	Total O 26 26	0	0
60	2D	28	Total O 28 28	0	0
60	2E	16	Total O 16 16	0	0
60	2F	16	Total O 16 16	0	0
60	2H	1	Total O 1 1	0	0
60	2I	4	Total O 4 4	0	0
60	2N	1	Total O 1 1	0	0
60	2P	14	Total O 14 14	0	0
60	2Q	2	Total O 2 2	0	0
60	2R	2	Total O 2 2	0	0
60	2T	6	Total O 6 6	0	0
60	2U	2	Total O 2 2	0	0
60	2V	2	Total O 2 2	0	0
60	2W	2	Total O 2 2	0	0
60	2X	5	Total O 5 5	0	0
60	2Y	1	Total O 1 1	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
60	2Z	2	Total O 2 2	0	0
60	20	7	Total O 7 7	0	0
60	21	12	Total O 12 12	0	0
60	22	1	Total O 1 1	0	0
60	23	1	Total O 1 1	0	0
60	25	4	Total O 4 4	0	0
60	26	1	Total O 1 1	0	0
60	27	4	Total O 4 4	0	0
60	28	6	Total O 6 6	0	0
60	29	1	Total O 1 1	0	0
60	2a	377	Total O 377 377	0	0
60	2d	1	Total O 1 1	0	0
60	2e	2	Total O 2 2	0	0
60	2g	1	Total O 1 1	0	0
60	2i	1	Total O 1 1	0	0
60	2j	4	Total O 4 4	0	0
60	2l	5	Total O 5 5	0	0
60	2o	1	Total O 1 1	0	0
60	2p	2	Total O 2 2	0	0
60	2q	1	Total O 1 1	0	0
60	2r	1	Total O 1 1	0	0

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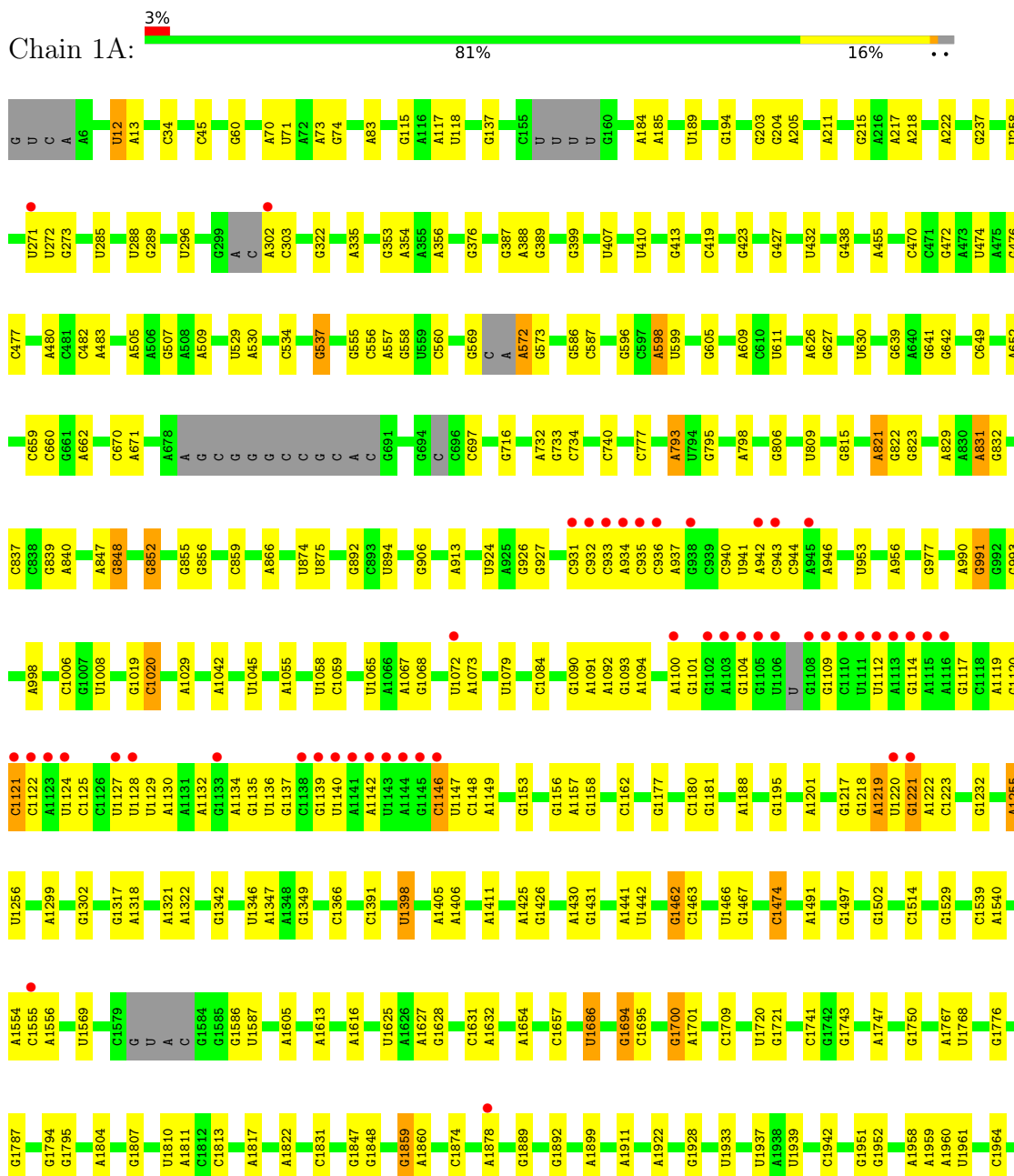
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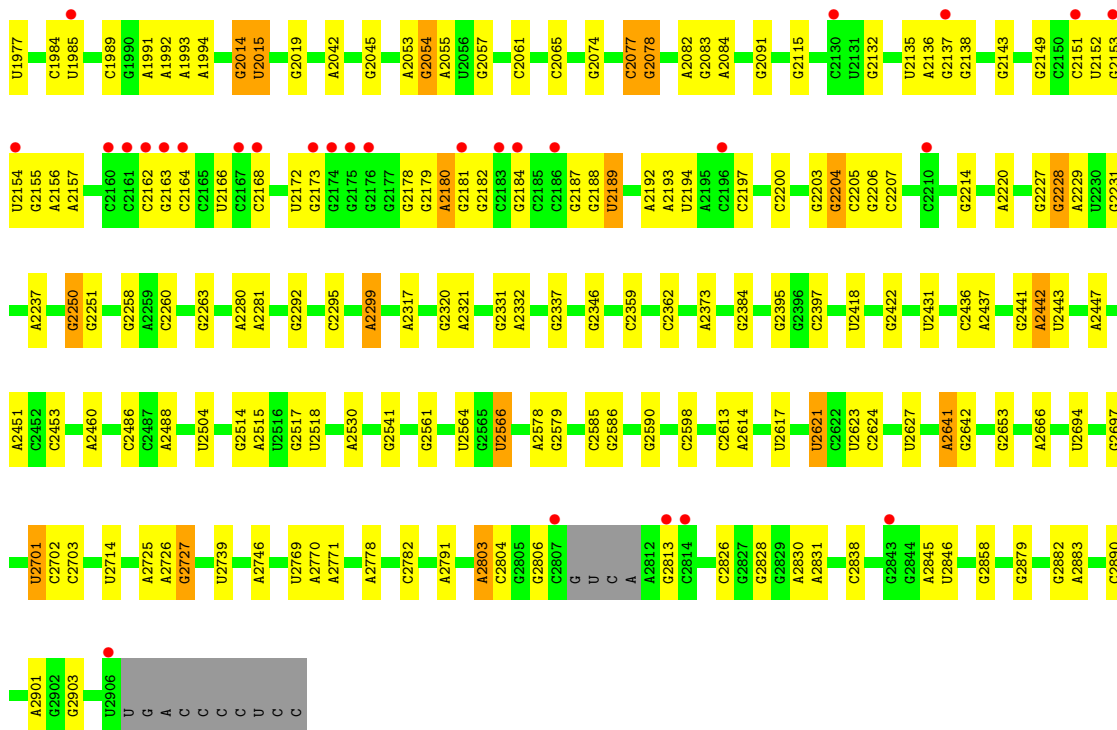
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
60	2t	4	Total O 4 4	0	0
60	2u	1	Total O 1 1	0	0
60	2v	1	Total O 1 1	0	0
60	2w	2	Total O 2 2	0	0
60	2x	7	Total O 7 7	0	0
60	2y	19	Total O 19 19	0	0

3 Residue-property plots

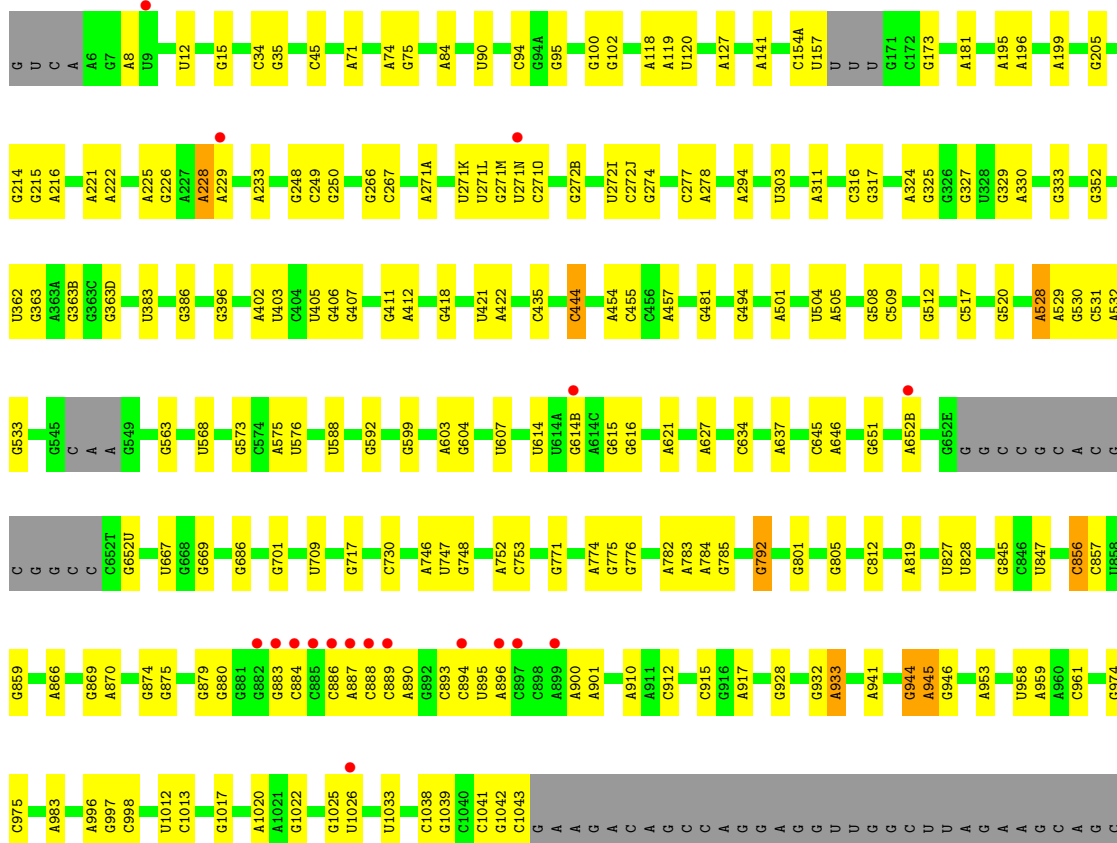
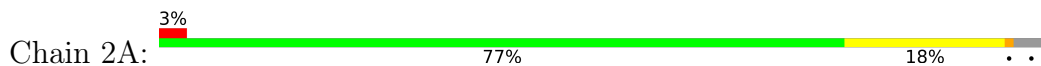
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

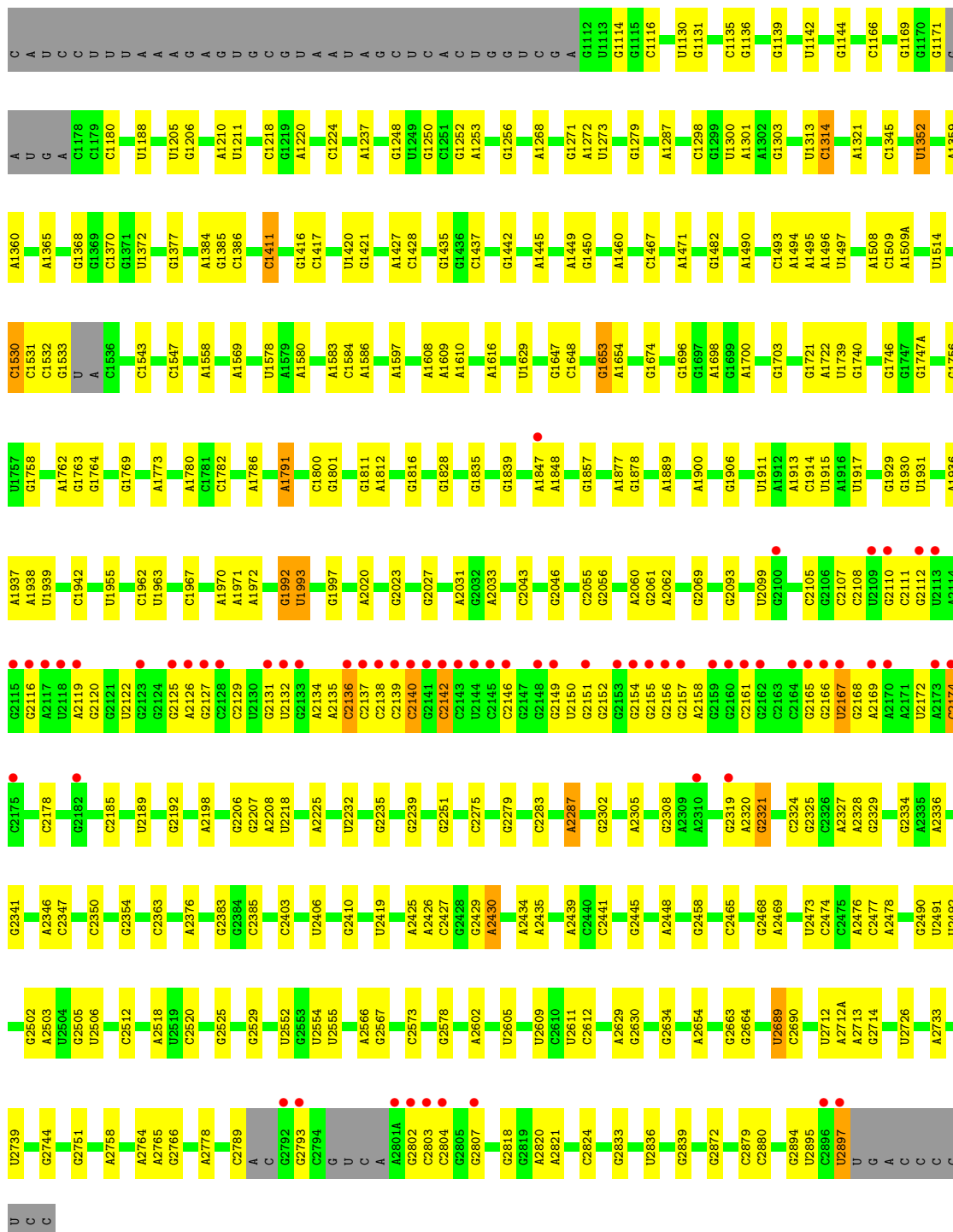
- Molecule 1: 23S Ribosomal RNA



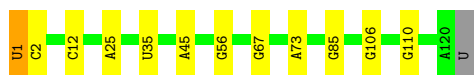
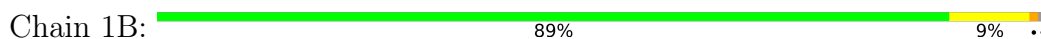


• Molecule 1: 23S Ribosomal RNA

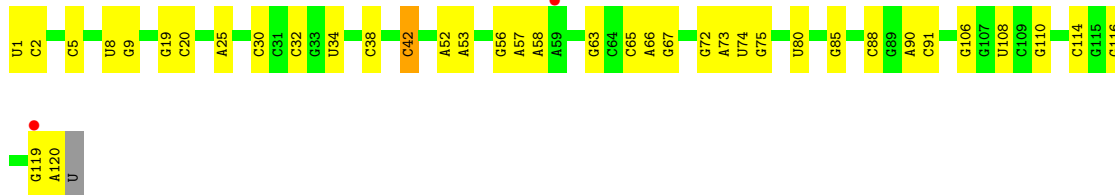




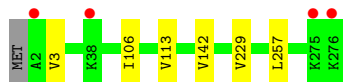
● Molecule 2: 5S Ribosomal RNA



● Molecule 2: 5S Ribosomal RNA



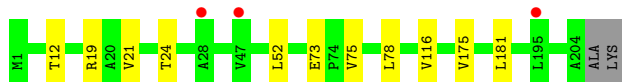
- Molecule 3: 50S ribosomal protein L2



- Molecule 3: 50S ribosomal protein L2



- Molecule 4: 50S ribosomal protein L3



- Molecule 4: 50S ribosomal protein L3



- Molecule 5: 50S ribosomal protein L4

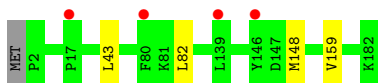


- Molecule 5: 50S ribosomal protein L4

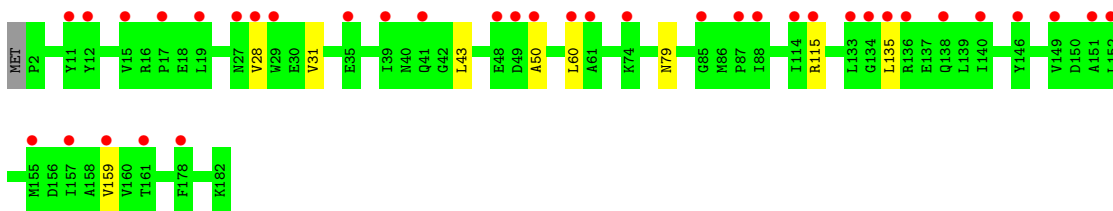




- Molecule 6: 50S ribosomal protein L5



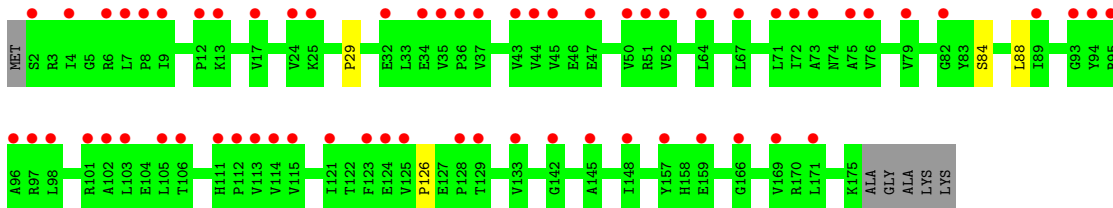
- Molecule 6: 50S ribosomal protein L5



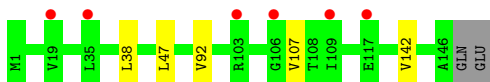
- Molecule 7: 50S ribosomal protein L6



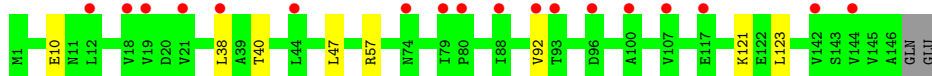
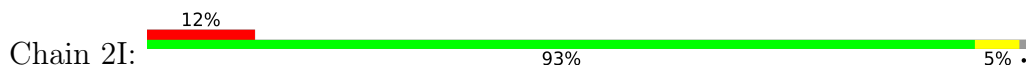
- Molecule 7: 50S ribosomal protein L6



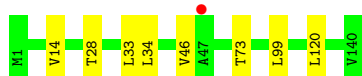
- Molecule 8: 50S ribosomal protein L9



- Molecule 8: 50S ribosomal protein L9



- Molecule 9: 50S ribosomal protein L13



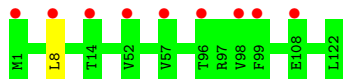
- Molecule 9: 50S ribosomal protein L13



- Molecule 10: 50S ribosomal protein L14



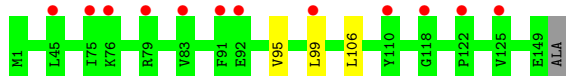
- Molecule 10: 50S ribosomal protein L14



- Molecule 11: 50S ribosomal protein L15



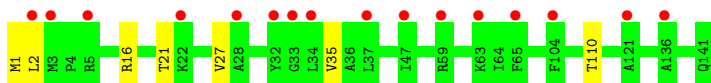
- Molecule 11: 50S ribosomal protein L15



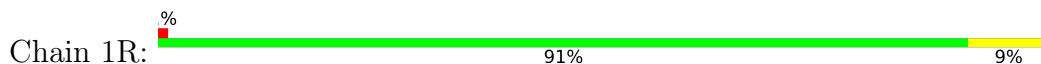
- Molecule 12: 50S ribosomal protein L16



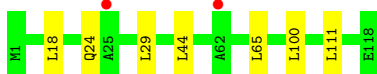
- Molecule 12: 50S ribosomal protein L16



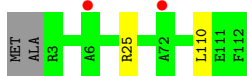
- Molecule 13: 50S ribosomal protein L17



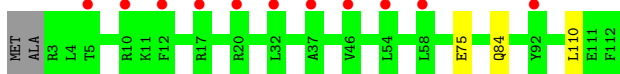
- Molecule 13: 50S ribosomal protein L17



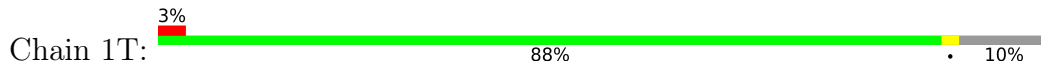
- Molecule 14: 50S ribosomal protein L18

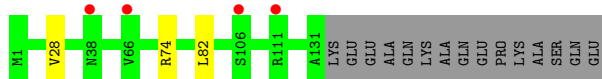


- Molecule 14: 50S ribosomal protein L18

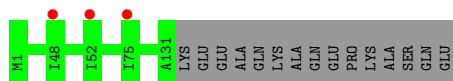


- Molecule 15: 50S ribosomal protein L19





- Molecule 15: 50S ribosomal protein L19



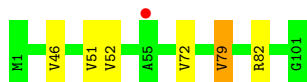
- Molecule 16: 50S ribosomal protein L20



- Molecule 16: 50S ribosomal protein L20



- Molecule 17: 50S ribosomal protein L21



- Molecule 17: 50S ribosomal protein L21

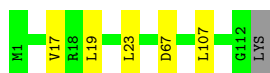


- Molecule 18: 50S ribosomal protein L22



- Molecule 18: 50S ribosomal protein L22

Chain 2W:  95%



• Molecule 19: 50S ribosomal protein L23

Chain 1X:  97%

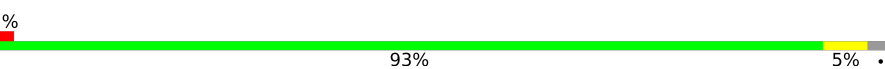


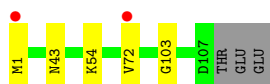
• Molecule 19: 50S ribosomal protein L23

Chain 2X:  97%

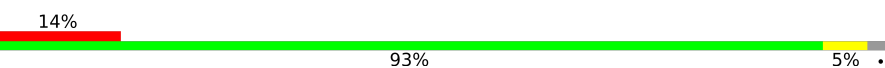


• Molecule 20: 50S ribosomal protein L24

Chain 1Y:  93%



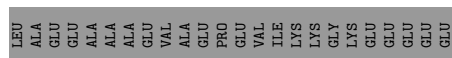
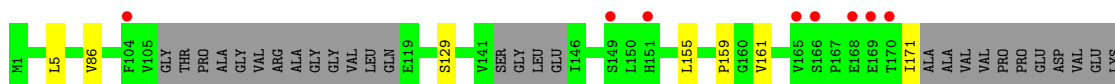
• Molecule 20: 50S ribosomal protein L24

Chain 2Y:  93%




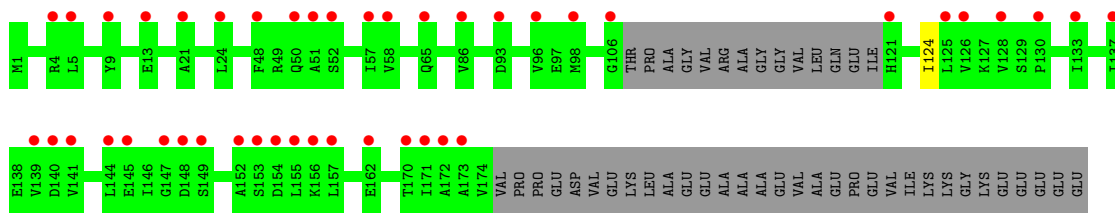
• Molecule 21: 50S ribosomal protein L25

Chain 1Z:  71%

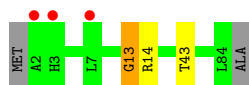


• Molecule 21: 50S ribosomal protein L25

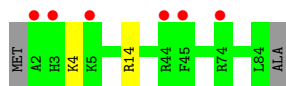
Chain 2Z:  77%



• Molecule 22: 50S ribosomal protein L27



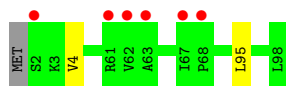
• Molecule 22: 50S ribosomal protein L27



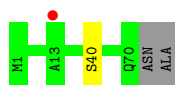
• Molecule 23: 50S ribosomal protein L28



• Molecule 23: 50S ribosomal protein L28



• Molecule 24: 50S ribosomal protein L29



• Molecule 24: 50S ribosomal protein L29





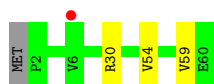
- Molecule 25: 50S ribosomal protein L30

Chain 13: 95%



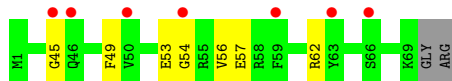
- Molecule 25: 50S ribosomal protein L30

Chain 23: 93%



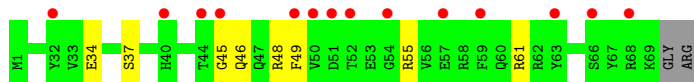
- Molecule 26: 50S ribosomal protein L31

Chain 14: 87%



- Molecule 26: 50S ribosomal protein L31

Chain 24: 86%



- Molecule 27: 50S ribosomal protein L32

Chain 15: 93%



- Molecule 27: 50S ribosomal protein L32

Chain 25: 92%



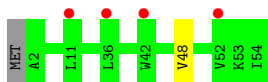
- Molecule 28: 50S ribosomal protein L33

Chain 16:  94% ..



- Molecule 28: 50S ribosomal protein L33

Chain 26:  96% ..



- Molecule 29: 50S ribosomal protein L34

Chain 17:  96% ..



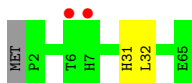
- Molecule 29: 50S ribosomal protein L34

Chain 27:  94% ..



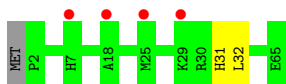
- Molecule 30: 50S ribosomal protein L35

Chain 18:  95% ..



- Molecule 30: 50S ribosomal protein L35

Chain 28:  95% ..

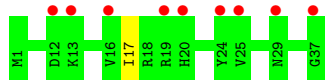


- Molecule 31: 50S ribosomal protein L36

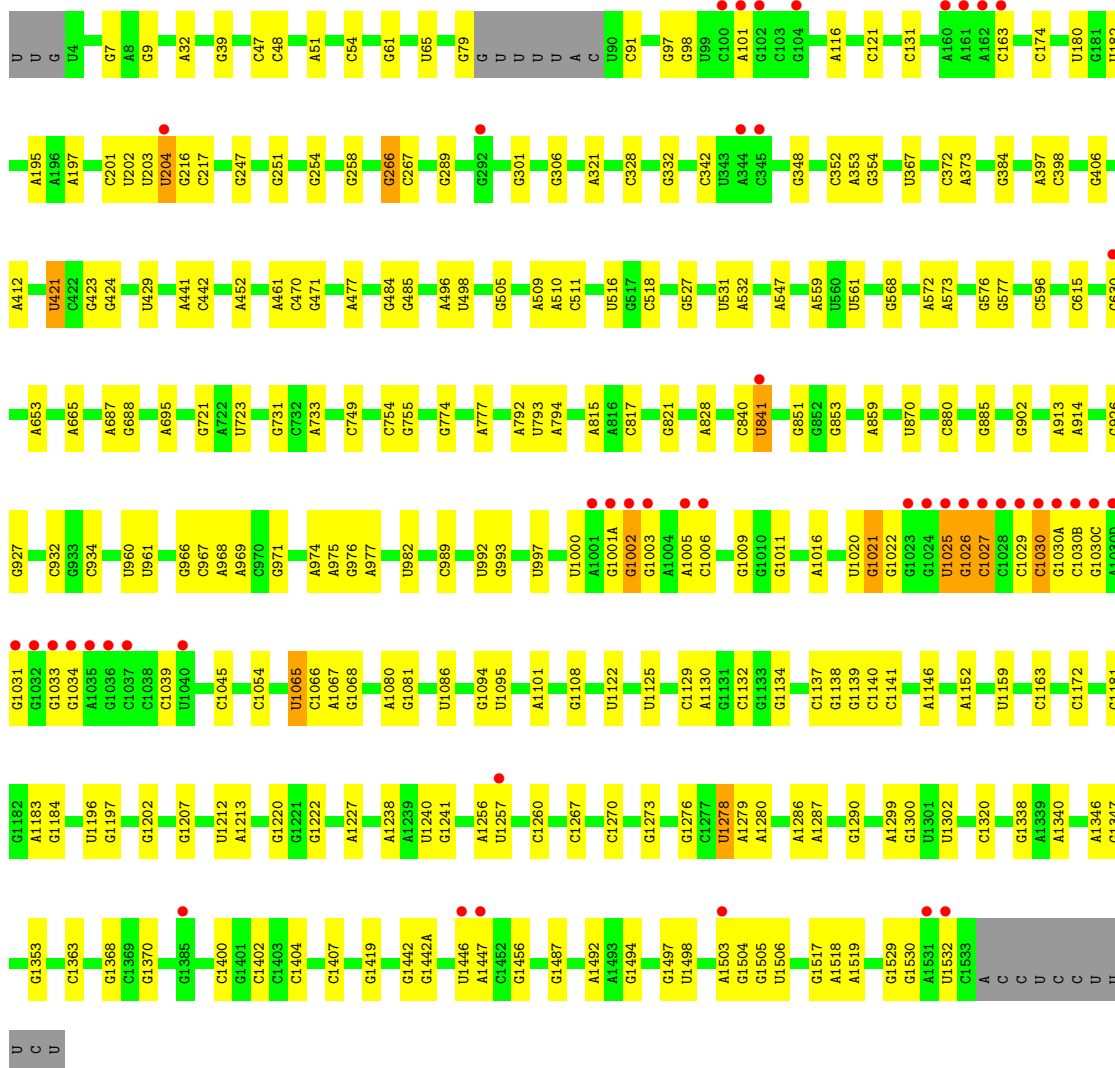
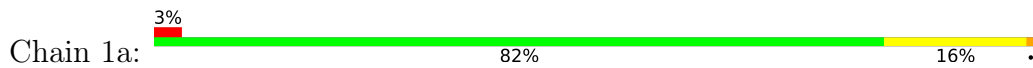
Chain 19:  100%

There are no outlier residues recorded for this chain.

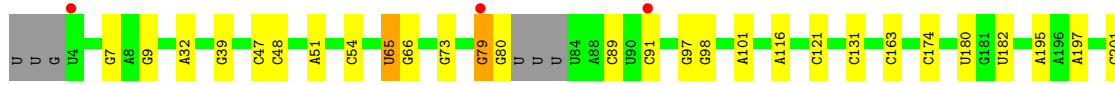
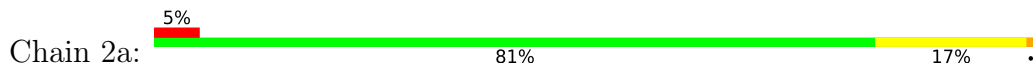
- Molecule 31: 50S ribosomal protein L36

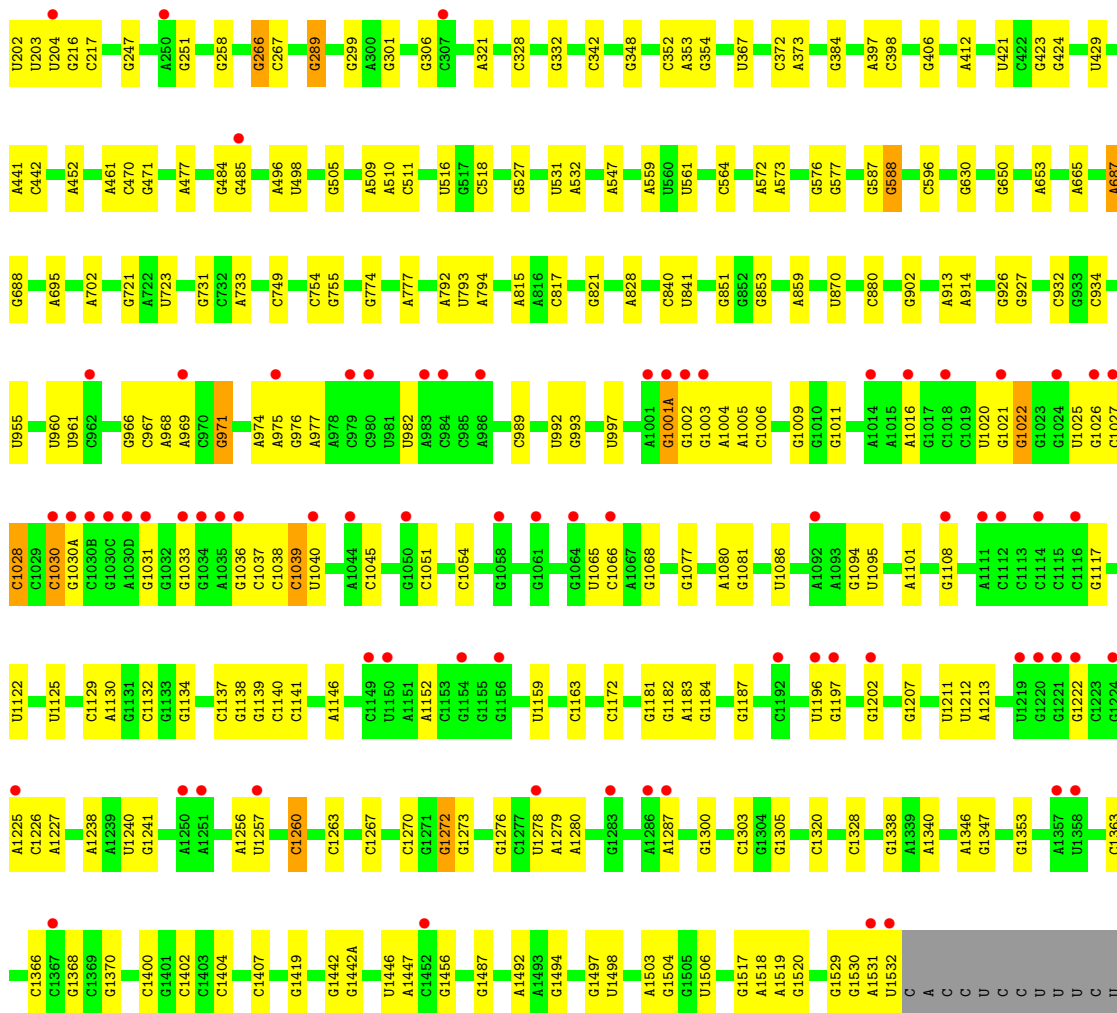


• Molecule 32: 16S Ribosomal RNA

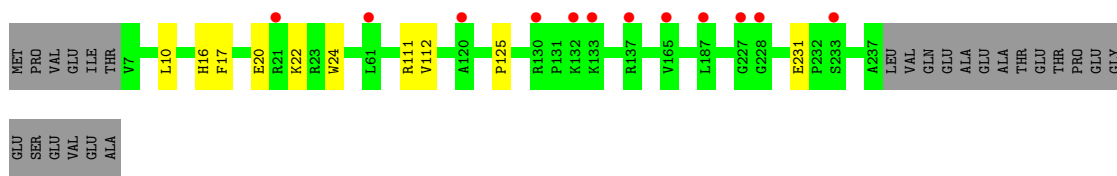
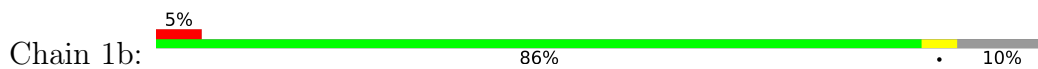


• Molecule 32: 16S Ribosomal RNA

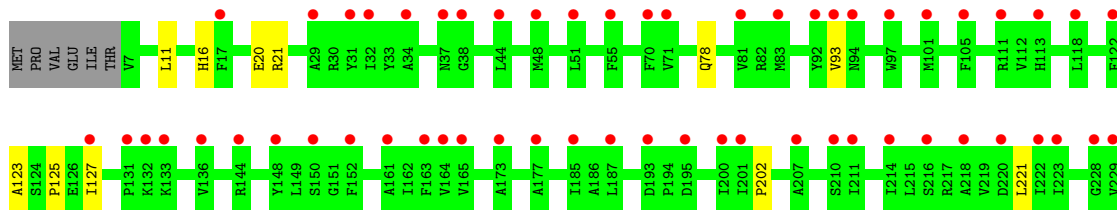
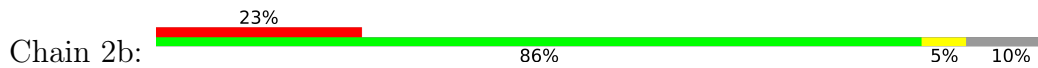


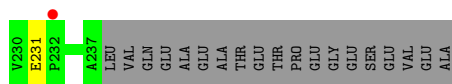


• Molecule 33: 30S ribosomal protein S2

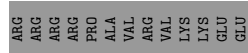
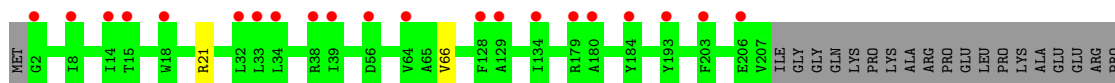
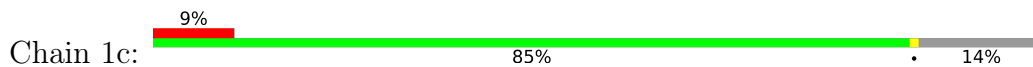


• Molecule 33: 30S ribosomal protein S2

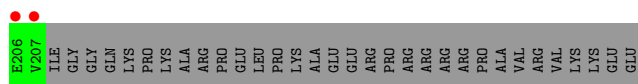
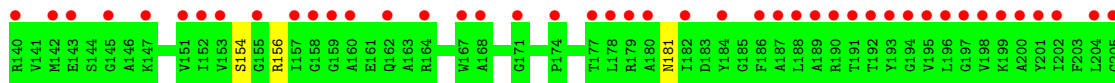
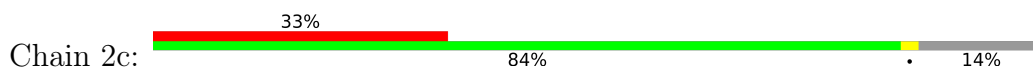




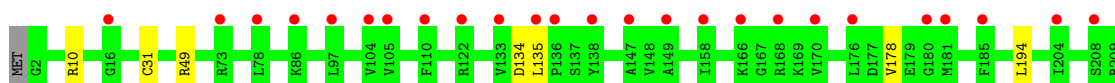
- Molecule 34: 30S ribosomal protein S3



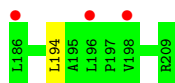
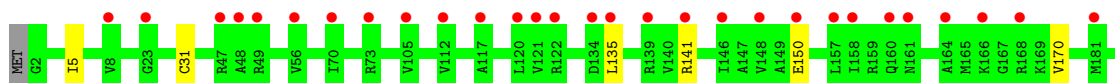
- Molecule 34: 30S ribosomal protein S3



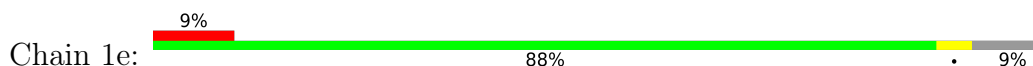
- Molecule 35: 30S ribosomal protein S4



- Molecule 35: 30S ribosomal protein S4

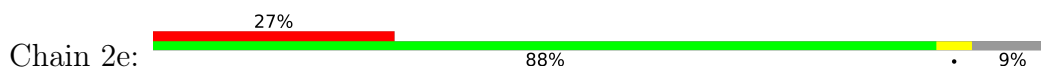


- Molecule 36: 30S ribosomal protein S5

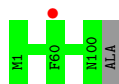




- Molecule 36: 30S ribosomal protein S5



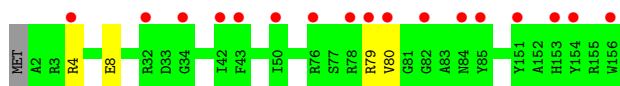
- Molecule 37: 30S ribosomal protein S6



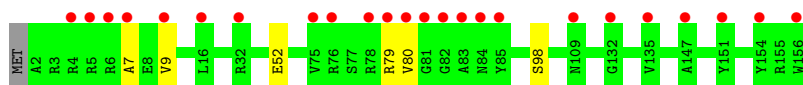
- Molecule 37: 30S ribosomal protein S6



- Molecule 38: 30S ribosomal protein S7

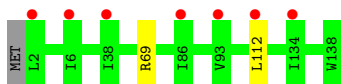


- Molecule 38: 30S ribosomal protein S7

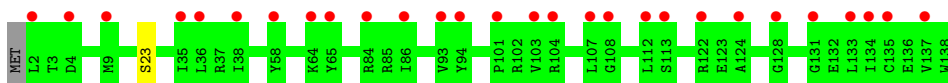


- Molecule 39: 30S ribosomal protein S8

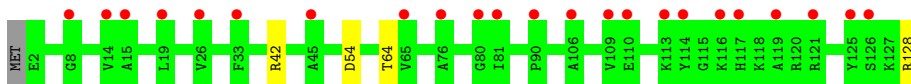




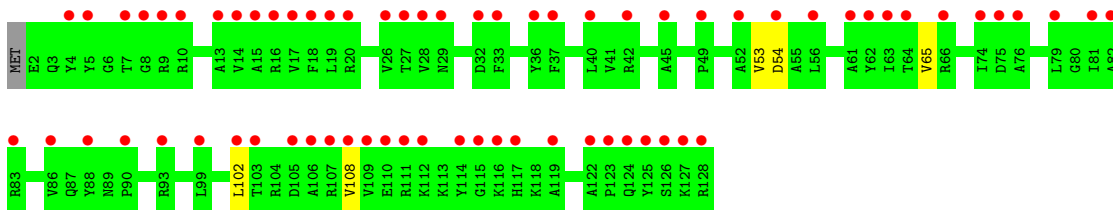
- Molecule 39: 30S ribosomal protein S8



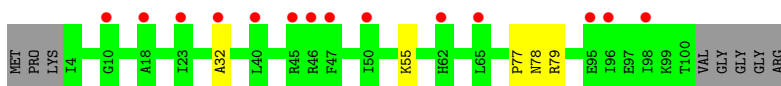
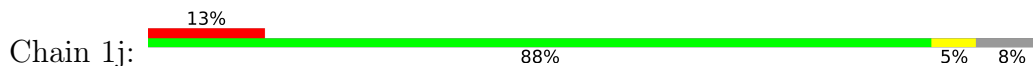
- Molecule 40: 30S ribosomal protein S9



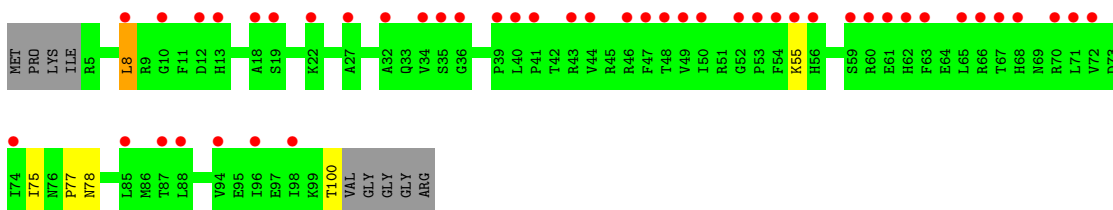
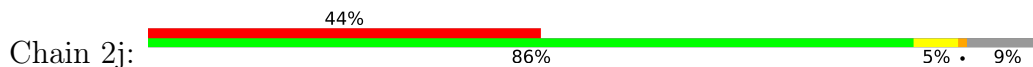
- Molecule 40: 30S ribosomal protein S9



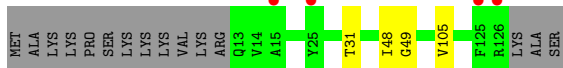
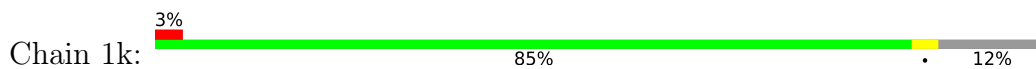
- Molecule 41: 30S ribosomal protein S10



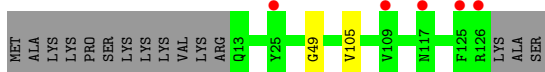
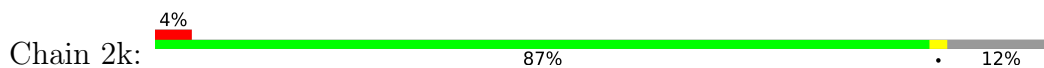
- Molecule 41: 30S ribosomal protein S10



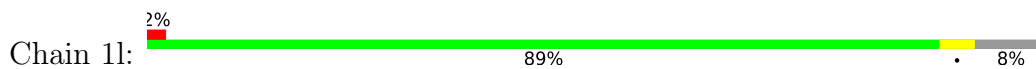
- Molecule 42: 30S ribosomal protein S11



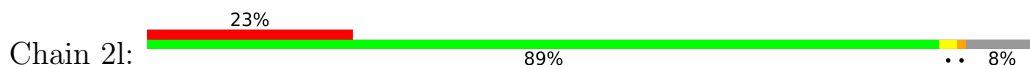
- Molecule 42: 30S ribosomal protein S11



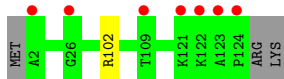
- Molecule 43: 30S ribosomal protein S12



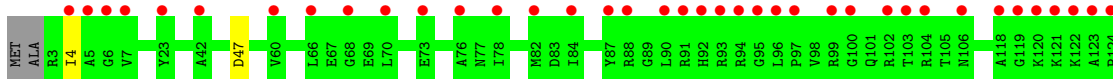
- Molecule 43: 30S ribosomal protein S12



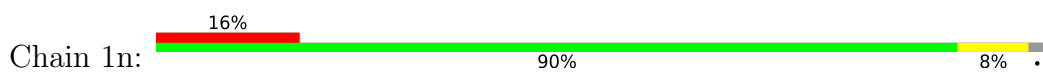
- Molecule 44: 30S ribosomal protein S13



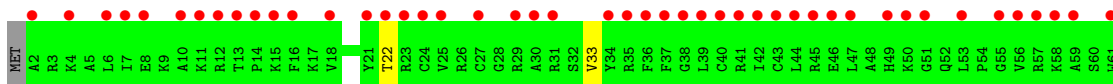
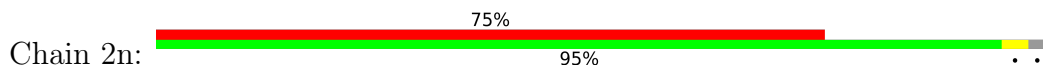
- Molecule 44: 30S ribosomal protein S13



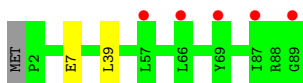
- Molecule 45: 30S ribosomal protein S14 type Z



- Molecule 45: 30S ribosomal protein S14 type Z



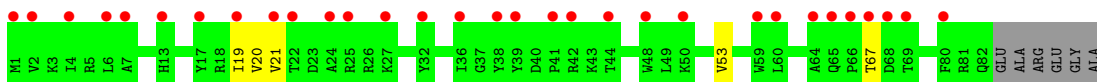
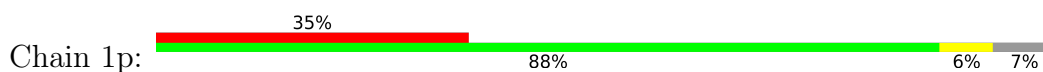
- Molecule 46: 30S ribosomal protein S15



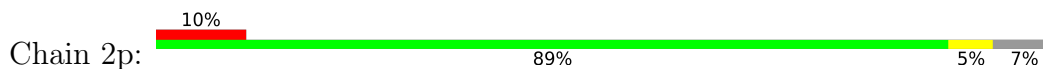
- Molecule 46: 30S ribosomal protein S15



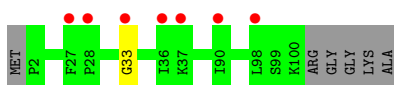
- Molecule 47: 30S ribosomal protein S16



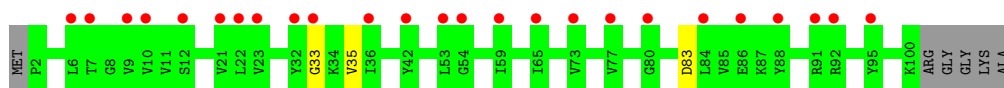
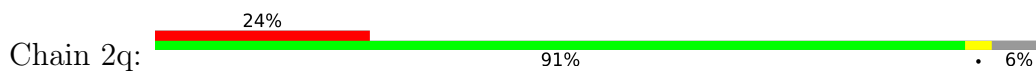
- Molecule 47: 30S ribosomal protein S16



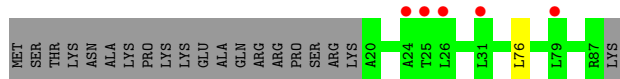
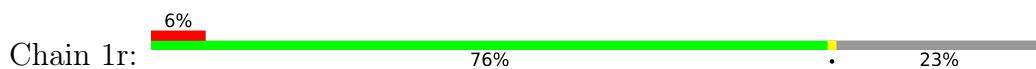
- Molecule 48: 30S ribosomal protein S17



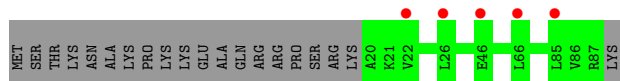
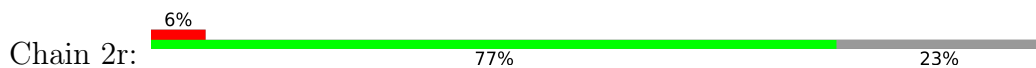
- Molecule 48: 30S ribosomal protein S17



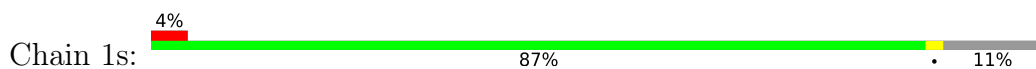
- Molecule 49: 30S ribosomal protein S18



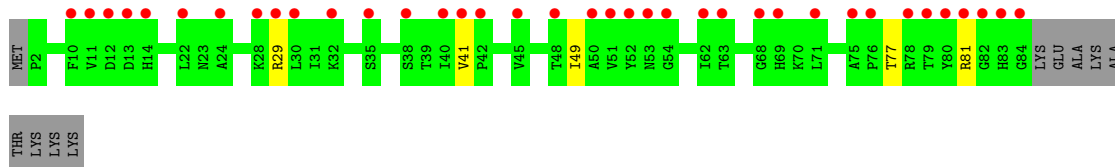
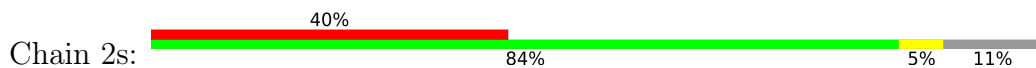
- Molecule 49: 30S ribosomal protein S18



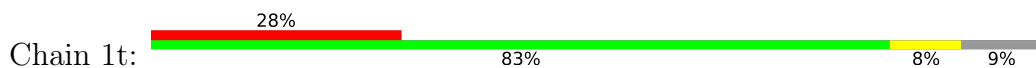
- Molecule 50: 30S ribosomal protein S19



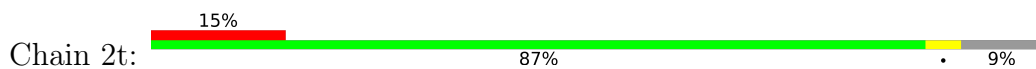
- Molecule 50: 30S ribosomal protein S19

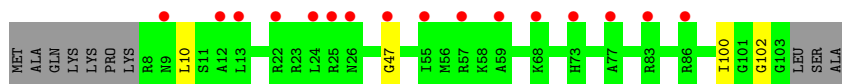


- Molecule 51: 30S ribosomal protein S20

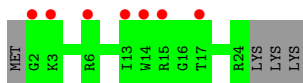
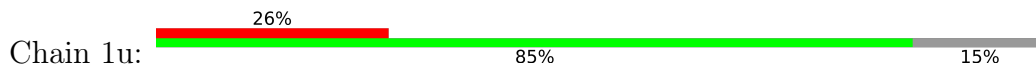


- Molecule 51: 30S ribosomal protein S20

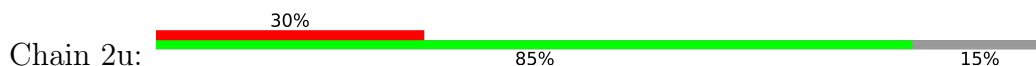




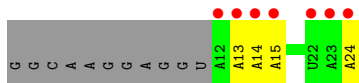
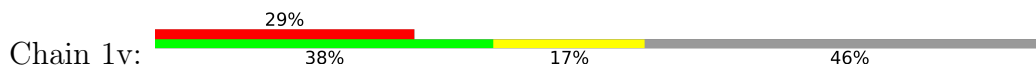
- Molecule 52: 30S ribosomal protein Thx



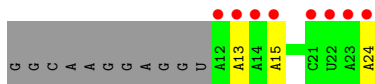
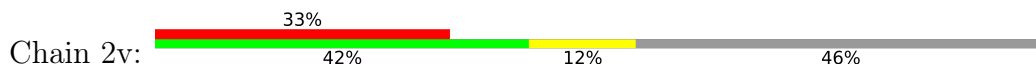
- Molecule 52: 30S ribosomal protein Thx



- Molecule 53: mRNA



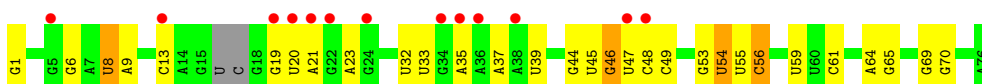
- Molecule 53: mRNA



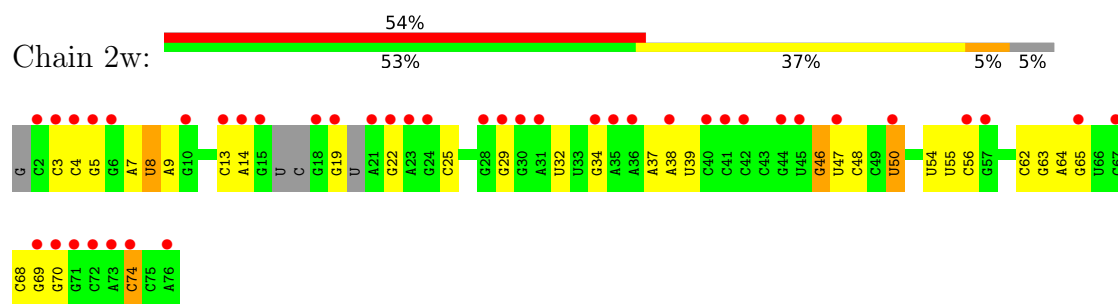
- Molecule 54: A-site and E-site tRNAs



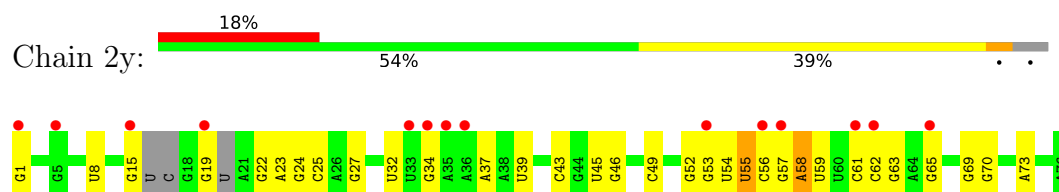
- Molecule 54: A-site and E-site tRNAs



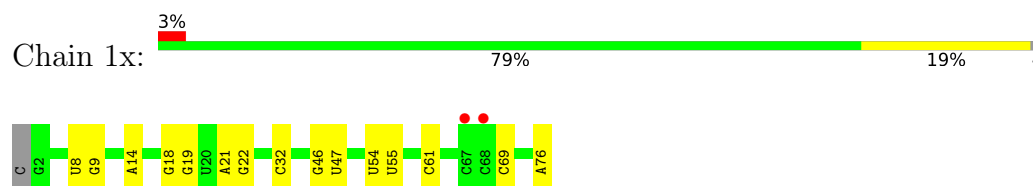
- Molecule 54: A-site and E-site tRNAs



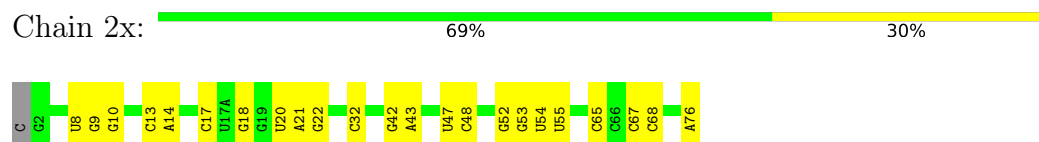
- Molecule 54: A-site and E-site tRNAs



- Molecule 55: P-site tRNA



- Molecule 55: P-site tRNA



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	209.70Å 450.05Å 624.09Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	122.01 – 2.50 198.78 – 2.50	Depositor EDS
% Data completeness (in resolution range)	97.8 (122.01-2.50) 97.8 (198.78-2.50)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.22 (at 2.52Å)	Xtrriage
Refinement program	PHENIX (phenix.refine: 1.8.2_1309)	Depositor
R, R_{free}	0.231 , 0.281 0.231 , 0.281	Depositor DCC
R_{free} test set	98495 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å ²)	47.4	Xtrriage
Anisotropy	0.174	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 57.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.41$, $\langle L^2 \rangle = 0.23$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	300910	wwPDB-VP
Average B, all atoms (Å ²)	60.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.58% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

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, 4OC, MA6, SF4, 2MU, MG, 5MU, 2MG, 2MA, 7MG, K, ZN, PSU, 4SU, 5MC, MIA, 0TD, M2G

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	0.61	0/69009	1.05	129/107712 (0.1%)
1	2A	0.52	1/67293 (0.0%)	1.03	84/105034 (0.1%)
2	1B	0.51	1/2882 (0.0%)	0.87	0/4494
2	2B	0.59	1/2879 (0.0%)	1.01	4/4487 (0.1%)
3	1D	0.44	0/2186	0.61	0/2944
3	2D	0.38	0/2186	0.61	0/2944
4	1E	0.43	0/1592	0.61	0/2149
4	2E	0.37	0/1592	0.59	0/2149
5	1F	0.40	0/1619	0.58	0/2193
5	2F	0.37	0/1615	0.58	0/2188
6	1G	0.34	0/1448	0.54	0/1957
6	2G	0.36	0/1453	0.58	0/1963
7	1H	0.36	0/1356	0.55	0/1834
7	2H	0.33	0/1356	0.55	0/1834
8	1I	0.31	0/1112	0.55	0/1514
8	2I	0.30	0/1079	0.54	0/1475
9	1N	0.39	0/1144	0.57	0/1543
9	2N	0.36	0/1144	0.58	0/1543
10	1O	0.42	0/943	0.58	0/1269
10	2O	0.35	0/943	0.54	0/1269
11	1P	0.39	0/1152	0.60	0/1533
11	2P	0.36	0/1152	0.62	0/1533
12	1Q	0.41	0/1143	0.57	0/1527
12	2Q	0.37	0/1143	0.60	0/1527
13	1R	0.43	0/982	0.63	0/1312
13	2R	0.38	0/982	0.60	0/1312
14	1S	0.34	0/883	0.56	0/1176
14	2S	0.38	0/880	0.59	0/1172
15	1T	0.39	0/1105	0.61	1/1477 (0.1%)
15	2T	0.36	0/1097	0.59	0/1468
16	1U	0.46	0/977	0.62	0/1301

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
16	2U	0.39	0/977	0.60	0/1301
17	1V	0.45	0/782	0.62	0/1049
17	2V	0.35	0/782	0.59	0/1049
18	1W	0.45	0/897	0.66	0/1205
18	2W	0.39	0/897	0.58	0/1205
19	1X	0.44	0/764	0.61	0/1025
19	2X	0.40	0/764	0.63	1/1025 (0.1%)
20	1Y	0.39	0/819	0.57	0/1095
20	2Y	0.35	0/819	0.56	0/1095
21	1Z	0.35	0/1267	0.59	0/1717
21	2Z	0.31	0/1299	0.53	0/1763
22	10	0.43	0/662	0.66	1/881 (0.1%)
22	20	0.33	0/662	0.56	0/881
23	11	0.39	0/762	0.58	0/1014
23	21	0.35	0/762	0.57	0/1014
24	12	0.35	0/590	0.56	0/781
24	22	0.33	0/590	0.51	0/781
25	13	0.41	0/474	0.60	0/635
25	23	0.33	0/469	0.57	0/630
26	14	0.35	0/565	0.69	1/761 (0.1%)
26	24	0.37	0/545	0.64	0/737
27	15	0.42	0/469	0.64	0/635
27	25	0.38	0/469	0.60	1/635 (0.2%)
28	16	0.44	0/460	0.56	0/613
28	26	0.35	0/456	0.51	0/608
29	17	0.44	0/426	0.70	0/561
29	27	0.42	0/426	0.66	0/561
30	18	0.41	0/525	0.59	0/691
30	28	0.39	0/525	0.60	0/691
31	19	0.42	0/310	0.60	0/407
31	29	0.38	0/310	0.60	0/407
32	1a	0.43	0/35795	0.92	40/55864 (0.1%)
32	2a	0.45	3/35886 (0.0%)	0.98	62/56005 (0.1%)
33	1b	0.31	0/1881	0.59	0/2542
33	2b	0.34	0/1860	0.57	0/2518
34	1c	0.28	0/1572	0.49	0/2126
34	2c	0.34	0/1566	0.55	0/2119
35	1d	0.31	0/1685	0.54	0/2262
35	2d	0.31	0/1704	0.52	0/2284
36	1e	0.31	0/1145	0.55	0/1543
36	2e	0.34	0/1149	0.61	0/1548
37	1f	0.32	0/823	0.53	0/1115
37	2f	0.32	0/829	0.51	0/1123

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
38	1g	0.29	0/1250	0.52	0/1679
38	2g	0.31	0/1254	0.54	0/1683
39	1h	0.30	0/1108	0.54	0/1494
39	2h	0.30	0/1108	0.55	0/1494
40	1i	0.31	0/1002	0.59	0/1346
40	2i	0.32	0/997	0.56	0/1343
41	1j	0.30	0/722	0.54	0/982
41	2j	0.34	0/727	0.59	1/988 (0.1%)
42	1k	0.30	0/844	0.55	0/1145
42	2k	0.31	0/848	0.52	0/1149
43	1l	0.34	0/937	0.54	0/1260
43	2l	0.32	0/937	0.59	1/1260 (0.1%)
44	1m	0.32	0/969	0.57	0/1302
44	2m	0.31	0/961	0.57	0/1291
45	1n	0.33	0/501	0.51	0/664
45	2n	0.31	0/501	0.53	0/664
46	1o	0.30	0/739	0.49	0/985
46	2o	0.30	0/739	0.51	0/985
47	1p	0.31	0/697	0.54	0/939
47	2p	0.31	0/693	0.53	0/935
48	1q	0.33	0/836	0.55	0/1117
48	2q	0.31	0/836	0.52	0/1117
49	1r	0.32	0/560	0.53	0/746
49	2r	0.30	0/560	0.51	0/746
50	1s	0.29	0/667	0.58	0/900
50	2s	0.38	0/661	0.66	0/893
51	1t	0.28	0/730	0.53	0/965
51	2t	0.30	0/729	0.54	0/965
52	1u	0.27	0/203	0.46	0/266
52	2u	0.34	0/203	0.50	0/266
53	1v	0.46	0/310	0.93	0/480
53	2v	0.60	0/310	0.91	0/480
54	1w	0.57	1/1606 (0.1%)	1.10	3/2497 (0.1%)
54	1y	0.56	1/1606 (0.1%)	1.13	9/2497 (0.4%)
54	2w	0.53	0/1556	1.12	2/2418 (0.1%)
54	2y	0.59	1/1583 (0.1%)	1.17	4/2459 (0.2%)
55	1x	0.57	3/1725 (0.2%)	1.16	16/2689 (0.6%)
55	2x	0.49	0/1725	1.06	8/2689 (0.3%)
All	All	0.49	12/316686 (0.0%)	0.92	368/474113 (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
43	2l	0	1

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
54	2y	1	G	OP3-P	-10.21	1.48	1.61
2	1B	1	U	OP3-P	-10.20	1.49	1.61
54	1y	1	G	OP3-P	-10.20	1.49	1.61
2	2B	1	U	OP3-P	-9.87	1.49	1.61
54	1w	1	G	OP3-P	-9.63	1.49	1.61
32	2a	1272	G	N1-C2	-9.38	1.30	1.37
32	2a	1272	G	C6-N1	-8.82	1.33	1.39
55	1x	14	A	N7-C5	-5.80	1.35	1.39
55	1x	22	G	N7-C5	5.47	1.42	1.39
32	2a	1263	C	N3-C4	-5.32	1.30	1.33
1	2A	2287	A	N9-C4	-5.20	1.34	1.37
55	1x	14	A	C8-N7	-5.06	1.28	1.31

All (368) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	2a	1263	C	N1-C2-O2	22.29	132.27	118.90
32	2a	1272	G	N3-C2-N2	21.80	135.16	119.90
32	2a	1272	G	C5-C6-O6	20.59	140.96	128.60
32	2a	1272	G	N1-C2-N2	-18.95	99.14	116.20
32	2a	1263	C	C2-N3-C4	15.04	127.42	119.90
1	1A	1686	U	O5'-P-OP2	-14.11	93.01	105.70
32	2a	1263	C	N3-C2-O2	-12.82	112.93	121.90
1	1A	1121	C	N1-C2-O2	12.15	126.19	118.90
32	2a	1272	G	N1-C6-O6	-12.10	112.64	119.90
32	2a	1272	G	C6-N1-C2	12.00	132.30	125.10
32	2a	1263	C	C5-C6-N1	11.97	126.99	121.00
1	1A	1132	A	N1-C6-N6	-11.68	111.59	118.60
1	1A	1109	G	C5-C6-O6	10.74	135.04	128.60
32	2a	1272	G	C5-C6-N1	-10.27	106.37	111.50
1	1A	1121	C	C2-N3-C4	10.09	124.94	119.90
55	1x	14	A	C4-C5-C6	10.08	122.04	117.00
1	1A	599	U	O5'-P-OP1	-10.05	96.65	105.70
32	2a	1263	C	C6-N1-C2	-9.80	116.38	120.30
1	1A	1020	C	N1-C2-O2	-9.76	113.04	118.90
1	1A	1807	G	O5'-P-OP2	-9.76	96.92	105.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
55	1x	14	A	C5-N7-C8	9.62	108.71	103.90
1	1A	611	U	O5'-P-OP2	-9.61	97.05	105.70
2	2B	80	U	O4'-C1'-N1	9.56	115.85	108.20
55	1x	46	G	C6-N1-C2	-9.00	119.70	125.10
32	1a	1034	G	N3-C2-N2	8.56	125.89	119.90
1	1A	2189	U	C2-N1-C1'	8.55	127.96	117.70
1	1A	1109	G	C6-N1-C2	8.53	130.22	125.10
1	1A	1398	U	O5'-P-OP1	-8.49	98.06	105.70
1	1A	537	G	O4'-C1'-N9	8.48	114.98	108.20
1	2A	2136	C	N1-C2-O2	8.47	123.98	118.90
1	2A	2473	U	C2-N1-C1'	8.45	127.84	117.70
32	2a	1001(A)	G	N3-C4-N9	8.41	131.04	126.00
1	1A	649	C	O5'-P-OP1	-8.39	98.15	105.70
32	1a	1030(B)	C	C2-N1-C1'	8.36	128.00	118.80
32	1a	1034	G	N9-C4-C5	-8.27	102.09	105.40
1	2A	1352	U	O5'-P-OP1	-8.26	98.27	105.70
54	1y	33	U	C2-N1-C1'	8.22	127.57	117.70
32	2a	1272	G	C2-N3-C4	-8.21	107.79	111.90
32	2a	1039	C	C5-C4-N4	-8.12	114.52	120.20
32	2a	79	G	C5-C6-O6	8.08	133.45	128.60
1	1A	1121	C	N3-C2-O2	-8.02	116.29	121.90
32	2a	1263	C	C4-C5-C6	-7.98	113.41	117.40
1	1A	848	G	O5'-P-OP2	-7.90	98.59	105.70
1	2A	2149	G	N3-C4-N9	7.89	130.74	126.00
32	2a	1263	C	C2-N1-C1'	7.83	127.42	118.80
32	1a	1030(B)	C	C6-N1-C2	-7.82	117.17	120.30
1	1A	798	A	O5'-P-OP1	-7.75	98.73	105.70
1	2A	2492	U	O5'-P-OP1	-7.74	98.74	105.70
19	2X	57	LEU	CA-CB-CG	7.70	133.00	115.30
32	2a	1263	C	C5-C4-N4	7.69	125.58	120.20
55	2x	14	A	C4-C5-C6	7.67	120.83	117.00
32	2a	1272	G	C4-N9-C1'	7.64	136.44	126.50
55	1x	22	G	C5-N7-C8	-7.57	100.52	104.30
32	2a	1272	G	C8-N9-C1'	-7.56	117.17	127.00
32	2a	1039	C	C2-N1-C1'	7.56	127.11	118.80
1	1A	2189	U	N1-C2-O2	7.55	128.09	122.80
1	1A	1232	G	N1-C6-O6	-7.54	115.37	119.90
1	1A	2504	U	O5'-P-OP1	-7.53	98.93	105.70
55	1x	14	A	C5-C6-N1	-7.51	113.95	117.70
55	1x	22	G	C4-C5-C6	-7.46	114.33	118.80
1	1A	2189	U	N3-C2-O2	-7.43	117.00	122.20
1	1A	2260	C	O5'-P-OP2	-7.39	99.05	105.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	1a	254	G	O5'-P-OP1	-7.30	99.13	105.70
1	1A	821	A	C8-N9-C4	-7.29	102.88	105.80
55	2x	14	A	C5-N7-C8	7.28	107.54	103.90
54	1y	56	C	N1-C2-O2	7.24	123.24	118.90
1	2A	801	G	O5'-P-OP2	-7.23	99.19	105.70
1	1A	1045	U	O5'-P-OP2	-7.19	99.23	105.70
32	1a	1034	G	C4-C5-N7	7.18	113.67	110.80
32	1a	1030	C	N1-C2-O2	7.08	123.15	118.90
32	1a	1034	G	C6-N1-C2	7.04	129.33	125.10
1	1A	1132	A	C5-C6-N6	7.03	129.32	123.70
32	2a	754	C	C2-N1-C1'	7.03	126.53	118.80
32	1a	1027	C	N3-C2-O2	-6.99	117.00	121.90
54	1y	33	U	N1-C2-O2	6.97	127.68	122.80
1	2A	2139	C	C2-N1-C1'	6.92	126.41	118.80
1	1A	2077	C	OP1-P-O3'	6.91	120.41	105.20
32	1a	1027	C	N3-C4-C5	-6.87	119.15	121.90
32	1a	1002	G	N3-C4-N9	6.82	130.09	126.00
32	1a	1034	G	N3-C4-N9	6.80	130.08	126.00
32	1a	1034	G	C8-N9-C1'	-6.76	118.21	127.00
1	2A	512	G	O4'-C1'-N9	6.75	113.60	108.20
1	1A	1020	C	C2-N1-C1'	-6.75	111.38	118.80
1	1A	2014	G	P-O3'-C3'	6.74	127.79	119.70
1	1A	1121	C	C6-N1-C2	-6.72	117.61	120.30
32	2a	1039	C	C6-N1-C1'	-6.70	112.76	120.80
1	2A	2473	U	N1-C2-O2	6.69	127.49	122.80
1	1A	2015	U	O5'-P-OP1	-6.67	99.70	105.70
32	2a	1004	A	N7-C8-N9	6.67	117.14	113.80
32	2a	754	C	N1-C2-O2	6.65	122.89	118.90
32	1a	1002	G	C4-N9-C1'	6.64	135.14	126.50
32	2a	1263	C	N1-C2-N3	-6.64	114.55	119.20
1	1A	840	A	O5'-P-OP2	-6.64	99.72	105.70
32	1a	1025	U	N1-C2-O2	6.64	127.44	122.80
1	1A	993	G	O5'-P-OP1	-6.63	99.73	105.70
1	2A	2492	U	O5'-P-OP2	6.56	118.57	110.70
1	1A	2727	G	O5'-P-OP2	-6.56	99.80	105.70
1	1A	215	G	O4'-C1'-N9	6.52	113.42	108.20
32	1a	1027	C	C5-C4-N4	6.51	124.76	120.20
32	1a	1002	G	C8-N9-C1'	-6.50	118.55	127.00
1	2A	2136	C	N3-C2-O2	-6.48	117.36	121.90
1	2A	2149	G	C8-N9-C1'	-6.48	118.58	127.00
1	2A	2149	G	C4-N9-C1'	6.47	134.91	126.50
54	1w	47	U	C2-N1-C1'	6.47	125.46	117.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1A	892	G	O4'-C1'-N9	6.45	113.36	108.20
1	1A	2566	U	O5'-P-OP1	-6.41	99.93	105.70
1	1A	1128	U	N3-C4-C5	6.39	118.43	114.60
32	2a	1263	C	N3-C4-N4	-6.38	113.53	118.00
32	1a	1034	G	C4-N9-C1'	6.35	134.76	126.50
1	2A	2149	G	N9-C4-C5	-6.35	102.86	105.40
54	1y	64	A	C5-C6-N6	6.35	128.78	123.70
1	2A	1698	A	O4'-C1'-N9	6.33	113.27	108.20
1	1A	1221	G	OP1-P-O3'	6.33	119.12	105.20
1	2A	1131	G	O4'-C1'-N9	6.32	113.26	108.20
1	1A	1121	C	C5-C4-N4	6.32	124.62	120.20
1	2A	2897	U	C2-N1-C1'	6.32	125.28	117.70
32	2a	588	G	O5'-P-OP2	-6.27	100.06	105.70
1	1A	1109	G	N3-C2-N2	6.26	124.28	119.90
1	1A	2054	G	C5-N7-C8	6.22	107.41	104.30
32	2a	1037	C	C6-N1-C2	-6.21	117.81	120.30
1	1A	2694	U	O5'-P-OP2	-6.19	100.13	105.70
1	1A	806	G	C5-C6-O6	-6.19	124.89	128.60
1	2A	2473	U	N3-C2-O2	-6.17	117.88	122.20
32	1a	1030(B)	C	C5-C6-N1	6.17	124.09	121.00
1	1A	1958	A	O4'-C1'-N9	6.16	113.13	108.20
1	2A	2430	A	O4'-C1'-N9	6.16	113.13	108.20
1	1A	809	U	C5-C4-O4	-6.15	122.21	125.90
55	1x	46	G	C5-C6-N1	6.15	114.57	111.50
54	1y	64	A	N1-C6-N6	-6.14	114.92	118.60
1	1A	1859	G	O5'-P-OP2	-6.13	100.19	105.70
54	2y	58	A	OP1-P-O3'	6.12	118.66	105.20
55	1x	22	G	C8-N9-C1'	6.11	134.95	127.00
32	1a	841	U	C5-C6-N1	6.11	125.75	122.70
1	1A	2180	A	N1-C2-N3	6.10	132.35	129.30
1	1A	2641	A	P-O3'-C3'	6.10	127.02	119.70
32	2a	1001(A)	G	N9-C4-C5	-6.10	102.96	105.40
1	2A	576	U	O5'-P-OP1	-6.09	100.22	105.70
54	1w	22	G	N1-C6-O6	6.05	123.53	119.90
1	2A	2174	C	C2-N1-C1'	6.05	125.45	118.80
32	2a	1366	C	C2-N3-C4	6.03	122.92	119.90
54	2y	22	G	N1-C6-O6	6.03	123.52	119.90
55	2x	14	A	C5-C6-N1	-6.03	114.69	117.70
1	2A	614	U	N3-C2-O2	-6.03	117.98	122.20
1	1A	2803	A	C2-N3-C4	6.00	113.60	110.60
1	2A	928	G	C8-N9-C4	-5.99	104.00	106.40
1	1A	572	A	P-O3'-C3'	5.98	126.87	119.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	2a	1039	C	N1-C2-O2	5.98	122.49	118.90
32	1a	266	G	P-O3'-C3'	5.97	126.87	119.70
1	1A	2180	A	P-O3'-C3'	5.97	126.86	119.70
1	2A	1372	U	C5-C4-O4	-5.96	122.32	125.90
1	2A	1314	C	C5-C6-N1	5.96	123.98	121.00
1	2A	783	A	C2-N3-C4	5.94	113.57	110.60
1	2A	2140	C	C2-N1-C1'	5.93	125.33	118.80
32	1a	1030	C	C2-N3-C4	5.92	122.86	119.90
55	1x	22	G	N3-C4-N9	-5.92	122.45	126.00
1	1A	1109	G	N1-C6-O6	-5.91	116.36	119.90
1	1A	894	U	C2-N1-C1'	5.89	124.77	117.70
32	2a	1187	G	N3-C4-N9	-5.89	122.47	126.00
1	1A	476	G	N1-C6-O6	-5.88	116.37	119.90
1	1A	605	G	C5-C6-O6	5.88	132.13	128.60
1	1A	1020	C	C6-N1-C1'	5.87	127.84	120.80
1	2A	2363	C	C6-N1-C2	5.87	122.65	120.30
32	2a	1039	C	N3-C4-N4	5.87	122.11	118.00
32	1a	1278	U	C5-C6-N1	5.87	125.63	122.70
1	1A	852	G	N9-C4-C5	-5.87	103.05	105.40
1	2A	1313	U	C2-N1-C1'	5.86	124.73	117.70
32	1a	1030(B)	C	N1-C2-O2	5.85	122.41	118.90
1	1A	2826	C	C6-N1-C2	-5.83	117.97	120.30
1	2A	2149	G	C6-C5-N7	-5.83	126.90	130.40
54	2w	50	U	C5-C4-O4	-5.82	122.41	125.90
32	2a	1030	C	N1-C2-O2	5.82	122.39	118.90
1	1A	2627	U	O5'-P-OP1	-5.81	100.47	105.70
1	2A	2139	C	C6-N1-C1'	-5.80	113.83	120.80
1	1A	1109	G	C5-C6-N1	-5.80	108.60	111.50
1	1A	1121	C	N3-C4-C5	-5.79	119.58	121.90
15	1T	82	LEU	CA-CB-CG	-5.79	101.99	115.30
1	1A	2858	G	O4'-C1'-N9	5.78	112.83	108.20
1	1A	2431	U	N3-C4-O4	-5.77	115.36	119.40
1	2A	1993	U	O5'-P-OP1	-5.76	100.51	105.70
55	1x	14	A	C8-N9-C1'	-5.76	117.33	127.70
1	1A	1121	C	C2-N1-C1'	5.75	125.13	118.80
55	2x	20	U	N1-C2-O2	5.75	126.83	122.80
55	1x	22	G	C5-C6-N1	5.75	114.38	111.50
1	2A	944	G	C4-N9-C1'	5.75	133.97	126.50
32	2a	266	G	N3-C4-C5	-5.74	125.73	128.60
1	1A	1232	G	C5-C6-O6	5.74	132.04	128.60
1	2A	2473	U	C6-N1-C1'	-5.74	113.17	121.20
32	2a	1054	C	C2-N1-C1'	5.73	125.11	118.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	2A	2689	U	P-O3'-C3'	5.72	126.57	119.70
1	2A	1992	G	P-O3'-C3'	5.72	126.56	119.70
1	1A	1121	C	C5-C6-N1	5.71	123.86	121.00
55	1x	22	G	N3-C4-C5	5.71	131.45	128.60
1	2A	856	C	C6-N1-C2	-5.70	118.02	120.30
1	1A	12	U	C2-N1-C1'	5.69	124.53	117.70
54	1y	33	U	N3-C2-O2	-5.69	118.22	122.20
32	2a	1225	A	C5-C6-N6	5.69	128.25	123.70
1	1A	1720	U	C5-C6-N1	-5.66	119.87	122.70
32	1a	1034	G	C6-C5-N7	-5.66	127.00	130.40
32	2a	299	G	C5-C6-O6	-5.66	125.21	128.60
55	2x	20	U	N3-C2-O2	-5.65	118.24	122.20
1	2A	2152	G	N3-C4-N9	5.64	129.38	126.00
2	2B	30	C	C6-N1-C2	-5.64	118.05	120.30
1	1A	322	G	C5-N7-C8	5.63	107.12	104.30
55	1x	22	G	C4-N9-C1'	-5.63	119.17	126.50
1	1A	2697	G	N1-C6-O6	-5.63	116.52	119.90
1	2A	746	A	O4'-C1'-N9	5.62	112.70	108.20
43	2l	29	GLY	N-CA-C	-5.62	99.05	113.10
1	1A	472	G	N1-C6-O6	5.62	123.27	119.90
1	1A	793	A	O4'-C1'-N9	5.61	112.69	108.20
1	2A	2174	C	N1-C2-O2	5.61	122.26	118.90
55	1x	14	A	C4-N9-C1'	5.60	136.38	126.30
1	1A	1991	A	OP1-P-O3'	5.59	117.50	105.20
1	2A	933	A	O4'-C1'-N9	5.58	112.66	108.20
1	1A	2299	A	O4'-C1'-N9	5.57	112.66	108.20
1	2A	228	A	P-O3'-C3'	5.57	126.39	119.70
32	2a	1054	C	O4'-C1'-N1	5.57	112.66	108.20
2	2B	1	U	C2-N1-C1'	5.57	124.38	117.70
32	1a	754	C	C2-N1-C1'	5.56	124.92	118.80
32	2a	299	G	N1-C6-O6	5.56	123.23	119.90
1	1A	598	A	O5'-P-OP1	-5.55	100.70	105.70
1	2A	1791	A	O5'-P-OP1	-5.55	100.71	105.70
1	2A	2107	C	C2-N3-C4	5.53	122.66	119.90
1	1A	399	G	O4'-C1'-N9	5.53	112.62	108.20
54	2w	74	C	N1-C2-O2	5.53	122.22	118.90
1	2A	444	C	O5'-P-OP1	-5.50	100.75	105.70
1	1A	2078	G	O4'-C1'-N9	-5.50	103.80	108.20
1	1A	1694	G	O4'-C1'-N9	-5.49	103.81	108.20
32	2a	1028	C	C2-N3-C4	5.49	122.65	119.90
1	2A	747	U	O5'-P-OP1	-5.49	100.76	105.70
1	1A	2442	A	C2-N3-C4	5.49	113.34	110.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	2a	1028	C	C5-C6-N1	5.48	123.74	121.00
1	1A	1342	G	O5'-P-OP2	-5.47	100.77	105.70
1	1A	1700	G	C8-N9-C4	-5.47	104.21	106.40
55	2x	17	C	C2-N1-C1'	5.46	124.81	118.80
1	1A	587	C	N1-C2-O2	-5.46	115.63	118.90
1	2A	1313	U	O4'-C1'-N1	5.46	112.56	108.20
1	1A	472	G	C5-C6-O6	-5.45	125.33	128.60
1	1A	356	A	N1-C6-N6	-5.44	115.33	118.60
1	1A	1657	C	N1-C2-O2	5.44	122.17	118.90
26	14	54	GLY	N-CA-C	5.44	126.70	113.10
1	1A	184	A	P-O3'-C3'	5.44	126.22	119.70
1	2A	1372	U	N3-C4-O4	5.43	123.20	119.40
1	2A	2712	U	O4'-C1'-N1	5.43	112.54	108.20
32	1a	1026	G	O4'-C1'-N9	5.43	112.54	108.20
55	1x	22	G	N1-C6-O6	-5.41	116.65	119.90
1	1A	795	G	O4'-C1'-N9	5.41	112.53	108.20
54	1y	56	C	C2-N3-C4	5.40	122.60	119.90
32	2a	1001(A)	G	C4-C5-N7	5.40	112.96	110.80
54	1y	33	U	C6-N1-C1'	-5.40	113.64	121.20
1	1A	732	A	C8-N9-C4	-5.39	103.64	105.80
1	1A	2613	C	C6-N1-C2	-5.38	118.15	120.30
32	1a	1021	G	O4'-C1'-N9	5.38	112.50	108.20
32	2a	754	C	N3-C2-O2	-5.38	118.14	121.90
1	1A	1462	G	O4'-C1'-N9	5.37	112.50	108.20
32	1a	1002	G	N3-C4-C5	-5.37	125.92	128.60
1	2A	2149	G	C4-C5-N7	5.37	112.95	110.80
32	2a	79	G	N1-C6-O6	-5.37	116.68	119.90
1	2A	226	G	O4'-C1'-N9	5.36	112.49	108.20
1	1A	2701	U	P-O3'-C3'	5.35	126.12	119.70
32	2a	1001(A)	G	C8-N9-C1'	-5.34	120.06	127.00
54	2y	58	A	P-O3'-C3'	5.34	126.11	119.70
32	2a	1022	G	N3-C2-N2	5.33	123.63	119.90
1	2A	792	G	O4'-C1'-N9	-5.33	103.94	108.20
32	2a	289	G	O5'-P-OP2	-5.32	100.91	105.70
1	1A	605	G	N1-C6-O6	-5.32	116.71	119.90
32	2a	1004	A	C8-N9-C4	-5.32	103.67	105.80
1	1A	2431	U	N1-C2-O2	5.31	126.52	122.80
1	2A	1314	C	C6-N1-C2	-5.31	118.18	120.30
1	1A	1177	G	O4'-C1'-N9	5.31	112.45	108.20
1	2A	1279	G	O5'-P-OP2	-5.31	100.92	105.70
1	2A	1698	A	C6-C5-N7	-5.31	128.59	132.30
1	1A	2189	U	C6-N1-C1'	-5.30	113.77	121.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
55	1x	46	G	C5-C6-O6	-5.30	125.42	128.60
32	1a	1065	U	P-O3'-C3'	5.30	126.06	119.70
1	1A	2697	G	C6-C5-N7	5.29	133.57	130.40
32	2a	1001(A)	G	C4-N9-C1'	5.29	133.38	126.50
1	1A	831	A	N9-C4-C5	5.29	107.92	105.80
1	1A	1874	C	N1-C2-O2	-5.29	115.73	118.90
32	1a	841	U	C6-N1-C2	-5.28	117.83	121.00
32	1a	1025	U	N3-C2-O2	-5.27	118.51	122.20
1	2A	912	C	C6-N1-C2	-5.27	118.19	120.30
32	2a	65	U	P-O3'-C3'	5.27	126.02	119.70
32	2a	1001(A)	G	N3-C4-C5	-5.26	125.97	128.60
32	1a	1030	C	N3-C2-O2	-5.26	118.22	121.90
1	2A	945	A	O4'-C1'-N9	5.26	112.41	108.20
1	1A	2074	G	N1-C6-O6	-5.26	116.75	119.90
1	1A	285	U	O4'-C1'-N1	5.26	112.40	108.20
1	2A	141	A	N7-C8-N9	5.25	116.43	113.80
32	2a	1260	C	C6-N1-C2	-5.25	118.20	120.30
1	2A	2142	C	C2-N1-C1'	5.25	124.58	118.80
1	2A	1530	C	P-O3'-C3'	5.25	126.00	119.70
1	2A	528	A	P-O3'-C3'	5.23	125.98	119.70
41	2j	8	LEU	CA-CB-CG	5.23	127.34	115.30
1	2A	646	A	O4'-C1'-N9	5.23	112.38	108.20
1	1A	2331	G	C5-N7-C8	-5.22	101.69	104.30
1	2A	383	U	O4'-C1'-N1	5.22	112.38	108.20
1	1A	2054	G	C4-C5-N7	-5.22	108.71	110.80
1	2A	2152	G	C5-C6-O6	-5.21	125.47	128.60
32	2a	754	C	C6-N1-C1'	-5.21	114.54	120.80
1	1A	1219	A	P-O3'-C3'	5.21	125.96	119.70
1	1A	2883	A	O4'-C1'-N9	5.20	112.36	108.20
1	2A	845	G	C4-N9-C1'	5.20	133.26	126.50
1	2A	528	A	OP1-P-O3'	5.20	116.64	105.20
1	1A	856	G	N1-C6-O6	-5.19	116.78	119.90
1	1A	1709	C	N3-C2-O2	-5.19	118.27	121.90
1	1A	855	G	O5'-P-OP2	-5.18	101.04	105.70
32	1a	421	U	C2-N1-C1'	5.18	123.92	117.70
32	2a	299	G	C6-C5-N7	-5.18	127.29	130.40
1	1A	815	G	C5-C6-O6	5.18	131.71	128.60
32	2a	687	A	P-O3'-C3'	5.17	125.91	119.70
1	1A	2074	G	C5-C6-O6	5.17	131.70	128.60
32	1a	1067	A	P-O3'-C3'	5.16	125.90	119.70
54	1w	60	U	N3-C2-O2	-5.16	118.59	122.20
1	2A	2427	C	O5'-P-OP1	-5.16	101.06	105.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	2a	266	G	P-O3'-C3'	5.16	125.89	119.70
32	2a	955	U	C2-N3-C4	5.16	130.09	127.00
22	10	13	GLY	N-CA-C	5.15	125.98	113.10
1	2A	228	A	OP1-P-O3'	5.15	116.54	105.20
1	1A	734	C	C6-N1-C2	-5.14	118.24	120.30
1	1A	2258	G	C8-N9-C4	5.14	108.46	106.40
32	1a	204	U	N1-C2-O2	5.14	126.40	122.80
55	2x	17	C	C6-N1-C2	-5.14	118.24	120.30
32	1a	615	C	C6-N1-C2	-5.13	118.25	120.30
1	1A	2598	C	C6-N1-C2	-5.12	118.25	120.30
1	2A	1377	G	N1-C6-O6	-5.12	116.83	119.90
1	2A	1411	C	C2-N1-C1'	5.12	124.43	118.80
1	1A	991	G	O5'-P-OP1	-5.11	101.10	105.70
1	1A	1255	A	P-O3'-C3'	5.11	125.84	119.70
1	2A	748	G	C4-N9-C1'	-5.11	119.86	126.50
54	1y	56	C	N3-C2-O2	-5.10	118.33	121.90
2	2B	42	C	N1-C2-O2	5.10	121.96	118.90
1	1A	2204	G	N3-C4-N9	-5.09	122.94	126.00
1	1A	2701	U	C6-N1-C2	-5.09	117.94	121.00
1	1A	2228	G	C4-N9-C1'	5.09	133.12	126.50
1	2A	912	C	N1-C2-O2	5.09	121.95	118.90
1	2A	1597	A	N1-C6-N6	-5.09	115.55	118.60
54	2y	43	C	C2-N1-C1'	5.09	124.39	118.80
32	2a	971	G	C4-C5-N7	-5.08	108.77	110.80
1	2A	2512	C	N1-C2-O2	-5.08	115.85	118.90
32	1a	1034	G	N1-C2-N3	-5.07	120.86	123.90
1	1A	419	C	O5'-P-OP1	-5.07	101.14	105.70
1	1A	1810	U	O4'-C1'-N1	5.07	112.25	108.20
1	1A	815	G	N1-C6-O6	-5.06	116.86	119.90
1	2A	2046	G	C8-N9-C1'	-5.06	120.42	127.00
1	1A	740	C	N1-C2-O2	5.06	121.93	118.90
1	1A	1474	C	N3-C2-O2	-5.06	118.36	121.90
27	25	58	LEU	CA-CB-CG	5.06	126.93	115.30
32	1a	1030(B)	C	C6-N1-C1'	-5.05	114.73	120.80
1	1A	410	U	C2-N1-C1'	-5.05	111.64	117.70
1	1A	2838	C	N1-C2-O2	-5.05	115.87	118.90
1	1A	2250	G	N3-C4-N9	5.05	129.03	126.00
1	2A	2804	C	C6-N1-C2	-5.05	118.28	120.30
1	1A	2621	U	C5-C6-N1	-5.05	120.18	122.70
1	2A	1698	A	N1-C6-N6	5.04	121.63	118.60
1	2A	944	G	C8-N9-C1'	-5.04	120.45	127.00
1	2A	1298	C	O5'-P-OP2	-5.04	101.16	105.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1A	12	U	C5-C6-N1	5.04	125.22	122.70
32	2a	299	G	C4-C5-N7	5.04	112.81	110.80
1	2A	928	G	N7-C8-N9	5.03	115.62	113.10
55	2x	14	A	C8-N9-C1'	-5.02	118.66	127.70
1	1A	560	C	N3-C2-O2	-5.02	118.38	121.90
32	1a	913	A	P-O3'-C3'	5.02	125.72	119.70
1	2A	1653	G	P-O3'-C3'	5.02	125.72	119.70
1	2A	2321	G	C4-N9-C1'	5.01	133.01	126.50
1	2A	2139	C	N1-C2-O2	5.01	121.91	118.90
1	2A	2167	U	N1-C2-O2	5.01	126.31	122.80
32	2a	913	A	P-O3'-C3'	5.01	125.71	119.70
1	1A	1146	C	C2-N1-C1'	5.00	124.30	118.80

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
43	2l	92	0TD	Mainchain

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%)	11 (4%)	2 (1%)	22	39
4	1E	202/206 (98%)	193 (96%)	8 (4%)	1 (0%)	29	48
4	2E	202/206 (98%)	194 (96%)	7 (4%)	1 (0%)	29	48

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
5	1F	201/210 (96%)	198 (98%)	2 (1%)	1 (0%)	29	48
5	2F	201/210 (96%)	197 (98%)	2 (1%)	2 (1%)	15	28
6	1G	179/182 (98%)	170 (95%)	9 (5%)	0	100	100
6	2G	179/182 (98%)	168 (94%)	10 (6%)	1 (1%)	25	43
7	1H	172/180 (96%)	164 (95%)	7 (4%)	1 (1%)	25	43
7	2H	172/180 (96%)	158 (92%)	12 (7%)	2 (1%)	13	24
8	1I	144/148 (97%)	132 (92%)	12 (8%)	0	100	100
8	2I	144/148 (97%)	128 (89%)	14 (10%)	2 (1%)	11	20
9	1N	138/140 (99%)	134 (97%)	4 (3%)	0	100	100
9	2N	138/140 (99%)	133 (96%)	4 (3%)	1 (1%)	22	39
10	1O	120/122 (98%)	112 (93%)	8 (7%)	0	100	100
10	2O	120/122 (98%)	114 (95%)	6 (5%)	0	100	100
11	1P	147/150 (98%)	139 (95%)	8 (5%)	0	100	100
11	2P	147/150 (98%)	137 (93%)	10 (7%)	0	100	100
12	1Q	139/141 (99%)	133 (96%)	6 (4%)	0	100	100
12	2Q	139/141 (99%)	131 (94%)	7 (5%)	1 (1%)	22	39
13	1R	116/118 (98%)	111 (96%)	5 (4%)	0	100	100
13	2R	116/118 (98%)	112 (97%)	4 (3%)	0	100	100
14	1S	108/112 (96%)	106 (98%)	2 (2%)	0	100	100
14	2S	108/112 (96%)	105 (97%)	2 (2%)	1 (1%)	17	31
15	1T	129/146 (88%)	123 (95%)	6 (5%)	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%)	1 (1%)	1 (1%)	15	28
17	2V	99/101 (98%)	97 (98%)	1 (1%)	1 (1%)	15	28
18	1W	110/113 (97%)	110 (100%)	0	0	100	100
18	2W	110/113 (97%)	110 (100%)	0	0	100	100
19	1X	93/96 (97%)	90 (97%)	3 (3%)	0	100	100
19	2X	93/96 (97%)	88 (95%)	4 (4%)	1 (1%)	14	26
20	1Y	105/110 (96%)	98 (93%)	5 (5%)	2 (2%)	8	13

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
20	2Y	105/110 (96%)	99 (94%)	4 (4%)	2 (2%)	8	13
21	1Z	148/206 (72%)	136 (92%)	11 (7%)	1 (1%)	22	39
21	2Z	156/206 (76%)	141 (90%)	15 (10%)	0	100	100
22	10	81/85 (95%)	80 (99%)	0	1 (1%)	13	24
22	20	81/85 (95%)	77 (95%)	3 (4%)	1 (1%)	13	24
23	11	95/98 (97%)	92 (97%)	3 (3%)	0	100	100
23	21	95/98 (97%)	91 (96%)	4 (4%)	0	100	100
24	12	68/72 (94%)	68 (100%)	0	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%)	53 (93%)	3 (5%)	1 (2%)	8	14
26	14	67/71 (94%)	58 (87%)	4 (6%)	5 (8%)	1	1
26	24	67/71 (94%)	53 (79%)	10 (15%)	4 (6%)	1	1
27	15	57/60 (95%)	56 (98%)	1 (2%)	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%)	50 (98%)	1 (2%)	0	100	100
29	17	46/49 (94%)	44 (96%)	2 (4%)	0	100	100
29	27	46/49 (94%)	44 (96%)	1 (2%)	1 (2%)	6	10
30	18	62/65 (95%)	62 (100%)	0	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%)	200 (87%)	22 (10%)	7 (3%)	4	5
33	2b	229/256 (90%)	202 (88%)	19 (8%)	8 (4%)	3	4
34	1c	204/239 (85%)	188 (92%)	15 (7%)	1 (0%)	29	48
34	2c	204/239 (85%)	187 (92%)	15 (7%)	2 (1%)	15	28
35	1d	206/209 (99%)	196 (95%)	9 (4%)	1 (0%)	29	48
35	2d	206/209 (99%)	197 (96%)	8 (4%)	1 (0%)	29	48
36	1e	146/162 (90%)	137 (94%)	6 (4%)	3 (2%)	7	11
36	2e	146/162 (90%)	139 (95%)	5 (3%)	2 (1%)	11	20

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
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%)	144 (94%)	6 (4%)	3 (2%)	7	12
38	2g	153/156 (98%)	143 (94%)	7 (5%)	3 (2%)	7	12
39	1h	135/138 (98%)	133 (98%)	2 (2%)	0	100	100
39	2h	135/138 (98%)	131 (97%)	4 (3%)	0	100	100
40	1i	125/128 (98%)	115 (92%)	9 (7%)	1 (1%)	19	35
40	2i	125/128 (98%)	114 (91%)	10 (8%)	1 (1%)	19	35
41	1j	95/105 (90%)	86 (90%)	4 (4%)	5 (5%)	2	2
41	2j	94/105 (90%)	85 (90%)	5 (5%)	4 (4%)	2	3
42	1k	112/129 (87%)	106 (95%)	4 (4%)	2 (2%)	8	14
42	2k	112/129 (87%)	107 (96%)	3 (3%)	2 (2%)	8	14
43	1l	119/132 (90%)	115 (97%)	4 (3%)	0	100	100
43	2l	119/132 (90%)	112 (94%)	7 (6%)	0	100	100
44	1m	121/126 (96%)	114 (94%)	7 (6%)	0	100	100
44	2m	120/126 (95%)	110 (92%)	9 (8%)	1 (1%)	19	35
45	1n	58/61 (95%)	56 (97%)	2 (3%)	0	100	100
45	2n	58/61 (95%)	55 (95%)	3 (5%)	0	100	100
46	1o	86/89 (97%)	82 (95%)	4 (5%)	0	100	100
46	2o	86/89 (97%)	81 (94%)	4 (5%)	1 (1%)	13	24
47	1p	80/88 (91%)	76 (95%)	3 (4%)	1 (1%)	12	21
47	2p	80/88 (91%)	76 (95%)	3 (4%)	1 (1%)	12	21
48	1q	97/105 (92%)	93 (96%)	3 (3%)	1 (1%)	15	28
48	2q	97/105 (92%)	94 (97%)	2 (2%)	1 (1%)	15	28
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%)	75 (93%)	5 (6%)	1 (1%)	13	24
50	2s	81/93 (87%)	74 (91%)	5 (6%)	2 (2%)	5	8
51	1t	94/106 (89%)	87 (93%)	0	7 (7%)	1	1
51	2t	94/106 (89%)	86 (92%)	4 (4%)	4 (4%)	2	3
52	1u	21/27 (78%)	21 (100%)	0	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
52	2u	21/27 (78%)	21 (100%)	0	0	100	100
All	All	11370/12128 (94%)	10779 (95%)	488 (4%)	103 (1%)	17	31

All (103) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
5	1F	130	ALA
7	1H	126	PRO
21	1Z	159	PRO
26	14	62	ARG
33	1b	10	LEU
38	1g	79	ARG
40	1i	54	ASP
41	1j	55	LYS
50	1s	81	ARG
51	1t	10	LEU
51	1t	100	ILE
5	2F	21	ALA
5	2F	130	ALA
7	2H	126	PRO
8	2I	10	GLU
17	2V	79	VAL
26	24	55	ARG
26	24	61	ARG
29	27	46	VAL
33	2b	16	HIS
33	2b	123	ALA
34	2c	181	ASN
38	2g	79	ARG
44	2m	4	ILE
50	2s	81	ARG
51	2t	10	LEU
17	1V	79	VAL
26	14	45	GLY
26	14	56	VAL
42	1k	49	GLY
3	2D	69	ARG
6	2G	50	ALA
8	2I	40	THR
14	2S	84	GLN
26	24	45	GLY
40	2i	54	ASP

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Mol	Chain	Res	Type
51	2t	47	GLY
4	1E	52	LEU
22	10	13	GLY
33	1b	17	PHE
38	1g	80	VAL
41	1j	32	ALA
41	1j	77	PRO
41	1j	78	ASN
51	1t	47	GLY
51	1t	96	GLY
51	1t	102	GLY
4	2E	52	LEU
9	2N	2	LYS
19	2X	2	LYS
26	24	46	GLN
33	2b	125	PRO
36	2e	37	ARG
41	2j	77	PRO
48	2q	33	GLY
50	2s	29	ARG
26	14	57	GLU
33	1b	16	HIS
33	1b	20	GLU
33	1b	22	LYS
34	1c	66	VAL
35	1d	178	VAL
36	1e	86	ALA
51	1t	95	ALA
3	2D	3	VAL
20	2Y	103	GLY
33	2b	20	GLU
33	2b	78	GLN
34	2c	156	ARG
38	2g	7	ALA
38	2g	80	VAL
41	2j	78	ASN
51	2t	100	ILE
20	1Y	54	LYS
26	14	53	GLU
33	1b	231	GLU
41	1j	79	ARG
42	1k	105	VAL

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Mol	Chain	Res	Type
20	2Y	57	GLN
22	20	4	LYS
33	2b	21	ARG
33	2b	231	GLU
41	2j	55	LYS
42	2k	49	GLY
46	2o	88	ARG
38	1g	4	ARG
51	1t	9	ASN
7	2H	29	PRO
36	2e	69	VAL
42	2k	105	VAL
47	2p	53	VAL
48	1q	33	GLY
25	23	59	VAL
51	2t	102	GLY
20	1Y	103	GLY
36	1e	69	VAL
36	1e	85	GLY
47	1p	53	VAL
33	2b	202	PRO
41	2j	75	ILE
12	2Q	27	VAL
35	2d	5	ILE
33	1b	125	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	215/218 (99%)	209 (97%)	6 (3%)	43 70
3	2D	215/218 (99%)	208 (97%)	7 (3%)	38 64
4	1E	164/166 (99%)	154 (94%)	10 (6%)	18 36
4	2E	164/166 (99%)	154 (94%)	10 (6%)	18 36
5	1F	160/166 (96%)	150 (94%)	10 (6%)	18 34

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
5	2F	159/166 (96%)	150 (94%)	9 (6%)	20	39
6	1G	143/156 (92%)	139 (97%)	4 (3%)	43	70
6	2G	143/156 (92%)	135 (94%)	8 (6%)	21	40
7	1H	144/148 (97%)	141 (98%)	3 (2%)	53	78
7	2H	144/148 (97%)	142 (99%)	2 (1%)	67	86
8	1I	113/124 (91%)	108 (96%)	5 (4%)	28	52
8	2I	105/124 (85%)	99 (94%)	6 (6%)	20	39
9	1N	118/119 (99%)	110 (93%)	8 (7%)	16	30
9	2N	118/119 (99%)	109 (92%)	9 (8%)	13	25
10	1O	100/100 (100%)	98 (98%)	2 (2%)	55	79
10	2O	100/100 (100%)	99 (99%)	1 (1%)	76	90
11	1P	115/116 (99%)	109 (95%)	6 (5%)	23	44
11	2P	115/116 (99%)	112 (97%)	3 (3%)	46	72
12	1Q	111/111 (100%)	108 (97%)	3 (3%)	44	71
12	2Q	111/111 (100%)	105 (95%)	6 (5%)	22	42
13	1R	101/101 (100%)	90 (89%)	11 (11%)	6	12
13	2R	101/101 (100%)	94 (93%)	7 (7%)	15	30
14	1S	86/88 (98%)	84 (98%)	2 (2%)	50	76
14	2S	85/88 (97%)	83 (98%)	2 (2%)	49	74
15	1T	115/127 (91%)	113 (98%)	2 (2%)	60	82
15	2T	113/127 (89%)	113 (100%)	0	100	100
16	1U	93/94 (99%)	92 (99%)	1 (1%)	73	89
16	2U	93/94 (99%)	91 (98%)	2 (2%)	52	77
17	1V	80/82 (98%)	74 (92%)	6 (8%)	13	26
17	2V	80/82 (98%)	74 (92%)	6 (8%)	13	26
18	1W	90/92 (98%)	85 (94%)	5 (6%)	21	40
18	2W	90/92 (98%)	85 (94%)	5 (6%)	21	40
19	1X	77/78 (99%)	75 (97%)	2 (3%)	46	72
19	2X	77/78 (99%)	76 (99%)	1 (1%)	69	87
20	1Y	85/91 (93%)	82 (96%)	3 (4%)	36	62
20	2Y	85/91 (93%)	82 (96%)	3 (4%)	36	62

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
21	1Z	135/179 (75%)	129 (96%)	6 (4%)	28	52
21	2Z	137/179 (76%)	136 (99%)	1 (1%)	84	94
22	10	65/67 (97%)	63 (97%)	2 (3%)	40	67
22	20	65/67 (97%)	64 (98%)	1 (2%)	65	85
23	11	80/83 (96%)	79 (99%)	1 (1%)	69	87
23	21	80/83 (96%)	78 (98%)	2 (2%)	47	73
24	12	65/67 (97%)	64 (98%)	1 (2%)	65	85
24	22	65/67 (97%)	65 (100%)	0	100	100
25	13	51/52 (98%)	49 (96%)	2 (4%)	32	57
25	23	50/52 (96%)	48 (96%)	2 (4%)	31	56
26	14	59/63 (94%)	58 (98%)	1 (2%)	60	82
26	24	53/63 (84%)	49 (92%)	4 (8%)	13	26
27	15	50/52 (96%)	47 (94%)	3 (6%)	19	37
27	25	50/52 (96%)	47 (94%)	3 (6%)	19	37
28	16	51/52 (98%)	49 (96%)	2 (4%)	32	57
28	26	50/52 (96%)	49 (98%)	1 (2%)	55	79
29	17	41/42 (98%)	40 (98%)	1 (2%)	49	74
29	27	41/42 (98%)	40 (98%)	1 (2%)	49	74
30	18	54/55 (98%)	52 (96%)	2 (4%)	34	60
30	28	54/55 (98%)	52 (96%)	2 (4%)	34	60
31	19	34/34 (100%)	34 (100%)	0	100	100
31	29	34/34 (100%)	33 (97%)	1 (3%)	42	69
33	1b	192/220 (87%)	189 (98%)	3 (2%)	62	84
33	2b	187/220 (85%)	183 (98%)	4 (2%)	53	78
34	1c	142/188 (76%)	141 (99%)	1 (1%)	84	94
34	2c	140/188 (74%)	137 (98%)	3 (2%)	53	78
35	1d	169/181 (93%)	163 (96%)	6 (4%)	35	61
35	2d	173/181 (96%)	167 (96%)	6 (4%)	36	62
36	1e	113/123 (92%)	110 (97%)	3 (3%)	44	71
36	2e	114/123 (93%)	110 (96%)	4 (4%)	36	62
37	1f	84/90 (93%)	84 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
37	2f	85/90 (94%)	83 (98%)	2 (2%)	49	74
38	1g	119/127 (94%)	118 (99%)	1 (1%)	81	93
38	2g	120/127 (94%)	117 (98%)	3 (2%)	47	73
39	1h	114/119 (96%)	112 (98%)	2 (2%)	59	81
39	2h	114/119 (96%)	113 (99%)	1 (1%)	78	92
40	1i	90/99 (91%)	87 (97%)	3 (3%)	38	64
40	2i	89/99 (90%)	85 (96%)	4 (4%)	27	51
41	1j	66/92 (72%)	66 (100%)	0	100	100
41	2j	69/92 (75%)	67 (97%)	2 (3%)	42	69
42	1k	82/99 (83%)	80 (98%)	2 (2%)	49	74
42	2k	83/99 (84%)	83 (100%)	0	100	100
43	1l	96/108 (89%)	92 (96%)	4 (4%)	30	54
43	2l	96/108 (89%)	94 (98%)	2 (2%)	53	78
44	1m	93/101 (92%)	92 (99%)	1 (1%)	73	89
44	2m	92/101 (91%)	91 (99%)	1 (1%)	73	89
45	1n	49/50 (98%)	44 (90%)	5 (10%)	7	14
45	2n	49/50 (98%)	47 (96%)	2 (4%)	30	55
46	1o	78/80 (98%)	76 (97%)	2 (3%)	46	72
46	2o	78/80 (98%)	77 (99%)	1 (1%)	69	87
47	1p	69/74 (93%)	65 (94%)	4 (6%)	20	38
47	2p	68/74 (92%)	65 (96%)	3 (4%)	28	52
48	1q	94/97 (97%)	94 (100%)	0	100	100
48	2q	94/97 (97%)	92 (98%)	2 (2%)	53	78
49	1r	59/77 (77%)	58 (98%)	1 (2%)	60	82
49	2r	59/77 (77%)	59 (100%)	0	100	100
50	1s	69/80 (86%)	68 (99%)	1 (1%)	67	86
50	2s	67/80 (84%)	64 (96%)	3 (4%)	27	51
51	1t	70/82 (85%)	69 (99%)	1 (1%)	67	86
51	2t	70/82 (85%)	70 (100%)	0	100	100
52	1u	18/22 (82%)	18 (100%)	0	100	100
52	2u	18/22 (82%)	18 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	9303/10064 (92%)	9005 (97%)	298 (3%)	39 65

All (298) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	1D	3	VAL
3	1D	106	ILE
3	1D	113	VAL
3	1D	142	VAL
3	1D	229	VAL
3	1D	257	LEU
4	1E	12	THR
4	1E	19	ARG
4	1E	21	VAL
4	1E	24	THR
4	1E	73	GLU
4	1E	75	VAL
4	1E	78	LEU
4	1E	116	VAL
4	1E	175	VAL
4	1E	181	LEU
5	1F	53	THR
5	1F	57	VAL
5	1F	74	ARG
5	1F	106	ARG
5	1F	125	LEU
5	1F	132	VAL
5	1F	170	LEU
5	1F	183	VAL
5	1F	192	LEU
5	1F	201	VAL
6	1G	43	LEU
6	1G	82	LEU
6	1G	148	MET
6	1G	159	VAL
7	1H	51	ARG
7	1H	71	LEU
7	1H	129	THR
8	1I	38	LEU
8	1I	47	LEU
8	1I	92	VAL
8	1I	107	VAL

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Mol	Chain	Res	Type
8	1I	142	VAL
9	1N	14	VAL
9	1N	28	THR
9	1N	33	LEU
9	1N	34	LEU
9	1N	46	VAL
9	1N	73	THR
9	1N	99	LEU
9	1N	120	LEU
10	1O	10	VAL
10	1O	108	GLU
11	1P	65	ARG
11	1P	95	VAL
11	1P	98	GLU
11	1P	106	LEU
11	1P	112	LEU
11	1P	125	VAL
12	1Q	35	VAL
12	1Q	109	VAL
12	1Q	110	THR
13	1R	6	SER
13	1R	24	GLN
13	1R	29	LEU
13	1R	36	THR
13	1R	44	LEU
13	1R	54	LEU
13	1R	65	LEU
13	1R	79	LEU
13	1R	100	LEU
13	1R	111	LEU
13	1R	114	VAL
14	1S	25	ARG
14	1S	110	LEU
15	1T	28	VAL
15	1T	74	ARG
16	1U	74	LEU
17	1V	46	VAL
17	1V	51	VAL
17	1V	52	VAL
17	1V	72	VAL
17	1V	79	VAL
17	1V	82	ARG

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Mol	Chain	Res	Type
18	1W	17	VAL
18	1W	19	LEU
18	1W	23	LEU
18	1W	67	ASP
18	1W	107	LEU
19	1X	35	THR
19	1X	57	LEU
20	1Y	1	MET
20	1Y	43	ASN
20	1Y	72	VAL
21	1Z	5	LEU
21	1Z	86	VAL
21	1Z	129	SER
21	1Z	155	LEU
21	1Z	161	VAL
21	1Z	171	ILE
22	10	14	ARG
22	10	43	THR
23	11	35	THR
24	12	40	SER
25	13	23	LEU
25	13	54	VAL
26	14	49	PHE
27	15	6	VAL
27	15	16	ARG
27	15	29	THR
28	16	37	ARG
28	16	48	VAL
29	17	43	THR
30	18	31	HIS
30	18	32	LEU
33	1b	24	TRP
33	1b	111	ARG
33	1b	112	VAL
34	1c	21	ARG
35	1d	10	ARG
35	1d	31	CYS
35	1d	49	ARG
35	1d	134	ASP
35	1d	135	LEU
35	1d	194	LEU
36	1e	31	LEU

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Mol	Chain	Res	Type
36	1e	41	VAL
36	1e	56	GLN
38	1g	8	GLU
39	1h	69	ARG
39	1h	112	LEU
40	1i	42	ARG
40	1i	64	THR
40	1i	128	ARG
42	1k	31	THR
42	1k	48	ILE
43	1l	27	LEU
43	1l	36	VAL
43	1l	83	VAL
43	1l	84	LEU
44	1m	102	ARG
45	1n	3	ARG
45	1n	6	LEU
45	1n	22	THR
45	1n	23	ARG
45	1n	33	VAL
46	1o	7	GLU
46	1o	39	LEU
47	1p	19	ILE
47	1p	20	VAL
47	1p	21	VAL
47	1p	67	THR
49	1r	76	LEU
50	1s	41	VAL
51	1t	13	LEU
3	2D	94	LEU
3	2D	106	ILE
3	2D	113	VAL
3	2D	134	ARG
3	2D	142	VAL
3	2D	259	THR
3	2D	276	LYS
4	2E	12	THR
4	2E	21	VAL
4	2E	24	THR
4	2E	52	LEU
4	2E	75	VAL
4	2E	78	LEU

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Mol	Chain	Res	Type
4	2E	116	VAL
4	2E	163	GLU
4	2E	175	VAL
4	2E	181	LEU
5	2F	53	THR
5	2F	70	THR
5	2F	74	ARG
5	2F	106	ARG
5	2F	170	LEU
5	2F	183	VAL
5	2F	192	LEU
5	2F	197	ASP
5	2F	201	VAL
6	2G	28	VAL
6	2G	31	VAL
6	2G	43	LEU
6	2G	60	LEU
6	2G	79	ASN
6	2G	115	ARG
6	2G	135	LEU
6	2G	159	VAL
7	2H	84	SER
7	2H	88	LEU
8	2I	38	LEU
8	2I	47	LEU
8	2I	57	ARG
8	2I	92	VAL
8	2I	121	LYS
8	2I	123	LEU
9	2N	14	VAL
9	2N	28	THR
9	2N	33	LEU
9	2N	34	LEU
9	2N	46	VAL
9	2N	67	LEU
9	2N	87	LEU
9	2N	99	LEU
9	2N	120	LEU
10	2O	8	LEU
11	2P	95	VAL
11	2P	99	LEU
11	2P	106	LEU

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Mol	Chain	Res	Type
12	2Q	1	MET
12	2Q	2	LEU
12	2Q	16	ARG
12	2Q	21	THR
12	2Q	35	VAL
12	2Q	110	THR
13	2R	18	LEU
13	2R	24	GLN
13	2R	29	LEU
13	2R	44	LEU
13	2R	65	LEU
13	2R	100	LEU
13	2R	111	LEU
14	2S	75	GLU
14	2S	110	LEU
16	2U	36	ARG
16	2U	74	LEU
17	2V	43	GLU
17	2V	46	VAL
17	2V	51	VAL
17	2V	72	VAL
17	2V	79	VAL
17	2V	82	ARG
18	2W	17	VAL
18	2W	19	LEU
18	2W	23	LEU
18	2W	67	ASP
18	2W	107	LEU
19	2X	57	LEU
20	2Y	28	LYS
20	2Y	72	VAL
20	2Y	90	LEU
21	2Z	124	ILE
22	20	14	ARG
23	21	4	VAL
23	21	95	LEU
25	23	30	ARG
25	23	54	VAL
26	24	34	GLU
26	24	37	SER
26	24	48	ARG
26	24	49	PHE

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Mol	Chain	Res	Type
27	25	6	VAL
27	25	16	ARG
27	25	29	THR
28	26	48	VAL
29	27	39	ARG
30	28	31	HIS
30	28	32	LEU
31	29	17	ILE
33	2b	11	LEU
33	2b	93	VAL
33	2b	127	ILE
33	2b	221	LEU
34	2c	70	VAL
34	2c	124	ILE
34	2c	154	SER
35	2d	31	CYS
35	2d	135	LEU
35	2d	141	ARG
35	2d	150	GLU
35	2d	170	VAL
35	2d	194	LEU
36	2e	13	ILE
36	2e	31	LEU
36	2e	41	VAL
36	2e	64	ARG
37	2f	21	LEU
37	2f	72	VAL
38	2g	9	VAL
38	2g	52	GLU
38	2g	98	SER
39	2h	23	SER
40	2i	53	VAL
40	2i	65	VAL
40	2i	102	LEU
40	2i	108	VAL
41	2j	8	LEU
41	2j	100	THR
43	2l	27	LEU
43	2l	83	VAL
44	2m	47	ASP
45	2n	22	THR
45	2n	33	VAL

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Mol	Chain	Res	Type
46	2o	39	LEU
47	2p	2	VAL
47	2p	21	VAL
47	2p	67	THR
48	2q	35	VAL
48	2q	83	ASP
50	2s	41	VAL
50	2s	49	ILE
50	2s	77	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (95) such sidechains are listed below:

Mol	Chain	Res	Type
4	1E	48	GLN
5	1F	8	GLN
8	1I	105	HIS
13	1R	71	GLN
19	1X	31	HIS
19	1X	82	GLN
20	1Y	6	HIS
20	1Y	43	ASN
23	11	56	GLN
24	12	9	GLN
25	13	32	GLN
34	1c	6	HIS
34	1c	162	GLN
34	1c	181	ASN
35	1d	116	GLN
35	1d	119	GLN
35	1d	123	HIS
35	1d	125	HIS
36	1e	78	HIS
37	1f	100	ASN
38	1g	28	ASN
38	1g	86	GLN
40	1i	3	GLN
40	1i	31	GLN
40	1i	34	ASN
40	1i	58	HIS
40	1i	89	ASN
40	1i	124	GLN
41	1j	56	HIS

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Mol	Chain	Res	Type
42	1k	99	GLN
43	1l	99	HIS
47	1p	16	HIS
48	1q	26	GLN
50	1s	23	ASN
50	1s	69	HIS
50	1s	83	HIS
3	2D	87	ASN
4	2E	48	GLN
5	2F	69	HIS
6	2G	41	GLN
9	2N	38	HIS
10	2O	3	GLN
12	2Q	12	GLN
12	2Q	13	GLN
12	2Q	57	HIS
12	2Q	123	HIS
13	2R	13	HIS
14	2S	38	GLN
15	2T	79	HIS
16	2U	81	HIS
16	2U	117	GLN
18	2W	60	ASN
19	2X	31	HIS
19	2X	82	GLN
20	2Y	6	HIS
21	2Z	55	HIS
21	2Z	73	GLN
22	20	35	ASN
23	21	56	GLN
24	22	9	GLN
24	22	65	ASN
26	24	46	GLN
33	2b	40	HIS
33	2b	94	ASN
33	2b	140	HIS
34	2c	6	HIS
34	2c	37	GLN
34	2c	98	ASN
34	2c	104	GLN
35	2d	119	GLN
35	2d	123	HIS

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Mol	Chain	Res	Type
35	2d	125	HIS
35	2d	161	ASN
36	2e	73	ASN
36	2e	78	HIS
36	2e	130	ASN
37	2f	64	GLN
37	2f	73	ASN
38	2g	28	ASN
38	2g	86	GLN
38	2g	109	ASN
39	2h	78	GLN
40	2i	3	GLN
40	2i	58	HIS
40	2i	89	ASN
40	2i	124	GLN
42	2k	22	HIS
42	2k	78	GLN
43	2l	49	ASN
43	2l	99	HIS
44	2m	12	ASN
44	2m	77	ASN
46	2o	28	GLN
50	2s	47	HIS
51	2t	75	ASN

5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	1A	2861/2915 (98%)	414 (14%)	43 (1%)
1	2A	2788/2915 (95%)	510 (18%)	28 (1%)
2	1B	120/121 (99%)	11 (9%)	1 (0%)
2	2B	118/121 (97%)	35 (29%)	0
32	1a	1494/1521 (98%)	241 (16%)	0
32	2a	1498/1521 (98%)	253 (16%)	0
53	1v	12/24 (50%)	4 (33%)	0
53	2v	12/24 (50%)	3 (25%)	0
54	1w	71/76 (93%)	22 (30%)	0
54	1y	71/76 (93%)	23 (32%)	0
54	2w	68/76 (89%)	27 (39%)	0
54	2y	69/76 (90%)	23 (33%)	0
55	1x	75/77 (97%)	8 (10%)	0

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Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
55	2x	75/77 (97%)	16 (21%)	0
All	All	9332/9620 (97%)	1590 (17%)	72 (0%)

All (1590) 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	60	G
1	1A	70	A
1	1A	71	U
1	1A	73	A
1	1A	74	G
1	1A	83	A
1	1A	117	A
1	1A	118	U
1	1A	137	G
1	1A	185	A
1	1A	189	U
1	1A	194	G
1	1A	203	G
1	1A	204	G
1	1A	205	A
1	1A	211	A
1	1A	217	A
1	1A	218	A
1	1A	222	A
1	1A	237	G
1	1A	258	U
1	1A	271	U
1	1A	272	U
1	1A	273	G
1	1A	288	U
1	1A	289	G
1	1A	296	U
1	1A	303	C
1	1A	335	A
1	1A	353	G
1	1A	354	A
1	1A	376	G

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Mol	Chain	Res	Type
1	1A	387	G
1	1A	388	A
1	1A	389	G
1	1A	407	U
1	1A	413	G
1	1A	423	G
1	1A	427	G
1	1A	432	U
1	1A	438	G
1	1A	455	A
1	1A	470	C
1	1A	474	U
1	1A	477	C
1	1A	480	A
1	1A	482	C
1	1A	483	A
1	1A	505	A
1	1A	507	G
1	1A	529	U
1	1A	530	A
1	1A	534	C
1	1A	537	G
1	1A	555	G
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	639	G
1	1A	641	G
1	1A	642	G
1	1A	652	A
1	1A	659	C
1	1A	660	C
1	1A	662	A

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Mol	Chain	Res	Type
1	1A	670	C
1	1A	671	A
1	1A	697	C
1	1A	716	G
1	1A	733	G
1	1A	777	C
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	848	G
1	1A	852	G
1	1A	859	C
1	1A	866	A
1	1A	874	U
1	1A	875	U
1	1A	906	G
1	1A	913	A
1	1A	924	U
1	1A	926	G
1	1A	927	G
1	1A	931	C
1	1A	932	C
1	1A	933	C
1	1A	934	A
1	1A	935	C
1	1A	936	C
1	1A	937	A
1	1A	940	C
1	1A	941	U
1	1A	942	A
1	1A	943	C
1	1A	944	C
1	1A	946	A
1	1A	953	U
1	1A	956	A
1	1A	977	G
1	1A	990	A
1	1A	991	G

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Mol	Chain	Res	Type
1	1A	998	A
1	1A	1006	C
1	1A	1008	U
1	1A	1019	G
1	1A	1020	C
1	1A	1029	A
1	1A	1042	A
1	1A	1055	A
1	1A	1058	U
1	1A	1059	C
1	1A	1068	G
1	1A	1072	U
1	1A	1073	A
1	1A	1079	U
1	1A	1084	C
1	1A	1090	G
1	1A	1091	A
1	1A	1092	A
1	1A	1093	G
1	1A	1094	A
1	1A	1100	A
1	1A	1101	G
1	1A	1104	G
1	1A	1112	U
1	1A	1114	G
1	1A	1117	G
1	1A	1119	A
1	1A	1120	G
1	1A	1121	C
1	1A	1122	C
1	1A	1124	U
1	1A	1125	C
1	1A	1127	U
1	1A	1129	U
1	1A	1130	A
1	1A	1134	A
1	1A	1135	G
1	1A	1136	U
1	1A	1137	G
1	1A	1139	G
1	1A	1140	U
1	1A	1142	A

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Mol	Chain	Res	Type
1	1A	1146	C
1	1A	1147	U
1	1A	1148	C
1	1A	1149	A
1	1A	1153	G
1	1A	1156	G
1	1A	1157	A
1	1A	1158	G
1	1A	1162	C
1	1A	1180	C
1	1A	1181	G
1	1A	1195	G
1	1A	1201	A
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	1256	U
1	1A	1299	A
1	1A	1302	G
1	1A	1317	G
1	1A	1318	A
1	1A	1322	A
1	1A	1346	U
1	1A	1347	A
1	1A	1349	G
1	1A	1366	C
1	1A	1391	C
1	1A	1398	U
1	1A	1405	A
1	1A	1406	A
1	1A	1411	A
1	1A	1426	G
1	1A	1430	A
1	1A	1431	G
1	1A	1441	A
1	1A	1442	U
1	1A	1462	G
1	1A	1463	C

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Mol	Chain	Res	Type
1	1A	1466	U
1	1A	1467	G
1	1A	1474	C
1	1A	1491	A
1	1A	1497	G
1	1A	1502	G
1	1A	1514	C
1	1A	1529	G
1	1A	1539	C
1	1A	1540	A
1	1A	1554	A
1	1A	1555	C
1	1A	1556	A
1	1A	1569	U
1	1A	1586	G
1	1A	1587	U
1	1A	1605	A
1	1A	1613	A
1	1A	1616	A
1	1A	1625	U
1	1A	1627	A
1	1A	1628	G
1	1A	1631	C
1	1A	1632	A
1	1A	1654	A
1	1A	1686	U
1	1A	1694	G
1	1A	1695	C
1	1A	1701	A
1	1A	1721	G
1	1A	1741	C
1	1A	1743	G
1	1A	1747	A
1	1A	1750	G
1	1A	1767	A
1	1A	1768	U
1	1A	1776	G
1	1A	1787	G
1	1A	1794	G
1	1A	1795	G
1	1A	1804	A
1	1A	1811	A

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Mol	Chain	Res	Type
1	1A	1813	C
1	1A	1817	A
1	1A	1822	A
1	1A	1831	C
1	1A	1847	G
1	1A	1848	G
1	1A	1859	G
1	1A	1860	A
1	1A	1878	A
1	1A	1889	G
1	1A	1892	G
1	1A	1899	A
1	1A	1911	A
1	1A	1922	A
1	1A	1928	G
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	2014	G
1	1A	2015	U
1	1A	2019	G
1	1A	2042	A
1	1A	2045	G
1	1A	2053	A
1	1A	2054	G
1	1A	2055	A
1	1A	2057	G
1	1A	2061	C
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

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Mol	Chain	Res	Type
1	1A	2115	G
1	1A	2132	G
1	1A	2135	U
1	1A	2136	A
1	1A	2137	G
1	1A	2138	G
1	1A	2143	G
1	1A	2149	G
1	1A	2151	C
1	1A	2152	U
1	1A	2153	G
1	1A	2154	U
1	1A	2155	G
1	1A	2156	A
1	1A	2157	A
1	1A	2162	C
1	1A	2163	G
1	1A	2164	C
1	1A	2166	U
1	1A	2168	C
1	1A	2172	U
1	1A	2173	G
1	1A	2178	G
1	1A	2179	G
1	1A	2180	A
1	1A	2181	G
1	1A	2182	G
1	1A	2184	G
1	1A	2187	G
1	1A	2188	G
1	1A	2189	U
1	1A	2193	A
1	1A	2194	U
1	1A	2197	C
1	1A	2200	C
1	1A	2203	G
1	1A	2204	G
1	1A	2206	G
1	1A	2207	C
1	1A	2214	G
1	1A	2220	A
1	1A	2227	G

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Mol	Chain	Res	Type
1	1A	2228	G
1	1A	2229	A
1	1A	2231	G
1	1A	2237	A
1	1A	2250	G
1	1A	2251	G
1	1A	2280	A
1	1A	2281	A
1	1A	2292	G
1	1A	2295	C
1	1A	2299	A
1	1A	2317	A
1	1A	2320	G
1	1A	2321	A
1	1A	2332	A
1	1A	2337	G
1	1A	2346	G
1	1A	2359	C
1	1A	2362	C
1	1A	2373	A
1	1A	2384	G
1	1A	2395	G
1	1A	2397	C
1	1A	2418	U
1	1A	2422	G
1	1A	2436	C
1	1A	2437	A
1	1A	2441	G
1	1A	2442	A
1	1A	2443	U
1	1A	2447	A
1	1A	2451	A
1	1A	2453	C
1	1A	2460	A
1	1A	2486	C
1	1A	2488	A
1	1A	2514	G
1	1A	2517	G
1	1A	2518	U
1	1A	2530	A
1	1A	2541	G
1	1A	2561	G

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Mol	Chain	Res	Type
1	1A	2566	U
1	1A	2578	A
1	1A	2579	G
1	1A	2585	C
1	1A	2586	G
1	1A	2590	G
1	1A	2614	A
1	1A	2621	U
1	1A	2623	U
1	1A	2624	C
1	1A	2641	A
1	1A	2642	G
1	1A	2653	G
1	1A	2666	A
1	1A	2701	U
1	1A	2702	C
1	1A	2703	C
1	1A	2714	U
1	1A	2725	A
1	1A	2726	A
1	1A	2727	G
1	1A	2739	U
1	1A	2746	A
1	1A	2770	A
1	1A	2771	A
1	1A	2778	A
1	1A	2782	C
1	1A	2791	A
1	1A	2803	A
1	1A	2804	C
1	1A	2806	G
1	1A	2813	G
1	1A	2828	G
1	1A	2830	A
1	1A	2831	A
1	1A	2845	A
1	1A	2846	U
1	1A	2879	G
1	1A	2882	G
1	1A	2890	C
1	1A	2901	A
1	1A	2903	G

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Mol	Chain	Res	Type
2	1B	2	C
2	1B	12	C
2	1B	25	A
2	1B	35	U
2	1B	45	A
2	1B	56	G
2	1B	67	G
2	1B	73	A
2	1B	85	G
2	1B	106	G
2	1B	110	G
32	1a	7	G
32	1a	9	G
32	1a	32	A
32	1a	39	G
32	1a	47	C
32	1a	48	C
32	1a	51	A
32	1a	54	C
32	1a	61	G
32	1a	65	U
32	1a	79	G
32	1a	91	C
32	1a	97	G
32	1a	98	G
32	1a	101	A
32	1a	116	A
32	1a	121	C
32	1a	131	C
32	1a	163	C
32	1a	174	C
32	1a	180	U
32	1a	182	U
32	1a	195	A
32	1a	197	A
32	1a	201	C
32	1a	202	U
32	1a	203	U
32	1a	204	U
32	1a	216	G
32	1a	217	C
32	1a	247	G

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Mol	Chain	Res	Type
32	1a	251	G
32	1a	258	G
32	1a	266	G
32	1a	267	C
32	1a	289	G
32	1a	301	G
32	1a	306	G
32	1a	321	A
32	1a	328	C
32	1a	332	G
32	1a	342	C
32	1a	348	G
32	1a	352	C
32	1a	353	A
32	1a	354	G
32	1a	367	U
32	1a	372	C
32	1a	373	A
32	1a	384	G
32	1a	397	A
32	1a	398	C
32	1a	406	G
32	1a	412	A
32	1a	421	U
32	1a	423	G
32	1a	424	G
32	1a	429	U
32	1a	441	A
32	1a	442	C
32	1a	452	A
32	1a	461	A
32	1a	470	C
32	1a	471	G
32	1a	477	A
32	1a	484	G
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

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Mol	Chain	Res	Type
32	1a	518	C
32	1a	531	U
32	1a	532	A
32	1a	547	A
32	1a	559	A
32	1a	561	U
32	1a	568	G
32	1a	572	A
32	1a	573	A
32	1a	576	G
32	1a	577	G
32	1a	596	C
32	1a	630	G
32	1a	653	A
32	1a	665	A
32	1a	687	A
32	1a	688	G
32	1a	695	A
32	1a	721	G
32	1a	723	U
32	1a	731	G
32	1a	733	A
32	1a	749	C
32	1a	755	G
32	1a	774	G
32	1a	777	A
32	1a	792	A
32	1a	793	U
32	1a	794	A
32	1a	815	A
32	1a	817	C
32	1a	821	G
32	1a	828	A
32	1a	840	C
32	1a	841	U
32	1a	851	G
32	1a	853	G
32	1a	859	A
32	1a	870	U
32	1a	880	C
32	1a	885	G
32	1a	902	G

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Mol	Chain	Res	Type
32	1a	914	A
32	1a	926	G
32	1a	927	G
32	1a	932	C
32	1a	934	C
32	1a	960	U
32	1a	961	U
32	1a	968	A
32	1a	969	A
32	1a	971	G
32	1a	974	A
32	1a	975	A
32	1a	976	G
32	1a	977	A
32	1a	982	U
32	1a	989	C
32	1a	992	U
32	1a	993	G
32	1a	997	U
32	1a	1000	U
32	1a	1001(A)	G
32	1a	1002	G
32	1a	1003	G
32	1a	1005	A
32	1a	1006	C
32	1a	1009	G
32	1a	1011	G
32	1a	1016	A
32	1a	1020	U
32	1a	1021	G
32	1a	1022	G
32	1a	1025	U
32	1a	1026	G
32	1a	1027	C
32	1a	1029	C
32	1a	1030	C
32	1a	1030(A)	G
32	1a	1030(C)	G
32	1a	1031	G
32	1a	1033	G
32	1a	1039	C
32	1a	1045	C

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Mol	Chain	Res	Type
32	1a	1054	C
32	1a	1065	U
32	1a	1066	C
32	1a	1068	G
32	1a	1080	A
32	1a	1081	G
32	1a	1086	U
32	1a	1094	G
32	1a	1095	U
32	1a	1101	A
32	1a	1108	G
32	1a	1122	U
32	1a	1125	U
32	1a	1129	C
32	1a	1130	A
32	1a	1132	C
32	1a	1134	G
32	1a	1137	C
32	1a	1138	G
32	1a	1139	G
32	1a	1140	C
32	1a	1141	C
32	1a	1146	A
32	1a	1152	A
32	1a	1159	U
32	1a	1163	C
32	1a	1172	C
32	1a	1181	G
32	1a	1183	A
32	1a	1184	G
32	1a	1196	U
32	1a	1197	G
32	1a	1202	G
32	1a	1212	U
32	1a	1213	A
32	1a	1220	G
32	1a	1222	G
32	1a	1227	A
32	1a	1238	A
32	1a	1240	U
32	1a	1241	G
32	1a	1256	A

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Mol	Chain	Res	Type
32	1a	1257	U
32	1a	1260	C
32	1a	1267	C
32	1a	1270	C
32	1a	1273	G
32	1a	1276	G
32	1a	1278	U
32	1a	1279	A
32	1a	1280	A
32	1a	1286	A
32	1a	1287	A
32	1a	1290	G
32	1a	1299	A
32	1a	1300	G
32	1a	1302	U
32	1a	1320	C
32	1a	1338	G
32	1a	1340	A
32	1a	1346	A
32	1a	1347	G
32	1a	1353	G
32	1a	1363	C
32	1a	1368	G
32	1a	1370	G
32	1a	1419	G
32	1a	1442	G
32	1a	1442(A)	G
32	1a	1446	U
32	1a	1447	A
32	1a	1456	G
32	1a	1487	G
32	1a	1492	A
32	1a	1494	G
32	1a	1497	G
32	1a	1503	A
32	1a	1504	G
32	1a	1505	G
32	1a	1506	U
32	1a	1517	G
32	1a	1529	G
32	1a	1530	G
32	1a	1532	U

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Mol	Chain	Res	Type
53	1v	13	A
53	1v	14	A
53	1v	15	A
53	1v	24	A
54	1w	2	C
54	1w	6	G
54	1w	8	4SU
54	1w	14	A
54	1w	19	G
54	1w	20	U
54	1w	21	A
54	1w	23	A
54	1w	24	G
54	1w	45	U
54	1w	46	7MG
54	1w	47	U
54	1w	48	C
54	1w	50	U
54	1w	62	C
54	1w	64	A
54	1w	67	C
54	1w	68	C
54	1w	70	G
54	1w	72	C
54	1w	73	A
54	1w	74	C
55	1x	9	G
55	1x	18	G
55	1x	19	G
55	1x	21	A
55	1x	47	U
55	1x	61	C
55	1x	69	C
55	1x	76	A
54	1y	6	G
54	1y	8	4SU
54	1y	9	A
54	1y	13	C
54	1y	19	G
54	1y	20	U
54	1y	21	A
54	1y	23	A

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Mol	Chain	Res	Type
54	1y	35	A
54	1y	44	G
54	1y	45	U
54	1y	46	7MG
54	1y	47	U
54	1y	48	C
54	1y	49	C
54	1y	53	G
54	1y	54	5MU
54	1y	56	C
54	1y	59	U
54	1y	61	C
54	1y	65	G
54	1y	69	G
54	1y	70	G
1	2A	8	A
1	2A	12	U
1	2A	15	G
1	2A	34	C
1	2A	35	G
1	2A	45	C
1	2A	71	A
1	2A	74	A
1	2A	75	G
1	2A	84	A
1	2A	90	U
1	2A	94	C
1	2A	95	G
1	2A	100	G
1	2A	102	G
1	2A	118	A
1	2A	119	A
1	2A	120	U
1	2A	127	A
1	2A	154(A)	C
1	2A	157	U
1	2A	173	G
1	2A	181	A
1	2A	196	A
1	2A	199	A
1	2A	205	G
1	2A	214	G

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Mol	Chain	Res	Type
1	2A	215	G
1	2A	216	A
1	2A	221	A
1	2A	222	A
1	2A	225	A
1	2A	228	A
1	2A	229	A
1	2A	233	A
1	2A	248	G
1	2A	249	C
1	2A	250	G
1	2A	267	C
1	2A	271(A)	A
1	2A	271(K)	U
1	2A	271(L)	U
1	2A	271(M)	G
1	2A	271(N)	U
1	2A	271(O)	C
1	2A	272(B)	G
1	2A	272(I)	U
1	2A	272(J)	C
1	2A	274	G
1	2A	277	C
1	2A	278	A
1	2A	294	A
1	2A	303	U
1	2A	311	A
1	2A	316	C
1	2A	317	G
1	2A	324	A
1	2A	325	G
1	2A	327	G
1	2A	329	G
1	2A	330	A
1	2A	333	G
1	2A	352	G
1	2A	362	U
1	2A	363	G
1	2A	363(B)	G
1	2A	363(D)	G
1	2A	386	G
1	2A	396	G

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Mol	Chain	Res	Type
1	2A	402	A
1	2A	403	U
1	2A	405	U
1	2A	406	G
1	2A	407	G
1	2A	411	G
1	2A	412	A
1	2A	418	G
1	2A	421	U
1	2A	422	A
1	2A	435	C
1	2A	444	C
1	2A	454	A
1	2A	455	C
1	2A	457	A
1	2A	481	G
1	2A	494	G
1	2A	501	A
1	2A	504	U
1	2A	505	A
1	2A	508	G
1	2A	509	C
1	2A	517	C
1	2A	520	G
1	2A	529	A
1	2A	530	G
1	2A	531	C
1	2A	532	A
1	2A	533	G
1	2A	563	G
1	2A	568	U
1	2A	573	G
1	2A	575	A
1	2A	588	U
1	2A	592	G
1	2A	599	G
1	2A	603	A
1	2A	604	G
1	2A	607	U
1	2A	614(B)	G
1	2A	615	G
1	2A	616	G

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Mol	Chain	Res	Type
1	2A	621	A
1	2A	627	A
1	2A	634	C
1	2A	637	A
1	2A	645	C
1	2A	651	G
1	2A	652(B)	A
1	2A	652(U)	G
1	2A	667	U
1	2A	669	G
1	2A	686	G
1	2A	701	G
1	2A	709	U
1	2A	717	G
1	2A	730	C
1	2A	752	A
1	2A	753	C
1	2A	771	G
1	2A	775	G
1	2A	776	G
1	2A	782	A
1	2A	784	A
1	2A	785	G
1	2A	792	G
1	2A	805	G
1	2A	812	C
1	2A	819	A
1	2A	827	U
1	2A	828	U
1	2A	847	U
1	2A	857	C
1	2A	859	G
1	2A	866	A
1	2A	869	G
1	2A	870	A
1	2A	874	G
1	2A	875	G
1	2A	879	G
1	2A	880	G
1	2A	884	C
1	2A	886	C
1	2A	887	A

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Mol	Chain	Res	Type
1	2A	888	C
1	2A	889	C
1	2A	890	A
1	2A	893	C
1	2A	894	C
1	2A	895	U
1	2A	896	A
1	2A	900	A
1	2A	901	A
1	2A	910	A
1	2A	915	C
1	2A	917	A
1	2A	932	G
1	2A	933	A
1	2A	941	A
1	2A	944	G
1	2A	945	A
1	2A	946	G
1	2A	953	A
1	2A	958	U
1	2A	959	A
1	2A	961	C
1	2A	974	G
1	2A	975	C
1	2A	983	A
1	2A	996	A
1	2A	997	G
1	2A	998	C
1	2A	1012	U
1	2A	1013	C
1	2A	1017	G
1	2A	1020	A
1	2A	1022	G
1	2A	1025	G
1	2A	1026	U
1	2A	1033	U
1	2A	1038	C
1	2A	1039	G
1	2A	1041	C
1	2A	1042	G
1	2A	1043	C
1	2A	1114	G

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Mol	Chain	Res	Type
1	2A	1116	C
1	2A	1130	U
1	2A	1135	C
1	2A	1136	G
1	2A	1139	G
1	2A	1142	U
1	2A	1144	G
1	2A	1166	C
1	2A	1169	G
1	2A	1171	G
1	2A	1180	C
1	2A	1188	U
1	2A	1205	U
1	2A	1206	G
1	2A	1210	A
1	2A	1211	U
1	2A	1218	C
1	2A	1220	A
1	2A	1224	C
1	2A	1237	A
1	2A	1248	G
1	2A	1250	G
1	2A	1252	G
1	2A	1253	A
1	2A	1256	G
1	2A	1268	A
1	2A	1271	G
1	2A	1272	A
1	2A	1273	U
1	2A	1287	A
1	2A	1300	U
1	2A	1301	A
1	2A	1303	G
1	2A	1314	C
1	2A	1321	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	1370	C

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Mol	Chain	Res	Type
1	2A	1384	A
1	2A	1385	G
1	2A	1386	C
1	2A	1411	C
1	2A	1416	G
1	2A	1417	C
1	2A	1420	U
1	2A	1421	G
1	2A	1427	A
1	2A	1428	C
1	2A	1435	G
1	2A	1437	C
1	2A	1445	A
1	2A	1449	A
1	2A	1450	G
1	2A	1460	A
1	2A	1467	C
1	2A	1471	A
1	2A	1482	G
1	2A	1490	A
1	2A	1493	C
1	2A	1494	A
1	2A	1495	A
1	2A	1496	A
1	2A	1497	U
1	2A	1508	A
1	2A	1509	C
1	2A	1509(A)	A
1	2A	1514	U
1	2A	1531	C
1	2A	1532	C
1	2A	1533	G
1	2A	1543	C
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

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Mol	Chain	Res	Type
1	2A	1609	A
1	2A	1610	A
1	2A	1616	A
1	2A	1629	U
1	2A	1647	G
1	2A	1648	C
1	2A	1654	A
1	2A	1674	G
1	2A	1696	G
1	2A	1700	A
1	2A	1703	G
1	2A	1721	G
1	2A	1722	A
1	2A	1739	U
1	2A	1740	G
1	2A	1746	G
1	2A	1747(A)	G
1	2A	1756	G
1	2A	1758	G
1	2A	1762	A
1	2A	1763	G
1	2A	1764	G
1	2A	1769	G
1	2A	1773	A
1	2A	1780	A
1	2A	1782	C
1	2A	1786	A
1	2A	1791	A
1	2A	1800	C
1	2A	1801	G
1	2A	1811	G
1	2A	1812	A
1	2A	1816	G
1	2A	1828	G
1	2A	1835	G
1	2A	1839	G
1	2A	1847	A
1	2A	1848	A
1	2A	1857	G
1	2A	1877	A
1	2A	1878	G
1	2A	1889	A

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Mol	Chain	Res	Type
1	2A	1900	A
1	2A	1906	G
1	2A	1913	A
1	2A	1914	C
1	2A	1929	G
1	2A	1930	G
1	2A	1931	U
1	2A	1936	A
1	2A	1937	A
1	2A	1938	A
1	2A	1955	U
1	2A	1963	U
1	2A	1967	C
1	2A	1970	A
1	2A	1971	A
1	2A	1972	A
1	2A	1992	G
1	2A	1993	U
1	2A	1997	G
1	2A	2020	A
1	2A	2023	G
1	2A	2027	G
1	2A	2031	A
1	2A	2033	A
1	2A	2043	C
1	2A	2055	C
1	2A	2056	G
1	2A	2060	A
1	2A	2061	G
1	2A	2062	A
1	2A	2069	G
1	2A	2093	G
1	2A	2099	U
1	2A	2105	C
1	2A	2108	C
1	2A	2110	G
1	2A	2111	C
1	2A	2112	G
1	2A	2116	G
1	2A	2119	A
1	2A	2120	G
1	2A	2122	U

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Mol	Chain	Res	Type
1	2A	2125	G
1	2A	2126	A
1	2A	2127	G
1	2A	2129	C
1	2A	2131	G
1	2A	2132	U
1	2A	2134	A
1	2A	2135	A
1	2A	2136	C
1	2A	2137	C
1	2A	2138	C
1	2A	2140	C
1	2A	2142	C
1	2A	2146	C
1	2A	2150	U
1	2A	2151	G
1	2A	2154	G
1	2A	2155	G
1	2A	2156	G
1	2A	2157	G
1	2A	2158	A
1	2A	2161	C
1	2A	2165	G
1	2A	2166	G
1	2A	2167	U
1	2A	2168	G
1	2A	2169	A
1	2A	2172	U
1	2A	2174	C
1	2A	2178	C
1	2A	2185	C
1	2A	2189	U
1	2A	2192	G
1	2A	2198	A
1	2A	2206	G
1	2A	2207	G
1	2A	2208	A
1	2A	2218	U
1	2A	2225	A
1	2A	2232	U
1	2A	2235	G
1	2A	2239	G

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Mol	Chain	Res	Type
1	2A	2275	C
1	2A	2279	G
1	2A	2283	C
1	2A	2287	A
1	2A	2302	G
1	2A	2305	A
1	2A	2308	G
1	2A	2319	G
1	2A	2320	A
1	2A	2321	G
1	2A	2324	C
1	2A	2325	G
1	2A	2327	A
1	2A	2328	A
1	2A	2329	G
1	2A	2334	G
1	2A	2336	A
1	2A	2341	G
1	2A	2346	A
1	2A	2347	C
1	2A	2350	C
1	2A	2354	G
1	2A	2376	A
1	2A	2383	G
1	2A	2385	C
1	2A	2403	C
1	2A	2406	U
1	2A	2410	G
1	2A	2419	U
1	2A	2425	A
1	2A	2426	A
1	2A	2429	G
1	2A	2430	A
1	2A	2434	A
1	2A	2435	A
1	2A	2439	A
1	2A	2441	C
1	2A	2445	G
1	2A	2448	A
1	2A	2458	G
1	2A	2465	C
1	2A	2468	G

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Mol	Chain	Res	Type
1	2A	2469	A
1	2A	2474	C
1	2A	2476	A
1	2A	2477	C
1	2A	2478	A
1	2A	2490	G
1	2A	2491	U
1	2A	2502	G
1	2A	2505	G
1	2A	2506	U
1	2A	2518	A
1	2A	2520	C
1	2A	2525	G
1	2A	2529	G
1	2A	2554	U
1	2A	2555	U
1	2A	2566	A
1	2A	2567	G
1	2A	2573	C
1	2A	2578	G
1	2A	2602	A
1	2A	2609	U
1	2A	2611	U
1	2A	2612	C
1	2A	2629	A
1	2A	2630	G
1	2A	2634	G
1	2A	2654	A
1	2A	2663	G
1	2A	2664	G
1	2A	2689	U
1	2A	2690	C
1	2A	2712(A)	A
1	2A	2713	A
1	2A	2714	G
1	2A	2726	U
1	2A	2733	A
1	2A	2739	U
1	2A	2744	G
1	2A	2751	G
1	2A	2758	A
1	2A	2764	A

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Mol	Chain	Res	Type
1	2A	2765	A
1	2A	2766	G
1	2A	2778	A
1	2A	2789	C
1	2A	2793	G
1	2A	2802	G
1	2A	2803	C
1	2A	2807	G
1	2A	2818	G
1	2A	2820	A
1	2A	2821	A
1	2A	2824	C
1	2A	2833	G
1	2A	2836	U
1	2A	2839	G
1	2A	2872	G
1	2A	2879	C
1	2A	2880	C
1	2A	2894	G
1	2A	2895	U
1	2A	2897	U
2	2B	2	C
2	2B	5	C
2	2B	8	U
2	2B	9	G
2	2B	19	G
2	2B	20	C
2	2B	25	A
2	2B	32	C
2	2B	34	U
2	2B	38	C
2	2B	42	C
2	2B	52	A
2	2B	53	A
2	2B	56	G
2	2B	57	A
2	2B	58	A
2	2B	63	G
2	2B	65	C
2	2B	66	A
2	2B	67	G
2	2B	72	G

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Mol	Chain	Res	Type
2	2B	73	A
2	2B	74	U
2	2B	75	G
2	2B	85	G
2	2B	88	C
2	2B	90	A
2	2B	91	C
2	2B	106	G
2	2B	108	U
2	2B	110	G
2	2B	114	C
2	2B	116	G
2	2B	119	G
2	2B	120	A
32	2a	7	G
32	2a	9	G
32	2a	32	A
32	2a	39	G
32	2a	47	C
32	2a	48	C
32	2a	51	A
32	2a	54	C
32	2a	65	U
32	2a	66	G
32	2a	73	G
32	2a	79	G
32	2a	80	G
32	2a	89	C
32	2a	91	C
32	2a	97	G
32	2a	98	G
32	2a	101	A
32	2a	116	A
32	2a	121	C
32	2a	131	C
32	2a	163	C
32	2a	174	C
32	2a	180	U
32	2a	182	U
32	2a	195	A
32	2a	197	A
32	2a	201	C

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Mol	Chain	Res	Type
32	2a	202	U
32	2a	203	U
32	2a	204	U
32	2a	216	G
32	2a	217	C
32	2a	247	G
32	2a	251	G
32	2a	258	G
32	2a	266	G
32	2a	267	C
32	2a	289	G
32	2a	301	G
32	2a	306	G
32	2a	321	A
32	2a	328	C
32	2a	332	G
32	2a	342	C
32	2a	348	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	384	G
32	2a	397	A
32	2a	398	C
32	2a	406	G
32	2a	412	A
32	2a	421	U
32	2a	423	G
32	2a	424	G
32	2a	429	U
32	2a	441	A
32	2a	442	C
32	2a	452	A
32	2a	461	A
32	2a	470	C
32	2a	471	G
32	2a	477	A
32	2a	484	G
32	2a	485	G

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Mol	Chain	Res	Type
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	531	U
32	2a	532	A
32	2a	547	A
32	2a	559	A
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	587	G
32	2a	588	G
32	2a	596	C
32	2a	630	G
32	2a	650	G
32	2a	653	A
32	2a	665	A
32	2a	687	A
32	2a	688	G
32	2a	695	A
32	2a	702	A
32	2a	721	G
32	2a	723	U
32	2a	731	G
32	2a	733	A
32	2a	749	C
32	2a	755	G
32	2a	774	G
32	2a	777	A
32	2a	792	A
32	2a	793	U
32	2a	794	A
32	2a	815	A
32	2a	817	C
32	2a	821	G

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Mol	Chain	Res	Type
32	2a	828	A
32	2a	840	C
32	2a	841	U
32	2a	851	G
32	2a	853	G
32	2a	859	A
32	2a	870	U
32	2a	880	C
32	2a	902	G
32	2a	914	A
32	2a	926	G
32	2a	927	G
32	2a	932	C
32	2a	934	C
32	2a	960	U
32	2a	961	U
32	2a	968	A
32	2a	969	A
32	2a	971	G
32	2a	974	A
32	2a	975	A
32	2a	976	G
32	2a	977	A
32	2a	982	U
32	2a	989	C
32	2a	992	U
32	2a	993	G
32	2a	997	U
32	2a	1001(A)	G
32	2a	1002	G
32	2a	1003	G
32	2a	1005	A
32	2a	1006	C
32	2a	1009	G
32	2a	1011	G
32	2a	1016	A
32	2a	1020	U
32	2a	1021	G
32	2a	1022	G
32	2a	1025	U
32	2a	1026	G
32	2a	1027	C

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Mol	Chain	Res	Type
32	2a	1028	C
32	2a	1030	C
32	2a	1030(A)	G
32	2a	1031	G
32	2a	1033	G
32	2a	1036	G
32	2a	1038	C
32	2a	1039	C
32	2a	1040	U
32	2a	1045	C
32	2a	1051	C
32	2a	1065	U
32	2a	1066	C
32	2a	1068	G
32	2a	1077	G
32	2a	1080	A
32	2a	1081	G
32	2a	1086	U
32	2a	1094	G
32	2a	1095	U
32	2a	1101	A
32	2a	1108	G
32	2a	1117	G
32	2a	1122	U
32	2a	1125	U
32	2a	1129	C
32	2a	1130	A
32	2a	1132	C
32	2a	1134	G
32	2a	1137	C
32	2a	1138	G
32	2a	1139	G
32	2a	1140	C
32	2a	1141	C
32	2a	1146	A
32	2a	1152	A
32	2a	1159	U
32	2a	1163	C
32	2a	1172	C
32	2a	1181	G
32	2a	1182	G
32	2a	1183	A

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Mol	Chain	Res	Type
32	2a	1184	G
32	2a	1196	U
32	2a	1197	G
32	2a	1202	G
32	2a	1211	U
32	2a	1212	U
32	2a	1213	A
32	2a	1222	G
32	2a	1226	C
32	2a	1227	A
32	2a	1238	A
32	2a	1240	U
32	2a	1241	G
32	2a	1256	A
32	2a	1257	U
32	2a	1260	C
32	2a	1267	C
32	2a	1270	C
32	2a	1272	G
32	2a	1273	G
32	2a	1276	G
32	2a	1278	U
32	2a	1279	A
32	2a	1280	A
32	2a	1287	A
32	2a	1300	G
32	2a	1303	C
32	2a	1305	G
32	2a	1320	C
32	2a	1328	C
32	2a	1338	G
32	2a	1340	A
32	2a	1346	A
32	2a	1347	G
32	2a	1353	G
32	2a	1363	C
32	2a	1368	G
32	2a	1370	G
32	2a	1419	G
32	2a	1442	G
32	2a	1442(A)	G
32	2a	1446	U

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Mol	Chain	Res	Type
32	2a	1447	A
32	2a	1456	G
32	2a	1487	G
32	2a	1492	A
32	2a	1494	G
32	2a	1497	G
32	2a	1503	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
32	2a	1531	A
32	2a	1532	U
53	2v	13	A
53	2v	15	A
53	2v	24	A
54	2w	3	C
54	2w	4	C
54	2w	5	G
54	2w	7	A
54	2w	8	4SU
54	2w	9	A
54	2w	13	C
54	2w	14	A
54	2w	19	G
54	2w	22	G
54	2w	25	C
54	2w	29	G
54	2w	34	G
54	2w	38	A
54	2w	46	7MG
54	2w	47	U
54	2w	48	C
54	2w	50	U
54	2w	56	C
54	2w	62	C
54	2w	63	G
54	2w	64	A
54	2w	65	G
54	2w	68	C

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Mol	Chain	Res	Type
54	2w	69	G
54	2w	70	G
54	2w	74	C
55	2x	9	G
55	2x	10	G
55	2x	13	C
55	2x	18	G
55	2x	21	A
55	2x	22	G
55	2x	42	G
55	2x	43	A
55	2x	47	U
55	2x	48	C
55	2x	52	G
55	2x	53	G
55	2x	65	C
55	2x	67	C
55	2x	68	C
55	2x	76	A
54	2y	15	G
54	2y	19	G
54	2y	23	A
54	2y	24	G
54	2y	25	C
54	2y	27	G
54	2y	34	G
54	2y	45	U
54	2y	49	C
54	2y	52	G
54	2y	53	G
54	2y	55	PSU
54	2y	56	C
54	2y	57	G
54	2y	58	A
54	2y	59	U
54	2y	61	C
54	2y	62	C
54	2y	63	G
54	2y	65	G
54	2y	69	G
54	2y	70	G
54	2y	73	A

All (72) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	1A	12	U
1	1A	115	G
1	1A	185	A
1	1A	271	U
1	1A	302	A
1	1A	509	A
1	1A	572	A
1	1A	596	G
1	1A	793	A
1	1A	821	A
1	1A	847	A
1	1A	913	A
1	1A	941	U
1	1A	1019	G
1	1A	1065	U
1	1A	1067	A
1	1A	1093	G
1	1A	1119	A
1	1A	1188	A
1	1A	1201	A
1	1A	1219	A
1	1A	1220	U
1	1A	1221	G
1	1A	1255	A
1	1A	1321	A
1	1A	1347	A
1	1A	1425	A
1	1A	1466	U
1	1A	1554	A
1	1A	1654	A
1	1A	1700	G
1	1A	2014	G
1	1A	2156	A
1	1A	2180	A
1	1A	2192	A
1	1A	2203	G
1	1A	2205	C
1	1A	2418	U
1	1A	2442	A
1	1A	2451	A
1	1A	2641	A
1	1A	2701	U

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Mol	Chain	Res	Type
1	1A	2769	U
2	1B	1	U
1	2A	34	C
1	2A	195	A
1	2A	196	A
1	2A	228	A
1	2A	266	G
1	2A	271(K)	U
1	2A	271(M)	G
1	2A	277	C
1	2A	528	A
1	2A	752	A
1	2A	774	A
1	2A	827	U
1	2A	856	C
1	2A	883	G
1	2A	900	A
1	2A	1210	A
1	2A	1420	U
1	2A	1442	G
1	2A	1530	C
1	2A	1608	A
1	2A	1653	G
1	2A	1913	A
1	2A	1992	G
1	2A	2119	A
1	2A	2126	A
1	2A	2406	U
1	2A	2439	A
1	2A	2689	U

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	2MA	1A	2515	1,56	17,25,26	1.06	1 (5%)	17,37,40	1.11	2 (11%)
55	PSU	1x	55	55,56	18,21,22	1.34	2 (11%)	22,30,33	1.85	3 (13%)
1	PSU	2A	1917	1	18,21,22	1.34	2 (11%)	22,30,33	1.82	3 (13%)
55	4SU	1x	8	55	18,21,22	2.02	5 (27%)	26,30,33	1.60	6 (23%)
32	PSU	1a	516	32	18,21,22	1.40	3 (16%)	22,30,33	1.75	5 (22%)
32	5MC	2a	1404	32	18,22,23	1.00	2 (11%)	26,32,35	1.18	3 (11%)
1	5MU	2A	1939	1,56	19,22,23	1.46	6 (31%)	28,32,35	2.50	6 (21%)
54	4SU	1y	8	54	18,21,22	1.63	4 (22%)	26,30,33	1.83	5 (19%)
32	4OC	2a	1402	56,32	20,23,24	0.81	0	26,32,35	1.07	1 (3%)
54	PSU	2y	55	54	18,21,22	1.31	3 (16%)	22,30,33	1.78	5 (22%)
1	5MC	2A	1962	1,56	18,22,23	0.99	2 (11%)	26,32,35	1.31	3 (11%)
32	5MC	2a	1400	32	18,22,23	0.96	2 (11%)	26,32,35	1.21	2 (7%)
54	7MG	1y	46	54	22,26,27	1.35	4 (18%)	29,39,42	2.49	6 (20%)
54	MIA	1y	37	54	18,24,32	1.13	2 (11%)	18,35,47	1.32	2 (11%)
1	5MU	2A	1915	1	19,22,23	1.46	4 (21%)	28,32,35	2.20	6 (21%)
32	2MG	1a	1207	32	18,26,27	0.98	1 (5%)	16,38,41	1.02	1 (6%)
54	PSU	2w	39	54	18,21,22	1.33	2 (11%)	22,30,33	1.67	3 (13%)
32	UR3	2a	1498	32	19,22,23	1.06	2 (10%)	26,32,35	1.54	2 (7%)
54	PSU	1y	55	54	18,21,22	1.31	2 (11%)	22,30,33	1.97	4 (18%)
54	7MG	2y	46	54	22,26,27	1.45	4 (18%)	29,39,42	2.67	7 (24%)
54	MIA	1w	37	54	24,31,32	2.23	3 (12%)	26,44,47	2.60	9 (34%)
1	2MU	1A	2564	1,56	19,22,24	1.18	2 (10%)	26,31,36	1.91	6 (23%)
54	MIA	2y	37	54	18,24,32	1.10	2 (11%)	18,35,47	1.31	3 (16%)
54	PSU	2y	39	54	18,21,22	1.33	2 (11%)	22,30,33	1.79	3 (13%)
32	5MC	2a	1407	32	18,22,23	0.96	2 (11%)	26,32,35	1.20	4 (15%)
55	5MU	1x	54	55,56	19,22,23	1.45	6 (31%)	28,32,35	1.87	6 (21%)
1	PSU	2A	2605	1	18,21,22	1.23	2 (11%)	22,30,33	2.03	5 (22%)
32	5MC	2a	967	32	18,22,23	0.98	1 (5%)	26,32,35	1.16	4 (15%)
54	MIA	2w	37	54	20,27,32	1.73	3 (15%)	22,39,47	1.88	7 (31%)
32	UR3	1a	1498	32	19,22,23	1.09	1 (5%)	26,32,35	1.57	4 (15%)
54	PSU	2w	55	54,56	18,21,22	1.36	2 (11%)	22,30,33	1.80	3 (13%)
32	7MG	2a	527	56,32	22,26,27	1.35	5 (22%)	29,39,42	2.49	6 (20%)
32	PSU	2a	516	32	18,21,22	1.31	2 (11%)	22,30,33	1.76	4 (18%)
32	MA6	2a	1519	32	19,26,27	1.04	1 (5%)	18,38,41	1.79	4 (22%)
32	5MC	1a	1407	32	18,22,23	0.98	2 (11%)	26,32,35	1.25	4 (15%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
54	PSU	1y	39	54	18,21,22	1.39	2 (11%)	22,30,33	1.71	3 (13%)
43	0TD	1l	92	43	7,9,10	5.97	5 (71%)	6,11,13	4.08	2 (33%)
1	PSU	1A	2617	1,56	18,21,22	1.49	3 (16%)	22,30,33	1.96	4 (18%)
55	5MC	1x	32	55	18,22,23	1.02	2 (11%)	26,32,35	1.22	2 (7%)
32	4OC	1a	1402	32	20,23,24	0.78	0	26,32,35	1.01	2 (7%)
54	4SU	1w	8	54	18,21,22	1.72	4 (22%)	26,30,33	1.93	5 (19%)
54	5MU	2y	54	54	19,22,23	1.50	4 (21%)	28,32,35	2.09	9 (32%)
1	5MU	1A	1961	1,56	19,22,23	1.32	4 (21%)	28,32,35	2.57	6 (21%)
55	5MC	2x	32	55	18,22,23	0.99	2 (11%)	26,32,35	1.17	3 (11%)
54	PSU	1w	32	54,56	18,21,22	1.33	2 (11%)	22,30,33	1.86	3 (13%)
1	2MU	2A	2552	1,56	19,22,24	1.30	2 (10%)	26,31,36	1.75	5 (19%)
1	5MC	1A	1984	1,56	18,22,23	0.97	2 (11%)	26,32,35	1.22	5 (19%)
54	4SU	2y	8	54	18,21,22	1.77	4 (22%)	26,30,33	2.18	5 (19%)
54	PSU	1y	32	54	18,21,22	1.38	3 (16%)	22,30,33	1.75	3 (13%)
54	7MG	1w	46	54	22,26,27	1.50	4 (18%)	29,39,42	2.42	6 (20%)
32	MA6	1a	1519	32	19,26,27	1.10	1 (5%)	18,38,41	1.58	4 (22%)
54	PSU	2w	32	54	18,21,22	1.35	2 (11%)	22,30,33	1.84	3 (13%)
32	5MC	1a	1404	32	18,22,23	1.00	2 (11%)	26,32,35	1.19	3 (11%)
54	4SU	2w	8	54	18,21,22	1.72	4 (22%)	26,30,33	2.40	5 (19%)
32	5MC	1a	1400	32	18,22,23	0.94	2 (11%)	26,32,35	1.18	2 (7%)
54	5MU	2w	54	54	19,22,23	1.38	4 (21%)	28,32,35	1.87	6 (21%)
1	4OC	2A	1920	1	19,22,24	0.78	0	26,31,35	0.83	0
32	M2G	2a	966	32	20,27,28	1.40	3 (15%)	22,40,43	0.99	2 (9%)
1	PSU	2A	1911	1	18,21,22	1.40	2 (11%)	22,30,33	1.70	4 (18%)
1	PSU	1A	1939	1	18,21,22	1.40	4 (22%)	22,30,33	1.96	3 (13%)
1	5MC	2A	1942	1	18,22,23	0.98	1 (5%)	26,32,35	1.11	2 (7%)
54	PSU	2y	32	54	18,21,22	1.33	2 (11%)	22,30,33	1.79	4 (18%)
1	5MU	1A	1937	1	19,22,23	1.35	5 (26%)	28,32,35	2.15	7 (25%)
32	MA6	1a	1518	32	19,26,27	0.91	1 (5%)	18,38,41	1.73	6 (33%)
54	PSU	1w	39	54	18,21,22	1.35	2 (11%)	22,30,33	1.81	3 (13%)
55	5MU	2x	54	55	19,22,23	1.39	4 (21%)	28,32,35	2.18	6 (21%)
1	5MC	1A	1964	1,56	18,22,23	0.90	2 (11%)	26,32,35	1.24	2 (7%)
54	5MU	1y	54	54	19,22,23	1.55	6 (31%)	28,32,35	1.97	6 (21%)
43	0TD	2l	92	43	7,9,10	5.80	2 (28%)	6,11,13	2.19	1 (16%)
1	PSU	1A	1933	1	18,21,22	1.32	2 (11%)	22,30,33	1.91	3 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
32	2MG	2a	1207	32	18,26,27	0.90	1 (5%)	16,38,41	1.15	2 (12%)
32	7MG	1a	527	56,32	22,26,27	1.50	4 (18%)	29,39,42	2.36	8 (27%)
1	OMG	2A	2251	1,55,56	18,26,27	0.93	1 (5%)	19,38,41	1.20	3 (15%)
54	PSU	1w	55	54	18,21,22	1.33	2 (11%)	22,30,33	1.84	3 (13%)
1	OMG	1A	2263	1,55,56	18,26,27	0.99	1 (5%)	19,38,41	1.08	3 (15%)
55	4SU	2x	8	55	18,21,22	1.94	6 (33%)	26,30,33	1.41	5 (19%)
55	PSU	2x	55	55	18,21,22	1.36	2 (11%)	22,30,33	1.83	3 (13%)
32	MA6	2a	1518	32	19,26,27	0.99	1 (5%)	18,38,41	1.74	5 (27%)
32	M2G	1a	966	32	20,27,28	1.53	3 (15%)	22,40,43	0.90	2 (9%)
32	5MC	1a	967	32	18,22,23	0.96	2 (11%)	26,32,35	1.16	3 (11%)
54	5MU	1w	54	54	19,22,23	1.47	5 (26%)	28,32,35	2.04	6 (21%)
1	4OC	1A	1942	1	19,22,24	0.81	0	26,31,35	0.94	1 (3%)
54	7MG	2w	46	54	22,26,27	1.42	3 (13%)	29,39,42	2.37	7 (24%)
1	2MA	2A	2503	1,56	17,25,26	1.07	1 (5%)	17,37,40	0.97	2 (11%)

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	2MA	1A	2515	1,56	-	2/3/25/26	0/3/3/3
55	PSU	1x	55	55,56	-	0/7/25/26	0/2/2/2
1	PSU	2A	1917	1	-	0/7/25/26	0/2/2/2
55	4SU	1x	8	55	-	0/7/25/26	0/2/2/2
32	PSU	1a	516	32	-	0/7/25/26	0/2/2/2
32	5MC	2a	1404	32	-	0/7/25/26	0/2/2/2
1	5MU	2A	1939	1,56	-	0/7/25/26	0/2/2/2
54	4SU	1y	8	54	-	3/7/25/26	0/2/2/2
32	4OC	2a	1402	56,32	-	2/9/29/30	0/2/2/2
54	PSU	2y	55	54	-	3/7/25/26	0/2/2/2
1	5MC	2A	1962	1,56	-	0/7/25/26	0/2/2/2
32	5MC	2a	1400	32	-	0/7/25/26	0/2/2/2
54	7MG	1y	46	54	-	2/7/37/38	0/3/3/3
54	MIA	1y	37	54	-	0/3/25/34	0/3/3/3
1	5MU	2A	1915	1	-	0/7/25/26	0/2/2/2
32	2MG	1a	1207	32	-	0/5/27/28	0/3/3/3
54	PSU	2w	39	54	-	0/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
32	UR3	2a	1498	32	-	0/7/25/26	0/2/2/2
54	PSU	1y	55	54	-	1/7/25/26	0/2/2/2
54	7MG	2y	46	54	-	3/7/37/38	0/3/3/3
54	MIA	1w	37	54	-	2/11/33/34	0/3/3/3
1	2MU	1A	2564	1,56	-	0/9/27/28	0/2/2/2
54	MIA	2y	37	54	-	3/3/25/34	0/3/3/3
54	PSU	2y	39	54	-	0/7/25/26	0/2/2/2
32	5MC	2a	1407	32	-	0/7/25/26	0/2/2/2
55	5MU	1x	54	55,56	-	0/7/25/26	0/2/2/2
1	PSU	2A	2605	1	-	0/7/25/26	0/2/2/2
32	5MC	2a	967	32	-	0/7/25/26	0/2/2/2
54	MIA	2w	37	54	-	1/7/29/34	0/3/3/3
32	UR3	1a	1498	32	-	0/7/25/26	0/2/2/2
54	PSU	2w	55	54,56	-	0/7/25/26	0/2/2/2
32	7MG	2a	527	56,32	-	3/7/37/38	0/3/3/3
32	PSU	2a	516	32	-	0/7/25/26	0/2/2/2
32	MA6	2a	1519	32	-	3/7/29/30	0/3/3/3
32	5MC	1a	1407	32	-	0/7/25/26	0/2/2/2
54	PSU	1y	39	54	-	0/7/25/26	0/2/2/2
43	0TD	1l	92	43	-	3/7/12/14	-
1	PSU	1A	2617	1,56	-	0/7/25/26	0/2/2/2
55	5MC	1x	32	55	-	0/7/25/26	0/2/2/2
32	4OC	1a	1402	32	-	3/9/29/30	0/2/2/2
54	4SU	1w	8	54	-	0/7/25/26	0/2/2/2
54	5MU	2y	54	54	-	2/7/25/26	0/2/2/2
1	5MU	1A	1961	1,56	-	0/7/25/26	0/2/2/2
55	5MC	2x	32	55	-	0/7/25/26	0/2/2/2
54	PSU	1w	32	54,56	-	0/7/25/26	0/2/2/2
1	2MU	2A	2552	1,56	-	0/9/27/28	0/2/2/2
1	5MC	1A	1984	1,56	-	0/7/25/26	0/2/2/2
54	4SU	2y	8	54	-	1/7/25/26	0/2/2/2
54	PSU	1y	32	54	-	0/7/25/26	0/2/2/2
54	7MG	1w	46	54	-	3/7/37/38	0/3/3/3
32	MA6	1a	1519	32	-	4/7/29/30	0/3/3/3
54	PSU	2w	32	54	-	0/7/25/26	0/2/2/2
32	5MC	1a	1404	32	-	0/7/25/26	0/2/2/2
54	4SU	2w	8	54	-	1/7/25/26	0/2/2/2
32	5MC	1a	1400	32	-	2/7/25/26	0/2/2/2
54	5MU	2w	54	54	-	0/7/25/26	0/2/2/2
1	4OC	2A	1920	1	-	0/9/27/30	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
32	M2G	2a	966	32	-	0/7/29/30	0/3/3/3
1	PSU	2A	1911	1	-	0/7/25/26	0/2/2/2
1	PSU	1A	1939	1	-	0/7/25/26	0/2/2/2
1	5MC	2A	1942	1	-	0/7/25/26	0/2/2/2
54	PSU	2y	32	54	-	1/7/25/26	0/2/2/2
1	5MU	1A	1937	1	-	0/7/25/26	0/2/2/2
32	MA6	1a	1518	32	-	2/7/29/30	0/3/3/3
54	PSU	1w	39	54	-	1/7/25/26	0/2/2/2
55	5MU	2x	54	55	-	0/7/25/26	0/2/2/2
1	5MC	1A	1964	1,56	-	0/7/25/26	0/2/2/2
54	5MU	1y	54	54	-	3/7/25/26	0/2/2/2
43	0TD	2l	92	43	-	1/7/12/14	-
1	PSU	1A	1933	1	-	0/7/25/26	0/2/2/2
32	2MG	2a	1207	32	-	0/5/27/28	0/3/3/3
32	7MG	1a	527	56,32	-	2/7/37/38	0/3/3/3
1	OMG	2A	2251	1,55,56	-	0/5/27/28	0/3/3/3
54	PSU	1w	55	54	-	0/7/25/26	0/2/2/2
1	OMG	1A	2263	1,55,56	-	0/5/27/28	0/3/3/3
55	4SU	2x	8	55	-	1/7/25/26	0/2/2/2
55	PSU	2x	55	55	-	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
32	5MC	1a	967	32	-	0/7/25/26	0/2/2/2
54	5MU	1w	54	54	-	0/7/25/26	0/2/2/2
1	4OC	1A	1942	1	-	1/9/27/30	0/2/2/2
54	7MG	2w	46	54	-	4/7/37/38	0/3/3/3
1	2MA	2A	2503	1,56	-	1/3/25/26	0/3/3/3

All (215) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
43	2l	92	0TD	CB-SB	-14.90	1.67	1.82
43	1l	92	0TD	CB-SB	-14.81	1.67	1.82
54	1w	37	MIA	C13-C14	7.24	1.53	1.32
54	1w	37	MIA	C2-S10	-6.78	1.70	1.75
54	2w	37	MIA	C2-S10	-6.02	1.70	1.75
32	1a	966	M2G	C2-N3	4.88	1.36	1.30
55	1x	8	4SU	C4-N3	-4.79	1.32	1.37
54	2y	8	4SU	C4-S4	-4.56	1.59	1.68
32	2a	966	M2G	C2-N3	4.54	1.36	1.30
55	2x	8	4SU	C4-N3	-4.51	1.32	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
54	2w	8	4SU	C4-S4	-4.49	1.59	1.68
54	1w	8	4SU	C4-S4	-4.29	1.60	1.68
32	1a	527	7MG	C4-N9	-3.98	1.33	1.37
55	2x	8	4SU	C4-S4	-3.94	1.60	1.68
54	1y	8	4SU	C4-S4	-3.90	1.61	1.68
54	1y	32	PSU	C6-C5	3.90	1.39	1.35
54	2w	55	PSU	C6-C5	3.86	1.39	1.35
54	1y	39	PSU	C6-C5	3.82	1.39	1.35
54	2w	46	7MG	C4-N9	-3.82	1.33	1.37
54	1w	55	PSU	C6-C5	3.82	1.39	1.35
55	2x	55	PSU	C6-C5	3.75	1.39	1.35
55	1x	8	4SU	C2-N3	-3.71	1.31	1.38
54	1w	46	7MG	C4-N9	-3.70	1.33	1.37
55	1x	8	4SU	C4-S4	-3.65	1.61	1.68
54	2y	32	PSU	C6-C5	3.64	1.39	1.35
1	2A	1911	PSU	C6-C5	3.63	1.39	1.35
32	2a	516	PSU	C6-C5	3.51	1.39	1.35
54	2w	39	PSU	C6-C5	3.51	1.39	1.35
54	1w	39	PSU	C6-C5	3.47	1.39	1.35
32	1a	516	PSU	C6-C5	3.42	1.39	1.35
54	2w	32	PSU	C6-C5	3.39	1.39	1.35
54	2y	46	7MG	C5-C4	3.39	1.49	1.38
54	2y	39	PSU	C6-C5	3.37	1.39	1.35
54	2y	54	5MU	C2-N1	3.37	1.43	1.38
1	2A	2605	PSU	C6-C5	3.36	1.39	1.35
1	2A	1917	PSU	C6-C5	3.36	1.39	1.35
54	1y	55	PSU	C6-C5	3.32	1.39	1.35
55	1x	55	PSU	C6-C5	3.26	1.39	1.35
54	1y	8	4SU	C4-N3	-3.22	1.34	1.37
43	1l	92	0TD	CSB-SB	-3.20	1.73	1.79
54	1w	46	7MG	C5-C4	3.18	1.48	1.38
54	1w	32	PSU	C6-C5	3.15	1.39	1.35
54	1y	46	7MG	C5-C4	3.13	1.48	1.38
1	2A	1942	5MC	C6-C5	3.13	1.39	1.34
32	2a	1404	5MC	C6-C5	3.09	1.39	1.34
54	1y	54	5MU	C6-C5	3.07	1.39	1.34
55	1x	8	4SU	C5-C4	-3.07	1.38	1.42
32	1a	527	7MG	C5-C4	3.06	1.48	1.38
54	1w	8	4SU	C4-N3	-3.05	1.34	1.37
55	2x	54	5MU	C6-C5	3.03	1.39	1.34
54	2w	46	7MG	C5-C4	3.02	1.47	1.38
54	1w	54	5MU	C6-C5	3.00	1.39	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
54	2y	46	7MG	C8-N9	3.00	1.47	1.46
32	1a	966	M2G	C2-N2	2.98	1.40	1.35
55	2x	8	4SU	C5-C4	-2.98	1.38	1.42
1	1A	1939	PSU	C6-C5	2.96	1.38	1.35
32	2a	527	7MG	C5-C4	2.96	1.47	1.38
1	1A	1933	PSU	C6-C5	2.94	1.38	1.35
1	1A	2263	OMG	C6-N1	-2.94	1.33	1.37
1	1A	2617	PSU	C4-N3	-2.94	1.33	1.38
32	1a	967	5MC	C6-C5	2.92	1.39	1.34
55	2x	32	5MC	C6-C5	2.91	1.39	1.34
32	1a	1404	5MC	C6-C5	2.90	1.39	1.34
32	2a	527	7MG	C4-N9	-2.88	1.34	1.37
54	2y	8	4SU	C4-N3	-2.87	1.34	1.37
54	2w	8	4SU	C2-N1	2.87	1.43	1.38
1	1A	1939	PSU	C4-N3	-2.86	1.33	1.38
54	2w	54	5MU	C6-C5	2.86	1.39	1.34
32	1a	1407	5MC	C6-C5	2.86	1.39	1.34
55	2x	8	4SU	C2-N3	-2.86	1.32	1.38
55	1x	32	5MC	C6-C5	2.85	1.39	1.34
55	1x	54	5MU	C6-C5	2.83	1.39	1.34
55	1x	54	5MU	C4-N3	-2.80	1.33	1.38
1	2A	1915	5MU	C6-C5	2.80	1.39	1.34
54	2w	8	4SU	C4-N3	-2.80	1.34	1.37
54	1y	54	5MU	C2-N1	2.79	1.42	1.38
1	1A	2617	PSU	C2-N1	-2.79	1.32	1.36
1	2A	1939	5MU	C4-C5	2.79	1.49	1.44
1	1A	1961	5MU	C6-C5	2.78	1.39	1.34
1	1A	1933	PSU	C4-N3	-2.78	1.33	1.38
1	2A	1939	5MU	C6-C5	2.78	1.39	1.34
32	1a	1400	5MC	C6-C5	2.77	1.39	1.34
1	2A	1915	5MU	C2-N1	2.76	1.42	1.38
32	2a	967	5MC	C6-C5	2.76	1.39	1.34
32	2a	1400	5MC	C6-C5	2.75	1.39	1.34
54	1y	37	MIA	C5-C4	2.73	1.48	1.40
54	2y	55	PSU	C6-C5	2.72	1.38	1.35
54	2w	46	7MG	C8-N9	2.71	1.47	1.46
54	1y	54	5MU	C4-N3	-2.71	1.33	1.38
1	2A	1915	5MU	C4-C5	2.71	1.49	1.44
54	1w	46	7MG	C8-N9	2.71	1.47	1.46
32	1a	1498	UR3	C2-N1	2.69	1.42	1.38
32	1a	516	PSU	C4-N3	-2.68	1.33	1.38
54	2w	37	MIA	C5-C4	2.68	1.48	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
54	2y	8	4SU	C2-N1	2.67	1.42	1.38
43	1l	92	0TD	CA-N	-2.67	1.39	1.47
54	1w	8	4SU	C5-C4	-2.67	1.39	1.42
55	2x	54	5MU	C4-C5	2.66	1.49	1.44
54	2y	54	5MU	C6-C5	2.66	1.39	1.34
54	2y	37	MIA	C5-C4	2.66	1.48	1.40
1	2A	1962	5MC	C6-N1	-2.65	1.33	1.38
32	2a	966	M2G	C2-N2	2.65	1.40	1.35
54	2y	8	4SU	C5-C4	-2.63	1.39	1.42
54	1w	54	5MU	C2-N1	2.63	1.42	1.38
1	2A	1939	5MU	C4-N3	-2.63	1.34	1.38
54	1w	54	5MU	C4-C5	2.63	1.49	1.44
32	1a	1207	2MG	C6-N1	-2.62	1.34	1.37
1	1A	1984	5MC	C6-N1	-2.61	1.33	1.38
54	1y	54	5MU	C4-C5	2.61	1.49	1.44
54	1y	39	PSU	C4-N3	-2.61	1.34	1.38
54	1w	54	5MU	C4-N3	-2.59	1.34	1.38
43	2l	92	0TD	OD2-CG	-2.59	1.22	1.30
1	1A	1937	5MU	C6-C5	2.59	1.38	1.34
1	1A	2617	PSU	C2-N3	-2.59	1.33	1.37
1	1A	2515	2MA	C2-N3	2.59	1.36	1.31
54	2y	37	MIA	C2-N3	2.59	1.36	1.32
32	2a	1518	MA6	C5-C4	2.59	1.47	1.40
1	1A	1961	5MU	C4-N3	-2.58	1.34	1.38
54	1w	39	PSU	C4-N3	-2.57	1.34	1.38
54	1w	37	MIA	C5-C4	2.56	1.47	1.40
1	2A	1962	5MC	C6-C5	2.55	1.38	1.34
54	2y	46	7MG	C6-N1	-2.55	1.34	1.38
43	1l	92	0TD	OD2-CG	-2.54	1.22	1.30
32	2a	1407	5MC	C6-N1	-2.54	1.33	1.38
54	2y	39	PSU	C4-N3	-2.54	1.34	1.38
54	2w	32	PSU	C4-N3	-2.54	1.34	1.38
1	2A	2503	2MA	C2-N3	2.53	1.36	1.31
1	2A	1911	PSU	C4-N3	-2.53	1.34	1.38
55	1x	32	5MC	C6-N1	-2.52	1.33	1.38
32	1a	1519	MA6	C5-C4	2.51	1.47	1.40
43	1l	92	0TD	CB-CG	-2.50	1.47	1.52
54	1y	37	MIA	C2-N3	2.49	1.36	1.32
54	1w	46	7MG	C6-N1	-2.49	1.34	1.38
1	1A	1964	5MC	C6-C5	2.48	1.38	1.34
32	2a	1519	MA6	C5-C4	2.48	1.47	1.40
1	1A	1937	5MU	C4-N3	-2.48	1.34	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
54	2w	39	PSU	C4-N3	-2.47	1.34	1.38
54	2w	54	5MU	C4-C5	2.47	1.48	1.44
55	2x	55	PSU	C4-N3	-2.47	1.34	1.38
1	1A	2564	2MU	C4-N3	-2.47	1.34	1.38
54	2y	55	PSU	C4-N3	-2.46	1.34	1.38
54	1w	32	PSU	C4-N3	-2.46	1.34	1.38
54	2y	54	5MU	C4-C5	2.45	1.48	1.44
54	2y	54	5MU	C4-N3	-2.45	1.34	1.38
54	1y	46	7MG	C8-N9	2.44	1.47	1.46
32	1a	966	M2G	C6-N1	-2.43	1.34	1.37
32	1a	527	7MG	C8-N9	2.43	1.47	1.46
55	1x	54	5MU	C4-C5	2.43	1.48	1.44
54	2w	54	5MU	C2-N1	2.42	1.42	1.38
54	2w	55	PSU	C4-N3	-2.40	1.34	1.38
32	2a	1498	UR3	C2-N1	2.40	1.42	1.38
54	2w	37	MIA	C6-N1	2.39	1.36	1.32
32	2a	527	7MG	C6-N1	-2.39	1.34	1.38
55	1x	55	PSU	C4-N3	-2.39	1.34	1.38
1	1A	1961	5MU	C6-N1	-2.38	1.34	1.38
1	2A	2552	2MU	C4-N3	-2.37	1.34	1.38
1	2A	1915	5MU	C4-N3	-2.37	1.34	1.38
54	1y	55	PSU	C4-N3	-2.37	1.34	1.38
32	1a	527	7MG	C6-N1	-2.37	1.34	1.38
32	2a	1407	5MC	C6-C5	2.36	1.38	1.34
55	1x	8	4SU	O2-C2	2.36	1.27	1.23
54	2w	8	4SU	C5-C4	-2.35	1.39	1.42
1	2A	2552	2MU	C5-C4	2.35	1.48	1.43
1	2A	1917	PSU	C4-N3	-2.34	1.34	1.38
54	1y	46	7MG	C4-N9	-2.33	1.35	1.37
32	1a	1518	MA6	C5-C4	2.32	1.47	1.40
54	2y	32	PSU	C4-N3	-2.31	1.34	1.38
32	2a	1400	5MC	C6-N1	-2.31	1.34	1.38
54	1y	8	4SU	C5-C4	-2.30	1.39	1.42
54	1y	46	7MG	C6-N1	-2.29	1.34	1.38
1	2A	2605	PSU	C4-N3	-2.28	1.34	1.38
32	2a	1207	2MG	C6-N1	-2.28	1.34	1.37
1	2A	1939	5MU	C6-N1	-2.28	1.34	1.38
54	1w	8	4SU	C2-N1	2.27	1.42	1.38
1	2A	2251	OMG	C6-N1	-2.25	1.34	1.37
1	1A	1984	5MC	C6-C5	2.25	1.38	1.34
1	1A	1937	5MU	C4-C5	2.25	1.48	1.44
32	1a	1400	5MC	C6-N1	-2.23	1.34	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	2A	1939	5MU	C2-N3	-2.23	1.34	1.38
54	1y	32	PSU	C4-N3	-2.23	1.34	1.38
1	1A	1937	5MU	C2-N1	2.22	1.42	1.38
55	2x	54	5MU	C4-N3	-2.22	1.34	1.38
32	2a	1498	UR3	C6-C5	2.21	1.40	1.35
32	1a	967	5MC	C6-N1	-2.20	1.34	1.38
32	2a	516	PSU	C4-N3	-2.18	1.34	1.38
32	2a	527	7MG	C5-C6	2.17	1.49	1.43
1	1A	1964	5MC	C6-N1	-2.17	1.34	1.38
1	1A	2564	2MU	C2-N3	-2.17	1.34	1.38
32	1a	1404	5MC	C6-N1	-2.16	1.34	1.38
1	1A	1939	PSU	C2-N1	-2.16	1.33	1.36
54	1w	55	PSU	C4-N3	-2.15	1.34	1.38
1	1A	1961	5MU	C2-N3	-2.14	1.34	1.38
1	1A	1937	5MU	C6-N1	-2.13	1.34	1.38
54	2y	55	PSU	C2-N1	-2.13	1.33	1.36
54	1y	54	5MU	C2-N3	-2.13	1.34	1.38
32	1a	1407	5MC	C6-N1	-2.12	1.34	1.38
55	1x	54	5MU	C2-N3	-2.11	1.34	1.38
54	2w	54	5MU	C4-N3	-2.11	1.34	1.38
32	2a	966	M2G	C6-N1	-2.11	1.34	1.37
54	2y	46	7MG	C2-N3	2.10	1.38	1.33
55	1x	54	5MU	C2-N1	2.10	1.41	1.38
32	1a	516	PSU	C2-N3	-2.09	1.33	1.37
1	2A	1939	5MU	C2-N1	2.08	1.41	1.38
55	1x	54	5MU	C6-N1	-2.07	1.34	1.38
55	2x	8	4SU	O2-C2	2.04	1.26	1.23
32	2a	1404	5MC	C6-N1	-2.04	1.34	1.38
55	2x	54	5MU	C6-N1	-2.04	1.34	1.38
54	1y	54	5MU	C6-N1	-2.03	1.34	1.38
55	2x	8	4SU	C2-N1	2.03	1.41	1.38
54	1w	54	5MU	C2-N3	-2.03	1.34	1.38
54	1y	8	4SU	C6-C5	2.03	1.39	1.35
54	1y	32	PSU	C4-C5	2.02	1.49	1.44
55	2x	32	5MC	C6-N1	-2.02	1.34	1.38
32	2a	527	7MG	C8-N9	2.02	1.47	1.46
1	1A	1939	PSU	C2-N3	-2.01	1.34	1.37

All (335) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	2y	46	7MG	N9-C4-N3	9.86	140.22	125.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	1y	46	7MG	N9-C4-N3	8.92	138.80	125.47
54	1w	46	7MG	N9-C4-N3	8.59	138.32	125.47
32	2a	527	7MG	N9-C4-N3	8.32	137.91	125.47
54	1w	37	MIA	C12-C13-C14	-8.21	111.17	127.14
32	1a	527	7MG	N9-C4-N3	8.19	137.72	125.47
54	2w	46	7MG	N9-C4-N3	7.55	136.76	125.47
54	2w	8	4SU	C4-N3-C2	-7.47	120.08	127.34
43	1l	92	0TD	CB-CA-N	-6.95	94.29	109.10
43	1l	92	0TD	CSB-SB-CB	6.63	114.44	102.44
1	1A	1961	5MU	C5-C4-N3	6.54	120.89	115.31
54	2w	8	4SU	C5-C4-N3	6.45	120.67	114.69
1	1A	1961	5MU	O4-C4-C5	-6.35	117.54	124.90
1	2A	1939	5MU	C4-N3-C2	-6.27	119.23	127.35
1	1A	1961	5MU	C4-N3-C2	-6.22	119.29	127.35
54	1y	55	PSU	N1-C2-N3	6.21	122.17	115.13
1	1A	1939	PSU	N1-C2-N3	6.15	122.10	115.13
54	2y	8	4SU	C4-N3-C2	-6.09	121.42	127.34
54	2y	8	4SU	C5-C4-N3	6.09	120.34	114.69
1	1A	2617	PSU	N1-C2-N3	6.01	121.94	115.13
32	2a	1498	UR3	C4-N3-C2	-5.98	118.93	124.56
55	2x	55	PSU	N1-C2-N3	5.95	121.87	115.13
1	2A	1939	5MU	C5-C4-N3	5.94	120.38	115.31
54	2w	32	PSU	N1-C2-N3	5.92	121.83	115.13
32	1a	1498	UR3	C4-N3-C2	-5.77	119.13	124.56
1	1A	1933	PSU	N1-C2-N3	5.75	121.64	115.13
55	1x	55	PSU	N1-C2-N3	5.73	121.62	115.13
54	1w	32	PSU	N1-C2-N3	5.73	121.62	115.13
1	2A	1917	PSU	N1-C2-N3	5.71	121.60	115.13
54	1w	39	PSU	N1-C2-N3	5.69	121.58	115.13
54	2y	46	7MG	C5-C4-N3	-5.68	117.31	128.13
1	2A	2605	PSU	N1-C2-N3	5.67	121.55	115.13
54	2y	32	PSU	N1-C2-N3	5.58	121.45	115.13
32	2a	527	7MG	N9-C8-N7	-5.57	95.42	103.38
1	2A	1939	5MU	C5-C6-N1	-5.57	117.61	123.34
54	2y	39	PSU	N1-C2-N3	5.56	121.43	115.13
54	2w	55	PSU	N1-C2-N3	5.53	121.39	115.13
54	1y	39	PSU	N1-C2-N3	5.51	121.37	115.13
54	1w	8	4SU	C4-N3-C2	-5.51	121.99	127.34
54	1y	8	4SU	C4-N3-C2	-5.50	122.00	127.34
1	2A	1915	5MU	C4-N3-C2	-5.48	120.26	127.35
1	2A	1915	5MU	C5-C4-N3	5.47	119.98	115.31
54	1y	32	PSU	N1-C2-N3	5.47	121.32	115.13

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
55	2x	54	5MU	C4-N3-C2	-5.46	120.28	127.35
54	1w	55	PSU	N1-C2-N3	5.42	121.27	115.13
1	1A	1937	5MU	C4-N3-C2	-5.42	120.34	127.35
1	2A	1911	PSU	N1-C2-N3	5.39	121.24	115.13
54	1w	8	4SU	C5-C4-N3	5.38	119.68	114.69
54	2w	46	7MG	N9-C8-N7	-5.37	95.70	103.38
32	1a	516	PSU	N1-C2-N3	5.35	121.19	115.13
55	2x	54	5MU	N3-C2-N1	5.31	121.94	114.89
32	2a	516	PSU	N1-C2-N3	5.31	121.15	115.13
54	1w	54	5MU	N3-C2-N1	5.26	121.87	114.89
54	1y	46	7MG	N9-C8-N7	-5.21	95.92	103.38
54	2w	39	PSU	N1-C2-N3	5.18	121.00	115.13
32	2a	527	7MG	C5-C4-N3	-5.16	118.30	128.13
54	1w	46	7MG	N9-C8-N7	-5.14	96.03	103.38
54	1w	54	5MU	C4-N3-C2	-5.11	120.73	127.35
1	1A	2564	2MU	N3-C2-N1	5.07	121.62	114.89
43	2l	92	0TD	CSB-SB-CB	5.07	111.61	102.44
54	1y	46	7MG	C5-C4-N3	-5.03	118.54	128.13
54	2y	55	PSU	N1-C2-N3	5.02	120.82	115.13
1	1A	1937	5MU	C5-C4-N3	4.94	119.53	115.31
1	2A	1939	5MU	N3-C2-N1	4.92	121.42	114.89
1	1A	1937	5MU	N3-C2-N1	4.92	121.42	114.89
1	1A	1961	5MU	C5-C6-N1	-4.90	118.30	123.34
32	1a	527	7MG	N9-C8-N7	-4.89	96.38	103.38
54	1y	54	5MU	C4-N3-C2	-4.88	121.04	127.35
32	1a	527	7MG	C5-C4-N3	-4.83	118.92	128.13
54	1y	54	5MU	N3-C2-N1	4.83	121.30	114.89
1	2A	2552	2MU	N3-C2-N1	4.73	121.17	114.89
1	1A	2564	2MU	C4-N3-C2	-4.72	120.36	126.58
54	2y	46	7MG	N9-C8-N7	-4.66	96.71	103.38
54	2y	46	7MG	C2-N3-C4	4.65	120.58	112.30
54	2w	46	7MG	C5-C4-N3	-4.63	119.30	128.13
1	1A	1961	5MU	N3-C2-N1	4.61	121.00	114.89
1	2A	2605	PSU	C4-N3-C2	-4.60	119.70	126.34
55	1x	54	5MU	N3-C2-N1	4.60	121.00	114.89
54	2y	54	5MU	C5-C4-N3	4.60	119.23	115.31
32	2a	1519	MA6	N1-C6-N6	4.59	121.88	117.06
1	2A	1915	5MU	N3-C2-N1	4.54	120.92	114.89
1	2A	1939	5MU	O4-C4-C5	-4.53	119.65	124.90
55	1x	54	5MU	C4-N3-C2	-4.52	121.50	127.35
54	2y	54	5MU	C4-N3-C2	-4.48	121.55	127.35
54	1w	46	7MG	C5-C4-N3	-4.45	119.64	128.13

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	2A	1915	5MU	O4-C4-C5	-4.44	119.75	124.90
54	1w	54	5MU	C5-C4-N3	4.43	119.10	115.31
54	1y	54	5MU	C5-C4-N3	4.39	119.05	115.31
32	1a	1400	5MC	C5-C6-N1	-4.37	118.84	123.34
55	2x	54	5MU	C5-C4-N3	4.35	119.02	115.31
32	2a	527	7MG	C2-N3-C4	4.34	120.04	112.30
54	1w	37	MIA	C15-C14-C13	-4.34	110.11	122.65
54	2w	37	MIA	C2-N3-C4	4.33	121.29	115.32
1	1A	1937	5MU	O4-C4-C5	-4.32	119.90	124.90
54	1y	8	4SU	N3-C2-N1	4.22	120.49	114.89
54	1w	37	MIA	C2-N3-C4	4.22	121.14	115.32
1	2A	2552	2MU	C4-N3-C2	-4.22	121.02	126.58
54	2w	54	5MU	C4-N3-C2	-4.21	121.90	127.35
54	2w	54	5MU	O4-C4-C5	-4.20	120.03	124.90
54	1y	46	7MG	C2-N3-C4	4.20	119.78	112.30
1	1A	1933	PSU	C4-N3-C2	-4.18	120.32	126.34
1	1A	2617	PSU	C4-N3-C2	-4.17	120.33	126.34
1	1A	1964	5MC	C5-C6-N1	-4.15	119.06	123.34
55	2x	54	5MU	O4-C4-C5	-4.15	120.10	124.90
54	2y	8	4SU	C5-C4-S4	-4.13	119.15	124.47
54	2w	8	4SU	N3-C2-N1	4.11	120.35	114.89
55	1x	8	4SU	C6-C5-C4	-4.10	116.40	119.95
54	2y	54	5MU	N3-C2-N1	4.08	120.31	114.89
1	2A	1915	5MU	C5-C6-N1	-4.06	119.16	123.34
54	2w	54	5MU	N3-C2-N1	4.04	120.25	114.89
32	1a	967	5MC	C5-C6-N1	-4.03	119.19	123.34
54	2w	54	5MU	C5-C4-N3	4.03	118.75	115.31
54	1y	8	4SU	C5-C4-N3	4.01	118.41	114.69
54	1w	37	MIA	C5-C6-N1	-4.00	117.48	120.81
54	2w	37	MIA	C5-C6-N1	-3.99	117.50	120.81
54	2y	54	5MU	O4-C4-C5	-3.97	120.30	124.90
1	2A	1962	5MC	C5-C6-N1	-3.97	119.25	123.34
1	1A	1939	PSU	C4-N3-C2	-3.94	120.66	126.34
54	2w	46	7MG	C2-N3-C4	3.92	119.29	112.30
55	1x	54	5MU	C5-C4-N3	3.90	118.64	115.31
32	2a	1400	5MC	C5-C6-N1	-3.85	119.37	123.34
54	1w	32	PSU	C4-N3-C2	-3.84	120.81	126.34
54	2w	32	PSU	C4-N3-C2	-3.83	120.82	126.34
54	1y	54	5MU	C5-C6-N1	-3.82	119.40	123.34
55	2x	8	4SU	C1'-N1-C2	3.82	124.49	117.57
54	1w	55	PSU	O2-C2-N1	-3.82	118.59	122.79
1	1A	1939	PSU	O2-C2-N1	-3.77	118.64	122.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	1a	1404	5MC	C5-C6-N1	-3.76	119.47	123.34
55	1x	55	PSU	C4-N3-C2	-3.76	120.93	126.34
32	1a	527	7MG	C2-N3-C4	3.75	118.97	112.30
54	1y	55	PSU	C4-N3-C2	-3.73	120.97	126.34
54	1y	55	PSU	O2-C2-N1	-3.73	118.69	122.79
54	2y	55	PSU	C4-N3-C2	-3.71	120.99	126.34
55	1x	54	5MU	C5-C6-N1	-3.70	119.53	123.34
32	2a	967	5MC	C5-C6-N1	-3.69	119.55	123.34
54	2w	8	4SU	C5-C4-S4	-3.68	119.73	124.47
54	1w	54	5MU	O4-C4-C5	-3.68	120.64	124.90
32	1a	1519	MA6	N1-C6-N6	3.66	120.91	117.06
55	2x	55	PSU	C4-N3-C2	-3.65	121.08	126.34
32	1a	1407	5MC	C5-C6-N1	-3.65	119.59	123.34
54	2y	37	MIA	N3-C2-N1	-3.64	122.98	128.68
54	1w	37	MIA	C16-C14-C13	-3.63	112.16	122.65
54	1w	37	MIA	C12-N6-C6	-3.63	117.18	122.55
55	1x	8	4SU	O2-C2-N1	3.62	127.60	122.79
1	2A	1917	PSU	C4-N3-C2	-3.62	121.12	126.34
55	2x	54	5MU	C5-C6-N1	-3.62	119.61	123.34
54	2y	32	PSU	C4-N3-C2	-3.62	121.13	126.34
54	2w	55	PSU	C4-N3-C2	-3.61	121.14	126.34
1	2A	1942	5MC	C5-C6-N1	-3.59	119.64	123.34
54	2y	39	PSU	C4-N3-C2	-3.59	121.17	126.34
32	2a	516	PSU	C4-N3-C2	-3.58	121.18	126.34
54	2y	55	PSU	O2-C2-N1	-3.58	118.85	122.79
32	1a	1518	MA6	C4-C5-N7	-3.56	105.69	109.40
54	1y	37	MIA	N3-C2-N1	-3.56	123.11	128.68
1	2A	1917	PSU	O2-C2-N1	-3.55	118.88	122.79
54	1w	8	4SU	N3-C2-N1	3.55	119.60	114.89
54	1w	39	PSU	O2-C2-N1	-3.53	118.91	122.79
54	2w	39	PSU	C4-N3-C2	-3.53	121.26	126.34
54	1w	54	5MU	C5-C6-N1	-3.52	119.72	123.34
1	1A	2564	2MU	O2-C2-N1	-3.52	118.11	122.79
54	1w	32	PSU	O2-C2-N1	-3.51	118.92	122.79
54	1w	39	PSU	C4-N3-C2	-3.51	121.28	126.34
54	2y	8	4SU	N3-C2-N1	3.49	119.53	114.89
1	1A	1937	5MU	C5-C6-N1	-3.49	119.75	123.34
55	2x	54	5MU	O2-C2-N1	-3.47	118.17	122.79
1	1A	2617	PSU	O2-C2-N1	-3.47	118.97	122.79
32	2a	1518	MA6	C9-N6-C6	-3.46	109.05	119.51
32	1a	516	PSU	C4-N3-C2	-3.45	121.36	126.34
32	2a	1518	MA6	N3-C2-N1	-3.43	123.32	128.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	1a	1518	MA6	N3-C2-N1	-3.43	123.32	128.68
32	2a	1519	MA6	N3-C2-N1	-3.42	123.33	128.68
54	2y	54	5MU	C1'-N1-C2	3.42	123.75	117.57
54	1y	54	5MU	O4-C4-C5	-3.41	120.94	124.90
54	1w	46	7MG	C2-N3-C4	3.41	118.38	112.30
54	1w	55	PSU	C4-N3-C2	-3.39	121.45	126.34
1	1A	1933	PSU	O2-C2-N1	-3.37	119.08	122.79
54	1y	32	PSU	C4-N3-C2	-3.37	121.49	126.34
55	1x	32	5MC	C5-C6-N1	-3.35	119.89	123.34
54	1w	46	7MG	C5-C4-N9	-3.35	102.00	106.35
32	2a	1404	5MC	C5-C6-N1	-3.34	119.90	123.34
1	1A	2564	2MU	O4-C4-C5	-3.32	119.33	125.16
55	2x	8	4SU	C5-C4-N3	3.29	117.74	114.69
54	2y	39	PSU	O2-C2-N1	-3.24	119.22	122.79
54	1y	39	PSU	C4-N3-C2	-3.22	121.70	126.34
32	1a	1519	MA6	C9-N6-C6	-3.19	109.85	119.51
54	2w	37	MIA	C12-N6-C6	-3.19	120.12	122.87
1	2A	1911	PSU	C4-N3-C2	-3.19	121.75	126.34
54	2y	54	5MU	C1'-N1-C6	-3.18	115.83	121.12
54	1w	8	4SU	C5-C4-S4	-3.18	120.38	124.47
54	1w	37	MIA	C2-N1-C6	3.17	122.86	117.19
55	1x	54	5MU	O4-C4-C5	-3.17	121.23	124.90
1	1A	2564	2MU	C5-C4-N3	3.16	119.56	114.84
32	2a	516	PSU	O2-C2-N1	-3.15	119.32	122.79
54	1y	32	PSU	O2-C2-N1	-3.15	119.33	122.79
1	2A	2552	2MU	O2-C2-N1	-3.14	118.61	122.79
32	2a	1518	MA6	C4-C5-N7	-3.13	106.14	109.40
1	2A	2605	PSU	O2-C2-N1	-3.10	119.38	122.79
32	2a	1407	5MC	C5-C4-N3	-3.09	118.34	121.67
1	1A	1961	5MU	O2-C2-N1	-3.09	118.68	122.79
32	1a	1518	MA6	C9-N6-C6	-3.07	110.23	119.51
54	2w	55	PSU	O2-C2-N1	-3.07	119.42	122.79
54	2w	32	PSU	O2-C2-N1	-3.06	119.42	122.79
55	1x	32	5MC	C5-C4-N3	-3.06	118.38	121.67
54	2w	37	MIA	C4-C5-N7	-3.04	106.23	109.40
55	1x	55	PSU	O2-C2-N1	-3.04	119.45	122.79
32	2a	1407	5MC	C5-C6-N1	-3.03	120.22	123.34
54	2w	8	4SU	C1'-N1-C2	3.02	123.04	117.57
55	1x	8	4SU	C1'-N1-C2	3.02	123.03	117.57
32	2a	1519	MA6	C9-N6-C6	-3.00	110.44	119.51
54	2y	46	7MG	C5-C4-N9	-3.00	102.46	106.35
54	2y	32	PSU	O2-C2-N1	-2.99	119.50	122.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	2A	1939	5MU	O2-C2-N1	-2.96	118.85	122.79
32	2a	527	7MG	C5-C6-N1	2.95	116.19	110.99
32	1a	1519	MA6	C4-C5-N7	-2.93	106.34	109.40
55	2x	55	PSU	O2-C2-N1	-2.91	119.59	122.79
55	2x	32	5MC	C5-C6-N1	-2.90	120.36	123.34
1	1A	2515	2MA	C8-N7-C5	2.86	108.44	102.99
54	2y	54	5MU	C5-C6-N1	-2.86	120.39	123.34
54	1y	46	7MG	C5-C4-N9	-2.85	102.65	106.35
54	1y	37	MIA	C4-C5-N7	-2.85	106.43	109.40
1	1A	1964	5MC	C5-C4-N3	-2.83	118.62	121.67
54	2w	37	MIA	C2-N1-C6	2.81	122.21	117.19
1	2A	1911	PSU	O2-C2-N1	-2.79	119.72	122.79
32	1a	1404	5MC	C5-C4-N3	-2.77	118.68	121.67
32	2a	1404	5MC	C5-C4-N3	-2.75	118.71	121.67
1	1A	1937	5MU	O2-C2-N1	-2.74	119.14	122.79
1	1A	1984	5MC	C5-C4-N3	-2.72	118.74	121.67
32	1a	1498	UR3	C1'-N1-C2	2.70	121.55	116.99
55	2x	32	5MC	C5-C4-N3	-2.70	118.76	121.67
1	2A	2552	2MU	C5-C4-N3	2.66	118.83	114.84
1	1A	1984	5MC	C5-C6-N1	-2.66	120.60	123.34
1	1A	1942	4OC	O2-C2-N3	-2.65	118.02	122.33
32	2a	1207	2MG	C8-N7-C5	2.64	108.03	102.99
1	1A	2515	2MA	C5-C6-N1	2.63	118.56	114.02
32	1a	1519	MA6	N3-C2-N1	-2.63	124.57	128.68
1	2A	1942	5MC	C5-C4-N3	-2.61	118.85	121.67
32	1a	1407	5MC	C5-C4-N3	-2.61	118.86	121.67
32	2a	1519	MA6	C4-C5-N7	-2.61	106.68	109.40
54	2y	54	5MU	O2-C2-N3	-2.59	116.67	121.50
32	2a	1400	5MC	C5-C4-N3	-2.59	118.88	121.67
1	2A	2503	2MA	C5-C6-N1	2.59	118.49	114.02
1	2A	2251	OMG	C8-N7-C5	2.58	107.91	102.99
54	2w	54	5MU	C5-C6-N1	-2.58	120.69	123.34
32	2a	1498	UR3	C6-N1-C2	-2.57	119.49	121.79
1	1A	2263	OMG	C5-C6-N1	2.57	118.49	113.95
32	1a	516	PSU	O2-C2-N1	-2.56	119.97	122.79
32	1a	527	7MG	C5-C6-N1	2.56	115.50	110.99
54	1w	37	MIA	N3-C2-N1	-2.56	122.27	126.98
32	1a	1207	2MG	C8-N7-C5	2.56	107.87	102.99
54	1w	37	MIA	C4-C5-N7	-2.56	106.73	109.40
54	2w	46	7MG	C5-C6-N1	2.55	115.49	110.99
1	2A	2552	2MU	O4-C4-C5	-2.54	120.69	125.16
1	2A	1962	5MC	C5-C4-N3	-2.53	118.95	121.67

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	2a	1518	MA6	C10-N6-C9	-2.53	107.98	116.12
55	1x	8	4SU	C4-N3-C2	2.52	129.79	127.34
54	1y	8	4SU	C5-C4-S4	-2.50	121.25	124.47
32	2a	1402	4OC	C6-C5-C4	2.48	120.00	116.96
32	1a	516	PSU	C6-C5-C4	-2.44	116.49	118.20
1	2A	2605	PSU	C6-C5-C4	-2.44	116.49	118.20
1	1A	1984	5MC	O2-C2-N3	-2.43	118.39	122.33
32	1a	1402	4OC	C6-C5-C4	2.42	119.92	116.96
32	1a	1518	MA6	C10-N6-C9	-2.40	108.38	116.12
54	2w	37	MIA	N3-C2-N1	-2.40	122.57	126.98
1	1A	2564	2MU	C2'-C1'-N1	-2.39	109.59	114.22
32	1a	1402	4OC	CM4-N4-C4	-2.38	117.80	122.45
32	2a	1407	5MC	O2-C2-N3	-2.37	118.48	122.33
55	2x	8	4SU	O2-C2-N1	2.37	125.93	122.79
1	2A	2251	OMG	C5-C6-N1	2.36	118.13	113.95
54	2w	54	5MU	C5M-C5-C4	2.36	121.36	118.77
32	1a	1404	5MC	O2-C2-N3	-2.36	118.50	122.33
1	1A	2617	PSU	C5-C6-N1	-2.33	118.61	122.11
32	2a	527	7MG	CM7-N7-C5	2.33	132.42	126.40
32	2a	967	5MC	C5-C4-N3	-2.33	119.16	121.67
32	1a	1498	UR3	C3U-N3-C4	2.33	121.21	117.89
1	2A	2503	2MA	C8-N7-C5	2.32	107.42	102.99
32	1a	527	7MG	C5-C4-N9	-2.32	103.33	106.35
54	2y	37	MIA	C4-C5-N7	-2.31	106.99	109.40
55	1x	8	4SU	C5-C4-N3	2.28	116.80	114.69
32	1a	967	5MC	C5-C4-N3	-2.27	119.22	121.67
54	1w	8	4SU	C1'-N1-C2	2.27	121.67	117.57
32	1a	966	M2G	C8-N7-C5	2.26	107.29	102.99
54	2y	54	5MU	C5M-C5-C4	2.25	121.25	118.77
55	1x	54	5MU	O2-C2-N1	-2.25	119.79	122.79
32	2a	967	5MC	CM5-C5-C6	-2.24	119.85	122.85
54	1y	46	7MG	C5-C6-N1	2.24	114.93	110.99
54	2y	8	4SU	C1'-N1-C2	2.24	121.62	117.57
1	2A	2251	OMG	O6-C6-C5	-2.23	120.01	124.37
1	2A	2605	PSU	O4-C4-C5	-2.23	118.21	124.05
32	1a	527	7MG	CM7-N7-C5	2.23	132.15	126.40
32	1a	1400	5MC	C5-C4-N3	-2.22	119.28	121.67
32	2a	966	M2G	C8-N7-C5	2.21	107.20	102.99
55	2x	32	5MC	O2-C2-N3	-2.21	118.75	122.33
32	1a	1407	5MC	O2-C2-N3	-2.20	118.75	122.33
32	2a	1404	5MC	O2-C2-N3	-2.20	118.75	122.33
1	1A	2263	OMG	C8-N7-C5	2.19	107.16	102.99

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	2w	39	PSU	O2-C2-N1	-2.19	120.38	122.79
54	1y	54	5MU	O2-C2-N3	-2.17	117.45	121.50
32	1a	966	M2G	C5-C6-N1	2.17	117.79	113.95
54	1w	54	5MU	O2-C2-N1	-2.17	119.91	122.79
1	1A	1984	5MC	C1'-N1-C6	-2.16	117.52	121.12
32	1a	527	7MG	O6-C6-C5	-2.16	122.23	127.54
54	1y	39	PSU	O2-C2-N1	-2.16	120.41	122.79
54	2w	46	7MG	O6-C6-C5	-2.14	122.30	127.54
32	1a	1498	UR3	C6-N1-C2	-2.13	119.88	121.79
1	2A	1962	5MC	N4-C4-N3	2.13	122.36	118.48
32	2a	967	5MC	O2-C2-N3	-2.12	118.89	122.33
55	2x	8	4SU	C1'-N1-C6	-2.12	116.23	120.84
54	2w	37	MIA	N6-C6-N1	2.11	121.13	118.50
54	1y	8	4SU	C1'-N1-C2	2.11	121.38	117.57
32	1a	967	5MC	O2-C2-N3	-2.10	118.91	122.33
55	2x	8	4SU	C6-C5-C4	-2.10	118.13	119.95
32	2a	1407	5MC	CM5-C5-C6	-2.10	120.04	122.85
1	2A	1911	PSU	C6-C5-C4	-2.10	116.73	118.20
54	2y	46	7MG	C5-C6-N1	2.10	114.69	110.99
1	1A	1984	5MC	CM5-C5-C6	-2.10	120.04	122.85
54	1w	46	7MG	O6-C6-C5	-2.10	122.39	127.54
1	1A	1937	5MU	C5M-C5-C4	2.09	121.06	118.77
54	1y	55	PSU	O4'-C1'-C2'	2.07	108.07	105.14
54	2y	32	PSU	O4'-C1'-C2'	2.07	108.06	105.14
54	2y	55	PSU	C6-C5-C4	-2.07	116.75	118.20
32	1a	1518	MA6	C1'-N9-C4	-2.06	123.01	126.64
54	2y	46	7MG	CM7-N7-C5	2.06	131.71	126.40
54	2y	55	PSU	O4'-C1'-C2'	2.06	108.05	105.14
55	1x	8	4SU	O2-C2-N3	-2.06	117.67	121.50
32	1a	1407	5MC	CM5-C5-C6	-2.06	120.10	122.85
1	1A	2263	OMG	O6-C6-C5	-2.05	120.37	124.37
54	2y	37	MIA	C2-N1-C6	2.04	122.24	118.75
32	2a	516	PSU	O4'-C1'-C2'	2.04	108.02	105.14
32	2a	1207	2MG	C5-C6-N1	2.03	117.53	113.95
54	2w	46	7MG	CM7-N7-C5	2.03	131.63	126.40
32	2a	966	M2G	C5-C6-N1	2.01	117.51	113.95
32	1a	516	PSU	O4'-C1'-C2'	2.01	107.98	105.14
32	2a	1518	MA6	C1'-N9-C4	-2.01	123.11	126.64
32	1a	1518	MA6	C10-N6-C6	-2.01	113.43	119.51
1	2A	1915	5MU	C5M-C5-C4	2.01	120.98	118.77

There are no chirality outliers.

All (65) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
32	1a	1518	MA6	C5-C6-N6-C10
32	1a	1519	MA6	O4'-C4'-C5'-O5'
43	1l	92	0TD	SB-CB-CG-OD2
32	2a	1402	4OC	O4'-C4'-C5'-O5'
32	2a	1519	MA6	O4'-C4'-C5'-O5'
54	1w	37	MIA	C12-C13-C14-C16
54	2y	37	MIA	C3'-C4'-C5'-O5'
54	1y	46	7MG	C4'-C5'-O5'-P
54	1y	54	5MU	O4'-C4'-C5'-O5'
54	2y	55	PSU	C2'-C1'-C5-C6
54	2y	55	PSU	O4'-C1'-C5-C6
32	1a	1400	5MC	O4'-C4'-C5'-O5'
32	1a	1402	4OC	O4'-C4'-C5'-O5'
32	1a	1519	MA6	C3'-C4'-C5'-O5'
32	2a	1402	4OC	C3'-C4'-C5'-O5'
32	2a	1519	MA6	C3'-C4'-C5'-O5'
54	1y	54	5MU	C3'-C4'-C5'-O5'
32	1a	1400	5MC	C3'-C4'-C5'-O5'
54	1y	8	4SU	C3'-C4'-C5'-O5'
54	1y	8	4SU	O4'-C4'-C5'-O5'
54	2w	46	7MG	O4'-C4'-C5'-O5'
54	2w	46	7MG	C3'-C4'-C5'-O5'
32	1a	527	7MG	C3'-C4'-C5'-O5'
32	1a	1402	4OC	C3'-C4'-C5'-O5'
54	2y	46	7MG	O4'-C1'-N9-C4
32	2a	527	7MG	C3'-C4'-C5'-O5'
54	2y	37	MIA	O4'-C4'-C5'-O5'
32	1a	1518	MA6	C5-C6-N6-C9
54	2w	46	7MG	C2'-C1'-N9-C8
32	1a	527	7MG	O4'-C4'-C5'-O5'
54	2y	32	PSU	O4'-C4'-C5'-O5'
43	1l	92	0TD	CG-CB-SB-CSB
43	2l	92	0TD	CG-CB-SB-CSB
54	1w	46	7MG	C2'-C1'-N9-C8
54	2y	46	7MG	C2'-C1'-N9-C8
32	2a	527	7MG	O4'-C4'-C5'-O5'
54	2y	46	7MG	O4'-C1'-N9-C8
32	1a	1519	MA6	C5-C6-N6-C10
32	2a	1518	MA6	C5-C6-N6-C10
32	2a	1519	MA6	C5-C6-N6-C10
54	1w	46	7MG	C4'-C5'-O5'-P
54	1y	8	4SU	C4'-C5'-O5'-P

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Mol	Chain	Res	Type	Atoms
32	1a	1519	MA6	C4'-C5'-O5'-P
32	1a	1402	4OC	C3'-C2'-O2'-CM2
54	2y	37	MIA	C4'-C5'-O5'-P
54	1y	46	7MG	C2'-C1'-N9-C8
1	2A	2503	2MA	O4'-C4'-C5'-O5'
54	2y	54	5MU	C2'-C1'-N1-C2
54	2y	54	5MU	C2'-C1'-N1-C6
54	1w	39	PSU	O4'-C1'-C5-C4
54	1y	55	PSU	O4'-C1'-C5-C4
32	2a	527	7MG	C4'-C5'-O5'-P
55	2x	8	4SU	C2'-C1'-N1-C2
1	1A	2515	2MA	C4'-C5'-O5'-P
54	2w	46	7MG	O4'-C1'-N9-C8
43	1l	92	0TD	SB-CB-CG-OD1
1	1A	1942	4OC	C2'-C1'-N1-C2
54	2w	8	4SU	C2'-C1'-N1-C2
54	1w	37	MIA	N3-C2-S10-C11
1	1A	2515	2MA	O4'-C4'-C5'-O5'
54	2y	55	PSU	O4'-C4'-C5'-O5'
54	1w	46	7MG	O4'-C1'-N9-C8
54	2w	37	MIA	N1-C6-N6-C12
54	2y	8	4SU	C2'-C1'-N1-C2
54	1y	54	5MU	C4'-C5'-O5'-P

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 2853 ligands modelled in this entry, 2851 are monoatomic - leaving 2 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
59	SF4	1d	501	35	0,12,12	-	-	-		
59	SF4	2d	501	35	0,12,12	-	-	-		

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
59	SF4	1d	501	35	-	-	0/6/5/5
59	SF4	2d	501	35	-	-	0/6/5/5

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

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, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	1A	2860/2915 (98%)	0.70	76 (2%) 54 58	24, 43, 91, 103	0
1	2A	2789/2915 (95%)	0.09	81 (2%) 51 55	28, 48, 89, 106	0
2	1B	120/121 (99%)	0.63	0 100 100	39, 61, 72, 90	0
2	2B	120/121 (99%)	-0.04	2 (1%) 70 72	45, 68, 77, 91	0
3	1D	275/276 (99%)	0.64	4 (1%) 73 75	25, 42, 58, 80	0
3	2D	275/276 (99%)	0.45	4 (1%) 73 75	28, 45, 61, 78	0
4	1E	204/206 (99%)	0.68	3 (1%) 73 75	23, 46, 66, 80	0
4	2E	204/206 (99%)	0.60	5 (2%) 57 61	26, 50, 67, 80	0
5	1F	203/210 (96%)	0.83	2 (0%) 82 84	22, 51, 76, 91	0
5	2F	203/210 (96%)	0.28	1 (0%) 91 91	27, 56, 76, 91	0
6	1G	181/182 (99%)	0.66	4 (2%) 62 65	48, 69, 80, 92	0
6	2G	181/182 (99%)	1.21	37 (20%) 1 0	54, 73, 81, 93	0
7	1H	174/180 (96%)	0.65	1 (0%) 89 90	47, 64, 74, 83	0
7	2H	174/180 (96%)	1.85	64 (36%) 0 0	54, 70, 78, 83	0
8	1I	146/148 (98%)	0.50	6 (4%) 37 40	49, 73, 82, 85	0
8	2I	146/148 (98%)	0.87	18 (12%) 4 3	50, 73, 82, 86	0
9	1N	140/140 (100%)	0.91	1 (0%) 87 89	31, 48, 67, 77	0
9	2N	140/140 (100%)	0.61	5 (3%) 42 46	37, 53, 71, 80	0
10	1O	122/122 (100%)	0.46	1 (0%) 86 87	23, 40, 60, 74	0
10	2O	122/122 (100%)	0.90	9 (7%) 14 15	45, 59, 72, 81	0
11	1P	149/150 (99%)	0.85	1 (0%) 87 89	24, 53, 75, 81	0
11	2P	149/150 (99%)	0.59	12 (8%) 12 12	29, 58, 76, 85	0
12	1Q	141/141 (100%)	0.79	2 (1%) 75 77	33, 51, 68, 77	0
12	2Q	141/141 (100%)	1.01	16 (11%) 5 4	37, 56, 73, 79	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
13	1R	118/118 (100%)	0.67	1 (0%) 86 87	29, 40, 55, 62	0
13	2R	118/118 (100%)	0.37	2 (1%) 70 72	31, 43, 58, 65	0
14	1S	110/112 (98%)	0.76	2 (1%) 68 71	49, 62, 72, 77	0
14	2S	110/112 (98%)	0.88	11 (10%) 7 6	55, 66, 75, 79	0
15	1T	131/146 (89%)	0.58	4 (3%) 49 52	38, 50, 72, 77	0
15	2T	131/146 (89%)	0.52	3 (2%) 60 63	43, 53, 74, 78	0
16	1U	116/118 (98%)	1.04	3 (2%) 56 59	26, 39, 55, 73	0
16	2U	116/118 (98%)	0.27	1 (0%) 84 86	33, 46, 61, 73	0
17	1V	101/101 (100%)	0.94	1 (0%) 82 84	28, 51, 67, 76	0
17	2V	101/101 (100%)	0.29	3 (2%) 50 53	33, 57, 70, 76	0
18	1W	112/113 (99%)	0.92	1 (0%) 84 86	26, 37, 55, 88	0
18	2W	112/113 (99%)	0.34	0 100 100	30, 41, 57, 88	0
19	1X	95/96 (98%)	0.81	1 (1%) 80 82	30, 44, 63, 75	0
19	2X	95/96 (98%)	0.29	2 (2%) 63 66	34, 49, 65, 76	0
20	1Y	107/110 (97%)	0.79	2 (1%) 66 69	45, 57, 74, 83	0
20	2Y	107/110 (97%)	0.95	15 (14%) 2 2	48, 61, 76, 86	0
21	1Z	154/206 (74%)	0.63	8 (5%) 27 29	38, 64, 86, 96	0
21	2Z	160/206 (77%)	1.52	44 (27%) 0 0	72, 83, 93, 99	0
22	10	83/85 (97%)	0.77	3 (3%) 42 46	25, 38, 59, 71	0
22	20	83/85 (97%)	0.90	6 (7%) 15 16	41, 66, 78, 82	0
23	11	97/98 (98%)	0.53	2 (2%) 63 66	23, 44, 71, 77	0
23	21	97/98 (98%)	0.79	6 (6%) 20 21	38, 58, 74, 82	0
24	12	70/72 (97%)	0.82	1 (1%) 75 77	40, 57, 66, 79	0
24	22	70/72 (97%)	0.19	1 (1%) 75 77	46, 61, 69, 78	0
25	13	59/60 (98%)	0.89	0 100 100	29, 45, 69, 83	0
25	23	59/60 (98%)	0.52	1 (1%) 70 72	36, 51, 72, 87	0
26	14	69/71 (97%)	0.69	7 (10%) 7 6	64, 79, 89, 97	0
26	24	69/71 (97%)	1.17	14 (20%) 1 0	70, 80, 89, 97	0
27	15	59/60 (98%)	0.97	1 (1%) 70 72	25, 36, 57, 72	0
27	25	59/60 (98%)	0.21	0 100 100	30, 40, 60, 71	0
28	16	53/54 (98%)	0.71	0 100 100	38, 51, 64, 74	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
28	26	53/54 (98%)	0.67	4 (7%) 14 14	42, 54, 65, 71	0
29	17	48/49 (97%)	0.92	3 (6%) 20 21	24, 31, 58, 69	0
29	27	48/49 (97%)	0.70	4 (8%) 11 11	28, 35, 58, 70	0
30	18	64/65 (98%)	0.84	2 (3%) 49 52	33, 42, 50, 66	0
30	28	64/65 (98%)	0.84	4 (6%) 20 21	38, 46, 53, 67	0
31	19	37/37 (100%)	0.88	0 100 100	37, 50, 67, 68	0
31	29	37/37 (100%)	1.57	9 (24%) 0 0	46, 54, 71, 72	0
32	1a	1488/1521 (97%)	0.37	47 (3%) 47 51	42, 72, 92, 103	0
32	2a	1491/1521 (98%)	0.42	76 (5%) 28 29	44, 74, 93, 103	0
33	1b	231/256 (90%)	0.50	12 (5%) 27 29	69, 82, 89, 94	0
33	2b	231/256 (90%)	1.28	58 (25%) 0 0	72, 83, 89, 94	0
34	1c	206/239 (86%)	0.83	21 (10%) 6 6	67, 80, 86, 92	0
34	2c	206/239 (86%)	1.82	79 (38%) 0 0	69, 82, 88, 93	0
35	1d	208/209 (99%)	0.94	25 (12%) 4 4	56, 72, 80, 87	0
35	2d	208/209 (99%)	1.13	32 (15%) 2 1	58, 71, 80, 88	0
36	1e	148/162 (91%)	0.88	14 (9%) 8 8	56, 72, 80, 86	0
36	2e	148/162 (91%)	1.66	43 (29%) 0 0	59, 74, 83, 87	0
37	1f	100/101 (99%)	0.31	1 (1%) 82 84	50, 66, 76, 78	0
37	2f	100/101 (99%)	0.22	1 (1%) 82 84	60, 72, 80, 86	0
38	1g	155/156 (99%)	0.87	17 (10%) 5 5	62, 74, 83, 100	0
38	2g	155/156 (99%)	1.02	24 (15%) 2 1	65, 76, 84, 102	0
39	1h	137/138 (99%)	0.65	7 (5%) 28 29	60, 72, 78, 83	0
39	2h	137/138 (99%)	1.16	28 (20%) 1 0	64, 74, 80, 84	0
40	1i	127/128 (99%)	1.09	23 (18%) 1 1	51, 75, 83, 87	0
40	2i	127/128 (99%)	2.37	68 (53%) 0 0	71, 85, 91, 92	0
41	1j	97/105 (92%)	0.89	14 (14%) 2 2	59, 78, 90, 95	0
41	2j	96/105 (91%)	2.16	46 (47%) 0 0	74, 87, 94, 98	0
42	1k	114/129 (88%)	0.66	4 (3%) 44 47	52, 69, 80, 83	0
42	2k	114/129 (88%)	0.57	5 (4%) 34 37	55, 71, 81, 87	0
43	1l	121/132 (91%)	0.62	3 (2%) 57 61	53, 64, 74, 77	0
43	2l	121/132 (91%)	1.34	30 (24%) 0 0	55, 67, 75, 80	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
44	1m	123/126 (97%)	0.60	7 (5%) 23 25	54, 69, 78, 82	0
44	2m	122/126 (96%)	1.65	38 (31%) 0 0	73, 84, 90, 94	0
45	1n	60/61 (98%)	1.13	10 (16%) 1 1	57, 69, 78, 82	0
45	2n	60/61 (98%)	3.35	46 (76%) 0 0	78, 85, 93, 95	0
46	1o	88/89 (98%)	0.61	5 (5%) 23 25	56, 69, 78, 82	0
46	2o	88/89 (98%)	0.60	5 (5%) 23 25	57, 70, 80, 83	0
47	1p	82/88 (93%)	1.76	31 (37%) 0 0	58, 70, 80, 83	0
47	2p	82/88 (93%)	1.00	9 (10%) 5 5	59, 69, 81, 82	0
48	1q	99/105 (94%)	0.78	7 (7%) 16 16	57, 70, 79, 82	0
48	2q	99/105 (94%)	1.21	25 (25%) 0 0	60, 70, 79, 82	0
49	1r	68/88 (77%)	0.56	5 (7%) 14 15	60, 68, 79, 82	0
49	2r	68/88 (77%)	0.50	5 (7%) 14 15	60, 70, 80, 82	0
50	1s	83/93 (89%)	0.74	4 (4%) 30 32	70, 79, 86, 91	0
50	2s	83/93 (89%)	2.16	37 (44%) 0 0	74, 81, 88, 94	0
51	1t	96/106 (90%)	1.38	30 (31%) 0 0	58, 71, 80, 86	0
51	2t	96/106 (90%)	1.04	16 (16%) 1 1	59, 71, 81, 85	0
52	1u	23/27 (85%)	1.42	7 (30%) 0 0	65, 74, 78, 80	0
52	2u	23/27 (85%)	1.96	8 (34%) 0 0	68, 75, 80, 83	0
53	1v	13/24 (54%)	2.65	7 (53%) 0 0	60, 74, 92, 98	0
53	2v	13/24 (54%)	3.37	8 (61%) 0 0	65, 78, 95, 98	0
54	1w	67/76 (88%)	1.86	19 (28%) 0 0	44, 89, 97, 101	0
54	1y	67/76 (88%)	0.98	13 (19%) 1 1	37, 91, 97, 101	0
54	2w	65/76 (85%)	2.68	41 (63%) 0 0	56, 96, 101, 104	0
54	2y	66/76 (86%)	1.20	14 (21%) 0 0	51, 95, 99, 100	0
55	1x	72/77 (93%)	0.31	2 (2%) 53 56	33, 66, 84, 87	0
55	2x	72/77 (93%)	0.23	0 100 100	52, 81, 90, 95	0
All	All	20875/21748 (95%)	0.69	1604 (7%) 13 13	22, 63, 88, 106	0

All (1604) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
45	2n	25	VAL	12.6
38	2g	82	GLY	10.7

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Mol	Chain	Res	Type	RSRZ
44	1m	124	PRO	10.0
44	2m	124	PRO	10.0
54	2w	71	G	9.6
54	1w	70	G	9.2
36	2e	12	LEU	8.9
50	2s	80	TYR	8.6
45	2n	39	LEU	8.4
45	2n	34	TYR	8.4
5	2F	208	GLY	8.4
40	2i	115	GLY	8.3
54	2y	36	A	8.3
32	2a	1030(B)	C	8.2
54	2w	70	G	8.0
50	2s	79	THR	7.9
44	2m	123	ALA	7.8
21	2Z	144	LEU	7.8
54	1w	71	G	7.7
21	2Z	149	SER	7.6
34	2c	198	VAL	7.5
34	2c	182	ILE	7.3
40	2i	7	THR	7.3
45	2n	38	GLY	7.3
41	2j	47	PHE	7.2
33	2b	165	VAL	7.2
6	2G	29	TRP	7.2
1	2A	229	A	7.1
34	2c	157	ILE	7.1
54	2w	72	C	7.0
44	2m	119	GLY	7.0
34	2c	8	ILE	7.0
53	2v	14	A	6.7
1	2A	883	G	6.6
34	2c	155	GLY	6.6
50	2s	82	GLY	6.5
26	24	49	PHE	6.5
33	2b	118	LEU	6.5
53	2v	24	A	6.5
34	2c	124	ILE	6.5
36	2e	90	VAL	6.5
1	2A	2154	G	6.3
7	2H	45	VAL	6.3
44	2m	120	LYS	6.2

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Mol	Chain	Res	Type	RSRZ
41	2j	85	LEU	6.1
21	2Z	155	LEU	6.1
38	2g	83	ALA	6.1
50	2s	41	VAL	6.1
54	1w	44	G	6.0
21	2Z	141	VAL	6.0
41	2j	72	VAL	6.0
43	2l	39	VAL	6.0
51	1t	9	ASN	6.0
44	2m	90	LEU	6.0
54	2w	4	C	5.9
50	2s	50	ALA	5.9
45	2n	13	THR	5.9
51	1t	13	LEU	5.9
7	2H	72	ILE	5.9
1	2A	2155	G	5.9
44	1m	2	ALA	5.9
32	1a	1030(B)	C	5.8
32	2a	1030(A)	G	5.8
32	1a	1001(A)	G	5.8
40	2i	17	VAL	5.8
54	2w	31	A	5.8
36	2e	94	ALA	5.7
54	1y	35	A	5.6
34	2c	53	ALA	5.6
40	1i	14	VAL	5.6
40	2i	36	TYR	5.6
44	2m	60	VAL	5.6
53	2v	12	A	5.6
40	2i	76	ALA	5.5
38	2g	81	GLY	5.5
44	2m	87	TYR	5.5
1	1A	2162	C	5.5
54	2w	3	C	5.5
41	2j	50	ILE	5.5
38	1g	79	ARG	5.5
1	1A	1141	A	5.4
52	2u	6	ARG	5.4
38	2g	80	VAL	5.4
40	2i	114	TYR	5.4
36	2e	29	GLY	5.4
45	2n	42	ILE	5.3

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Mol	Chain	Res	Type	RSRZ
38	2g	16	LEU	5.3
34	2c	194	GLY	5.3
33	2b	92	TYR	5.3
54	2w	13	C	5.3
7	2H	128	PRO	5.3
7	2H	52	VAL	5.3
53	2v	23	A	5.3
7	2H	102	ALA	5.3
7	2H	35	VAL	5.2
1	2A	2802	G	5.2
41	2j	48	THR	5.2
45	2n	50	LYS	5.2
40	2i	61	ALA	5.2
26	24	63	TYR	5.2
45	2n	36	PHE	5.2
53	1v	14	A	5.2
41	2j	55	LYS	5.2
1	2A	2145	C	5.1
6	2G	28	VAL	5.1
20	2Y	45	VAL	5.1
33	2b	81	VAL	5.1
12	2Q	33	GLY	5.1
34	2c	145	GLY	5.1
21	2Z	139	VAL	5.1
54	1w	69	G	5.1
41	2j	71	LEU	5.1
1	2A	2139	C	5.1
38	2g	156	TRP	5.1
40	2i	52	ALA	5.1
38	2g	4	ARG	5.1
50	2s	13	ASP	5.1
54	1w	72	C	5.1
54	2y	34	G	5.0
32	2a	1035	A	5.0
44	2m	118	ALA	5.0
40	2i	14	VAL	5.0
32	1a	163	C	5.0
45	2n	58	LYS	5.0
26	14	66	SER	5.0
54	2y	35	A	5.0
34	2c	6	HIS	5.0
39	1h	93	VAL	4.9

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Mol	Chain	Res	Type	RSRZ
45	2n	6	LEU	4.9
43	2l	95	GLY	4.9
53	1v	24	A	4.9
26	24	50	VAL	4.9
45	2n	53	LEU	4.9
40	2i	125	TYR	4.9
41	2j	74	ILE	4.9
44	1m	123	ALA	4.9
1	2A	888	C	4.9
23	2l	2	SER	4.9
40	2i	9	ARG	4.8
1	2A	885	C	4.8
38	1g	80	VAL	4.8
53	1v	12	A	4.8
51	1t	12	ALA	4.8
20	2Y	5	MET	4.8
44	2m	82	MET	4.8
38	2g	7	ALA	4.8
40	2i	79	LEU	4.8
41	2j	65	LEU	4.8
33	2b	136	VAL	4.8
43	2l	55	VAL	4.8
1	1A	936	C	4.8
33	2b	152	PHE	4.8
44	2m	122	LYS	4.8
40	2i	15	ALA	4.8
41	2j	54	PHE	4.8
32	1a	1036	G	4.7
32	2a	1036	G	4.7
1	2A	884	C	4.7
7	2H	105	LEU	4.7
26	24	51	ASP	4.7
21	2Z	57	ILE	4.7
1	2A	896	A	4.7
18	1W	112	GLY	4.7
32	2a	1034	G	4.7
41	2j	10	GLY	4.7
33	2b	101	MET	4.7
1	2A	887	A	4.7
6	1G	139	LEU	4.7
41	2j	39	PRO	4.7
34	2c	180	ALA	4.7

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Mol	Chain	Res	Type	RSRZ
22	20	45	PHE	4.7
48	1q	27	PHE	4.7
38	2g	6	ARG	4.6
53	2v	13	A	4.6
40	1i	106	ALA	4.6
51	1t	14	LYS	4.6
40	2i	109	VAL	4.6
35	1d	180	GLY	4.6
1	1A	1142	A	4.6
40	2i	103	THR	4.6
50	2s	63	THR	4.6
1	1A	2163	G	4.6
54	1w	20	U	4.6
1	2A	2133	G	4.6
38	1g	82	GLY	4.6
40	2i	127	LYS	4.6
1	1A	1140	U	4.5
34	2c	188	LEU	4.5
44	2m	102	ARG	4.5
45	2n	24	CYS	4.5
21	2Z	173	ALA	4.5
50	2s	14	HIS	4.5
7	2H	98	LEU	4.5
1	2A	2153	G	4.5
53	2v	22	U	4.5
33	2b	214	ILE	4.5
53	1v	23	A	4.5
44	2m	96	LEU	4.5
45	2n	44	LEU	4.5
38	1g	156	TRP	4.4
34	1c	15	THR	4.4
32	2a	1033	G	4.4
40	2i	81	ILE	4.4
34	2c	167	TRP	4.4
36	2e	86	ALA	4.4
39	2h	2	LEU	4.4
36	2e	109	ILE	4.4
1	2A	2149	G	4.4
54	1w	4	C	4.4
45	2n	47	LEU	4.4
1	2A	2160	G	4.4
45	2n	61	TRP	4.4

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Mol	Chain	Res	Type	RSRZ
7	2H	115	VAL	4.4
40	2i	106	ALA	4.4
45	1n	2	ALA	4.4
1	1A	2153	G	4.4
7	2H	123	PHE	4.4
40	2i	116	LYS	4.3
7	2H	37	VAL	4.3
40	2i	126	SER	4.3
44	2m	100	GLY	4.3
20	2Y	65	ALA	4.3
35	2d	168	ARG	4.3
40	2i	128	ARG	4.3
14	2S	32	LEU	4.3
36	2e	31	LEU	4.3
1	2A	2141	G	4.3
6	2G	11	TYR	4.3
33	2b	187	LEU	4.3
1	1A	1115	A	4.3
1	2A	2146	C	4.3
44	2m	97	PRO	4.3
45	2n	37	PHE	4.3
36	2e	80	ILE	4.3
51	1t	70	SER	4.3
48	2q	80	GLY	4.3
40	2i	86	VAL	4.3
32	2a	1001(A)	G	4.3
33	2b	34	ALA	4.3
48	2q	92	ARG	4.3
50	2s	75	ALA	4.3
1	1A	1110	C	4.2
34	1c	39	ILE	4.2
32	1a	1002	G	4.2
54	1y	34	G	4.2
54	2w	2	C	4.2
45	2n	10	ALA	4.2
33	2b	200	ILE	4.2
51	2t	9	ASN	4.2
32	1a	162	A	4.2
54	2w	5	G	4.2
32	1a	1257	U	4.2
21	1Z	169	GLU	4.2
36	2e	115	VAL	4.2

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Mol	Chain	Res	Type	RSRZ
47	1p	1	MET	4.2
42	1k	25	TYR	4.2
45	2n	12	ARG	4.2
41	2j	98	ILE	4.2
22	20	3	HIS	4.2
36	2e	81	GLU	4.2
1	1A	1138	C	4.2
1	1A	1144	A	4.2
31	29	16	VAL	4.2
36	2e	10	MET	4.2
40	2i	27	THR	4.2
54	1w	73	A	4.2
54	1y	13	C	4.2
54	1y	36	A	4.2
50	2s	52	TYR	4.2
34	2c	60	ALA	4.1
34	2c	160	ALA	4.1
1	1A	932	C	4.1
54	1w	2	C	4.1
44	2m	78	ILE	4.1
45	2n	29	ARG	4.1
1	2A	2127	G	4.1
21	2Z	125	LEU	4.1
44	2m	6	GLY	4.1
4	2E	52	LEU	4.1
44	2m	68	GLY	4.1
45	2n	51	GLY	4.1
32	1a	204	U	4.1
32	1a	1023	G	4.1
52	2u	15	ARG	4.1
1	1A	933	C	4.1
33	2b	37	ASN	4.1
21	2Z	170	THR	4.1
39	2h	93	VAL	4.1
40	2i	49	PRO	4.1
53	1v	22	U	4.1
34	2c	197	GLY	4.1
40	2i	124	GLN	4.1
54	2w	69	G	4.1
54	2w	56	C	4.1
35	2d	164	ALA	4.1
7	2H	6	ARG	4.1

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Mol	Chain	Res	Type	RSRZ
41	2j	40	LEU	4.0
32	1a	160	A	4.0
1	1A	2173	G	4.0
32	1a	1026	G	4.0
32	2a	1220	G	4.0
21	2Z	96	VAL	4.0
29	17	48	LYS	4.0
32	1a	161	A	4.0
50	1s	40	ILE	4.0
32	2a	1150	U	4.0
47	1p	2	VAL	4.0
48	2q	23	VAL	4.0
54	1w	3	C	4.0
34	2c	189	ALA	4.0
1	1A	931	C	4.0
40	2i	123	PRO	4.0
26	24	54	GLY	4.0
38	2g	85	TYR	4.0
40	2i	83	ARG	4.0
50	2s	81	ARG	4.0
12	2Q	22	LYS	4.0
51	1t	69	GLY	4.0
1	1A	1112	U	4.0
38	2g	32	ARG	4.0
40	1i	117	HIS	4.0
36	2e	22	GLY	4.0
41	1j	98	ILE	3.9
45	2n	7	ILE	3.9
32	2a	1532	U	3.9
54	2w	28	G	3.9
21	2Z	148	ASP	3.9
34	2c	206	GLU	3.9
50	2s	71	LEU	3.9
35	2d	158	ILE	3.9
1	1A	2167	C	3.9
51	1t	71	THR	3.9
43	2l	68	ALA	3.9
1	1A	934	A	3.9
1	1A	1105	G	3.9
36	2e	11	ILE	3.9
1	2A	2804	C	3.9
41	2j	13	HIS	3.9

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Mol	Chain	Res	Type	RSRZ
54	2w	73	A	3.9
1	2A	2116	G	3.9
7	2H	76	VAL	3.9
34	1c	193	TYR	3.9
19	2X	92	LEU	3.9
33	2b	122	PHE	3.9
20	2Y	44	ILE	3.9
34	2c	158	GLY	3.9
1	2A	886	C	3.9
6	2G	19	LEU	3.9
52	2u	16	GLY	3.8
34	2c	134	ILE	3.8
47	1p	19	ILE	3.8
36	1e	10	MET	3.8
50	2s	24	ALA	3.8
51	1t	67	ALA	3.8
21	2Z	52	SER	3.8
32	1a	1447	A	3.8
21	2Z	50	GLN	3.8
7	2H	113	VAL	3.8
33	1b	165	VAL	3.8
39	2h	128	GLY	3.8
32	1a	1033	G	3.8
32	1a	1028	C	3.8
12	2Q	65	PHE	3.8
47	2p	9	PHE	3.8
34	2c	202	ILE	3.8
33	2b	228	GLY	3.8
38	2g	76	ARG	3.8
34	2c	33	LEU	3.8
35	2d	146	ILE	3.8
54	2w	6	G	3.8
52	2u	11	GLY	3.8
35	1d	208	SER	3.8
31	29	13	LYS	3.8
34	2c	4	LYS	3.8
41	1j	46	ARG	3.8
54	1y	24	G	3.8
12	2Q	37	LEU	3.8
32	1a	1001	A	3.8
41	2j	67	THR	3.8
43	2l	56	ALA	3.7

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Mol	Chain	Res	Type	RSRZ
38	1g	84	ASN	3.7
32	2a	1061	G	3.7
54	2w	29	G	3.7
34	2c	87	LEU	3.7
40	2i	37	PHE	3.7
47	1p	80	PHE	3.7
47	1p	38	TYR	3.7
1	2A	2174	C	3.7
21	2Z	152	ALA	3.7
35	2d	48	ALA	3.7
34	2c	205	GLY	3.7
1	2A	882	G	3.7
3	1D	276	LYS	3.7
32	1a	1031	G	3.7
6	2G	39	ILE	3.7
50	2s	12	ASP	3.7
1	2A	2128	C	3.7
7	2H	142	GLY	3.7
32	1a	1030(C)	G	3.7
54	1y	47	U	3.7
7	2H	166	GLY	3.7
38	1g	153	HIS	3.7
7	2H	157	TYR	3.7
48	2q	9	VAL	3.7
1	1A	1555	C	3.7
40	2i	18	PHE	3.6
41	1j	47	PHE	3.6
38	2g	79	ARG	3.6
51	1t	24	LEU	3.6
6	2G	41	GLN	3.6
54	2w	30	G	3.6
44	2m	94	ARG	3.6
36	2e	13	ILE	3.6
41	2j	96	ILE	3.6
50	2s	35	SER	3.6
51	1t	16	HIS	3.6
47	1p	21	VAL	3.6
32	2a	1531	A	3.6
21	2Z	137	ILE	3.6
1	2A	2140	C	3.6
33	2b	51	LEU	3.6
42	2k	25	TYR	3.6

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Mol	Chain	Res	Type	RSRZ
50	2s	51	VAL	3.6
7	2H	47	GLU	3.6
21	2Z	140	ASP	3.6
1	1A	1145	G	3.6
40	2i	45	ALA	3.6
11	2P	91	PHE	3.6
32	1a	344	A	3.6
54	1w	14	A	3.6
45	2n	40	CYS	3.6
1	2A	2159	G	3.6
3	2D	2	ALA	3.6
6	1G	146	TYR	3.6
8	2I	100	ALA	3.6
34	2c	153	VAL	3.6
47	1p	39	TYR	3.6
45	2n	35	ARG	3.5
33	2b	32	ILE	3.5
51	1t	72	LEU	3.5
7	2H	145	ALA	3.5
44	2m	5	ALA	3.5
32	1a	1446	U	3.5
40	2i	99	LEU	3.5
51	1t	20	LEU	3.5
35	1d	147	ALA	3.5
36	1e	95	ALA	3.5
1	1A	2151	C	3.5
7	2H	24	VAL	3.5
40	2i	62	TYR	3.5
40	2i	82	ALA	3.5
36	2e	33	VAL	3.5
6	2G	146	TYR	3.5
38	2g	154	TYR	3.5
8	2I	88	ILE	3.5
7	2H	106	THR	3.5
38	2g	147	ALA	3.5
36	2e	133	TYR	3.5
53	2v	21	C	3.5
1	2A	1026	U	3.5
34	2c	178	LEU	3.5
32	2a	1002	G	3.5
36	2e	8	GLU	3.5
40	2i	90	PRO	3.5

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Mol	Chain	Res	Type	RSRZ
47	1p	66	PRO	3.5
51	1t	8	ARG	3.5
53	1v	13	A	3.5
1	1A	943	C	3.5
38	2g	84	ASN	3.5
48	2q	22	LEU	3.5
11	2P	92	GLU	3.5
21	2Z	172	ALA	3.5
36	2e	131	ILE	3.4
50	2s	30	LEU	3.4
12	2Q	136	ALA	3.4
43	2l	28	LYS	3.4
6	2G	149	VAL	3.4
47	2p	20	VAL	3.4
1	1A	1109	G	3.4
32	1a	1531	A	3.4
41	2j	56	HIS	3.4
14	2S	5	THR	3.4
52	2u	14	TRP	3.4
39	2h	122	ARG	3.4
6	2G	157	ILE	3.4
26	14	59	PHE	3.4
33	2b	201	ILE	3.4
52	2u	5	ASP	3.4
32	2a	1219	U	3.4
32	1a	1029	C	3.4
32	2a	1018	C	3.4
33	2b	71	VAL	3.4
36	2e	84	PHE	3.4
48	2q	36	ILE	3.4
1	2A	2113	U	3.4
14	2S	54	LEU	3.4
3	2D	38	LYS	3.4
35	2d	117	ALA	3.4
32	1a	1024	G	3.4
23	2l	62	VAL	3.4
46	2o	27	VAL	3.4
30	28	29	LYS	3.4
26	14	54	GLY	3.4
34	2c	41	GLY	3.4
34	2c	191	THR	3.4
40	2i	4	TYR	3.4

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Mol	Chain	Res	Type	RSRZ
40	2i	88	TYR	3.4
54	1w	67	C	3.4
39	2h	104	ARG	3.4
34	2c	5	ILE	3.3
34	2c	196	LEU	3.3
41	2j	63	PHE	3.3
47	1p	7	ALA	3.3
1	2A	2138	C	3.3
36	2e	20	GLN	3.3
51	1t	76	ALA	3.3
34	2c	190	ARG	3.3
41	2j	62	HIS	3.3
36	2e	105	VAL	3.3
21	2Z	156	LYS	3.3
41	2j	88	LEU	3.3
1	2A	2157	G	3.3
54	2w	45	U	3.3
44	2m	104	ARG	3.3
40	1i	116	LYS	3.3
40	2i	28	VAL	3.3
43	2l	41	ARG	3.3
33	2b	161	ALA	3.3
34	2c	199	LYS	3.3
40	1i	8	GLY	3.3
8	2I	19	VAL	3.3
47	1p	42	ARG	3.3
7	2H	171	LEU	3.3
49	2r	85	LEU	3.3
1	1A	942	A	3.3
1	2A	2144	U	3.3
32	1a	1037	C	3.3
7	2H	93	GLY	3.3
23	11	2	SER	3.3
29	17	46	VAL	3.3
40	1i	26	VAL	3.3
43	2l	62	SER	3.3
43	2l	25	PRO	3.3
51	1t	68	LYS	3.3
6	2G	178	PHE	3.3
7	2H	73	ALA	3.3
34	2c	186	PHE	3.3
44	1m	26	GLY	3.3

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Mol	Chain	Res	Type	RSRZ
1	1A	1878	A	3.3
47	1p	27	LYS	3.3
7	2H	44	VAL	3.3
27	15	60	VAL	3.3
35	1d	133	VAL	3.3
34	2c	174	PRO	3.2
45	2n	49	HIS	3.2
47	1p	22	THR	3.2
33	2b	38	GLY	3.2
1	2A	2136	C	3.2
40	2i	5	TYR	3.2
41	2j	49	VAL	3.2
47	1p	59	TRP	3.2
13	2R	62	ALA	3.2
36	1e	132	ALA	3.2
1	1A	271	U	3.2
32	2a	1257	U	3.2
47	1p	4	ILE	3.2
35	1d	138	TYR	3.2
31	29	25	VAL	3.2
38	2g	5	ARG	3.2
50	1s	67	VAL	3.2
45	2n	2	ALA	3.2
45	2n	30	ALA	3.2
7	2H	133	VAL	3.2
28	26	52	VAL	3.2
31	29	20	HIS	3.2
44	2m	103	THR	3.2
1	1A	1128	U	3.2
1	1A	1143	U	3.2
41	2j	59	SER	3.2
26	24	40	HIS	3.2
45	2n	18	VAL	3.2
1	2A	2173	A	3.2
7	2H	103	LEU	3.2
12	2Q	104	PHE	3.2
1	1A	935	C	3.2
26	24	32	TYR	3.2
34	1c	184	TYR	3.2
34	2c	48	TYR	3.2
34	2c	147	LYS	3.2
35	1d	135	LEU	3.2

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Mol	Chain	Res	Type	RSRZ
42	2k	126	ARG	3.2
1	2A	2132	U	3.2
4	2E	134	ILE	3.2
6	2G	88	ILE	3.2
12	2Q	32	TYR	3.1
36	2e	135	THR	3.1
7	2H	159	GLU	3.1
32	2a	1040	U	3.1
32	2a	1286	A	3.1
45	2n	27	CYS	3.1
52	1u	14	TRP	3.1
34	2c	187	ALA	3.1
35	2d	135	LEU	3.1
48	2q	95	TYR	3.1
48	1q	90	ILE	3.1
1	1A	2174	G	3.1
22	10	3	HIS	3.1
40	2i	93	ARG	3.1
34	2c	192	THR	3.1
36	2e	138	ALA	3.1
39	2h	64	LYS	3.1
39	2h	112	LEU	3.1
52	1u	17	THR	3.1
36	2e	125	SER	3.1
1	1A	1111	U	3.1
32	1a	345	C	3.1
32	2a	1202	G	3.1
54	2w	65	G	3.1
6	2G	152	LEU	3.1
21	2Z	51	ALA	3.1
7	2H	101	ARG	3.1
45	2n	46	GLU	3.1
20	2Y	1	MET	3.1
47	1p	41	PRO	3.1
1	1A	1139	G	3.1
34	2c	179	ARG	3.1
41	1j	32	ALA	3.1
43	2l	48	PRO	3.1
54	2y	61	C	3.1
44	2m	88	ARG	3.1
21	1Z	170	THR	3.1
1	1A	1104	G	3.1

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Mol	Chain	Res	Type	RSRZ
1	1A	2184	G	3.1
1	2A	2123	G	3.1
50	2s	69	HIS	3.1
54	1y	20	U	3.1
44	2m	93	ARG	3.1
45	2n	41	ARG	3.1
1	1A	1122	C	3.1
1	1A	1146	C	3.1
32	1a	1027	C	3.1
7	2H	64	LEU	3.1
50	2s	22	LEU	3.1
7	2H	43	VAL	3.1
1	1A	2154	U	3.0
40	2i	66	ARG	3.0
44	2m	91	ARG	3.0
51	1t	80	ARG	3.0
54	2w	22	G	3.0
50	2s	84	GLY	3.0
1	2A	2803	C	3.0
6	2G	35	GLU	3.0
40	1i	65	VAL	3.0
53	2v	15	A	3.0
1	1A	1106	U	3.0
26	24	59	PHE	3.0
36	2e	89	ILE	3.0
38	1g	85	TYR	3.0
47	2p	48	TRP	3.0
26	24	45	GLY	3.0
32	1a	1030(A)	G	3.0
50	2s	68	GLY	3.0
33	2b	207	ALA	3.0
35	2d	120	LEU	3.0
34	2c	164	ARG	3.0
40	2i	122	ALA	3.0
6	2G	159	VAL	3.0
17	2V	72	VAL	3.0
40	2i	108	VAL	3.0
44	1m	122	LYS	3.0
43	2l	94	PRO	3.0
34	1c	206	GLU	3.0
45	2n	11	LYS	3.0
7	2H	71	LEU	3.0

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Mol	Chain	Res	Type	RSRZ
44	2m	76	ALA	3.0
32	2a	1149	C	3.0
34	2c	128	PHE	3.0
34	2c	171	GLY	3.0
32	2a	983	A	3.0
53	1v	15	A	3.0
36	2e	78	HIS	3.0
43	2l	64	TYR	3.0
50	2s	83	HIS	3.0
21	2Z	157	LEU	3.0
1	2A	2162	G	3.0
7	2H	79	VAL	3.0
7	2H	125	VAL	3.0
32	1a	1003	G	3.0
20	2Y	43	ASN	3.0
33	2b	55	PHE	3.0
47	1p	17	TYR	3.0
54	2w	38	A	3.0
12	2Q	121	ALA	3.0
34	1c	32	LEU	3.0
47	1p	24	ALA	3.0
11	2P	79	ARG	3.0
1	2A	2793	G	3.0
54	2w	34	G	3.0
32	2a	1030	C	3.0
34	1c	134	ILE	3.0
35	2d	134	ASP	3.0
33	1b	233	SER	3.0
40	1i	126	SER	3.0
6	2G	151	ALA	3.0
6	2G	85	GLY	3.0
38	1g	34	GLY	3.0
41	2j	60	ARG	3.0
38	2g	75	VAL	2.9
36	2e	50	GLU	2.9
33	2b	70	PHE	2.9
44	2m	121	LYS	2.9
7	2H	7	LEU	2.9
39	2h	65	TYR	2.9
41	2j	87	THR	2.9
7	2H	32	GLU	2.9
9	2N	10	GLU	2.9

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Mol	Chain	Res	Type	RSRZ
7	2H	50	VAL	2.9
48	2q	21	VAL	2.9
50	2s	45	VAL	2.9
32	1a	1532	U	2.9
35	1d	110	PHE	2.9
36	1e	89	ILE	2.9
9	2N	102	ALA	2.9
12	2Q	28	ALA	2.9
43	2l	27	LEU	2.9
7	2H	114	VAL	2.9
45	1n	61	TRP	2.9
33	2b	127	ILE	2.9
8	2l	74	ASN	2.9
7	2H	36	PRO	2.9
40	2i	13	ALA	2.9
1	2A	2896	C	2.9
49	1r	26	LEU	2.9
55	1x	67	C	2.9
34	2c	23	TYR	2.9
50	2s	40	ILE	2.9
6	2G	135	LEU	2.9
7	2H	34	GLU	2.9
35	2d	47	ARG	2.9
54	2y	56	C	2.9
40	1i	113	LYS	2.9
54	2y	15	G	2.9
32	2a	1251	A	2.9
39	2h	4	ASP	2.9
43	2l	32	PHE	2.9
54	1y	38	A	2.9
6	2G	161	THR	2.9
19	1X	95	LEU	2.9
34	2c	132	ARG	2.9
41	2j	32	ALA	2.9
7	2H	111	HIS	2.9
48	2q	32	TYR	2.9
51	1t	74	LYS	2.9
11	2P	125	VAL	2.9
39	2h	135	CYS	2.9
51	2t	47	GLY	2.9
1	1A	1114	G	2.9
1	1A	2176	G	2.9

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Mol	Chain	Res	Type	RSRZ
21	2Z	133	ILE	2.9
40	2i	33	PHE	2.9
48	1q	36	ILE	2.9
6	2G	136	ARG	2.9
41	2j	70	ARG	2.9
33	2b	173	ALA	2.9
34	2c	200	ALA	2.9
47	1p	44	THR	2.9
1	2A	2161	C	2.8
8	1I	117	GLU	2.8
32	2a	1114	C	2.8
51	1t	75	ASN	2.8
45	1n	7	ILE	2.8
8	2I	38	LEU	2.8
32	1a	1035	A	2.8
54	1w	5	G	2.8
40	2i	75	ASP	2.8
45	2n	56	VAL	2.8
46	1o	69	TYR	2.8
7	2H	13	LYS	2.8
6	2G	87	PRO	2.8
51	2t	55	ILE	2.8
21	2Z	5	LEU	2.8
40	2i	110	GLU	2.8
40	2i	105	ASP	2.8
1	1A	2181	G	2.8
54	1w	15	G	2.8
30	28	25	MET	2.8
8	1I	19	VAL	2.8
8	2I	144	VAL	2.8
39	2h	58	TYR	2.8
1	1A	2164	C	2.8
23	21	68	PRO	2.8
32	2a	204	U	2.8
7	2H	96	ALA	2.8
45	2n	4	LYS	2.8
21	2Z	126	VAL	2.8
45	2n	8	GLU	2.8
22	20	5	LYS	2.8
32	2a	307	C	2.8
36	2e	21	ALA	2.8
11	2P	118	GLY	2.8

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Mol	Chain	Res	Type	RSRZ
33	1b	228	GLY	2.8
29	17	47	ARG	2.8
51	2t	73	HIS	2.8
32	2a	1196	U	2.8
54	2w	19	G	2.8
44	2m	84	ILE	2.8
33	1b	120	ALA	2.8
1	1A	2807	C	2.8
20	2Y	106	LEU	2.8
34	2c	9	GLY	2.8
21	2Z	145	GLU	2.8
35	2d	196	LEU	2.8
7	2H	8	PRO	2.8
43	2l	18	VAL	2.8
1	2A	652(B)	A	2.8
1	2A	2801(A)	A	2.8
39	2h	131	GLY	2.8
32	2a	1030(C)	G	2.8
35	1d	78	LEU	2.8
39	2h	133	LEU	2.8
35	2d	49	ARG	2.8
21	2Z	58	VAL	2.7
43	1l	43	VAL	2.7
6	2G	27	ASN	2.7
35	2d	161	ASN	2.7
32	2a	1092	A	2.7
40	2i	63	ILE	2.7
43	1l	7	ILE	2.7
49	2r	26	LEU	2.7
41	2j	46	ARG	2.7
51	1t	17	ARG	2.7
1	2A	2807	G	2.7
32	2a	1108	G	2.7
54	2w	44	G	2.7
51	1t	18	GLN	2.7
6	2G	140	ILE	2.7
8	2I	79	ILE	2.7
14	2S	37	ALA	2.7
23	21	63	ALA	2.7
33	2b	29	ALA	2.7
33	2b	31	TYR	2.7
46	1o	87	ILE	2.7

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Mol	Chain	Res	Type	RSRZ
51	1t	55	ILE	2.7
1	1A	1116	A	2.7
21	1Z	168	GLU	2.7
7	2H	112	PRO	2.7
34	2c	120	VAL	2.7
36	2e	114	GLY	2.7
36	2e	107	ARG	2.7
1	1A	1124	U	2.7
26	24	57	GLU	2.7
47	1p	32	TYR	2.7
1	2A	2119	A	2.7
6	2G	138	GLN	2.7
36	1e	81	GLU	2.7
1	2A	2151	G	2.7
32	2a	1224	G	2.7
50	2s	48	THR	2.7
54	2y	33	U	2.7
34	1c	14	ILE	2.7
7	2H	94	TYR	2.7
12	2Q	2	LEU	2.7
35	1d	176	LEU	2.7
39	2h	134	ILE	2.7
44	2m	4	ILE	2.7
38	1g	154	TYR	2.7
1	2A	1847	A	2.7
6	2G	48	GLU	2.7
7	2H	82	GLY	2.7
32	2a	975	A	2.7
38	1g	78	ARG	2.7
8	2I	142	VAL	2.7
32	2a	980	C	2.7
7	1H	2	SER	2.7
21	1Z	149	SER	2.7
1	2A	2112	G	2.7
10	2O	8	LEU	2.7
35	2d	186	LEU	2.7
48	2q	59	ILE	2.7
41	2j	68	HIS	2.7
34	1c	179	ARG	2.7
45	2n	14	PRO	2.7
1	1A	1100	A	2.7
41	2j	61	GLU	2.7

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Mol	Chain	Res	Type	RSRZ
54	1w	13	C	2.7
54	2w	42	C	2.7
42	1k	125	PHE	2.7
45	1n	16	PHE	2.7
45	2n	45	ARG	2.7
33	1b	132	LYS	2.7
41	2j	22	LYS	2.7
45	2n	55	GLY	2.7
6	2G	17	PRO	2.7
47	2p	59	TRP	2.7
1	1A	1103	A	2.6
34	2c	44	GLU	2.6
12	1Q	81	VAL	2.6
35	1d	149	ALA	2.6
1	2A	2118	U	2.6
50	2s	54	GLY	2.6
1	2A	2148	G	2.6
32	1a	1034	G	2.6
29	27	47	ARG	2.6
7	2H	75	ALA	2.6
32	2a	1001	A	2.6
41	1j	18	ALA	2.6
1	1A	1127	U	2.6
47	2p	19	ILE	2.6
50	2s	62	ILE	2.6
51	1t	62	LEU	2.6
40	1i	33	PHE	2.6
35	1d	105	VAL	2.6
54	1w	10	G	2.6
54	2w	18	G	2.6
20	2Y	80	GLY	2.6
42	2k	117	ASN	2.6
50	2s	53	ASN	2.6
24	22	60	LEU	2.6
32	2a	1016	A	2.6
32	2a	1250	A	2.6
34	1c	33	LEU	2.6
34	2c	131	ARG	2.6
38	1g	32	ARG	2.6
51	2t	22	ARG	2.6
32	2a	962	C	2.6
34	2c	19	GLU	2.6

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Mol	Chain	Res	Type	RSRZ
50	2s	38	SER	2.6
35	2d	148	VAL	2.6
41	2j	36	GLY	2.6
9	2N	93	THR	2.6
32	1a	1032	G	2.6
33	2b	220	ASP	2.6
35	2d	157	LEU	2.6
34	2c	10	PHE	2.6
43	2l	72	GLY	2.6
33	2b	229	VAL	2.6
36	1e	134	ALA	2.6
36	2e	16	THR	2.6
38	2g	9	VAL	2.6
41	2j	27	ALA	2.6
48	2q	73	VAL	2.6
32	2a	1358	U	2.6
48	1q	28	PRO	2.6
45	2n	16	PHE	2.6
50	2s	10	PHE	2.6
1	2A	2156	G	2.6
32	2a	79	G	2.6
2	2B	59	A	2.6
40	1i	125	TYR	2.6
43	2l	69	TYR	2.6
34	1c	64	VAL	2.6
47	1p	60	LEU	2.6
54	2w	47	U	2.6
33	2b	185	ILE	2.6
21	2Z	154	ASP	2.6
32	2a	250	A	2.6
37	2f	55	ASP	2.6
40	2i	20	ARG	2.6
41	2j	52	GLY	2.6
47	1p	68	ASP	2.6
54	2w	35	A	2.6
6	2G	12	TYR	2.6
1	1A	1121	C	2.6
14	2S	58	LEU	2.5
40	2i	19	LEU	2.5
7	2H	4	ILE	2.5
15	2T	52	ILE	2.5
35	2d	160	GLN	2.5

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Mol	Chain	Res	Type	RSRZ
42	2k	125	PHE	2.5
33	2b	83	MET	2.5
34	1c	18	TRP	2.5
45	1n	34	TYR	2.5
54	2w	23	A	2.5
32	2a	1154	G	2.5
33	2b	218	ALA	2.5
1	1A	2196	C	2.5
47	1p	67	THR	2.5
54	2y	62	C	2.5
36	2e	123	LEU	2.5
46	1o	57	LEU	2.5
48	1q	98	LEU	2.5
48	2q	6	LEU	2.5
51	1t	23	ARG	2.5
40	2i	74	ILE	2.5
26	14	45	GLY	2.5
12	2Q	3	MET	2.5
21	2Z	153	SER	2.5
33	2b	210	SER	2.5
34	2c	72	LYS	2.5
35	1d	86	LYS	2.5
26	24	52	THR	2.5
34	2c	37	GLN	2.5
42	1k	15	ALA	2.5
12	2Q	59	ARG	2.5
1	1A	1133	G	2.5
21	1Z	165	VAL	2.5
32	2a	1021	G	2.5
32	2a	1197	G	2.5
40	1i	109	VAL	2.5
1	1A	2906	U	2.5
40	2i	32	ASP	2.5
34	1c	128	PHE	2.5
47	1p	13	HIS	2.5
47	1p	48	TRP	2.5
1	2A	2126	A	2.5
1	2A	2170	A	2.5
4	1E	195	LEU	2.5
6	2G	60	LEU	2.5
7	2H	67	LEU	2.5
39	1h	2	LEU	2.5

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Mol	Chain	Res	Type	RSRZ
4	2E	115	GLY	2.5
1	1A	1108	G	2.5
7	2H	89	ILE	2.5
32	2a	1156	G	2.5
54	2y	53	G	2.5
31	29	19	ARG	2.5
48	2q	91	ARG	2.5
22	10	7	LEU	2.5
34	1c	34	LEU	2.5
38	2g	109	ASN	2.5
39	2h	94	TYR	2.5
44	2m	23	TYR	2.5
48	2q	77	VAL	2.5
50	1s	71	LEU	2.5
1	1A	1072	U	2.5
1	2A	894	C	2.5
33	2b	211	ILE	2.5
39	2h	38	ILE	2.5
41	1j	96	ILE	2.5
54	2w	74	C	2.5
33	2b	48	MET	2.5
32	2a	1050	G	2.5
45	1n	17	LYS	2.5
54	2y	5	G	2.5
51	2t	59	ALA	2.5
34	2c	159	GLY	2.5
11	2P	99	LEU	2.5
39	2h	84	ARG	2.5
48	2q	12	SER	2.5
50	2s	78	ARG	2.5
52	1u	15	ARG	2.5
1	1A	945	A	2.5
32	2a	1357	A	2.5
37	1f	60	PHE	2.5
54	2w	21	A	2.5
1	2A	2110	G	2.5
36	2e	17	ALA	2.5
40	1i	76	ALA	2.5
46	1o	89	GLY	2.5
48	2q	33	GLY	2.5
33	1b	61	LEU	2.4
35	1d	97	LEU	2.4

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Mol	Chain	Res	Type	RSRZ
3	1D	275	LYS	2.4
40	2i	111	ARG	2.4
6	2G	15	VAL	2.4
8	2I	92	VAL	2.4
48	2q	10	VAL	2.4
32	1a	1025	U	2.4
34	1c	8	ILE	2.4
39	2h	35	ILE	2.4
52	1u	13	ILE	2.4
6	2G	49	ASP	2.4
32	1a	1005	A	2.4
32	2a	91	C	2.4
32	2a	1066	C	2.4
36	2e	93	PRO	2.4
50	2s	76	PRO	2.4
54	2w	67	C	2.4
31	29	37	GLY	2.4
40	2i	8	GLY	2.4
47	2p	64	ALA	2.4
6	2G	74	LYS	2.4
20	2Y	6	HIS	2.4
1	2A	2100	G	2.4
32	2a	1003	G	2.4
32	2a	1064	G	2.4
32	2a	1222	G	2.4
36	2e	43	LEU	2.4
33	2b	93	VAL	2.4
7	2H	124	GLU	2.4
36	1e	13	ILE	2.4
1	1A	1113	A	2.4
1	2A	2117	A	2.4
34	2c	162	GLN	2.4
35	1d	168	ARG	2.4
1	2A	889	C	2.4
1	2A	2137	C	2.4
40	1i	15	ALA	2.4
44	2m	66	LEU	2.4
43	2l	16	GLU	2.4
32	2a	1024	G	2.4
34	2c	142	MET	2.4
36	2e	14	ARG	2.4
7	2H	12	PRO	2.4

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Mol	Chain	Res	Type	RSRZ
33	2b	113	HIS	2.4
44	2m	92	HIS	2.4
54	1y	48	C	2.4
10	2O	52	VAL	2.4
29	27	46	VAL	2.4
35	1d	104	VAL	2.4
43	2l	13	LYS	2.4
33	1b	130	ARG	2.4
14	2S	92	TYR	2.4
40	1i	81	ILE	2.4
43	2l	63	GLY	2.4
45	2n	43	CYS	2.4
54	2w	15	G	2.4
54	2y	19	G	2.4
54	2y	65	G	2.4
12	2Q	63	LYS	2.4
45	2n	15	LYS	2.4
1	1A	2186	C	2.4
32	1a	1030	C	2.4
45	2n	23	ARG	2.4
52	1u	6	ARG	2.4
54	2w	14	A	2.4
34	2c	195	VAL	2.4
1	1A	1985	U	2.4
34	2c	152	ILE	2.4
39	1h	6	ILE	2.4
41	2j	41	PRO	2.4
7	2H	129	THR	2.4
31	29	12	ASP	2.4
49	1r	24	ALA	2.4
32	1a	102	G	2.4
10	1O	17	ARG	2.4
35	2d	141	ARG	2.4
12	2Q	34	LEU	2.4
39	1h	112	LEU	2.4
39	2h	36	LEU	2.4
21	2Z	147	GLY	2.4
39	2h	137	VAL	2.4
40	1i	80	GLY	2.4
40	1i	110	GLU	2.4
54	1y	21	A	2.4
43	2l	47	LYS	2.4

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Mol	Chain	Res	Type	RSRZ
12	2Q	47	ILE	2.4
20	1Y	1	MET	2.4
34	2c	39	ILE	2.4
21	1Z	104	PHE	2.4
50	2s	42	PRO	2.4
21	2Z	93	ASP	2.4
51	2t	12	ALA	2.4
49	1r	79	LEU	2.4
49	2r	46	GLU	2.4
1	2A	2165	G	2.3
54	2w	57	G	2.3
25	23	6	VAL	2.3
35	1d	170	VAL	2.3
42	2k	109	VAL	2.3
1	1A	2814	C	2.3
11	2P	122	PRO	2.3
33	1b	21	ARG	2.3
33	2b	111	ARG	2.3
40	2i	16	ARG	2.3
45	1n	57	ARG	2.3
22	10	2	ALA	2.3
48	2q	7	THR	2.3
21	2Z	24	LEU	2.3
48	1q	33	GLY	2.3
48	2q	53	LEU	2.3
51	2t	24	LEU	2.3
21	2Z	86	VAL	2.3
43	2l	58	VAL	2.3
22	20	44	ARG	2.3
35	2d	122	ARG	2.3
40	2i	107	ARG	2.3
41	2j	43	ARG	2.3
54	1w	65	G	2.3
54	2w	24	G	2.3
1	2A	2143	C	2.3
7	2H	9	ILE	2.3
54	2w	40	C	2.3
14	1S	72	ALA	2.3
33	1b	133	LYS	2.3
40	1i	45	ALA	2.3
40	1i	119	ALA	2.3
44	2m	42	ALA	2.3

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Mol	Chain	Res	Type	RSRZ
45	2n	59	ALA	2.3
9	2N	116	LEU	2.3
12	1Q	59	ARG	2.3
20	2Y	2	ARG	2.3
21	2Z	4	ARG	2.3
40	2i	10	ARG	2.3
51	2t	83	ARG	2.3
21	1Z	151	HIS	2.3
21	2Z	13	GLU	2.3
33	2b	164	VAL	2.3
41	2j	34	VAL	2.3
35	2d	181	MET	2.3
1	2A	897	C	2.3
1	2A	2115	G	2.3
1	2A	2319	G	2.3
32	2a	1283	G	2.3
33	2b	223	ILE	2.3
35	1d	185	PHE	2.3
24	12	13	ALA	2.3
38	2g	151	TYR	2.3
51	1t	59	ALA	2.3
26	24	44	THR	2.3
47	1p	69	THR	2.3
52	2u	17	THR	2.3
34	1c	38	ARG	2.3
7	2H	169	VAL	2.3
33	2b	232	PRO	2.3
36	1e	55	VAL	2.3
40	2i	26	VAL	2.3
20	2Y	75	ILE	2.3
36	1e	118	ILE	2.3
1	1A	2168	C	2.3
6	2G	50	ALA	2.3
34	1c	180	ALA	2.3
1	2A	614(B)	G	2.3
7	2H	97	ARG	2.3
21	2Z	9	TYR	2.3
32	2a	1026	G	2.3
34	2c	140	ARG	2.3
41	1j	10	GLY	2.3
34	2c	193	TYR	2.3
34	2c	201	TYR	2.3

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Mol	Chain	Res	Type	RSRZ
41	1j	45	ARG	2.3
51	2t	57	ARG	2.3
54	2y	57	G	2.3
40	1i	19	LEU	2.3
47	2p	74	LEU	2.3
6	2G	155	MET	2.3
54	2w	50	U	2.3
15	2T	48	ILE	2.3
35	2d	70	ILE	2.3
41	1j	50	ILE	2.3
10	2O	96	THR	2.3
45	1n	13	THR	2.3
1	1A	2130	C	2.3
16	1U	69	CYS	2.3
11	2P	45	LEU	2.3
47	2p	73	LEU	2.3
49	1r	31	LEU	2.3
54	2w	76	A	2.3
10	2O	98	VAL	2.3
1	1A	1220	U	2.3
15	1T	111	ARG	2.3
45	2n	31	ARG	2.3
11	2P	76	LYS	2.3
36	2e	121	LYS	2.3
8	1I	106	GLY	2.3
48	2q	54	GLY	2.3
23	2l	67	ILE	2.3
33	2b	222	ILE	2.3
36	2e	129	ILE	2.3
33	2b	163	PHE	2.3
33	2b	193	ASP	2.3
6	2G	133	LEU	2.3
31	29	24	TYR	2.3
34	2c	184	TYR	2.3
39	2h	107	LEU	2.3
46	1o	66	LEU	2.3
51	2t	13	LEU	2.3
1	2A	2310	A	2.2
29	27	23	ARG	2.2
33	2b	131	PRO	2.2
1	2A	2166	G	2.2
54	1y	5	G	2.2

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Mol	Chain	Res	Type	RSRZ
8	2I	21	VAL	2.2
21	2Z	106	GLY	2.2
21	2Z	128	VAL	2.2
33	1b	227	GLY	2.2
35	2d	8	VAL	2.2
33	2b	216	SER	2.2
41	2j	35	SER	2.2
35	1d	158	ILE	2.2
36	2e	30	ALA	2.2
39	1h	38	ILE	2.2
47	1p	64	ALA	2.2
8	2I	93	THR	2.2
21	2Z	121	HIS	2.2
8	2I	12	LEU	2.2
11	2P	110	TYR	2.2
26	24	68	ARG	2.2
35	1d	122	ARG	2.2
47	1p	25	ARG	2.2
41	2j	53	PRO	2.2
32	2a	1112	C	2.2
32	2a	986	A	2.2
34	1c	2	GLY	2.2
34	2c	136	GLN	2.2
44	2m	106	ASN	2.2
34	2c	138	VAL	2.2
35	1d	181	MET	2.2
35	2d	105	VAL	2.2
1	2A	9	U	2.2
41	2j	19	SER	2.2
32	2a	485	G	2.2
54	2w	10	G	2.2
36	2e	118	ILE	2.2
3	2D	15	PHE	2.2
12	2Q	5	ARG	2.2
14	2S	10	ARG	2.2
33	2b	144	ARG	2.2
50	2s	29	ARG	2.2
17	2V	71	LEU	2.2
34	2c	12	LEU	2.2
48	2q	84	LEU	2.2
50	1s	22	LEU	2.2
51	1t	10	LEU	2.2

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Mol	Chain	Res	Type	RSRZ
34	2c	28	GLN	2.2
5	1F	131	GLY	2.2
1	1A	2161	C	2.2
55	1x	68	C	2.2
26	24	66	SER	2.2
35	2d	56	VAL	2.2
39	2h	9	MET	2.2
41	2j	94	VAL	2.2
1	2A	2169	A	2.2
32	2a	1014	A	2.2
48	1q	37	LYS	2.2
7	2H	121	ILE	2.2
35	2d	73	ARG	2.2
36	1e	21	ALA	2.2
38	1g	76	ARG	2.2
43	2l	15	ARG	2.2
43	2l	26	ALA	2.2
45	1n	41	ARG	2.2
51	1t	15	ARG	2.2
10	2O	99	PHE	2.2
33	2b	17	PHE	2.2
38	1g	43	PHE	2.2
44	1m	109	THR	2.2
49	1r	25	THR	2.2
54	2y	1	G	2.2
4	2E	195	LEU	2.2
36	1e	49	PRO	2.2
41	2j	8	LEU	2.2
51	2t	26	ASN	2.2
7	2H	25	LYS	2.2
40	2i	112	LYS	2.2
21	1Z	166	SER	2.2
1	2A	2164	C	2.2
22	20	74	ARG	2.2
51	1t	22	ARG	2.2
32	2a	4	U	2.2
30	28	7	HIS	2.2
13	2R	25	ALA	2.2
21	2Z	21	ALA	2.2
54	1w	23	A	2.2
8	2I	117	GLU	2.2
21	2Z	162	GLU	2.2

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Mol	Chain	Res	Type	RSRZ
35	2d	150	GLU	2.2
47	1p	65	GLN	2.2
34	2c	91	LEU	2.2
34	2c	204	LEU	2.2
51	1t	64	ASP	2.2
1	1A	938	G	2.2
1	1A	1221	G	2.2
1	1A	2843	G	2.2
32	2a	1031	G	2.2
35	1d	73	ARG	2.2
38	2g	78	ARG	2.2
40	1i	114	TYR	2.2
40	1i	121	ARG	2.2
42	1k	126	ARG	2.2
7	2H	2	SER	2.2
33	2b	150	SER	2.2
8	2I	18	VAL	2.2
11	2P	83	VAL	2.2
34	2c	151	VAL	2.2
9	2N	8	GLN	2.2
26	14	46	GLN	2.2
34	2c	71	ALA	2.2
34	2c	168	ALA	2.2
48	2q	86	GLU	2.2
6	2G	114	ILE	2.2
21	2Z	171	ILE	2.2
1	1A	302	A	2.2
1	2A	899	A	2.2
32	1a	1030(D)	A	2.2
43	2l	93	LEU	2.2
49	2r	66	LEU	2.2
7	2H	51	ARG	2.2
8	1I	103	ARG	2.2
1	1A	2137	G	2.2
1	2A	2125	G	2.2
1	2A	2131	G	2.2
1	2A	2897	U	2.2
32	1a	841	U	2.2
36	2e	55	VAL	2.2
43	2l	104	VAL	2.2
50	2s	32	LYS	2.2
14	1S	6	ALA	2.2

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Mol	Chain	Res	Type	RSRZ
43	2l	30	ALA	2.2
46	2o	16	ALA	2.2
15	2T	75	ILE	2.2
39	1h	86	ILE	2.2
39	1h	134	ILE	2.2
6	1G	80	PHE	2.2
6	2G	115	ARG	2.2
7	2H	95	ARG	2.2
14	2S	20	ARG	2.2
21	2Z	48	PHE	2.2
38	1g	4	ARG	2.2
38	2g	132	GLY	2.2
32	1a	101	A	2.2
32	2a	1044	A	2.2
41	1j	40	LEU	2.2
44	2m	70	LEU	2.2
47	1p	50	LYS	2.1
17	2V	91	TYR	2.1
20	2Y	35	TYR	2.1
45	2n	21	TYR	2.1
28	26	42	TRP	2.1
40	2i	54	ASP	2.1
8	1I	109	ILE	2.1
16	2U	17	ILE	2.1
30	18	6	THR	2.1
1	1A	2183	C	2.1
21	2Z	130	PRO	2.1
32	2a	979	C	2.1
44	2m	73	GLU	2.1
28	26	36	LEU	2.1
33	2b	44	LEU	2.1
33	2b	132	LYS	2.1
33	2b	133	LYS	2.1
15	1T	106	SER	2.1
32	2a	1225	A	2.1
32	2a	1287	A	2.1
10	2O	1	MET	2.1
40	2i	29	ASN	2.1
41	2j	66	ARG	2.1
45	2n	57	ARG	2.1
48	2q	88	TYR	2.1
1	2A	2167	U	2.1

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Mol	Chain	Res	Type	RSRZ
3	1D	2	ALA	2.1
7	2H	17	VAL	2.1
14	2S	46	VAL	2.1
22	20	2	ALA	2.1
34	2c	177	THR	2.1
36	1e	135	THR	2.1
1	2A	2792	G	2.1
11	2P	75	ILE	2.1
32	1a	630	G	2.1
38	1g	42	ILE	2.1
44	1m	121	LYS	2.1
48	2q	65	ILE	2.1
33	2b	105	PHE	2.1
8	1I	35	LEU	2.1
8	2I	44	LEU	2.1
32	1a	1006	C	2.1
32	2a	984	C	2.1
23	2l	61	ARG	2.1
32	1a	1503	A	2.1
33	2b	195	ASP	2.1
31	29	29	ASN	2.1
41	1j	95	GLU	2.1
35	1d	166	LYS	2.1
39	2h	108	GLY	2.1
5	1F	49	ALA	2.1
6	2G	61	ALA	2.1
13	1R	109	ALA	2.1
20	1Y	72	VAL	2.1
26	14	50	VAL	2.1
32	1a	1040	U	2.1
35	2d	121	VAL	2.1
54	1w	66	U	2.1
40	2i	40	LEU	2.1
40	2i	56	LEU	2.1
1	1A	2175	G	2.1
32	1a	104	G	2.1
1	1A	2160	C	2.1
1	2A	2175	C	2.1
8	2I	96	ASP	2.1
10	2O	108	GLU	2.1
32	1a	100	C	2.1
33	1b	137	ARG	2.1

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Mol	Chain	Res	Type	RSRZ
51	1t	73	HIS	2.1
54	1y	22	G	2.1
34	2c	143	GLU	2.1
41	2j	12	ASP	2.1
4	1E	28	ALA	2.1
9	1N	47	ALA	2.1
10	2O	57	VAL	2.1
16	1U	113	ALA	2.1
34	2c	139	GLN	2.1
34	2c	207	VAL	2.1
36	1e	17	ALA	2.1
43	2l	90	VAL	2.1
6	1G	17	PRO	2.1
40	2i	64	THR	2.1
20	2Y	38	ILE	2.1
40	2i	102	LEU	2.1
41	1j	62	HIS	2.1
15	1T	38	ASN	2.1
33	2b	94	ASN	2.1
6	2G	134	GLY	2.1
32	1a	292	G	2.1
32	2a	1367	C	2.1
29	27	1	MET	2.1
11	1P	125	VAL	2.1
34	2c	65	ALA	2.1
34	2c	7	PRO	2.1
36	1e	82	VAL	2.1
39	2h	103	VAL	2.1
40	1i	90	PRO	2.1
50	2s	11	VAL	2.1
14	2S	17	ARG	2.1
14	2S	12	PHE	2.1
34	1c	56	ASP	2.1
47	1p	36	ILE	2.1
28	26	11	LEU	2.1
39	2h	113	SER	2.1
47	1p	6	LEU	2.1
52	1u	2	GLY	2.1
21	2Z	65	GLN	2.1
1	2A	2182	G	2.1
3	1D	38	LYS	2.1
32	2a	1221	G	2.1

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Mol	Chain	Res	Type	RSRZ
34	1c	129	ALA	2.1
35	1d	136	PRO	2.1
35	2d	166	LYS	2.1
39	2h	124	ALA	2.1
40	2i	42	ARG	2.1
40	2i	119	ALA	2.1
43	2l	59	ARG	2.1
50	2s	28	LYS	2.1
51	2t	68	LYS	2.1
45	2n	22	THR	2.1
52	2u	8	THR	2.1
32	2a	1111	A	2.1
33	2b	148	TYR	2.1
38	1g	151	TYR	2.1
48	2q	42	TYR	2.1
40	2i	117	HIS	2.1
41	1j	65	LEU	2.1
4	2E	6	GLY	2.1
44	2m	95	GLY	2.1
46	2o	61	GLY	2.1
33	2b	97	TRP	2.1
35	2d	139	ARG	2.1
45	1n	12	ARG	2.1
17	1V	55	ALA	2.0
32	2a	1452	C	2.0
47	2p	70	ALA	2.0
3	2D	205	VAL	2.0
10	2O	14	THR	2.0
23	11	35	THR	2.0
38	2g	135	VAL	2.0
44	2m	7	VAL	2.0
2	2B	119	G	2.0
30	18	7	HIS	2.0
32	2a	1058	G	2.0
54	1y	19	G	2.0
35	1d	204	ILE	2.0
38	1g	50	ILE	2.0
39	2h	86	ILE	2.0
32	2a	1030(D)	A	2.0
46	2o	15	PHE	2.0
52	1u	3	LYS	2.0
51	2t	25	ARG	2.0

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Mol	Chain	Res	Type	RSRZ
21	2Z	98	MET	2.0
30	28	18	ALA	2.0
33	2b	177	ALA	2.0
39	2h	101	PRO	2.0
51	2t	77	ALA	2.0
1	2A	2142	C	2.0
4	1E	47	VAL	2.0
8	2I	107	VAL	2.0
20	2Y	24	VAL	2.0
32	2a	1027	C	2.0
32	2a	1116	C	2.0
35	2d	198	VAL	2.0
36	2e	34	VAL	2.0
41	2j	44	VAL	2.0
49	2r	22	VAL	2.0
54	2w	41	C	2.0
26	14	63	TYR	2.0
33	1b	187	LEU	2.0
35	2d	23	GLY	2.0
41	1j	23	ILE	2.0
36	2e	45	PHE	2.0
44	2m	99	ARG	2.0
1	1A	2813	G	2.0
32	1a	1385	G	2.0
1	1A	1123	A	2.0
8	2I	80	PRO	2.0
16	1U	61	TRP	2.0
41	2j	18	ALA	2.0
51	1t	40	ALA	2.0
1	2A	271(N)	U	2.0
1	2A	2109	U	2.0
15	1T	66	VAL	2.0
32	2a	1278	U	2.0
35	2d	112	VAL	2.0
19	2X	68	ARG	2.0
1	1A	2210	C	2.0
20	2Y	22	GLY	2.0
35	1d	16	GLY	2.0
43	2l	19	ARG	2.0
51	2t	86	ARG	2.0
7	2H	148	ILE	2.0
32	2a	1192	C	2.0

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Mol	Chain	Res	Type	RSRZ
46	2o	31	LEU	2.0
34	1c	203	PHE	2.0
43	1l	64	TYR	2.0
1	1A	1102	G	2.0
32	2a	969	A	2.0
54	2w	36	A	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, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q<0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
54	7MG	2y	46	24/25	0.65	0.20	68,95,99,128	0
54	5MU	2y	54	21/22	0.71	0.31	79,93,108,123	0
54	PSU	1y	55	20/21	0.72	0.20	72,89,99,120	0
54	4SU	2w	8	20/21	0.75	0.30	81,98,120,128	0
54	MIA	2y	37	22/30	0.76	0.27	72,86,94,120	0
54	PSU	2y	32	20/21	0.76	0.21	73,89,97,108	0
54	PSU	2w	55	20/21	0.76	0.29	80,94,98,113	0
54	7MG	2w	46	24/25	0.77	0.24	83,96,107,134	0
54	PSU	2y	55	20/21	0.77	0.28	80,96,115,118	0
54	7MG	1w	46	24/25	0.78	0.20	76,90,101,124	0
54	4SU	1y	8	20/21	0.79	0.23	80,98,105,114	0
54	5MU	1y	54	21/22	0.79	0.20	76,87,95,116	0
54	PSU	1w	55	20/21	0.80	0.22	72,81,90,98	0
54	7MG	1y	46	24/25	0.83	0.24	76,95,106,115	0
54	4SU	2y	8	20/21	0.83	0.12	87,94,106,113	0
54	4SU	1w	8	20/21	0.83	0.20	75,86,105,114	0
54	PSU	1y	32	20/21	0.84	0.23	69,87,94,95	0
55	4SU	2x	8	20/21	0.84	0.16	74,85,90,96	0
54	PSU	2y	39	20/21	0.85	0.23	78,84,100,112	0
32	2MG	2a	1207	24/25	0.85	0.17	74,85,90,98	0
54	5MU	2w	54	21/22	0.86	0.21	66,85,93,101	0
55	5MU	2x	54	21/22	0.86	0.24	71,87,95,100	0
32	M2G	2a	966	25/26	0.87	0.22	52,69,95,99	0
43	0TD	1l	92	10/11	0.87	0.23	61,64,70,74	0
54	MIA	1y	37	22/30	0.87	0.23	76,83,93,94	0
54	MIA	2w	37	25/30	0.88	0.28	70,82,91,110	0
55	PSU	2x	55	20/21	0.88	0.18	69,84,106,107	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
54	PSU	2w	32	20/21	0.90	0.32	69,85,94,103	0
32	5MC	2a	967	21/22	0.90	0.19	62,71,79,86	0
1	5MU	2A	1915	21/22	0.91	0.18	64,72,79,93	0
54	PSU	1y	39	20/21	0.91	0.18	71,81,89,95	0
54	PSU	2w	39	20/21	0.91	0.33	80,88,96,102	0
32	PSU	2a	516	20/21	0.92	0.15	65,72,79,83	0
55	5MC	2x	32	21/22	0.92	0.19	65,78,87,88	0
32	4OC	2a	1402	22/23	0.92	0.17	45,63,71,90	0
32	5MC	2a	1404	21/22	0.92	0.21	47,59,74,77	0
1	PSU	2A	1911	20/21	0.93	0.17	56,60,66,70	0
54	MIA	1w	37	29/30	0.93	0.22	43,62,74,78	0
54	PSU	1w	32	20/21	0.93	0.20	59,72,79,83	0
32	2MG	1a	1207	24/25	0.93	0.14	62,72,76,80	0
43	0TD	2l	92	10/11	0.93	0.23	65,68,73,79	0
54	PSU	1w	39	20/21	0.93	0.23	50,70,80,83	0
54	5MU	1w	54	21/22	0.94	0.16	55,67,78,79	0
1	PSU	2A	1917	20/21	0.94	0.20	56,65,75,76	0
55	PSU	1x	55	20/21	0.94	0.16	56,67,81,87	0
32	PSU	1a	516	20/21	0.94	0.16	63,70,78,78	0
32	7MG	2a	527	24/25	0.95	0.19	61,70,77,88	0
1	PSU	1A	1939	20/21	0.95	0.23	53,60,71,72	0
32	5MC	2a	1407	21/22	0.95	0.20	48,57,69,76	0
32	UR3	2a	1498	21/22	0.95	0.20	48,58,62,68	0
32	MA6	2a	1518	24/25	0.95	0.20	41,63,74,82	0
55	5MU	1x	54	21/22	0.95	0.14	57,71,79,83	0
32	MA6	2a	1519	24/25	0.95	0.25	47,65,74,81	0
1	4OC	2A	1920	21/23	0.95	0.23	46,57,62,72	0
1	5MU	1A	1937	21/22	0.95	0.18	56,67,75,82	0
55	4SU	1x	8	20/21	0.96	0.17	46,60,69,73	0
32	5MC	2a	1400	21/22	0.96	0.23	70,74,80,93	0
55	5MC	1x	32	21/22	0.96	0.21	44,54,67,73	0
32	M2G	1a	966	25/26	0.96	0.20	41,55,61,77	0
32	5MC	1a	967	21/22	0.96	0.21	51,58,67,70	0
1	4OC	1A	1942	21/23	0.96	0.20	42,55,61,65	0
32	7MG	1a	527	24/25	0.96	0.18	40,50,60,67	0
1	5MC	2A	1962	21/22	0.96	0.18	28,43,52,59	0
1	OMG	2A	2251	24/25	0.97	0.17	27,36,44,46	0
1	2MU	2A	2552	21/23	0.97	0.20	28,38,46,52	0
1	PSU	2A	2605	20/21	0.97	0.18	25,33,40,42	0
32	MA6	1a	1518	24/25	0.97	0.21	31,47,51,57	0
32	MA6	1a	1519	24/25	0.97	0.21	39,48,57,71	0
1	OMG	1A	2263	24/25	0.97	0.22	22,32,39,44	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
1	PSU	1A	1933	20/21	0.97	0.21	49,59,62,66	0
1	5MC	1A	1964	21/22	0.97	0.21	38,47,52,60	0
32	4OC	1a	1402	22/23	0.97	0.18	37,47,55,61	0
32	5MC	1a	1404	21/22	0.97	0.19	32,43,50,53	0
1	5MU	2A	1939	21/22	0.97	0.17	24,34,41,46	0
1	5MC	2A	1942	21/22	0.97	0.16	45,50,58,61	0
32	5MC	1a	1407	21/22	0.97	0.19	34,42,56,62	0
1	2MU	1A	2564	21/23	0.98	0.22	26,36,40,46	0
1	PSU	1A	2617	20/21	0.98	0.20	24,31,37,39	0
32	5MC	1a	1400	21/22	0.98	0.18	39,53,61,67	0
1	5MC	1A	1984	21/22	0.98	0.18	31,38,48,57	0
1	2MA	2A	2503	23/24	0.98	0.20	25,30,35,37	0
1	5MU	1A	1961	21/22	0.98	0.19	21,33,38,44	0
1	2MA	1A	2515	23/24	0.98	0.24	20,26,31,34	0
32	UR3	1a	1498	21/22	0.98	0.18	38,43,50,54	0

6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	2A	3871	1/1	-0.25	0.20	70,70,70,70	0
56	MG	1A	3786	1/1	0.18	0.32	81,81,81,81	0
56	MG	18	103	1/1	0.23	0.17	72,72,72,72	0
56	MG	1A	3830	1/1	0.24	0.16	66,66,66,66	0
56	MG	1A	3875	1/1	0.27	0.24	60,60,60,60	0
56	MG	2a	3028	1/1	0.38	0.23	84,84,84,84	0
56	MG	1A	3970	1/1	0.42	0.13	70,70,70,70	0
56	MG	1A	4088	1/1	0.46	0.07	57,57,57,57	0
56	MG	2a	3179	1/1	0.47	0.50	100,100,100,100	0
56	MG	2A	3892	1/1	0.48	0.31	78,78,78,78	0
56	MG	1A	3912	1/1	0.49	0.30	80,80,80,80	0
56	MG	2A	3854	1/1	0.50	0.09	77,77,77,77	0
56	MG	2A	3610	1/1	0.51	0.14	67,67,67,67	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
56	MG	2a	3168	1/1	0.51	0.10	78,78,78,78	0
56	MG	1B	3007	1/1	0.51	0.25	85,85,85,85	0
56	MG	2t	3001	1/1	0.52	0.15	60,60,60,60	0
56	MG	2x	102	1/1	0.52	0.17	77,77,77,77	0
56	MG	1A	3994	1/1	0.56	0.33	76,76,76,76	0
56	MG	2a	3181	1/1	0.56	0.10	69,69,69,69	0
56	MG	2A	3824	1/1	0.57	0.14	78,78,78,78	0
56	MG	1A	3989	1/1	0.57	0.08	60,60,60,60	0
56	MG	1a	1738	1/1	0.58	0.21	66,66,66,66	0
56	MG	1x	103	1/1	0.58	0.16	71,71,71,71	0
56	MG	2a	3166	1/1	0.58	0.13	84,84,84,84	0
56	MG	2A	3364	1/1	0.58	0.17	77,77,77,77	0
56	MG	1A	4054	1/1	0.58	0.13	81,81,81,81	0
56	MG	1A	3954	1/1	0.58	0.16	58,58,58,58	0
56	MG	1A	3272	1/1	0.58	0.30	60,60,60,60	0
56	MG	1A	4025	1/1	0.58	0.13	77,77,77,77	0
56	MG	1x	101	1/1	0.59	0.09	56,56,56,56	0
56	MG	1y	3004	1/1	0.59	0.15	86,86,86,86	0
56	MG	2A	3865	1/1	0.59	0.17	71,71,71,71	0
56	MG	2A	3850	1/1	0.60	0.10	59,59,59,59	0
56	MG	1a	1688	1/1	0.60	0.16	74,74,74,74	0
56	MG	1A	3446	1/1	0.60	0.18	61,61,61,61	0
56	MG	1a	1635	1/1	0.61	0.13	75,75,75,75	0
56	MG	2A	3540	1/1	0.61	0.13	47,47,47,47	0
56	MG	1A	4076	1/1	0.61	0.29	75,75,75,75	0
56	MG	1A	3698	1/1	0.61	0.11	73,73,73,73	0
56	MG	2A	3342	1/1	0.62	0.21	59,59,59,59	0
56	MG	2A	3872	1/1	0.62	0.07	44,44,44,44	0
56	MG	1A	4026	1/1	0.62	0.15	51,51,51,51	0
56	MG	1A	3926	1/1	0.62	0.10	53,53,53,53	0
56	MG	1A	3671	1/1	0.62	0.27	67,67,67,67	0
56	MG	1A	3834	1/1	0.63	0.34	69,69,69,69	0
56	MG	2A	3868	1/1	0.63	0.16	69,69,69,69	0
56	MG	1A	3940	1/1	0.63	0.12	48,48,48,48	0
56	MG	1A	3949	1/1	0.63	0.13	63,63,63,63	0
56	MG	2A	3374	1/1	0.64	0.26	65,65,65,65	0
56	MG	2A	3091	1/1	0.64	0.14	60,60,60,60	0
56	MG	1A	4044	1/1	0.64	0.25	79,79,79,79	0
56	MG	1A	3980	1/1	0.64	0.11	74,74,74,74	0
56	MG	2a	3103	1/1	0.64	0.16	76,76,76,76	0
56	MG	2a	3155	1/1	0.64	0.12	81,81,81,81	0
56	MG	2A	3453	1/1	0.65	0.15	45,45,45,45	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	1a	1788	1/1	0.65	0.10	69,69,69,69	0
56	MG	1a	1790	1/1	0.65	0.20	73,73,73,73	0
56	MG	1a	1672	1/1	0.65	0.17	73,73,73,73	0
56	MG	1A	3718	1/1	0.66	0.13	67,67,67,67	0
56	MG	2a	3026	1/1	0.66	0.17	64,64,64,64	0
56	MG	1A	3264	1/1	0.66	0.18	63,63,63,63	0
56	MG	2a	3063	1/1	0.66	0.15	74,74,74,74	0
56	MG	2a	3090	1/1	0.66	0.11	68,68,68,68	0
56	MG	1A	3555	1/1	0.66	0.26	60,60,60,60	0
56	MG	2w	107	1/1	0.66	0.22	75,75,75,75	0
56	MG	2a	3127	1/1	0.66	0.15	85,85,85,85	0
56	MG	1a	1766	1/1	0.67	0.17	76,76,76,76	0
56	MG	1a	1702	1/1	0.67	0.28	73,73,73,73	0
56	MG	2a	3204	1/1	0.67	0.44	86,86,86,86	0
56	MG	2a	3131	1/1	0.68	0.11	80,80,80,80	0
56	MG	2A	3891	1/1	0.68	0.15	71,71,71,71	0
56	MG	1A	4040	1/1	0.68	0.14	60,60,60,60	0
56	MG	1a	1775	1/1	0.68	0.19	76,76,76,76	0
56	MG	1A	4037	1/1	0.68	0.12	62,62,62,62	0
56	MG	1A	3969	1/1	0.69	0.14	66,66,66,66	0
56	MG	1B	3032	1/1	0.69	0.22	80,80,80,80	0
56	MG	2a	3142	1/1	0.69	0.15	74,74,74,74	0
56	MG	2a	3214	1/1	0.69	0.16	91,91,91,91	0
56	MG	2a	3228	1/1	0.69	0.11	86,86,86,86	0
56	MG	2A	3867	1/1	0.69	0.11	64,64,64,64	0
56	MG	1A	4007	1/1	0.69	0.09	86,86,86,86	0
56	MG	2a	3005	1/1	0.69	0.12	75,75,75,75	0
56	MG	1A	4068	1/1	0.70	0.18	48,48,48,48	0
56	MG	1A	4095	1/1	0.70	0.17	67,67,67,67	0
56	MG	1A	4072	1/1	0.70	0.38	62,62,62,62	0
56	MG	2a	3120	1/1	0.70	0.19	72,72,72,72	0
56	MG	1B	3029	1/1	0.70	0.28	66,66,66,66	0
56	MG	1A	4074	1/1	0.70	0.15	64,64,64,64	0
56	MG	2A	3535	1/1	0.70	0.17	59,59,59,59	0
56	MG	1A	3649	1/1	0.70	0.16	54,54,54,54	0
56	MG	2a	3030	1/1	0.70	0.19	61,61,61,61	0
56	MG	2A	3745	1/1	0.71	0.20	56,56,56,56	0
56	MG	2A	3810	1/1	0.71	0.20	51,51,51,51	0
56	MG	1A	3058	1/1	0.71	0.19	54,54,54,54	0
56	MG	2a	3137	1/1	0.71	0.18	79,79,79,79	0
56	MG	1a	1782	1/1	0.71	0.17	79,79,79,79	0
56	MG	2A	3568	1/1	0.71	0.14	46,46,46,46	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	2A	3466	1/1	0.71	0.36	65,65,65,65	0
56	MG	2B	3021	1/1	0.71	0.09	75,75,75,75	0
56	MG	1a	1617	1/1	0.72	0.18	63,63,63,63	0
56	MG	2A	3463	1/1	0.72	0.14	57,57,57,57	0
56	MG	2a	3146	1/1	0.72	0.32	84,84,84,84	0
56	MG	2A	3839	1/1	0.72	0.12	45,45,45,45	0
56	MG	1A	3824	1/1	0.72	0.16	70,70,70,70	0
56	MG	1A	3770	1/1	0.72	0.09	74,74,74,74	0
56	MG	2A	3291	1/1	0.72	0.15	56,56,56,56	0
56	MG	2a	3046	1/1	0.72	0.17	64,64,64,64	0
56	MG	2a	3192	1/1	0.72	0.20	63,63,63,63	0
56	MG	2a	3201	1/1	0.72	0.13	79,79,79,79	0
56	MG	1A	3976	1/1	0.72	0.14	72,72,72,72	0
56	MG	2A	3607	1/1	0.72	0.18	55,55,55,55	0
56	MG	1A	4024	1/1	0.72	0.12	71,71,71,71	0
56	MG	2A	3716	1/1	0.72	0.62	55,55,55,55	0
56	MG	2A	3876	1/1	0.72	0.30	66,66,66,66	0
56	MG	1A	3322	1/1	0.72	0.17	59,59,59,59	0
58	ZN	24	501	1/1	0.72	0.10	128,128,128,128	0
56	MG	1A	3616	1/1	0.73	0.17	40,40,40,40	0
56	MG	1G	3004	1/1	0.73	0.34	92,92,92,92	0
56	MG	1U	202	1/1	0.73	0.49	73,73,73,73	0
56	MG	2A	3691	1/1	0.73	0.31	68,68,68,68	0
56	MG	2A	3375	1/1	0.73	0.25	52,52,52,52	0
56	MG	2A	3053	1/1	0.73	0.20	54,54,54,54	0
56	MG	2A	3058	1/1	0.73	0.18	66,66,66,66	0
56	MG	1A	3795	1/1	0.73	0.23	51,51,51,51	0
56	MG	2A	3470	1/1	0.73	0.15	56,56,56,56	0
56	MG	2A	3488	1/1	0.73	0.21	65,65,65,65	0
56	MG	1A	3513	1/1	0.73	0.16	62,62,62,62	0
56	MG	2A	3307	1/1	0.73	0.16	68,68,68,68	0
56	MG	1A	3370	1/1	0.74	0.27	57,57,57,57	0
56	MG	1A	3730	1/1	0.74	0.17	43,43,43,43	0
56	MG	2A	3790	1/1	0.74	0.21	65,65,65,65	0
56	MG	1A	3257	1/1	0.74	0.24	68,68,68,68	0
56	MG	2A	3884	1/1	0.74	0.19	42,42,42,42	0
56	MG	2a	3104	1/1	0.74	0.19	75,75,75,75	0
56	MG	1A	3934	1/1	0.74	0.11	44,44,44,44	0
56	MG	1A	3774	1/1	0.74	0.17	55,55,55,55	0
56	MG	1A	3781	1/1	0.74	0.21	32,32,32,32	0
56	MG	2A	3406	1/1	0.74	0.27	55,55,55,55	0
56	MG	2a	3010	1/1	0.74	0.18	76,76,76,76	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	2A	3074	1/1	0.74	0.11	73,73,73,73	0
56	MG	1a	1676	1/1	0.74	0.18	67,67,67,67	0
56	MG	1O	204	1/1	0.75	0.12	58,58,58,58	0
56	MG	1A	3458	1/1	0.75	0.29	54,54,54,54	0
56	MG	2a	3013	1/1	0.75	0.11	78,78,78,78	0
56	MG	1A	4084	1/1	0.75	0.12	50,50,50,50	0
56	MG	2A	3656	1/1	0.75	0.17	77,77,77,77	0
56	MG	1a	1605	1/1	0.75	0.17	65,65,65,65	0
56	MG	1a	1811	1/1	0.75	0.08	77,77,77,77	0
56	MG	1w	105	1/1	0.75	0.10	87,87,87,87	0
56	MG	2a	3083	1/1	0.75	0.21	72,72,72,72	0
56	MG	1A	3432	1/1	0.75	0.14	54,54,54,54	0
56	MG	2A	3795	1/1	0.75	0.11	37,37,37,37	0
56	MG	1a	1753	1/1	0.75	0.10	59,59,59,59	0
56	MG	2a	3230	1/1	0.75	0.12	63,63,63,63	0
56	MG	2A	3818	1/1	0.75	0.31	66,66,66,66	0
56	MG	1A	3975	1/1	0.75	0.25	93,93,93,93	0
56	MG	2A	3829	1/1	0.75	0.12	59,59,59,59	0
56	MG	2y	3005	1/1	0.75	0.30	82,82,82,82	0
56	MG	2O	8001	1/1	0.75	0.10	65,65,65,65	0
56	MG	1a	1803	1/1	0.76	0.22	73,73,73,73	0
56	MG	1a	1612	1/1	0.76	0.09	74,74,74,74	0
56	MG	2A	3100	1/1	0.76	0.14	57,57,57,57	0
56	MG	2E	308	1/1	0.76	0.14	38,38,38,38	0
56	MG	2a	3138	1/1	0.76	0.24	79,79,79,79	0
56	MG	1A	3096	1/1	0.76	0.27	49,49,49,49	0
56	MG	28	102	1/1	0.76	0.18	52,52,52,52	0
56	MG	2a	3148	1/1	0.76	0.16	77,77,77,77	0
56	MG	1A	3787	1/1	0.76	0.14	55,55,55,55	0
56	MG	2A	3335	1/1	0.76	0.16	59,59,59,59	0
56	MG	2a	3012	1/1	0.76	0.14	71,71,71,71	0
56	MG	1A	3521	1/1	0.76	0.18	65,65,65,65	0
56	MG	2A	3577	1/1	0.76	0.12	56,56,56,56	0
56	MG	2A	3358	1/1	0.76	0.12	65,65,65,65	0
56	MG	1x	107	1/1	0.76	0.12	61,61,61,61	0
56	MG	2a	3034	1/1	0.76	0.17	72,72,72,72	0
56	MG	1A	3253	1/1	0.76	0.21	61,61,61,61	0
56	MG	2A	3039	1/1	0.76	0.16	55,55,55,55	0
56	MG	19	102	1/1	0.76	0.21	51,51,51,51	0
56	MG	2a	3088	1/1	0.76	0.20	62,62,62,62	0
56	MG	1A	4061	1/1	0.76	0.17	72,72,72,72	0
56	MG	2w	108	1/1	0.76	0.15	66,66,66,66	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	2a	3099	1/1	0.76	0.14	74,74,74,74	0
56	MG	2A	3754	1/1	0.76	0.13	45,45,45,45	0
56	MG	2A	3769	1/1	0.76	0.10	62,62,62,62	0
56	MG	1B	3024	1/1	0.77	0.10	50,50,50,50	0
56	MG	1W	201	1/1	0.77	0.38	57,57,57,57	0
56	MG	1A	3073	1/1	0.77	0.35	69,69,69,69	0
56	MG	1A	3879	1/1	0.77	0.16	51,51,51,51	0
56	MG	1A	3445	1/1	0.77	0.18	62,62,62,62	0
56	MG	2A	3332	1/1	0.77	0.34	62,62,62,62	0
56	MG	2a	3215	1/1	0.77	0.19	71,71,71,71	0
56	MG	1A	3869	1/1	0.77	0.20	56,56,56,56	0
56	MG	1O	207	1/1	0.77	0.12	65,65,65,65	0
56	MG	2a	3240	1/1	0.77	0.36	63,63,63,63	0
56	MG	1a	1829	1/1	0.77	0.20	73,73,73,73	0
56	MG	2A	3741	1/1	0.77	0.12	61,61,61,61	0
56	MG	2A	3520	1/1	0.77	0.11	65,65,65,65	0
56	MG	2A	3864	1/1	0.77	0.17	63,63,63,63	0
56	MG	2A	3748	1/1	0.77	0.10	57,57,57,57	0
56	MG	2a	3171	1/1	0.77	0.09	73,73,73,73	0
56	MG	2E	307	1/1	0.78	0.13	54,54,54,54	0
56	MG	1A	3996	1/1	0.78	0.12	43,43,43,43	0
56	MG	2A	3134	1/1	0.78	0.26	72,72,72,72	0
56	MG	2W	202	1/1	0.78	0.22	58,58,58,58	0
56	MG	2A	3813	1/1	0.78	0.11	48,48,48,48	0
56	MG	2A	3259	1/1	0.78	0.15	61,61,61,61	0
56	MG	1A	4103	1/1	0.78	0.22	67,67,67,67	0
56	MG	2A	3546	1/1	0.78	0.12	44,44,44,44	0
56	MG	1a	1823	1/1	0.78	0.21	68,68,68,68	0
56	MG	2A	3844	1/1	0.78	0.08	50,50,50,50	0
56	MG	1Z	302	1/1	0.78	0.16	67,67,67,67	0
56	MG	1a	1704	1/1	0.78	0.20	63,63,63,63	0
56	MG	1A	3218	1/1	0.78	0.22	62,62,62,62	0
56	MG	2a	3198	1/1	0.78	0.17	83,83,83,83	0
56	MG	1A	3711	1/1	0.78	0.15	61,61,61,61	0
56	MG	2a	3051	1/1	0.78	0.18	69,69,69,69	0
56	MG	1x	104	1/1	0.78	0.18	72,72,72,72	0
56	MG	2a	3076	1/1	0.78	0.15	73,73,73,73	0
56	MG	2A	3696	1/1	0.78	0.13	58,58,58,58	0
56	MG	1A	3913	1/1	0.78	0.24	80,80,80,80	0
56	MG	1a	1773	1/1	0.78	0.14	90,90,90,90	0
56	MG	2a	3096	1/1	0.78	0.14	65,65,65,65	0
56	MG	1A	3378	1/1	0.78	0.14	53,53,53,53	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	1A	3962	1/1	0.78	0.17	62,62,62,62	0
56	MG	1a	1784	1/1	0.78	0.25	74,74,74,74	0
56	MG	1A	3990	1/1	0.78	0.16	52,52,52,52	0
56	MG	1A	3933	1/1	0.78	0.10	47,47,47,47	0
56	MG	2A	3341	1/1	0.79	0.11	52,52,52,52	0
56	MG	1a	1755	1/1	0.79	0.12	74,74,74,74	0
56	MG	2a	3144	1/1	0.79	0.08	83,83,83,83	0
56	MG	2A	3615	1/1	0.79	0.13	51,51,51,51	0
56	MG	1A	3971	1/1	0.79	0.24	44,44,44,44	0
56	MG	2a	3153	1/1	0.79	0.17	74,74,74,74	0
56	MG	1A	3423	1/1	0.79	0.30	67,67,67,67	0
56	MG	1A	3261	1/1	0.79	0.25	55,55,55,55	0
56	MG	1A	3853	1/1	0.79	0.10	52,52,52,52	0
56	MG	2A	3056	1/1	0.79	0.17	60,60,60,60	0
56	MG	2a	3040	1/1	0.79	0.09	57,57,57,57	0
56	MG	1A	3708	1/1	0.79	0.16	76,76,76,76	0
56	MG	1A	4045	1/1	0.79	0.10	38,38,38,38	0
56	MG	1a	1671	1/1	0.79	0.15	66,66,66,66	0
56	MG	1A	3169	1/1	0.79	0.23	55,55,55,55	0
56	MG	1A	3992	1/1	0.79	0.23	75,75,75,75	0
56	MG	2A	3180	1/1	0.79	0.19	51,51,51,51	0
56	MG	2B	3005	1/1	0.79	0.13	53,53,53,53	0
56	MG	2B	3014	1/1	0.79	0.17	77,77,77,77	0
56	MG	2B	3019	1/1	0.79	0.12	76,76,76,76	0
56	MG	1A	3251	1/1	0.79	0.09	58,58,58,58	0
56	MG	2A	3812	1/1	0.79	0.13	47,47,47,47	0
56	MG	1A	3897	1/1	0.79	0.24	62,62,62,62	0
56	MG	2a	3122	1/1	0.79	0.16	73,73,73,73	0
56	MG	1A	3421	1/1	0.79	0.15	46,46,46,46	0
56	MG	1A	4021	1/1	0.79	0.23	66,66,66,66	0
56	MG	1A	3737	1/1	0.79	0.21	57,57,57,57	0
56	MG	1A	4010	1/1	0.80	0.20	26,26,26,26	0
56	MG	2a	3121	1/1	0.80	0.24	75,75,75,75	0
56	MG	1A	3238	1/1	0.80	0.17	57,57,57,57	0
56	MG	1x	102	1/1	0.80	0.21	63,63,63,63	0
56	MG	1a	1709	1/1	0.80	0.07	59,59,59,59	0
56	MG	1A	3182	1/1	0.80	0.12	55,55,55,55	0
56	MG	1a	1744	1/1	0.80	0.25	73,73,73,73	0
56	MG	2A	3766	1/1	0.80	0.11	52,52,52,52	0
56	MG	1A	3588	1/1	0.80	0.19	46,46,46,46	0
56	MG	1A	3614	1/1	0.80	0.13	39,39,39,39	0
56	MG	2A	3413	1/1	0.80	0.16	56,56,56,56	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	2A	3051	1/1	0.80	0.15	43,43,43,43	0
56	MG	1A	3741	1/1	0.80	0.18	45,45,45,45	0
56	MG	2a	3011	1/1	0.80	0.11	64,64,64,64	0
56	MG	1A	3363	1/1	0.80	0.28	60,60,60,60	0
56	MG	1B	3002	1/1	0.80	0.33	58,58,58,58	0
56	MG	1A	3464	1/1	0.80	0.21	45,45,45,45	0
56	MG	2A	3080	1/1	0.80	0.16	58,58,58,58	0
56	MG	1A	3468	1/1	0.80	0.32	68,68,68,68	0
56	MG	1a	1654	1/1	0.80	0.17	49,49,49,49	0
56	MG	2A	3101	1/1	0.80	0.15	59,59,59,59	0
56	MG	2A	3113	1/1	0.80	0.13	52,52,52,52	0
56	MG	1a	1656	1/1	0.80	0.21	75,75,75,75	0
56	MG	1A	4049	1/1	0.80	0.13	55,55,55,55	0
56	MG	2a	3070	1/1	0.80	0.15	61,61,61,61	0
56	MG	2A	3608	1/1	0.80	0.09	61,61,61,61	0
56	MG	1A	3492	1/1	0.80	0.29	52,52,52,52	0
56	MG	1A	3998	1/1	0.80	0.16	65,65,65,65	0
56	MG	2A	3642	1/1	0.80	0.18	47,47,47,47	0
56	MG	2A	3648	1/1	0.80	0.08	51,51,51,51	0
56	MG	2A	3880	1/1	0.80	0.13	65,65,65,65	0
56	MG	2y	3002	1/1	0.80	0.13	64,64,64,64	0
56	MG	1A	3006	1/1	0.80	0.33	57,57,57,57	0
56	MG	1e	201	1/1	0.80	0.12	79,79,79,79	0
56	MG	2A	3232	1/1	0.81	0.12	64,64,64,64	0
56	MG	1w	106	1/1	0.81	0.18	74,74,74,74	0
56	MG	2A	3265	1/1	0.81	0.17	59,59,59,59	0
56	MG	1A	4029	1/1	0.81	0.08	53,53,53,53	0
56	MG	2A	3295	1/1	0.81	0.14	63,63,63,63	0
56	MG	1a	1636	1/1	0.81	0.21	67,67,67,67	0
56	MG	2a	3108	1/1	0.81	0.21	78,78,78,78	0
56	MG	1a	1642	1/1	0.81	0.10	67,67,67,67	0
56	MG	1A	3207	1/1	0.81	0.28	54,54,54,54	0
56	MG	2A	3667	1/1	0.81	0.12	49,49,49,49	0
56	MG	1A	3144	1/1	0.81	0.19	52,52,52,52	0
56	MG	1a	1661	1/1	0.81	0.14	70,70,70,70	0
56	MG	2A	3029	1/1	0.81	0.22	44,44,44,44	0
56	MG	2A	3893	1/1	0.81	0.08	66,66,66,66	0
56	MG	2a	3140	1/1	0.81	0.06	57,57,57,57	0
56	MG	2A	3740	1/1	0.81	0.17	53,53,53,53	0
56	MG	2B	3008	1/1	0.81	0.18	58,58,58,58	0
56	MG	1a	1779	1/1	0.81	0.08	65,65,65,65	0
56	MG	1a	1663	1/1	0.81	0.15	76,76,76,76	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	1A	3344	1/1	0.81	0.27	64,64,64,64	0
56	MG	1A	3417	1/1	0.81	0.17	51,51,51,51	0
56	MG	1a	1789	1/1	0.81	0.15	72,72,72,72	0
56	MG	1A	3348	1/1	0.81	0.19	62,62,62,62	0
56	MG	2U	204	1/1	0.81	0.21	45,45,45,45	0
56	MG	2A	3780	1/1	0.81	0.22	80,80,80,80	0
56	MG	1a	1795	1/1	0.81	0.12	70,70,70,70	0
56	MG	2a	3183	1/1	0.81	0.10	76,76,76,76	0
56	MG	2A	3087	1/1	0.81	0.19	53,53,53,53	0
56	MG	1A	3349	1/1	0.81	0.20	44,44,44,44	0
56	MG	2A	3811	1/1	0.81	0.10	47,47,47,47	0
56	MG	2A	3474	1/1	0.81	0.19	55,55,55,55	0
56	MG	1a	1697	1/1	0.81	0.22	63,63,63,63	0
56	MG	2A	3515	1/1	0.81	0.11	55,55,55,55	0
56	MG	1A	3947	1/1	0.81	0.12	44,44,44,44	0
56	MG	2A	3828	1/1	0.81	0.13	80,80,80,80	0
56	MG	2a	3238	1/1	0.81	0.17	62,62,62,62	0
56	MG	1a	1620	1/1	0.81	0.15	66,66,66,66	0
56	MG	2A	3830	1/1	0.81	0.19	48,48,48,48	0
56	MG	2A	3832	1/1	0.81	0.16	54,54,54,54	0
56	MG	2A	3837	1/1	0.81	0.14	37,37,37,37	0
56	MG	1a	1625	1/1	0.81	0.26	63,63,63,63	0
56	MG	2A	3843	1/1	0.81	0.17	58,58,58,58	0
56	MG	2A	3152	1/1	0.81	0.11	62,62,62,62	0
56	MG	1a	1629	1/1	0.81	0.16	57,57,57,57	0
56	MG	2B	3003	1/1	0.82	0.20	74,74,74,74	0
56	MG	1A	3147	1/1	0.82	0.28	54,54,54,54	0
56	MG	1a	1677	1/1	0.82	0.11	68,68,68,68	0
56	MG	1A	3623	1/1	0.82	0.21	59,59,59,59	0
56	MG	1A	4031	1/1	0.82	0.15	54,54,54,54	0
56	MG	1v	3001	1/1	0.82	0.12	77,77,77,77	0
56	MG	2a	3135	1/1	0.82	0.19	62,62,62,62	0
56	MG	1A	3723	1/1	0.82	0.11	47,47,47,47	0
56	MG	2A	3220	1/1	0.82	0.27	68,68,68,68	0
56	MG	1A	3641	1/1	0.82	0.17	65,65,65,65	0
56	MG	1A	3531	1/1	0.82	0.16	67,67,67,67	0
56	MG	2a	3143	1/1	0.82	0.07	73,73,73,73	0
56	MG	2A	3556	1/1	0.82	0.17	43,43,43,43	0
56	MG	1A	4006	1/1	0.82	0.11	76,76,76,76	0
56	MG	2a	3004	1/1	0.82	0.16	57,57,57,57	0
56	MG	1A	3487	1/1	0.82	0.23	70,70,70,70	0
56	MG	1A	4008	1/1	0.82	0.14	56,56,56,56	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
56	MG	1A	4058	1/1	0.82	0.07	47,47,47,47	0
56	MG	2A	3836	1/1	0.82	0.23	42,42,42,42	0
56	MG	2A	3330	1/1	0.82	0.14	63,63,63,63	0
56	MG	1E	302	1/1	0.82	0.24	58,58,58,58	0
56	MG	1E	304	1/1	0.82	0.24	55,55,55,55	0
56	MG	2a	3182	1/1	0.82	0.09	71,71,71,71	0
56	MG	1a	1643	1/1	0.82	0.17	61,61,61,61	0
56	MG	1a	1651	1/1	0.82	0.11	56,56,56,56	0
56	MG	2a	3197	1/1	0.82	0.09	69,69,69,69	0
56	MG	2A	3345	1/1	0.82	0.19	59,59,59,59	0
56	MG	2A	3684	1/1	0.82	0.10	44,44,44,44	0
56	MG	2A	3686	1/1	0.82	0.14	57,57,57,57	0
56	MG	1E	310	1/1	0.82	0.09	42,42,42,42	0
56	MG	1A	3752	1/1	0.82	0.19	41,41,41,41	0
56	MG	2a	3074	1/1	0.82	0.09	63,63,63,63	0
56	MG	2A	3712	1/1	0.82	0.14	63,63,63,63	0
56	MG	2a	3234	1/1	0.82	0.13	66,66,66,66	0
56	MG	2a	3236	1/1	0.82	0.13	75,75,75,75	0
56	MG	1A	4064	1/1	0.82	0.13	66,66,66,66	0
56	MG	2A	3067	1/1	0.82	0.11	57,57,57,57	0
56	MG	1A	3440	1/1	0.82	0.17	50,50,50,50	0
56	MG	2a	3093	1/1	0.82	0.15	64,64,64,64	0
56	MG	1A	3863	1/1	0.82	0.23	50,50,50,50	0
56	MG	2A	3434	1/1	0.82	0.14	59,59,59,59	0
56	MG	1A	3002	1/1	0.82	0.24	59,59,59,59	0
56	MG	1a	1675	1/1	0.82	0.13	60,60,60,60	0
56	MG	2a	3105	1/1	0.82	0.17	45,45,45,45	0
56	MG	1a	1645	1/1	0.83	0.22	80,80,80,80	0
56	MG	1A	3692	1/1	0.83	0.29	64,64,64,64	0
56	MG	2A	3275	1/1	0.83	0.19	58,58,58,58	0
56	MG	2G	3001	1/1	0.83	0.16	51,51,51,51	0
56	MG	1A	3537	1/1	0.83	0.24	49,49,49,49	0
56	MG	1A	3894	1/1	0.83	0.11	73,73,73,73	0
56	MG	2A	3822	1/1	0.83	0.11	66,66,66,66	0
56	MG	1a	1781	1/1	0.83	0.11	71,71,71,71	0
56	MG	2A	3309	1/1	0.83	0.13	53,53,53,53	0
56	MG	2A	3320	1/1	0.83	0.15	54,54,54,54	0
56	MG	1A	3466	1/1	0.83	0.15	64,64,64,64	0
56	MG	2A	3052	1/1	0.83	0.16	58,58,58,58	0
56	MG	1A	3581	1/1	0.83	0.16	58,58,58,58	0
56	MG	1A	3794	1/1	0.83	0.28	61,61,61,61	0
56	MG	10	104	1/1	0.83	0.30	64,64,64,64	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
56	MG	1A	3978	1/1	0.83	0.09	65,65,65,65	0
56	MG	2A	3354	1/1	0.83	0.15	68,68,68,68	0
56	MG	1A	3183	1/1	0.83	0.17	54,54,54,54	0
56	MG	1A	4033	1/1	0.83	0.11	76,76,76,76	0
56	MG	1A	4113	1/1	0.83	0.24	56,56,56,56	0
56	MG	2a	3047	1/1	0.83	0.12	52,52,52,52	0
56	MG	1A	3332	1/1	0.83	0.32	56,56,56,56	0
56	MG	2a	3058	1/1	0.83	0.20	73,73,73,73	0
56	MG	2A	3700	1/1	0.83	0.19	65,65,65,65	0
56	MG	2A	3380	1/1	0.83	0.12	55,55,55,55	0
56	MG	1A	3248	1/1	0.83	0.26	47,47,47,47	0
56	MG	2a	3210	1/1	0.83	0.10	70,70,70,70	0
56	MG	1A	3507	1/1	0.83	0.21	51,51,51,51	0
56	MG	2a	3081	1/1	0.83	0.18	49,49,49,49	0
56	MG	2A	3112	1/1	0.83	0.17	42,42,42,42	0
56	MG	1A	3942	1/1	0.83	0.09	56,56,56,56	0
56	MG	2a	3231	1/1	0.83	0.11	68,68,68,68	0
56	MG	2A	3747	1/1	0.83	0.11	51,51,51,51	0
56	MG	1a	1710	1/1	0.83	0.13	77,77,77,77	0
56	MG	1A	3203	1/1	0.83	0.16	50,50,50,50	0
56	MG	2a	3097	1/1	0.83	0.13	72,72,72,72	0
56	MG	1A	3221	1/1	0.83	0.17	55,55,55,55	0
56	MG	2A	3208	1/1	0.83	0.14	57,57,57,57	0
56	MG	1A	3353	1/1	0.83	0.32	64,64,64,64	0
56	MG	2A	3490	1/1	0.83	0.14	61,61,61,61	0
56	MG	1A	3956	1/1	0.83	0.17	61,61,61,61	0
56	MG	2B	3016	1/1	0.83	0.13	81,81,81,81	0
56	MG	2A	3808	1/1	0.83	0.12	60,60,60,60	0
56	MG	2A	3360	1/1	0.84	0.12	63,63,63,63	0
56	MG	1A	3948	1/1	0.84	0.12	60,60,60,60	0
56	MG	2A	3717	1/1	0.84	0.15	39,39,39,39	0
56	MG	2A	3726	1/1	0.84	0.13	56,56,56,56	0
56	MG	1a	1610	1/1	0.84	0.46	79,79,79,79	0
56	MG	2A	3096	1/1	0.84	0.26	59,59,59,59	0
56	MG	1A	3395	1/1	0.84	0.16	42,42,42,42	0
56	MG	1a	1819	1/1	0.84	0.10	48,48,48,48	0
56	MG	1B	3025	1/1	0.84	0.16	77,77,77,77	0
56	MG	1A	3112	1/1	0.84	0.17	49,49,49,49	0
56	MG	1A	3087	1/1	0.84	0.22	32,32,32,32	0
56	MG	1A	3696	1/1	0.84	0.21	61,61,61,61	0
56	MG	2A	3169	1/1	0.84	0.22	73,73,73,73	0
56	MG	1a	1722	1/1	0.84	0.08	65,65,65,65	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	2D	305	1/1	0.84	0.20	50,50,50,50	0
56	MG	2E	306	1/1	0.84	0.09	67,67,67,67	0
56	MG	1a	1726	1/1	0.84	0.18	67,67,67,67	0
56	MG	2A	3802	1/1	0.84	0.13	56,56,56,56	0
56	MG	2A	3805	1/1	0.84	0.26	77,77,77,77	0
56	MG	1A	3576	1/1	0.84	0.25	57,57,57,57	0
56	MG	1A	3900	1/1	0.84	0.19	44,44,44,44	0
56	MG	2A	3247	1/1	0.84	0.12	51,51,51,51	0
56	MG	2W	203	1/1	0.84	0.25	59,59,59,59	0
56	MG	1a	1746	1/1	0.84	0.08	84,84,84,84	0
56	MG	2a	3003	1/1	0.84	0.16	64,64,64,64	0
56	MG	1a	1751	1/1	0.84	0.13	70,70,70,70	0
56	MG	2A	3266	1/1	0.84	0.12	59,59,59,59	0
56	MG	2a	3178	1/1	0.84	0.22	75,75,75,75	0
56	MG	2A	3821	1/1	0.84	0.18	79,79,79,79	0
56	MG	2A	3271	1/1	0.84	0.13	49,49,49,49	0
56	MG	2A	3823	1/1	0.84	0.15	73,73,73,73	0
56	MG	1A	3026	1/1	0.84	0.10	60,60,60,60	0
56	MG	2a	3020	1/1	0.84	0.13	71,71,71,71	0
56	MG	1A	3184	1/1	0.84	0.15	62,62,62,62	0
56	MG	1A	3917	1/1	0.84	0.17	80,80,80,80	0
56	MG	2a	3029	1/1	0.84	0.15	67,67,67,67	0
56	MG	1A	3438	1/1	0.84	0.21	50,50,50,50	0
56	MG	2A	3050	1/1	0.84	0.10	51,51,51,51	0
56	MG	2a	3035	1/1	0.84	0.12	63,63,63,63	0
56	MG	1V	203	1/1	0.84	0.26	67,67,67,67	0
56	MG	2a	3042	1/1	0.84	0.24	58,58,58,58	0
56	MG	1A	3377	1/1	0.84	0.21	54,54,54,54	0
56	MG	1X	101	1/1	0.84	0.17	40,40,40,40	0
56	MG	1A	3152	1/1	0.84	0.21	55,55,55,55	0
56	MG	2a	3056	1/1	0.84	0.14	63,63,63,63	0
56	MG	2A	3338	1/1	0.84	0.22	62,62,62,62	0
56	MG	1A	3627	1/1	0.84	0.13	62,62,62,62	0
56	MG	2l	202	1/1	0.84	0.09	70,70,70,70	0
56	MG	18	101	1/1	0.84	0.23	47,47,47,47	0
56	MG	2A	3857	1/1	0.84	0.13	47,47,47,47	0
56	MG	1A	3382	1/1	0.84	0.17	54,54,54,54	0
56	MG	2A	3353	1/1	0.84	0.18	65,65,65,65	0
56	MG	1A	3747	1/1	0.84	0.21	53,53,53,53	0
56	MG	2A	3698	1/1	0.84	0.12	51,51,51,51	0
56	MG	2A	3082	1/1	0.84	0.12	50,50,50,50	0
56	MG	1a	1689	1/1	0.85	0.12	73,73,73,73	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	1A	4043	1/1	0.85	0.10	50,50,50,50	0
56	MG	2A	3033	1/1	0.85	0.18	42,42,42,42	0
56	MG	2A	3362	1/1	0.85	0.12	68,68,68,68	0
56	MG	2a	3048	1/1	0.85	0.13	67,67,67,67	0
56	MG	1A	3083	1/1	0.85	0.26	44,44,44,44	0
56	MG	1S	3001	1/1	0.85	0.30	51,51,51,51	0
56	MG	1a	1706	1/1	0.85	0.20	60,60,60,60	0
56	MG	2a	3062	1/1	0.85	0.20	70,70,70,70	0
56	MG	1a	1708	1/1	0.85	0.16	68,68,68,68	0
56	MG	2a	3065	1/1	0.85	0.24	57,57,57,57	0
56	MG	2a	3069	1/1	0.85	0.10	62,62,62,62	0
56	MG	2A	3403	1/1	0.85	0.18	60,60,60,60	0
56	MG	1A	3361	1/1	0.85	0.11	49,49,49,49	0
56	MG	1A	4048	1/1	0.85	0.08	48,48,48,48	0
56	MG	1a	1718	1/1	0.85	0.11	70,70,70,70	0
56	MG	1A	3699	1/1	0.85	0.25	64,64,64,64	0
56	MG	1A	3856	1/1	0.85	0.20	47,47,47,47	0
56	MG	1Y	502	1/1	0.85	0.22	59,59,59,59	0
56	MG	1a	1743	1/1	0.85	0.12	73,73,73,73	0
56	MG	1A	3540	1/1	0.85	0.29	52,52,52,52	0
56	MG	2A	3088	1/1	0.85	0.11	49,49,49,49	0
56	MG	1A	3541	1/1	0.85	0.13	73,73,73,73	0
56	MG	2A	3501	1/1	0.85	0.12	59,59,59,59	0
56	MG	2A	3503	1/1	0.85	0.13	58,58,58,58	0
56	MG	1A	3127	1/1	0.85	0.44	51,51,51,51	0
56	MG	2A	3855	1/1	0.85	0.11	69,69,69,69	0
56	MG	2a	3119	1/1	0.85	0.15	71,71,71,71	0
56	MG	1A	3722	1/1	0.85	0.12	39,39,39,39	0
56	MG	1A	4071	1/1	0.85	0.15	26,26,26,26	0
56	MG	2A	3105	1/1	0.85	0.09	51,51,51,51	0
56	MG	2A	3543	1/1	0.85	0.14	34,34,34,34	0
56	MG	2A	3544	1/1	0.85	0.12	42,42,42,42	0
56	MG	2A	3110	1/1	0.85	0.16	58,58,58,58	0
56	MG	1a	1601	1/1	0.85	0.11	53,53,53,53	0
56	MG	1A	3560	1/1	0.85	0.22	55,55,55,55	0
56	MG	1A	3567	1/1	0.85	0.08	54,54,54,54	0
56	MG	2A	3147	1/1	0.85	0.29	58,58,58,58	0
56	MG	1A	3734	1/1	0.85	0.13	59,59,59,59	0
56	MG	1A	3016	1/1	0.85	0.33	51,51,51,51	0
56	MG	1A	3281	1/1	0.85	0.26	50,50,50,50	0
56	MG	2A	3627	1/1	0.85	0.17	50,50,50,50	0
56	MG	2A	3202	1/1	0.85	0.26	56,56,56,56	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	2A	3647	1/1	0.85	0.22	51,51,51,51	0
56	MG	1A	3302	1/1	0.85	0.21	56,56,56,56	0
56	MG	2A	3209	1/1	0.85	0.14	61,61,61,61	0
56	MG	1A	3242	1/1	0.85	0.24	43,43,43,43	0
56	MG	1A	3095	1/1	0.85	0.20	55,55,55,55	0
56	MG	2A	3245	1/1	0.85	0.37	59,59,59,59	0
56	MG	1A	3404	1/1	0.85	0.23	59,59,59,59	0
56	MG	1A	3333	1/1	0.85	0.11	52,52,52,52	0
56	MG	1B	3011	1/1	0.85	0.16	55,55,55,55	0
56	MG	2A	3699	1/1	0.85	0.09	76,76,76,76	0
56	MG	1A	3785	1/1	0.85	0.13	47,47,47,47	0
56	MG	2T	3002	1/1	0.85	0.15	58,58,58,58	0
56	MG	2A	3710	1/1	0.85	0.14	63,63,63,63	0
56	MG	1a	1815	1/1	0.85	0.07	64,64,64,64	0
56	MG	1A	3945	1/1	0.85	0.21	41,41,41,41	0
56	MG	1A	3057	1/1	0.85	0.22	54,54,54,54	0
56	MG	1A	3164	1/1	0.85	0.18	73,73,73,73	0
56	MG	2A	3734	1/1	0.85	0.14	57,57,57,57	0
56	MG	1b	3002	1/1	0.85	0.17	61,61,61,61	0
56	MG	2A	3308	1/1	0.85	0.11	49,49,49,49	0
56	MG	1A	3668	1/1	0.85	0.20	28,28,28,28	0
56	MG	1A	3518	1/1	0.85	0.17	48,48,48,48	0
56	MG	1w	103	1/1	0.85	0.14	57,57,57,57	0
56	MG	1E	307	1/1	0.85	0.19	70,70,70,70	0
56	MG	2g	8001	1/1	0.85	0.12	75,75,75,75	0
56	MG	2a	3022	1/1	0.85	0.09	72,72,72,72	0
56	MG	2q	201	1/1	0.85	0.17	76,76,76,76	0
56	MG	1A	3208	1/1	0.85	0.16	55,55,55,55	0
56	MG	1a	1674	1/1	0.85	0.17	72,72,72,72	0
56	MG	1E	311	1/1	0.85	0.20	42,42,42,42	0
56	MG	1F	302	1/1	0.85	0.16	47,47,47,47	0
56	MG	1A	3829	1/1	0.85	0.13	59,59,59,59	0
56	MG	1N	202	1/1	0.85	0.22	48,48,48,48	0
56	MG	2a	3036	1/1	0.85	0.18	83,83,83,83	0
56	MG	1f	3002	1/1	0.86	0.27	80,80,80,80	0
56	MG	2a	3080	1/1	0.86	0.11	50,50,50,50	0
56	MG	1l	202	1/1	0.86	0.13	69,69,69,69	0
56	MG	1A	3983	1/1	0.86	0.13	48,48,48,48	0
56	MG	1A	3607	1/1	0.86	0.17	35,35,35,35	0
56	MG	2A	3879	1/1	0.86	0.10	37,37,37,37	0
56	MG	1A	3326	1/1	0.86	0.18	41,41,41,41	0
56	MG	1A	3474	1/1	0.86	0.30	60,60,60,60	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	2A	3890	1/1	0.86	0.16	61,61,61,61	0
56	MG	2A	3402	1/1	0.86	0.17	50,50,50,50	0
56	MG	1A	3418	1/1	0.86	0.11	54,54,54,54	0
56	MG	2A	3195	1/1	0.86	0.21	56,56,56,56	0
56	MG	1A	3250	1/1	0.86	0.21	49,49,49,49	0
56	MG	2A	3432	1/1	0.86	0.19	60,60,60,60	0
56	MG	1A	3798	1/1	0.86	0.09	63,63,63,63	0
56	MG	2A	3452	1/1	0.86	0.19	42,42,42,42	0
56	MG	2A	3738	1/1	0.86	0.19	59,59,59,59	0
56	MG	1A	3999	1/1	0.86	0.20	55,55,55,55	0
56	MG	1a	1760	1/1	0.86	0.17	74,74,74,74	0
56	MG	1A	3384	1/1	0.86	0.22	57,57,57,57	0
56	MG	2A	3746	1/1	0.86	0.08	68,68,68,68	0
56	MG	2A	3008	1/1	0.86	0.14	49,49,49,49	0
56	MG	2A	3471	1/1	0.86	0.21	54,54,54,54	0
56	MG	1A	4073	1/1	0.86	0.10	42,42,42,42	0
56	MG	2A	3482	1/1	0.86	0.16	63,63,63,63	0
56	MG	1A	3728	1/1	0.86	0.24	26,26,26,26	0
56	MG	2A	3770	1/1	0.86	0.13	57,57,57,57	0
56	MG	2a	3145	1/1	0.86	0.20	76,76,76,76	0
56	MG	1A	3643	1/1	0.86	0.17	34,34,34,34	0
56	MG	2A	3493	1/1	0.86	0.38	53,53,53,53	0
56	MG	2a	3149	1/1	0.86	0.12	56,56,56,56	0
56	MG	2A	3792	1/1	0.86	0.10	51,51,51,51	0
56	MG	1A	3832	1/1	0.86	0.10	62,62,62,62	0
56	MG	1A	4012	1/1	0.86	0.20	34,34,34,34	0
56	MG	2A	3510	1/1	0.86	0.18	46,46,46,46	0
56	MG	2a	3170	1/1	0.86	0.10	80,80,80,80	0
56	MG	1a	1783	1/1	0.86	0.23	83,83,83,83	0
56	MG	2A	3518	1/1	0.86	0.09	52,52,52,52	0
56	MG	1A	3648	1/1	0.86	0.12	55,55,55,55	0
56	MG	2A	3526	1/1	0.86	0.09	41,41,41,41	0
56	MG	2a	3014	1/1	0.86	0.11	64,64,64,64	0
56	MG	2a	3017	1/1	0.86	0.09	66,66,66,66	0
56	MG	2A	3531	1/1	0.86	0.23	51,51,51,51	0
56	MG	2A	3294	1/1	0.86	0.12	52,52,52,52	0
56	MG	2a	3024	1/1	0.86	0.11	72,72,72,72	0
56	MG	1a	1786	1/1	0.86	0.09	64,64,64,64	0
56	MG	2A	3305	1/1	0.86	0.13	56,56,56,56	0
56	MG	1A	3851	1/1	0.86	0.13	62,62,62,62	0
56	MG	1A	3511	1/1	0.86	0.16	45,45,45,45	0
56	MG	2A	3826	1/1	0.86	0.11	54,54,54,54	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	2a	3221	1/1	0.86	0.13	60,60,60,60	0
56	MG	2A	3549	1/1	0.86	0.16	58,58,58,58	0
56	MG	1A	3566	1/1	0.86	0.31	72,72,72,72	0
56	MG	2A	3077	1/1	0.86	0.15	45,45,45,45	0
56	MG	2A	3326	1/1	0.86	0.10	64,64,64,64	0
56	MG	1A	3459	1/1	0.86	0.23	47,47,47,47	0
56	MG	1A	3679	1/1	0.86	0.25	39,39,39,39	0
56	MG	1B	3016	1/1	0.86	0.16	54,54,54,54	0
56	MG	1A	3761	1/1	0.86	0.09	51,51,51,51	0
56	MG	2j	8001	1/1	0.86	0.09	75,75,75,75	0
56	MG	1A	3129	1/1	0.86	0.23	51,51,51,51	0
56	MG	1A	3888	1/1	0.86	0.24	70,70,70,70	0
56	MG	2a	3060	1/1	0.86	0.11	63,63,63,63	0
56	MG	2w	101	1/1	0.86	0.20	73,73,73,73	0
56	MG	2w	104	1/1	0.86	0.14	69,69,69,69	0
56	MG	2A	3643	1/1	0.86	0.15	34,34,34,34	0
56	MG	2A	3644	1/1	0.86	0.21	64,64,64,64	0
56	MG	1a	1827	1/1	0.86	0.14	58,58,58,58	0
56	MG	1A	3343	1/1	0.86	0.34	59,59,59,59	0
56	MG	1A	3776	1/1	0.86	0.20	75,75,75,75	0
56	MG	1A	3530	1/1	0.86	0.21	63,63,63,63	0
56	MG	1A	3548	1/1	0.87	0.12	49,49,49,49	0
56	MG	1A	3768	1/1	0.87	0.17	61,61,61,61	0
56	MG	1A	3034	1/1	0.87	0.16	45,45,45,45	0
56	MG	1a	1745	1/1	0.87	0.16	55,55,55,55	0
56	MG	1x	110	1/1	0.87	0.14	52,52,52,52	0
56	MG	1x	114	1/1	0.87	0.10	82,82,82,82	0
56	MG	2A	3274	1/1	0.87	0.11	53,53,53,53	0
56	MG	1A	3166	1/1	0.87	0.22	38,38,38,38	0
56	MG	2A	3289	1/1	0.87	0.14	47,47,47,47	0
56	MG	1B	3026	1/1	0.87	0.21	42,42,42,42	0
56	MG	2A	3028	1/1	0.87	0.14	54,54,54,54	0
56	MG	1A	3357	1/1	0.87	0.22	56,56,56,56	0
56	MG	1a	1628	1/1	0.87	0.11	58,58,58,58	0
56	MG	1B	3031	1/1	0.87	0.12	67,67,67,67	0
56	MG	2A	3557	1/1	0.87	0.08	45,45,45,45	0
56	MG	1A	3151	1/1	0.87	0.23	47,47,47,47	0
56	MG	2A	3574	1/1	0.87	0.12	44,44,44,44	0
56	MG	1D	307	1/1	0.87	0.16	45,45,45,45	0
56	MG	2A	3579	1/1	0.87	0.18	60,60,60,60	0
56	MG	2A	3846	1/1	0.87	0.09	47,47,47,47	0
56	MG	2A	3849	1/1	0.87	0.18	44,44,44,44	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	2A	3596	1/1	0.87	0.11	47,47,47,47	0
56	MG	2A	3314	1/1	0.87	0.18	47,47,47,47	0
56	MG	1D	311	1/1	0.87	0.20	56,56,56,56	0
56	MG	1A	3783	1/1	0.87	0.22	34,34,34,34	0
56	MG	2A	3859	1/1	0.87	0.10	53,53,53,53	0
56	MG	2A	3860	1/1	0.87	0.12	59,59,59,59	0
56	MG	1A	3437	1/1	0.87	0.15	52,52,52,52	0
56	MG	2a	3106	1/1	0.87	0.16	62,62,62,62	0
56	MG	1a	1646	1/1	0.87	0.19	51,51,51,51	0
56	MG	2a	3116	1/1	0.87	0.08	67,67,67,67	0
56	MG	2A	3628	1/1	0.87	0.07	52,52,52,52	0
56	MG	2A	3629	1/1	0.87	0.13	43,43,43,43	0
56	MG	2A	3869	1/1	0.87	0.07	56,56,56,56	0
56	MG	1A	3386	1/1	0.87	0.21	54,54,54,54	0
56	MG	1A	3390	1/1	0.87	0.18	35,35,35,35	0
56	MG	2a	3128	1/1	0.87	0.12	87,87,87,87	0
56	MG	1A	4060	1/1	0.87	0.10	37,37,37,37	0
56	MG	2A	3646	1/1	0.87	0.15	55,55,55,55	0
56	MG	1A	3441	1/1	0.87	0.10	56,56,56,56	0
56	MG	2A	3883	1/1	0.87	0.34	56,56,56,56	0
56	MG	1A	3392	1/1	0.87	0.27	56,56,56,56	0
56	MG	2A	3085	1/1	0.87	0.12	44,44,44,44	0
56	MG	2A	3661	1/1	0.87	0.19	56,56,56,56	0
56	MG	1N	201	1/1	0.87	0.62	59,59,59,59	0
56	MG	1a	1794	1/1	0.87	0.14	52,52,52,52	0
56	MG	2A	3906	1/1	0.87	0.66	62,62,62,62	0
56	MG	1A	4066	1/1	0.87	0.11	71,71,71,71	0
56	MG	1A	3108	1/1	0.87	0.45	43,43,43,43	0
56	MG	1O	206	1/1	0.87	0.24	84,84,84,84	0
56	MG	2B	3009	1/1	0.87	0.16	61,61,61,61	0
56	MG	2A	3367	1/1	0.87	0.18	61,61,61,61	0
56	MG	1A	3447	1/1	0.87	0.15	46,46,46,46	0
56	MG	1a	1817	1/1	0.87	0.04	79,79,79,79	0
56	MG	2A	3707	1/1	0.87	0.06	61,61,61,61	0
56	MG	2a	3173	1/1	0.87	0.12	62,62,62,62	0
56	MG	2D	304	1/1	0.87	0.36	45,45,45,45	0
56	MG	1A	3451	1/1	0.87	0.16	47,47,47,47	0
56	MG	2A	3387	1/1	0.87	0.20	59,59,59,59	0
56	MG	2A	3715	1/1	0.87	0.13	46,46,46,46	0
56	MG	1a	1821	1/1	0.87	0.09	62,62,62,62	0
56	MG	1A	3946	1/1	0.87	0.13	49,49,49,49	0
56	MG	2A	3722	1/1	0.87	0.10	58,58,58,58	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	2A	3121	1/1	0.87	0.18	42,42,42,42	0
56	MG	2A	3731	1/1	0.87	0.14	57,57,57,57	0
56	MG	2A	3126	1/1	0.87	0.18	58,58,58,58	0
56	MG	1A	3154	1/1	0.87	0.54	51,51,51,51	0
56	MG	2A	3433	1/1	0.87	0.13	64,64,64,64	0
56	MG	2a	3002	1/1	0.87	0.10	50,50,50,50	0
56	MG	1A	3407	1/1	0.87	0.36	65,65,65,65	0
56	MG	1A	3645	1/1	0.87	0.21	37,37,37,37	0
56	MG	2A	3168	1/1	0.87	0.20	52,52,52,52	0
56	MG	2A	3458	1/1	0.87	0.11	65,65,65,65	0
56	MG	2a	3232	1/1	0.87	0.23	77,77,77,77	0
56	MG	1A	3372	1/1	0.87	0.24	58,58,58,58	0
56	MG	1A	3746	1/1	0.87	0.20	55,55,55,55	0
56	MG	1A	3546	1/1	0.87	0.19	45,45,45,45	0
56	MG	10	106	1/1	0.87	0.16	65,65,65,65	0
56	MG	2a	3016	1/1	0.87	0.14	66,66,66,66	0
56	MG	1A	4105	1/1	0.87	0.13	44,44,44,44	0
56	MG	2A	3475	1/1	0.87	0.16	44,44,44,44	0
56	MG	2A	3781	1/1	0.87	0.10	55,55,55,55	0
56	MG	1A	4027	1/1	0.87	0.09	50,50,50,50	0
56	MG	2A	3212	1/1	0.87	0.13	52,52,52,52	0
56	MG	2a	3027	1/1	0.87	0.17	61,61,61,61	0
56	MG	2A	3793	1/1	0.87	0.17	56,56,56,56	0
56	MG	1A	3751	1/1	0.87	0.27	48,48,48,48	0
56	MG	2A	3796	1/1	0.87	0.10	49,49,49,49	0
56	MG	2A	3224	1/1	0.87	0.22	52,52,52,52	0
56	MG	2A	3500	1/1	0.87	0.10	55,55,55,55	0
56	MG	1A	3666	1/1	0.87	0.16	34,34,34,34	0
56	MG	13	101	1/1	0.88	0.22	55,55,55,55	0
56	MG	2A	3733	1/1	0.88	0.13	50,50,50,50	0
56	MG	15	103	1/1	0.88	0.10	61,61,61,61	0
56	MG	2A	3073	1/1	0.88	0.11	36,36,36,36	0
56	MG	1A	3425	1/1	0.88	0.17	55,55,55,55	0
56	MG	1A	3428	1/1	0.88	0.16	51,51,51,51	0
56	MG	2A	3079	1/1	0.88	0.11	41,41,41,41	0
56	MG	19	101	1/1	0.88	0.26	49,49,49,49	0
56	MG	1A	3024	1/1	0.88	0.17	43,43,43,43	0
56	MG	2A	3381	1/1	0.88	0.13	53,53,53,53	0
56	MG	1A	3754	1/1	0.88	0.20	48,48,48,48	0
56	MG	2A	3756	1/1	0.88	0.18	42,42,42,42	0
56	MG	1A	3758	1/1	0.88	0.10	71,71,71,71	0
56	MG	1A	3545	1/1	0.88	0.16	67,67,67,67	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
56	MG	1B	3010	1/1	0.88	0.81	73,73,73,73	0
56	MG	2A	3410	1/1	0.88	0.16	55,55,55,55	0
56	MG	2A	3093	1/1	0.88	0.25	54,54,54,54	0
56	MG	2A	3789	1/1	0.88	0.10	49,49,49,49	0
56	MG	2A	3419	1/1	0.88	0.14	51,51,51,51	0
56	MG	2A	3422	1/1	0.88	0.15	58,58,58,58	0
56	MG	2A	3426	1/1	0.88	0.23	63,63,63,63	0
56	MG	1A	3654	1/1	0.88	0.24	36,36,36,36	0
56	MG	2a	3057	1/1	0.88	0.14	71,71,71,71	0
56	MG	1A	3918	1/1	0.88	0.13	56,56,56,56	0
56	MG	1A	3335	1/1	0.88	0.37	62,62,62,62	0
56	MG	1A	3929	1/1	0.88	0.15	42,42,42,42	0
56	MG	1A	3478	1/1	0.88	0.23	65,65,65,65	0
56	MG	2A	3111	1/1	0.88	0.16	54,54,54,54	0
56	MG	1A	3552	1/1	0.88	0.21	60,60,60,60	0
56	MG	2A	3465	1/1	0.88	0.22	55,55,55,55	0
56	MG	1A	3189	1/1	0.88	0.41	43,43,43,43	0
56	MG	2A	3814	1/1	0.88	0.29	55,55,55,55	0
56	MG	2A	3468	1/1	0.88	0.30	59,59,59,59	0
56	MG	2A	3117	1/1	0.88	0.28	63,63,63,63	0
56	MG	1A	3488	1/1	0.88	0.29	59,59,59,59	0
56	MG	1D	305	1/1	0.88	0.18	42,42,42,42	0
56	MG	1A	3693	1/1	0.88	0.18	40,40,40,40	0
56	MG	1A	3489	1/1	0.88	0.18	44,44,44,44	0
56	MG	2A	3827	1/1	0.88	0.12	58,58,58,58	0
56	MG	2A	3484	1/1	0.88	0.21	53,53,53,53	0
56	MG	1a	1812	1/1	0.88	0.07	70,70,70,70	0
56	MG	1A	3491	1/1	0.88	0.15	59,59,59,59	0
56	MG	1A	3792	1/1	0.88	0.14	35,35,35,35	0
56	MG	1E	306	1/1	0.88	0.15	31,31,31,31	0
56	MG	1A	3396	1/1	0.88	0.14	47,47,47,47	0
56	MG	1A	3704	1/1	0.88	0.24	49,49,49,49	0
56	MG	2a	3110	1/1	0.88	0.08	73,73,73,73	0
56	MG	1a	1669	1/1	0.88	0.23	73,73,73,73	0
56	MG	1a	1828	1/1	0.88	0.08	59,59,59,59	0
56	MG	1A	3123	1/1	0.88	0.24	54,54,54,54	0
56	MG	1A	3800	1/1	0.88	0.15	65,65,65,65	0
56	MG	1G	3003	1/1	0.88	0.11	66,66,66,66	0
56	MG	2A	3225	1/1	0.88	0.13	62,62,62,62	0
56	MG	2A	3227	1/1	0.88	0.18	57,57,57,57	0
56	MG	2A	3536	1/1	0.88	0.14	51,51,51,51	0
56	MG	1A	3709	1/1	0.88	0.31	52,52,52,52	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	2A	3234	1/1	0.88	0.14	52,52,52,52	0
56	MG	2A	3239	1/1	0.88	0.40	52,52,52,52	0
56	MG	2A	3243	1/1	0.88	0.10	52,52,52,52	0
56	MG	2A	3244	1/1	0.88	0.09	54,54,54,54	0
56	MG	1A	3206	1/1	0.88	0.14	55,55,55,55	0
56	MG	1n	102	1/1	0.88	0.24	66,66,66,66	0
56	MG	2A	3249	1/1	0.88	0.13	57,57,57,57	0
56	MG	2A	3255	1/1	0.88	0.15	59,59,59,59	0
56	MG	2A	3874	1/1	0.88	0.17	53,53,53,53	0
56	MG	2A	3875	1/1	0.88	0.51	76,76,76,76	0
56	MG	2a	3151	1/1	0.88	0.09	78,78,78,78	0
56	MG	1A	3590	1/1	0.88	0.21	37,37,37,37	0
56	MG	2A	3261	1/1	0.88	0.20	59,59,59,59	0
56	MG	2A	3591	1/1	0.88	0.06	50,50,50,50	0
56	MG	1w	101	1/1	0.88	0.14	64,64,64,64	0
56	MG	1a	1680	1/1	0.88	0.09	64,64,64,64	0
56	MG	2A	3885	1/1	0.88	0.33	54,54,54,54	0
56	MG	2A	3888	1/1	0.88	0.20	57,57,57,57	0
56	MG	2a	3174	1/1	0.88	0.35	69,69,69,69	0
56	MG	2a	3176	1/1	0.88	0.11	62,62,62,62	0
56	MG	1a	1686	1/1	0.88	0.09	54,54,54,54	0
56	MG	1A	3974	1/1	0.88	0.06	45,45,45,45	0
56	MG	1A	3591	1/1	0.88	0.13	52,52,52,52	0
56	MG	2A	3617	1/1	0.88	0.12	38,38,38,38	0
56	MG	2A	3286	1/1	0.88	0.20	55,55,55,55	0
56	MG	2B	3002	1/1	0.88	0.11	49,49,49,49	0
56	MG	1a	1694	1/1	0.88	0.11	58,58,58,58	0
56	MG	1a	1696	1/1	0.88	0.14	71,71,71,71	0
56	MG	1A	3408	1/1	0.88	0.19	60,60,60,60	0
56	MG	1Q	204	1/1	0.88	0.15	51,51,51,51	0
56	MG	2A	3301	1/1	0.88	0.11	60,60,60,60	0
56	MG	1A	3328	1/1	0.88	0.17	64,64,64,64	0
56	MG	1T	8001	1/1	0.88	0.10	63,63,63,63	0
56	MG	1y	3001	1/1	0.88	0.09	64,64,64,64	0
56	MG	2a	3224	1/1	0.88	0.20	74,74,74,74	0
56	MG	2a	3225	1/1	0.88	0.10	57,57,57,57	0
56	MG	1U	201	1/1	0.88	0.18	52,52,52,52	0
56	MG	2A	3313	1/1	0.88	0.22	64,64,64,64	0
56	MG	1A	3350	1/1	0.88	0.25	59,59,59,59	0
56	MG	2A	3317	1/1	0.88	0.13	55,55,55,55	0
56	MG	2A	3011	1/1	0.88	0.07	48,48,48,48	0
56	MG	2F	301	1/1	0.88	0.18	58,58,58,58	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	2A	3322	1/1	0.88	0.11	60,60,60,60	0
56	MG	1A	3527	1/1	0.88	0.30	40,40,40,40	0
56	MG	1A	3330	1/1	0.88	0.28	50,50,50,50	0
56	MG	1a	1721	1/1	0.88	0.11	58,58,58,58	0
56	MG	1A	3630	1/1	0.88	0.17	32,32,32,32	0
56	MG	1A	3745	1/1	0.88	0.23	19,19,19,19	0
56	MG	2r	102	1/1	0.88	0.10	73,73,73,73	0
56	MG	1A	4079	1/1	0.88	0.25	46,46,46,46	0
56	MG	1A	3878	1/1	0.88	0.23	33,33,33,33	0
56	MG	2w	102	1/1	0.88	0.16	62,62,62,62	0
56	MG	2A	3344	1/1	0.88	0.19	55,55,55,55	0
56	MG	1A	3227	1/1	0.88	0.29	42,42,42,42	0
56	MG	12	101	1/1	0.88	0.21	60,60,60,60	0
56	MG	2a	3007	1/1	0.88	0.11	71,71,71,71	0
56	MG	2A	3057	1/1	0.88	0.07	46,46,46,46	0
56	MG	2A	3723	1/1	0.88	0.10	50,50,50,50	0
56	MG	2y	3006	1/1	0.88	0.07	86,86,86,86	0
56	MG	2A	3356	1/1	0.88	0.30	55,55,55,55	0
56	MG	1A	3505	1/1	0.89	0.14	47,47,47,47	0
56	MG	2A	3205	1/1	0.89	0.22	52,52,52,52	0
56	MG	2A	3430	1/1	0.89	0.10	51,51,51,51	0
56	MG	2A	3759	1/1	0.89	0.12	46,46,46,46	0
56	MG	1A	3209	1/1	0.89	0.26	68,68,68,68	0
56	MG	1A	3569	1/1	0.89	0.25	54,54,54,54	0
56	MG	1X	105	1/1	0.89	0.13	47,47,47,47	0
56	MG	2A	3777	1/1	0.89	0.15	41,41,41,41	0
56	MG	2A	3438	1/1	0.89	0.19	68,68,68,68	0
56	MG	2A	3450	1/1	0.89	0.20	50,50,50,50	0
56	MG	2a	3033	1/1	0.89	0.14	63,63,63,63	0
56	MG	2A	3216	1/1	0.89	0.13	56,56,56,56	0
56	MG	1A	3764	1/1	0.89	0.18	31,31,31,31	0
56	MG	1A	3327	1/1	0.89	0.16	28,28,28,28	0
56	MG	2a	3038	1/1	0.89	0.13	68,68,68,68	0
56	MG	1A	3230	1/1	0.89	0.18	60,60,60,60	0
56	MG	1A	3997	1/1	0.89	0.14	39,39,39,39	0
56	MG	2A	3229	1/1	0.89	0.10	41,41,41,41	0
56	MG	1A	3694	1/1	0.89	0.17	61,61,61,61	0
56	MG	2A	3803	1/1	0.89	0.10	42,42,42,42	0
56	MG	2a	3050	1/1	0.89	0.20	61,61,61,61	0
56	MG	1A	3906	1/1	0.89	0.12	51,51,51,51	0
56	MG	1a	1714	1/1	0.89	0.14	66,66,66,66	0
56	MG	2A	3241	1/1	0.89	0.37	56,56,56,56	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	1A	3911	1/1	0.89	0.10	65,65,65,65	0
56	MG	2A	3479	1/1	0.89	0.17	54,54,54,54	0
56	MG	1A	3362	1/1	0.89	0.24	54,54,54,54	0
56	MG	1A	3231	1/1	0.89	0.23	51,51,51,51	0
56	MG	1A	3252	1/1	0.89	0.23	52,52,52,52	0
56	MG	2A	3819	1/1	0.89	0.13	64,64,64,64	0
56	MG	1A	3703	1/1	0.89	0.11	56,56,56,56	0
56	MG	2a	3071	1/1	0.89	0.08	75,75,75,75	0
56	MG	2A	3253	1/1	0.89	0.12	47,47,47,47	0
56	MG	2A	3498	1/1	0.89	0.11	55,55,55,55	0
56	MG	2A	3010	1/1	0.89	0.19	51,51,51,51	0
56	MG	1A	4018	1/1	0.89	0.15	67,67,67,67	0
56	MG	2A	3260	1/1	0.89	0.17	53,53,53,53	0
56	MG	2A	3507	1/1	0.89	0.14	64,64,64,64	0
56	MG	1a	1603	1/1	0.89	0.18	59,59,59,59	0
56	MG	2A	3512	1/1	0.89	0.12	53,53,53,53	0
56	MG	1A	3922	1/1	0.89	0.10	57,57,57,57	0
56	MG	1A	3461	1/1	0.89	0.31	44,44,44,44	0
56	MG	2A	3269	1/1	0.89	0.17	53,53,53,53	0
56	MG	1A	3609	1/1	0.89	0.14	50,50,50,50	0
56	MG	2A	3272	1/1	0.89	0.18	51,51,51,51	0
56	MG	2A	3040	1/1	0.89	0.18	52,52,52,52	0
56	MG	1A	3284	1/1	0.89	0.39	56,56,56,56	0
56	MG	2A	3282	1/1	0.89	0.24	63,63,63,63	0
56	MG	2A	3284	1/1	0.89	0.16	59,59,59,59	0
56	MG	1A	3080	1/1	0.89	0.26	42,42,42,42	0
56	MG	2a	3117	1/1	0.89	0.85	81,81,81,81	0
56	MG	1A	3937	1/1	0.89	0.24	31,31,31,31	0
56	MG	1a	1762	1/1	0.89	0.13	78,78,78,78	0
56	MG	1a	1627	1/1	0.89	0.14	55,55,55,55	0
56	MG	1A	3539	1/1	0.89	0.16	49,49,49,49	0
56	MG	2A	3562	1/1	0.89	0.11	37,37,37,37	0
56	MG	1A	3337	1/1	0.89	0.30	48,48,48,48	0
56	MG	2a	3129	1/1	0.89	0.10	59,59,59,59	0
56	MG	2a	3130	1/1	0.89	0.08	72,72,72,72	0
56	MG	2A	3573	1/1	0.89	0.11	42,42,42,42	0
56	MG	2A	3303	1/1	0.89	0.16	60,60,60,60	0
56	MG	2A	3304	1/1	0.89	0.17	60,60,60,60	0
56	MG	1a	1630	1/1	0.89	0.13	60,60,60,60	0
56	MG	2A	3590	1/1	0.89	0.08	64,64,64,64	0
56	MG	2a	3141	1/1	0.89	0.18	94,94,94,94	0
56	MG	1a	1631	1/1	0.89	0.24	54,54,54,54	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	1A	3307	1/1	0.89	0.32	45,45,45,45	0
56	MG	1A	3808	1/1	0.89	0.16	36,36,36,36	0
56	MG	2A	3878	1/1	0.89	0.10	49,49,49,49	0
56	MG	1a	1639	1/1	0.89	0.10	62,62,62,62	0
56	MG	1A	3637	1/1	0.89	0.19	50,50,50,50	0
56	MG	2A	3881	1/1	0.89	0.14	48,48,48,48	0
56	MG	2A	3315	1/1	0.89	0.22	54,54,54,54	0
56	MG	2a	3152	1/1	0.89	0.17	67,67,67,67	0
56	MG	1A	3639	1/1	0.89	0.23	41,41,41,41	0
56	MG	1A	3542	1/1	0.89	0.21	75,75,75,75	0
56	MG	2a	3156	1/1	0.89	0.13	69,69,69,69	0
56	MG	1A	3951	1/1	0.89	0.20	72,72,72,72	0
56	MG	1a	1648	1/1	0.89	0.16	59,59,59,59	0
56	MG	1G	3002	1/1	0.89	0.17	56,56,56,56	0
56	MG	1A	3429	1/1	0.89	0.15	48,48,48,48	0
56	MG	1a	1804	1/1	0.89	0.17	77,77,77,77	0
56	MG	2A	3896	1/1	0.89	0.18	39,39,39,39	0
56	MG	1A	3833	1/1	0.89	0.09	60,60,60,60	0
56	MG	1I	3001	1/1	0.89	0.11	70,70,70,70	0
56	MG	1A	3312	1/1	0.89	0.18	59,59,59,59	0
56	MG	2B	3004	1/1	0.89	0.13	69,69,69,69	0
56	MG	2A	3343	1/1	0.89	0.11	57,57,57,57	0
56	MG	1A	3968	1/1	0.89	0.09	62,62,62,62	0
56	MG	1O	202	1/1	0.89	0.49	67,67,67,67	0
56	MG	2B	3013	1/1	0.89	0.20	61,61,61,61	0
56	MG	2A	3670	1/1	0.89	0.12	70,70,70,70	0
56	MG	2A	3346	1/1	0.89	0.20	54,54,54,54	0
56	MG	1A	3131	1/1	0.89	0.17	72,72,72,72	0
56	MG	2a	3207	1/1	0.89	0.14	74,74,74,74	0
56	MG	1A	3324	1/1	0.89	0.25	55,55,55,55	0
56	MG	1a	1824	1/1	0.89	0.12	73,73,73,73	0
56	MG	2A	3118	1/1	0.89	0.13	50,50,50,50	0
56	MG	2E	304	1/1	0.89	0.12	46,46,46,46	0
56	MG	1a	1826	1/1	0.89	0.06	58,58,58,58	0
56	MG	1A	3325	1/1	0.89	0.21	64,64,64,64	0
56	MG	2A	3703	1/1	0.89	0.13	47,47,47,47	0
56	MG	1A	3858	1/1	0.89	0.13	30,30,30,30	0
56	MG	2F	302	1/1	0.89	0.15	53,53,53,53	0
56	MG	2A	3365	1/1	0.89	0.11	56,56,56,56	0
56	MG	1A	3660	1/1	0.89	0.25	31,31,31,31	0
56	MG	2A	3149	1/1	0.89	0.22	54,54,54,54	0
56	MG	2U	202	1/1	0.89	0.13	54,54,54,54	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
56	MG	1b	3001	1/1	0.89	0.15	83,83,83,83	0
56	MG	2A	3153	1/1	0.89	0.20	52,52,52,52	0
56	MG	1A	3867	1/1	0.89	0.14	69,69,69,69	0
56	MG	2Z	8001	1/1	0.89	0.07	78,78,78,78	0
56	MG	28	101	1/1	0.89	0.12	53,53,53,53	0
56	MG	1a	1681	1/1	0.89	0.25	54,54,54,54	0
56	MG	2A	3394	1/1	0.89	0.31	50,50,50,50	0
56	MG	1A	3352	1/1	0.89	0.22	64,64,64,64	0
56	MG	2A	3182	1/1	0.89	0.13	42,42,42,42	0
56	MG	2A	3189	1/1	0.89	0.11	52,52,52,52	0
56	MG	2a	3006	1/1	0.89	0.17	74,74,74,74	0
56	MG	2A	3407	1/1	0.89	0.12	61,61,61,61	0
56	MG	2A	3190	1/1	0.89	0.19	45,45,45,45	0
56	MG	2A	3194	1/1	0.89	0.24	67,67,67,67	0
56	MG	2A	3414	1/1	0.89	0.20	59,59,59,59	0
56	MG	2A	3417	1/1	0.89	0.10	41,41,41,41	0
56	MG	1A	3874	1/1	0.89	0.12	40,40,40,40	0
56	MG	1A	3110	1/1	0.90	0.12	42,42,42,42	0
56	MG	1a	1650	1/1	0.90	0.12	53,53,53,53	0
56	MG	1A	3944	1/1	0.90	0.15	60,60,60,60	0
56	MG	1A	4116	1/1	0.90	0.22	41,41,41,41	0
56	MG	1A	4135	1/1	0.90	0.23	44,44,44,44	0
56	MG	1A	3134	1/1	0.90	0.32	54,54,54,54	0
56	MG	25	105	1/1	0.90	0.09	58,58,58,58	0
56	MG	1A	3600	1/1	0.90	0.13	46,46,46,46	0
56	MG	2A	3006	1/1	0.90	0.23	56,56,56,56	0
56	MG	1a	1664	1/1	0.90	0.25	62,62,62,62	0
56	MG	1A	3397	1/1	0.90	0.23	47,47,47,47	0
56	MG	1A	3766	1/1	0.90	0.08	47,47,47,47	0
56	MG	2A	3678	1/1	0.90	0.09	49,49,49,49	0
56	MG	2A	3018	1/1	0.90	0.24	44,44,44,44	0
56	MG	1B	3014	1/1	0.90	0.13	63,63,63,63	0
56	MG	2A	3687	1/1	0.90	0.37	63,63,63,63	0
56	MG	2A	3323	1/1	0.90	0.13	56,56,56,56	0
56	MG	1A	3399	1/1	0.90	0.22	52,52,52,52	0
56	MG	1A	3210	1/1	0.90	0.16	42,42,42,42	0
56	MG	2A	3034	1/1	0.90	0.15	45,45,45,45	0
56	MG	1A	3258	1/1	0.90	0.17	33,33,33,33	0
56	MG	2A	3337	1/1	0.90	0.09	47,47,47,47	0
56	MG	1A	3259	1/1	0.90	0.16	40,40,40,40	0
56	MG	1A	3778	1/1	0.90	0.08	57,57,57,57	0
56	MG	1A	3963	1/1	0.90	0.23	60,60,60,60	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	1a	1684	1/1	0.90	0.14	60,60,60,60	0
56	MG	1A	3342	1/1	0.90	0.25	57,57,57,57	0
56	MG	1A	3497	1/1	0.90	0.20	33,33,33,33	0
56	MG	2A	3718	1/1	0.90	0.36	64,64,64,64	0
56	MG	1A	3499	1/1	0.90	0.11	49,49,49,49	0
56	MG	1a	1691	1/1	0.90	0.21	69,69,69,69	0
56	MG	2A	3063	1/1	0.90	0.12	67,67,67,67	0
56	MG	1A	3501	1/1	0.90	0.25	51,51,51,51	0
56	MG	1A	3973	1/1	0.90	0.10	85,85,85,85	0
56	MG	1A	3090	1/1	0.90	0.16	54,54,54,54	0
56	MG	1A	3419	1/1	0.90	0.15	60,60,60,60	0
56	MG	1A	3420	1/1	0.90	0.26	55,55,55,55	0
56	MG	1A	3075	1/1	0.90	0.11	28,28,28,28	0
56	MG	1A	3124	1/1	0.90	0.22	44,44,44,44	0
56	MG	2A	3370	1/1	0.90	0.23	50,50,50,50	0
56	MG	2a	3049	1/1	0.90	0.12	55,55,55,55	0
56	MG	1A	3519	1/1	0.90	0.16	49,49,49,49	0
56	MG	1A	3987	1/1	0.90	0.17	32,32,32,32	0
56	MG	2a	3053	1/1	0.90	0.09	66,66,66,66	0
56	MG	2A	3752	1/1	0.90	0.14	61,61,61,61	0
56	MG	1a	1713	1/1	0.90	0.08	68,68,68,68	0
56	MG	1A	3802	1/1	0.90	0.13	57,57,57,57	0
56	MG	2A	3757	1/1	0.90	0.11	52,52,52,52	0
56	MG	2A	3384	1/1	0.90	0.17	62,62,62,62	0
56	MG	1A	3185	1/1	0.90	0.24	47,47,47,47	0
56	MG	2a	3064	1/1	0.90	0.10	81,81,81,81	0
56	MG	2A	3391	1/1	0.90	0.18	58,58,58,58	0
56	MG	1A	3823	1/1	0.90	0.18	65,65,65,65	0
56	MG	2A	3399	1/1	0.90	0.15	60,60,60,60	0
56	MG	2A	3099	1/1	0.90	0.13	42,42,42,42	0
56	MG	1A	3525	1/1	0.90	0.17	58,58,58,58	0
56	MG	2A	3783	1/1	0.90	0.25	58,58,58,58	0
56	MG	2a	3077	1/1	0.90	0.21	61,61,61,61	0
56	MG	2A	3784	1/1	0.90	0.10	47,47,47,47	0
56	MG	2A	3787	1/1	0.90	0.04	64,64,64,64	0
56	MG	1A	3825	1/1	0.90	0.12	57,57,57,57	0
56	MG	1A	3070	1/1	0.90	0.15	41,41,41,41	0
56	MG	2A	3408	1/1	0.90	0.10	51,51,51,51	0
56	MG	1A	3299	1/1	0.90	0.20	61,61,61,61	0
56	MG	1A	3674	1/1	0.90	0.16	39,39,39,39	0
56	MG	1A	3234	1/1	0.90	0.42	54,54,54,54	0
56	MG	1Q	203	1/1	0.90	0.19	64,64,64,64	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	1A	3691	1/1	0.90	0.21	41,41,41,41	0
56	MG	1a	1752	1/1	0.90	0.13	68,68,68,68	0
56	MG	2A	3423	1/1	0.90	0.18	58,58,58,58	0
56	MG	2A	3424	1/1	0.90	0.19	50,50,50,50	0
56	MG	2A	3119	1/1	0.90	0.19	47,47,47,47	0
56	MG	1R	203	1/1	0.90	0.31	47,47,47,47	0
56	MG	1A	3839	1/1	0.90	0.08	66,66,66,66	0
56	MG	1A	3436	1/1	0.90	0.14	45,45,45,45	0
56	MG	2A	3815	1/1	0.90	0.14	48,48,48,48	0
56	MG	1A	3190	1/1	0.90	0.21	39,39,39,39	0
56	MG	1A	3308	1/1	0.90	0.26	51,51,51,51	0
56	MG	2A	3439	1/1	0.90	0.21	60,60,60,60	0
56	MG	2a	3126	1/1	0.90	0.09	69,69,69,69	0
56	MG	2A	3441	1/1	0.90	0.15	51,51,51,51	0
56	MG	2A	3445	1/1	0.90	0.24	55,55,55,55	0
56	MG	1A	3192	1/1	0.90	0.19	52,52,52,52	0
56	MG	1A	3859	1/1	0.90	0.19	44,44,44,44	0
56	MG	2A	3167	1/1	0.90	0.27	52,52,52,52	0
56	MG	1a	1777	1/1	0.90	0.16	55,55,55,55	0
56	MG	2A	3462	1/1	0.90	0.27	59,59,59,59	0
56	MG	1A	3862	1/1	0.90	0.22	43,43,43,43	0
56	MG	2A	3171	1/1	0.90	0.12	38,38,38,38	0
56	MG	1a	1780	1/1	0.90	0.11	74,74,74,74	0
56	MG	1A	3313	1/1	0.90	0.25	49,49,49,49	0
56	MG	1A	3544	1/1	0.90	0.17	47,47,47,47	0
56	MG	1A	3315	1/1	0.90	0.35	61,61,61,61	0
56	MG	1A	3871	1/1	0.90	0.26	49,49,49,49	0
56	MG	10	105	1/1	0.90	0.17	70,70,70,70	0
56	MG	2A	3478	1/1	0.90	0.15	50,50,50,50	0
56	MG	2A	3196	1/1	0.90	0.14	56,56,56,56	0
56	MG	2A	3480	1/1	0.90	0.21	65,65,65,65	0
56	MG	1A	3318	1/1	0.90	0.12	46,46,46,46	0
56	MG	1A	3245	1/1	0.90	0.27	64,64,64,64	0
56	MG	1A	3448	1/1	0.90	0.16	59,59,59,59	0
56	MG	13	102	1/1	0.90	0.23	53,53,53,53	0
56	MG	2a	3158	1/1	0.90	0.12	52,52,52,52	0
56	MG	2A	3492	1/1	0.90	0.17	54,54,54,54	0
56	MG	1A	4042	1/1	0.90	0.10	46,46,46,46	0
56	MG	16	101	1/1	0.90	0.25	45,45,45,45	0
56	MG	1A	3450	1/1	0.90	0.19	57,57,57,57	0
56	MG	1a	1806	1/1	0.90	0.13	66,66,66,66	0
56	MG	1a	1807	1/1	0.90	0.06	67,67,67,67	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	2A	3505	1/1	0.90	0.11	59,59,59,59	0
56	MG	1a	1809	1/1	0.90	0.08	56,56,56,56	0
56	MG	1A	3557	1/1	0.90	0.32	60,60,60,60	0
56	MG	1A	3890	1/1	0.90	0.16	57,57,57,57	0
56	MG	1A	3721	1/1	0.90	0.19	57,57,57,57	0
56	MG	2A	3238	1/1	0.90	0.39	56,56,56,56	0
56	MG	1A	3323	1/1	0.90	0.17	50,50,50,50	0
56	MG	1a	1818	1/1	0.90	0.08	54,54,54,54	0
56	MG	2A	3529	1/1	0.90	0.07	43,43,43,43	0
56	MG	1A	3564	1/1	0.90	0.19	40,40,40,40	0
56	MG	2a	3202	1/1	0.90	0.17	64,64,64,64	0
56	MG	1A	3901	1/1	0.90	0.20	43,43,43,43	0
56	MG	1a	1607	1/1	0.90	0.20	67,67,67,67	0
56	MG	1A	3724	1/1	0.90	0.21	58,58,58,58	0
56	MG	1A	3246	1/1	0.90	0.31	58,58,58,58	0
56	MG	1a	1615	1/1	0.90	0.11	67,67,67,67	0
56	MG	1A	3247	1/1	0.90	0.26	58,58,58,58	0
56	MG	2A	3895	1/1	0.90	0.15	46,46,46,46	0
56	MG	1A	3128	1/1	0.90	0.17	41,41,41,41	0
56	MG	2a	3227	1/1	0.90	0.12	59,59,59,59	0
56	MG	2A	3553	1/1	0.90	0.14	71,71,71,71	0
56	MG	2a	3229	1/1	0.90	0.15	69,69,69,69	0
56	MG	1A	3916	1/1	0.90	0.14	53,53,53,53	0
56	MG	1A	3572	1/1	0.90	0.12	55,55,55,55	0
56	MG	1d	502	1/1	0.90	0.22	67,67,67,67	0
56	MG	1A	3573	1/1	0.90	0.09	60,60,60,60	0
56	MG	2A	3571	1/1	0.90	0.08	35,35,35,35	0
56	MG	2A	3572	1/1	0.90	0.11	44,44,44,44	0
56	MG	2A	3268	1/1	0.90	0.18	63,63,63,63	0
56	MG	1A	3743	1/1	0.90	0.22	60,60,60,60	0
56	MG	1A	3744	1/1	0.90	0.28	74,74,74,74	0
56	MG	2j	8002	1/1	0.90	0.16	66,66,66,66	0
56	MG	2B	3017	1/1	0.90	0.11	65,65,65,65	0
56	MG	1A	3157	1/1	0.90	0.19	53,53,53,53	0
56	MG	1s	101	1/1	0.90	0.17	65,65,65,65	0
56	MG	2D	302	1/1	0.90	0.16	51,51,51,51	0
56	MG	1A	3931	1/1	0.90	0.17	55,55,55,55	0
56	MG	1A	3579	1/1	0.90	0.17	44,44,44,44	0
56	MG	2A	3605	1/1	0.90	0.15	51,51,51,51	0
56	MG	1A	4087	1/1	0.90	0.21	54,54,54,54	0
56	MG	1A	3465	1/1	0.90	0.18	60,60,60,60	0
56	MG	1A	4094	1/1	0.90	0.09	37,37,37,37	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	2y	3001	1/1	0.90	0.18	59,59,59,59	0
56	MG	2A	3290	1/1	0.90	0.19	50,50,50,50	0
56	MG	1w	110	1/1	0.90	0.11	66,66,66,66	0
56	MG	1A	3587	1/1	0.90	0.21	38,38,38,38	0
56	MG	1A	3089	1/1	0.90	0.26	48,48,48,48	0
56	MG	1A	3268	1/1	0.91	0.18	59,59,59,59	0
56	MG	2A	3065	1/1	0.91	0.20	57,57,57,57	0
56	MG	1A	3710	1/1	0.91	0.12	68,68,68,68	0
56	MG	1U	203	1/1	0.91	0.23	42,42,42,42	0
56	MG	2a	3001	1/1	0.91	0.22	57,57,57,57	0
56	MG	1a	1723	1/1	0.91	0.10	61,61,61,61	0
56	MG	1A	3939	1/1	0.91	0.14	53,53,53,53	0
56	MG	1a	1728	1/1	0.91	0.24	48,48,48,48	0
56	MG	1a	1735	1/1	0.91	0.18	57,57,57,57	0
56	MG	2A	3081	1/1	0.91	0.22	45,45,45,45	0
56	MG	1A	4053	1/1	0.91	0.37	37,37,37,37	0
56	MG	1A	3099	1/1	0.91	0.13	44,44,44,44	0
56	MG	1X	102	1/1	0.91	0.22	46,46,46,46	0
56	MG	1X	104	1/1	0.91	0.18	52,52,52,52	0
56	MG	2A	3089	1/1	0.91	0.12	46,46,46,46	0
56	MG	1A	4056	1/1	0.91	0.12	47,47,47,47	0
56	MG	2a	3015	1/1	0.91	0.11	62,62,62,62	0
56	MG	1A	3821	1/1	0.91	0.16	47,47,47,47	0
56	MG	1Z	301	1/1	0.91	0.27	56,56,56,56	0
56	MG	2A	3098	1/1	0.91	0.17	49,49,49,49	0
56	MG	1A	3274	1/1	0.91	0.17	36,36,36,36	0
56	MG	1A	3719	1/1	0.91	0.11	50,50,50,50	0
56	MG	2A	3730	1/1	0.91	0.18	43,43,43,43	0
56	MG	1A	3613	1/1	0.91	0.13	33,33,33,33	0
56	MG	2A	3732	1/1	0.91	0.13	42,42,42,42	0
56	MG	2A	3383	1/1	0.91	0.16	60,60,60,60	0
56	MG	2A	3104	1/1	0.91	0.11	53,53,53,53	0
56	MG	1a	1761	1/1	0.91	0.11	64,64,64,64	0
56	MG	1A	4065	1/1	0.91	0.18	51,51,51,51	0
56	MG	1A	3364	1/1	0.91	0.19	64,64,64,64	0
56	MG	1A	3365	1/1	0.91	0.31	53,53,53,53	0
56	MG	2a	3037	1/1	0.91	0.38	77,77,77,77	0
56	MG	1A	3279	1/1	0.91	0.17	38,38,38,38	0
56	MG	2a	3039	1/1	0.91	0.21	73,73,73,73	0
56	MG	1a	1776	1/1	0.91	0.12	91,91,91,91	0
56	MG	1A	3727	1/1	0.91	0.15	36,36,36,36	0
56	MG	1A	3953	1/1	0.91	0.10	46,46,46,46	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	2A	3753	1/1	0.91	0.13	45,45,45,45	0
56	MG	1A	3371	1/1	0.91	0.13	45,45,45,45	0
56	MG	1A	3835	1/1	0.91	0.18	59,59,59,59	0
56	MG	2A	3412	1/1	0.91	0.30	59,59,59,59	0
56	MG	2A	3129	1/1	0.91	0.14	50,50,50,50	0
56	MG	2A	3130	1/1	0.91	0.19	53,53,53,53	0
56	MG	2a	3054	1/1	0.91	0.14	65,65,65,65	0
56	MG	1A	3836	1/1	0.91	0.23	54,54,54,54	0
56	MG	2A	3138	1/1	0.91	0.15	59,59,59,59	0
56	MG	2A	3774	1/1	0.91	0.11	51,51,51,51	0
56	MG	1A	3143	1/1	0.91	0.17	55,55,55,55	0
56	MG	1A	3966	1/1	0.91	0.20	59,59,59,59	0
56	MG	1A	3846	1/1	0.91	0.12	53,53,53,53	0
56	MG	1a	1604	1/1	0.91	0.11	58,58,58,58	0
56	MG	2A	3155	1/1	0.91	0.12	59,59,59,59	0
56	MG	2a	3068	1/1	0.91	0.16	72,72,72,72	0
56	MG	1A	3104	1/1	0.91	0.27	40,40,40,40	0
56	MG	2A	3788	1/1	0.91	0.10	53,53,53,53	0
56	MG	1A	3431	1/1	0.91	0.13	52,52,52,52	0
56	MG	1A	3553	1/1	0.91	0.26	49,49,49,49	0
56	MG	2a	3075	1/1	0.91	0.15	49,49,49,49	0
56	MG	2A	3791	1/1	0.91	0.21	46,46,46,46	0
56	MG	1A	3857	1/1	0.91	0.36	48,48,48,48	0
56	MG	2a	3078	1/1	0.91	0.27	74,74,74,74	0
56	MG	1A	3229	1/1	0.91	0.23	33,33,33,33	0
56	MG	1A	3093	1/1	0.91	0.22	33,33,33,33	0
56	MG	2A	3186	1/1	0.91	0.14	54,54,54,54	0
56	MG	2a	3087	1/1	0.91	0.08	63,63,63,63	0
56	MG	2A	3187	1/1	0.91	0.17	50,50,50,50	0
56	MG	1A	3558	1/1	0.91	0.12	52,52,52,52	0
56	MG	1A	3383	1/1	0.91	0.15	55,55,55,55	0
56	MG	2A	3455	1/1	0.91	0.30	54,54,54,54	0
56	MG	2A	3809	1/1	0.91	0.08	59,59,59,59	0
56	MG	1a	1808	1/1	0.91	0.09	53,53,53,53	0
56	MG	2A	3459	1/1	0.91	0.13	62,62,62,62	0
56	MG	1B	3004	1/1	0.91	0.29	50,50,50,50	0
56	MG	1B	3006	1/1	0.91	0.15	45,45,45,45	0
56	MG	1A	3561	1/1	0.91	0.31	48,48,48,48	0
56	MG	1B	3009	1/1	0.91	0.16	43,43,43,43	0
56	MG	1A	3981	1/1	0.91	0.09	52,52,52,52	0
56	MG	2a	3112	1/1	0.91	0.10	54,54,54,54	0
56	MG	1A	3982	1/1	0.91	0.26	29,29,29,29	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	2A	3210	1/1	0.91	0.14	47,47,47,47	0
56	MG	2a	3118	1/1	0.91	0.12	65,65,65,65	0
56	MG	2A	3473	1/1	0.91	0.13	57,57,57,57	0
56	MG	1B	3012	1/1	0.91	0.18	55,55,55,55	0
56	MG	1A	3655	1/1	0.91	0.12	39,39,39,39	0
56	MG	1a	1641	1/1	0.91	0.18	58,58,58,58	0
56	MG	1A	3305	1/1	0.91	0.33	55,55,55,55	0
56	MG	1B	3020	1/1	0.91	0.22	82,82,82,82	0
56	MG	2A	3481	1/1	0.91	0.20	56,56,56,56	0
56	MG	1A	3661	1/1	0.91	0.13	32,32,32,32	0
56	MG	1A	3757	1/1	0.91	0.23	27,27,27,27	0
56	MG	2A	3230	1/1	0.91	0.13	48,48,48,48	0
56	MG	1a	1647	1/1	0.91	0.16	65,65,65,65	0
56	MG	2a	3136	1/1	0.91	0.28	73,73,73,73	0
56	MG	1A	3991	1/1	0.91	0.10	48,48,48,48	0
56	MG	1A	3149	1/1	0.91	0.15	33,33,33,33	0
56	MG	1A	3023	1/1	0.91	0.17	59,59,59,59	0
56	MG	1A	3995	1/1	0.91	0.21	73,73,73,73	0
56	MG	1B	3034	1/1	0.91	0.19	58,58,58,58	0
56	MG	2A	3502	1/1	0.91	0.09	43,43,43,43	0
56	MG	2A	3852	1/1	0.91	0.12	49,49,49,49	0
56	MG	1a	1660	1/1	0.91	0.12	74,74,74,74	0
56	MG	1A	3886	1/1	0.91	0.13	57,57,57,57	0
56	MG	1A	3762	1/1	0.91	0.12	60,60,60,60	0
56	MG	1A	3889	1/1	0.91	0.25	60,60,60,60	0
56	MG	2a	3150	1/1	0.91	0.05	78,78,78,78	0
56	MG	1a	1667	1/1	0.91	0.12	65,65,65,65	0
56	MG	2A	3861	1/1	0.91	0.13	36,36,36,36	0
56	MG	2A	3862	1/1	0.91	0.11	71,71,71,71	0
56	MG	1A	3235	1/1	0.91	0.25	66,66,66,66	0
56	MG	1A	3672	1/1	0.91	0.16	31,31,31,31	0
56	MG	1A	3571	1/1	0.91	0.21	57,57,57,57	0
56	MG	2a	3160	1/1	0.91	0.09	49,49,49,49	0
56	MG	1w	109	1/1	0.91	0.10	67,67,67,67	0
56	MG	1A	3512	1/1	0.91	0.17	50,50,50,50	0
56	MG	1A	3019	1/1	0.91	0.22	37,37,37,37	0
56	MG	2A	3267	1/1	0.91	0.11	58,58,58,58	0
56	MG	1A	3240	1/1	0.91	0.15	35,35,35,35	0
56	MG	2A	3539	1/1	0.91	0.16	62,62,62,62	0
56	MG	1A	3910	1/1	0.91	0.07	76,76,76,76	0
56	MG	1a	1678	1/1	0.91	0.18	63,63,63,63	0
56	MG	1x	105	1/1	0.91	0.11	62,62,62,62	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	1x	106	1/1	0.91	0.22	63,63,63,63	0
56	MG	1F	305	1/1	0.91	0.22	48,48,48,48	0
56	MG	1F	306	1/1	0.91	0.28	53,53,53,53	0
56	MG	2a	3188	1/1	0.91	0.12	68,68,68,68	0
56	MG	1A	4020	1/1	0.91	0.11	53,53,53,53	0
56	MG	1a	1685	1/1	0.91	0.14	51,51,51,51	0
56	MG	2A	3287	1/1	0.91	0.09	55,55,55,55	0
56	MG	1y	3002	1/1	0.91	0.16	75,75,75,75	0
56	MG	1A	3316	1/1	0.91	0.19	58,58,58,58	0
56	MG	2A	3001	1/1	0.91	0.19	47,47,47,47	0
56	MG	2A	3292	1/1	0.91	0.11	54,54,54,54	0
56	MG	2A	3005	1/1	0.91	0.22	48,48,48,48	0
56	MG	1a	1687	1/1	0.91	0.18	50,50,50,50	0
56	MG	2A	3299	1/1	0.91	0.12	51,51,51,51	0
56	MG	2a	3219	1/1	0.91	0.07	65,65,65,65	0
56	MG	2a	3220	1/1	0.91	0.12	66,66,66,66	0
56	MG	2A	3589	1/1	0.91	0.09	45,45,45,45	0
56	MG	1A	3580	1/1	0.91	0.27	39,39,39,39	0
56	MG	1A	3116	1/1	0.91	0.22	47,47,47,47	0
56	MG	2A	3594	1/1	0.91	0.09	38,38,38,38	0
56	MG	1A	3915	1/1	0.91	0.14	39,39,39,39	0
56	MG	2A	3603	1/1	0.91	0.14	50,50,50,50	0
56	MG	2A	3016	1/1	0.91	0.14	61,61,61,61	0
56	MG	1a	1692	1/1	0.91	0.09	69,69,69,69	0
56	MG	1A	3784	1/1	0.91	0.10	39,39,39,39	0
56	MG	1A	3697	1/1	0.91	0.14	51,51,51,51	0
56	MG	2A	3613	1/1	0.91	0.16	33,33,33,33	0
56	MG	2B	3020	1/1	0.91	0.20	78,78,78,78	0
56	MG	1A	3586	1/1	0.91	0.22	49,49,49,49	0
56	MG	2d	502	1/1	0.91	0.09	68,68,68,68	0
56	MG	1a	1698	1/1	0.91	0.07	52,52,52,52	0
56	MG	1A	3921	1/1	0.91	0.17	50,50,50,50	0
56	MG	2A	3316	1/1	0.91	0.17	54,54,54,54	0
56	MG	1A	4036	1/1	0.91	0.08	43,43,43,43	0
56	MG	2A	3641	1/1	0.91	0.25	57,57,57,57	0
56	MG	2A	3047	1/1	0.91	0.16	46,46,46,46	0
56	MG	1A	3320	1/1	0.91	0.23	60,60,60,60	0
56	MG	1a	1707	1/1	0.91	0.14	63,63,63,63	0
56	MG	2A	3325	1/1	0.91	0.10	63,63,63,63	0
56	MG	1A	3405	1/1	0.91	0.21	42,42,42,42	0
56	MG	2A	3329	1/1	0.91	0.41	56,56,56,56	0
56	MG	2R	201	1/1	0.91	0.11	48,48,48,48	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	2T	3001	1/1	0.91	0.13	53,53,53,53	0
56	MG	1Q	206	1/1	0.91	0.12	54,54,54,54	0
56	MG	1A	3262	1/1	0.91	0.14	49,49,49,49	0
56	MG	2A	3662	1/1	0.91	0.12	48,48,48,48	0
56	MG	1A	3705	1/1	0.91	0.09	42,42,42,42	0
56	MG	1A	3187	1/1	0.91	0.21	47,47,47,47	0
56	MG	1A	3180	1/1	0.92	0.21	36,36,36,36	0
56	MG	1A	4125	1/1	0.92	0.34	54,54,54,54	0
56	MG	1A	4128	1/1	0.92	0.32	43,43,43,43	0
56	MG	1A	4133	1/1	0.92	0.15	45,45,45,45	0
56	MG	2A	3671	1/1	0.92	0.10	46,46,46,46	0
56	MG	20	3003	1/1	0.92	0.09	58,58,58,58	0
56	MG	2A	3673	1/1	0.92	0.24	64,64,64,64	0
56	MG	27	101	1/1	0.92	0.20	51,51,51,51	0
56	MG	2A	3675	1/1	0.92	0.17	55,55,55,55	0
56	MG	2A	3676	1/1	0.92	0.09	48,48,48,48	0
56	MG	1A	4134	1/1	0.92	0.32	46,46,46,46	0
56	MG	2A	3363	1/1	0.92	0.22	65,65,65,65	0
56	MG	1A	3007	1/1	0.92	0.15	38,38,38,38	0
56	MG	1A	3469	1/1	0.92	0.23	53,53,53,53	0
56	MG	2A	3366	1/1	0.92	0.10	54,54,54,54	0
56	MG	2A	3693	1/1	0.92	0.11	35,35,35,35	0
56	MG	2A	3694	1/1	0.92	0.15	51,51,51,51	0
56	MG	2a	3008	1/1	0.92	0.26	68,68,68,68	0
56	MG	1a	1613	1/1	0.92	0.08	74,74,74,74	0
56	MG	1B	3003	1/1	0.92	0.23	56,56,56,56	0
56	MG	2A	3373	1/1	0.92	0.06	52,52,52,52	0
56	MG	1A	3470	1/1	0.92	0.17	47,47,47,47	0
56	MG	2A	3701	1/1	0.92	0.19	64,64,64,64	0
56	MG	1a	1787	1/1	0.92	0.07	72,72,72,72	0
56	MG	2A	3704	1/1	0.92	0.07	56,56,56,56	0
56	MG	2A	3378	1/1	0.92	0.15	62,62,62,62	0
56	MG	1A	3473	1/1	0.92	0.26	50,50,50,50	0
56	MG	1a	1623	1/1	0.92	0.14	60,60,60,60	0
56	MG	2A	3123	1/1	0.92	0.10	56,56,56,56	0
56	MG	1A	3647	1/1	0.92	0.22	29,29,29,29	0
56	MG	2A	3386	1/1	0.92	0.13	63,63,63,63	0
56	MG	1A	3550	1/1	0.92	0.19	38,38,38,38	0
56	MG	1A	3115	1/1	0.92	0.14	57,57,57,57	0
56	MG	1A	3213	1/1	0.92	0.12	42,42,42,42	0
56	MG	2A	3397	1/1	0.92	0.17	54,54,54,54	0
56	MG	1A	3756	1/1	0.92	0.20	39,39,39,39	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	2A	3400	1/1	0.92	0.25	56,56,56,56	0
56	MG	1A	3884	1/1	0.92	0.09	48,48,48,48	0
56	MG	2A	3148	1/1	0.92	0.16	52,52,52,52	0
56	MG	1A	3554	1/1	0.92	0.28	47,47,47,47	0
56	MG	1A	3480	1/1	0.92	0.10	52,52,52,52	0
56	MG	1B	3021	1/1	0.92	0.26	46,46,46,46	0
56	MG	1A	3482	1/1	0.92	0.16	50,50,50,50	0
56	MG	1A	3664	1/1	0.92	0.14	48,48,48,48	0
56	MG	1A	3665	1/1	0.92	0.10	60,60,60,60	0
56	MG	1a	1644	1/1	0.92	0.15	66,66,66,66	0
56	MG	2A	3416	1/1	0.92	0.15	59,59,59,59	0
56	MG	2A	3749	1/1	0.92	0.11	48,48,48,48	0
56	MG	1A	3483	1/1	0.92	0.17	46,46,46,46	0
56	MG	2A	3418	1/1	0.92	0.09	61,61,61,61	0
56	MG	1A	3898	1/1	0.92	0.19	50,50,50,50	0
56	MG	2a	3055	1/1	0.92	0.07	51,51,51,51	0
56	MG	1A	3288	1/1	0.92	0.12	43,43,43,43	0
56	MG	1A	3291	1/1	0.92	0.13	59,59,59,59	0
56	MG	1A	3903	1/1	0.92	0.17	40,40,40,40	0
56	MG	1A	4016	1/1	0.92	0.13	46,46,46,46	0
56	MG	2A	3429	1/1	0.92	0.11	65,65,65,65	0
56	MG	1A	3772	1/1	0.92	0.16	36,36,36,36	0
56	MG	2A	3771	1/1	0.92	0.13	39,39,39,39	0
56	MG	2A	3431	1/1	0.92	0.14	62,62,62,62	0
56	MG	2a	3066	1/1	0.92	0.14	54,54,54,54	0
56	MG	2A	3191	1/1	0.92	0.21	50,50,50,50	0
56	MG	1A	4019	1/1	0.92	0.20	42,42,42,42	0
56	MG	1A	3424	1/1	0.92	0.33	70,70,70,70	0
56	MG	1A	3376	1/1	0.92	0.21	51,51,51,51	0
56	MG	2a	3073	1/1	0.92	0.12	66,66,66,66	0
56	MG	1A	3298	1/1	0.92	0.15	43,43,43,43	0
56	MG	2A	3203	1/1	0.92	0.22	46,46,46,46	0
56	MG	1A	3680	1/1	0.92	0.19	44,44,44,44	0
56	MG	2A	3447	1/1	0.92	0.28	46,46,46,46	0
56	MG	2A	3207	1/1	0.92	0.14	44,44,44,44	0
56	MG	1a	1665	1/1	0.92	0.10	78,78,78,78	0
56	MG	1a	1666	1/1	0.92	0.14	59,59,59,59	0
56	MG	1A	3682	1/1	0.92	0.21	35,35,35,35	0
56	MG	2A	3211	1/1	0.92	0.10	43,43,43,43	0
56	MG	1a	1668	1/1	0.92	0.13	67,67,67,67	0
56	MG	2A	3798	1/1	0.92	0.28	52,52,52,52	0
56	MG	2A	3799	1/1	0.92	0.41	68,68,68,68	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	2A	3801	1/1	0.92	0.27	64,64,64,64	0
56	MG	1F	301	1/1	0.92	0.16	40,40,40,40	0
56	MG	1A	3686	1/1	0.92	0.20	35,35,35,35	0
56	MG	1F	303	1/1	0.92	0.17	38,38,38,38	0
56	MG	2A	3807	1/1	0.92	0.07	61,61,61,61	0
56	MG	1A	4028	1/1	0.92	0.12	69,69,69,69	0
56	MG	1A	3568	1/1	0.92	0.26	50,50,50,50	0
56	MG	1A	3130	1/1	0.92	0.23	41,41,41,41	0
56	MG	2a	3109	1/1	0.92	0.20	67,67,67,67	0
56	MG	1A	3381	1/1	0.92	0.14	43,43,43,43	0
56	MG	1A	3788	1/1	0.92	0.10	59,59,59,59	0
56	MG	2a	3114	1/1	0.92	0.13	51,51,51,51	0
56	MG	2a	3115	1/1	0.92	0.09	57,57,57,57	0
56	MG	1A	3101	1/1	0.92	0.12	44,44,44,44	0
56	MG	1A	3504	1/1	0.92	0.19	44,44,44,44	0
56	MG	2A	3477	1/1	0.92	0.34	56,56,56,56	0
56	MG	2A	3817	1/1	0.92	0.08	56,56,56,56	0
56	MG	1a	1682	1/1	0.92	0.27	66,66,66,66	0
56	MG	1A	3153	1/1	0.92	0.14	37,37,37,37	0
56	MG	1N	205	1/1	0.92	0.15	57,57,57,57	0
56	MG	1A	3340	1/1	0.92	0.27	58,58,58,58	0
56	MG	1A	3132	1/1	0.92	0.26	40,40,40,40	0
56	MG	1x	108	1/1	0.92	0.15	63,63,63,63	0
56	MG	2A	3248	1/1	0.92	0.13	42,42,42,42	0
56	MG	1A	3060	1/1	0.92	0.10	45,45,45,45	0
56	MG	1A	3391	1/1	0.92	0.20	41,41,41,41	0
56	MG	1x	115	1/1	0.92	0.15	75,75,75,75	0
56	MG	2A	3258	1/1	0.92	0.16	58,58,58,58	0
56	MG	1A	3810	1/1	0.92	0.15	45,45,45,45	0
56	MG	2A	3833	1/1	0.92	0.14	55,55,55,55	0
56	MG	1A	4051	1/1	0.92	0.23	38,38,38,38	0
56	MG	1y	3003	1/1	0.92	0.23	71,71,71,71	0
56	MG	1A	3941	1/1	0.92	0.15	46,46,46,46	0
56	MG	1R	202	1/1	0.92	0.18	38,38,38,38	0
56	MG	1A	3816	1/1	0.92	0.22	49,49,49,49	0
56	MG	1A	3818	1/1	0.92	0.18	57,57,57,57	0
56	MG	1a	1701	1/1	0.92	0.22	51,51,51,51	0
56	MG	1A	3310	1/1	0.92	0.18	40,40,40,40	0
56	MG	1a	1703	1/1	0.92	0.27	55,55,55,55	0
56	MG	2A	3519	1/1	0.92	0.17	33,33,33,33	0
56	MG	2A	3014	1/1	0.92	0.26	43,43,43,43	0
56	MG	2A	3523	1/1	0.92	0.13	27,27,27,27	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	1A	3063	1/1	0.92	0.20	38,38,38,38	0
56	MG	2A	3280	1/1	0.92	0.17	54,54,54,54	0
56	MG	2A	3017	1/1	0.92	0.24	52,52,52,52	0
56	MG	1a	1705	1/1	0.92	0.18	63,63,63,63	0
56	MG	2A	3863	1/1	0.92	0.05	58,58,58,58	0
56	MG	1A	3232	1/1	0.92	0.10	47,47,47,47	0
56	MG	1A	3523	1/1	0.92	0.26	44,44,44,44	0
56	MG	2A	3032	1/1	0.92	0.10	38,38,38,38	0
56	MG	1V	202	1/1	0.92	0.15	53,53,53,53	0
56	MG	1A	3595	1/1	0.92	0.21	59,59,59,59	0
56	MG	1A	3950	1/1	0.92	0.09	41,41,41,41	0
56	MG	1a	1712	1/1	0.92	0.19	67,67,67,67	0
56	MG	2A	3044	1/1	0.92	0.10	48,48,48,48	0
56	MG	2A	3555	1/1	0.92	0.10	43,43,43,43	0
56	MG	2A	3045	1/1	0.92	0.15	58,58,58,58	0
56	MG	1W	204	1/1	0.92	0.14	40,40,40,40	0
56	MG	2A	3560	1/1	0.92	0.19	63,63,63,63	0
56	MG	2a	3187	1/1	0.92	0.13	72,72,72,72	0
56	MG	1A	4067	1/1	0.92	0.14	56,56,56,56	0
56	MG	1a	1716	1/1	0.92	0.22	53,53,53,53	0
56	MG	1A	3201	1/1	0.92	0.24	45,45,45,45	0
56	MG	1a	1719	1/1	0.92	0.22	63,63,63,63	0
56	MG	2A	3055	1/1	0.92	0.15	46,46,46,46	0
56	MG	2A	3886	1/1	0.92	0.29	45,45,45,45	0
56	MG	1A	4069	1/1	0.92	0.12	42,42,42,42	0
56	MG	2a	3206	1/1	0.92	0.17	69,69,69,69	0
56	MG	2A	3311	1/1	0.92	0.12	63,63,63,63	0
56	MG	1A	3604	1/1	0.92	0.14	65,65,65,65	0
56	MG	2a	3213	1/1	0.92	0.18	69,69,69,69	0
56	MG	2A	3588	1/1	0.92	0.10	47,47,47,47	0
56	MG	1A	3720	1/1	0.92	0.17	53,53,53,53	0
56	MG	2a	3218	1/1	0.92	0.20	61,61,61,61	0
56	MG	1Y	503	1/1	0.92	0.15	78,78,78,78	0
56	MG	2A	3064	1/1	0.92	0.13	51,51,51,51	0
56	MG	1A	3202	1/1	0.92	0.15	32,32,32,32	0
56	MG	2a	3222	1/1	0.92	0.09	63,63,63,63	0
56	MG	2A	3066	1/1	0.92	0.10	41,41,41,41	0
56	MG	2A	3597	1/1	0.92	0.16	61,61,61,61	0
56	MG	1A	3401	1/1	0.92	0.21	35,35,35,35	0
56	MG	10	101	1/1	0.92	0.12	63,63,63,63	0
56	MG	2B	3006	1/1	0.92	0.23	59,59,59,59	0
56	MG	2A	3606	1/1	0.92	0.15	61,61,61,61	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	1A	4075	1/1	0.92	0.13	42,42,42,42	0
56	MG	2A	3075	1/1	0.92	0.19	37,37,37,37	0
56	MG	1A	3165	1/1	0.92	0.24	48,48,48,48	0
56	MG	1A	3533	1/1	0.92	0.18	36,36,36,36	0
56	MG	1A	3076	1/1	0.92	0.15	53,53,53,53	0
56	MG	2a	3239	1/1	0.92	0.14	65,65,65,65	0
56	MG	2A	3333	1/1	0.92	0.13	55,55,55,55	0
56	MG	2A	3625	1/1	0.92	0.14	69,69,69,69	0
56	MG	2A	3626	1/1	0.92	0.19	53,53,53,53	0
56	MG	1A	3848	1/1	0.92	0.14	56,56,56,56	0
56	MG	1A	3145	1/1	0.92	0.23	32,32,32,32	0
56	MG	13	103	1/1	0.92	0.21	47,47,47,47	0
56	MG	2E	303	1/1	0.92	0.12	49,49,49,49	0
56	MG	2r	101	1/1	0.92	0.16	68,68,68,68	0
56	MG	2A	3632	1/1	0.92	0.13	41,41,41,41	0
56	MG	2A	3635	1/1	0.92	0.18	43,43,43,43	0
56	MG	1A	3273	1/1	0.92	0.28	53,53,53,53	0
56	MG	1a	1759	1/1	0.92	0.13	64,64,64,64	0
56	MG	1A	3854	1/1	0.92	0.12	51,51,51,51	0
56	MG	1A	4098	1/1	0.92	0.21	45,45,45,45	0
56	MG	1A	3733	1/1	0.92	0.12	52,52,52,52	0
56	MG	2N	8001	1/1	0.92	0.17	47,47,47,47	0
56	MG	2x	104	1/1	0.92	0.24	60,60,60,60	0
56	MG	1A	3410	1/1	0.92	0.07	57,57,57,57	0
56	MG	2A	3351	1/1	0.92	0.11	54,54,54,54	0
56	MG	2A	3651	1/1	0.92	0.14	44,44,44,44	0
56	MG	1A	3634	1/1	0.92	0.18	44,44,44,44	0
58	ZN	14	501	1/1	0.92	0.11	99,99,99,99	0
56	MG	2T	3003	1/1	0.92	0.13	63,63,63,63	0
56	MG	1A	3367	1/1	0.93	0.23	57,57,57,57	0
56	MG	1A	4003	1/1	0.93	0.18	20,20,20,20	0
56	MG	1A	3669	1/1	0.93	0.10	34,34,34,34	0
56	MG	1a	1622	1/1	0.93	0.28	62,62,62,62	0
56	MG	2A	3090	1/1	0.93	0.07	60,60,60,60	0
56	MG	1B	3019	1/1	0.93	0.23	56,56,56,56	0
56	MG	2A	3645	1/1	0.93	0.16	40,40,40,40	0
56	MG	1a	1624	1/1	0.93	0.15	50,50,50,50	0
56	MG	2A	3095	1/1	0.93	0.19	39,39,39,39	0
56	MG	1A	3891	1/1	0.93	0.18	41,41,41,41	0
56	MG	2Y	502	1/1	0.93	0.25	54,54,54,54	0
56	MG	2A	3350	1/1	0.93	0.21	61,61,61,61	0
56	MG	20	3001	1/1	0.93	0.17	59,59,59,59	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	1A	3368	1/1	0.93	0.29	47,47,47,47	0
56	MG	1A	3896	1/1	0.93	0.22	47,47,47,47	0
56	MG	1A	4011	1/1	0.93	0.10	43,43,43,43	0
56	MG	2A	3666	1/1	0.93	0.10	34,34,34,34	0
56	MG	2A	3355	1/1	0.93	0.10	51,51,51,51	0
56	MG	1A	3236	1/1	0.93	0.35	37,37,37,37	0
56	MG	1A	3495	1/1	0.93	0.26	42,42,42,42	0
56	MG	1a	1633	1/1	0.93	0.21	60,60,60,60	0
56	MG	2A	3361	1/1	0.93	0.16	51,51,51,51	0
56	MG	1A	3071	1/1	0.93	0.31	38,38,38,38	0
56	MG	1A	3044	1/1	0.93	0.20	37,37,37,37	0
56	MG	2A	3682	1/1	0.93	0.15	70,70,70,70	0
56	MG	1a	1637	1/1	0.93	0.20	68,68,68,68	0
56	MG	1B	3033	1/1	0.93	0.17	56,56,56,56	0
56	MG	2A	3116	1/1	0.93	0.23	68,68,68,68	0
56	MG	2A	3688	1/1	0.93	0.09	38,38,38,38	0
56	MG	1a	1797	1/1	0.93	0.13	64,64,64,64	0
56	MG	1A	3373	1/1	0.93	0.24	52,52,52,52	0
56	MG	1D	304	1/1	0.93	0.19	30,30,30,30	0
56	MG	2A	3120	1/1	0.93	0.09	51,51,51,51	0
56	MG	1A	3904	1/1	0.93	0.17	36,36,36,36	0
56	MG	2a	3018	1/1	0.93	0.18	65,65,65,65	0
56	MG	2a	3019	1/1	0.93	0.11	57,57,57,57	0
56	MG	1A	4022	1/1	0.93	0.11	72,72,72,72	0
56	MG	1A	3683	1/1	0.93	0.19	40,40,40,40	0
56	MG	2A	3127	1/1	0.93	0.13	50,50,50,50	0
56	MG	2A	3382	1/1	0.93	0.07	50,50,50,50	0
56	MG	1A	3575	1/1	0.93	0.14	33,33,33,33	0
56	MG	1A	3278	1/1	0.93	0.20	51,51,51,51	0
56	MG	1E	305	1/1	0.93	0.22	57,57,57,57	0
56	MG	2A	3135	1/1	0.93	0.20	43,43,43,43	0
56	MG	2A	3388	1/1	0.93	0.18	56,56,56,56	0
56	MG	2A	3390	1/1	0.93	0.14	57,57,57,57	0
56	MG	2A	3136	1/1	0.93	0.18	45,45,45,45	0
56	MG	1A	3118	1/1	0.93	0.22	38,38,38,38	0
56	MG	2A	3719	1/1	0.93	0.20	57,57,57,57	0
56	MG	2A	3395	1/1	0.93	0.21	50,50,50,50	0
56	MG	2A	3396	1/1	0.93	0.09	56,56,56,56	0
56	MG	2A	3139	1/1	0.93	0.14	32,32,32,32	0
56	MG	2A	3727	1/1	0.93	0.15	51,51,51,51	0
56	MG	2A	3140	1/1	0.93	0.18	50,50,50,50	0
56	MG	1A	3329	1/1	0.93	0.15	43,43,43,43	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	1A	3280	1/1	0.93	0.26	50,50,50,50	0
56	MG	1A	4030	1/1	0.93	0.12	44,44,44,44	0
56	MG	1a	1820	1/1	0.93	0.08	57,57,57,57	0
56	MG	1A	3791	1/1	0.93	0.17	43,43,43,43	0
56	MG	2a	3052	1/1	0.93	0.15	62,62,62,62	0
56	MG	1A	3331	1/1	0.93	0.23	54,54,54,54	0
56	MG	2A	3160	1/1	0.93	0.25	44,44,44,44	0
56	MG	2A	3744	1/1	0.93	0.15	55,55,55,55	0
56	MG	2A	3411	1/1	0.93	0.17	53,53,53,53	0
56	MG	2A	3161	1/1	0.93	0.18	44,44,44,44	0
56	MG	2A	3165	1/1	0.93	0.35	49,49,49,49	0
56	MG	1A	4034	1/1	0.93	0.08	51,51,51,51	0
56	MG	1A	3244	1/1	0.93	0.21	49,49,49,49	0
56	MG	1A	3103	1/1	0.93	0.15	38,38,38,38	0
56	MG	1F	308	1/1	0.93	0.20	53,53,53,53	0
56	MG	2A	3178	1/1	0.93	0.24	57,57,57,57	0
56	MG	2A	3421	1/1	0.93	0.16	61,61,61,61	0
56	MG	2a	3067	1/1	0.93	0.15	65,65,65,65	0
56	MG	1A	3385	1/1	0.93	0.15	58,58,58,58	0
56	MG	1A	4041	1/1	0.93	0.14	36,36,36,36	0
56	MG	2A	3762	1/1	0.93	0.09	52,52,52,52	0
56	MG	2A	3183	1/1	0.93	0.17	56,56,56,56	0
56	MG	2A	3768	1/1	0.93	0.10	62,62,62,62	0
56	MG	2A	3425	1/1	0.93	0.16	58,58,58,58	0
56	MG	1A	3799	1/1	0.93	0.18	57,57,57,57	0
56	MG	1A	3334	1/1	0.93	0.26	56,56,56,56	0
56	MG	2A	3772	1/1	0.93	0.14	53,53,53,53	0
56	MG	2A	3773	1/1	0.93	0.06	63,63,63,63	0
56	MG	1A	3594	1/1	0.93	0.14	31,31,31,31	0
56	MG	1A	3805	1/1	0.93	0.23	54,54,54,54	0
56	MG	1A	3136	1/1	0.93	0.08	52,52,52,52	0
56	MG	2a	3086	1/1	0.93	0.11	57,57,57,57	0
56	MG	1A	3596	1/1	0.93	0.20	51,51,51,51	0
56	MG	1O	203	1/1	0.93	0.31	63,63,63,63	0
56	MG	2A	3437	1/1	0.93	0.14	67,67,67,67	0
56	MG	2a	3091	1/1	0.93	0.42	76,76,76,76	0
56	MG	2a	3092	1/1	0.93	0.13	51,51,51,51	0
56	MG	1t	3001	1/1	0.93	0.13	58,58,58,58	0
56	MG	2A	3197	1/1	0.93	0.12	57,57,57,57	0
56	MG	2A	3200	1/1	0.93	0.15	42,42,42,42	0
56	MG	1A	3815	1/1	0.93	0.27	44,44,44,44	0
56	MG	2a	3100	1/1	0.93	0.06	69,69,69,69	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
56	MG	1A	3598	1/1	0.93	0.13	51,51,51,51	0
56	MG	1A	3155	1/1	0.93	0.20	47,47,47,47	0
56	MG	2A	3451	1/1	0.93	0.19	56,56,56,56	0
56	MG	2A	3794	1/1	0.93	0.09	67,67,67,67	0
56	MG	1A	3051	1/1	0.93	0.28	50,50,50,50	0
56	MG	1A	3454	1/1	0.93	0.20	59,59,59,59	0
56	MG	1w	107	1/1	0.93	0.18	67,67,67,67	0
56	MG	1A	3341	1/1	0.93	0.30	55,55,55,55	0
56	MG	1A	3217	1/1	0.93	0.28	47,47,47,47	0
56	MG	1w	111	1/1	0.93	0.17	41,41,41,41	0
56	MG	1A	3535	1/1	0.93	0.20	45,45,45,45	0
56	MG	2A	3219	1/1	0.93	0.20	51,51,51,51	0
56	MG	2A	3806	1/1	0.93	0.11	66,66,66,66	0
56	MG	1A	3460	1/1	0.93	0.22	48,48,48,48	0
56	MG	1S	3002	1/1	0.93	0.17	49,49,49,49	0
56	MG	1A	3617	1/1	0.93	0.16	33,33,33,33	0
56	MG	1A	3158	1/1	0.93	0.19	56,56,56,56	0
56	MG	1a	1693	1/1	0.93	0.08	58,58,58,58	0
56	MG	1A	3219	1/1	0.93	0.16	37,37,37,37	0
56	MG	1A	3160	1/1	0.93	0.23	41,41,41,41	0
56	MG	1x	109	1/1	0.93	0.10	82,82,82,82	0
56	MG	1A	3729	1/1	0.93	0.26	42,42,42,42	0
56	MG	1x	112	1/1	0.93	0.14	71,71,71,71	0
56	MG	1x	113	1/1	0.93	0.19	62,62,62,62	0
56	MG	1A	3632	1/1	0.93	0.12	34,34,34,34	0
56	MG	1A	3840	1/1	0.93	0.11	63,63,63,63	0
56	MG	1A	3191	1/1	0.93	0.19	42,42,42,42	0
56	MG	2A	3485	1/1	0.93	0.23	63,63,63,63	0
56	MG	2A	3487	1/1	0.93	0.24	62,62,62,62	0
56	MG	2A	3246	1/1	0.93	0.12	65,65,65,65	0
56	MG	1A	3847	1/1	0.93	0.09	48,48,48,48	0
56	MG	1A	3967	1/1	0.93	0.15	65,65,65,65	0
56	MG	1A	3052	1/1	0.93	0.15	56,56,56,56	0
56	MG	1A	3406	1/1	0.93	0.29	47,47,47,47	0
56	MG	2A	3499	1/1	0.93	0.11	46,46,46,46	0
56	MG	2A	3254	1/1	0.93	0.51	53,53,53,53	0
56	MG	1A	3739	1/1	0.93	0.18	39,39,39,39	0
56	MG	1A	3195	1/1	0.93	0.21	40,40,40,40	0
56	MG	1A	3855	1/1	0.93	0.22	53,53,53,53	0
56	MG	1A	3742	1/1	0.93	0.13	64,64,64,64	0
56	MG	1A	3642	1/1	0.93	0.10	40,40,40,40	0
56	MG	2A	3262	1/1	0.93	0.16	57,57,57,57	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
56	MG	2a	3157	1/1	0.93	0.12	64,64,64,64	0
56	MG	2A	3848	1/1	0.93	0.10	36,36,36,36	0
56	MG	1A	4102	1/1	0.93	0.10	45,45,45,45	0
56	MG	2a	3161	1/1	0.93	0.21	91,91,91,91	0
56	MG	2a	3165	1/1	0.93	0.25	54,54,54,54	0
56	MG	1A	3260	1/1	0.93	0.12	39,39,39,39	0
56	MG	1A	3196	1/1	0.93	0.10	59,59,59,59	0
56	MG	11	101	1/1	0.93	0.13	38,38,38,38	0
56	MG	2A	3024	1/1	0.93	0.13	49,49,49,49	0
56	MG	2A	3856	1/1	0.93	0.32	41,41,41,41	0
56	MG	2A	3521	1/1	0.93	0.11	51,51,51,51	0
56	MG	11	103	1/1	0.93	0.09	65,65,65,65	0
56	MG	2a	3177	1/1	0.93	0.07	67,67,67,67	0
56	MG	1A	4110	1/1	0.93	0.13	56,56,56,56	0
56	MG	2A	3527	1/1	0.93	0.12	31,31,31,31	0
56	MG	1A	3476	1/1	0.93	0.16	52,52,52,52	0
56	MG	1A	3416	1/1	0.93	0.17	47,47,47,47	0
56	MG	2A	3534	1/1	0.93	0.19	40,40,40,40	0
56	MG	2A	3278	1/1	0.93	0.18	57,57,57,57	0
56	MG	1A	3866	1/1	0.93	0.17	46,46,46,46	0
56	MG	2a	3191	1/1	0.93	0.15	63,63,63,63	0
56	MG	2A	3281	1/1	0.93	0.16	63,63,63,63	0
56	MG	2a	3193	1/1	0.93	0.12	73,73,73,73	0
56	MG	2a	3195	1/1	0.93	0.13	41,41,41,41	0
56	MG	2a	3196	1/1	0.93	0.11	64,64,64,64	0
56	MG	15	102	1/1	0.93	0.19	39,39,39,39	0
56	MG	1a	1729	1/1	0.93	0.20	61,61,61,61	0
56	MG	2a	3199	1/1	0.93	0.11	72,72,72,72	0
56	MG	2A	3285	1/1	0.93	0.12	49,49,49,49	0
56	MG	2A	3041	1/1	0.93	0.20	49,49,49,49	0
56	MG	2A	3042	1/1	0.93	0.22	42,42,42,42	0
56	MG	2A	3552	1/1	0.93	0.18	59,59,59,59	0
56	MG	1a	1730	1/1	0.93	0.16	80,80,80,80	0
56	MG	1a	1733	1/1	0.93	0.14	58,58,58,58	0
56	MG	1A	3199	1/1	0.93	0.19	45,45,45,45	0
56	MG	1A	4129	1/1	0.93	0.23	42,42,42,42	0
56	MG	2A	3558	1/1	0.93	0.17	31,31,31,31	0
56	MG	2A	3293	1/1	0.93	0.13	50,50,50,50	0
56	MG	17	101	1/1	0.93	0.22	54,54,54,54	0
56	MG	2A	3563	1/1	0.93	0.14	49,49,49,49	0
56	MG	1A	4131	1/1	0.93	0.19	58,58,58,58	0
56	MG	2A	3569	1/1	0.93	0.09	49,49,49,49	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	1A	3986	1/1	0.93	0.24	22,22,22,22	0
56	MG	2A	3300	1/1	0.93	0.14	55,55,55,55	0
56	MG	2A	3054	1/1	0.93	0.19	54,54,54,54	0
56	MG	1A	3066	1/1	0.93	0.17	35,35,35,35	0
56	MG	1a	1749	1/1	0.93	0.15	45,45,45,45	0
56	MG	2A	3901	1/1	0.93	0.31	59,59,59,59	0
56	MG	2A	3903	1/1	0.93	0.14	58,58,58,58	0
56	MG	1A	3753	1/1	0.93	0.27	34,34,34,34	0
56	MG	2A	3907	1/1	0.93	0.16	57,57,57,57	0
56	MG	2a	3235	1/1	0.93	0.06	71,71,71,71	0
56	MG	2B	3001	1/1	0.93	0.16	62,62,62,62	0
56	MG	2A	3583	1/1	0.93	0.16	69,69,69,69	0
56	MG	1A	3266	1/1	0.93	0.22	52,52,52,52	0
56	MG	1A	3656	1/1	0.93	0.09	46,46,46,46	0
56	MG	1A	3877	1/1	0.93	0.15	39,39,39,39	0
56	MG	1a	1757	1/1	0.93	0.10	48,48,48,48	0
56	MG	2A	3312	1/1	0.93	0.12	51,51,51,51	0
56	MG	1A	3484	1/1	0.93	0.13	54,54,54,54	0
56	MG	1A	3485	1/1	0.93	0.18	48,48,48,48	0
56	MG	2A	3599	1/1	0.93	0.18	51,51,51,51	0
56	MG	2q	202	1/1	0.93	0.06	78,78,78,78	0
56	MG	2A	3069	1/1	0.93	0.14	40,40,40,40	0
56	MG	2A	3071	1/1	0.93	0.06	52,52,52,52	0
56	MG	2A	3072	1/1	0.93	0.10	46,46,46,46	0
56	MG	2A	3318	1/1	0.93	0.15	48,48,48,48	0
56	MG	1A	3017	1/1	0.93	0.14	54,54,54,54	0
56	MG	2A	3321	1/1	0.93	0.13	54,54,54,54	0
56	MG	2w	106	1/1	0.93	0.12	60,60,60,60	0
56	MG	2A	3612	1/1	0.93	0.07	39,39,39,39	0
56	MG	1A	3270	1/1	0.93	0.25	59,59,59,59	0
56	MG	2x	101	1/1	0.93	0.10	42,42,42,42	0
56	MG	1a	1765	1/1	0.93	0.11	49,49,49,49	0
56	MG	2x	103	1/1	0.93	0.13	64,64,64,64	0
56	MG	1A	3565	1/1	0.93	0.32	71,71,71,71	0
56	MG	1a	1767	1/1	0.93	0.12	66,66,66,66	0
56	MG	1a	1769	1/1	0.93	0.11	55,55,55,55	0
56	MG	2y	3004	1/1	0.93	0.19	59,59,59,59	0
56	MG	1a	1771	1/1	0.93	0.08	70,70,70,70	0
56	MG	1a	1772	1/1	0.93	0.13	39,39,39,39	0
57	K	2A	3496	1/1	0.93	0.09	73,73,73,73	0
56	MG	2A	3084	1/1	0.93	0.10	45,45,45,45	0
56	MG	2A	3630	1/1	0.93	0.16	69,69,69,69	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	1A	4052	1/1	0.94	0.18	31,31,31,31	0
56	MG	1A	3015	1/1	0.94	0.16	40,40,40,40	0
56	MG	1A	3657	1/1	0.94	0.18	27,27,27,27	0
56	MG	1a	1737	1/1	0.94	0.11	66,66,66,66	0
56	MG	1A	4055	1/1	0.94	0.09	33,33,33,33	0
56	MG	1a	1742	1/1	0.94	0.08	51,51,51,51	0
56	MG	2A	3614	1/1	0.94	0.14	36,36,36,36	0
56	MG	1A	3086	1/1	0.94	0.42	50,50,50,50	0
56	MG	2P	201	1/1	0.94	0.13	45,45,45,45	0
56	MG	2A	3324	1/1	0.94	0.09	41,41,41,41	0
56	MG	1A	3114	1/1	0.94	0.17	57,57,57,57	0
56	MG	1A	3779	1/1	0.94	0.10	56,56,56,56	0
56	MG	2A	3328	1/1	0.94	0.20	39,39,39,39	0
56	MG	1A	3065	1/1	0.94	0.22	33,33,33,33	0
56	MG	2U	203	1/1	0.94	0.25	46,46,46,46	0
56	MG	1a	1747	1/1	0.94	0.14	49,49,49,49	0
56	MG	1A	3927	1/1	0.94	0.10	47,47,47,47	0
56	MG	1a	1750	1/1	0.94	0.10	85,85,85,85	0
56	MG	1A	3018	1/1	0.94	0.14	33,33,33,33	0
56	MG	2A	3638	1/1	0.94	0.18	43,43,43,43	0
56	MG	1A	3398	1/1	0.94	0.31	58,58,58,58	0
56	MG	1A	3667	1/1	0.94	0.20	61,61,61,61	0
56	MG	23	101	1/1	0.94	0.31	61,61,61,61	0
56	MG	25	101	1/1	0.94	0.15	55,55,55,55	0
56	MG	25	103	1/1	0.94	0.21	52,52,52,52	0
56	MG	25	104	1/1	0.94	0.11	43,43,43,43	0
56	MG	2A	3339	1/1	0.94	0.20	51,51,51,51	0
56	MG	1a	1754	1/1	0.94	0.09	51,51,51,51	0
56	MG	1A	3282	1/1	0.94	0.17	30,30,30,30	0
56	MG	10	102	1/1	0.94	0.12	44,44,44,44	0
56	MG	10	103	1/1	0.94	0.18	45,45,45,45	0
56	MG	1A	3936	1/1	0.94	0.11	31,31,31,31	0
56	MG	1A	3004	1/1	0.94	0.19	34,34,34,34	0
56	MG	2A	3652	1/1	0.94	0.12	41,41,41,41	0
56	MG	2A	3347	1/1	0.94	0.24	51,51,51,51	0
56	MG	2A	3659	1/1	0.94	0.07	59,59,59,59	0
56	MG	2A	3348	1/1	0.94	0.20	48,48,48,48	0
56	MG	1A	3938	1/1	0.94	0.08	55,55,55,55	0
56	MG	1a	1764	1/1	0.94	0.06	59,59,59,59	0
56	MG	1A	3120	1/1	0.94	0.18	42,42,42,42	0
56	MG	1A	3092	1/1	0.94	0.21	50,50,50,50	0
56	MG	1A	3479	1/1	0.94	0.17	38,38,38,38	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	2A	3672	1/1	0.94	0.23	45,45,45,45	0
56	MG	1A	3678	1/1	0.94	0.12	61,61,61,61	0
56	MG	1A	3943	1/1	0.94	0.19	81,81,81,81	0
56	MG	2A	3107	1/1	0.94	0.10	46,46,46,46	0
56	MG	1A	4083	1/1	0.94	0.15	44,44,44,44	0
56	MG	2A	3681	1/1	0.94	0.08	50,50,50,50	0
56	MG	1A	3295	1/1	0.94	0.14	48,48,48,48	0
56	MG	1A	3053	1/1	0.94	0.17	52,52,52,52	0
56	MG	2A	3685	1/1	0.94	0.09	53,53,53,53	0
56	MG	1A	3021	1/1	0.94	0.17	45,45,45,45	0
56	MG	16	103	1/1	0.94	0.12	54,54,54,54	0
56	MG	1a	1778	1/1	0.94	0.17	64,64,64,64	0
56	MG	1A	4092	1/1	0.94	0.22	37,37,37,37	0
56	MG	2A	3368	1/1	0.94	0.06	47,47,47,47	0
56	MG	2a	3031	1/1	0.94	0.19	49,49,49,49	0
56	MG	2A	3369	1/1	0.94	0.07	47,47,47,47	0
56	MG	1A	3300	1/1	0.94	0.18	61,61,61,61	0
56	MG	1A	3801	1/1	0.94	0.17	28,28,28,28	0
56	MG	1A	4096	1/1	0.94	0.14	30,30,30,30	0
56	MG	2A	3122	1/1	0.94	0.13	39,39,39,39	0
56	MG	2A	3376	1/1	0.94	0.13	58,58,58,58	0
56	MG	2A	3702	1/1	0.94	0.07	49,49,49,49	0
56	MG	1A	3570	1/1	0.94	0.22	54,54,54,54	0
56	MG	2A	3124	1/1	0.94	0.10	48,48,48,48	0
56	MG	2a	3045	1/1	0.94	0.06	65,65,65,65	0
56	MG	1A	3415	1/1	0.94	0.30	59,59,59,59	0
56	MG	2A	3708	1/1	0.94	0.11	53,53,53,53	0
56	MG	1A	3486	1/1	0.94	0.19	42,42,42,42	0
56	MG	2A	3128	1/1	0.94	0.19	48,48,48,48	0
56	MG	1A	4104	1/1	0.94	0.15	30,30,30,30	0
56	MG	1A	3074	1/1	0.94	0.21	27,27,27,27	0
56	MG	2A	3132	1/1	0.94	0.22	56,56,56,56	0
56	MG	1a	1606	1/1	0.94	0.17	65,65,65,65	0
56	MG	2A	3389	1/1	0.94	0.11	58,58,58,58	0
56	MG	1A	4109	1/1	0.94	0.21	49,49,49,49	0
56	MG	1a	1791	1/1	0.94	0.09	54,54,54,54	0
56	MG	1A	3574	1/1	0.94	0.18	43,43,43,43	0
56	MG	1A	4111	1/1	0.94	0.17	34,34,34,34	0
56	MG	2A	3728	1/1	0.94	0.09	58,58,58,58	0
56	MG	2a	3061	1/1	0.94	0.19	54,54,54,54	0
56	MG	1A	4112	1/1	0.94	0.17	42,42,42,42	0
56	MG	2A	3143	1/1	0.94	0.12	56,56,56,56	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	2A	3398	1/1	0.94	0.30	55,55,55,55	0
56	MG	2A	3144	1/1	0.94	0.19	45,45,45,45	0
56	MG	1a	1798	1/1	0.94	0.14	56,56,56,56	0
56	MG	2A	3737	1/1	0.94	0.13	72,72,72,72	0
56	MG	1A	3695	1/1	0.94	0.09	57,57,57,57	0
56	MG	1A	3958	1/1	0.94	0.10	44,44,44,44	0
56	MG	1A	3959	1/1	0.94	0.14	56,56,56,56	0
56	MG	1a	1621	1/1	0.94	0.15	42,42,42,42	0
56	MG	2a	3072	1/1	0.94	0.14	53,53,53,53	0
56	MG	1A	3351	1/1	0.94	0.29	49,49,49,49	0
56	MG	1A	3819	1/1	0.94	0.11	48,48,48,48	0
56	MG	1A	3303	1/1	0.94	0.17	33,33,33,33	0
56	MG	2A	3163	1/1	0.94	0.13	56,56,56,56	0
56	MG	1A	3490	1/1	0.94	0.11	50,50,50,50	0
56	MG	2A	3751	1/1	0.94	0.12	61,61,61,61	0
56	MG	1a	1813	1/1	0.94	0.12	58,58,58,58	0
56	MG	2A	3415	1/1	0.94	0.10	50,50,50,50	0
56	MG	2a	3082	1/1	0.94	0.14	54,54,54,54	0
56	MG	1A	3304	1/1	0.94	0.29	55,55,55,55	0
56	MG	2a	3085	1/1	0.94	0.11	65,65,65,65	0
56	MG	1A	3701	1/1	0.94	0.09	48,48,48,48	0
56	MG	1A	3036	1/1	0.94	0.19	31,31,31,31	0
56	MG	2A	3172	1/1	0.94	0.09	47,47,47,47	0
56	MG	2A	3174	1/1	0.94	0.15	53,53,53,53	0
56	MG	2A	3763	1/1	0.94	0.12	52,52,52,52	0
56	MG	2A	3765	1/1	0.94	0.13	53,53,53,53	0
56	MG	2A	3175	1/1	0.94	0.06	65,65,65,65	0
56	MG	2a	3095	1/1	0.94	0.11	71,71,71,71	0
56	MG	2A	3177	1/1	0.94	0.16	63,63,63,63	0
56	MG	1A	3585	1/1	0.94	0.08	66,66,66,66	0
56	MG	1A	3358	1/1	0.94	0.22	33,33,33,33	0
56	MG	1B	3005	1/1	0.94	0.16	55,55,55,55	0
56	MG	2A	3428	1/1	0.94	0.15	52,52,52,52	0
56	MG	1A	3707	1/1	0.94	0.21	29,29,29,29	0
56	MG	2A	3185	1/1	0.94	0.08	45,45,45,45	0
56	MG	1A	3163	1/1	0.94	0.29	52,52,52,52	0
56	MG	2a	3107	1/1	0.94	0.14	57,57,57,57	0
56	MG	2A	3778	1/1	0.94	0.18	52,52,52,52	0
56	MG	1A	3498	1/1	0.94	0.14	46,46,46,46	0
56	MG	2A	3188	1/1	0.94	0.07	36,36,36,36	0
56	MG	2A	3782	1/1	0.94	0.08	51,51,51,51	0
56	MG	1A	3977	1/1	0.94	0.33	56,56,56,56	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	1A	3100	1/1	0.94	0.18	60,60,60,60	0
56	MG	1A	3979	1/1	0.94	0.09	73,73,73,73	0
56	MG	1A	3043	1/1	0.94	0.19	39,39,39,39	0
56	MG	1A	3714	1/1	0.94	0.18	46,46,46,46	0
56	MG	2A	3442	1/1	0.94	0.14	50,50,50,50	0
56	MG	1B	3018	1/1	0.94	0.15	37,37,37,37	0
56	MG	1A	3716	1/1	0.94	0.20	28,28,28,28	0
56	MG	2A	3198	1/1	0.94	0.14	61,61,61,61	0
56	MG	1A	3502	1/1	0.94	0.26	49,49,49,49	0
56	MG	1A	3985	1/1	0.94	0.16	23,23,23,23	0
56	MG	1l	203	1/1	0.94	0.14	63,63,63,63	0
56	MG	1A	3503	1/1	0.94	0.17	32,32,32,32	0
56	MG	1A	3850	1/1	0.94	0.17	53,53,53,53	0
56	MG	1a	1652	1/1	0.94	0.21	63,63,63,63	0
56	MG	1A	3102	1/1	0.94	0.17	54,54,54,54	0
56	MG	1B	3028	1/1	0.94	0.08	61,61,61,61	0
56	MG	1A	3852	1/1	0.94	0.14	33,33,33,33	0
56	MG	1A	3597	1/1	0.94	0.18	50,50,50,50	0
56	MG	2a	3139	1/1	0.94	0.11	73,73,73,73	0
56	MG	1a	1662	1/1	0.94	0.12	67,67,67,67	0
56	MG	2A	3469	1/1	0.94	0.11	55,55,55,55	0
56	MG	1A	3167	1/1	0.94	0.15	41,41,41,41	0
56	MG	1A	3133	1/1	0.94	0.19	44,44,44,44	0
56	MG	2A	3472	1/1	0.94	0.18	60,60,60,60	0
56	MG	1A	3510	1/1	0.94	0.11	45,45,45,45	0
56	MG	1D	302	1/1	0.94	0.44	55,55,55,55	0
56	MG	1D	303	1/1	0.94	0.14	37,37,37,37	0
56	MG	2A	3476	1/1	0.94	0.13	41,41,41,41	0
56	MG	1A	3214	1/1	0.94	0.09	42,42,42,42	0
56	MG	1A	3434	1/1	0.94	0.14	48,48,48,48	0
56	MG	1a	1670	1/1	0.94	0.11	59,59,59,59	0
56	MG	2A	3233	1/1	0.94	0.14	32,32,32,32	0
56	MG	1A	3435	1/1	0.94	0.10	53,53,53,53	0
56	MG	2A	3235	1/1	0.94	0.17	50,50,50,50	0
56	MG	2A	3236	1/1	0.94	0.07	53,53,53,53	0
56	MG	2A	3825	1/1	0.94	0.12	58,58,58,58	0
56	MG	1D	309	1/1	0.94	0.18	46,46,46,46	0
56	MG	1a	1673	1/1	0.94	0.13	67,67,67,67	0
56	MG	2a	3164	1/1	0.94	0.21	73,73,73,73	0
56	MG	1A	3861	1/1	0.94	0.17	33,33,33,33	0
56	MG	2A	3489	1/1	0.94	0.17	41,41,41,41	0
56	MG	1E	301	1/1	0.94	0.19	37,37,37,37	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	1A	4002	1/1	0.94	0.20	33,33,33,33	0
56	MG	1A	3317	1/1	0.94	0.17	47,47,47,47	0
56	MG	2a	3172	1/1	0.94	0.09	66,66,66,66	0
56	MG	2A	3495	1/1	0.94	0.15	51,51,51,51	0
56	MG	2A	3497	1/1	0.94	0.12	63,63,63,63	0
56	MG	1A	3732	1/1	0.94	0.23	64,64,64,64	0
56	MG	1A	3615	1/1	0.94	0.16	25,25,25,25	0
56	MG	1A	3216	1/1	0.94	0.42	50,50,50,50	0
56	MG	1E	309	1/1	0.94	0.15	50,50,50,50	0
56	MG	2a	3180	1/1	0.94	0.11	73,73,73,73	0
56	MG	1a	1683	1/1	0.94	0.14	61,61,61,61	0
56	MG	1A	3319	1/1	0.94	0.14	63,63,63,63	0
56	MG	1A	3870	1/1	0.94	0.12	39,39,39,39	0
56	MG	2a	3186	1/1	0.94	0.12	53,53,53,53	0
56	MG	2A	3256	1/1	0.94	0.31	53,53,53,53	0
56	MG	2A	3853	1/1	0.94	0.12	50,50,50,50	0
56	MG	2a	3189	1/1	0.94	0.16	48,48,48,48	0
56	MG	2A	3257	1/1	0.94	0.19	65,65,65,65	0
56	MG	1A	3738	1/1	0.94	0.12	43,43,43,43	0
56	MG	2A	3004	1/1	0.94	0.24	48,48,48,48	0
56	MG	2a	3194	1/1	0.94	0.11	68,68,68,68	0
56	MG	1A	3170	1/1	0.94	0.15	39,39,39,39	0
56	MG	1A	3626	1/1	0.94	0.14	44,44,44,44	0
56	MG	1A	3876	1/1	0.94	0.18	49,49,49,49	0
56	MG	1a	1690	1/1	0.94	0.14	70,70,70,70	0
56	MG	1A	3374	1/1	0.94	0.15	55,55,55,55	0
56	MG	1A	3442	1/1	0.94	0.27	56,56,56,56	0
56	MG	2A	3015	1/1	0.94	0.20	43,43,43,43	0
56	MG	1A	3631	1/1	0.94	0.20	32,32,32,32	0
56	MG	2A	3270	1/1	0.94	0.10	53,53,53,53	0
56	MG	2A	3532	1/1	0.94	0.14	65,65,65,65	0
56	MG	1A	3881	1/1	0.94	0.18	37,37,37,37	0
56	MG	1A	3443	1/1	0.94	0.27	54,54,54,54	0
56	MG	2A	3022	1/1	0.94	0.27	47,47,47,47	0
56	MG	2A	3023	1/1	0.94	0.05	48,48,48,48	0
56	MG	1A	3321	1/1	0.94	0.34	51,51,51,51	0
56	MG	2A	3541	1/1	0.94	0.14	30,30,30,30	0
56	MG	1A	3171	1/1	0.94	0.33	53,53,53,53	0
56	MG	1A	3749	1/1	0.94	0.15	41,41,41,41	0
56	MG	2A	3030	1/1	0.94	0.13	51,51,51,51	0
56	MG	2A	3547	1/1	0.94	0.09	37,37,37,37	0
56	MG	2A	3283	1/1	0.94	0.24	61,61,61,61	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	1A	3172	1/1	0.94	0.22	43,43,43,43	0
56	MG	1A	3640	1/1	0.94	0.17	53,53,53,53	0
56	MG	1A	3077	1/1	0.94	0.09	35,35,35,35	0
56	MG	2A	3887	1/1	0.94	0.08	48,48,48,48	0
56	MG	2A	3036	1/1	0.94	0.14	54,54,54,54	0
56	MG	2A	3288	1/1	0.94	0.11	49,49,49,49	0
56	MG	1A	4032	1/1	0.94	0.07	68,68,68,68	0
56	MG	1A	3222	1/1	0.94	0.16	56,56,56,56	0
56	MG	1A	3755	1/1	0.94	0.20	36,36,36,36	0
56	MG	1P	202	1/1	0.94	0.11	31,31,31,31	0
56	MG	2A	3564	1/1	0.94	0.15	31,31,31,31	0
56	MG	2A	3897	1/1	0.94	0.32	57,57,57,57	0
56	MG	2a	3241	1/1	0.94	0.10	41,41,41,41	0
56	MG	2A	3899	1/1	0.94	0.21	45,45,45,45	0
56	MG	2A	3565	1/1	0.94	0.16	36,36,36,36	0
56	MG	2A	3043	1/1	0.94	0.12	53,53,53,53	0
56	MG	1A	3267	1/1	0.94	0.15	57,57,57,57	0
56	MG	1A	3452	1/1	0.94	0.23	58,58,58,58	0
56	MG	1A	3225	1/1	0.94	0.22	52,52,52,52	0
56	MG	1A	3759	1/1	0.94	0.18	24,24,24,24	0
56	MG	1A	3061	1/1	0.94	0.35	62,62,62,62	0
56	MG	2A	3575	1/1	0.94	0.11	39,39,39,39	0
56	MG	1A	3141	1/1	0.94	0.16	35,35,35,35	0
56	MG	2v	3002	1/1	0.94	0.09	77,77,77,77	0
56	MG	1A	3651	1/1	0.94	0.22	32,32,32,32	0
56	MG	2B	3007	1/1	0.94	0.25	55,55,55,55	0
56	MG	2A	3580	1/1	0.94	0.23	49,49,49,49	0
56	MG	1S	3003	1/1	0.94	0.13	59,59,59,59	0
56	MG	2A	3306	1/1	0.94	0.12	58,58,58,58	0
56	MG	1a	1720	1/1	0.94	0.12	67,67,67,67	0
56	MG	1A	3653	1/1	0.94	0.19	27,27,27,27	0
56	MG	1A	3387	1/1	0.94	0.25	54,54,54,54	0
56	MG	2B	3018	1/1	0.94	0.18	65,65,65,65	0
56	MG	2A	3593	1/1	0.94	0.16	30,30,30,30	0
56	MG	2A	3310	1/1	0.94	0.15	62,62,62,62	0
56	MG	1A	3769	1/1	0.94	0.24	29,29,29,29	0
56	MG	2A	3061	1/1	0.94	0.12	49,49,49,49	0
56	MG	1A	3082	1/1	0.94	0.27	49,49,49,49	0
56	MG	1U	206	1/1	0.94	0.12	32,32,32,32	0
56	MG	2y	3007	1/1	0.94	0.15	68,68,68,68	0
56	MG	2E	301	1/1	0.94	0.17	50,50,50,50	0
56	MG	2A	3604	1/1	0.94	0.20	64,64,64,64	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	1U	208	1/1	0.94	0.23	38,38,38,38	0
56	MG	23	102	1/1	0.95	0.21	48,48,48,48	0
56	MG	1A	3993	1/1	0.95	0.14	37,37,37,37	0
56	MG	1A	4122	1/1	0.95	0.13	41,41,41,41	0
56	MG	2A	3420	1/1	0.95	0.37	43,43,43,43	0
56	MG	2A	3222	1/1	0.95	0.17	38,38,38,38	0
56	MG	2A	3697	1/1	0.95	0.18	34,34,34,34	0
56	MG	1A	4123	1/1	0.95	0.22	35,35,35,35	0
56	MG	1A	4124	1/1	0.95	0.36	46,46,46,46	0
56	MG	1A	3211	1/1	0.95	0.14	49,49,49,49	0
56	MG	1A	3892	1/1	0.95	0.13	39,39,39,39	0
56	MG	2A	3019	1/1	0.95	0.15	38,38,38,38	0
56	MG	1a	1727	1/1	0.95	0.16	49,49,49,49	0
56	MG	1A	3148	1/1	0.95	0.63	48,48,48,48	0
56	MG	1A	3493	1/1	0.95	0.20	36,36,36,36	0
56	MG	1A	3717	1/1	0.95	0.17	22,22,22,22	0
56	MG	1a	1731	1/1	0.95	0.16	50,50,50,50	0
56	MG	2A	3711	1/1	0.95	0.17	56,56,56,56	0
56	MG	1A	3638	1/1	0.95	0.06	53,53,53,53	0
56	MG	1A	4000	1/1	0.95	0.18	34,34,34,34	0
56	MG	2A	3240	1/1	0.95	0.13	40,40,40,40	0
56	MG	1A	3797	1/1	0.95	0.14	53,53,53,53	0
56	MG	1A	3249	1/1	0.95	0.30	56,56,56,56	0
56	MG	2A	3440	1/1	0.95	0.20	43,43,43,43	0
56	MG	2A	3721	1/1	0.95	0.18	46,46,46,46	0
56	MG	1a	1741	1/1	0.95	0.08	34,34,34,34	0
56	MG	1A	4005	1/1	0.95	0.11	50,50,50,50	0
56	MG	2A	3724	1/1	0.95	0.06	57,57,57,57	0
56	MG	2A	3444	1/1	0.95	0.29	49,49,49,49	0
56	MG	2a	3023	1/1	0.95	0.08	47,47,47,47	0
56	MG	1A	3902	1/1	0.95	0.21	33,33,33,33	0
56	MG	1A	3496	1/1	0.95	0.16	38,38,38,38	0
56	MG	2A	3729	1/1	0.95	0.12	41,41,41,41	0
56	MG	2A	3449	1/1	0.95	0.38	47,47,47,47	0
56	MG	18	102	1/1	0.95	0.30	50,50,50,50	0
56	MG	1A	3562	1/1	0.95	0.21	24,24,24,24	0
56	MG	2A	3251	1/1	0.95	0.10	42,42,42,42	0
56	MG	1B	3008	1/1	0.95	0.14	57,57,57,57	0
56	MG	1A	3005	1/1	0.95	0.16	41,41,41,41	0
56	MG	1A	3907	1/1	0.95	0.23	54,54,54,54	0
56	MG	1a	1602	1/1	0.95	0.10	72,72,72,72	0
56	MG	2A	3460	1/1	0.95	0.36	64,64,64,64	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	1A	3215	1/1	0.95	0.06	65,65,65,65	0
56	MG	1A	4014	1/1	0.95	0.08	34,34,34,34	0
56	MG	1B	3013	1/1	0.95	0.09	55,55,55,55	0
56	MG	1A	3079	1/1	0.95	0.17	57,57,57,57	0
56	MG	1A	3725	1/1	0.95	0.14	52,52,52,52	0
56	MG	1a	1608	1/1	0.95	0.18	60,60,60,60	0
56	MG	2A	3263	1/1	0.95	0.13	55,55,55,55	0
56	MG	2A	3264	1/1	0.95	0.10	62,62,62,62	0
56	MG	1A	3726	1/1	0.95	0.06	48,48,48,48	0
56	MG	1A	3812	1/1	0.95	0.17	45,45,45,45	0
56	MG	1A	3813	1/1	0.95	0.21	56,56,56,56	0
56	MG	2A	3062	1/1	0.95	0.20	61,61,61,61	0
56	MG	2A	3758	1/1	0.95	0.23	58,58,58,58	0
56	MG	1A	3125	1/1	0.95	0.26	41,41,41,41	0
56	MG	1B	3023	1/1	0.95	0.18	54,54,54,54	0
56	MG	1A	3255	1/1	0.95	0.24	47,47,47,47	0
56	MG	2A	3764	1/1	0.95	0.11	66,66,66,66	0
56	MG	1A	3919	1/1	0.95	0.18	38,38,38,38	0
56	MG	2a	3059	1/1	0.95	0.13	74,74,74,74	0
56	MG	2A	3273	1/1	0.95	0.14	51,51,51,51	0
56	MG	2A	3767	1/1	0.95	0.09	56,56,56,56	0
56	MG	1A	3256	1/1	0.95	0.10	57,57,57,57	0
56	MG	2A	3068	1/1	0.95	0.14	56,56,56,56	0
56	MG	2A	3483	1/1	0.95	0.16	55,55,55,55	0
56	MG	2A	3276	1/1	0.95	0.18	55,55,55,55	0
56	MG	1A	3062	1/1	0.95	0.23	59,59,59,59	0
56	MG	1A	3924	1/1	0.95	0.09	50,50,50,50	0
56	MG	1A	3402	1/1	0.95	0.23	54,54,54,54	0
56	MG	2A	3776	1/1	0.95	0.13	44,44,44,44	0
56	MG	1a	1774	1/1	0.95	0.11	60,60,60,60	0
56	MG	1A	3081	1/1	0.95	0.18	34,34,34,34	0
56	MG	2A	3779	1/1	0.95	0.08	56,56,56,56	0
56	MG	2A	3491	1/1	0.95	0.30	55,55,55,55	0
56	MG	1A	3928	1/1	0.95	0.20	31,31,31,31	0
56	MG	1A	3508	1/1	0.95	0.14	36,36,36,36	0
56	MG	2A	3078	1/1	0.95	0.20	25,25,25,25	0
56	MG	1B	3035	1/1	0.95	0.11	59,59,59,59	0
56	MG	2A	3786	1/1	0.95	0.09	48,48,48,48	0
56	MG	1A	3457	1/1	0.95	0.15	59,59,59,59	0
56	MG	1a	1632	1/1	0.95	0.18	52,52,52,52	0
56	MG	1A	3932	1/1	0.95	0.19	45,45,45,45	0
56	MG	1a	1634	1/1	0.95	0.17	27,27,27,27	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	1A	3826	1/1	0.95	0.14	42,42,42,42	0
56	MG	2A	3086	1/1	0.95	0.22	44,44,44,44	0
56	MG	2A	3504	1/1	0.95	0.09	36,36,36,36	0
56	MG	1A	3827	1/1	0.95	0.25	50,50,50,50	0
56	MG	2a	3089	1/1	0.95	0.06	65,65,65,65	0
56	MG	2A	3506	1/1	0.95	0.25	31,31,31,31	0
56	MG	1A	4038	1/1	0.95	0.07	45,45,45,45	0
56	MG	2A	3797	1/1	0.95	0.15	52,52,52,52	0
56	MG	2A	3508	1/1	0.95	0.10	60,60,60,60	0
56	MG	2A	3297	1/1	0.95	0.20	51,51,51,51	0
56	MG	2A	3800	1/1	0.95	0.08	67,67,67,67	0
56	MG	1a	1638	1/1	0.95	0.14	58,58,58,58	0
56	MG	1D	308	1/1	0.95	0.11	48,48,48,48	0
56	MG	1a	1640	1/1	0.95	0.05	58,58,58,58	0
56	MG	1A	3009	1/1	0.95	0.12	24,24,24,24	0
56	MG	2A	3094	1/1	0.95	0.17	44,44,44,44	0
56	MG	1D	310	1/1	0.95	0.34	39,39,39,39	0
56	MG	2A	3522	1/1	0.95	0.08	59,59,59,59	0
56	MG	1a	1792	1/1	0.95	0.05	59,59,59,59	0
56	MG	1a	1793	1/1	0.95	0.25	82,82,82,82	0
56	MG	1A	3012	1/1	0.95	0.16	30,30,30,30	0
56	MG	1A	3831	1/1	0.95	0.15	70,70,70,70	0
56	MG	2a	3111	1/1	0.95	0.14	76,76,76,76	0
56	MG	1A	3029	1/1	0.95	0.24	38,38,38,38	0
56	MG	1A	3515	1/1	0.95	0.10	29,29,29,29	0
56	MG	1a	1799	1/1	0.95	0.08	49,49,49,49	0
56	MG	1a	1800	1/1	0.95	0.12	70,70,70,70	0
56	MG	1a	1801	1/1	0.95	0.07	53,53,53,53	0
56	MG	1A	3159	1/1	0.95	0.15	39,39,39,39	0
56	MG	1A	4046	1/1	0.95	0.13	30,30,30,30	0
56	MG	1a	1805	1/1	0.95	0.08	47,47,47,47	0
56	MG	1A	4047	1/1	0.95	0.27	50,50,50,50	0
56	MG	1E	308	1/1	0.95	0.11	34,34,34,34	0
56	MG	2a	3125	1/1	0.95	0.10	65,65,65,65	0
56	MG	2A	3545	1/1	0.95	0.14	52,52,52,52	0
56	MG	1A	3583	1/1	0.95	0.37	42,42,42,42	0
56	MG	1A	3193	1/1	0.95	0.21	34,34,34,34	0
56	MG	1A	3838	1/1	0.95	0.25	45,45,45,45	0
56	MG	2A	3550	1/1	0.95	0.15	44,44,44,44	0
56	MG	1a	1657	1/1	0.95	0.23	57,57,57,57	0
56	MG	2a	3132	1/1	0.95	0.21	63,63,63,63	0
56	MG	2A	3831	1/1	0.95	0.10	45,45,45,45	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	1A	3013	1/1	0.95	0.33	35,35,35,35	0
56	MG	1A	3088	1/1	0.95	0.11	47,47,47,47	0
56	MG	2A	3327	1/1	0.95	0.12	50,50,50,50	0
56	MG	1A	3844	1/1	0.95	0.17	54,54,54,54	0
56	MG	1A	3055	1/1	0.95	0.27	43,43,43,43	0
56	MG	2A	3842	1/1	0.95	0.13	59,59,59,59	0
56	MG	2A	3559	1/1	0.95	0.14	39,39,39,39	0
56	MG	1A	3589	1/1	0.95	0.23	52,52,52,52	0
56	MG	2A	3845	1/1	0.95	0.13	42,42,42,42	0
56	MG	2A	3561	1/1	0.95	0.09	62,62,62,62	0
56	MG	2A	3331	1/1	0.95	0.18	56,56,56,56	0
56	MG	1F	307	1/1	0.95	0.13	50,50,50,50	0
56	MG	1A	3526	1/1	0.95	0.24	53,53,53,53	0
56	MG	2A	3334	1/1	0.95	0.08	64,64,64,64	0
56	MG	1G	3001	1/1	0.95	0.15	41,41,41,41	0
56	MG	1A	3675	1/1	0.95	0.16	32,32,32,32	0
56	MG	2A	3570	1/1	0.95	0.13	53,53,53,53	0
56	MG	2A	3133	1/1	0.95	0.11	49,49,49,49	0
56	MG	1A	3269	1/1	0.95	0.12	52,52,52,52	0
56	MG	2A	3340	1/1	0.95	0.26	51,51,51,51	0
56	MG	1A	4063	1/1	0.95	0.08	57,57,57,57	0
56	MG	2a	3159	1/1	0.95	0.09	71,71,71,71	0
56	MG	1A	3528	1/1	0.95	0.17	45,45,45,45	0
56	MG	2A	3137	1/1	0.95	0.09	42,42,42,42	0
56	MG	1A	3955	1/1	0.95	0.14	30,30,30,30	0
56	MG	1A	3233	1/1	0.95	0.13	49,49,49,49	0
56	MG	1A	3001	1/1	0.95	0.17	42,42,42,42	0
56	MG	2A	3866	1/1	0.95	0.11	42,42,42,42	0
56	MG	2A	3587	1/1	0.95	0.11	37,37,37,37	0
56	MG	1A	3532	1/1	0.95	0.23	36,36,36,36	0
56	MG	1A	3140	1/1	0.95	0.14	43,43,43,43	0
56	MG	2A	3349	1/1	0.95	0.87	58,58,58,58	0
56	MG	2A	3146	1/1	0.95	0.15	43,43,43,43	0
56	MG	2a	3175	1/1	0.95	0.13	46,46,46,46	0
56	MG	1f	3001	1/1	0.95	0.20	34,34,34,34	0
56	MG	1A	4070	1/1	0.95	0.13	56,56,56,56	0
56	MG	1A	3760	1/1	0.95	0.22	35,35,35,35	0
56	MG	1A	3687	1/1	0.95	0.18	31,31,31,31	0
56	MG	1A	3475	1/1	0.95	0.11	42,42,42,42	0
56	MG	2A	3602	1/1	0.95	0.14	42,42,42,42	0
56	MG	1P	204	1/1	0.95	0.21	47,47,47,47	0
56	MG	2A	3359	1/1	0.95	0.05	56,56,56,56	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	1A	3763	1/1	0.95	0.15	52,52,52,52	0
56	MG	1A	3603	1/1	0.95	0.28	39,39,39,39	0
56	MG	2A	3162	1/1	0.95	0.17	53,53,53,53	0
56	MG	1A	3765	1/1	0.95	0.13	25,25,25,25	0
56	MG	1A	3037	1/1	0.95	0.41	40,40,40,40	0
56	MG	1w	104	1/1	0.95	0.13	69,69,69,69	0
56	MG	1A	4081	1/1	0.95	0.22	44,44,44,44	0
56	MG	1A	4082	1/1	0.95	0.25	38,38,38,38	0
56	MG	1A	3277	1/1	0.95	0.20	38,38,38,38	0
56	MG	2A	3894	1/1	0.95	0.15	55,55,55,55	0
56	MG	2A	3616	1/1	0.95	0.15	46,46,46,46	0
56	MG	1w	108	1/1	0.95	0.07	63,63,63,63	0
56	MG	2A	3619	1/1	0.95	0.16	37,37,37,37	0
56	MG	2A	3620	1/1	0.95	0.10	65,65,65,65	0
56	MG	2A	3173	1/1	0.95	0.09	51,51,51,51	0
56	MG	2a	3203	1/1	0.95	0.14	62,62,62,62	0
56	MG	1A	3608	1/1	0.95	0.20	51,51,51,51	0
56	MG	1A	3204	1/1	0.95	0.27	26,26,26,26	0
56	MG	2A	3176	1/1	0.95	0.13	46,46,46,46	0
56	MG	2A	3910	1/1	0.95	0.27	57,57,57,57	0
56	MG	2a	3211	1/1	0.95	0.13	61,61,61,61	0
56	MG	1A	3610	1/1	0.95	0.23	54,54,54,54	0
56	MG	1A	4091	1/1	0.95	0.16	49,49,49,49	0
56	MG	2A	3631	1/1	0.95	0.11	39,39,39,39	0
56	MG	2A	3379	1/1	0.95	0.21	53,53,53,53	0
56	MG	2A	3634	1/1	0.95	0.17	34,34,34,34	0
56	MG	1A	3059	1/1	0.95	0.15	48,48,48,48	0
56	MG	2A	3637	1/1	0.95	0.11	42,42,42,42	0
56	MG	1a	1695	1/1	0.95	0.15	68,68,68,68	0
56	MG	2A	3640	1/1	0.95	0.26	45,45,45,45	0
56	MG	2B	3010	1/1	0.95	0.22	73,73,73,73	0
56	MG	1U	204	1/1	0.95	0.22	38,38,38,38	0
56	MG	1U	205	1/1	0.95	0.16	35,35,35,35	0
56	MG	1A	4093	1/1	0.95	0.27	35,35,35,35	0
56	MG	1a	1699	1/1	0.95	0.28	40,40,40,40	0
56	MG	1A	3094	1/1	0.95	0.10	52,52,52,52	0
56	MG	1A	3777	1/1	0.95	0.13	55,55,55,55	0
56	MG	2a	3233	1/1	0.95	0.44	68,68,68,68	0
56	MG	1A	3430	1/1	0.95	0.10	47,47,47,47	0
56	MG	1A	3243	1/1	0.95	0.15	53,53,53,53	0
56	MG	2D	301	1/1	0.95	0.15	57,57,57,57	0
56	MG	2A	3649	1/1	0.95	0.09	69,69,69,69	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	2D	303	1/1	0.95	0.15	35,35,35,35	0
56	MG	2A	3193	1/1	0.95	0.06	55,55,55,55	0
56	MG	2A	3393	1/1	0.95	0.09	48,48,48,48	0
56	MG	2a	3242	1/1	0.95	0.20	55,55,55,55	0
56	MG	2a	3243	1/1	0.95	0.13	64,64,64,64	0
56	MG	1A	4099	1/1	0.95	0.21	41,41,41,41	0
56	MG	2e	3001	1/1	0.95	0.08	79,79,79,79	0
56	MG	2A	3657	1/1	0.95	0.13	39,39,39,39	0
56	MG	1A	3780	1/1	0.95	0.16	21,21,21,21	0
56	MG	2E	305	1/1	0.95	0.11	40,40,40,40	0
56	MG	2A	3660	1/1	0.95	0.08	45,45,45,45	0
56	MG	2n	502	1/1	0.95	0.06	86,86,86,86	0
56	MG	1A	3880	1/1	0.95	0.17	30,30,30,30	0
56	MG	1x	116	1/1	0.95	0.12	59,59,59,59	0
56	MG	2E	309	1/1	0.95	0.09	60,60,60,60	0
56	MG	2A	3663	1/1	0.95	0.05	64,64,64,64	0
56	MG	1A	3119	1/1	0.95	0.25	51,51,51,51	0
56	MG	2v	3001	1/1	0.95	0.09	69,69,69,69	0
56	MG	1A	3883	1/1	0.95	0.16	68,68,68,68	0
56	MG	2A	3669	1/1	0.95	0.12	42,42,42,42	0
56	MG	2A	3201	1/1	0.95	0.10	51,51,51,51	0
56	MG	1A	4108	1/1	0.95	0.23	48,48,48,48	0
56	MG	2w	105	1/1	0.95	0.31	70,70,70,70	0
56	MG	2Q	3002	1/1	0.95	0.16	44,44,44,44	0
56	MG	1a	1711	1/1	0.95	0.17	65,65,65,65	0
56	MG	1A	3283	1/1	0.95	0.17	40,40,40,40	0
56	MG	2A	3003	1/1	0.95	0.28	43,43,43,43	0
56	MG	1A	3040	1/1	0.95	0.20	36,36,36,36	0
56	MG	1A	3287	1/1	0.95	0.18	30,30,30,30	0
56	MG	2A	3680	1/1	0.95	0.05	62,62,62,62	0
56	MG	1A	3179	1/1	0.95	0.21	36,36,36,36	0
56	MG	2A	3007	1/1	0.95	0.10	43,43,43,43	0
56	MG	2y	3003	1/1	0.95	0.11	70,70,70,70	0
56	MG	2A	3683	1/1	0.95	0.12	62,62,62,62	0
56	MG	2X	103	1/1	0.95	0.11	46,46,46,46	0
56	MG	1a	1717	1/1	0.95	0.15	64,64,64,64	0
56	MG	2A	3213	1/1	0.95	0.23	45,45,45,45	0
57	K	1A	3584	1/1	0.95	0.13	58,58,58,58	0
56	MG	2A	3215	1/1	0.95	0.17	37,37,37,37	0
56	MG	1A	3289	1/1	0.95	0.09	52,52,52,52	0
56	MG	2A	3218	1/1	0.95	0.19	61,61,61,61	0
56	MG	1a	1796	1/1	0.96	0.06	59,59,59,59	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	2A	3103	1/1	0.96	0.15	42,42,42,42	0
56	MG	1A	3463	1/1	0.96	0.16	53,53,53,53	0
56	MG	1B	3037	1/1	0.96	0.15	40,40,40,40	0
56	MG	1A	3529	1/1	0.96	0.19	43,43,43,43	0
56	MG	2A	3509	1/1	0.96	0.16	38,38,38,38	0
56	MG	2A	3109	1/1	0.96	0.15	37,37,37,37	0
56	MG	1A	3275	1/1	0.96	0.13	44,44,44,44	0
56	MG	2a	3032	1/1	0.96	0.10	60,60,60,60	0
56	MG	2A	3514	1/1	0.96	0.13	32,32,32,32	0
56	MG	1A	3360	1/1	0.96	0.16	31,31,31,31	0
56	MG	1A	4035	1/1	0.96	0.11	46,46,46,46	0
56	MG	1A	3612	1/1	0.96	0.12	41,41,41,41	0
56	MG	1A	3045	1/1	0.96	0.20	36,36,36,36	0
56	MG	1A	3920	1/1	0.96	0.14	44,44,44,44	0
56	MG	2A	3775	1/1	0.96	0.12	38,38,38,38	0
56	MG	1A	3409	1/1	0.96	0.23	60,60,60,60	0
56	MG	1A	3807	1/1	0.96	0.15	38,38,38,38	0
56	MG	2a	3044	1/1	0.96	0.19	57,57,57,57	0
56	MG	1D	312	1/1	0.96	0.27	42,42,42,42	0
56	MG	1A	3923	1/1	0.96	0.14	47,47,47,47	0
56	MG	2A	3528	1/1	0.96	0.34	57,57,57,57	0
56	MG	1A	3106	1/1	0.96	0.19	25,25,25,25	0
56	MG	1A	3713	1/1	0.96	0.18	62,62,62,62	0
56	MG	1a	1814	1/1	0.96	0.26	55,55,55,55	0
56	MG	2A	3125	1/1	0.96	0.16	44,44,44,44	0
56	MG	1A	3536	1/1	0.96	0.17	37,37,37,37	0
56	MG	1A	3412	1/1	0.96	0.21	52,52,52,52	0
56	MG	2A	3537	1/1	0.96	0.12	35,35,35,35	0
56	MG	1A	3618	1/1	0.96	0.07	56,56,56,56	0
56	MG	1A	3930	1/1	0.96	0.15	30,30,30,30	0
56	MG	1A	3622	1/1	0.96	0.16	36,36,36,36	0
56	MG	2A	3131	1/1	0.96	0.11	42,42,42,42	0
56	MG	1a	1658	1/1	0.96	0.13	57,57,57,57	0
56	MG	1a	1822	1/1	0.96	0.11	54,54,54,54	0
56	MG	1A	3817	1/1	0.96	0.19	45,45,45,45	0
56	MG	1A	3471	1/1	0.96	0.17	57,57,57,57	0
56	MG	1A	3414	1/1	0.96	0.19	39,39,39,39	0
56	MG	1A	3820	1/1	0.96	0.11	41,41,41,41	0
56	MG	1A	3150	1/1	0.96	0.22	50,50,50,50	0
56	MG	1A	3047	1/1	0.96	0.15	21,21,21,21	0
56	MG	1A	4057	1/1	0.96	0.19	40,40,40,40	0
56	MG	2A	3141	1/1	0.96	0.09	51,51,51,51	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	2A	3142	1/1	0.96	0.17	41,41,41,41	0
56	MG	2A	3804	1/1	0.96	0.06	31,31,31,31	0
56	MG	1A	3122	1/1	0.96	0.22	44,44,44,44	0
56	MG	1A	3048	1/1	0.96	0.20	48,48,48,48	0
56	MG	1A	3228	1/1	0.96	0.20	41,41,41,41	0
56	MG	1A	3636	1/1	0.96	0.07	38,38,38,38	0
56	MG	1A	3254	1/1	0.96	0.22	53,53,53,53	0
56	MG	1A	3481	1/1	0.96	0.14	39,39,39,39	0
56	MG	1G	3005	1/1	0.96	0.10	66,66,66,66	0
56	MG	1A	3551	1/1	0.96	0.16	37,37,37,37	0
56	MG	2a	3079	1/1	0.96	0.11	59,59,59,59	0
56	MG	1A	3285	1/1	0.96	0.22	39,39,39,39	0
56	MG	2A	3156	1/1	0.96	0.15	48,48,48,48	0
56	MG	2A	3159	1/1	0.96	0.16	53,53,53,53	0
56	MG	2A	3816	1/1	0.96	0.25	57,57,57,57	0
56	MG	2a	3084	1/1	0.96	0.10	44,44,44,44	0
56	MG	1A	3422	1/1	0.96	0.24	38,38,38,38	0
56	MG	1N	203	1/1	0.96	0.19	48,48,48,48	0
56	MG	1N	204	1/1	0.96	0.51	64,64,64,64	0
56	MG	1A	3138	1/1	0.96	0.23	36,36,36,36	0
56	MG	1O	201	1/1	0.96	0.11	63,63,63,63	0
56	MG	2A	3576	1/1	0.96	0.15	39,39,39,39	0
56	MG	2A	3166	1/1	0.96	0.29	47,47,47,47	0
56	MG	1A	3175	1/1	0.96	0.21	40,40,40,40	0
56	MG	1A	3736	1/1	0.96	0.15	46,46,46,46	0
56	MG	1A	3176	1/1	0.96	0.16	37,37,37,37	0
56	MG	2A	3584	1/1	0.96	0.24	37,37,37,37	0
56	MG	2A	3585	1/1	0.96	0.10	43,43,43,43	0
56	MG	1O	205	1/1	0.96	0.08	44,44,44,44	0
56	MG	1A	3952	1/1	0.96	0.18	46,46,46,46	0
56	MG	2a	3101	1/1	0.96	0.15	56,56,56,56	0
56	MG	1A	3646	1/1	0.96	0.18	32,32,32,32	0
56	MG	1P	201	1/1	0.96	0.13	26,26,26,26	0
56	MG	2A	3835	1/1	0.96	0.09	43,43,43,43	0
56	MG	1A	3426	1/1	0.96	0.14	50,50,50,50	0
56	MG	1A	3740	1/1	0.96	0.17	28,28,28,28	0
56	MG	2A	3838	1/1	0.96	0.16	47,47,47,47	0
56	MG	1Q	201	1/1	0.96	0.20	36,36,36,36	0
56	MG	1Q	202	1/1	0.96	0.20	46,46,46,46	0
56	MG	1A	3427	1/1	0.96	0.14	44,44,44,44	0
56	MG	2A	3598	1/1	0.96	0.15	48,48,48,48	0
56	MG	2A	3372	1/1	0.96	0.24	41,41,41,41	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	1A	4080	1/1	0.96	0.24	23,23,23,23	0
56	MG	1Q	205	1/1	0.96	0.17	39,39,39,39	0
56	MG	1A	3139	1/1	0.96	0.14	48,48,48,48	0
56	MG	1A	3292	1/1	0.96	0.17	56,56,56,56	0
56	MG	2A	3851	1/1	0.96	0.08	46,46,46,46	0
56	MG	1A	3960	1/1	0.96	0.18	23,23,23,23	0
56	MG	1x	111	1/1	0.96	0.12	66,66,66,66	0
56	MG	1A	3849	1/1	0.96	0.26	44,44,44,44	0
56	MG	2a	3123	1/1	0.96	0.10	54,54,54,54	0
56	MG	1A	3652	1/1	0.96	0.21	31,31,31,31	0
56	MG	1A	3563	1/1	0.96	0.26	43,43,43,43	0
56	MG	2A	3192	1/1	0.96	0.19	44,44,44,44	0
56	MG	2A	3858	1/1	0.96	0.13	43,43,43,43	0
56	MG	1A	3293	1/1	0.96	0.24	50,50,50,50	0
56	MG	2A	3385	1/1	0.96	0.24	52,52,52,52	0
56	MG	1A	3380	1/1	0.96	0.27	48,48,48,48	0
56	MG	1A	3294	1/1	0.96	0.19	52,52,52,52	0
56	MG	2a	3133	1/1	0.96	0.13	54,54,54,54	0
56	MG	2a	3134	1/1	0.96	0.15	64,64,64,64	0
56	MG	1A	3494	1/1	0.96	0.21	39,39,39,39	0
56	MG	1A	3658	1/1	0.96	0.24	37,37,37,37	0
56	MG	2A	3621	1/1	0.96	0.09	51,51,51,51	0
56	MG	1A	3972	1/1	0.96	0.16	60,60,60,60	0
56	MG	1A	3659	1/1	0.96	0.15	23,23,23,23	0
56	MG	1U	207	1/1	0.96	0.20	31,31,31,31	0
56	MG	1A	3156	1/1	0.96	0.22	40,40,40,40	0
56	MG	1V	201	1/1	0.96	0.25	49,49,49,49	0
56	MG	1A	4100	1/1	0.96	0.16	47,47,47,47	0
56	MG	1A	4101	1/1	0.96	0.20	39,39,39,39	0
56	MG	1A	3181	1/1	0.96	0.14	54,54,54,54	0
56	MG	1W	202	1/1	0.96	0.24	50,50,50,50	0
56	MG	1A	3662	1/1	0.96	0.14	30,30,30,30	0
56	MG	2A	3401	1/1	0.96	0.16	52,52,52,52	0
56	MG	2A	3012	1/1	0.96	0.13	39,39,39,39	0
56	MG	1A	3091	1/1	0.96	0.22	43,43,43,43	0
56	MG	2A	3404	1/1	0.96	0.10	53,53,53,53	0
56	MG	2A	3405	1/1	0.96	0.24	33,33,33,33	0
56	MG	2a	3154	1/1	0.96	0.11	68,68,68,68	0
56	MG	1A	3113	1/1	0.96	0.14	35,35,35,35	0
56	MG	2A	3214	1/1	0.96	0.11	56,56,56,56	0
56	MG	1A	4106	1/1	0.96	0.17	29,29,29,29	0
56	MG	1A	4107	1/1	0.96	0.26	42,42,42,42	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	1X	106	1/1	0.96	0.19	29,29,29,29	0
56	MG	1a	1725	1/1	0.96	0.20	55,55,55,55	0
56	MG	2A	3020	1/1	0.96	0.08	49,49,49,49	0
56	MG	2a	3162	1/1	0.96	0.08	62,62,62,62	0
56	MG	2a	3163	1/1	0.96	0.10	72,72,72,72	0
56	MG	1A	3865	1/1	0.96	0.36	43,43,43,43	0
56	MG	2A	3223	1/1	0.96	0.19	44,44,44,44	0
56	MG	2A	3653	1/1	0.96	0.18	58,58,58,58	0
56	MG	2a	3167	1/1	0.96	0.09	69,69,69,69	0
56	MG	2A	3654	1/1	0.96	0.09	62,62,62,62	0
56	MG	2A	3655	1/1	0.96	0.12	65,65,65,65	0
56	MG	1A	3263	1/1	0.96	0.18	52,52,52,52	0
56	MG	2A	3900	1/1	0.96	0.34	44,44,44,44	0
56	MG	1A	3237	1/1	0.96	0.19	38,38,38,38	0
56	MG	2A	3658	1/1	0.96	0.13	55,55,55,55	0
56	MG	2A	3905	1/1	0.96	0.23	38,38,38,38	0
56	MG	2A	3226	1/1	0.96	0.10	58,58,58,58	0
56	MG	1A	3868	1/1	0.96	0.15	47,47,47,47	0
56	MG	2A	3909	1/1	0.96	0.15	43,43,43,43	0
56	MG	2A	3228	1/1	0.96	0.18	65,65,65,65	0
56	MG	1A	3388	1/1	0.96	0.20	42,42,42,42	0
56	MG	1A	3084	1/1	0.96	0.15	34,34,34,34	0
56	MG	2A	3664	1/1	0.96	0.15	54,54,54,54	0
56	MG	2A	3031	1/1	0.96	0.06	45,45,45,45	0
56	MG	2a	3185	1/1	0.96	0.15	47,47,47,47	0
56	MG	1a	1732	1/1	0.96	0.16	48,48,48,48	0
56	MG	1A	4115	1/1	0.96	0.35	51,51,51,51	0
56	MG	1A	3670	1/1	0.96	0.16	32,32,32,32	0
56	MG	2A	3035	1/1	0.96	0.10	31,31,31,31	0
56	MG	1a	1736	1/1	0.96	0.12	57,57,57,57	0
56	MG	1A	4120	1/1	0.96	0.16	44,44,44,44	0
56	MG	2B	3011	1/1	0.96	0.31	67,67,67,67	0
56	MG	2B	3012	1/1	0.96	0.23	55,55,55,55	0
56	MG	2A	3674	1/1	0.96	0.17	55,55,55,55	0
56	MG	1A	3872	1/1	0.96	0.23	33,33,33,33	0
56	MG	1A	3033	1/1	0.96	0.17	36,36,36,36	0
56	MG	2A	3242	1/1	0.96	0.16	52,52,52,52	0
56	MG	1A	3444	1/1	0.96	0.22	63,63,63,63	0
56	MG	2a	3200	1/1	0.96	0.14	76,76,76,76	0
56	MG	2A	3436	1/1	0.96	0.17	49,49,49,49	0
56	MG	1A	3346	1/1	0.96	0.19	48,48,48,48	0
56	MG	1A	3767	1/1	0.96	0.14	41,41,41,41	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	1A	3394	1/1	0.96	0.16	35,35,35,35	0
56	MG	2A	3046	1/1	0.96	0.11	48,48,48,48	0
56	MG	1A	3677	1/1	0.96	0.15	29,29,29,29	0
56	MG	2a	3208	1/1	0.96	0.30	75,75,75,75	0
56	MG	1A	3509	1/1	0.96	0.29	45,45,45,45	0
56	MG	2A	3250	1/1	0.96	0.11	41,41,41,41	0
56	MG	2A	3690	1/1	0.96	0.13	61,61,61,61	0
56	MG	2E	302	1/1	0.96	0.09	52,52,52,52	0
56	MG	1A	3771	1/1	0.96	0.18	49,49,49,49	0
56	MG	2a	3217	1/1	0.96	0.07	61,61,61,61	0
56	MG	2A	3446	1/1	0.96	0.27	45,45,45,45	0
56	MG	2A	3252	1/1	0.96	0.30	52,52,52,52	0
56	MG	1A	3882	1/1	0.96	0.17	36,36,36,36	0
56	MG	1A	4140	1/1	0.96	0.18	31,31,31,31	0
56	MG	1A	3241	1/1	0.96	0.17	44,44,44,44	0
56	MG	1A	3773	1/1	0.96	0.07	41,41,41,41	0
56	MG	1A	3885	1/1	0.96	0.15	37,37,37,37	0
56	MG	2A	3454	1/1	0.96	0.21	58,58,58,58	0
56	MG	1A	3186	1/1	0.96	0.32	39,39,39,39	0
56	MG	2A	3456	1/1	0.96	0.36	60,60,60,60	0
56	MG	1A	3681	1/1	0.96	0.07	34,34,34,34	0
56	MG	1A	4004	1/1	0.96	0.15	29,29,29,29	0
56	MG	1A	3162	1/1	0.96	0.43	44,44,44,44	0
56	MG	1A	3271	1/1	0.96	0.12	50,50,50,50	0
56	MG	1A	3685	1/1	0.96	0.23	60,60,60,60	0
56	MG	1a	1763	1/1	0.96	0.10	55,55,55,55	0
56	MG	1A	3514	1/1	0.96	0.20	53,53,53,53	0
56	MG	2a	3237	1/1	0.96	0.07	66,66,66,66	0
56	MG	1A	3188	1/1	0.96	0.17	49,49,49,49	0
56	MG	1A	3895	1/1	0.96	0.14	61,61,61,61	0
56	MG	1A	3782	1/1	0.96	0.19	25,25,25,25	0
56	MG	2W	201	1/1	0.96	0.14	57,57,57,57	0
56	MG	1B	3015	1/1	0.96	0.18	58,58,58,58	0
56	MG	1a	1770	1/1	0.96	0.10	60,60,60,60	0
56	MG	2a	3244	1/1	0.96	0.18	43,43,43,43	0
56	MG	2X	101	1/1	0.96	0.10	37,37,37,37	0
56	MG	2X	102	1/1	0.96	0.16	56,56,56,56	0
56	MG	1A	4013	1/1	0.96	0.13	33,33,33,33	0
56	MG	1a	1611	1/1	0.96	0.16	22,22,22,22	0
56	MG	1B	3017	1/1	0.96	0.31	50,50,50,50	0
56	MG	2l	201	1/1	0.96	0.14	66,66,66,66	0
56	MG	2A	3076	1/1	0.96	0.27	35,35,35,35	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	1A	3516	1/1	0.96	0.11	25,25,25,25	0
56	MG	1a	1614	1/1	0.96	0.17	45,45,45,45	0
56	MG	2A	3277	1/1	0.96	0.17	50,50,50,50	0
56	MG	1A	3592	1/1	0.96	0.20	21,21,21,21	0
56	MG	2A	3279	1/1	0.96	0.28	53,53,53,53	0
56	MG	1a	1616	1/1	0.96	0.12	55,55,55,55	0
56	MG	1A	3899	1/1	0.96	0.16	52,52,52,52	0
56	MG	1a	1618	1/1	0.96	0.17	48,48,48,48	0
56	MG	2A	3735	1/1	0.96	0.10	55,55,55,55	0
56	MG	1A	3453	1/1	0.96	0.17	57,57,57,57	0
56	MG	1B	3022	1/1	0.96	0.19	60,60,60,60	0
56	MG	2A	3739	1/1	0.96	0.10	59,59,59,59	0
56	MG	1A	3400	1/1	0.96	0.16	54,54,54,54	0
56	MG	1A	3041	1/1	0.96	0.23	38,38,38,38	0
56	MG	2A	3743	1/1	0.96	0.16	75,75,75,75	0
56	MG	1A	3354	1/1	0.96	0.38	68,68,68,68	0
56	MG	1A	3790	1/1	0.96	0.18	25,25,25,25	0
56	MG	1a	1626	1/1	0.96	0.13	61,61,61,61	0
56	MG	1B	3027	1/1	0.96	0.22	35,35,35,35	0
56	MG	2A	3494	1/1	0.96	0.27	50,50,50,50	0
56	MG	1A	3524	1/1	0.96	0.16	47,47,47,47	0
56	MG	2A	3750	1/1	0.96	0.26	47,47,47,47	0
56	MG	1A	3403	1/1	0.96	0.17	27,27,27,27	0
56	MG	1B	3030	1/1	0.96	0.15	59,59,59,59	0
56	MG	1A	3908	1/1	0.96	0.09	65,65,65,65	0
56	MG	1A	3356	1/1	0.96	0.14	39,39,39,39	0
56	MG	2A	3755	1/1	0.96	0.14	50,50,50,50	0
56	MG	1A	3117	1/1	0.96	0.38	39,39,39,39	0
56	MG	2A	3298	1/1	0.96	0.12	41,41,41,41	0
58	ZN	2Y	501	1/1	0.96	0.13	81,81,81,81	0
56	MG	1A	3796	1/1	0.96	0.18	34,34,34,34	0
58	ZN	26	501	1/1	0.96	0.14	60,60,60,60	0
58	ZN	2n	501	1/1	0.96	0.09	107,107,107,107	0
56	MG	2A	3179	1/1	0.97	0.17	59,59,59,59	0
56	MG	1A	4015	1/1	0.97	0.14	37,37,37,37	0
56	MG	2A	3665	1/1	0.97	0.09	52,52,52,52	0
56	MG	1A	3750	1/1	0.97	0.21	29,29,29,29	0
56	MG	1A	4017	1/1	0.97	0.19	36,36,36,36	0
56	MG	1A	3049	1/1	0.97	0.23	26,26,26,26	0
56	MG	2A	3037	1/1	0.97	0.14	35,35,35,35	0
56	MG	2A	3038	1/1	0.97	0.16	31,31,31,31	0
56	MG	1a	1655	1/1	0.97	0.07	43,43,43,43	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	1A	4127	1/1	0.97	0.19	34,34,34,34	0
56	MG	2A	3336	1/1	0.97	0.18	53,53,53,53	0
56	MG	1A	3676	1/1	0.97	0.21	24,24,24,24	0
56	MG	1A	3925	1/1	0.97	0.17	14,14,14,14	0
56	MG	1a	1659	1/1	0.97	0.26	62,62,62,62	0
56	MG	1A	4130	1/1	0.97	0.18	38,38,38,38	0
56	MG	1A	3602	1/1	0.97	0.25	25,25,25,25	0
56	MG	1A	3837	1/1	0.97	0.23	21,21,21,21	0
56	MG	1A	3226	1/1	0.97	0.31	47,47,47,47	0
56	MG	2a	3094	1/1	0.97	0.12	68,68,68,68	0
56	MG	2A	3048	1/1	0.97	0.12	41,41,41,41	0
56	MG	2A	3877	1/1	0.97	0.19	28,28,28,28	0
56	MG	1T	8002	1/1	0.97	0.14	58,58,58,58	0
56	MG	2a	3098	1/1	0.97	0.14	46,46,46,46	0
56	MG	1A	3198	1/1	0.97	0.20	41,41,41,41	0
56	MG	1A	4137	1/1	0.97	0.18	44,44,44,44	0
56	MG	1A	4138	1/1	0.97	0.26	43,43,43,43	0
56	MG	2A	3689	1/1	0.97	0.08	71,71,71,71	0
56	MG	1A	3543	1/1	0.97	0.17	73,73,73,73	0
56	MG	1A	4142	1/1	0.97	0.17	42,42,42,42	0
56	MG	2A	3692	1/1	0.97	0.17	56,56,56,56	0
56	MG	2A	3206	1/1	0.97	0.17	56,56,56,56	0
56	MG	1A	3842	1/1	0.97	0.27	26,26,26,26	0
56	MG	2A	3889	1/1	0.97	0.11	49,49,49,49	0
56	MG	1A	3126	1/1	0.97	0.20	41,41,41,41	0
56	MG	2A	3511	1/1	0.97	0.17	24,24,24,24	0
56	MG	1A	3845	1/1	0.97	0.17	38,38,38,38	0
56	MG	2a	3113	1/1	0.97	0.14	46,46,46,46	0
56	MG	1A	3177	1/1	0.97	0.27	38,38,38,38	0
56	MG	1A	3935	1/1	0.97	0.07	50,50,50,50	0
56	MG	2A	3516	1/1	0.97	0.14	56,56,56,56	0
56	MG	2A	3517	1/1	0.97	0.12	42,42,42,42	0
56	MG	1A	3178	1/1	0.97	0.26	21,21,21,21	0
56	MG	1A	3684	1/1	0.97	0.27	32,32,32,32	0
56	MG	2A	3705	1/1	0.97	0.32	57,57,57,57	0
56	MG	1A	3449	1/1	0.97	0.12	41,41,41,41	0
56	MG	2A	3902	1/1	0.97	0.14	43,43,43,43	0
56	MG	1a	1802	1/1	0.97	0.07	52,52,52,52	0
56	MG	2A	3709	1/1	0.97	0.14	33,33,33,33	0
56	MG	1A	3549	1/1	0.97	0.13	38,38,38,38	0
56	MG	2A	3217	1/1	0.97	0.22	64,64,64,64	0
56	MG	2A	3908	1/1	0.97	0.14	44,44,44,44	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
56	MG	2A	3524	1/1	0.97	0.11	48,48,48,48	0
56	MG	2A	3713	1/1	0.97	0.45	67,67,67,67	0
56	MG	1W	205	1/1	0.97	0.15	39,39,39,39	0
56	MG	1A	3064	1/1	0.97	0.20	53,53,53,53	0
56	MG	1A	3689	1/1	0.97	0.23	51,51,51,51	0
56	MG	1A	3690	1/1	0.97	0.14	28,28,28,28	0
56	MG	2A	3530	1/1	0.97	0.15	37,37,37,37	0
56	MG	2A	3720	1/1	0.97	0.11	41,41,41,41	0
56	MG	1A	3142	1/1	0.97	0.24	23,23,23,23	0
56	MG	1A	3205	1/1	0.97	0.20	42,42,42,42	0
56	MG	2A	3371	1/1	0.97	0.11	48,48,48,48	0
56	MG	1a	1810	1/1	0.97	0.07	51,51,51,51	0
56	MG	2A	3725	1/1	0.97	0.11	49,49,49,49	0
56	MG	1A	3500	1/1	0.97	0.18	38,38,38,38	0
56	MG	1A	3032	1/1	0.97	0.18	31,31,31,31	0
56	MG	2A	3538	1/1	0.97	0.19	35,35,35,35	0
56	MG	1Y	504	1/1	0.97	0.41	48,48,48,48	0
56	MG	1A	3621	1/1	0.97	0.11	48,48,48,48	0
56	MG	2a	3147	1/1	0.97	0.13	49,49,49,49	0
56	MG	1A	3020	1/1	0.97	0.15	25,25,25,25	0
56	MG	2A	3542	1/1	0.97	0.16	39,39,39,39	0
56	MG	1Z	303	1/1	0.97	0.17	56,56,56,56	0
56	MG	1A	3556	1/1	0.97	0.33	42,42,42,42	0
56	MG	1A	3624	1/1	0.97	0.17	28,28,28,28	0
56	MG	1A	3625	1/1	0.97	0.17	19,19,19,19	0
56	MG	1A	3864	1/1	0.97	0.15	35,35,35,35	0
56	MG	2A	3548	1/1	0.97	0.17	38,38,38,38	0
56	MG	1A	3456	1/1	0.97	0.22	48,48,48,48	0
56	MG	1A	3078	1/1	0.97	0.22	31,31,31,31	0
56	MG	2A	3742	1/1	0.97	0.09	49,49,49,49	0
56	MG	2A	3551	1/1	0.97	0.14	39,39,39,39	0
56	MG	1A	3629	1/1	0.97	0.21	32,32,32,32	0
56	MG	1A	3559	1/1	0.97	0.27	34,34,34,34	0
56	MG	2A	3554	1/1	0.97	0.10	39,39,39,39	0
56	MG	1A	3957	1/1	0.97	0.11	55,55,55,55	0
56	MG	1A	3706	1/1	0.97	0.23	40,40,40,40	0
56	MG	1A	3146	1/1	0.97	0.16	36,36,36,36	0
56	MG	1A	3506	1/1	0.97	0.19	42,42,42,42	0
56	MG	2A	3392	1/1	0.97	0.11	55,55,55,55	0
56	MG	2F	303	1/1	0.97	0.21	48,48,48,48	0
56	MG	2a	3169	1/1	0.97	0.08	51,51,51,51	0
56	MG	2F	304	1/1	0.97	0.50	53,53,53,53	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
56	MG	1A	3265	1/1	0.97	0.10	63,63,63,63	0
56	MG	2A	3097	1/1	0.97	0.13	56,56,56,56	0
56	MG	1A	3107	1/1	0.97	0.18	35,35,35,35	0
56	MG	1A	4062	1/1	0.97	0.12	14,14,14,14	0
56	MG	2Q	3001	1/1	0.97	0.15	50,50,50,50	0
56	MG	1A	3964	1/1	0.97	0.15	45,45,45,45	0
56	MG	16	104	1/1	0.97	0.21	53,53,53,53	0
56	MG	2A	3567	1/1	0.97	0.08	50,50,50,50	0
56	MG	1A	3239	1/1	0.97	0.17	30,30,30,30	0
56	MG	2A	3760	1/1	0.97	0.56	58,58,58,58	0
56	MG	2U	201	1/1	0.97	0.24	40,40,40,40	0
56	MG	2A	3761	1/1	0.97	0.23	46,46,46,46	0
56	MG	1D	301	1/1	0.97	0.27	46,46,46,46	0
56	MG	2a	3184	1/1	0.97	0.16	54,54,54,54	0
56	MG	1A	3712	1/1	0.97	0.08	40,40,40,40	0
56	MG	2A	3106	1/1	0.97	0.09	59,59,59,59	0
56	MG	1A	3375	1/1	0.97	0.18	43,43,43,43	0
56	MG	2A	3108	1/1	0.97	0.23	44,44,44,44	0
56	MG	1A	3301	1/1	0.97	0.05	54,54,54,54	0
56	MG	1A	3715	1/1	0.97	0.09	54,54,54,54	0
56	MG	1A	3014	1/1	0.97	0.20	31,31,31,31	0
56	MG	1w	102	1/1	0.97	0.17	61,61,61,61	0
56	MG	1A	3336	1/1	0.97	0.27	41,41,41,41	0
56	MG	2A	3114	1/1	0.97	0.18	55,55,55,55	0
56	MG	2A	3582	1/1	0.97	0.11	51,51,51,51	0
56	MG	2A	3115	1/1	0.97	0.11	51,51,51,51	0
56	MG	1A	3379	1/1	0.97	0.21	37,37,37,37	0
56	MG	1A	3121	1/1	0.97	0.20	43,43,43,43	0
56	MG	2A	3586	1/1	0.97	0.09	53,53,53,53	0
56	MG	1A	3339	1/1	0.97	0.14	51,51,51,51	0
56	MG	1A	3098	1/1	0.97	0.18	25,25,25,25	0
56	MG	1A	3472	1/1	0.97	0.24	56,56,56,56	0
56	MG	1a	1724	1/1	0.97	0.10	36,36,36,36	0
56	MG	1A	3887	1/1	0.97	0.23	31,31,31,31	0
56	MG	2A	3592	1/1	0.97	0.20	57,57,57,57	0
56	MG	1a	1609	1/1	0.97	0.11	54,54,54,54	0
56	MG	2a	3209	1/1	0.97	0.14	77,77,77,77	0
56	MG	2A	3785	1/1	0.97	0.26	45,45,45,45	0
56	MG	1A	4078	1/1	0.97	0.33	41,41,41,41	0
56	MG	2A	3595	1/1	0.97	0.11	49,49,49,49	0
56	MG	1A	3520	1/1	0.97	0.24	41,41,41,41	0
56	MG	1A	3168	1/1	0.97	0.14	42,42,42,42	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	1A	3522	1/1	0.97	0.16	49,49,49,49	0
56	MG	1A	3578	1/1	0.97	0.27	33,33,33,33	0
56	MG	2A	3600	1/1	0.97	0.15	40,40,40,40	0
56	MG	2A	3601	1/1	0.97	0.15	39,39,39,39	0
56	MG	1A	3803	1/1	0.97	0.39	44,44,44,44	0
56	MG	1A	3804	1/1	0.97	0.10	40,40,40,40	0
56	MG	2a	3223	1/1	0.97	0.16	52,52,52,52	0
56	MG	1A	3306	1/1	0.97	0.47	38,38,38,38	0
56	MG	1A	3806	1/1	0.97	0.17	34,34,34,34	0
56	MG	2a	3226	1/1	0.97	0.07	64,64,64,64	0
56	MG	1a	1619	1/1	0.97	0.13	62,62,62,62	0
56	MG	1A	4089	1/1	0.97	0.15	36,36,36,36	0
56	MG	1a	1739	1/1	0.97	0.05	36,36,36,36	0
56	MG	1A	3135	1/1	0.97	0.23	32,32,32,32	0
56	MG	2A	3611	1/1	0.97	0.16	62,62,62,62	0
56	MG	1A	3054	1/1	0.97	0.23	39,39,39,39	0
56	MG	1A	3582	1/1	0.97	0.20	54,54,54,54	0
56	MG	2a	3025	1/1	0.97	0.18	57,57,57,57	0
56	MG	1A	3345	1/1	0.97	0.28	47,47,47,47	0
56	MG	1A	3309	1/1	0.97	0.29	33,33,33,33	0
56	MG	1A	3347	1/1	0.97	0.24	44,44,44,44	0
56	MG	1A	4097	1/1	0.97	0.15	47,47,47,47	0
56	MG	1a	1748	1/1	0.97	0.11	43,43,43,43	0
56	MG	2A	3443	1/1	0.97	0.28	50,50,50,50	0
56	MG	1A	3735	1/1	0.97	0.18	41,41,41,41	0
56	MG	2A	3622	1/1	0.97	0.25	63,63,63,63	0
56	MG	2A	3623	1/1	0.97	0.10	48,48,48,48	0
56	MG	2A	3624	1/1	0.97	0.10	32,32,32,32	0
56	MG	2A	3145	1/1	0.97	0.15	36,36,36,36	0
56	MG	2A	3002	1/1	0.97	0.30	57,57,57,57	0
56	MG	2A	3296	1/1	0.97	0.20	45,45,45,45	0
56	MG	2i	8001	1/1	0.97	0.12	51,51,51,51	0
56	MG	1A	3433	1/1	0.97	0.16	47,47,47,47	0
56	MG	1A	3905	1/1	0.97	0.16	46,46,46,46	0
56	MG	2a	3041	1/1	0.97	0.26	50,50,50,50	0
56	MG	1A	3137	1/1	0.97	0.20	33,33,33,33	0
56	MG	2a	3043	1/1	0.97	0.08	64,64,64,64	0
56	MG	2A	3151	1/1	0.97	0.18	40,40,40,40	0
56	MG	1A	3311	1/1	0.97	0.25	48,48,48,48	0
56	MG	2A	3633	1/1	0.97	0.24	55,55,55,55	0
56	MG	2A	3302	1/1	0.97	0.19	66,66,66,66	0
56	MG	1A	3010	1/1	0.97	0.20	39,39,39,39	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	1A	3909	1/1	0.97	0.20	40,40,40,40	0
56	MG	2A	3457	1/1	0.97	0.34	57,57,57,57	0
56	MG	1a	1756	1/1	0.97	0.14	72,72,72,72	0
56	MG	2A	3157	1/1	0.97	0.14	58,58,58,58	0
56	MG	2w	103	1/1	0.97	0.10	56,56,56,56	0
56	MG	1A	3220	1/1	0.97	0.23	41,41,41,41	0
56	MG	1a	1758	1/1	0.97	0.06	56,56,56,56	0
56	MG	1A	3822	1/1	0.97	0.16	48,48,48,48	0
56	MG	2A	3834	1/1	0.97	0.10	40,40,40,40	0
56	MG	1N	206	1/1	0.97	0.29	42,42,42,42	0
56	MG	1A	3534	1/1	0.97	0.18	33,33,33,33	0
56	MG	2A	3467	1/1	0.97	0.09	60,60,60,60	0
56	MG	2A	3164	1/1	0.97	0.25	53,53,53,53	0
56	MG	1A	3593	1/1	0.97	0.18	56,56,56,56	0
56	MG	2x	105	1/1	0.97	0.15	57,57,57,57	0
56	MG	2A	3841	1/1	0.97	0.16	30,30,30,30	0
56	MG	2A	3650	1/1	0.97	0.14	41,41,41,41	0
56	MG	1A	3194	1/1	0.97	0.26	43,43,43,43	0
56	MG	1A	3173	1/1	0.97	0.17	42,42,42,42	0
56	MG	1A	4009	1/1	0.97	0.21	27,27,27,27	0
56	MG	1A	3224	1/1	0.97	0.19	50,50,50,50	0
56	MG	1A	3538	1/1	0.97	0.13	54,54,54,54	0
56	MG	1a	1768	1/1	0.97	0.06	53,53,53,53	0
56	MG	2A	3026	1/1	0.97	0.19	36,36,36,36	0
56	MG	1A	4114	1/1	0.97	0.21	34,34,34,34	0
56	MG	1A	3355	1/1	0.97	0.26	47,47,47,47	0
56	MG	1A	3748	1/1	0.97	0.23	25,25,25,25	0
58	ZN	25	102	1/1	0.97	0.31	68,68,68,68	0
56	MG	1A	3599	1/1	0.97	0.16	21,21,21,21	0
58	ZN	29	101	1/1	0.97	0.08	73,73,73,73	0
56	MG	1a	1649	1/1	0.97	0.12	45,45,45,45	0
59	SF4	2d	501	8/8	0.97	0.11	61,71,85,99	0
56	MG	2A	3677	1/1	0.98	0.32	35,35,35,35	0
56	MG	1A	3359	1/1	0.98	0.14	38,38,38,38	0
56	MG	2A	3679	1/1	0.98	0.11	41,41,41,41	0
56	MG	1A	4001	1/1	0.98	0.19	17,17,17,17	0
56	MG	2A	3820	1/1	0.98	0.07	49,49,49,49	0
56	MG	1A	3809	1/1	0.98	0.30	51,51,51,51	0
56	MG	1l	201	1/1	0.98	0.16	43,43,43,43	0
56	MG	1A	3467	1/1	0.98	0.16	45,45,45,45	0
56	MG	2A	3181	1/1	0.98	0.22	40,40,40,40	0
56	MG	20	3002	1/1	0.98	0.07	63,63,63,63	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	2A	3070	1/1	0.98	0.24	42,42,42,42	0
56	MG	1A	3873	1/1	0.98	0.21	35,35,35,35	0
56	MG	2A	3184	1/1	0.98	0.25	48,48,48,48	0
56	MG	1A	4077	1/1	0.98	0.19	11,11,11,11	0
56	MG	1A	3811	1/1	0.98	0.22	45,45,45,45	0
56	MG	1A	3393	1/1	0.98	0.18	50,50,50,50	0
56	MG	1A	3700	1/1	0.98	0.20	16,16,16,16	0
56	MG	2A	3427	1/1	0.98	0.13	45,45,45,45	0
56	MG	1A	3814	1/1	0.98	0.17	45,45,45,45	0
56	MG	1A	3039	1/1	0.98	0.17	36,36,36,36	0
56	MG	2A	3695	1/1	0.98	0.09	38,38,38,38	0
56	MG	1A	3031	1/1	0.98	0.17	31,31,31,31	0
56	MG	1A	3276	1/1	0.98	0.14	49,49,49,49	0
56	MG	1A	4085	1/1	0.98	0.22	21,21,21,21	0
56	MG	1A	4086	1/1	0.98	0.33	43,43,43,43	0
56	MG	2A	3840	1/1	0.98	0.18	43,43,43,43	0
56	MG	1A	3650	1/1	0.98	0.20	35,35,35,35	0
56	MG	2A	3435	1/1	0.98	0.07	49,49,49,49	0
56	MG	2a	3009	1/1	0.98	0.07	60,60,60,60	0
56	MG	2A	3083	1/1	0.98	0.43	49,49,49,49	0
56	MG	2A	3566	1/1	0.98	0.14	33,33,33,33	0
56	MG	1X	103	1/1	0.98	0.26	40,40,40,40	0
56	MG	1A	3025	1/1	0.98	0.17	41,41,41,41	0
56	MG	2A	3847	1/1	0.98	0.06	42,42,42,42	0
56	MG	2A	3706	1/1	0.98	0.12	47,47,47,47	0
56	MG	2A	3199	1/1	0.98	0.18	50,50,50,50	0
56	MG	1A	3042	1/1	0.98	0.18	40,40,40,40	0
56	MG	1A	4090	1/1	0.98	0.29	37,37,37,37	0
56	MG	1A	3067	1/1	0.98	0.18	51,51,51,51	0
56	MG	1A	3366	1/1	0.98	0.17	38,38,38,38	0
56	MG	2a	3021	1/1	0.98	0.14	65,65,65,65	0
56	MG	2A	3204	1/1	0.98	0.17	48,48,48,48	0
56	MG	1A	3068	1/1	0.98	0.24	38,38,38,38	0
56	MG	2A	3714	1/1	0.98	0.23	39,39,39,39	0
56	MG	1A	3517	1/1	0.98	0.14	37,37,37,37	0
56	MG	2A	3092	1/1	0.98	0.27	43,43,43,43	0
56	MG	2A	3578	1/1	0.98	0.09	39,39,39,39	0
56	MG	1A	3605	1/1	0.98	0.20	32,32,32,32	0
56	MG	1A	3606	1/1	0.98	0.23	36,36,36,36	0
56	MG	2A	3581	1/1	0.98	0.17	25,25,25,25	0
56	MG	1A	3477	1/1	0.98	0.25	48,48,48,48	0
56	MG	1D	306	1/1	0.98	0.21	32,32,32,32	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	1A	3069	1/1	0.98	0.25	20,20,20,20	0
56	MG	1A	4023	1/1	0.98	0.14	47,47,47,47	0
56	MG	1A	3439	1/1	0.98	0.14	40,40,40,40	0
56	MG	1A	3893	1/1	0.98	0.18	17,17,17,17	0
56	MG	2a	3190	1/1	0.98	0.07	66,66,66,66	0
56	MG	1A	3369	1/1	0.98	0.19	57,57,57,57	0
56	MG	2A	3870	1/1	0.98	0.18	33,33,33,33	0
56	MG	1I	102	1/1	0.98	0.10	36,36,36,36	0
56	MG	1A	3663	1/1	0.98	0.18	28,28,28,28	0
56	MG	2A	3873	1/1	0.98	0.12	40,40,40,40	0
56	MG	1A	3611	1/1	0.98	0.23	25,25,25,25	0
56	MG	2A	3461	1/1	0.98	0.26	52,52,52,52	0
56	MG	1A	3338	1/1	0.98	0.20	49,49,49,49	0
56	MG	2A	3221	1/1	0.98	0.10	48,48,48,48	0
56	MG	2A	3464	1/1	0.98	0.40	54,54,54,54	0
56	MG	1a	1679	1/1	0.98	0.10	73,73,73,73	0
56	MG	2A	3736	1/1	0.98	0.13	67,67,67,67	0
56	MG	1A	3961	1/1	0.98	0.18	38,38,38,38	0
56	MG	1A	3775	1/1	0.98	0.21	27,27,27,27	0
56	MG	1A	3212	1/1	0.98	0.37	32,32,32,32	0
56	MG	1A	3003	1/1	0.98	0.15	27,27,27,27	0
56	MG	1A	3965	1/1	0.98	0.14	67,67,67,67	0
56	MG	1A	3028	1/1	0.98	0.24	34,34,34,34	0
56	MG	1A	3174	1/1	0.98	0.14	38,38,38,38	0
56	MG	1A	3314	1/1	0.98	0.16	33,33,33,33	0
56	MG	1A	3841	1/1	0.98	0.15	27,27,27,27	0
56	MG	1A	4039	1/1	0.98	0.15	21,21,21,21	0
56	MG	2A	3009	1/1	0.98	0.13	31,31,31,31	0
56	MG	2a	3216	1/1	0.98	0.12	65,65,65,65	0
56	MG	1a	1785	1/1	0.98	0.09	55,55,55,55	0
56	MG	2A	3609	1/1	0.98	0.16	42,42,42,42	0
56	MG	1A	3072	1/1	0.98	0.26	19,19,19,19	0
56	MG	2A	3237	1/1	0.98	0.15	39,39,39,39	0
56	MG	1F	304	1/1	0.98	0.25	40,40,40,40	0
56	MG	2A	3357	1/1	0.98	0.10	39,39,39,39	0
56	MG	1A	4117	1/1	0.98	0.22	39,39,39,39	0
56	MG	1A	4118	1/1	0.98	0.24	36,36,36,36	0
56	MG	1A	4119	1/1	0.98	0.23	34,34,34,34	0
56	MG	1A	3619	1/1	0.98	0.20	31,31,31,31	0
56	MG	2A	3904	1/1	0.98	0.19	41,41,41,41	0
56	MG	2A	3618	1/1	0.98	0.08	39,39,39,39	0
56	MG	2A	3486	1/1	0.98	0.36	55,55,55,55	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	1A	4121	1/1	0.98	0.17	34,34,34,34	0
56	MG	1A	3673	1/1	0.98	0.15	29,29,29,29	0
56	MG	1A	3105	1/1	0.98	0.17	40,40,40,40	0
56	MG	2A	3021	1/1	0.98	0.11	28,28,28,28	0
56	MG	1A	3413	1/1	0.98	0.21	36,36,36,36	0
56	MG	1A	3035	1/1	0.98	0.23	20,20,20,20	0
56	MG	1A	4126	1/1	0.98	0.18	45,45,45,45	0
56	MG	2A	3025	1/1	0.98	0.27	42,42,42,42	0
56	MG	1A	3290	1/1	0.98	0.24	46,46,46,46	0
56	MG	2A	3027	1/1	0.98	0.32	48,48,48,48	0
56	MG	1A	3197	1/1	0.98	0.19	52,52,52,52	0
56	MG	1A	3789	1/1	0.98	0.11	29,29,29,29	0
56	MG	1A	3914	1/1	0.98	0.10	53,53,53,53	0
56	MG	1A	4050	1/1	0.98	0.23	32,32,32,32	0
56	MG	1A	3011	1/1	0.98	0.13	46,46,46,46	0
56	MG	2A	3377	1/1	0.98	0.15	57,57,57,57	0
56	MG	2A	3636	1/1	0.98	0.15	59,59,59,59	0
56	MG	2f	3001	1/1	0.98	0.19	41,41,41,41	0
56	MG	1A	3030	1/1	0.98	0.18	34,34,34,34	0
56	MG	2B	3015	1/1	0.98	0.19	50,50,50,50	0
56	MG	1A	3628	1/1	0.98	0.27	28,28,28,28	0
56	MG	1A	4136	1/1	0.98	0.16	40,40,40,40	0
56	MG	1A	3455	1/1	0.98	0.12	47,47,47,47	0
56	MG	1A	3984	1/1	0.98	0.16	34,34,34,34	0
56	MG	1A	4139	1/1	0.98	0.15	35,35,35,35	0
56	MG	1a	1715	1/1	0.98	0.11	49,49,49,49	0
56	MG	1A	3200	1/1	0.98	0.27	23,23,23,23	0
56	MG	1A	4141	1/1	0.98	0.36	50,50,50,50	0
56	MG	2A	3513	1/1	0.98	0.15	34,34,34,34	0
56	MG	2A	3150	1/1	0.98	0.35	39,39,39,39	0
56	MG	2a	3102	1/1	0.98	0.14	58,58,58,58	0
56	MG	1A	3223	1/1	0.98	0.14	32,32,32,32	0
56	MG	1B	3001	1/1	0.98	0.30	48,48,48,48	0
56	MG	1A	3296	1/1	0.98	0.24	58,58,58,58	0
56	MG	2A	3154	1/1	0.98	0.14	48,48,48,48	0
56	MG	1a	1816	1/1	0.98	0.13	48,48,48,48	0
56	MG	1A	4059	1/1	0.98	0.20	21,21,21,21	0
56	MG	1A	3988	1/1	0.98	0.07	68,68,68,68	0
56	MG	2A	3158	1/1	0.98	0.17	41,41,41,41	0
56	MG	1A	3633	1/1	0.98	0.16	58,58,58,58	0
56	MG	1A	3860	1/1	0.98	0.18	47,47,47,47	0
56	MG	2A	3525	1/1	0.98	0.13	34,34,34,34	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	1A	3297	1/1	0.98	0.29	32,32,32,32	0
56	MG	1R	201	1/1	0.98	0.13	30,30,30,30	0
56	MG	1A	3635	1/1	0.98	0.11	32,32,32,32	0
56	MG	1A	3161	1/1	0.98	0.27	38,38,38,38	0
56	MG	1a	1825	1/1	0.98	0.18	37,37,37,37	0
56	MG	1A	3038	1/1	0.98	0.13	50,50,50,50	0
56	MG	1A	3462	1/1	0.98	0.13	32,32,32,32	0
56	MG	1A	3389	1/1	0.98	0.20	53,53,53,53	0
56	MG	2A	3668	1/1	0.98	0.12	45,45,45,45	0
56	MG	2Q	3003	1/1	0.98	0.17	51,51,51,51	0
56	MG	2a	3124	1/1	0.98	0.13	61,61,61,61	0
56	MG	2A	3059	1/1	0.98	0.17	46,46,46,46	0
56	MG	2A	3170	1/1	0.98	0.14	54,54,54,54	0
58	ZN	1n	101	1/1	0.98	0.12	71,71,71,71	0
56	MG	2A	3060	1/1	0.98	0.10	53,53,53,53	0
56	MG	2A	3409	1/1	0.98	0.23	47,47,47,47	0
56	MG	1A	3111	1/1	0.98	0.15	40,40,40,40	0
56	MG	1A	3050	1/1	0.98	0.28	32,32,32,32	0
56	MG	1a	1734	1/1	0.98	0.08	67,67,67,67	0
56	MG	1A	3547	1/1	0.98	0.14	53,53,53,53	0
59	SF4	1d	501	8/8	0.98	0.13	59,71,76,86	0
56	MG	2V	201	1/1	0.98	0.16	53,53,53,53	0
56	MG	2A	3319	1/1	0.99	0.07	49,49,49,49	0
56	MG	1A	3731	1/1	0.99	0.18	17,17,17,17	0
56	MG	2a	3212	1/1	0.99	0.12	51,51,51,51	0
56	MG	1a	1653	1/1	0.99	0.13	54,54,54,54	0
56	MG	1A	3056	1/1	0.99	0.27	28,28,28,28	0
56	MG	1A	3022	1/1	0.99	0.14	21,21,21,21	0
56	MG	1A	3644	1/1	0.99	0.22	33,33,33,33	0
56	MG	1A	3702	1/1	0.99	0.15	34,34,34,34	0
56	MG	1P	203	1/1	0.99	0.27	30,30,30,30	0
56	MG	2A	3882	1/1	0.99	0.13	44,44,44,44	0
56	MG	1A	3411	1/1	0.99	0.18	43,43,43,43	0
56	MG	1a	1740	1/1	0.99	0.17	35,35,35,35	0
56	MG	1A	3843	1/1	0.99	0.21	31,31,31,31	0
56	MG	2A	3102	1/1	0.99	0.04	56,56,56,56	0
56	MG	2A	3231	1/1	0.99	0.14	49,49,49,49	0
56	MG	1A	3688	1/1	0.99	0.15	15,15,15,15	0
56	MG	1A	3109	1/1	0.99	0.20	35,35,35,35	0
56	MG	1W	203	1/1	0.99	0.24	30,30,30,30	0
56	MG	2A	3013	1/1	0.99	0.20	44,44,44,44	0
56	MG	1A	3620	1/1	0.99	0.19	25,25,25,25	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	1A	3286	1/1	0.99	0.41	49,49,49,49	0
56	MG	1A	3828	1/1	0.99	0.21	34,34,34,34	0
56	MG	1A	3027	1/1	0.99	0.20	33,33,33,33	0
56	MG	1E	303	1/1	0.99	0.16	26,26,26,26	0
56	MG	2A	3049	1/1	0.99	0.16	23,23,23,23	0
56	MG	2A	3898	1/1	0.99	0.13	28,28,28,28	0
56	MG	1A	3793	1/1	0.99	0.24	37,37,37,37	0
56	MG	2A	3448	1/1	0.99	0.20	49,49,49,49	0
56	MG	1A	3046	1/1	0.99	0.17	32,32,32,32	0
56	MG	1A	4132	1/1	0.99	0.23	39,39,39,39	0
56	MG	1A	3097	1/1	0.99	0.11	35,35,35,35	0
56	MG	1A	3577	1/1	0.99	0.17	27,27,27,27	0
58	ZN	1Y	501	1/1	0.99	0.19	60,60,60,60	0
56	MG	1a	1700	1/1	0.99	0.26	50,50,50,50	0
58	ZN	19	103	1/1	0.99	0.19	44,44,44,44	0
56	MG	1n	103	1/1	0.99	0.23	48,48,48,48	0
56	MG	2A	3639	1/1	0.99	0.17	34,34,34,34	0
56	MG	1A	3601	1/1	0.99	0.18	11,11,11,11	0
56	MG	1B	3036	1/1	0.99	0.10	36,36,36,36	0
56	MG	2a	3205	1/1	0.99	0.23	70,70,70,70	0
56	MG	1A	3085	1/1	0.99	0.26	30,30,30,30	0
56	MG	2A	3352	1/1	0.99	0.14	53,53,53,53	0
56	MG	1A	3008	1/1	0.99	0.18	26,26,26,26	0
56	MG	2A	3533	1/1	0.99	0.12	48,48,48,48	0
58	ZN	15	101	1/1	1.00	0.27	37,37,37,37	0
58	ZN	16	102	1/1	1.00	0.22	44,44,44,44	0

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

There are no such residues in this entry.