



Full wwPDB X-ray Structure Validation Report ⓘ

Jan 2, 2024 – 07:31 pm GMT

PDB ID : 5F8K
Title : Crystal structure of the Bac7(1-16) antimicrobial peptide bound to the *Thermus thermophilus* 70S ribosome
Authors : Seefeldt, A.C.; Graf, M.; Perebaskine, N.; Nguyen, F.; Arenz, S.; Mardirossian, M.; Scocchi, M.; Wilson, D.N.; Innis, C.A.
Deposited on : 2015-12-09
Resolution : 2.80 Å(reported)

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

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

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 : 1.8.4, CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.36
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.36

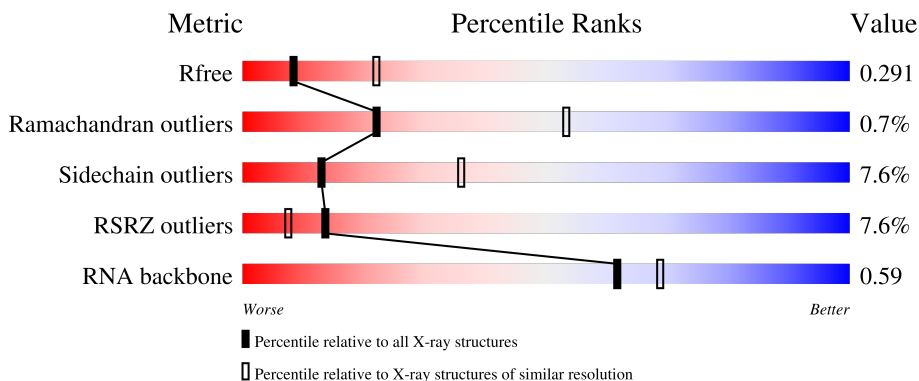
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 Å.

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



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

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments 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: 9%; 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: 5%; height: 10px; background-color: grey;"></div> </div> <p style="margin-left: 20px;">9% 81% 16% ..</p>
1	2A	2915	<div style="display: flex; align-items: center;"> <div style="width: 10%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 82%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 15%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 5%; height: 10px; background-color: grey;"></div> </div> <p style="margin-left: 20px;">10% 82% 15% ..</p>
2	1B	120	<div style="display: flex; align-items: center;"> <div style="width: 2%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 92%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 8%; height: 10px; background-color: yellow;"></div> </div> <p style="margin-left: 20px;">2% 92% 8%</p>
2	2B	120	<div style="display: flex; align-items: center;"> <div style="width: 9%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 94%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 5%; height: 10px; background-color: yellow;"></div> </div> <p style="margin-left: 20px;">9% 94% 5% .</p>
3	1D	275	<div style="display: flex; align-items: center;"> <div style="width: 92%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 8%; height: 10px; background-color: yellow;"></div> </div> <p style="margin-left: 20px;">92% 8%</p>

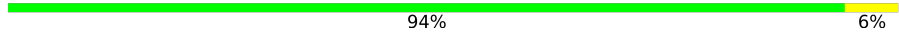

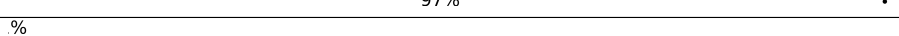


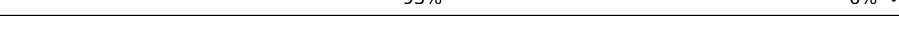
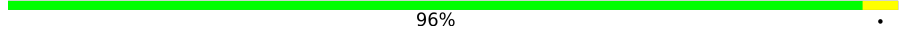

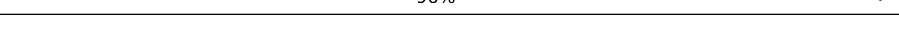
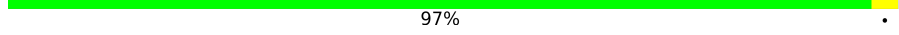

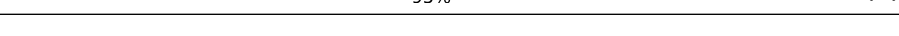
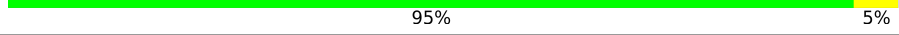

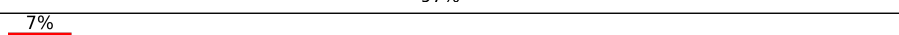



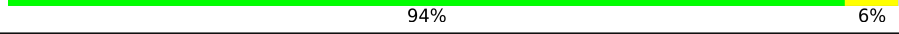
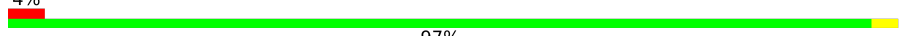
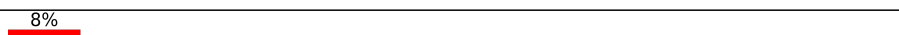
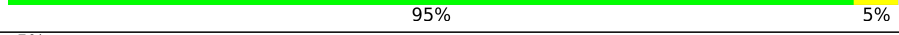

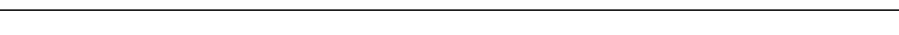
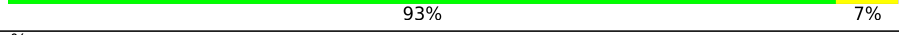
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Mol	Chain	Length	Quality of chain
3	2D	275	93% 7%
4	1E	204	91% 9%
4	2E	204	92% 8%
5	1F	203	95% 5%
5	2F	203	96% .
6	1G	181	94% 6% .
6	2G	181	17% 93% 7% .
7	1H	174	94% 6%
7	2H	174	20% 93% 7% .
8	1I	147	6% 91% 9%
8	2I	147	10% 89% 10% .
9	1N	140	94% 6%
9	2N	140	90% 10%
10	1O	122	94% 6%
10	2O	122	97% .
11	1P	149	2% 95% 5%
11	2P	149	5% 95% 5%
12	1Q	141	93% 7%
12	2Q	141	95% 5%
13	1R	118	92% 8%
13	2R	118	93% 7%
14	1S	110	96% . .
14	2S	110	11% 95% 5%
15	1T	131	2% 96% .
15	2T	131	3% 93% 7%

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Mol	Chain	Length	Quality of chain
16	1U	116	 94% 6%
16	2U	116	 5% 97%
17	1V	101	 % 89% 10%
17	2V	101	 5% 93% 6%
18	1W	112	 96%
18	2W	112	 2% 96%
19	1X	95	 97%
19	2X	95	 % 95%
20	1Y	107	 95% 5%
20	2Y	107	 5% 97%
21	1Z	203	 7% 90% 10%
21	2Z	203	 13% 93% 6%
22	10	77	 % 94% 6%
22	20	77	 4% 97%
23	11	97	 8% 95% 5%
23	21	97	 5% 93% 7%
24	12	70	 93% 7%
24	22	70	 % 93% 7%
25	13	59	 95% 5%
25	23	59	 8% 95% 5%
26	14	69	 14% 87% 12%
26	24	69	 45% 88% 12%
27	15	59	 95% 5%
27	25	59	 3% 98%
28	16	53	 98%

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Mol	Chain	Length	Quality of chain
28	26	53	6% 91% 9%
29	17	48	96% .
29	27	48	2% 98% .
30	18	64	92% 8%
30	28	64	91% 9%
31	19	37	97% .
31	29	37	100%
32	1a	1520	8% 83% 14% ..
32	2a	1520	10% 82% 15% ..
33	1b	231	15% 87% 12% .
33	2b	231	28% 89% 11%
34	1c	206	6% 95% 5%
34	2c	206	17% 95% 5%
35	1d	208	4% 95% 5%
35	2d	208	10% 94% 6%
36	1e	148	4% 93% 7%
36	2e	148	4% 94% 6%
37	1f	100	2% 97% .
37	2f	100	4% 90% 10%
38	1g	155	9% 92% 8%
38	2g	155	13% 95% 5% .
39	1h	137	% 97% .
39	2h	137	4% 96% .
40	1i	127	13% 91% 9%
40	2i	127	26% 87% 12% .





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Mol	Chain	Length	Quality of chain
41	1j	97	16% 90% 10%
41	2j	97	25% 91% 8%
42	1k	114	10% 96% .
42	2k	114	11% 96% .
43	1l	122	7% 96% .
43	2l	122	3% 94% 6%
44	1m	116	12% 92% 8%
44	2m	116	10% 90% 9%
45	1n	60	7% 90% 10%
45	2n	60	20% 95% 5%
46	1o	88	% 95% 5%
46	2o	88	% 92% 7%
47	1p	82	7% 87% 13%
47	2p	82	9% 85% 15%
48	1q	99	% 97% .
48	2q	99	% 96% .
49	1r	68	12% 96% .
49	2r	68	16% 94% 6%
50	1s	83	2% 90% 10%
50	2s	83	19% 94% 6%
51	1t	98	2% 90% 6%
51	2t	98	4% 92% 7%
52	1u	23	96% .
52	2u	23	30% 100%
53	1v	3	100%

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Mol	Chain	Length	Quality of chain
53	2v	3	 100%
54	1x	76	 3% 68% 32%
54	2x	76	 22% 78% 22%
55	1y	16	 75% 19% 6%
55	2y	16	 81% 12% 6%

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	1A	8888	-	-	-	X
56	MG	1a	1660	-	-	-	X
56	MG	2A	3061	-	-	-	X
56	MG	2A	3074	-	-	-	X
56	MG	2A	3079	-	-	-	X
56	MG	2A	3092	-	-	-	X
56	MG	2A	3093	-	-	-	X
56	MG	2A	3098	-	-	-	X
56	MG	2A	3125	-	-	-	X
56	MG	2A	3243	-	-	-	X
56	MG	2A	3603	-	-	-	X
56	MG	2A	3686	-	-	-	X
56	MG	2A	3690	-	-	-	X
56	MG	2A	3699	-	-	-	X
56	MG	2A	3742	-	-	-	X
56	MG	2A	3744	-	-	-	X
56	MG	2A	3763	-	-	-	X
56	MG	2A	3775	-	-	-	X
56	MG	2A	3803	-	-	-	X
56	MG	2A	3856	-	-	-	X
56	MG	2A	3866	-	-	-	X
56	MG	2A	3899	-	-	-	X
56	MG	2A	3967	-	-	-	X
56	MG	2B	3014	-	-	-	X
56	MG	2B	3017	-	-	-	X
56	MG	2H	8001	-	-	-	X
56	MG	2H	8002	-	-	-	X
56	MG	2a	1610	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
56	MG	2a	1635	-	-	-	X
56	MG	2a	1646	-	-	-	X
56	MG	2a	1660	-	-	-	X
56	MG	2a	1667	-	-	-	X
56	MG	2a	1680	-	-	-	X
56	MG	2a	1718	-	-	-	X
56	MG	2a	1719	-	-	-	X
56	MG	2a	1725	-	-	-	X
56	MG	2a	1758	-	-	-	X
56	MG	2a	1780	-	-	-	X
56	MG	2a	1805	-	-	-	X
56	MG	2a	1807	-	-	-	X
56	MG	2h	3002	-	-	-	X
56	MG	2l	201	-	-	-	X
56	MG	2x	104	-	-	-	X

2 Entry composition [i](#)

There are 60 unique types of molecules in this entry. The entry contains 296108 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a RNA chain called 23S ribosomal RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
1	1A	2872	Total	C	N	O	P	0	0	0
			61872	27540	11574	19886	2872			
1	2A	2867	Total	C	N	O	P	0	0	0
			61761	27491	11552	19852	2866			

- 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
			2575	1145	476	834	120			
2	2B	120	Total	C	N	O	P	0	0	0
			2571	1146	476	831	118			

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
4	1E	204	Total	C	N	O	S	0	0	0
			1559	985	298	270	6			
4	2E	204	Total	C	N	O	S	0	0	0
			1559	985	298	270	6			

- Molecule 5 is a protein called 50S ribosomal protein L4.

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

- Molecule 53 is a RNA chain called mRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
53	1v	3	Total	C	N	O	P	0	0	0
			65	29	12	21	3			
53	2v	3	Total	C	N	O	P	0	0	0
			65	29	12	21	3			

- Molecule 54 is a RNA chain called tRNAiMet.

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

- Molecule 55 is a protein called Cathelicidin-3.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
55	1y	16	Total	C	N	O	0	0	0
			147	90	40	17			
55	2y	16	Total	C	N	O	0	0	0
			147	90	40	17			

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
56	1A	973	Total	Mg	0	0
			973	973		
56	1B	27	Total	Mg	0	0
			27	27		
56	1D	14	Total	Mg	0	0
			14	14		
56	1E	7	Total	Mg	0	0
			7	7		
56	1F	10	Total	Mg	0	0
			10	10		
56	1G	3	Total	Mg	0	0
			3	3		
56	1H	2	Total	Mg	0	0
			2	2		
56	1N	4	Total	Mg	0	0
			4	4		
56	1P	4	Total	Mg	0	0
			4	4		

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
56	1Q	6	Total Mg 6 6	0	0
56	1R	4	Total Mg 4 4	0	0
56	1S	1	Total Mg 1 1	0	0
56	1T	1	Total Mg 1 1	0	0
56	1U	3	Total Mg 3 3	0	0
56	1V	3	Total Mg 3 3	0	0
56	1W	3	Total Mg 3 3	0	0
56	1X	1	Total Mg 1 1	0	0
56	10	8	Total Mg 8 8	0	0
56	11	2	Total Mg 2 2	0	0
56	13	2	Total Mg 2 2	0	0
56	15	7	Total Mg 7 7	0	0
56	17	2	Total Mg 2 2	0	0
56	18	1	Total Mg 1 1	0	0
56	19	3	Total Mg 3 3	0	0
56	1a	240	Total Mg 240 240	0	0
56	1b	1	Total Mg 1 1	0	0
56	1d	5	Total Mg 5 5	0	0
56	1e	1	Total Mg 1 1	0	0
56	1f	1	Total Mg 1 1	0	0
56	1g	1	Total Mg 1 1	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
56	1h	1	Total 1	Mg 1	0	0
56	1i	1	Total 1	Mg 1	0	0
56	1l	3	Total 3	Mg 3	0	0
56	1n	1	Total 1	Mg 1	0	0
56	1o	2	Total 2	Mg 2	0	0
56	1q	1	Total 1	Mg 1	0	0
56	1t	1	Total 1	Mg 1	0	0
56	1x	13	Total 13	Mg 13	0	0
56	2A	986	Total 986	Mg 986	0	0
56	2B	25	Total 25	Mg 25	0	0
56	2D	17	Total 17	Mg 17	0	0
56	2E	6	Total 6	Mg 6	0	0
56	2F	9	Total 9	Mg 9	0	0
56	2G	3	Total 3	Mg 3	0	0
56	2H	2	Total 2	Mg 2	0	0
56	2N	3	Total 3	Mg 3	0	0
56	2P	3	Total 3	Mg 3	0	0
56	2Q	4	Total 4	Mg 4	0	0
56	2R	2	Total 2	Mg 2	0	0
56	2S	1	Total 1	Mg 1	0	0
56	2U	7	Total 7	Mg 7	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
56	2V	1	Total 1	Mg 1	0	0
56	2W	1	Total 1	Mg 1	0	0
56	2X	2	Total 2	Mg 2	0	0
56	2Y	2	Total 2	Mg 2	0	0
56	20	5	Total 5	Mg 5	0	0
56	23	2	Total 2	Mg 2	0	0
56	25	3	Total 3	Mg 3	0	0
56	27	2	Total 2	Mg 2	0	0
56	28	1	Total 1	Mg 1	0	0
56	29	2	Total 2	Mg 2	0	0
56	2a	221	Total 221	Mg 221	0	0
56	2b	1	Total 1	Mg 1	0	0
56	2d	4	Total 4	Mg 4	0	0
56	2e	1	Total 1	Mg 1	0	0
56	2f	1	Total 1	Mg 1	0	0
56	2g	1	Total 1	Mg 1	0	0
56	2h	2	Total 2	Mg 2	0	0
56	2i	1	Total 1	Mg 1	0	0
56	2j	1	Total 1	Mg 1	0	0
56	2l	2	Total 2	Mg 2	0	0
56	2n	1	Total 1	Mg 1	0	0

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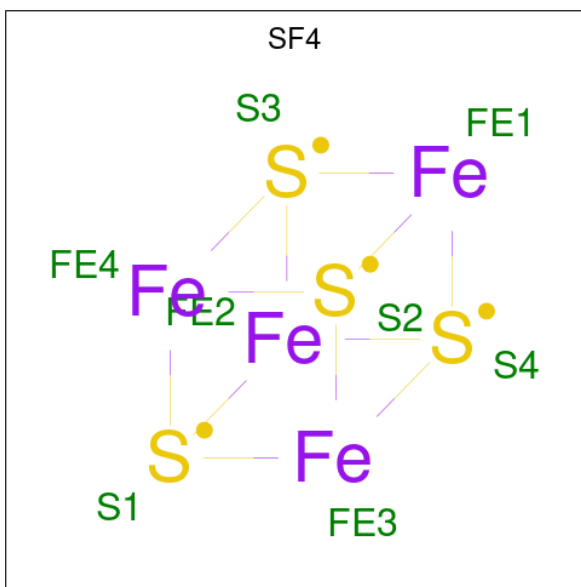
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
56	2o	1	Total 1	Mg 1	0	0
56	2t	1	Total 1	Mg 1	0	0
56	2v	1	Total 1	Mg 1	0	0
56	2x	12	Total 12	Mg 12	0	0

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
57	1Y	1	Total 1	Zn 1	0	0
57	14	1	Total 1	Zn 1	0	0
57	15	1	Total 1	Zn 1	0	0
57	16	1	Total 1	Zn 1	0	0
57	19	1	Total 1	Zn 1	0	0
57	1n	1	Total 1	Zn 1	0	0
57	2Y	1	Total 1	Zn 1	0	0
57	24	1	Total 1	Zn 1	0	0
57	25	1	Total 1	Zn 1	0	0
57	26	1	Total 1	Zn 1	0	0
57	29	1	Total 1	Zn 1	0	0
57	2n	1	Total 1	Zn 1	0	0

- Molecule 58 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe₄S₄).



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

- Molecule 59 is POTASSIUM ION (three-letter code: K) (formula: K).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
59	1x	1	Total	K	0	0
			1	1		
59	2A	1	Total	K	0	0
			1	1		

- Molecule 60 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
60	1A	1795	Total	O	0	0
			1795	1795		
60	1B	49	Total	O	0	0
			49	49		
60	1D	23	Total	O	0	0
			23	23		
60	1E	16	Total	O	0	0
			16	16		
60	1F	9	Total	O	0	0
			9	9		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
60	1G	2	Total 2	O 2	0	0
60	1H	4	Total 4	O 4	0	0
60	1N	8	Total 8	O 8	0	0
60	1P	14	Total 14	O 14	0	0
60	1Q	6	Total 6	O 6	0	0
60	1R	6	Total 6	O 6	0	0
60	1T	5	Total 5	O 5	0	0
60	1U	3	Total 3	O 3	0	0
60	1V	6	Total 6	O 6	0	0
60	1W	1	Total 1	O 1	0	0
60	1X	6	Total 6	O 6	0	0
60	1Y	4	Total 4	O 4	0	0
60	10	5	Total 5	O 5	0	0
60	11	5	Total 5	O 5	0	0
60	13	1	Total 1	O 1	0	0
60	15	3	Total 3	O 3	0	0
60	16	1	Total 1	O 1	0	0
60	17	2	Total 2	O 2	0	0
60	18	8	Total 8	O 8	0	0
60	19	2	Total 2	O 2	0	0
60	1a	408	Total 408	O 408	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
60	1d	8	Total 8	O 8	0	0
60	1e	3	Total 3	O 3	0	0
60	1f	1	Total 1	O 1	0	0
60	1h	1	Total 1	O 1	0	0
60	1j	1	Total 1	O 1	0	0
60	1l	4	Total 4	O 4	0	0
60	1m	1	Total 1	O 1	0	0
60	1o	2	Total 2	O 2	0	0
60	1p	1	Total 1	O 1	0	0
60	1t	2	Total 2	O 2	0	0
60	1v	2	Total 2	O 2	0	0
60	1x	5	Total 5	O 5	0	0
60	1y	2	Total 2	O 2	0	0
60	2A	1787	Total 1787	O 1787	0	0
60	2B	46	Total 46	O 46	0	0
60	2D	20	Total 20	O 20	0	0
60	2E	15	Total 15	O 15	0	0
60	2F	11	Total 11	O 11	0	0
60	2G	2	Total 2	O 2	0	0
60	2H	4	Total 4	O 4	0	0
60	2N	8	Total 8	O 8	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
60	2P	17	Total 17	O 17	0	0
60	2Q	4	Total 4	O 4	0	0
60	2R	6	Total 6	O 6	0	0
60	2T	4	Total 4	O 4	0	0
60	2U	5	Total 5	O 5	0	0
60	2V	3	Total 3	O 3	0	0
60	2W	1	Total 1	O 1	0	0
60	2X	5	Total 5	O 5	0	0
60	2Y	8	Total 8	O 8	0	0
60	20	9	Total 9	O 9	0	0
60	21	2	Total 2	O 2	0	0
60	23	2	Total 2	O 2	0	0
60	25	2	Total 2	O 2	0	0
60	26	1	Total 1	O 1	0	0
60	27	2	Total 2	O 2	0	0
60	28	9	Total 9	O 9	0	0
60	29	4	Total 4	O 4	0	0
60	2a	408	Total 408	O 408	0	0
60	2d	7	Total 7	O 7	0	0
60	2e	4	Total 4	O 4	0	0
60	2f	1	Total 1	O 1	0	0

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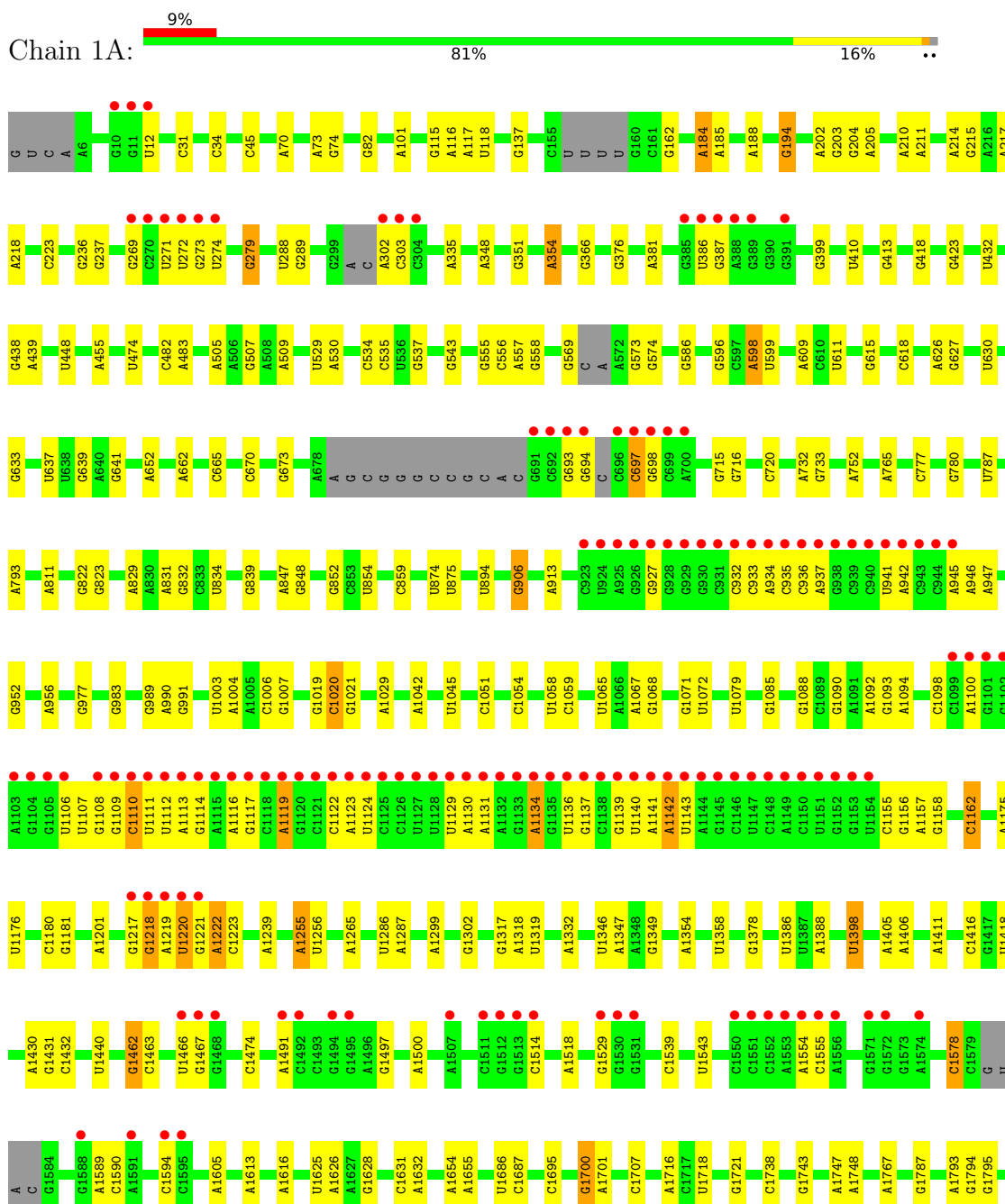
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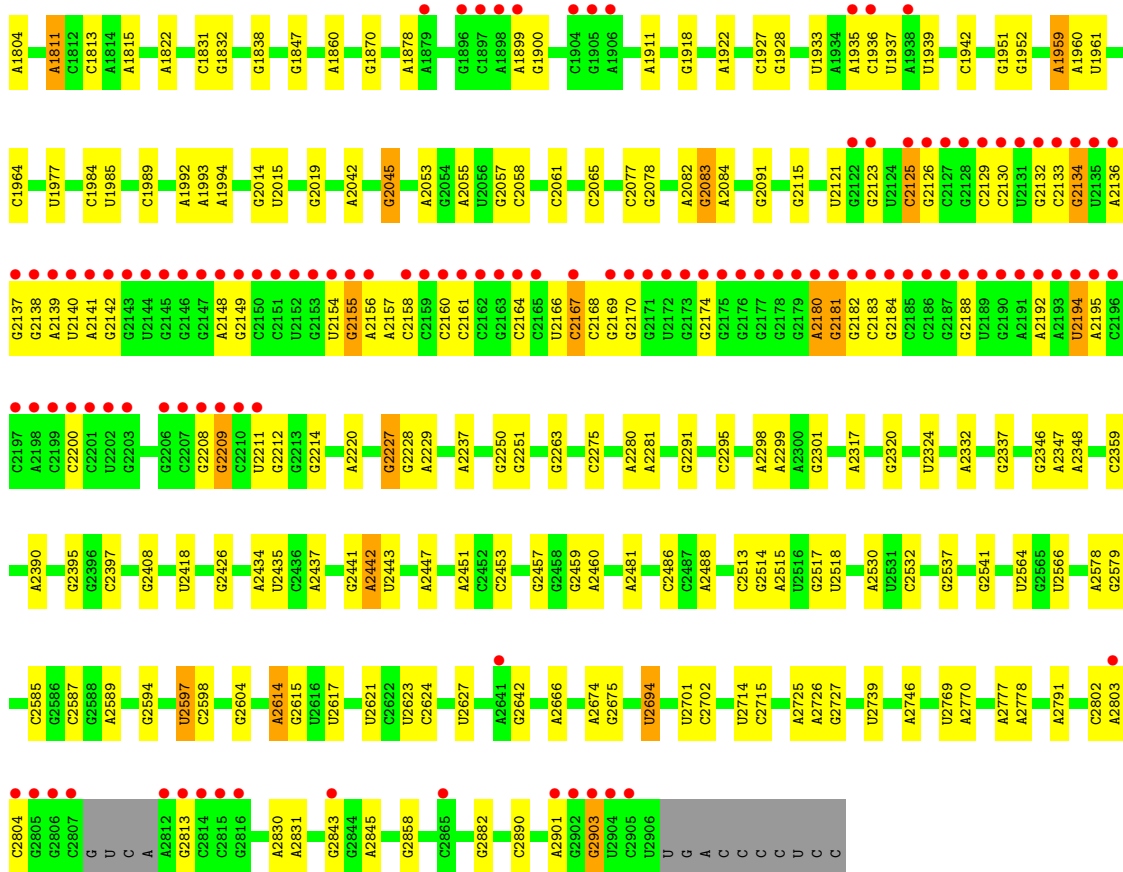
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
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60	2j	2	Total O 2 2	0	0
60	2l	7	Total O 7 7	0	0
60	2m	1	Total O 1 1	0	0
60	2n	1	Total O 1 1	0	0
60	2t	1	Total O 1 1	0	0
60	2v	3	Total O 3 3	0	0
60	2x	4	Total O 4 4	0	0
60	2y	4	Total O 4 4	0	0

3 Residue-property plots [i](#)

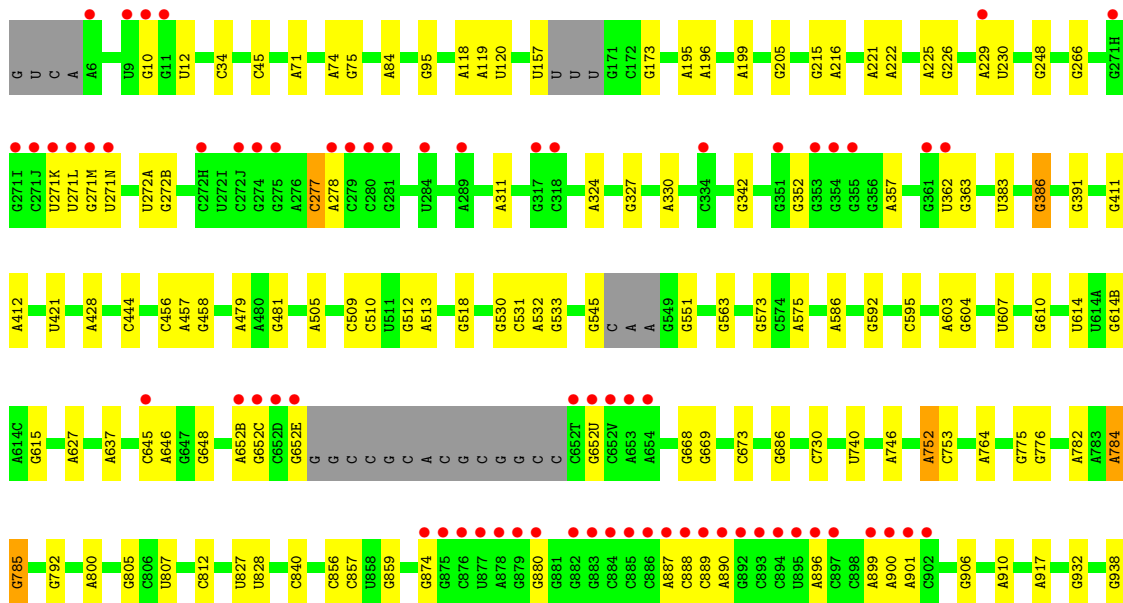
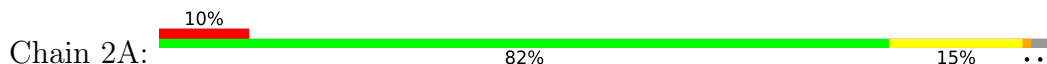
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

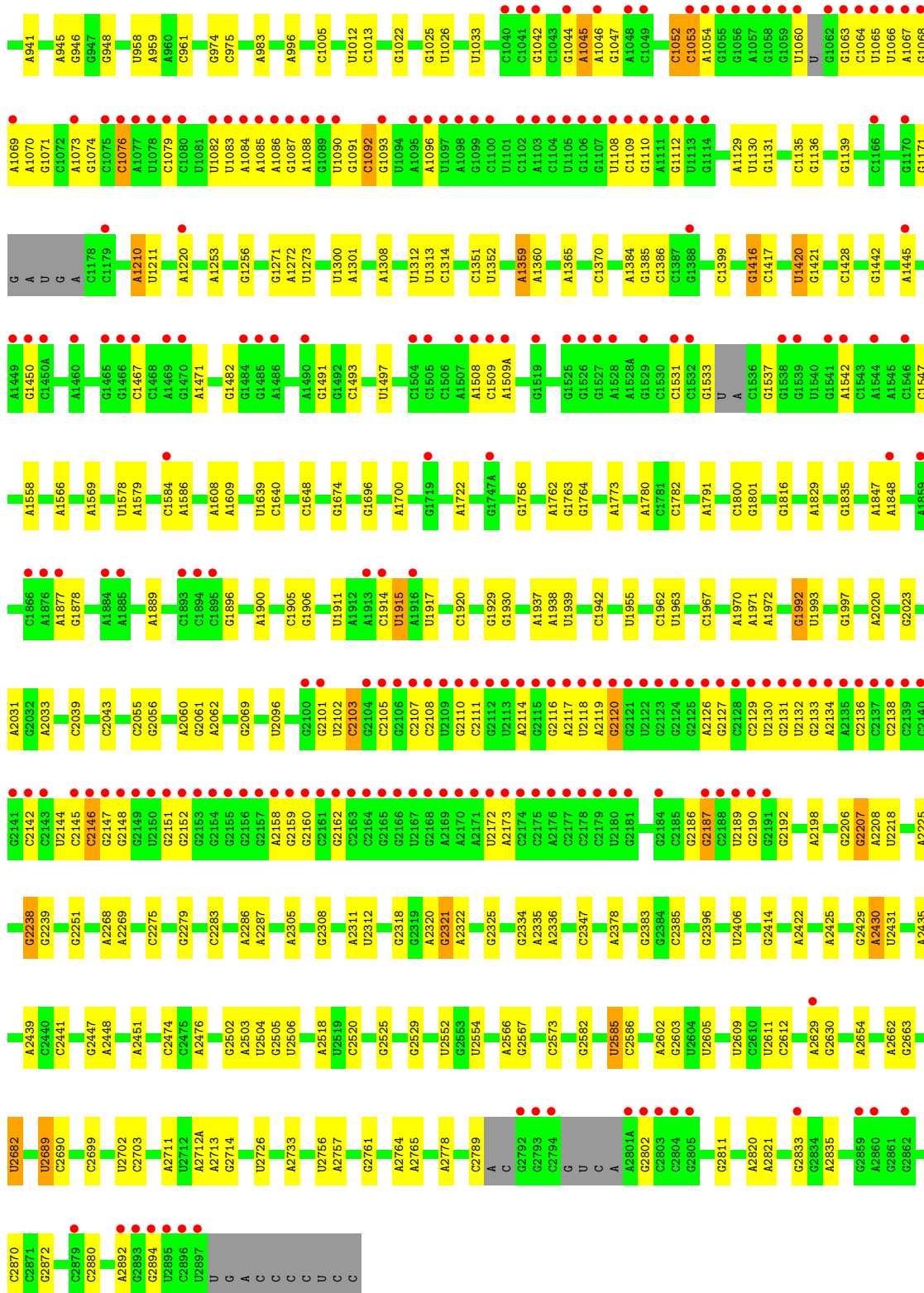
- Molecule 1: 23S ribosomal RNA





● Molecule 1: 23S ribosomal RNA



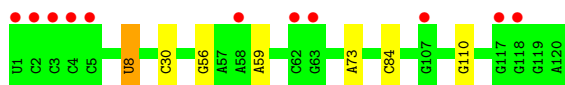


• Molecule 2: 5S ribosomal RNA





- Molecule 2: 5S ribosomal RNA



- Molecule 3: 50S ribosomal protein L2



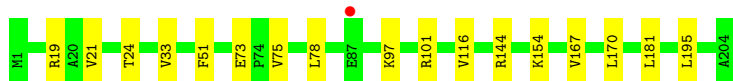
- Molecule 3: 50S ribosomal protein L2



- Molecule 4: 50S ribosomal protein L3



- Molecule 4: 50S ribosomal protein L3



- Molecule 5: 50S ribosomal protein L4



- Molecule 5: 50S ribosomal protein L4

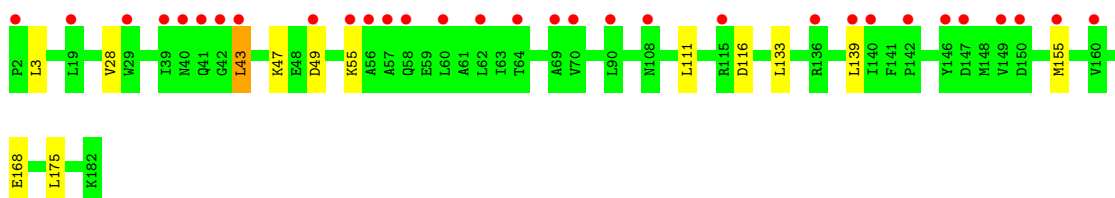




- Molecule 6: 50S ribosomal protein L5



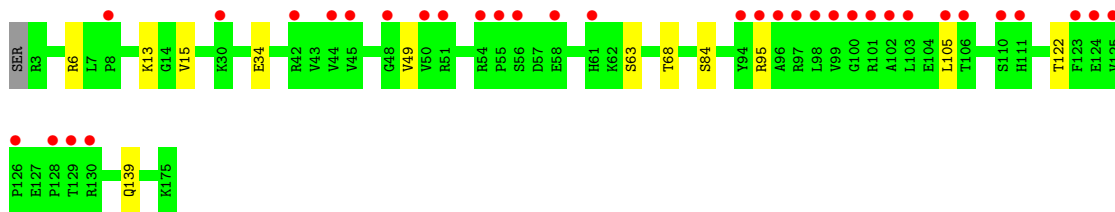
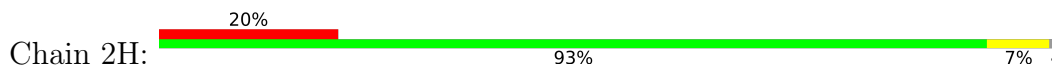
- Molecule 6: 50S ribosomal protein L5



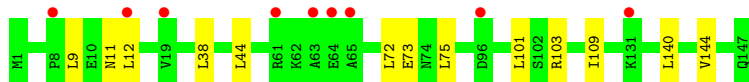
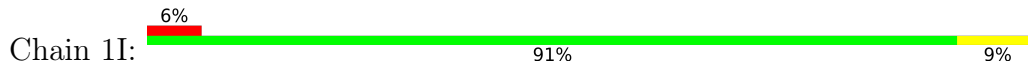
- Molecule 7: 50S ribosomal protein L6



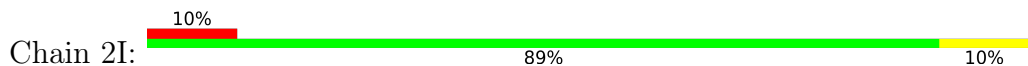
- Molecule 7: 50S ribosomal protein L6



- Molecule 8: 50S ribosomal protein L9



- Molecule 8: 50S ribosomal protein L9





- Molecule 9: 50S ribosomal protein L13



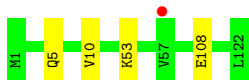
- Molecule 9: 50S ribosomal protein L13



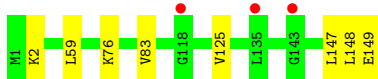
- Molecule 10: 50S ribosomal protein L14



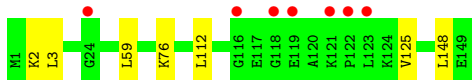
- Molecule 10: 50S ribosomal protein L14



- Molecule 11: 50S ribosomal protein L15

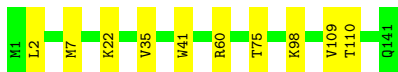


- Molecule 11: 50S ribosomal protein L15



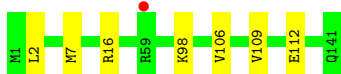
- Molecule 12: 50S ribosomal protein L16

Chain 1Q:  93% 7%



- Molecule 12: 50S ribosomal protein L16

Chain 2Q:  95% 5%



- Molecule 13: 50S ribosomal protein L17

Chain 1R:  92% 8%



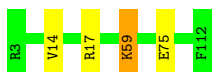
- Molecule 13: 50S ribosomal protein L17

Chain 2R:  93% 7%



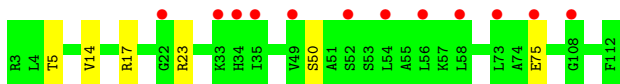
- Molecule 14: 50S ribosomal protein L18

Chain 1S:  96%



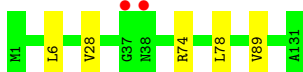
- Molecule 14: 50S ribosomal protein L18

Chain 2S:  95% 5%

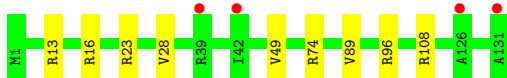


- Molecule 15: 50S ribosomal protein L19

Chain 1T:  96%



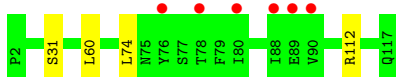
- Molecule 15: 50S ribosomal protein L19



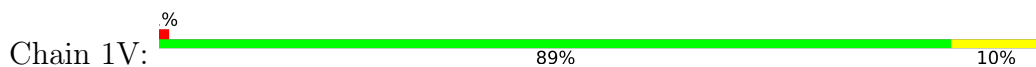
- Molecule 16: 50S ribosomal protein L20



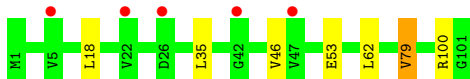
- Molecule 16: 50S ribosomal protein L20



- Molecule 17: 50S ribosomal protein L21



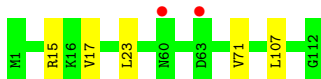
- Molecule 17: 50S ribosomal protein L21



- Molecule 18: 50S ribosomal protein L22



- Molecule 18: 50S ribosomal protein L22



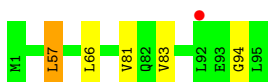
- Molecule 19: 50S ribosomal protein L23

Chain 1X:  97%



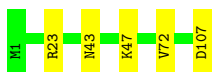
- Molecule 19: 50S ribosomal protein L23

Chain 2X:  95%



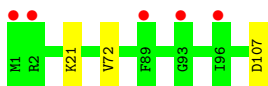
- Molecule 20: 50S ribosomal protein L24

Chain 1Y:  95%




- Molecule 20: 50S ribosomal protein L24

Chain 2Y:  97%




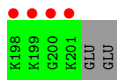
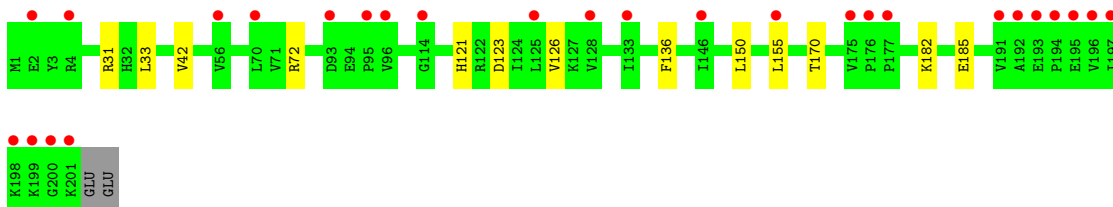
- Molecule 21: 50S ribosomal protein L25

Chain 1Z:  90%



- Molecule 21: 50S ribosomal protein L25

Chain 2Z:  93%



- Molecule 22: 50S ribosomal protein L27

Chain 10:  94%



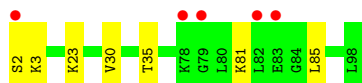
- Molecule 22: 50S ribosomal protein L27



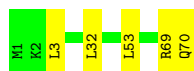
- Molecule 23: 50S ribosomal protein L28



- Molecule 23: 50S ribosomal protein L28



- Molecule 24: 50S ribosomal protein L29



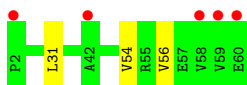
- Molecule 24: 50S ribosomal protein L29



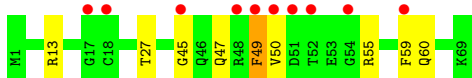
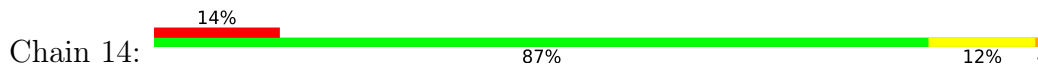
- Molecule 25: 50S ribosomal protein L30



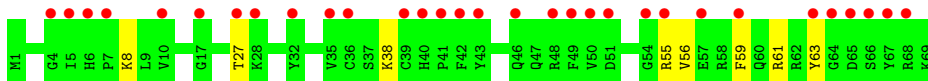
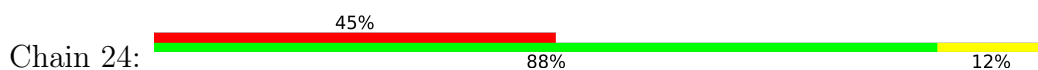
- Molecule 25: 50S ribosomal protein L30



- Molecule 26: 50S ribosomal protein L31



- Molecule 26: 50S ribosomal protein L31



- Molecule 27: 50S ribosomal protein L32



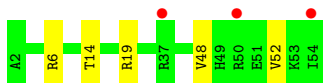
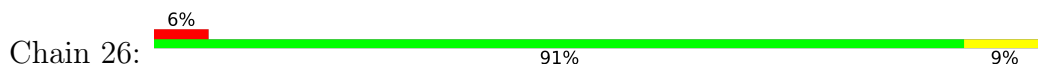
- Molecule 27: 50S ribosomal protein L32



- Molecule 28: 50S ribosomal protein L33



- Molecule 28: 50S ribosomal protein L33



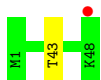
- Molecule 29: 50S ribosomal protein L34

Chain 17:  96%



- Molecule 29: 50S ribosomal protein L34

Chain 27:  98%



- Molecule 30: 50S ribosomal protein L35

Chain 18:  92%



- Molecule 30: 50S ribosomal protein L35

Chain 28:  91%



- Molecule 31: 50S ribosomal protein L36

Chain 19:  97%




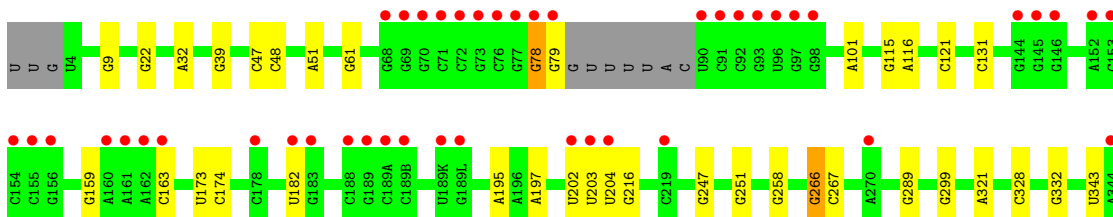
- Molecule 31: 50S ribosomal protein L36

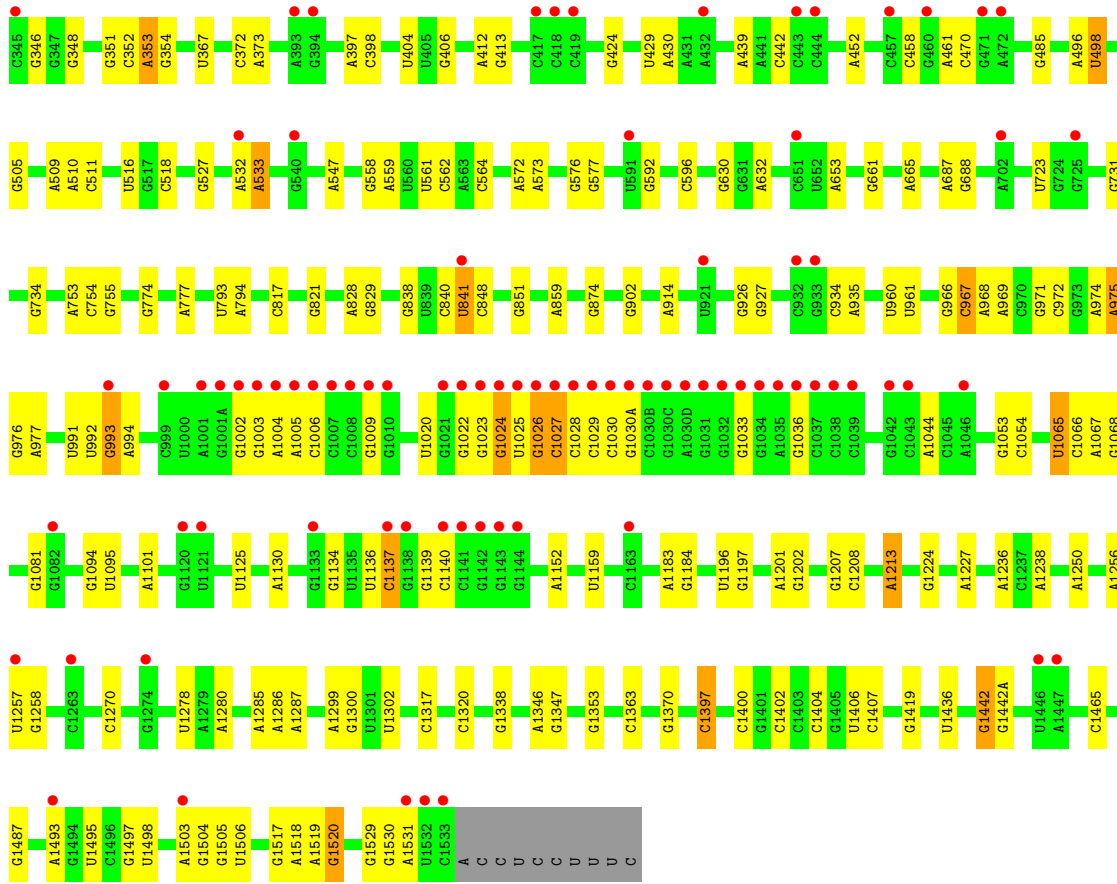
Chain 29:  100%

There are no outlier residues recorded for this chain.

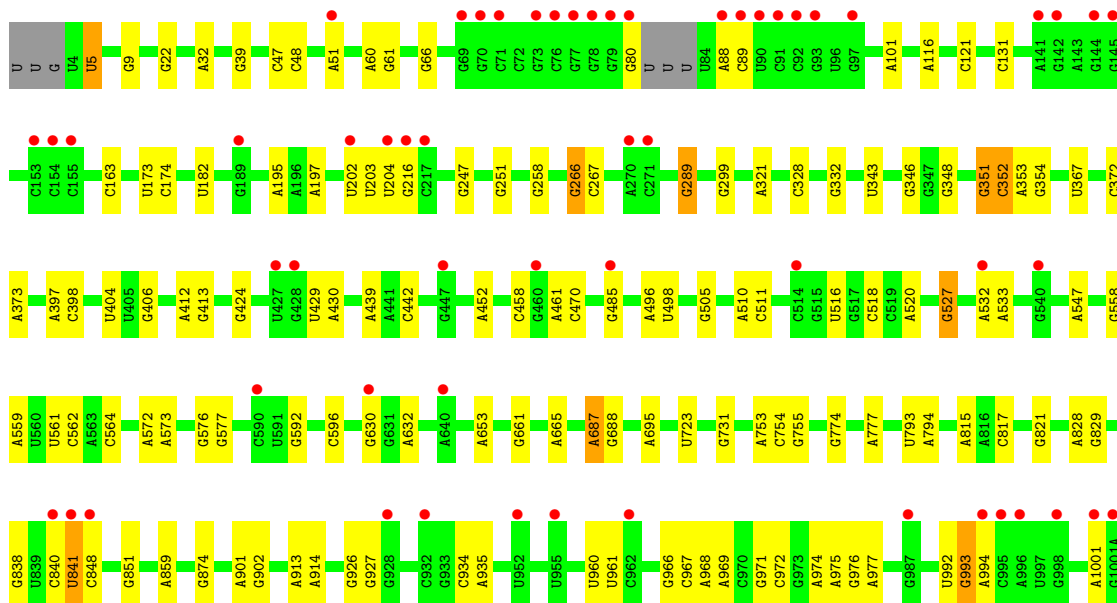
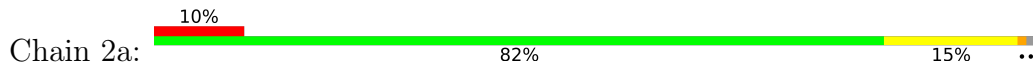
- Molecule 32: 16S ribosomal RNA

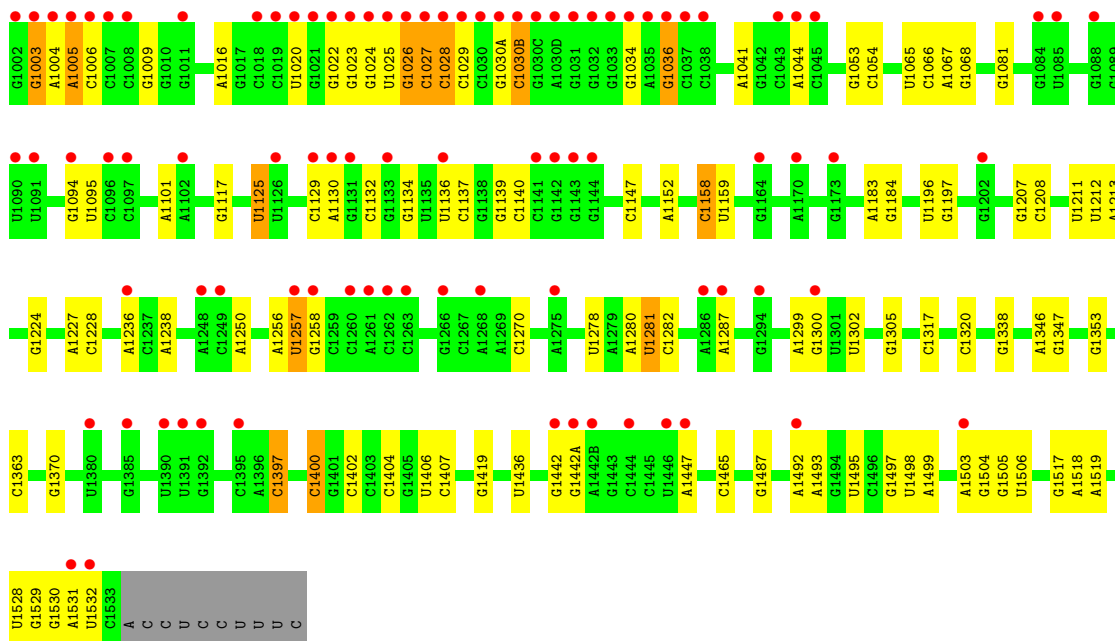
Chain 1a:  83%



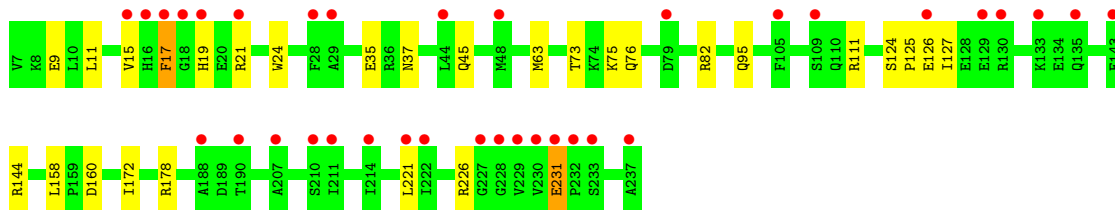
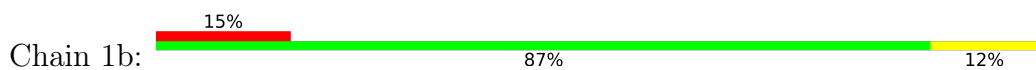


● Molecule 32: 16S ribosomal RNA

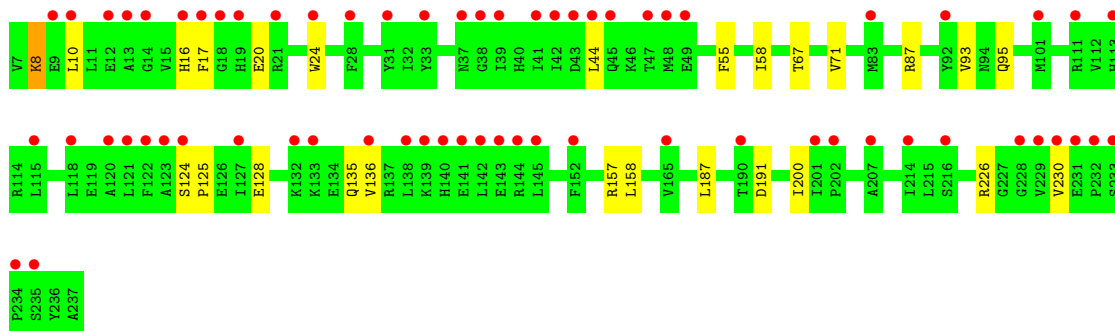
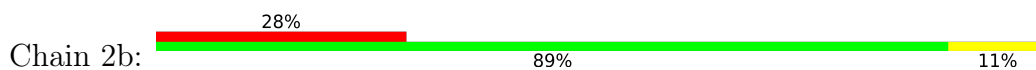




- Molecule 33: 30S ribosomal protein S2



- Molecule 33: 30S ribosomal protein S2

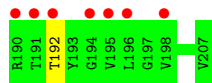
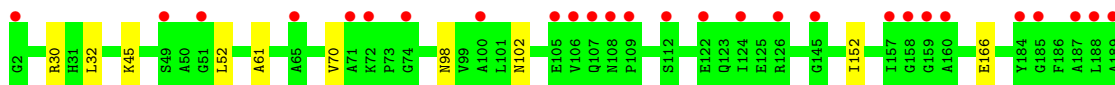


- Molecule 34: 30S ribosomal protein S3





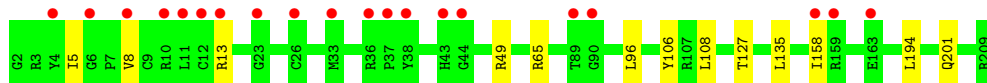
- Molecule 34: 30S ribosomal protein S3



- Molecule 35: 30S ribosomal protein S4



- Molecule 35: 30S ribosomal protein S4



- Molecule 36: 30S ribosomal protein S5



- Molecule 36: 30S ribosomal protein S5

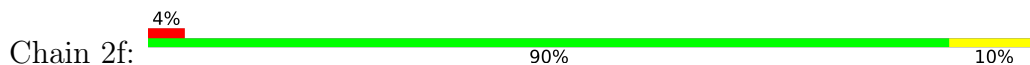


- Molecule 37: 30S ribosomal protein S6

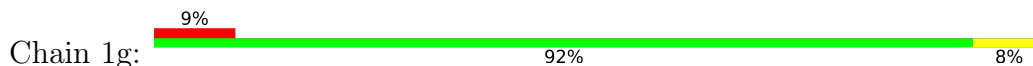




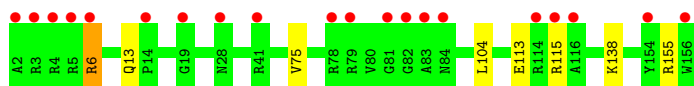
- Molecule 37: 30S ribosomal protein S6



- Molecule 38: 30S ribosomal protein S7



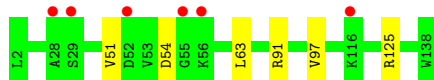
- Molecule 38: 30S ribosomal protein S7



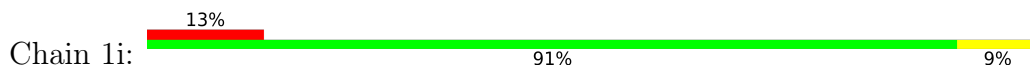
- Molecule 39: 30S ribosomal protein S8



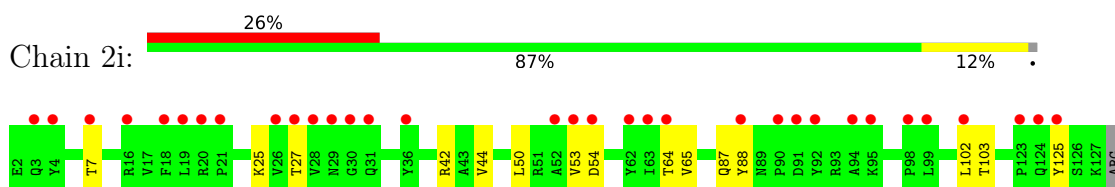
- Molecule 39: 30S ribosomal protein S8



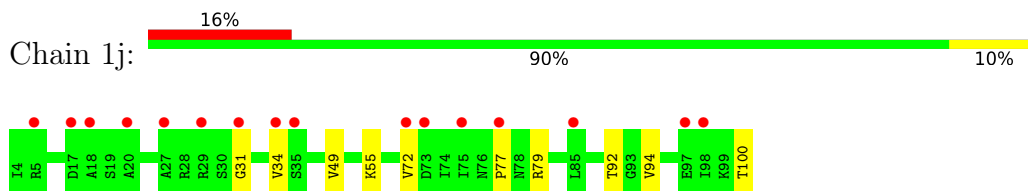
- Molecule 40: 30S ribosomal protein S9



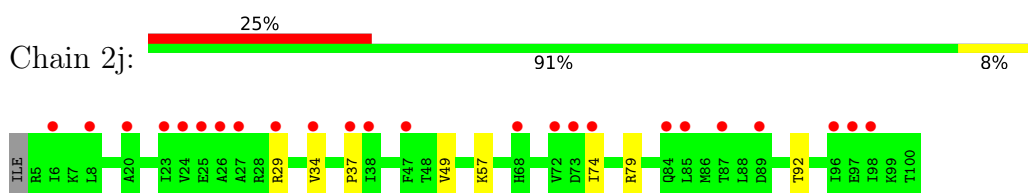
- Molecule 40: 30S ribosomal protein S9



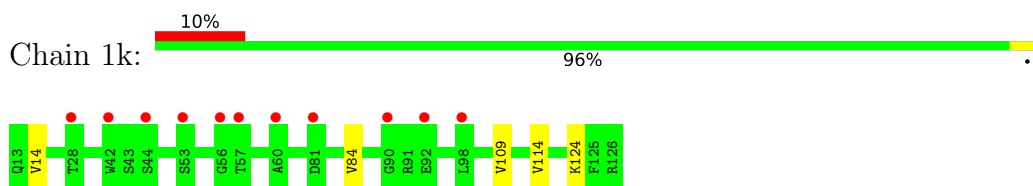
- Molecule 41: 30S ribosomal protein S10



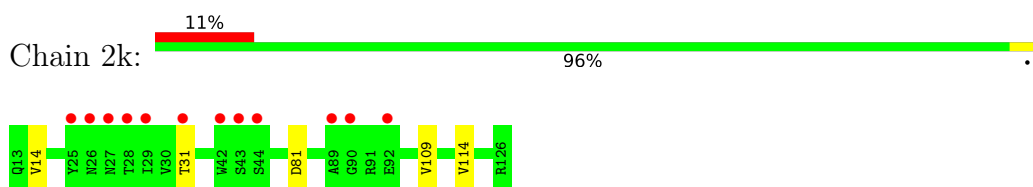
- Molecule 41: 30S ribosomal protein S10



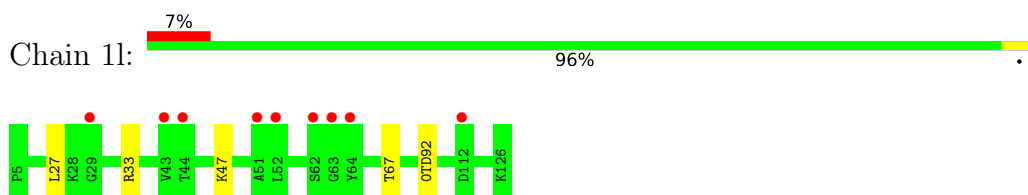
- Molecule 42: 30S ribosomal protein S11



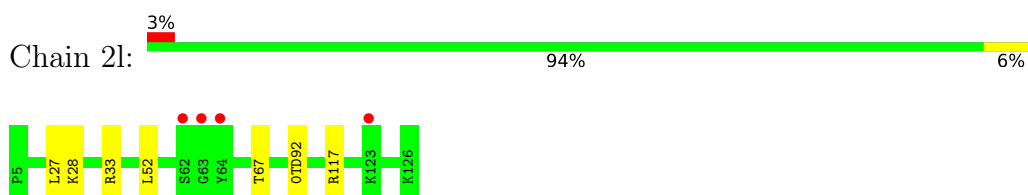
- Molecule 42: 30S ribosomal protein S11



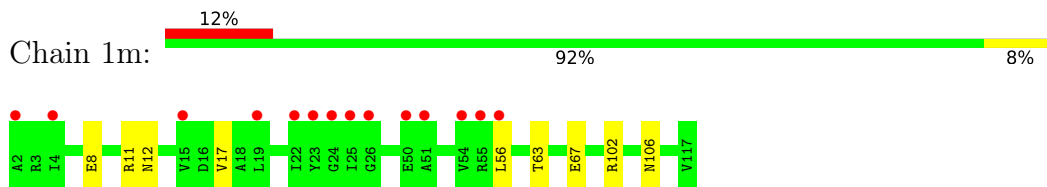
- Molecule 43: 30S ribosomal protein S12



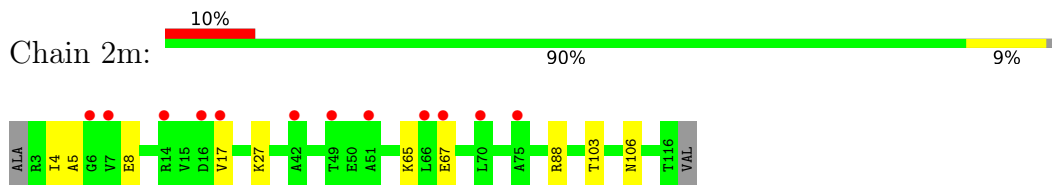
- Molecule 43: 30S ribosomal protein S12



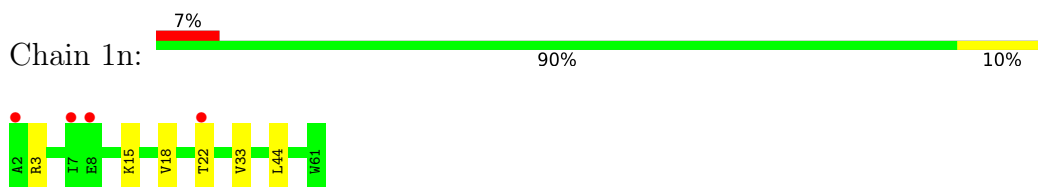
- Molecule 44: 30S ribosomal protein S13



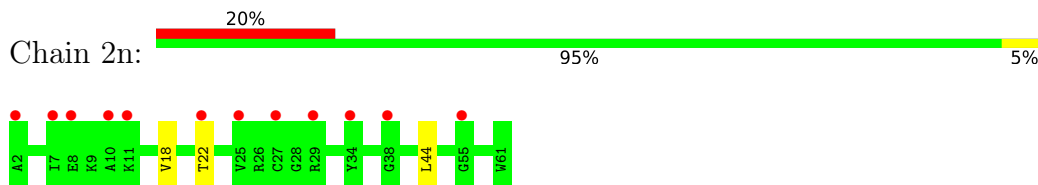
- Molecule 44: 30S ribosomal protein S13



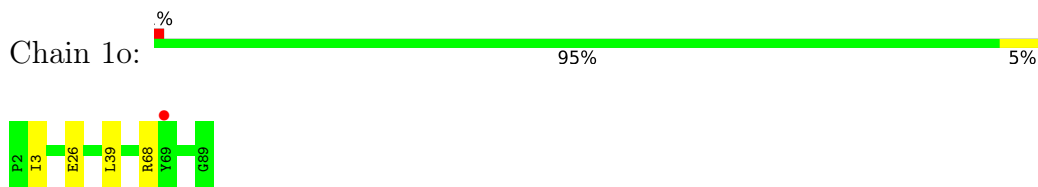
- Molecule 45: 30S ribosomal protein S14 type Z



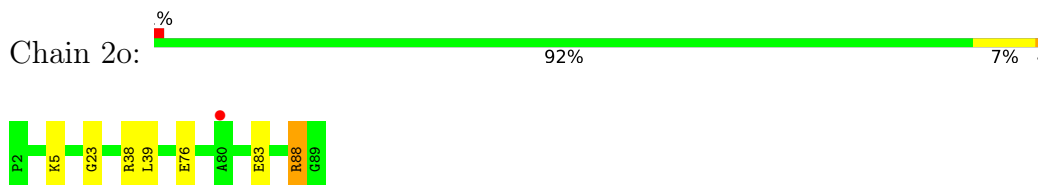
- Molecule 45: 30S ribosomal protein S14 type Z



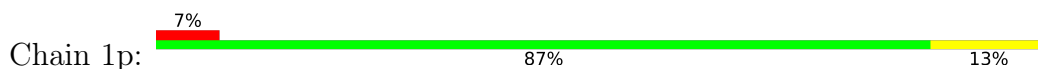
- Molecule 46: 30S ribosomal protein S15

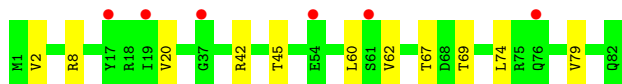


- Molecule 46: 30S ribosomal protein S15

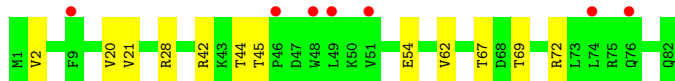
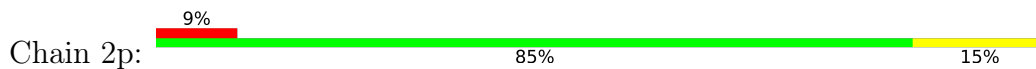


- Molecule 47: 30S ribosomal protein S16





- Molecule 47: 30S ribosomal protein S16



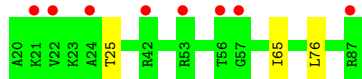
- Molecule 48: 30S ribosomal protein S17



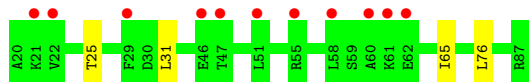
- Molecule 48: 30S ribosomal protein S17



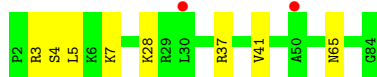
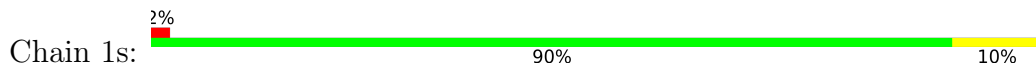
- Molecule 49: 30S ribosomal protein S18



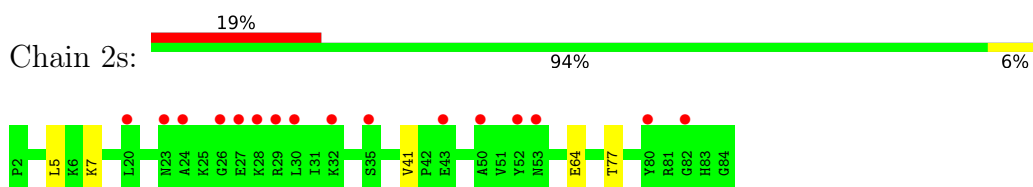
- Molecule 49: 30S ribosomal protein S18



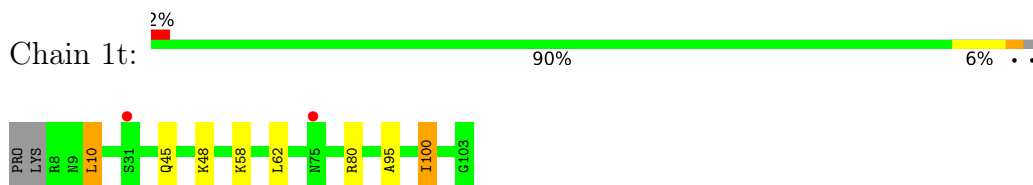
- Molecule 50: 30S ribosomal protein S19



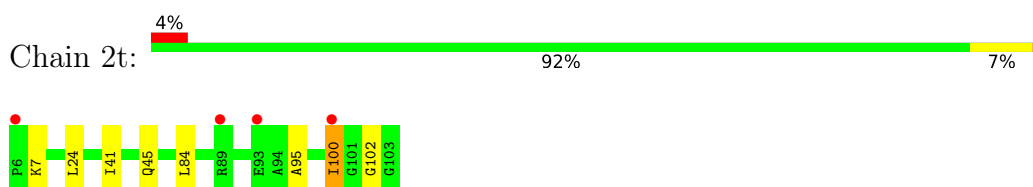
- Molecule 50: 30S ribosomal protein S19



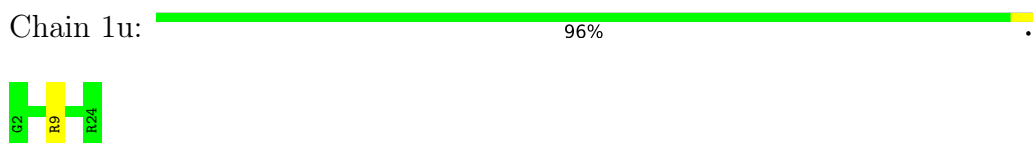
- Molecule 51: 30S ribosomal protein S20



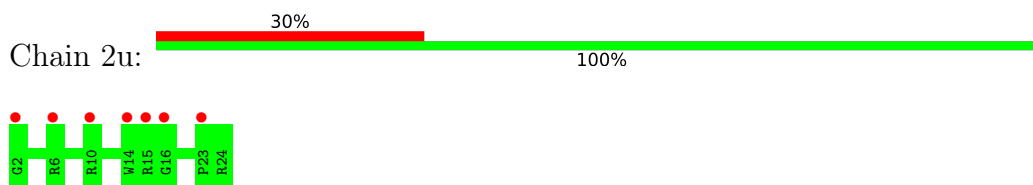
- Molecule 51: 30S ribosomal protein S20



- Molecule 52: 30S ribosomal protein Thx



- Molecule 52: 30S ribosomal protein Thx



- Molecule 53: mRNA



There are no outlier residues recorded for this chain.

- Molecule 53: mRNA



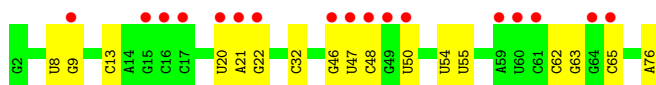
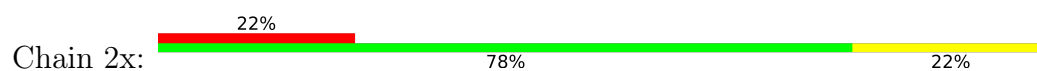
There are no outlier residues recorded for this chain.

- Molecule 54: tRNAⁱMet

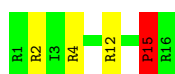
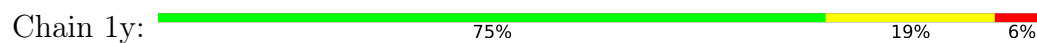




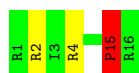
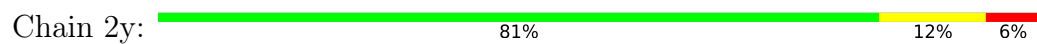
- Molecule 54: tRNAiMet



- Molecule 55: Cathelicidin-3



- Molecule 55: Cathelicidin-3



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	209.96Å 450.13Å 622.82Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.62 – 2.80 48.98 – 2.80	Depositor EDS
% Data completeness (in resolution range)	99.5 (48.62-2.80) 99.6 (48.98-2.80)	Depositor EDS
R_{merge}	0.51	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.14 (at 2.81Å)	Xtrriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.249 , 0.292 0.248 , 0.291	Depositor DCC
R_{free} test set	70217 reflections (4.93%)	wwPDB-VP
Wilson B-factor (Å ²)	42.0	Xtrriage
Anisotropy	0.182	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 48.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.38$, $\langle L^2 \rangle = 0.20$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.84	EDS
Total number of atoms	296108	wwPDB-VP
Average B, all atoms (Å ²)	44.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.60% 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, 4SU, 5MC, M2G, K, 7MG, MG, 2MG, UR3, 2MA, OMC, MA6, 4OC, 5MU, ZN, SF4, 0TD, PSU, OMU

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	0.54	0/69034	1.07	167/107758 (0.2%)
1	2A	0.44	0/68906	0.97	77/107556 (0.1%)
2	1B	0.46	0/2879	1.03	11/4490 (0.2%)
2	2B	0.41	0/2874	0.97	2/4482 (0.0%)
3	1D	0.39	0/2181	0.64	1/2940 (0.0%)
3	2D	0.34	0/2186	0.61	0/2944
4	1E	0.38	0/1592	0.61	0/2149
4	2E	0.34	0/1592	0.62	0/2149
5	1F	0.36	0/1619	0.60	0/2193
5	2F	0.32	0/1615	0.56	0/2188
6	1G	0.33	0/1451	0.61	0/1961
6	2G	0.31	0/1449	0.60	0/1957
7	1H	0.34	0/1356	0.55	0/1834
7	2H	0.31	0/1350	0.54	0/1826
8	1I	0.31	0/1109	0.62	0/1512
8	2I	0.29	0/1091	0.58	0/1490
9	1N	0.36	0/1148	0.60	0/1547
9	2N	0.30	0/1144	0.55	0/1543
10	1O	0.41	0/943	0.61	0/1269
10	2O	0.35	0/943	0.58	0/1269
11	1P	0.35	0/1152	0.62	0/1533
11	2P	0.31	0/1152	0.57	0/1533
12	1Q	0.44	1/1143 (0.1%)	0.64	2/1527 (0.1%)
12	2Q	0.32	0/1143	0.54	0/1527
13	1R	0.37	0/982	0.61	0/1312
13	2R	0.32	0/982	0.57	0/1312
14	1S	0.32	0/887	0.59	0/1180
14	2S	0.31	0/880	0.58	0/1172
15	1T	0.34	0/1105	0.60	0/1477
15	2T	0.32	0/1097	0.58	0/1468
16	1U	0.37	0/977	0.58	0/1301

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
16	2U	0.31	0/977	0.53	0/1301
17	1V	0.37	0/786	0.60	0/1053
17	2V	0.32	0/782	0.60	0/1049
18	1W	0.39	0/897	0.60	0/1205
18	2W	0.32	0/897	0.55	0/1205
19	1X	0.39	0/764	0.60	0/1025
19	2X	0.34	0/764	0.63	1/1025 (0.1%)
20	1Y	0.38	0/823	0.62	0/1099
20	2Y	0.33	0/823	0.63	0/1100
21	1Z	0.33	0/1620	0.57	0/2200
21	2Z	0.32	0/1590	0.58	0/2162
22	10	0.36	0/616	0.61	0/821
22	20	0.33	0/616	0.58	0/821
23	11	0.36	0/761	0.57	0/1013
23	21	0.33	0/766	0.56	0/1018
24	12	0.35	0/590	0.63	1/781 (0.1%)
24	22	0.31	0/594	0.53	0/785
25	13	0.35	0/474	0.57	0/635
25	23	0.30	0/469	0.53	0/630
26	14	0.35	0/559	0.68	0/754
26	24	0.37	0/549	0.67	0/741
27	15	0.39	0/473	0.63	0/639
27	25	0.31	0/469	0.61	1/635 (0.2%)
28	16	0.36	0/460	0.59	0/613
28	26	0.34	0/456	0.57	0/608
29	17	0.41	0/426	0.65	0/561
29	27	0.36	0/426	0.55	0/561
30	18	0.38	0/525	0.61	0/691
30	28	0.34	0/525	0.57	0/691
31	19	0.36	0/310	0.61	0/407
31	29	0.31	0/310	0.58	0/407
32	1a	0.41	0/35795	0.99	69/55864 (0.1%)
32	2a	0.40	1/35890 (0.0%)	1.00	91/56012 (0.2%)
33	1b	0.34	0/1876	0.63	0/2533
33	2b	0.33	0/1860	0.59	0/2518
34	1c	0.31	0/1582	0.57	0/2137
34	2c	0.31	0/1566	0.58	0/2119
35	1d	0.32	0/1695	0.60	0/2274
35	2d	0.29	0/1698	0.55	0/2277
36	1e	0.32	0/1149	0.58	0/1548
36	2e	0.32	0/1149	0.58	0/1548
37	1f	0.32	0/827	0.57	0/1120
37	2f	0.31	0/829	0.57	0/1123

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
38	1g	0.32	0/1254	0.55	0/1683
38	2g	0.29	0/1248	0.52	0/1676
39	1h	0.30	0/1118	0.58	0/1506
39	2h	0.30	0/1108	0.56	0/1494
40	1i	0.30	0/1005	0.58	0/1351
40	2i	0.32	0/985	0.57	0/1329
41	1j	0.32	0/732	0.58	0/993
41	2j	0.32	0/723	0.60	0/984
42	1k	0.33	0/849	0.59	0/1150
42	2k	0.36	0/848	0.61	0/1149
43	1l	0.31	0/937	0.56	0/1260
43	2l	0.31	0/937	0.61	0/1260
44	1m	0.29	0/924	0.60	0/1242
44	2m	0.31	0/905	0.58	0/1217
45	1n	0.31	0/501	0.55	0/664
45	2n	0.33	0/501	0.55	0/664
46	1o	0.31	0/739	0.58	0/985
46	2o	0.29	0/739	0.52	0/985
47	1p	0.30	0/697	0.56	0/939
47	2p	0.31	0/693	0.55	0/935
48	1q	0.32	0/836	0.60	0/1117
48	2q	0.31	0/836	0.56	0/1117
49	1r	0.30	0/560	0.56	0/746
49	2r	0.31	0/560	0.56	0/746
50	1s	0.30	0/663	0.61	0/895
50	2s	0.29	0/660	0.60	0/893
51	1t	0.31	0/734	0.57	0/969
51	2t	0.29	0/736	0.54	0/976
52	1u	0.28	0/203	0.57	0/266
52	2u	0.30	0/203	0.57	0/266
53	1v	0.45	0/72	0.91	0/110
53	2v	0.48	0/72	1.04	0/110
54	1x	0.42	0/1725	0.94	0/2689
54	2x	0.40	0/1725	0.96	3/2689 (0.1%)
55	1y	0.37	0/152	0.83	1/203 (0.5%)
55	2y	0.33	0/152	0.87	1/203 (0.5%)
All	All	0.43	2/312307 (0.0%)	0.92	428/467169 (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
26	24	0	1
33	1b	0	1
55	1y	0	1
55	2y	0	1
All	All	0	4

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	1Q	41	TRP	NE1-CE2	6.34	1.45	1.37
32	2a	1034	G	N9-C4	5.00	1.42	1.38

All (428) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	2a	1208	C	O5'-P-OP1	-31.64	72.74	110.70
32	1a	1520	G	O5'-P-OP1	-30.14	74.54	110.70
32	2a	1208	C	OP1-P-OP2	-27.27	78.69	119.60
32	1a	1520	G	OP1-P-OP2	-26.36	80.06	119.60
32	1a	1520	G	O5'-P-OP2	19.44	134.03	110.70
32	2a	1208	C	O5'-P-OP2	17.89	132.16	110.70
32	2a	1207	2MG	OP1-P-O3'	13.62	135.16	105.20
32	2a	1207	2MG	OP2-P-O3'	-12.53	77.64	105.20
1	1A	720	C	C2-N3-C4	-12.23	113.79	119.90
1	1A	787	U	O5'-P-OP2	-11.63	95.24	105.70
1	1A	834	U	O5'-P-OP1	-11.59	95.27	105.70
32	1a	558	G	O5'-P-OP1	-11.56	95.29	105.70
1	2A	1639	U	O5'-P-OP2	-10.79	95.99	105.70
32	1a	1495	U	N1-C2-O2	10.76	130.33	122.80
1	1A	1686	U	O5'-P-OP2	-10.56	96.19	105.70
32	2a	351	G	OP1-P-O3'	-10.39	82.33	105.20
32	2a	404	U	N1-C2-O2	10.16	129.91	122.80
1	1A	2694	U	O5'-P-OP2	-10.05	96.65	105.70
1	2A	2711	A	O5'-P-OP1	-9.70	96.97	105.70
2	1B	75	G	C6-N1-C2	-9.56	119.36	125.10
1	1A	1045	U	O5'-P-OP2	-9.54	97.12	105.70
1	1A	2227	G	C4-N9-C1'	-9.53	114.12	126.50
1	2A	673	C	C2-N3-C4	-9.51	115.15	119.90
1	2A	2682	U	O5'-P-OP2	-9.46	97.18	105.70
1	1A	2188	G	N3-C4-N9	-9.08	120.55	126.00
32	2a	1495	U	N1-C2-O2	8.97	129.08	122.80
1	1A	2083	G	O5'-P-OP2	-8.90	97.69	105.70
32	2a	352	C	OP1-P-OP2	8.89	132.94	119.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	2A	948	G	O5'-P-OP1	-8.85	97.73	105.70
1	1A	854	U	C2-N3-C4	-8.73	121.76	127.00
32	1a	343	U	C2-N1-C1'	-8.67	107.30	117.70
32	2a	351	G	OP2-P-O3'	-8.63	86.20	105.20
1	1A	2227	G	C8-N9-C1'	8.63	138.22	127.00
1	1A	2442	A	O5'-P-OP2	-8.53	98.03	105.70
1	1A	932	C	C6-N1-C2	-8.49	116.90	120.30
32	2a	299	G	C5-C6-O6	-8.40	123.56	128.60
32	2a	558	G	O5'-P-OP1	-8.39	98.14	105.70
32	1a	404	U	N1-C2-O2	8.39	128.67	122.80
32	1a	841	U	C5-C6-N1	8.28	126.84	122.70
1	1A	354	A	C2-N3-C4	-8.24	106.48	110.60
32	1a	1137	C	C6-N1-C2	-8.22	117.01	120.30
32	1a	1436	U	C2-N3-C4	-8.19	122.08	127.00
32	1a	1465	C	C2-N3-C4	-8.19	115.81	119.90
1	1A	82	G	N9-C4-C5	-8.16	102.14	105.40
32	2a	1034	G	C5-C6-N1	8.03	115.51	111.50
32	2a	1034	G	N3-C4-C5	-8.00	124.60	128.60
32	2a	343	U	C5-C4-O4	7.98	130.69	125.90
1	2A	785	G	O5'-P-OP2	-7.92	98.57	105.70
1	1A	354	A	N1-C2-N3	7.90	133.25	129.30
1	1A	2058	C	O5'-P-OP1	-7.89	98.60	105.70
32	2a	343	U	N3-C4-O4	-7.86	113.90	119.40
32	2a	343	U	C2-N1-C1'	-7.77	108.38	117.70
1	1A	952	G	C5-C6-O6	7.75	133.25	128.60
1	2A	807	U	C2-N3-C4	-7.74	122.36	127.00
32	2a	1465	C	C2-N3-C4	-7.54	116.13	119.90
32	2a	1034	G	C6-N1-C2	-7.54	120.58	125.10
32	1a	1495	U	N3-C2-O2	-7.53	116.93	122.20
32	1a	299	G	C5-C6-O6	-7.46	124.12	128.60
55	2y	15	PRO	O-C-N	-7.46	110.76	122.70
1	1A	1700	G	P-O3'-C3'	7.46	128.65	119.70
1	2A	906	G	C5-C6-O6	7.46	133.07	128.60
32	1a	1397	C	N1-C2-O2	7.45	123.37	118.90
32	2a	1027	C	C6-N1-C2	-7.43	117.33	120.30
32	1a	1495	U	C2-N1-C1'	7.42	126.60	117.70
1	1A	1358	U	C5-C4-O4	7.41	130.35	125.90
1	1A	952	G	N3-C4-N9	-7.39	121.57	126.00
1	1A	2858	G	O4'-C1'-N9	7.29	114.03	108.20
2	1B	102	A	C6-N1-C2	-7.28	114.23	118.60
32	1a	343	U	O4'-C1'-N1	7.24	114.00	108.20
32	2a	1001	A	O4'-C1'-N9	7.18	113.94	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	2a	1034	G	N3-C4-N9	7.15	130.29	126.00
1	1A	2604	G	O5'-P-OP1	-7.15	99.27	105.70
1	2A	740	U	O5'-P-OP2	-7.12	99.29	105.70
1	1A	2227	G	N3-C4-N9	-7.08	121.75	126.00
32	2a	1125	U	C2-N1-C1'	7.06	126.17	117.70
2	1B	59	A	C6-N1-C2	-7.04	114.38	118.60
2	1B	24	G	N3-C4-C5	-7.03	125.09	128.60
32	2a	1034	G	C2-N3-C4	6.99	115.39	111.90
1	1A	2188	G	C8-N9-C1'	6.96	136.05	127.00
1	1A	720	C	N3-C4-C5	6.94	124.68	121.90
1	1A	1378	G	O5'-P-OP1	-6.93	99.47	105.70
1	1A	932	C	C5-C6-N1	6.91	124.46	121.00
32	2a	1436	U	C2-N3-C4	-6.88	122.87	127.00
1	1A	2188	G	C6-C5-N7	6.87	134.52	130.40
1	1A	194	G	O5'-P-OP2	-6.84	99.54	105.70
1	1A	2802	C	C2-N1-C1'	-6.84	111.28	118.80
1	1A	2188	G	C4-N9-C1'	-6.83	117.63	126.50
1	1A	2188	G	N9-C4-C5	6.81	108.12	105.40
1	1A	101	A	N1-C6-N6	6.79	122.67	118.60
32	2a	993	G	N3-C4-N9	6.79	130.07	126.00
19	2X	57	LEU	CA-CB-CG	6.78	130.88	115.30
32	1a	1397	C	C2-N1-C1'	6.77	126.24	118.80
1	2A	1092	C	N1-C2-O2	6.76	122.96	118.90
32	1a	1137	C	C5-C6-N1	6.75	124.38	121.00
32	2a	404	U	C2-N1-C1'	6.73	125.77	117.70
1	1A	848	G	O5'-P-OP2	-6.72	99.65	105.70
32	2a	1003	G	C8-N9-C4	-6.72	103.71	106.40
1	1A	2459	G	C6-N1-C2	-6.71	121.07	125.10
1	2A	383	U	N1-C2-O2	6.69	127.48	122.80
1	1A	215	G	C2-N3-C4	6.68	115.24	111.90
1	2A	1416	G	O4'-C1'-N9	6.67	113.54	108.20
32	2a	299	G	N1-C6-O6	6.66	123.90	119.90
32	2a	993	G	N3-C4-C5	-6.64	125.28	128.60
1	1A	952	G	N9-C4-C5	6.62	108.05	105.40
32	1a	343	U	C6-N1-C1'	6.62	130.47	121.20
1	1A	537	G	O4'-C1'-N9	6.62	113.50	108.20
1	1A	418	G	C6-N1-C2	-6.62	121.13	125.10
32	2a	993	G	C4-N9-C1'	6.59	135.07	126.50
1	2A	2130	U	C5-C6-N1	6.54	125.97	122.70
1	1A	1140	U	O4'-C1'-N1	6.52	113.41	108.20
32	1a	1436	U	C5-C4-O4	-6.49	122.01	125.90
32	2a	1397	C	C2-N1-C1'	6.49	125.94	118.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1A	2188	G	C5-C6-O6	6.48	132.49	128.60
32	2a	1030(B)	C	C2-N1-C1'	6.47	125.92	118.80
32	2a	404	U	N3-C2-O2	-6.47	117.67	122.20
32	2a	299	G	C4-C5-N7	6.46	113.38	110.80
55	1y	15	PRO	O-C-N	-6.45	112.38	122.70
1	2A	807	U	C5-C4-O4	-6.41	122.05	125.90
32	1a	78	G	C8-N9-C1'	6.40	135.32	127.00
1	1A	215	G	N1-C2-N2	6.38	121.94	116.20
1	1A	720	C	N1-C2-N3	6.36	123.65	119.20
1	1A	2227	G	N3-C4-C5	6.36	131.78	128.60
32	2a	1003	G	N3-C4-C5	-6.36	125.42	128.60
1	2A	2102	U	N1-C2-O2	6.34	127.24	122.80
1	2A	1835	G	C4-N9-C1'	6.34	134.74	126.50
1	1A	1462	G	O4'-C1'-N9	6.33	113.26	108.20
1	1A	2180	A	O4'-C1'-N9	6.32	113.25	108.20
1	2A	2689	U	N3-C2-O2	-6.30	117.79	122.20
32	2a	1003	G	C4-N9-C1'	6.29	134.68	126.50
1	2A	1076	C	O4'-C1'-N1	6.28	113.23	108.20
1	2A	2447	G	C6-N1-C2	-6.28	121.33	125.10
1	1A	2136	A	N1-C6-N6	-6.28	114.83	118.60
1	1A	2390	A	C4-C5-C6	6.28	120.14	117.00
1	1A	410	U	N1-C2-O2	6.28	127.19	122.80
1	1A	1134	A	O4'-C1'-N9	6.28	113.22	108.20
32	2a	299	G	C6-C5-N7	-6.28	126.64	130.40
32	1a	343	U	C5-C4-O4	6.25	129.65	125.90
1	1A	2802	C	C6-N1-C1'	6.25	128.30	120.80
32	1a	533	A	N1-C6-N6	6.25	122.35	118.60
32	1a	1406	U	C2-N3-C4	-6.23	123.26	127.00
2	2B	59	A	C6-N1-C2	-6.22	114.87	118.60
32	2a	5	U	C2-N1-C1'	6.22	125.17	117.70
1	1A	1398	U	O5'-P-OP1	-6.21	100.11	105.70
1	2A	1052	C	C2-N1-C1'	6.20	125.62	118.80
32	2a	346	G	C6-N1-C2	-6.20	121.38	125.10
1	2A	2699	C	C6-N1-C2	6.19	122.78	120.30
1	1A	2903	G	N3-C4-N9	-6.19	122.29	126.00
1	2A	1835	G	C8-N9-C1'	-6.19	118.96	127.00
1	2A	2187	G	C6-C5-N7	-6.18	126.69	130.40
32	2a	1030(B)	C	N1-C2-O2	6.18	122.61	118.90
1	1A	1386	U	C2-N3-C4	-6.16	123.30	127.00
32	1a	1465	C	N3-C4-C5	6.15	124.36	121.90
1	1A	82	G	C2-N3-C4	-6.14	108.83	111.90
32	2a	1228	C	N1-C2-O2	6.14	122.59	118.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	2A	1087	G	N3-C4-N9	-6.10	122.34	126.00
1	1A	1110	C	C5-C6-N1	6.09	124.05	121.00
32	2a	1036	G	N7-C8-N9	6.08	116.14	113.10
2	1B	24	G	C6-N1-C2	-6.07	121.46	125.10
1	2A	1053	C	P-O3'-C3'	6.07	126.98	119.70
32	2a	343	U	C6-N1-C1'	6.07	129.69	121.20
32	1a	1024	G	N3-C4-N9	6.06	129.64	126.00
1	1A	598	A	O5'-P-OP1	-6.06	100.25	105.70
32	1a	78	G	C4-N9-C1'	-6.06	118.63	126.50
32	2a	1028	C	C6-N1-C2	-6.05	117.88	120.30
1	1A	2188	G	C4-C5-N7	-6.03	108.39	110.80
1	1A	720	C	N1-C2-O2	-6.02	115.29	118.90
32	1a	1024	G	C8-N9-C1'	-6.02	119.17	127.00
32	1a	1024	G	C4-N9-C1'	6.02	134.32	126.50
1	1A	1418	U	C2-N1-C1'	6.01	124.91	117.70
32	1a	498	U	C5-C4-O4	6.00	129.50	125.90
32	1a	1495	U	C5-C6-N1	6.00	125.70	122.70
1	1A	2161	C	C5-C6-N1	5.99	124.00	121.00
1	2A	2103	C	C6-N1-C2	-5.99	117.90	120.30
32	2a	5	U	N3-C2-O2	-5.99	118.01	122.20
1	1A	2125	C	N1-C2-O2	5.98	122.48	118.90
1	1A	2227	G	C6-C5-N7	5.97	133.99	130.40
1	1A	1578	C	C6-N1-C2	-5.96	117.92	120.30
32	2a	1005	A	C8-N9-C4	-5.96	103.42	105.80
32	1a	299	G	C4-C5-N7	5.96	113.18	110.80
2	1B	75	G	C5-C6-O6	-5.96	125.03	128.60
1	2A	1087	G	C8-N9-C1'	5.94	134.72	127.00
1	1A	215	G	C6-C5-N7	5.93	133.96	130.40
1	1A	637	U	O4'-C1'-N1	5.93	112.94	108.20
32	1a	1285	A	P-O3'-C3'	5.93	126.81	119.70
32	2a	1495	U	C2-N1-C1'	5.91	124.79	117.70
1	1A	952	G	C4-C5-N7	-5.91	108.44	110.80
32	1a	1495	U	C2-N3-C4	5.90	130.54	127.00
32	2a	1495	U	N3-C2-O2	-5.87	118.09	122.20
1	1A	952	G	C6-C5-N7	5.86	133.92	130.40
32	2a	346	G	C5-C6-N1	5.84	114.42	111.50
1	1A	1959	A	N1-C6-N6	-5.84	115.09	118.60
1	2A	277	C	N1-C2-O2	5.84	122.40	118.90
2	1B	75	G	N3-C4-C5	-5.84	125.68	128.60
1	1A	2136	A	C8-N9-C4	-5.83	103.47	105.80
32	2a	1465	C	C5-C4-N4	-5.82	116.12	120.20
1	2A	2430	A	O5'-P-OP2	-5.82	100.46	105.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	2a	5	U	N1-C2-O2	5.82	126.88	122.80
32	1a	841	U	C6-N1-C2	-5.82	117.51	121.00
1	2A	1992	G	P-O3'-C3'	5.82	126.68	119.70
32	2a	1228	C	N3-C2-O2	-5.81	117.83	121.90
32	1a	1397	C	N3-C2-O2	-5.80	117.84	121.90
32	2a	1026	G	N7-C8-N9	5.79	116.00	113.10
1	1A	217	A	C5-N7-C8	-5.78	101.01	103.90
1	2A	752	A	P-O3'-C3'	5.78	126.63	119.70
32	1a	78	G	O4'-C1'-N9	5.77	112.81	108.20
32	2a	266	G	P-O3'-C3'	5.77	126.62	119.70
1	1A	1440	U	O5'-P-OP1	-5.76	100.51	105.70
1	1A	2157	A	N1-C6-N6	5.76	122.06	118.60
32	2a	1024	G	C2-N3-C4	5.75	114.78	111.90
32	2a	754	C	C2-N1-C1'	5.75	125.12	118.80
32	1a	343	U	C5-C6-N1	-5.75	119.83	122.70
32	2a	346	G	C5-C6-O6	-5.74	125.16	128.60
1	2A	1313	U	C2-N1-C1'	5.73	124.58	117.70
32	1a	533	A	C5-C6-N6	-5.71	119.13	123.70
1	2A	673	C	N3-C4-C5	5.71	124.18	121.90
1	2A	2144	U	O4'-C1'-N1	5.71	112.76	108.20
32	1a	343	U	N3-C4-O4	-5.70	115.41	119.40
1	1A	529	U	C2-N1-C1'	5.70	124.54	117.70
32	1a	533	A	C6-C5-N7	-5.69	128.32	132.30
1	2A	2451	A	C5-N7-C8	-5.68	101.06	103.90
1	1A	989	G	N7-C8-N9	5.68	115.94	113.10
1	1A	2209	G	C5-C6-O6	-5.67	125.20	128.60
1	2A	1052	C	N1-C2-O2	5.67	122.30	118.90
54	2x	22	G	C5-N7-C8	-5.67	101.47	104.30
1	1A	780	G	C5-N7-C8	5.66	107.13	104.30
32	1a	1067	A	P-O3'-C3'	5.66	126.49	119.70
1	1A	215	G	N1-C2-N3	-5.66	120.51	123.90
32	2a	1406	U	C2-N3-C4	-5.66	123.61	127.00
32	2a	1067	A	P-O3'-C3'	5.64	126.47	119.70
1	1A	2123	G	O4'-C1'-N9	5.64	112.71	108.20
1	1A	1718	U	O5'-P-OP2	-5.63	100.63	105.70
1	2A	383	U	N3-C2-O2	-5.63	118.26	122.20
2	1B	75	G	C5-C6-N1	5.63	114.31	111.50
32	2a	1281	U	C2-N1-C1'	5.63	124.45	117.70
32	2a	993	G	C8-N9-C1'	-5.62	119.69	127.00
1	1A	2275	C	N1-C2-O2	-5.61	115.53	118.90
2	1B	24	G	N3-C4-N9	5.61	129.37	126.00
1	2A	1087	G	C4-N9-C1'	-5.60	119.22	126.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	1a	1397	C	C6-N1-C2	-5.58	118.07	120.30
32	2a	299	G	N9-C4-C5	-5.58	103.17	105.40
1	1A	2136	A	N9-C4-C5	5.57	108.03	105.80
1	1A	2802	C	O4'-C1'-N1	5.57	112.66	108.20
1	2A	512	G	O4'-C1'-N9	5.57	112.66	108.20
32	2a	1034	G	C5-C6-O6	-5.57	125.26	128.60
2	2B	8	U	C5-C6-N1	5.57	125.48	122.70
1	1A	1838	G	C2-N3-C4	-5.56	109.12	111.90
1	2A	2102	U	N3-C2-O2	-5.56	118.31	122.20
1	1A	1811	A	O5'-P-OP1	-5.56	100.70	105.70
1	2A	673	C	C5-C4-N4	-5.56	116.31	120.20
1	1A	2903	G	N9-C4-C5	5.55	107.62	105.40
2	1B	102	A	N1-C2-N3	5.55	132.07	129.30
1	1A	215	G	N9-C4-C5	5.55	107.62	105.40
1	2A	1092	C	C2-N1-C1'	5.54	124.89	118.80
32	1a	1065	U	P-O3'-C3'	5.54	126.34	119.70
1	1A	31	C	O5'-P-OP1	-5.53	100.72	105.70
1	1A	2589	A	O5'-P-OP1	-5.53	100.72	105.70
1	1A	2903	G	C6-C5-N7	5.53	133.72	130.40
1	1A	1054	C	C6-N1-C2	-5.53	118.09	120.30
1	2A	226	G	C4-N9-C1'	-5.52	119.32	126.50
32	1a	1465	C	C5-C4-N4	-5.52	116.33	120.20
32	2a	1158	C	C6-N1-C2	-5.52	118.09	120.30
32	2a	1005	A	N7-C8-N9	5.52	116.56	113.80
1	1A	215	G	O4'-C1'-N9	5.52	112.61	108.20
1	1A	2181	G	O4'-C1'-N9	5.51	112.61	108.20
32	2a	841	U	C5-C6-N1	5.51	125.45	122.70
32	1a	266	G	P-O3'-C3'	5.50	126.31	119.70
32	1a	993	G	C4-N9-C1'	5.50	133.65	126.50
32	1a	991	U	P-O3'-C3'	5.49	126.28	119.70
27	25	58	LEU	CA-CB-CG	5.49	127.92	115.30
32	2a	1026	G	C5-N7-C8	-5.49	101.56	104.30
1	1A	1398	U	O5'-P-OP2	5.48	117.28	110.70
32	1a	1442	G	N3-C4-C5	-5.47	125.86	128.60
1	2A	2870	C	C6-N1-C2	-5.47	118.11	120.30
32	2a	299	G	N3-C4-N9	5.46	129.28	126.00
1	1A	952	G	C8-N9-C1'	5.46	134.10	127.00
1	1A	1222	A	O5'-P-OP1	-5.46	100.78	105.70
1	1A	2167	C	C5-C6-N1	5.46	123.73	121.00
32	2a	289	G	O5'-P-OP2	5.45	117.24	110.70
32	2a	520	A	N9-C4-C5	5.45	107.98	105.80
32	2a	1436	U	C5-C4-O4	-5.45	122.63	125.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1A	101	A	C4-C5-C6	5.44	119.72	117.00
1	1A	215	G	C8-N9-C1'	5.44	134.07	127.00
1	2A	1312	U	C5-C4-O4	5.44	129.16	125.90
54	2x	47	U	C5-C6-N1	5.44	125.42	122.70
1	2A	2207	G	N7-C8-N9	5.42	115.81	113.10
32	2a	1158	C	C2-N1-C1'	5.42	124.76	118.80
1	2A	2321	G	P-O3'-C3'	5.41	126.19	119.70
1	1A	2183	C	C5-C6-N1	5.41	123.70	121.00
1	2A	513	A	N1-C6-N6	5.39	121.83	118.60
1	1A	215	G	N3-C4-N9	-5.39	122.77	126.00
1	1A	223	C	N1-C2-O2	5.38	122.13	118.90
1	1A	184	A	P-O3'-C3'	5.38	126.16	119.70
1	1A	2057	G	O5'-P-OP1	-5.37	100.86	105.70
32	2a	404	U	C5-C6-N1	5.37	125.39	122.70
1	1A	2390	A	N1-C6-N6	5.37	121.82	118.60
1	2A	2120	G	N3-C4-N9	5.36	129.22	126.00
32	2a	901	A	N1-C6-N6	5.36	121.82	118.60
1	1A	854	U	N1-C2-N3	5.36	118.12	114.90
1	1A	82	G	C8-N9-C4	5.36	108.54	106.40
1	1A	2459	G	C5-C6-N1	5.35	114.18	111.50
1	1A	1418	U	C5-C4-O4	-5.35	122.69	125.90
1	2A	784	A	P-O3'-C3'	5.34	126.11	119.70
32	1a	1201	A	P-O3'-C3'	5.34	126.11	119.70
1	1A	2627	U	O5'-P-OP1	-5.33	100.90	105.70
1	1A	1020	C	O5'-P-OP1	-5.33	100.90	105.70
1	1A	1815	A	O5'-P-OP2	-5.33	100.90	105.70
32	1a	299	G	N9-C4-C5	-5.33	103.27	105.40
32	1a	404	U	N3-C2-O2	-5.33	118.47	122.20
1	1A	2188	G	N3-C4-C5	5.33	131.26	128.60
32	1a	754	C	C2-N1-C1'	5.32	124.65	118.80
32	2a	343	U	O4'-C1'-N1	5.32	112.45	108.20
1	2A	1992	G	N3-C4-C5	-5.30	125.95	128.60
1	2A	1351	C	OP1-P-O3'	5.29	116.85	105.20
32	2a	1030(B)	C	C5-C6-N1	5.29	123.65	121.00
32	1a	404	U	C2-N1-C1'	5.29	124.05	117.70
1	1A	906	G	C8-N9-C4	5.29	108.52	106.40
1	2A	2144	U	C2-N1-C1'	5.29	124.04	117.70
1	1A	697	C	C5-C6-N1	5.28	123.64	121.00
1	2A	1359	A	C2-N3-C4	5.28	113.24	110.60
32	1a	1024	G	C6-C5-N7	-5.28	127.23	130.40
1	1A	2587	C	O5'-P-OP2	-5.27	100.95	105.70
32	2a	60	A	P-O3'-C3'	5.27	126.02	119.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1A	854	U	C5-C4-O4	-5.26	122.74	125.90
1	1A	2457	G	N1-C6-O6	-5.26	116.74	119.90
1	1A	2134	G	N3-C4-C5	-5.26	125.97	128.60
1	1A	1162	C	C2-N1-C1'	5.25	124.58	118.80
32	1a	975	A	O4'-C1'-N9	-5.25	104.00	108.20
1	1A	236	G	C8-N9-C4	5.25	108.50	106.40
1	1A	2045	G	O5'-P-OP1	-5.25	100.98	105.70
1	1A	1220	U	P-O3'-C3'	5.25	125.99	119.70
32	1a	346	G	C5-C6-O6	-5.24	125.45	128.60
1	2A	2318	G	C4-N9-C1'	5.24	133.31	126.50
1	2A	1045	A	C2-N3-C4	5.23	113.22	110.60
1	2A	2146	C	O4'-C1'-N1	5.23	112.38	108.20
32	2a	404	U	C2-N3-C4	5.23	130.14	127.00
1	1A	1716	A	C8-N9-C4	-5.23	103.71	105.80
1	2A	386	G	C6-N1-C2	-5.22	121.97	125.10
12	1Q	41	TRP	CD2-CE2-CZ2	5.22	128.56	122.30
1	1A	82	G	C4-C5-N7	5.22	112.89	110.80
1	1A	697	C	N1-C2-O2	5.21	122.03	118.90
32	1a	353	A	OP2-P-O3'	5.21	116.67	105.20
32	2a	1027	C	N3-C2-O2	-5.21	118.25	121.90
1	1A	1119	A	C2-N3-C4	5.21	113.21	110.60
1	2A	2114	A	C8-N9-C4	-5.21	103.72	105.80
1	1A	2194	U	C5-C4-O4	5.20	129.02	125.90
32	2a	1026	G	C8-N9-C4	-5.20	104.32	106.40
54	2x	46	G	C6-N1-C2	-5.20	121.98	125.10
32	2a	1036	G	C8-N9-C4	-5.20	104.32	106.40
1	1A	1687	C	O4'-C1'-N1	5.20	112.36	108.20
1	1A	847	A	N1-C6-N6	-5.20	115.48	118.60
32	1a	1213	A	N1-C6-N6	-5.19	115.48	118.60
1	1A	1239	A	N1-C6-N6	-5.19	115.49	118.60
32	1a	1067	A	C8-N9-C4	-5.19	103.72	105.80
1	1A	2155	G	O4'-C1'-N9	5.18	112.35	108.20
1	1A	1110	C	C2-N1-C1'	5.18	124.50	118.80
1	1A	215	G	C4-N9-C1'	-5.18	119.77	126.50
1	1A	599	U	O5'-P-OP1	-5.18	101.04	105.70
1	1A	1388	A	O5'-P-OP2	-5.17	101.04	105.70
1	1A	665	C	C6-N1-C2	-5.17	118.23	120.30
1	1A	1707	C	N3-C4-N4	-5.17	114.38	118.00
32	1a	1442	G	P-O3'-C3'	5.17	125.90	119.70
1	1A	752	A	N1-C6-N6	5.16	121.70	118.60
32	2a	1397	C	C6-N1-C1'	-5.16	114.61	120.80
1	1A	1220	U	OP1-P-O3'	5.15	116.54	105.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1A	952	G	O4'-C1'-N9	5.14	112.31	108.20
1	1A	2192	A	O4'-C1'-N9	5.14	112.31	108.20
32	2a	266	G	C4-N9-C1'	5.14	133.18	126.50
32	1a	533	A	C4-C5-C6	5.13	119.57	117.00
1	2A	2378	A	N1-C6-N6	5.13	121.68	118.60
1	1A	101	A	N9-C4-C5	-5.13	103.75	105.80
32	2a	1257	U	O4'-C1'-N1	5.13	112.30	108.20
1	1A	1255	A	P-O3'-C3'	5.13	125.85	119.70
12	1Q	41	TRP	CE2-CD2-CG	5.13	111.40	107.30
1	2A	458	G	O4'-C1'-N9	5.12	112.29	108.20
1	2A	277	C	C2-N1-C1'	5.11	124.42	118.80
1	2A	1416	G	C4-N9-C1'	-5.11	119.86	126.50
32	2a	520	A	C8-N9-C4	-5.11	103.76	105.80
32	1a	1026	G	O4'-C1'-N9	5.11	112.29	108.20
1	1A	1142	A	O4'-C1'-N9	5.10	112.28	108.20
32	1a	1027	C	C5-C6-N1	5.10	123.55	121.00
1	2A	2187	G	N3-C4-N9	5.10	129.06	126.00
1	1A	1134	A	C4-N9-C1'	5.09	135.47	126.30
3	1D	155	LEU	CA-CB-CG	5.09	127.02	115.30
32	1a	78	G	N3-C4-N9	-5.09	122.95	126.00
32	1a	1036	G	C4-N9-C1'	5.09	133.12	126.50
1	1A	203	G	O4'-C1'-N9	5.08	112.27	108.20
1	1A	2597	U	OP1-P-O3'	5.08	116.37	105.20
1	2A	2318	G	C8-N9-C4	-5.08	104.37	106.40
1	1A	637	U	C2-N1-C1'	5.08	123.79	117.70
1	1A	1218	G	O4'-C1'-N9	5.08	112.26	108.20
1	1A	1738	C	N3-C2-O2	-5.08	118.35	121.90
1	1A	2155	G	C4-N9-C1'	-5.07	119.91	126.50
32	2a	1016	A	N1-C6-N6	5.07	121.64	118.60
2	1B	24	G	C4-N9-C1'	5.07	133.09	126.50
32	1a	115	G	P-O3'-C3'	5.07	125.78	119.70
1	2A	614	U	C2-N1-C1'	5.06	123.78	117.70
1	2A	2585	U	OP1-P-O3'	5.06	116.34	105.20
32	1a	533	A	C6-N1-C2	-5.06	115.56	118.60
1	2A	2238	G	N3-C4-C5	-5.06	126.07	128.60
32	2a	913	A	P-O3'-C3'	5.06	125.77	119.70
1	1A	137	G	C8-N9-C1'	-5.06	120.43	127.00
1	1A	2014	G	O5'-P-OP1	-5.05	101.15	105.70
32	2a	687	A	P-O3'-C3'	5.05	125.76	119.70
1	1A	2513	C	C2-N1-C1'	-5.05	113.25	118.80
1	1A	2903	G	N3-C2-N2	-5.05	116.37	119.90
1	1A	101	A	C8-N9-C1'	-5.05	118.61	127.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	2A	1835	G	O4'-C1'-N9	-5.05	104.16	108.20
32	2a	1465	C	N3-C4-C5	5.04	123.92	121.90
1	1A	1007	G	OP1-P-O3'	5.04	116.29	105.20
1	1A	1098	C	C6-N1-C2	-5.04	118.28	120.30
1	2A	1420	U	P-O3'-C3'	5.04	125.75	119.70
1	1A	2614	A	P-O3'-C3'	5.04	125.74	119.70
32	2a	1004	A	O4'-C1'-N9	5.03	112.23	108.20
1	1A	894	U	C2-N1-C1'	5.03	123.73	117.70
24	12	69	ARG	N-CA-C	5.03	124.58	111.00
1	1A	1332	A	C8-N9-C4	5.02	107.81	105.80
1	1A	611	U	O5'-P-OP2	-5.02	101.18	105.70
1	1A	279	G	O4'-C1'-N9	-5.02	104.19	108.20
1	1A	765	A	N1-C6-N6	5.01	121.61	118.60
1	2A	906	G	N9-C4-C5	5.01	107.41	105.40
1	2A	1131	G	O4'-C1'-N9	5.01	112.21	108.20
1	1A	399	G	O4'-C1'-N9	5.01	112.21	108.20
1	2A	226	G	C8-N9-C1'	5.01	133.51	127.00
1	2A	800	A	O5'-P-OP1	-5.01	101.19	105.70
1	2A	2114	A	N7-C8-N9	5.01	116.30	113.80
1	2A	391	G	C6-N1-C2	-5.00	122.10	125.10
32	1a	993	G	N3-C4-N9	5.00	129.00	126.00
1	2A	1210	A	P-O3'-C3'	5.00	125.70	119.70

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
33	1b	231	GLU	Peptide
55	1y	15	PRO	Mainchain
26	24	59	PHE	Peptide
55	2y	15	PRO	Mainchain

5.2 Too-close contacts

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

5.3 Torsion angles

5.3.1 Protein backbone

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	273/275 (99%)	259 (95%)	13 (5%)	1 (0%)	34	66
3	2D	273/275 (99%)	261 (96%)	12 (4%)	0	100	100
4	1E	202/204 (99%)	193 (96%)	8 (4%)	1 (0%)	29	61
4	2E	202/204 (99%)	192 (95%)	9 (4%)	1 (0%)	29	61
5	1F	201/203 (99%)	196 (98%)	5 (2%)	0	100	100
5	2F	201/203 (99%)	192 (96%)	8 (4%)	1 (0%)	29	61
6	1G	179/181 (99%)	161 (90%)	16 (9%)	2 (1%)	14	41
6	2G	179/181 (99%)	164 (92%)	14 (8%)	1 (1%)	25	56
7	1H	172/174 (99%)	161 (94%)	11 (6%)	0	100	100
7	2H	171/174 (98%)	161 (94%)	10 (6%)	0	100	100
8	1I	145/147 (99%)	130 (90%)	12 (8%)	3 (2%)	7	23
8	2I	144/147 (98%)	131 (91%)	13 (9%)	0	100	100
9	1N	138/140 (99%)	135 (98%)	3 (2%)	0	100	100
9	2N	138/140 (99%)	136 (99%)	2 (1%)	0	100	100
10	1O	120/122 (98%)	113 (94%)	6 (5%)	1 (1%)	19	49
10	2O	120/122 (98%)	113 (94%)	6 (5%)	1 (1%)	19	49
11	1P	147/149 (99%)	137 (93%)	10 (7%)	0	100	100
11	2P	147/149 (99%)	138 (94%)	9 (6%)	0	100	100
12	1Q	139/141 (99%)	133 (96%)	6 (4%)	0	100	100
12	2Q	139/141 (99%)	133 (96%)	6 (4%)	0	100	100
13	1R	116/118 (98%)	110 (95%)	6 (5%)	0	100	100
13	2R	116/118 (98%)	109 (94%)	7 (6%)	0	100	100
14	1S	108/110 (98%)	102 (94%)	5 (5%)	1 (1%)	17	46
14	2S	108/110 (98%)	103 (95%)	5 (5%)	0	100	100
15	1T	129/131 (98%)	122 (95%)	7 (5%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
15	2T	129/131 (98%)	123 (95%)	6 (5%)	0	100	100
16	1U	114/116 (98%)	112 (98%)	2 (2%)	0	100	100
16	2U	114/116 (98%)	112 (98%)	2 (2%)	0	100	100
17	1V	99/101 (98%)	95 (96%)	3 (3%)	1 (1%)	15	44
17	2V	99/101 (98%)	95 (96%)	3 (3%)	1 (1%)	15	44
18	1W	110/112 (98%)	106 (96%)	4 (4%)	0	100	100
18	2W	110/112 (98%)	108 (98%)	2 (2%)	0	100	100
19	1X	93/95 (98%)	90 (97%)	2 (2%)	1 (1%)	14	41
19	2X	93/95 (98%)	88 (95%)	4 (4%)	1 (1%)	14	41
20	1Y	105/107 (98%)	98 (93%)	7 (7%)	0	100	100
20	2Y	105/107 (98%)	100 (95%)	5 (5%)	0	100	100
21	1Z	201/203 (99%)	186 (92%)	15 (8%)	0	100	100
21	2Z	199/203 (98%)	184 (92%)	15 (8%)	0	100	100
22	10	75/77 (97%)	70 (93%)	5 (7%)	0	100	100
22	20	75/77 (97%)	70 (93%)	5 (7%)	0	100	100
23	11	95/97 (98%)	94 (99%)	1 (1%)	0	100	100
23	21	95/97 (98%)	93 (98%)	1 (1%)	1 (1%)	14	41
24	12	68/70 (97%)	66 (97%)	2 (3%)	0	100	100
24	22	68/70 (97%)	66 (97%)	2 (3%)	0	100	100
25	13	57/59 (97%)	55 (96%)	2 (4%)	0	100	100
25	23	57/59 (97%)	54 (95%)	3 (5%)	0	100	100
26	14	67/69 (97%)	55 (82%)	8 (12%)	4 (6%)	1	4
26	24	67/69 (97%)	52 (78%)	14 (21%)	1 (2%)	10	33
27	15	57/59 (97%)	54 (95%)	3 (5%)	0	100	100
27	25	57/59 (97%)	54 (95%)	3 (5%)	0	100	100
28	16	51/53 (96%)	49 (96%)	2 (4%)	0	100	100
28	26	51/53 (96%)	49 (96%)	2 (4%)	0	100	100
29	17	46/48 (96%)	44 (96%)	2 (4%)	0	100	100
29	27	46/48 (96%)	44 (96%)	2 (4%)	0	100	100
30	18	62/64 (97%)	60 (97%)	2 (3%)	0	100	100
30	28	62/64 (97%)	59 (95%)	3 (5%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
31	19	35/37 (95%)	35 (100%)	0	0	100	100
31	29	35/37 (95%)	35 (100%)	0	0	100	100
33	1b	229/231 (99%)	201 (88%)	20 (9%)	8 (4%)	3	12
33	2b	229/231 (99%)	198 (86%)	24 (10%)	7 (3%)	4	14
34	1c	204/206 (99%)	185 (91%)	17 (8%)	2 (1%)	15	44
34	2c	204/206 (99%)	186 (91%)	16 (8%)	2 (1%)	15	44
35	1d	206/208 (99%)	188 (91%)	18 (9%)	0	100	100
35	2d	206/208 (99%)	188 (91%)	18 (9%)	0	100	100
36	1e	146/148 (99%)	138 (94%)	6 (4%)	2 (1%)	11	34
36	2e	146/148 (99%)	139 (95%)	7 (5%)	0	100	100
37	1f	98/100 (98%)	92 (94%)	6 (6%)	0	100	100
37	2f	98/100 (98%)	92 (94%)	6 (6%)	0	100	100
38	1g	153/155 (99%)	148 (97%)	5 (3%)	0	100	100
38	2g	153/155 (99%)	145 (95%)	7 (5%)	1 (1%)	22	53
39	1h	135/137 (98%)	130 (96%)	5 (4%)	0	100	100
39	2h	135/137 (98%)	129 (96%)	6 (4%)	0	100	100
40	1i	125/127 (98%)	112 (90%)	12 (10%)	1 (1%)	19	49
40	2i	124/127 (98%)	109 (88%)	13 (10%)	2 (2%)	9	31
41	1j	95/97 (98%)	82 (86%)	10 (10%)	3 (3%)	4	13
41	2j	94/97 (97%)	83 (88%)	9 (10%)	2 (2%)	7	23
42	1k	112/114 (98%)	100 (89%)	12 (11%)	0	100	100
42	2k	112/114 (98%)	100 (89%)	12 (11%)	0	100	100
43	1l	119/122 (98%)	114 (96%)	5 (4%)	0	100	100
43	2l	119/122 (98%)	115 (97%)	4 (3%)	0	100	100
44	1m	114/116 (98%)	102 (90%)	9 (8%)	3 (3%)	5	18
44	2m	112/116 (97%)	96 (86%)	13 (12%)	3 (3%)	5	17
45	1n	58/60 (97%)	54 (93%)	4 (7%)	0	100	100
45	2n	58/60 (97%)	54 (93%)	4 (7%)	0	100	100
46	1o	86/88 (98%)	84 (98%)	2 (2%)	0	100	100
46	2o	86/88 (98%)	81 (94%)	3 (4%)	2 (2%)	6	21
47	1p	80/82 (98%)	77 (96%)	3 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
47	2p	80/82 (98%)	76 (95%)	4 (5%)	0	100	100
48	1q	97/99 (98%)	89 (92%)	7 (7%)	1 (1%)	15	44
48	2q	97/99 (98%)	90 (93%)	6 (6%)	1 (1%)	15	44
49	1r	66/68 (97%)	60 (91%)	5 (8%)	1 (2%)	10	33
49	2r	66/68 (97%)	61 (92%)	4 (6%)	1 (2%)	10	33
50	1s	81/83 (98%)	72 (89%)	8 (10%)	1 (1%)	13	39
50	2s	81/83 (98%)	73 (90%)	7 (9%)	1 (1%)	13	39
51	1t	94/98 (96%)	85 (90%)	6 (6%)	3 (3%)	4	13
51	2t	96/98 (98%)	87 (91%)	5 (5%)	4 (4%)	3	9
52	1u	21/23 (91%)	19 (90%)	2 (10%)	0	100	100
52	2u	21/23 (91%)	19 (90%)	2 (10%)	0	100	100
55	1y	14/16 (88%)	13 (93%)	0	1 (7%)	1	2
55	2y	14/16 (88%)	13 (93%)	0	1 (7%)	1	2
All	All	11468/11680 (98%)	10719 (94%)	673 (6%)	76 (1%)	22	53

All (76) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
8	1I	11	ASN
14	1S	59	LYS
33	1b	17	PHE
33	1b	21	ARG
33	1b	37	ASN
34	1c	108	ASN
36	1e	96	PRO
40	1i	127	LYS
41	1j	79	ARG
44	1m	67	GLU
48	1q	49	GLU
51	1t	95	ALA
4	2E	51	PHE
5	2F	21	ALA
6	2G	43	LEU
23	2I	3	LYS
33	2b	8	LYS
33	2b	17	PHE
33	2b	124	SER

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Mol	Chain	Res	Type
34	2c	98	ASN
40	2i	44	VAL
40	2i	54	ASP
51	2t	95	ALA
3	1D	274	ARG
6	1G	43	LEU
8	1I	72	LEU
8	1I	73	GLU
19	1X	94	GLY
26	14	45	GLY
26	14	47	GLN
26	14	49	PHE
26	14	55	ARG
33	1b	95	GLN
33	1b	127	ILE
44	1m	12	ASN
49	1r	25	THR
55	1y	15	PRO
17	2V	79	VAL
19	2X	94	GLY
26	24	55	ARG
33	2b	10	LEU
33	2b	125	PRO
34	2c	61	ALA
41	2j	79	ARG
44	2m	67	GLU
49	2r	25	THR
55	2y	15	PRO
4	1E	52	LEU
6	1G	51	ARG
17	1V	79	VAL
33	1b	125	PRO
44	1m	106	ASN
50	1s	7	LYS
10	2O	5	GLN
44	2m	106	ASN
51	2t	7	LYS
10	1O	5	GLN
33	1b	11	LEU
34	1c	98	ASN
51	1t	10	LEU
33	2b	20	GLU

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Mol	Chain	Res	Type
33	2b	95	GLN
48	2q	49	GLU
50	2s	7	LYS
38	2g	6	ARG
44	2m	5	ALA
46	2o	88	ARG
51	2t	100	ILE
41	1j	77	PRO
51	1t	100	ILE
36	1e	97	GLY
46	2o	23	GLY
33	1b	124	SER
41	1j	31	GLY
51	2t	102	GLY
41	2j	37	PRO

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	1D	214/217 (99%)	193 (90%)	21 (10%)	8	24
3	2D	215/217 (99%)	197 (92%)	18 (8%)	11	31
4	1E	164/165 (99%)	146 (89%)	18 (11%)	6	19
4	2E	164/165 (99%)	148 (90%)	16 (10%)	8	24
5	1F	160/161 (99%)	149 (93%)	11 (7%)	15	41
5	2F	159/161 (99%)	151 (95%)	8 (5%)	24	56
6	1G	144/155 (93%)	134 (93%)	10 (7%)	15	41
6	2G	142/155 (92%)	129 (91%)	13 (9%)	9	27
7	1H	144/145 (99%)	133 (92%)	11 (8%)	13	36
7	2H	143/145 (99%)	131 (92%)	12 (8%)	11	31
8	1I	111/123 (90%)	101 (91%)	10 (9%)	9	28
8	2I	108/123 (88%)	93 (86%)	15 (14%)	3	11

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
9	1N	119/119 (100%)	110 (92%)	9 (8%)	13	36
9	2N	118/119 (99%)	104 (88%)	14 (12%)	5	16
10	1O	100/100 (100%)	94 (94%)	6 (6%)	19	48
10	2O	100/100 (100%)	97 (97%)	3 (3%)	41	75
11	1P	115/116 (99%)	107 (93%)	8 (7%)	15	40
11	2P	115/116 (99%)	108 (94%)	7 (6%)	18	48
12	1Q	111/111 (100%)	102 (92%)	9 (8%)	11	33
12	2Q	111/111 (100%)	104 (94%)	7 (6%)	18	46
13	1R	101/101 (100%)	91 (90%)	10 (10%)	8	23
13	2R	101/101 (100%)	93 (92%)	8 (8%)	12	34
14	1S	87/87 (100%)	83 (95%)	4 (5%)	27	60
14	2S	85/87 (98%)	79 (93%)	6 (7%)	14	39
15	1T	115/115 (100%)	110 (96%)	5 (4%)	29	62
15	2T	113/115 (98%)	104 (92%)	9 (8%)	12	34
16	1U	93/93 (100%)	86 (92%)	7 (8%)	13	37
16	2U	93/93 (100%)	89 (96%)	4 (4%)	29	62
17	1V	81/82 (99%)	70 (86%)	11 (14%)	3	11
17	2V	80/82 (98%)	73 (91%)	7 (9%)	10	29
18	1W	90/91 (99%)	85 (94%)	5 (6%)	21	51
18	2W	90/91 (99%)	85 (94%)	5 (6%)	21	51
19	1X	77/77 (100%)	75 (97%)	2 (3%)	46	79
19	2X	77/77 (100%)	73 (95%)	4 (5%)	23	55
20	1Y	86/88 (98%)	81 (94%)	5 (6%)	20	50
20	2Y	86/88 (98%)	83 (96%)	3 (4%)	36	70
21	1Z	169/176 (96%)	149 (88%)	20 (12%)	5	16
21	2Z	165/176 (94%)	152 (92%)	13 (8%)	12	34
22	10	61/62 (98%)	56 (92%)	5 (8%)	11	33
22	20	61/62 (98%)	59 (97%)	2 (3%)	38	72
23	11	79/82 (96%)	74 (94%)	5 (6%)	18	46
23	21	81/82 (99%)	75 (93%)	6 (7%)	13	37
24	12	65/66 (98%)	61 (94%)	4 (6%)	18	47

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
24	22	66/66 (100%)	61 (92%)	5 (8%)	13	36
25	13	51/51 (100%)	48 (94%)	3 (6%)	19	49
25	23	50/51 (98%)	47 (94%)	3 (6%)	19	48
26	14	58/62 (94%)	52 (90%)	6 (10%)	7	21
26	24	54/62 (87%)	48 (89%)	6 (11%)	6	19
27	15	51/51 (100%)	48 (94%)	3 (6%)	19	49
27	25	50/51 (98%)	49 (98%)	1 (2%)	55	84
28	16	51/51 (100%)	50 (98%)	1 (2%)	55	84
28	26	50/51 (98%)	45 (90%)	5 (10%)	7	22
29	17	41/41 (100%)	39 (95%)	2 (5%)	25	57
29	27	41/41 (100%)	40 (98%)	1 (2%)	49	81
30	18	54/54 (100%)	49 (91%)	5 (9%)	9	26
30	28	54/54 (100%)	48 (89%)	6 (11%)	6	19
31	19	34/34 (100%)	33 (97%)	1 (3%)	42	76
31	29	34/34 (100%)	34 (100%)	0	100	100
33	1b	191/199 (96%)	169 (88%)	22 (12%)	5	17
33	2b	187/199 (94%)	167 (89%)	20 (11%)	6	20
34	1c	144/160 (90%)	135 (94%)	9 (6%)	18	46
34	2c	140/160 (88%)	131 (94%)	9 (6%)	17	45
35	1d	171/180 (95%)	161 (94%)	10 (6%)	20	50
35	2d	172/180 (96%)	159 (92%)	13 (8%)	13	36
36	1e	114/114 (100%)	106 (93%)	8 (7%)	15	40
36	2e	114/114 (100%)	105 (92%)	9 (8%)	12	34
37	1f	85/90 (94%)	82 (96%)	3 (4%)	36	70
37	2f	85/90 (94%)	75 (88%)	10 (12%)	5	16
38	1g	120/126 (95%)	108 (90%)	12 (10%)	7	22
38	2g	119/126 (94%)	111 (93%)	8 (7%)	16	43
39	1h	116/118 (98%)	112 (97%)	4 (3%)	37	71
39	2h	114/118 (97%)	108 (95%)	6 (5%)	22	54
40	1i	91/98 (93%)	80 (88%)	11 (12%)	5	15
40	2i	88/98 (90%)	75 (85%)	13 (15%)	3	9

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
41	1j	68/87 (78%)	61 (90%)	7 (10%)	7	21
41	2j	68/87 (78%)	62 (91%)	6 (9%)	10	29
42	1k	83/86 (96%)	78 (94%)	5 (6%)	19	48
42	2k	83/86 (96%)	78 (94%)	5 (6%)	19	48
43	1l	96/102 (94%)	92 (96%)	4 (4%)	30	63
43	2l	96/102 (94%)	90 (94%)	6 (6%)	18	46
44	1m	90/94 (96%)	84 (93%)	6 (7%)	16	43
44	2m	87/94 (93%)	80 (92%)	7 (8%)	12	34
45	1n	49/49 (100%)	43 (88%)	6 (12%)	5	15
45	2n	49/49 (100%)	46 (94%)	3 (6%)	18	48
46	1o	78/79 (99%)	74 (95%)	4 (5%)	24	55
46	2o	78/79 (99%)	72 (92%)	6 (8%)	13	35
47	1p	69/71 (97%)	58 (84%)	11 (16%)	2	7
47	2p	68/71 (96%)	56 (82%)	12 (18%)	2	5
48	1q	94/94 (100%)	92 (98%)	2 (2%)	53	84
48	2q	94/94 (100%)	91 (97%)	3 (3%)	39	73
49	1r	59/59 (100%)	57 (97%)	2 (3%)	37	71
49	2r	59/59 (100%)	56 (95%)	3 (5%)	24	55
50	1s	68/72 (94%)	61 (90%)	7 (10%)	7	21
50	2s	67/72 (93%)	63 (94%)	4 (6%)	19	48
51	1t	71/76 (93%)	64 (90%)	7 (10%)	8	23
51	2t	70/76 (92%)	65 (93%)	5 (7%)	14	39
52	1u	18/18 (100%)	17 (94%)	1 (6%)	21	51
52	2u	18/18 (100%)	18 (100%)	0	100	100
55	1y	16/16 (100%)	13 (81%)	3 (19%)	1	5
55	2y	16/16 (100%)	14 (88%)	2 (12%)	4	14
All	All	9395/9728 (97%)	8677 (92%)	718 (8%)	13	36

All (718) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	1D	3	VAL
3	1D	13	ARG

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Mol	Chain	Res	Type
3	1D	37	LEU
3	1D	61	LEU
3	1D	88	ARG
3	1D	94	LEU
3	1D	103	ARG
3	1D	111	LEU
3	1D	113	VAL
3	1D	138	VAL
3	1D	155	LEU
3	1D	162	SER
3	1D	173	VAL
3	1D	193	VAL
3	1D	200	ASP
3	1D	211	ARG
3	1D	217	ARG
3	1D	221	VAL
3	1D	229	VAL
3	1D	242	ARG
3	1D	253	GLN
4	1E	21	VAL
4	1E	33	VAL
4	1E	45	THR
4	1E	47	VAL
4	1E	49	LEU
4	1E	75	VAL
4	1E	77	ILE
4	1E	78	LEU
4	1E	89	ASP
4	1E	101	ARG
4	1E	116	VAL
4	1E	119	ARG
4	1E	127	ASP
4	1E	144	ARG
4	1E	154	LYS
4	1E	175	VAL
4	1E	178	GLU
4	1E	181	LEU
5	1F	18	ARG
5	1F	33	LEU
5	1F	53	THR
5	1F	60	SER
5	1F	74	ARG

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Mol	Chain	Res	Type
5	1F	88	VAL
5	1F	110	LEU
5	1F	170	LEU
5	1F	175	THR
5	1F	191	ARG
5	1F	192	LEU
6	1G	28	VAL
6	1G	43	LEU
6	1G	45	GLU
6	1G	53	LEU
6	1G	79	ASN
6	1G	82	LEU
6	1G	136	ARG
6	1G	153	ARG
6	1G	167	GLU
6	1G	175	LEU
7	1H	2	SER
7	1H	13	LYS
7	1H	23	ARG
7	1H	32	GLU
7	1H	45	VAL
7	1H	47	GLU
7	1H	98	LEU
7	1H	104	GLU
7	1H	105	LEU
7	1H	107	VAL
7	1H	172	LYS
8	1I	9	LEU
8	1I	12	LEU
8	1I	38	LEU
8	1I	44	LEU
8	1I	75	LEU
8	1I	101	LEU
8	1I	103	ARG
8	1I	109	ILE
8	1I	140	LEU
8	1I	144	VAL
9	1N	5	VAL
9	1N	8	GLN
9	1N	33	LEU
9	1N	34	LEU
9	1N	48	MET

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Mol	Chain	Res	Type
9	1N	83	LYS
9	1N	99	LEU
9	1N	133	GLN
9	1N	140	VAL
10	1O	8	LEU
10	1O	24	VAL
10	1O	26	LYS
10	1O	69	ILE
10	1O	80	ASP
10	1O	94	ARG
11	1P	2	LYS
11	1P	59	LEU
11	1P	76	LYS
11	1P	83	VAL
11	1P	125	VAL
11	1P	147	LEU
11	1P	148	LEU
11	1P	149	GLU
12	1Q	2	LEU
12	1Q	7	MET
12	1Q	22	LYS
12	1Q	35	VAL
12	1Q	60	ARG
12	1Q	75	THR
12	1Q	98	LYS
12	1Q	109	VAL
12	1Q	110	THR
13	1R	29	LEU
13	1R	33	ARG
13	1R	36	THR
13	1R	44	LEU
13	1R	54	LEU
13	1R	65	LEU
13	1R	75	LEU
13	1R	96	ARG
13	1R	100	LEU
13	1R	111	LEU
14	1S	14	VAL
14	1S	17	ARG
14	1S	59	LYS
14	1S	75	GLU
15	1T	6	LEU

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Mol	Chain	Res	Type
15	1T	28	VAL
15	1T	74	ARG
15	1T	78	LEU
15	1T	89	VAL
16	1U	5	LYS
16	1U	8	VAL
16	1U	52	ARG
16	1U	74	LEU
16	1U	84	LYS
16	1U	104	GLN
16	1U	117	GLN
17	1V	1	MET
17	1V	7	THR
17	1V	21	ARG
17	1V	44	LYS
17	1V	46	VAL
17	1V	52	VAL
17	1V	61	VAL
17	1V	79	VAL
17	1V	82	ARG
17	1V	91	TYR
17	1V	95	LEU
18	1W	17	VAL
18	1W	19	LEU
18	1W	67	ASP
18	1W	100	THR
18	1W	107	LEU
19	1X	66	LEU
19	1X	68	ARG
20	1Y	23	ARG
20	1Y	43	ASN
20	1Y	47	LYS
20	1Y	72	VAL
20	1Y	107	ASP
21	1Z	11	GLU
21	1Z	18	LEU
21	1Z	20	ARG
21	1Z	28	MET
21	1Z	33	LEU
21	1Z	42	VAL
21	1Z	61	LEU
21	1Z	72	ARG

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Mol	Chain	Res	Type
21	1Z	76	LEU
21	1Z	86	VAL
21	1Z	91	LEU
21	1Z	103	ARG
21	1Z	126	VAL
21	1Z	150	LEU
21	1Z	155	LEU
21	1Z	162	GLU
21	1Z	185	GLU
21	1Z	193	GLU
21	1Z	202	GLU
21	1Z	203	GLU
22	10	11	ARG
22	10	14	ARG
22	10	39	ARG
22	10	43	THR
22	10	59	LEU
23	11	21	ARG
23	11	30	VAL
23	11	76	ARG
23	11	81	LYS
23	11	83	GLU
24	12	3	LEU
24	12	32	LEU
24	12	53	LEU
24	12	70	GLN
25	13	8	LEU
25	13	23	LEU
25	13	54	VAL
26	14	13	ARG
26	14	27	THR
26	14	49	PHE
26	14	50	VAL
26	14	59	PHE
26	14	60	GLN
27	15	6	VAL
27	15	16	ARG
27	15	58	LEU
28	16	48	VAL
29	17	24	THR
29	17	43	THR
30	18	14	VAL

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Mol	Chain	Res	Type
30	18	30	ARG
30	18	31	HIS
30	18	32	LEU
30	18	34	TRP
31	19	35	ARG
33	1b	9	GLU
33	1b	15	VAL
33	1b	17	PHE
33	1b	19	HIS
33	1b	24	TRP
33	1b	35	GLU
33	1b	45	GLN
33	1b	63	MET
33	1b	73	THR
33	1b	75	LYS
33	1b	76	GLN
33	1b	82	ARG
33	1b	111	ARG
33	1b	126	GLU
33	1b	144	ARG
33	1b	158	LEU
33	1b	160	ASP
33	1b	172	ILE
33	1b	178	ARG
33	1b	221	LEU
33	1b	226	ARG
33	1b	231	GLU
34	1c	3	ASN
34	1c	54	ARG
34	1c	64	VAL
34	1c	70	VAL
34	1c	89	GLU
34	1c	104	GLN
34	1c	105	GLU
34	1c	161	GLU
34	1c	192	THR
35	1d	31	CYS
35	1d	85	LYS
35	1d	86	LYS
35	1d	107	ARG
35	1d	108	LEU
35	1d	122	ARG

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Mol	Chain	Res	Type
35	1d	127	THR
35	1d	135	LEU
35	1d	158	ILE
35	1d	173	TRP
36	1e	10	MET
36	1e	20	GLN
36	1e	34	VAL
36	1e	41	VAL
36	1e	68	GLU
36	1e	69	VAL
36	1e	78	HIS
36	1e	150	ARG
37	1f	46	ARG
37	1f	63	TYR
37	1f	70	ASP
38	1g	6	ARG
38	1g	8	GLU
38	1g	10	ARG
38	1g	13	GLN
38	1g	15	ASP
38	1g	56	GLN
38	1g	75	VAL
38	1g	104	LEU
38	1g	113	GLU
38	1g	136	LYS
38	1g	143	ARG
38	1g	155	ARG
39	1h	26	VAL
39	1h	51	VAL
39	1h	52	ASP
39	1h	63	LEU
40	1i	14	VAL
40	1i	25	LYS
40	1i	51	ARG
40	1i	56	LEU
40	1i	65	VAL
40	1i	66	ARG
40	1i	81	ILE
40	1i	86	VAL
40	1i	87	GLN
40	1i	103	THR
40	1i	125	TYR

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Mol	Chain	Res	Type
41	1j	34	VAL
41	1j	49	VAL
41	1j	55	LYS
41	1j	72	VAL
41	1j	92	THR
41	1j	94	VAL
41	1j	100	THR
42	1k	14	VAL
42	1k	84	VAL
42	1k	109	VAL
42	1k	114	VAL
42	1k	124	LYS
43	1l	27	LEU
43	1l	33	ARG
43	1l	47	LYS
43	1l	67	THR
44	1m	8	GLU
44	1m	11	ARG
44	1m	17	VAL
44	1m	56	LEU
44	1m	63	THR
44	1m	102	ARG
45	1n	3	ARG
45	1n	15	LYS
45	1n	18	VAL
45	1n	22	THR
45	1n	33	VAL
45	1n	44	LEU
46	1o	3	ILE
46	1o	26	GLU
46	1o	39	LEU
46	1o	68	ARG
47	1p	2	VAL
47	1p	8	ARG
47	1p	20	VAL
47	1p	42	ARG
47	1p	45	THR
47	1p	60	LEU
47	1p	62	VAL
47	1p	67	THR
47	1p	69	THR
47	1p	74	LEU

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Mol	Chain	Res	Type
47	1p	79	VAL
48	1q	16	GLN
48	1q	87	LYS
49	1r	65	ILE
49	1r	76	LEU
50	1s	3	ARG
50	1s	4	SER
50	1s	5	LEU
50	1s	28	LYS
50	1s	37	ARG
50	1s	41	VAL
50	1s	65	ASN
51	1t	10	LEU
51	1t	45	GLN
51	1t	48	LYS
51	1t	58	LYS
51	1t	62	LEU
51	1t	80	ARG
51	1t	100	ILE
52	1u	9	ARG
55	1y	2	ARG
55	1y	4	ARG
55	1y	12	ARG
3	2D	3	VAL
3	2D	37	LEU
3	2D	61	LEU
3	2D	94	LEU
3	2D	103	ARG
3	2D	109	ASP
3	2D	111	LEU
3	2D	113	VAL
3	2D	155	LEU
3	2D	193	VAL
3	2D	211	ARG
3	2D	217	ARG
3	2D	221	VAL
3	2D	229	VAL
3	2D	242	ARG
3	2D	253	GLN
3	2D	274	ARG
3	2D	276	LYS
4	2E	19	ARG

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Mol	Chain	Res	Type
4	2E	21	VAL
4	2E	24	THR
4	2E	33	VAL
4	2E	73	GLU
4	2E	75	VAL
4	2E	78	LEU
4	2E	97	LYS
4	2E	101	ARG
4	2E	116	VAL
4	2E	144	ARG
4	2E	154	LYS
4	2E	167	VAL
4	2E	170	LEU
4	2E	181	LEU
4	2E	195	LEU
5	2F	33	LEU
5	2F	57	VAL
5	2F	74	ARG
5	2F	112	MET
5	2F	158	THR
5	2F	175	THR
5	2F	192	LEU
5	2F	201	VAL
6	2G	3	LEU
6	2G	28	VAL
6	2G	43	LEU
6	2G	47	LYS
6	2G	49	ASP
6	2G	55	LYS
6	2G	111	LEU
6	2G	116	ASP
6	2G	133	LEU
6	2G	139	LEU
6	2G	155	MET
6	2G	168	GLU
6	2G	175	LEU
7	2H	6	ARG
7	2H	13	LYS
7	2H	15	VAL
7	2H	34	GLU
7	2H	49	VAL
7	2H	63	SER

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Mol	Chain	Res	Type
7	2H	68	THR
7	2H	84	SER
7	2H	95	ARG
7	2H	105	LEU
7	2H	122	THR
7	2H	139	GLN
8	2I	15	VAL
8	2I	38	LEU
8	2I	43	ASN
8	2I	44	LEU
8	2I	48	GLU
8	2I	50	ARG
8	2I	66	GLU
8	2I	75	LEU
8	2I	85	GLU
8	2I	92	VAL
8	2I	101	LEU
8	2I	116	LEU
8	2I	129	THR
8	2I	140	LEU
8	2I	144	VAL
9	2N	5	VAL
9	2N	28	THR
9	2N	34	LEU
9	2N	58	ASP
9	2N	62	VAL
9	2N	67	LEU
9	2N	74	ARG
9	2N	87	LEU
9	2N	97	ARG
9	2N	99	LEU
9	2N	119	ARG
9	2N	131	GLN
9	2N	133	GLN
9	2N	140	VAL
10	2O	10	VAL
10	2O	53	LYS
10	2O	108	GLU
11	2P	2	LYS
11	2P	3	LEU
11	2P	59	LEU
11	2P	76	LYS

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Mol	Chain	Res	Type
11	2P	112	LEU
11	2P	125	VAL
11	2P	148	LEU
12	2Q	2	LEU
12	2Q	7	MET
12	2Q	16	ARG
12	2Q	98	LYS
12	2Q	106	VAL
12	2Q	109	VAL
12	2Q	112	GLU
13	2R	18	LEU
13	2R	36	THR
13	2R	44	LEU
13	2R	65	LEU
13	2R	75	LEU
13	2R	79	LEU
13	2R	96	ARG
13	2R	100	LEU
14	2S	5	THR
14	2S	14	VAL
14	2S	17	ARG
14	2S	23	ARG
14	2S	50	SER
14	2S	75	GLU
15	2T	13	ARG
15	2T	16	ARG
15	2T	23	ARG
15	2T	28	VAL
15	2T	49	VAL
15	2T	74	ARG
15	2T	89	VAL
15	2T	96	ARG
15	2T	108	ARG
16	2U	31	SER
16	2U	60	LEU
16	2U	74	LEU
16	2U	112	ARG
17	2V	18	LEU
17	2V	35	LEU
17	2V	46	VAL
17	2V	53	GLU
17	2V	62	LEU

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Mol	Chain	Res	Type
17	2V	79	VAL
17	2V	100	ARG
18	2W	15	ARG
18	2W	17	VAL
18	2W	23	LEU
18	2W	71	VAL
18	2W	107	LEU
19	2X	57	LEU
19	2X	66	LEU
19	2X	81	VAL
19	2X	83	VAL
20	2Y	21	LYS
20	2Y	72	VAL
20	2Y	107	ASP
21	2Z	31	ARG
21	2Z	33	LEU
21	2Z	42	VAL
21	2Z	72	ARG
21	2Z	121	HIS
21	2Z	123	ASP
21	2Z	126	VAL
21	2Z	136	PHE
21	2Z	150	LEU
21	2Z	155	LEU
21	2Z	170	THR
21	2Z	182	LYS
21	2Z	185	GLU
22	20	14	ARG
22	20	39	ARG
23	21	2	SER
23	21	23	LYS
23	21	30	VAL
23	21	35	THR
23	21	81	LYS
23	21	85	LEU
24	22	3	LEU
24	22	26	ARG
24	22	32	LEU
24	22	40	SER
24	22	53	LEU
25	23	31	LEU
25	23	54	VAL

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Mol	Chain	Res	Type
25	23	56	VAL
26	24	8	LYS
26	24	27	THR
26	24	38	LYS
26	24	56	VAL
26	24	61	ARG
26	24	63	TYR
27	25	58	LEU
28	26	6	ARG
28	26	14	THR
28	26	19	ARG
28	26	48	VAL
28	26	52	VAL
29	27	43	THR
30	28	23	VAL
30	28	26	LYS
30	28	31	HIS
30	28	34	TRP
30	28	46	ARG
30	28	56	GLU
33	2b	8	LYS
33	2b	16	HIS
33	2b	24	TRP
33	2b	44	LEU
33	2b	55	PHE
33	2b	58	ILE
33	2b	67	THR
33	2b	71	VAL
33	2b	87	ARG
33	2b	93	VAL
33	2b	128	GLU
33	2b	135	GLN
33	2b	136	VAL
33	2b	157	ARG
33	2b	158	LEU
33	2b	187	LEU
33	2b	191	ASP
33	2b	200	ILE
33	2b	226	ARG
33	2b	230	VAL
34	2c	30	ARG
34	2c	32	LEU

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Mol	Chain	Res	Type
34	2c	45	LYS
34	2c	52	LEU
34	2c	70	VAL
34	2c	102	ASN
34	2c	152	ILE
34	2c	166	GLU
34	2c	192	THR
35	2d	5	ILE
35	2d	8	VAL
35	2d	13	ARG
35	2d	49	ARG
35	2d	65	ARG
35	2d	96	LEU
35	2d	106	TYR
35	2d	108	LEU
35	2d	127	THR
35	2d	135	LEU
35	2d	158	ILE
35	2d	194	LEU
35	2d	201	GLN
36	2e	24	ARG
36	2e	31	LEU
36	2e	34	VAL
36	2e	41	VAL
36	2e	68	GLU
36	2e	69	VAL
36	2e	72	GLN
36	2e	75	THR
36	2e	91	LEU
37	2f	17	SER
37	2f	22	GLU
37	2f	28	ARG
37	2f	40	VAL
37	2f	46	ARG
37	2f	63	TYR
37	2f	75	LEU
37	2f	81	ILE
37	2f	92	LYS
37	2f	95	GLU
38	2g	6	ARG
38	2g	13	GLN
38	2g	75	VAL

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Mol	Chain	Res	Type
38	2g	104	LEU
38	2g	113	GLU
38	2g	115	ARG
38	2g	138	LYS
38	2g	155	ARG
39	2h	51	VAL
39	2h	54	ASP
39	2h	63	LEU
39	2h	91	ARG
39	2h	97	VAL
39	2h	125	ARG
40	2i	7	THR
40	2i	25	LYS
40	2i	27	THR
40	2i	42	ARG
40	2i	50	LEU
40	2i	53	VAL
40	2i	64	THR
40	2i	65	VAL
40	2i	87	GLN
40	2i	88	TYR
40	2i	102	LEU
40	2i	103	THR
40	2i	125	TYR
41	2j	29	ARG
41	2j	34	VAL
41	2j	49	VAL
41	2j	57	LYS
41	2j	74	ILE
41	2j	92	THR
42	2k	14	VAL
42	2k	31	THR
42	2k	81	ASP
42	2k	109	VAL
42	2k	114	VAL
43	2l	27	LEU
43	2l	28	LYS
43	2l	33	ARG
43	2l	52	LEU
43	2l	67	THR
43	2l	117	ARG
44	2m	4	ILE

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Mol	Chain	Res	Type
44	2m	8	GLU
44	2m	17	VAL
44	2m	27	LYS
44	2m	65	LYS
44	2m	88	ARG
44	2m	103	THR
45	2n	18	VAL
45	2n	22	THR
45	2n	44	LEU
46	2o	5	LYS
46	2o	38	ARG
46	2o	39	LEU
46	2o	76	GLU
46	2o	83	GLU
46	2o	88	ARG
47	2p	2	VAL
47	2p	20	VAL
47	2p	21	VAL
47	2p	28	ARG
47	2p	42	ARG
47	2p	44	THR
47	2p	45	THR
47	2p	54	GLU
47	2p	62	VAL
47	2p	67	THR
47	2p	69	THR
47	2p	72	ARG
48	2q	6	LEU
48	2q	57	VAL
48	2q	74	LEU
49	2r	31	LEU
49	2r	65	ILE
49	2r	76	LEU
50	2s	5	LEU
50	2s	41	VAL
50	2s	64	GLU
50	2s	77	THR
51	2t	24	LEU
51	2t	41	ILE
51	2t	45	GLN
51	2t	84	LEU
51	2t	100	ILE

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Mol	Chain	Res	Type
55	2y	2	ARG
55	2y	4	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (96) such sidechains are listed below:

Mol	Chain	Res	Type
3	1D	253	GLN
4	1E	48	GLN
5	1F	8	GLN
5	1F	75	HIS
5	1F	203	GLN
8	1I	104	GLN
9	1N	133	GLN
13	1R	24	GLN
13	1R	71	GLN
15	1T	58	ASN
16	1U	104	GLN
20	1Y	6	HIS
20	1Y	43	ASN
20	1Y	92	ASN
21	1Z	34	ASN
21	1Z	54	HIS
21	1Z	73	GLN
24	12	70	GLN
25	13	32	GLN
26	14	60	GLN
34	1c	6	HIS
34	1c	104	GLN
34	1c	176	HIS
35	1d	77	ASN
35	1d	119	GLN
35	1d	123	HIS
35	1d	129	ASN
36	1e	20	GLN
37	1f	100	ASN
38	1g	28	ASN
38	1g	56	GLN
38	1g	110	GLN
38	1g	148	ASN
40	1i	3	GLN
40	1i	34	ASN
40	1i	73	GLN

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Mol	Chain	Res	Type
40	1i	87	GLN
41	1j	56	HIS
41	1j	84	GLN
43	1l	80	HIS
43	1l	99	HIS
46	1o	28	GLN
48	1q	16	GLN
50	1s	23	ASN
50	1s	69	HIS
50	1s	83	HIS
3	2D	253	GLN
5	2F	69	HIS
5	2F	203	GLN
6	2G	79	ASN
8	2I	133	HIS
12	2Q	141	GLN
17	2V	64	HIS
18	2W	60	ASN
19	2X	31	HIS
19	2X	82	GLN
21	2Z	73	GLN
21	2Z	121	HIS
22	20	70	GLN
23	21	19	GLN
25	23	32	GLN
26	24	20	ASN
26	24	46	GLN
33	2b	19	HIS
33	2b	76	GLN
33	2b	135	GLN
34	2c	6	HIS
34	2c	136	GLN
34	2c	176	HIS
35	2d	77	ASN
35	2d	116	GLN
35	2d	119	GLN
35	2d	123	HIS
35	2d	160	GLN
35	2d	161	ASN
35	2d	201	GLN
36	2e	78	HIS
36	2e	141	GLN

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Mol	Chain	Res	Type
37	2f	73	ASN
37	2f	100	ASN
38	2g	11	GLN
38	2g	28	ASN
38	2g	68	ASN
38	2g	86	GLN
40	2i	3	GLN
40	2i	31	GLN
40	2i	73	GLN
40	2i	117	HIS
41	2j	69	ASN
44	2m	62	ASN
46	2o	28	GLN
48	2q	26	GLN
50	2s	23	ASN
50	2s	47	HIS
50	2s	69	HIS
50	2s	83	HIS

5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	1A	2864/2915 (98%)	407 (14%)	38 (1%)
1	2A	2857/2915 (98%)	408 (14%)	33 (1%)
2	1B	119/120 (99%)	5 (4%)	0
2	2B	118/120 (98%)	6 (5%)	0
32	1a	1494/1520 (98%)	208 (13%)	0
32	2a	1498/1520 (98%)	220 (14%)	0
53	1v	2/3 (66%)	0	0
53	2v	2/3 (66%)	0	0
54	1x	75/76 (98%)	20 (26%)	0
54	2x	75/76 (98%)	10 (13%)	0
All	All	9104/9268 (98%)	1284 (14%)	71 (0%)

All (1284) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	1A	12	U
1	1A	34	C
1	1A	45	C
1	1A	70	A

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Mol	Chain	Res	Type
1	1A	73	A
1	1A	74	G
1	1A	116	A
1	1A	117	A
1	1A	118	U
1	1A	162	G
1	1A	185	A
1	1A	188	A
1	1A	194	G
1	1A	202	A
1	1A	204	G
1	1A	205	A
1	1A	210	A
1	1A	211	A
1	1A	214	A
1	1A	218	A
1	1A	237	G
1	1A	269	G
1	1A	271	U
1	1A	272	U
1	1A	273	G
1	1A	274	U
1	1A	279	G
1	1A	288	U
1	1A	289	G
1	1A	303	C
1	1A	335	A
1	1A	348	A
1	1A	351	G
1	1A	354	A
1	1A	366	G
1	1A	376	G
1	1A	381	A
1	1A	386	U
1	1A	387	G
1	1A	413	G
1	1A	423	G
1	1A	432	U
1	1A	438	G
1	1A	439	A
1	1A	448	U
1	1A	455	A

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Mol	Chain	Res	Type
1	1A	474	U
1	1A	482	C
1	1A	483	A
1	1A	505	A
1	1A	507	G
1	1A	530	A
1	1A	534	C
1	1A	535	C
1	1A	543	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	574	G
1	1A	586	G
1	1A	596	G
1	1A	598	A
1	1A	609	A
1	1A	615	G
1	1A	618	C
1	1A	626	A
1	1A	627	G
1	1A	630	U
1	1A	633	G
1	1A	639	G
1	1A	641	G
1	1A	652	A
1	1A	662	A
1	1A	670	C
1	1A	673	G
1	1A	693	G
1	1A	694	G
1	1A	697	C
1	1A	698	G
1	1A	715	G
1	1A	716	G
1	1A	733	G
1	1A	777	C
1	1A	822	G
1	1A	823	G

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Mol	Chain	Res	Type
1	1A	829	A
1	1A	831	A
1	1A	832	G
1	1A	839	G
1	1A	852	G
1	1A	859	C
1	1A	874	U
1	1A	875	U
1	1A	906	G
1	1A	927	G
1	1A	933	C
1	1A	934	A
1	1A	935	C
1	1A	936	C
1	1A	937	A
1	1A	942	A
1	1A	945	A
1	1A	946	A
1	1A	947	A
1	1A	956	A
1	1A	977	G
1	1A	983	G
1	1A	990	A
1	1A	991	G
1	1A	1003	U
1	1A	1004	A
1	1A	1006	C
1	1A	1019	G
1	1A	1020	C
1	1A	1021	G
1	1A	1029	A
1	1A	1042	A
1	1A	1051	C
1	1A	1058	U
1	1A	1059	C
1	1A	1068	G
1	1A	1071	G
1	1A	1072	U
1	1A	1079	U
1	1A	1085	G
1	1A	1088	G
1	1A	1090	G

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Mol	Chain	Res	Type
1	1A	1092	A
1	1A	1093	G
1	1A	1094	A
1	1A	1100	A
1	1A	1106	U
1	1A	1107	U
1	1A	1108	G
1	1A	1109	G
1	1A	1110	C
1	1A	1111	U
1	1A	1112	U
1	1A	1113	A
1	1A	1114	G
1	1A	1116	A
1	1A	1117	G
1	1A	1119	A
1	1A	1122	C
1	1A	1123	A
1	1A	1124	U
1	1A	1129	U
1	1A	1130	A
1	1A	1131	A
1	1A	1134	A
1	1A	1136	U
1	1A	1137	G
1	1A	1139	G
1	1A	1141	A
1	1A	1142	A
1	1A	1143	U
1	1A	1155	C
1	1A	1156	G
1	1A	1158	G
1	1A	1162	C
1	1A	1175	A
1	1A	1176	U
1	1A	1180	C
1	1A	1181	G
1	1A	1217	G
1	1A	1218	G
1	1A	1219	A
1	1A	1220	U
1	1A	1221	G

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Mol	Chain	Res	Type
1	1A	1222	A
1	1A	1223	C
1	1A	1256	U
1	1A	1265	A
1	1A	1287	A
1	1A	1299	A
1	1A	1302	G
1	1A	1317	G
1	1A	1318	A
1	1A	1319	U
1	1A	1346	U
1	1A	1347	A
1	1A	1349	G
1	1A	1354	A
1	1A	1398	U
1	1A	1405	A
1	1A	1406	A
1	1A	1411	A
1	1A	1416	C
1	1A	1430	A
1	1A	1431	G
1	1A	1432	C
1	1A	1462	G
1	1A	1463	C
1	1A	1466	U
1	1A	1467	G
1	1A	1474	C
1	1A	1491	A
1	1A	1497	G
1	1A	1500	A
1	1A	1514	C
1	1A	1518	A
1	1A	1529	G
1	1A	1539	C
1	1A	1543	U
1	1A	1554	A
1	1A	1555	C
1	1A	1578	C
1	1A	1589	A
1	1A	1590	C
1	1A	1594	C
1	1A	1605	A

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Mol	Chain	Res	Type
1	1A	1613	A
1	1A	1616	A
1	1A	1625	U
1	1A	1626	A
1	1A	1628	G
1	1A	1631	C
1	1A	1632	A
1	1A	1654	A
1	1A	1655	A
1	1A	1695	C
1	1A	1701	A
1	1A	1721	G
1	1A	1743	G
1	1A	1747	A
1	1A	1748	A
1	1A	1767	A
1	1A	1787	G
1	1A	1793	A
1	1A	1794	G
1	1A	1795	G
1	1A	1804	A
1	1A	1811	A
1	1A	1813	C
1	1A	1822	A
1	1A	1831	C
1	1A	1832	G
1	1A	1847	G
1	1A	1860	A
1	1A	1870	G
1	1A	1878	A
1	1A	1899	A
1	1A	1900	G
1	1A	1911	A
1	1A	1918	G
1	1A	1922	A
1	1A	1927	C
1	1A	1928	G
1	1A	1935	A
1	1A	1936	C
1	1A	1951	G
1	1A	1952	G
1	1A	1959	A

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Mol	Chain	Res	Type
1	1A	1960	A
1	1A	1977	U
1	1A	1985	U
1	1A	1989	C
1	1A	1992	A
1	1A	1993	A
1	1A	1994	A
1	1A	2015	U
1	1A	2019	G
1	1A	2042	A
1	1A	2045	G
1	1A	2053	A
1	1A	2055	A
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
1	1A	2115	G
1	1A	2121	U
1	1A	2125	C
1	1A	2126	G
1	1A	2129	C
1	1A	2130	C
1	1A	2132	G
1	1A	2133	C
1	1A	2134	G
1	1A	2137	G
1	1A	2138	G
1	1A	2139	A
1	1A	2140	U
1	1A	2141	A
1	1A	2142	G
1	1A	2148	A
1	1A	2149	G
1	1A	2154	U
1	1A	2155	G
1	1A	2156	A
1	1A	2158	C

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Mol	Chain	Res	Type
1	1A	2160	C
1	1A	2164	C
1	1A	2166	U
1	1A	2167	C
1	1A	2168	C
1	1A	2169	G
1	1A	2170	G
1	1A	2174	G
1	1A	2180	A
1	1A	2181	G
1	1A	2182	G
1	1A	2184	G
1	1A	2194	U
1	1A	2195	A
1	1A	2200	C
1	1A	2208	G
1	1A	2209	G
1	1A	2211	U
1	1A	2212	G
1	1A	2214	G
1	1A	2220	A
1	1A	2227	G
1	1A	2228	G
1	1A	2229	A
1	1A	2237	A
1	1A	2250	G
1	1A	2251	G
1	1A	2280	A
1	1A	2281	A
1	1A	2291	G
1	1A	2295	C
1	1A	2298	A
1	1A	2299	A
1	1A	2301	G
1	1A	2317	A
1	1A	2320	G
1	1A	2324	U
1	1A	2332	A
1	1A	2337	G
1	1A	2346	G
1	1A	2347	A
1	1A	2348	A

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Mol	Chain	Res	Type
1	1A	2359	C
1	1A	2395	G
1	1A	2397	C
1	1A	2408	G
1	1A	2418	U
1	1A	2426	G
1	1A	2434	A
1	1A	2435	U
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	2481	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	2532	C
1	1A	2537	G
1	1A	2541	G
1	1A	2566	U
1	1A	2578	A
1	1A	2579	G
1	1A	2585	C
1	1A	2594	G
1	1A	2597	U
1	1A	2598	C
1	1A	2614	A
1	1A	2615	G
1	1A	2621	U
1	1A	2623	U
1	1A	2624	C
1	1A	2642	G
1	1A	2666	A
1	1A	2674	A
1	1A	2675	G

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Mol	Chain	Res	Type
1	1A	2694	U
1	1A	2701	U
1	1A	2702	C
1	1A	2714	U
1	1A	2715	C
1	1A	2725	A
1	1A	2726	A
1	1A	2727	G
1	1A	2739	U
1	1A	2746	A
1	1A	2770	A
1	1A	2777	A
1	1A	2778	A
1	1A	2791	A
1	1A	2803	A
1	1A	2804	C
1	1A	2813	G
1	1A	2830	A
1	1A	2831	A
1	1A	2843	G
1	1A	2845	A
1	1A	2882	G
1	1A	2890	C
1	1A	2901	A
1	1A	2903	G
2	1B	2	C
2	1B	30	C
2	1B	56	G
2	1B	73	A
2	1B	110	G
32	1a	9	G
32	1a	22	G
32	1a	32	A
32	1a	39	G
32	1a	47	C
32	1a	48	C
32	1a	51	A
32	1a	61	G
32	1a	78	G
32	1a	79	G
32	1a	101	A
32	1a	116	A

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Mol	Chain	Res	Type
32	1a	121	C
32	1a	131	C
32	1a	159	G
32	1a	163	C
32	1a	173	U
32	1a	174	C
32	1a	182	U
32	1a	195	A
32	1a	197	A
32	1a	202	U
32	1a	203	U
32	1a	204	U
32	1a	216	G
32	1a	247	G
32	1a	251	G
32	1a	258	G
32	1a	266	G
32	1a	267	C
32	1a	289	G
32	1a	321	A
32	1a	328	C
32	1a	332	G
32	1a	348	G
32	1a	351	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	397	A
32	1a	398	C
32	1a	406	G
32	1a	412	A
32	1a	413	G
32	1a	424	G
32	1a	429	U
32	1a	430	A
32	1a	439	A
32	1a	442	C
32	1a	452	A
32	1a	458	C

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Mol	Chain	Res	Type
32	1a	461	A
32	1a	470	C
32	1a	485	G
32	1a	496	A
32	1a	498	U
32	1a	505	G
32	1a	509	A
32	1a	510	A
32	1a	511	C
32	1a	518	C
32	1a	532	A
32	1a	533	A
32	1a	547	A
32	1a	559	A
32	1a	561	U
32	1a	562	C
32	1a	564	C
32	1a	572	A
32	1a	573	A
32	1a	576	G
32	1a	577	G
32	1a	592	G
32	1a	596	C
32	1a	630	G
32	1a	632	A
32	1a	653	A
32	1a	661	G
32	1a	665	A
32	1a	687	A
32	1a	688	G
32	1a	723	U
32	1a	731	G
32	1a	734	G
32	1a	753	A
32	1a	755	G
32	1a	774	G
32	1a	777	A
32	1a	793	U
32	1a	794	A
32	1a	817	C
32	1a	821	G
32	1a	828	A

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Mol	Chain	Res	Type
32	1a	829	G
32	1a	838	G
32	1a	840	C
32	1a	841	U
32	1a	848	C
32	1a	851	G
32	1a	859	A
32	1a	874	G
32	1a	902	G
32	1a	914	A
32	1a	926	G
32	1a	927	G
32	1a	934	C
32	1a	935	A
32	1a	960	U
32	1a	961	U
32	1a	967	5MC
32	1a	968	A
32	1a	969	A
32	1a	971	G
32	1a	972	C
32	1a	974	A
32	1a	975	A
32	1a	976	G
32	1a	977	A
32	1a	992	U
32	1a	993	G
32	1a	994	A
32	1a	1002	G
32	1a	1003	G
32	1a	1004	A
32	1a	1005	A
32	1a	1006	C
32	1a	1009	G
32	1a	1020	U
32	1a	1022	G
32	1a	1023	G
32	1a	1024	G
32	1a	1025	U
32	1a	1026	G
32	1a	1027	C
32	1a	1028	C

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Mol	Chain	Res	Type
32	1a	1029	C
32	1a	1030	C
32	1a	1030(A)	G
32	1a	1033	G
32	1a	1044	A
32	1a	1053	G
32	1a	1054	C
32	1a	1065	U
32	1a	1066	C
32	1a	1068	G
32	1a	1081	G
32	1a	1094	G
32	1a	1095	U
32	1a	1101	A
32	1a	1125	U
32	1a	1130	A
32	1a	1134	G
32	1a	1136	U
32	1a	1137	C
32	1a	1139	G
32	1a	1140	C
32	1a	1152	A
32	1a	1159	U
32	1a	1183	A
32	1a	1184	G
32	1a	1196	U
32	1a	1197	G
32	1a	1202	G
32	1a	1208	C
32	1a	1213	A
32	1a	1224	G
32	1a	1227	A
32	1a	1236	A
32	1a	1238	A
32	1a	1250	A
32	1a	1256	A
32	1a	1257	U
32	1a	1258	G
32	1a	1270	C
32	1a	1278	U
32	1a	1280	A
32	1a	1286	A

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Mol	Chain	Res	Type
32	1a	1287	A
32	1a	1299	A
32	1a	1300	G
32	1a	1302	U
32	1a	1317	C
32	1a	1320	C
32	1a	1338	G
32	1a	1346	A
32	1a	1347	G
32	1a	1353	G
32	1a	1363	C
32	1a	1370	G
32	1a	1397	C
32	1a	1419	G
32	1a	1442	G
32	1a	1442(A)	G
32	1a	1487	G
32	1a	1493	A
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	1520	G
32	1a	1529	G
32	1a	1530	G
32	1a	1531	A
54	1x	3	C
54	1x	6	G
54	1x	9	G
54	1x	14	A
54	1x	16	C
54	1x	19	G
54	1x	20	U
54	1x	21	A
54	1x	30	G
54	1x	34	C
54	1x	42	G
54	1x	44	A
54	1x	47	U
54	1x	50	U

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Mol	Chain	Res	Type
54	1x	60	U
54	1x	63	G
54	1x	69	C
54	1x	72	A
54	1x	75	C
54	1x	76	A
1	2A	10	G
1	2A	12	U
1	2A	34	C
1	2A	45	C
1	2A	71	A
1	2A	74	A
1	2A	75	G
1	2A	84	A
1	2A	95	G
1	2A	118	A
1	2A	119	A
1	2A	120	U
1	2A	157	U
1	2A	173	G
1	2A	196	A
1	2A	199	A
1	2A	205	G
1	2A	215	G
1	2A	216	A
1	2A	221	A
1	2A	222	A
1	2A	225	A
1	2A	229	A
1	2A	230	U
1	2A	248	G
1	2A	271(K)	U
1	2A	271(L)	U
1	2A	271(M)	G
1	2A	271(N)	U
1	2A	272(A)	U
1	2A	272(B)	G
1	2A	277	C
1	2A	278	A
1	2A	311	A
1	2A	324	A
1	2A	327	G

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Mol	Chain	Res	Type
1	2A	330	A
1	2A	342	G
1	2A	352	G
1	2A	357	A
1	2A	362	U
1	2A	363	G
1	2A	386	G
1	2A	411	G
1	2A	412	A
1	2A	421	U
1	2A	428	A
1	2A	444	C
1	2A	456	C
1	2A	457	A
1	2A	479	A
1	2A	481	G
1	2A	505	A
1	2A	509	C
1	2A	510	C
1	2A	518	G
1	2A	530	G
1	2A	531	C
1	2A	532	A
1	2A	533	G
1	2A	545	G
1	2A	551	G
1	2A	563	G
1	2A	573	G
1	2A	575	A
1	2A	586	A
1	2A	592	G
1	2A	595	C
1	2A	603	A
1	2A	604	G
1	2A	607	U
1	2A	610	G
1	2A	614(B)	G
1	2A	615	G
1	2A	627	A
1	2A	637	A
1	2A	645	C
1	2A	646	A

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Mol	Chain	Res	Type
1	2A	648	G
1	2A	652(B)	A
1	2A	652(C)	G
1	2A	652(E)	G
1	2A	652(U)	G
1	2A	668	G
1	2A	669	G
1	2A	686	G
1	2A	730	C
1	2A	753	C
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	827	U
1	2A	828	U
1	2A	857	C
1	2A	859	G
1	2A	874	G
1	2A	880	G
1	2A	887	A
1	2A	888	C
1	2A	889	C
1	2A	890	A
1	2A	896	A
1	2A	899	A
1	2A	900	A
1	2A	901	A
1	2A	910	A
1	2A	917	A
1	2A	932	G
1	2A	938	G
1	2A	941	A
1	2A	945	A
1	2A	946	G
1	2A	958	U
1	2A	959	A
1	2A	961	C

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Mol	Chain	Res	Type
1	2A	974	G
1	2A	975	C
1	2A	983	A
1	2A	996	A
1	2A	1005	C
1	2A	1012	U
1	2A	1013	C
1	2A	1022	G
1	2A	1025	G
1	2A	1026	U
1	2A	1033	U
1	2A	1042	G
1	2A	1044	G
1	2A	1045	A
1	2A	1046	A
1	2A	1047	G
1	2A	1052	C
1	2A	1053	C
1	2A	1054	A
1	2A	1060	U
1	2A	1063	G
1	2A	1064	C
1	2A	1065	U
1	2A	1066	U
1	2A	1068	G
1	2A	1069	A
1	2A	1070	A
1	2A	1071	G
1	2A	1073	A
1	2A	1074	G
1	2A	1076	C
1	2A	1079	C
1	2A	1082	U
1	2A	1083	U
1	2A	1084	A
1	2A	1085	A
1	2A	1086	A
1	2A	1088	A
1	2A	1090	U
1	2A	1091	G
1	2A	1092	C
1	2A	1093	G

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Mol	Chain	Res	Type
1	2A	1096	A
1	2A	1108	U
1	2A	1109	C
1	2A	1110	G
1	2A	1112	G
1	2A	1129	A
1	2A	1130	U
1	2A	1135	C
1	2A	1136	G
1	2A	1139	G
1	2A	1171	G
1	2A	1211	U
1	2A	1220	A
1	2A	1253	A
1	2A	1256	G
1	2A	1271	G
1	2A	1272	A
1	2A	1273	U
1	2A	1300	U
1	2A	1301	A
1	2A	1308	A
1	2A	1314	C
1	2A	1352	U
1	2A	1359	A
1	2A	1360	A
1	2A	1365	A
1	2A	1370	C
1	2A	1384	A
1	2A	1385	G
1	2A	1386	C
1	2A	1416	G
1	2A	1417	C
1	2A	1420	U
1	2A	1421	G
1	2A	1428	C
1	2A	1445	A
1	2A	1450	G
1	2A	1467	C
1	2A	1471	A
1	2A	1482	G
1	2A	1493	C
1	2A	1497	U

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Mol	Chain	Res	Type
1	2A	1508	A
1	2A	1509	C
1	2A	1509(A)	A
1	2A	1531	C
1	2A	1533	G
1	2A	1537	G
1	2A	1542	A
1	2A	1547	C
1	2A	1558	A
1	2A	1566	A
1	2A	1569	A
1	2A	1578	U
1	2A	1579	A
1	2A	1584	C
1	2A	1586	A
1	2A	1608	A
1	2A	1609	A
1	2A	1640	C
1	2A	1648	C
1	2A	1674	G
1	2A	1696	G
1	2A	1700	A
1	2A	1722	A
1	2A	1756	G
1	2A	1762	A
1	2A	1763	G
1	2A	1764	G
1	2A	1773	A
1	2A	1780	A
1	2A	1782	C
1	2A	1791	A
1	2A	1800	C
1	2A	1801	G
1	2A	1816	G
1	2A	1829	A
1	2A	1847	A
1	2A	1848	A
1	2A	1877	A
1	2A	1878	G
1	2A	1889	A
1	2A	1896	G
1	2A	1900	A

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Mol	Chain	Res	Type
1	2A	1905	C
1	2A	1906	G
1	2A	1914	C
1	2A	1915	5MU
1	2A	1929	G
1	2A	1930	G
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	1993	U
1	2A	1997	G
1	2A	2020	A
1	2A	2023	G
1	2A	2031	A
1	2A	2033	A
1	2A	2039	C
1	2A	2043	C
1	2A	2055	C
1	2A	2056	G
1	2A	2060	A
1	2A	2061	G
1	2A	2062	A
1	2A	2069	G
1	2A	2096	U
1	2A	2101	G
1	2A	2103	C
1	2A	2105	C
1	2A	2107	C
1	2A	2108	C
1	2A	2110	G
1	2A	2111	C
1	2A	2116	G
1	2A	2117	A
1	2A	2118	U
1	2A	2119	A
1	2A	2120	G
1	2A	2126	A

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Mol	Chain	Res	Type
1	2A	2127	G
1	2A	2129	C
1	2A	2131	G
1	2A	2132	U
1	2A	2133	G
1	2A	2134	A
1	2A	2136	C
1	2A	2138	C
1	2A	2142	C
1	2A	2145	C
1	2A	2146	C
1	2A	2147	G
1	2A	2148	G
1	2A	2151	G
1	2A	2152	G
1	2A	2158	A
1	2A	2159	G
1	2A	2160	G
1	2A	2162	G
1	2A	2172	U
1	2A	2173	A
1	2A	2186	G
1	2A	2187	G
1	2A	2189	U
1	2A	2190	G
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	2238	G
1	2A	2239	G
1	2A	2268	A
1	2A	2269	A
1	2A	2275	C
1	2A	2279	G
1	2A	2283	C
1	2A	2286	A
1	2A	2287	A
1	2A	2305	A

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Mol	Chain	Res	Type
1	2A	2308	G
1	2A	2311	A
1	2A	2312	U
1	2A	2320	A
1	2A	2321	G
1	2A	2322	A
1	2A	2325	G
1	2A	2334	G
1	2A	2335	A
1	2A	2336	A
1	2A	2347	C
1	2A	2383	G
1	2A	2385	C
1	2A	2396	G
1	2A	2406	U
1	2A	2414	G
1	2A	2422	A
1	2A	2425	A
1	2A	2429	G
1	2A	2430	A
1	2A	2431	U
1	2A	2435	A
1	2A	2439	A
1	2A	2441	C
1	2A	2448	A
1	2A	2474	C
1	2A	2476	A
1	2A	2502	G
1	2A	2504	U
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	2566	A
1	2A	2567	G
1	2A	2573	C
1	2A	2582	G
1	2A	2585	U
1	2A	2586	C

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Mol	Chain	Res	Type
1	2A	2602	A
1	2A	2603	G
1	2A	2609	U
1	2A	2611	U
1	2A	2612	C
1	2A	2629	A
1	2A	2630	G
1	2A	2654	A
1	2A	2662	A
1	2A	2663	G
1	2A	2682	U
1	2A	2689	U
1	2A	2690	C
1	2A	2702	U
1	2A	2703	C
1	2A	2712(A)	A
1	2A	2713	A
1	2A	2714	G
1	2A	2726	U
1	2A	2733	A
1	2A	2757	A
1	2A	2761	G
1	2A	2764	A
1	2A	2765	A
1	2A	2778	A
1	2A	2789	C
1	2A	2802	G
1	2A	2811	G
1	2A	2820	A
1	2A	2821	A
1	2A	2833	G
1	2A	2835	A
1	2A	2872	G
1	2A	2880	C
1	2A	2892	A
1	2A	2894	G
2	2B	8	U
2	2B	30	C
2	2B	56	G
2	2B	73	A
2	2B	84	C
2	2B	110	G

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Mol	Chain	Res	Type
32	2a	5	U
32	2a	9	G
32	2a	22	G
32	2a	32	A
32	2a	39	G
32	2a	47	C
32	2a	48	C
32	2a	51	A
32	2a	61	G
32	2a	66	G
32	2a	80	G
32	2a	88	A
32	2a	89	C
32	2a	101	A
32	2a	116	A
32	2a	121	C
32	2a	131	C
32	2a	163	C
32	2a	173	U
32	2a	174	C
32	2a	182	U
32	2a	195	A
32	2a	197	A
32	2a	202	U
32	2a	203	U
32	2a	204	U
32	2a	216	G
32	2a	247	G
32	2a	251	G
32	2a	258	G
32	2a	266	G
32	2a	267	C
32	2a	289	G
32	2a	321	A
32	2a	328	C
32	2a	332	G
32	2a	348	G
32	2a	351	G
32	2a	352	C
32	2a	353	A
32	2a	354	G
32	2a	367	U

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Mol	Chain	Res	Type
32	2a	372	C
32	2a	373	A
32	2a	397	A
32	2a	398	C
32	2a	406	G
32	2a	412	A
32	2a	413	G
32	2a	424	G
32	2a	429	U
32	2a	430	A
32	2a	439	A
32	2a	442	C
32	2a	452	A
32	2a	458	C
32	2a	461	A
32	2a	470	C
32	2a	485	G
32	2a	496	A
32	2a	498	U
32	2a	505	G
32	2a	510	A
32	2a	511	C
32	2a	518	C
32	2a	527	7MG
32	2a	532	A
32	2a	533	A
32	2a	547	A
32	2a	559	A
32	2a	561	U
32	2a	562	C
32	2a	564	C
32	2a	572	A
32	2a	573	A
32	2a	576	G
32	2a	577	G
32	2a	592	G
32	2a	596	C
32	2a	630	G
32	2a	632	A
32	2a	653	A
32	2a	661	G
32	2a	665	A

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Mol	Chain	Res	Type
32	2a	687	A
32	2a	688	G
32	2a	695	A
32	2a	723	U
32	2a	731	G
32	2a	753	A
32	2a	755	G
32	2a	774	G
32	2a	777	A
32	2a	793	U
32	2a	794	A
32	2a	815	A
32	2a	817	C
32	2a	821	G
32	2a	828	A
32	2a	829	G
32	2a	838	G
32	2a	840	C
32	2a	841	U
32	2a	848	C
32	2a	851	G
32	2a	859	A
32	2a	874	G
32	2a	902	G
32	2a	914	A
32	2a	926	G
32	2a	927	G
32	2a	934	C
32	2a	935	A
32	2a	960	U
32	2a	961	U
32	2a	968	A
32	2a	969	A
32	2a	971	G
32	2a	972	C
32	2a	974	A
32	2a	975	A
32	2a	976	G
32	2a	977	A
32	2a	992	U
32	2a	993	G
32	2a	994	A

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Mol	Chain	Res	Type
32	2a	1003	G
32	2a	1005	A
32	2a	1006	C
32	2a	1009	G
32	2a	1020	U
32	2a	1022	G
32	2a	1023	G
32	2a	1025	U
32	2a	1026	G
32	2a	1027	C
32	2a	1028	C
32	2a	1029	C
32	2a	1030(A)	G
32	2a	1030(B)	C
32	2a	1036	G
32	2a	1041	A
32	2a	1044	A
32	2a	1053	G
32	2a	1054	C
32	2a	1065	U
32	2a	1066	C
32	2a	1068	G
32	2a	1081	G
32	2a	1094	G
32	2a	1095	U
32	2a	1101	A
32	2a	1117	G
32	2a	1125	U
32	2a	1129	C
32	2a	1130	A
32	2a	1132	C
32	2a	1134	G
32	2a	1136	U
32	2a	1137	C
32	2a	1139	G
32	2a	1140	C
32	2a	1147	C
32	2a	1152	A
32	2a	1158	C
32	2a	1159	U
32	2a	1183	A
32	2a	1184	G

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Mol	Chain	Res	Type
32	2a	1196	U
32	2a	1197	G
32	2a	1211	U
32	2a	1212	U
32	2a	1213	A
32	2a	1224	G
32	2a	1227	A
32	2a	1236	A
32	2a	1238	A
32	2a	1250	A
32	2a	1256	A
32	2a	1257	U
32	2a	1258	G
32	2a	1270	C
32	2a	1278	U
32	2a	1280	A
32	2a	1281	U
32	2a	1282	C
32	2a	1287	A
32	2a	1299	A
32	2a	1300	G
32	2a	1302	U
32	2a	1305	G
32	2a	1317	C
32	2a	1320	C
32	2a	1338	G
32	2a	1346	A
32	2a	1347	G
32	2a	1353	G
32	2a	1363	C
32	2a	1370	G
32	2a	1397	C
32	2a	1400	5MC
32	2a	1419	G
32	2a	1442	G
32	2a	1442(A)	G
32	2a	1447	A
32	2a	1487	G
32	2a	1492	A
32	2a	1493	A
32	2a	1497	G
32	2a	1499	A

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Mol	Chain	Res	Type
32	2a	1503	A
32	2a	1504	G
32	2a	1505	G
32	2a	1506	U
32	2a	1517	G
32	2a	1528	U
32	2a	1529	G
32	2a	1530	G
32	2a	1531	A
32	2a	1532	U
54	2x	9	G
54	2x	13	C
54	2x	20	U
54	2x	21	A
54	2x	48	C
54	2x	50	U
54	2x	62	C
54	2x	63	G
54	2x	65	C
54	2x	76	A

All (71) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	1A	115	G
1	1A	184	A
1	1A	185	A
1	1A	188	A
1	1A	302	A
1	1A	386	U
1	1A	509	A
1	1A	732	A
1	1A	793	A
1	1A	811	A
1	1A	874	U
1	1A	913	A
1	1A	934	A
1	1A	935	C
1	1A	941	U
1	1A	1019	G
1	1A	1065	U
1	1A	1067	A

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Mol	Chain	Res	Type
1	1A	1093	G
1	1A	1116	A
1	1A	1157	A
1	1A	1201	A
1	1A	1219	A
1	1A	1220	U
1	1A	1221	G
1	1A	1255	A
1	1A	1286	U
1	1A	1466	U
1	1A	1654	A
1	1A	1700	G
1	1A	2148	A
1	1A	2227	G
1	1A	2418	U
1	1A	2434	A
1	1A	2442	A
1	1A	2623	U
1	1A	2701	U
1	1A	2769	U
1	2A	195	A
1	2A	196	A
1	2A	266	G
1	2A	271(M)	G
1	2A	277	C
1	2A	746	A
1	2A	752	A
1	2A	764	A
1	2A	827	U
1	2A	840	C
1	2A	856	C
1	2A	974	G
1	2A	1053	C
1	2A	1065	U
1	2A	1067	A
1	2A	1073	A
1	2A	1210	A
1	2A	1399	C
1	2A	1420	U
1	2A	1442	G
1	2A	1491	G
1	2A	1608	A

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Mol	Chain	Res	Type
1	2A	1992	G
1	2A	2126	A
1	2A	2172	U
1	2A	2206	G
1	2A	2321	G
1	2A	2406	U
1	2A	2430	A
1	2A	2585	U
1	2A	2611	U
1	2A	2689	U
1	2A	2756	U

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
43	0TD	1l	92	43	7,9,10	2.23	2 (28%)	6,11,13	2.83	4 (66%)
32	4OC	1a	1402	32	20,23,24	2.47	8 (40%)	26,32,35	0.97	2 (7%)
1	OMU	1A	2564	1,56	19,22,23	6.67	10 (52%)	26,31,34	2.34	7 (26%)
43	0TD	2l	92	43	7,9,10	1.97	1 (14%)	6,11,13	2.86	4 (66%)
32	5MC	1a	1404	32	18,22,23	0.98	1 (5%)	26,32,35	1.16	4 (15%)
32	7MG	1a	527	56,32	22,26,27	2.33	7 (31%)	29,39,42	1.94	9 (31%)
32	MA6	1a	1518	32	19,26,27	1.01	2 (10%)	18,38,41	4.93	3 (16%)
1	5MC	2A	1962	1,56	18,22,23	1.07	2 (11%)	26,32,35	1.13	3 (11%)
1	5MC	2A	1942	1	18,22,23	1.08	1 (5%)	26,32,35	1.32	5 (19%)
32	5MC	2a	1404	32	18,22,23	0.93	1 (5%)	26,32,35	1.27	5 (19%)
54	PSU	1x	55	54	18,21,22	1.51	3 (16%)	22,30,33	1.50	1 (4%)
1	2MA	2A	2503	1,56	17,25,26	1.85	4 (23%)	17,37,40	1.36	3 (17%)
32	MA6	2a	1518	32	19,26,27	1.04	1 (5%)	18,38,41	5.11	3 (16%)
1	PSU	1A	2617	1	18,21,22	1.16	1 (5%)	22,30,33	1.53	4 (18%)

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	1.83	4 (22%)	16,38,41	1.18	2 (12%)
32	5MC	1a	1400	32	18,22,23	0.91	0	26,32,35	1.26	4 (15%)
32	MA6	2a	1519	32	19,26,27	0.97	1 (5%)	18,38,41	5.18	3 (16%)
32	M2G	1a	966	32	20,27,28	3.08	6 (30%)	22,40,43	1.29	4 (18%)
54	5MU	1x	54	54	19,22,23	0.86	1 (5%)	28,32,35	1.14	2 (7%)
1	5MU	1A	1937	1	19,22,23	1.15	1 (5%)	28,32,35	1.48	5 (17%)
32	5MC	2a	1407	32	18,22,23	1.13	3 (16%)	26,32,35	1.16	3 (11%)
1	PSU	2A	2605	1	18,21,22	1.01	2 (11%)	22,30,33	1.56	3 (13%)
1	OMU	2A	2552	1,56	19,22,23	6.66	10 (52%)	26,31,34	2.28	7 (26%)
1	5MC	1A	1964	1,56	18,22,23	0.94	1 (5%)	26,32,35	1.30	3 (11%)
32	UR3	1a	1498	32	19,22,23	2.02	3 (15%)	26,32,35	1.51	3 (11%)
1	PSU	1A	1939	1,56	18,21,22	1.40	3 (16%)	22,30,33	1.53	3 (13%)
32	4OC	2a	1402	32	20,23,24	2.51	8 (40%)	26,32,35	1.58	3 (11%)
54	4SU	1x	8	54	18,21,22	1.19	1 (5%)	26,30,33	0.89	1 (3%)
32	5MC	1a	1407	32	18,22,23	1.07	1 (5%)	26,32,35	1.33	5 (19%)
32	7MG	2a	527	32	22,26,27	2.46	7 (31%)	29,39,42	1.86	8 (27%)
1	5MC	1A	1984	1,56	18,22,23	1.01	1 (5%)	26,32,35	1.39	5 (19%)
1	OMC	2A	1920	1	19,22,23	2.48	7 (36%)	26,31,34	0.94	1 (3%)
1	5MU	2A	1939	1	19,22,23	1.05	2 (10%)	28,32,35	1.24	3 (10%)
32	M2G	2a	966	32	20,27,28	3.29	6 (30%)	22,40,43	1.30	4 (18%)
54	5MC	2x	32	54	18,22,23	1.09	2 (11%)	26,32,35	1.22	4 (15%)
54	5MU	2x	54	54	19,22,23	0.97	2 (10%)	28,32,35	1.07	2 (7%)
1	5MU	1A	1961	1	19,22,23	0.71	0	28,32,35	1.14	4 (14%)
1	OMG	2A	2251	1,54	18,26,27	1.85	5 (27%)	19,38,41	1.60	4 (21%)
1	PSU	1A	1933	1	18,21,22	1.10	2 (11%)	22,30,33	1.65	4 (18%)
32	MA6	1a	1519	32	19,26,27	0.98	2 (10%)	18,38,41	5.30	3 (16%)
32	UR3	2a	1498	32	19,22,23	2.05	4 (21%)	26,32,35	1.34	3 (11%)
54	4SU	2x	8	54	18,21,22	1.24	3 (16%)	26,30,33	1.07	1 (3%)
54	5MC	1x	32	54	18,22,23	1.13	3 (16%)	26,32,35	1.28	3 (11%)
32	5MC	2a	967	32	18,22,23	0.88	0	26,32,35	1.31	4 (15%)
1	PSU	2A	1911	1	18,21,22	1.32	3 (16%)	22,30,33	1.59	2 (9%)
1	5MU	2A	1915	1	19,22,23	1.25	2 (10%)	28,32,35	1.36	4 (14%)
1	2MA	1A	2515	1,56	17,25,26	1.82	4 (23%)	17,37,40	1.50	3 (17%)
32	5MC	2a	1400	32	18,22,23	1.08	1 (5%)	26,32,35	1.27	4 (15%)
1	OMC	1A	1942	1	19,22,23	2.45	7 (36%)	26,31,34	0.91	1 (3%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	PSU	2A	1917	1	18,21,22	1.32	3 (16%)	22,30,33	1.53	3 (13%)
32	2MG	1a	1207	32	18,26,27	1.94	5 (27%)	16,38,41	1.63	4 (25%)
32	5MC	1a	967	32	18,22,23	1.14	2 (11%)	26,32,35	1.22	4 (15%)
32	PSU	2a	516	32	18,21,22	1.34	3 (16%)	22,30,33	1.92	5 (22%)
1	OMG	1A	2263	1,54	18,26,27	1.88	7 (38%)	19,38,41	1.59	5 (26%)
32	PSU	1a	516	32	18,21,22	1.47	3 (16%)	22,30,33	2.31	6 (27%)
54	PSU	2x	55	56,54	18,21,22	1.53	3 (16%)	22,30,33	1.55	4 (18%)

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
43	0TD	1l	92	43	-	2/7/12/14	-
32	4OC	1a	1402	32	-	2/9/29/30	0/2/2/2
1	OMU	1A	2564	1,56	-	0/9/27/28	0/2/2/2
43	0TD	2l	92	43	-	5/7/12/14	-
32	5MC	1a	1404	32	-	0/7/25/26	0/2/2/2
32	7MG	1a	527	56,32	-	2/7/37/38	0/3/3/3
32	MA6	1a	1518	32	-	0/7/29/30	0/3/3/3
1	5MC	2A	1962	1,56	-	0/7/25/26	0/2/2/2
1	5MC	2A	1942	1	-	0/7/25/26	0/2/2/2
32	5MC	2a	1404	32	-	0/7/25/26	0/2/2/2
54	PSU	1x	55	54	-	0/7/25/26	0/2/2/2
1	2MA	2A	2503	1,56	-	2/3/25/26	0/3/3/3
32	MA6	2a	1518	32	-	0/7/29/30	0/3/3/3
1	PSU	1A	2617	1	-	0/7/25/26	0/2/2/2
32	2MG	2a	1207	32	-	0/5/27/28	0/3/3/3
32	5MC	1a	1400	32	-	2/7/25/26	0/2/2/2
32	MA6	2a	1519	32	-	2/7/29/30	0/3/3/3
32	M2G	1a	966	32	-	0/7/29/30	0/3/3/3
54	5MU	1x	54	54	-	0/7/25/26	0/2/2/2
1	5MU	1A	1937	1	-	2/7/25/26	0/2/2/2
32	5MC	2a	1407	32	-	0/7/25/26	0/2/2/2
1	PSU	2A	2605	1	-	0/7/25/26	0/2/2/2
1	OMU	2A	2552	1,56	-	1/9/27/28	0/2/2/2
1	5MC	1A	1964	1,56	-	0/7/25/26	0/2/2/2
32	UR3	1a	1498	32	-	0/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	PSU	1A	1939	1,56	-	0/7/25/26	0/2/2/2
32	4OC	2a	1402	32	-	2/9/29/30	0/2/2/2
54	4SU	1x	8	54	-	0/7/25/26	0/2/2/2
32	5MC	1a	1407	32	-	0/7/25/26	0/2/2/2
32	7MG	2a	527	32	-	2/7/37/38	0/3/3/3
1	5MC	1A	1984	1,56	-	0/7/25/26	0/2/2/2
1	OMC	2A	1920	1	-	0/9/27/28	0/2/2/2
1	5MU	2A	1939	1	-	0/7/25/26	0/2/2/2
32	M2G	2a	966	32	-	0/7/29/30	0/3/3/3
54	5MC	2x	32	54	-	0/7/25/26	0/2/2/2
54	5MU	2x	54	54	-	0/7/25/26	0/2/2/2
1	5MU	1A	1961	1	-	0/7/25/26	0/2/2/2
1	OMG	2A	2251	1,54	-	1/5/27/28	0/3/3/3
1	PSU	1A	1933	1	-	0/7/25/26	0/2/2/2
32	MA6	1a	1519	32	-	4/7/29/30	0/3/3/3
32	UR3	2a	1498	32	-	0/7/25/26	0/2/2/2
54	4SU	2x	8	54	-	0/7/25/26	0/2/2/2
54	5MC	1x	32	54	-	0/7/25/26	0/2/2/2
32	5MC	2a	967	32	-	0/7/25/26	0/2/2/2
1	PSU	2A	1911	1	-	0/7/25/26	0/2/2/2
1	5MU	2A	1915	1	-	5/7/25/26	0/2/2/2
1	2MA	1A	2515	1,56	-	1/3/25/26	0/3/3/3
32	5MC	2a	1400	32	-	2/7/25/26	0/2/2/2
1	OMC	1A	1942	1	-	1/9/27/28	0/2/2/2
1	PSU	2A	1917	1	-	0/7/25/26	0/2/2/2
32	2MG	1a	1207	32	-	0/5/27/28	0/3/3/3
32	5MC	1a	967	32	-	2/7/25/26	0/2/2/2
32	PSU	2a	516	32	-	1/7/25/26	0/2/2/2
1	OMG	1A	2263	1,54	-	2/5/27/28	0/3/3/3
32	PSU	1a	516	32	-	1/7/25/26	0/2/2/2
54	PSU	2x	55	56,54	-	0/7/25/26	0/2/2/2

All (178) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	1A	2564	OMU	C5-C4	15.74	1.78	1.43
1	2A	2552	OMU	C5-C4	15.47	1.77	1.43
1	2A	2552	OMU	C4-N3	-14.70	1.12	1.38
1	1A	2564	OMU	C4-N3	-14.50	1.12	1.38
32	2a	966	M2G	C2-N3	12.15	1.45	1.30
32	1a	966	M2G	C2-N3	11.16	1.44	1.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	2A	2552	OMU	C6-C5	-10.23	1.11	1.35
1	1A	2564	OMU	C6-C5	-10.16	1.11	1.35
1	1A	2564	OMU	C6-N1	8.61	1.58	1.38
1	1A	2564	OMU	C3'-C2'	-8.56	1.33	1.52
1	2A	2552	OMU	C6-N1	8.52	1.58	1.38
1	2A	2552	OMU	C3'-C2'	-8.32	1.34	1.52
1	2A	2552	OMU	O4'-C1'	6.46	1.57	1.42
1	2A	2552	OMU	O4'-C4'	-6.38	1.30	1.45
1	1A	2564	OMU	O4'-C4'	-6.21	1.31	1.45
1	1A	2564	OMU	O4'-C1'	6.18	1.56	1.42
32	2a	527	7MG	C5-N7	6.07	1.42	1.35
32	1a	527	7MG	C5-N7	5.94	1.42	1.35
1	2A	1920	OMC	C4-N4	5.93	1.47	1.33
1	1A	1942	OMC	C4-N4	5.61	1.47	1.33
1	2A	2503	2MA	C2-N3	5.35	1.42	1.31
1	1A	2564	OMU	C1'-N1	-5.29	1.32	1.47
32	2a	1498	UR3	C6-C5	5.28	1.47	1.35
32	1a	1402	4OC	C4-N4	5.20	1.46	1.35
32	2a	1402	4OC	C4-N4	5.17	1.46	1.35
1	1A	2515	2MA	C2-N3	5.17	1.42	1.31
1	2A	2552	OMU	C1'-N1	-5.13	1.32	1.47
32	1a	1498	UR3	C6-C5	5.01	1.46	1.35
32	1a	1498	UR3	C2-N1	4.99	1.45	1.38
32	2a	966	M2G	C2-N2	4.89	1.44	1.35
43	1l	92	0TD	CB-SB	-4.82	1.77	1.82
32	1a	1207	2MG	C2-N1	4.77	1.44	1.36
1	1A	1942	OMC	C2-N3	4.75	1.46	1.36
32	2a	1498	UR3	C2-N1	4.70	1.45	1.38
1	1A	1942	OMC	C6-C5	4.69	1.45	1.35
32	2a	1207	2MG	C2-N1	4.64	1.44	1.36
32	1a	966	M2G	C2-N2	4.63	1.44	1.35
1	2A	1920	OMC	C2-N3	4.63	1.45	1.36
32	2a	527	7MG	C4-N3	4.62	1.45	1.34
32	2a	1402	4OC	C2-N3	4.62	1.45	1.36
1	2A	1920	OMC	C6-C5	4.57	1.45	1.35
32	2a	527	7MG	C2-N3	4.55	1.44	1.33
54	1x	8	4SU	C4-S4	-4.52	1.59	1.68
32	1a	1402	4OC	C6-C5	4.48	1.45	1.35
32	1a	527	7MG	C8-N9	4.45	1.48	1.46
32	2a	527	7MG	C8-N9	4.45	1.48	1.46
1	2A	2251	OMG	C2-N3	4.35	1.43	1.33
32	1a	1207	2MG	C2-N2	4.35	1.43	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	1a	1402	4OC	C2-N3	4.28	1.45	1.36
1	1A	2564	OMU	C3'-C4'	4.25	1.63	1.53
54	1x	55	PSU	C2-N1	4.24	1.42	1.36
1	2A	1915	5MU	C2-N1	4.21	1.45	1.38
32	1a	527	7MG	C4-N3	4.20	1.44	1.34
32	2a	1402	4OC	C4-N3	4.19	1.40	1.32
32	1a	527	7MG	C2-N3	4.19	1.43	1.33
1	1A	1937	5MU	C2-N1	4.18	1.45	1.38
32	2a	966	M2G	C4-N3	4.14	1.47	1.37
32	2a	1207	2MG	C2-N2	4.10	1.42	1.33
1	1A	1939	PSU	C2-N1	4.04	1.42	1.36
32	1a	1402	4OC	C4-N3	4.00	1.39	1.32
43	2l	92	0TD	CB-SB	-3.99	1.78	1.82
32	1a	516	PSU	C2-N1	3.98	1.42	1.36
32	2a	516	PSU	C2-N1	3.98	1.42	1.36
1	1A	2263	OMG	C2-N3	3.94	1.42	1.33
32	1a	1498	UR3	C2-N3	3.93	1.46	1.39
32	2a	1402	4OC	C6-C5	3.93	1.44	1.35
54	2x	55	PSU	C2-N1	3.89	1.42	1.36
1	2A	2552	OMU	C3'-C4'	3.89	1.62	1.53
32	2a	1498	UR3	C2-N3	3.77	1.46	1.39
1	2A	1917	PSU	C2-N1	3.73	1.41	1.36
32	2a	1402	4OC	C5-C4	3.69	1.48	1.40
32	1a	966	M2G	C4-N3	3.66	1.46	1.37
1	1A	1942	OMC	C2-N1	3.57	1.47	1.40
1	2A	2251	OMG	C4-N3	3.55	1.46	1.37
1	2A	1920	OMC	C2-N1	3.54	1.47	1.40
32	2a	1402	4OC	C2-N1	3.45	1.47	1.40
32	1a	1402	4OC	C5-C4	3.42	1.48	1.40
1	1A	2617	PSU	C2-N1	3.30	1.41	1.36
1	2A	1911	PSU	C2-N1	3.26	1.41	1.36
54	2x	55	PSU	C4-N3	3.22	1.44	1.38
32	2a	527	7MG	C2-N2	3.20	1.41	1.34
32	1a	527	7MG	C5-C6	3.20	1.51	1.43
1	1A	2515	2MA	C5-C4	-3.16	1.35	1.43
1	1A	2263	OMG	C5-C4	-3.16	1.35	1.43
32	2a	527	7MG	C5-C6	3.15	1.51	1.43
32	1a	1207	2MG	C4-N3	3.15	1.45	1.37
1	2A	2503	2MA	C5-C4	-3.11	1.35	1.43
1	2A	1920	OMC	O2-C2	-3.10	1.18	1.23
32	1a	1402	4OC	C2-N1	3.07	1.46	1.40
1	1A	2263	OMG	C4-N3	3.06	1.44	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	1a	967	5MC	C2-N1	3.05	1.46	1.40
1	2A	1939	5MU	C2-N1	3.04	1.43	1.38
32	1a	1402	4OC	O2-C2	-3.02	1.18	1.23
1	2A	1942	5MC	C2-N1	3.00	1.46	1.40
32	2a	1402	4OC	O2-C2	-2.98	1.18	1.23
54	2x	8	4SU	C2-N1	2.97	1.43	1.38
32	2a	1207	2MG	C4-N3	2.92	1.44	1.37
1	2A	2251	OMG	C5-C4	-2.91	1.35	1.43
32	2a	1400	5MC	C2-N1	2.89	1.46	1.40
32	2a	1402	4OC	CM4-N4	-2.89	1.40	1.45
54	1x	55	PSU	C6-N1	2.87	1.41	1.36
1	2A	2552	OMU	O2'-C2'	2.84	1.49	1.42
1	2A	1920	OMC	C4-N3	2.83	1.40	1.34
1	2A	2503	2MA	C4-N3	2.82	1.44	1.37
1	2A	1911	PSU	C4-N3	2.82	1.44	1.38
32	1a	527	7MG	C2-N2	2.80	1.40	1.34
54	2x	8	4SU	C2-N3	2.79	1.42	1.38
32	2a	1518	MA6	C2-N3	2.79	1.36	1.32
54	1x	55	PSU	C4-N3	2.76	1.44	1.38
1	1A	1942	OMC	C4-N3	2.76	1.40	1.34
32	1a	966	M2G	C2-N1	2.75	1.43	1.36
32	1a	1402	4OC	CM4-N4	-2.74	1.40	1.45
1	1A	2263	OMG	C6-N1	2.72	1.41	1.37
32	2a	527	7MG	C2-N1	2.70	1.44	1.37
1	1A	1942	OMC	O2-C2	-2.68	1.18	1.23
54	2x	32	5MC	C2-N1	2.66	1.45	1.40
32	1a	516	PSU	C6-N1	2.66	1.40	1.36
32	1a	966	M2G	C5-C4	-2.65	1.36	1.43
54	2x	8	4SU	C4-S4	-2.64	1.63	1.68
1	1A	1933	PSU	C2-N1	2.64	1.40	1.36
32	1a	1519	MA6	C2-N3	2.64	1.36	1.32
32	1a	1407	5MC	C2-N1	2.64	1.45	1.40
32	2a	966	M2G	C2-N1	2.63	1.43	1.36
54	2x	55	PSU	C6-N1	2.62	1.40	1.36
32	1a	516	PSU	O4'-C1'	-2.60	1.40	1.43
32	2a	966	M2G	C5-C4	-2.60	1.36	1.43
1	1A	1984	5MC	C2-N1	2.59	1.45	1.40
1	1A	1939	PSU	C4-N3	2.58	1.43	1.38
32	2a	1519	MA6	C2-N3	2.58	1.36	1.32
1	1A	1942	OMC	C5-C4	2.58	1.48	1.42
54	2x	54	5MU	C2-N1	2.57	1.42	1.38
54	1x	32	5MC	C2-N1	2.51	1.45	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	1A	2515	2MA	C4-N3	2.49	1.43	1.37
32	2a	1407	5MC	C2-N1	2.49	1.45	1.40
32	1a	1518	MA6	C2-N3	2.48	1.36	1.32
32	2a	516	PSU	C6-N1	2.48	1.40	1.36
1	2A	1920	OMC	C5-C4	2.47	1.48	1.42
1	1A	1939	PSU	C6-N1	2.46	1.40	1.36
1	2A	1962	5MC	C2-N3	2.45	1.41	1.36
1	2A	1917	PSU	C6-N1	2.41	1.40	1.36
1	1A	2564	OMU	O2'-C2'	2.38	1.48	1.42
32	1a	967	5MC	C2-N3	2.37	1.41	1.36
54	1x	54	5MU	C2-N1	2.36	1.42	1.38
1	2A	1915	5MU	C2-N3	2.36	1.42	1.38
32	2a	516	PSU	O4'-C1'	-2.35	1.40	1.43
1	1A	1964	5MC	C2-N1	2.35	1.45	1.40
1	1A	2515	2MA	C2-N1	2.34	1.43	1.36
32	1a	527	7MG	C2-N1	2.32	1.43	1.37
54	2x	54	5MU	C2-N3	2.30	1.42	1.38
32	2a	1207	2MG	CM2-N2	-2.28	1.41	1.45
1	2A	1911	PSU	C6-N1	2.27	1.40	1.36
1	2A	1962	5MC	C2-N1	2.27	1.44	1.40
54	1x	32	5MC	C2-N3	2.26	1.40	1.36
1	2A	1939	5MU	C2-N3	2.24	1.42	1.38
32	2a	966	M2G	C5-C6	2.23	1.51	1.47
1	1A	2263	OMG	C2-N1	2.22	1.43	1.37
1	1A	2263	OMG	C8-N7	2.20	1.38	1.35
1	2A	2503	2MA	C2-N1	2.19	1.43	1.36
32	1a	966	M2G	C5-C6	2.18	1.51	1.47
32	1a	1518	MA6	C5-C4	-2.18	1.35	1.40
1	2A	2251	OMG	C6-N1	2.17	1.41	1.37
1	2A	1917	PSU	C4-N3	2.16	1.42	1.38
1	1A	2263	OMG	C2-N2	2.16	1.39	1.34
54	2x	32	5MC	C6-C5	2.14	1.38	1.34
1	2A	2605	PSU	C4-N3	2.12	1.42	1.38
1	1A	1933	PSU	C4-N3	2.11	1.42	1.38
32	1a	1207	2MG	CM2-N2	-2.09	1.41	1.45
54	1x	32	5MC	C6-C5	2.08	1.38	1.34
32	2a	1407	5MC	C2-N3	2.08	1.40	1.36
1	2A	2605	PSU	C2-N1	2.07	1.39	1.36
43	1l	92	0TD	CA-N	-2.05	1.41	1.47
32	1a	1519	MA6	C5-C4	-2.04	1.35	1.40
32	2a	1407	5MC	C6-C5	2.04	1.37	1.34
1	2A	2251	OMG	C2-N2	2.03	1.39	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	1a	1404	5MC	C2-N3	2.03	1.40	1.36
32	2a	1498	UR3	O2-C2	-2.03	1.18	1.22
32	1a	1207	2MG	C5-C4	-2.03	1.37	1.43
32	2a	1404	5MC	C4-N4	2.02	1.39	1.34

All (206) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	1a	1519	MA6	N1-C6-N6	-20.95	95.00	117.06
32	2a	1519	MA6	N1-C6-N6	-20.61	95.36	117.06
32	2a	1518	MA6	N1-C6-N6	-20.06	95.95	117.06
32	1a	1518	MA6	N1-C6-N6	-19.20	96.85	117.06
32	1a	516	PSU	C6-C5-C4	8.15	123.89	118.20
1	1A	2564	OMU	C5-C4-N3	7.18	125.58	114.84
1	2A	2552	OMU	C5-C4-N3	7.02	125.33	114.84
32	2a	516	PSU	C6-C5-C4	6.31	122.61	118.20
32	1a	1518	MA6	C1'-N9-C4	-6.07	115.98	126.64
32	1a	1519	MA6	C1'-N9-C4	-5.85	116.37	126.64
32	2a	1518	MA6	C1'-N9-C4	-5.79	116.47	126.64
1	1A	2564	OMU	C4-N3-C2	-5.57	119.24	126.58
32	2a	1518	MA6	N3-C2-N1	-5.37	120.29	128.68
32	2a	1519	MA6	N3-C2-N1	-5.25	120.47	128.68
1	2A	2552	OMU	C4-N3-C2	-5.25	119.66	126.58
32	2a	1402	4OC	CM4-N4-C4	-5.22	112.25	122.45
32	1a	1518	MA6	N3-C2-N1	-5.20	120.55	128.68
32	1a	1519	MA6	N3-C2-N1	-5.18	120.58	128.68
32	2a	1519	MA6	C1'-N9-C4	-5.16	117.58	126.64
1	1A	1933	PSU	C6-C5-C4	5.08	121.75	118.20
54	1x	55	PSU	C6-C5-C4	4.95	121.66	118.20
32	1a	1498	UR3	C4-N3-C2	-4.91	119.94	124.56
1	2A	1911	PSU	C6-C5-C4	4.89	121.61	118.20
1	1A	1939	PSU	C6-C5-C4	4.80	121.55	118.20
32	1a	527	7MG	C5-C6-N1	4.80	119.44	110.99
43	2l	92	0TD	OD2-CG-CB	4.73	123.36	113.15
32	2a	527	7MG	C5-C6-N1	4.69	119.26	110.99
54	2x	55	PSU	C6-C5-C4	4.44	121.31	118.20
1	2A	2605	PSU	C6-C5-C4	4.40	121.27	118.20
1	2A	1917	PSU	C6-C5-C4	4.39	121.27	118.20
32	1a	527	7MG	C2-N3-C4	4.26	119.88	112.30
1	1A	2617	PSU	C6-C5-C4	4.22	121.15	118.20
32	2a	1498	UR3	C4-N3-C2	-4.20	120.61	124.56
32	2a	527	7MG	C2-N3-C4	4.15	119.70	112.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	1a	527	7MG	C5-C4-N9	3.93	111.44	106.35
43	1l	92	0TD	OD2-CG-CB	3.89	121.54	113.15
1	1A	2564	OMU	N3-C2-N1	3.75	119.87	114.89
1	2A	2251	OMG	C5-C6-N1	3.72	120.52	113.95
43	1l	92	0TD	CSB-SB-CB	3.70	109.13	102.44
1	2A	2552	OMU	N3-C2-N1	3.65	119.74	114.89
1	1A	2515	2MA	CM2-C2-N1	3.65	124.35	116.23
1	1A	1984	5MC	C5-C4-N3	3.60	125.56	121.67
1	2A	1939	5MU	C6-C5-C4	3.58	121.03	118.03
32	1a	527	7MG	C5-C4-N3	-3.56	121.34	128.13
32	2a	967	5MC	C5-C4-N3	3.49	125.44	121.67
32	2a	966	M2G	C5-C6-N1	3.47	120.08	113.95
1	1A	1964	5MC	C5-C4-N3	3.47	125.41	121.67
32	2a	527	7MG	C5-C4-N3	-3.45	121.56	128.13
32	2a	967	5MC	C5-C6-N1	-3.43	119.81	123.34
32	2a	1400	5MC	C5-C4-N3	3.41	125.36	121.67
32	1a	516	PSU	C6-N1-C2	-3.40	119.20	122.68
32	1a	967	5MC	C5-C4-N3	3.39	125.34	121.67
32	2a	1402	4OC	C5-C4-N4	-3.38	115.72	122.61
32	1a	1400	5MC	C5-C6-N1	-3.37	119.87	123.34
54	1x	32	5MC	C5-C6-N1	-3.35	119.89	123.34
32	1a	516	PSU	N1-C2-N3	3.35	118.93	115.13
32	2a	1404	5MC	C5-C6-N1	-3.35	119.89	123.34
1	2A	2503	2MA	C5-C6-N1	3.35	119.79	114.02
1	2A	1939	5MU	C4-N3-C2	-3.28	123.11	127.35
1	1A	1964	5MC	C5-C6-N1	-3.27	119.97	123.34
32	2a	527	7MG	C5-C4-N9	3.27	110.59	106.35
32	1a	1400	5MC	C5-C4-N3	3.27	125.20	121.67
1	1A	2263	OMG	C5-C6-N1	3.25	119.69	113.95
32	1a	1407	5MC	C5-C6-N1	-3.25	120.00	123.34
1	2A	1942	5MC	C5-C4-N3	3.23	125.16	121.67
54	2x	54	5MU	C6-C5-C4	3.23	120.73	118.03
32	1a	1498	UR3	C1'-N1-C2	3.22	122.43	116.99
1	2A	1915	5MU	C6-C5-C4	3.20	120.71	118.03
1	1A	1937	5MU	C6-C5-C4	3.19	120.70	118.03
32	1a	1207	2MG	C5-C6-N1	3.18	119.57	113.95
1	1A	2564	OMU	O4-C4-C5	-3.17	119.59	125.16
54	2x	32	5MC	C5-C4-N3	3.16	125.08	121.67
54	1x	8	4SU	C4-N3-C2	-3.15	124.28	127.34
1	1A	1984	5MC	C5-C6-N1	-3.14	120.11	123.34
32	1a	1407	5MC	C5-C4-N3	3.10	125.02	121.67
1	1A	1961	5MU	C4-N3-C2	-3.09	123.36	127.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	2A	2251	OMG	C2-N1-C6	-3.08	119.42	125.10
32	1a	1404	5MC	C5-C4-N3	3.08	125.00	121.67
32	1a	966	M2G	C5-C6-N1	3.07	119.38	113.95
1	1A	2515	2MA	C5-C6-N1	3.06	119.30	114.02
54	1x	32	5MC	C4-N3-C2	-3.05	116.56	120.69
1	1A	2564	OMU	O4-C4-N3	-3.05	114.83	119.31
1	1A	1937	5MU	C4-N3-C2	-3.05	123.41	127.35
32	2a	1400	5MC	C5-C6-N1	-3.05	120.20	123.34
43	2l	92	0TD	CSB-SB-CB	3.04	107.94	102.44
1	2A	2552	OMU	O4-C4-C5	-3.04	119.82	125.16
54	2x	8	4SU	C6-C5-C4	3.04	122.58	119.95
1	2A	2552	OMU	O4-C4-N3	-3.03	114.85	119.31
1	2A	2552	OMU	C6-C5-C4	-3.02	115.39	119.52
1	1A	2263	OMG	C8-N7-C5	3.00	108.71	102.99
54	1x	32	5MC	C5-C4-N3	3.00	124.91	121.67
1	2A	1962	5MC	C5-C4-N3	3.00	124.91	121.67
1	1A	1933	PSU	O2-C2-N1	-2.99	119.50	122.79
54	1x	54	5MU	C6-C5-C4	2.98	120.53	118.03
54	2x	32	5MC	C5-C6-N1	-2.96	120.29	123.34
1	2A	1942	5MC	C5-C6-N1	-2.96	120.30	123.34
32	2a	1407	5MC	C5-C6-N1	-2.90	120.36	123.34
32	1a	1404	5MC	C5-C6-N1	-2.89	120.36	123.34
43	1l	92	0TD	CB-CA-N	-2.88	102.96	109.10
32	2a	516	PSU	N1-C2-N3	2.86	118.37	115.13
54	2x	54	5MU	C4-N3-C2	-2.85	123.66	127.35
1	1A	1964	5MC	C4-N3-C2	-2.84	116.85	120.69
32	1a	1207	2MG	C8-N7-C5	2.83	108.38	102.99
1	2A	1942	5MC	C4-N3-C2	-2.81	116.88	120.69
32	2a	1404	5MC	C5-C4-N3	2.81	124.70	121.67
32	1a	967	5MC	C5-C6-N1	-2.80	120.45	123.34
1	1A	2564	OMU	C6-C5-C4	-2.80	115.69	119.52
1	1A	1984	5MC	C4-N3-C2	-2.80	116.90	120.69
32	2a	1407	5MC	C5-C4-N3	2.80	124.69	121.67
43	2l	92	0TD	OD2-CG-OD1	-2.79	117.75	124.09
32	2a	1207	2MG	C5-C6-N1	2.79	118.88	113.95
54	1x	54	5MU	C4-N3-C2	-2.78	123.76	127.35
1	2A	2251	OMG	O6-C6-C5	-2.76	118.97	124.37
1	1A	2515	2MA	C8-N7-C5	2.76	108.25	102.99
32	2a	1400	5MC	C4-N3-C2	-2.72	117.01	120.69
32	2a	966	M2G	C2-N1-C6	-2.72	119.20	123.71
1	1A	2263	OMG	C2-N1-C6	-2.72	120.10	125.10
1	1A	2263	OMG	N2-C2-N1	2.71	122.48	116.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	2A	2503	2MA	C8-N7-C5	2.71	108.15	102.99
32	2a	1207	2MG	C8-N7-C5	2.70	108.13	102.99
32	2a	1498	UR3	C1'-N1-C2	2.69	121.53	116.99
1	2A	1962	5MC	C5-C6-N1	-2.69	120.57	123.34
54	2x	55	PSU	O2-C2-N1	-2.68	119.84	122.79
1	1A	1937	5MU	C1'-N1-C2	2.68	122.42	117.57
1	2A	1911	PSU	O2-C2-N1	-2.68	119.84	122.79
32	2a	966	M2G	C8-N7-C5	2.67	108.08	102.99
1	2A	1915	5MU	C4-N3-C2	-2.66	123.90	127.35
32	2a	967	5MC	C4-N3-C2	-2.66	117.09	120.69
32	2a	1404	5MC	C4-N3-C2	-2.65	117.10	120.69
1	2A	2605	PSU	O2-C2-N1	-2.65	119.87	122.79
32	2a	527	7MG	C4-C5-N7	2.65	109.21	105.53
32	1a	967	5MC	C4-N3-C2	-2.64	117.11	120.69
1	2A	2503	2MA	CM2-C2-N1	2.64	122.11	116.23
54	2x	32	5MC	C4-N3-C2	-2.64	117.12	120.69
32	1a	1400	5MC	C4-N3-C2	-2.64	117.12	120.69
1	1A	2617	PSU	O4-C4-N3	-2.64	115.06	120.12
32	1a	966	M2G	C2-N1-C6	-2.63	119.34	123.71
1	2A	2251	OMG	C8-N7-C5	2.63	108.00	102.99
32	1a	1407	5MC	C4-N3-C2	-2.62	117.15	120.69
32	2a	1498	UR3	C6-N1-C2	-2.61	119.45	121.79
1	1A	1961	5MU	C6-C5-C4	2.55	120.16	118.03
32	1a	1402	4OC	CM4-N4-C4	-2.54	117.48	122.45
32	2a	516	PSU	O4'-C1'-C2'	2.48	108.64	105.14
1	2A	2552	OMU	O2-C2-N1	-2.47	119.50	122.79
32	2a	1402	4OC	C6-C5-C4	2.46	119.97	116.96
32	1a	1402	4OC	CM2-O2'-C2'	2.46	120.98	114.52
32	1a	1407	5MC	N4-C4-N3	-2.45	114.00	118.48
32	1a	966	M2G	C8-N7-C5	2.45	107.65	102.99
1	2A	1917	PSU	O4-C4-N3	-2.44	115.44	120.12
32	1a	516	PSU	O4'-C1'-C2'	2.44	108.58	105.14
32	1a	527	7MG	C4-C5-N7	2.42	108.89	105.53
1	2A	1962	5MC	C4-N3-C2	-2.42	117.41	120.69
1	2A	1917	PSU	O2-C2-N1	-2.42	120.13	122.79
32	1a	527	7MG	N9-C8-N7	2.41	106.82	103.38
32	2a	1404	5MC	CM5-C5-C6	-2.40	119.64	122.85
1	2A	1915	5MU	C1'-N1-C2	2.40	121.91	117.57
32	1a	1404	5MC	C4-N3-C2	-2.40	117.45	120.69
32	1a	527	7MG	C2-N1-C6	-2.33	120.84	125.10
1	1A	1937	5MU	C1'-N1-C6	-2.33	117.24	121.12
43	1l	92	0TD	OD2-CG-OD1	-2.32	118.82	124.09

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	2A	1942	5MC	CM5-C5-C6	-2.32	119.75	122.85
32	2a	1407	5MC	C4-N3-C2	-2.31	117.56	120.69
1	1A	2564	OMU	O2-C2-N1	-2.28	119.75	122.79
32	2a	516	PSU	C6-N1-C2	-2.26	120.37	122.68
54	2x	55	PSU	O4-C4-N3	-2.23	115.84	120.12
1	2A	1920	OMC	O2-C2-N3	-2.23	118.71	122.33
1	1A	1984	5MC	N4-C4-N3	-2.22	114.42	118.48
32	2a	516	PSU	O4-C4-N3	-2.21	115.88	120.12
32	1a	527	7MG	N2-C2-N1	2.19	121.39	116.71
43	2l	92	0TD	CB-CA-N	-2.19	104.42	109.10
32	2a	1404	5MC	N4-C4-N3	-2.19	114.48	118.48
32	2a	527	7MG	O6-C6-C5	-2.19	122.17	127.54
1	1A	1939	PSU	O2-C2-N1	-2.18	120.39	122.79
32	2a	967	5MC	N4-C4-N3	-2.17	114.51	118.48
32	1a	1404	5MC	N4-C4-N3	-2.16	114.53	118.48
1	1A	2263	OMG	O6-C6-C5	-2.15	120.18	124.37
32	1a	1407	5MC	CM5-C5-C6	-2.15	119.98	122.85
32	1a	516	PSU	C5-C6-N1	-2.15	118.89	122.11
1	1A	1984	5MC	CM5-C5-C6	-2.14	119.99	122.85
32	1a	1207	2MG	O3'-C3'-C2'	2.14	118.75	111.82
1	1A	1937	5MU	C5-C4-N3	2.13	117.13	115.31
1	1A	1961	5MU	C5-C6-N1	-2.12	121.15	123.34
32	1a	516	PSU	O4-C4-N3	-2.11	116.07	120.12
32	1a	527	7MG	C6-C5-C4	-2.11	118.27	122.62
32	1a	966	M2G	O6-C6-C5	-2.10	120.27	124.37
32	1a	1400	5MC	N4-C4-N3	-2.09	114.66	118.48
1	1A	1939	PSU	O4-C4-N3	-2.09	116.11	120.12
1	2A	2605	PSU	O4-C4-N3	-2.09	116.11	120.12
1	1A	2617	PSU	O2-C2-N1	-2.09	120.49	122.79
32	2a	527	7MG	C2-N1-C6	-2.09	121.30	125.10
1	1A	1933	PSU	N1-C2-N3	2.08	117.49	115.13
1	1A	1933	PSU	O4'-C1'-C2'	2.08	108.08	105.14
1	1A	1942	OMC	O2-C2-N3	-2.07	118.97	122.33
1	1A	2617	PSU	C4-N3-C2	-2.07	123.36	126.34
1	2A	1939	5MU	C5-C6-N1	-2.06	121.21	123.34
54	2x	32	5MC	N4-C4-N3	-2.06	114.71	118.48
54	2x	55	PSU	C4-N3-C2	-2.06	123.36	126.34
32	1a	1207	2MG	O6-C6-C5	-2.06	120.36	124.37
32	1a	1498	UR3	C3U-N3-C4	2.06	120.83	117.89
32	1a	967	5MC	N4-C4-N3	-2.04	114.75	118.48
1	1A	1961	5MU	C5-C4-N3	2.04	117.05	115.31
32	2a	966	M2G	O6-C6-C5	-2.04	120.39	124.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	2A	1942	5MC	N4-C4-N3	-2.03	114.77	118.48
1	2A	1915	5MU	O2-C2-N1	2.03	125.48	122.79
32	2a	1400	5MC	N4-C4-N3	-2.03	114.78	118.48
32	2a	527	7MG	N2-C2-N1	2.02	121.02	116.71

There are no chirality outliers.

All (44) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	1A	1937	5MU	O4'-C1'-N1-C2
1	1A	1937	5MU	O4'-C1'-N1-C6
1	1A	2263	OMG	C1'-C2'-O2'-CM2
32	1a	967	5MC	O4'-C4'-C5'-O5'
32	1a	967	5MC	C3'-C4'-C5'-O5'
32	1a	1402	4OC	O4'-C4'-C5'-O5'
1	2A	1915	5MU	O4'-C1'-N1-C2
1	2A	1915	5MU	O4'-C1'-N1-C6
1	2A	1915	5MU	C3'-C4'-C5'-O5'
1	2A	1915	5MU	O4'-C4'-C5'-O5'
32	2a	527	7MG	C3'-C4'-C5'-O5'
32	2a	1402	4OC	O4'-C4'-C5'-O5'
43	2l	92	0TD	CA-CB-CG-OD2
43	2l	92	0TD	CA-CB-CG-OD1
43	2l	92	0TD	SB-CB-CG-OD2
32	1a	527	7MG	C3'-C4'-C5'-O5'
32	1a	1402	4OC	C3'-C4'-C5'-O5'
32	1a	1519	MA6	O4'-C4'-C5'-O5'
32	1a	1519	MA6	C3'-C4'-C5'-O5'
1	2A	2503	2MA	O4'-C4'-C5'-O5'
1	2A	2503	2MA	C3'-C4'-C5'-O5'
32	2a	1402	4OC	C3'-C4'-C5'-O5'
32	2a	527	7MG	O4'-C4'-C5'-O5'
32	2a	1519	MA6	O4'-C4'-C5'-O5'
32	2a	1519	MA6	C3'-C4'-C5'-O5'
32	1a	527	7MG	O4'-C4'-C5'-O5'
32	2a	1400	5MC	O4'-C4'-C5'-O5'
32	1a	1519	MA6	C5-C6-N6-C9
32	2a	1400	5MC	C3'-C4'-C5'-O5'
43	1l	92	0TD	CA-CB-CG-OD2
1	2A	1915	5MU	C4'-C5'-O5'-P
1	1A	2515	2MA	O4'-C4'-C5'-O5'
1	2A	2552	OMU	O4'-C4'-C5'-O5'

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Mol	Chain	Res	Type	Atoms
43	2l	92	0TD	CA-CB-SB-CSB
1	2A	2251	OMG	C4'-C5'-O5'-P
32	1a	1400	5MC	O4'-C4'-C5'-O5'
1	1A	1942	OMC	C2'-C1'-N1-C2
32	1a	516	PSU	O4'-C4'-C5'-O5'
43	1l	92	0TD	CG-CB-SB-CSB
43	2l	92	0TD	CG-CB-SB-CSB
32	1a	1400	5MC	C3'-C4'-C5'-O5'
32	2a	516	PSU	O4'-C4'-C5'-O5'
1	1A	2263	OMG	C4'-C5'-O5'-P
32	1a	1519	MA6	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 2719 ligands modelled in this entry, 2717 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	$\# Z > 2$
58	SF4	1d	501	35	0,12,12	-	-	-		
58	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
58	SF4	1d	501	35	-	-	0/6/5/5
58	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	2861/2915 (98%)	0.58	252 (8%) 10 5	6, 22, 80, 93	0
1	2A	2856/2915 (97%)	0.72	286 (10%) 7 4	19, 41, 80, 92	0
2	1B	120/120 (100%)	0.26	2 (1%) 70 63	18, 35, 49, 69	0
2	2B	120/120 (100%)	0.76	11 (9%) 9 5	43, 60, 69, 73	0
3	1D	275/275 (100%)	-0.24	0 100 100	7, 23, 36, 52	0
3	2D	275/275 (100%)	-0.09	0 100 100	19, 36, 47, 63	0
4	1E	204/204 (100%)	-0.17	0 100 100	7, 29, 47, 56	0
4	2E	204/204 (100%)	-0.00	1 (0%) 91 88	19, 41, 55, 63	0
5	1F	203/203 (100%)	-0.14	3 (1%) 73 68	7, 28, 53, 70	0
5	2F	203/203 (100%)	0.02	1 (0%) 91 88	24, 50, 63, 73	0
6	1G	181/181 (100%)	-0.07	0 100 100	28, 44, 55, 69	0
6	2G	181/181 (100%)	0.84	31 (17%) 1 1	56, 65, 74, 77	0
7	1H	174/174 (100%)	-0.09	0 100 100	23, 38, 49, 54	0
7	2H	173/174 (99%)	0.98	34 (19%) 1 0	50, 62, 69, 71	0
8	1I	147/147 (100%)	0.52	9 (6%) 21 13	31, 54, 66, 70	0
8	2I	146/147 (99%)	0.58	14 (9%) 8 4	39, 58, 68, 76	0
9	1N	140/140 (100%)	-0.20	1 (0%) 87 84	14, 26, 44, 58	0
9	2N	140/140 (100%)	0.02	2 (1%) 75 70	28, 47, 59, 63	0
10	1O	122/122 (100%)	-0.15	0 100 100	14, 26, 41, 49	0
10	2O	122/122 (100%)	-0.00	1 (0%) 86 81	30, 40, 51, 56	0
11	1P	149/149 (100%)	0.14	3 (2%) 65 56	7, 32, 48, 64	0
11	2P	149/149 (100%)	0.42	7 (4%) 31 22	24, 50, 64, 71	0
12	1Q	141/141 (100%)	-0.11	0 100 100	14, 26, 42, 59	0
12	2Q	141/141 (100%)	0.01	1 (0%) 87 84	31, 47, 57, 65	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
13	1R	118/118 (100%)	-0.21	0 100 100	14, 22, 36, 47	0
13	2R	118/118 (100%)	-0.13	0 100 100	25, 37, 46, 55	0
14	1S	110/110 (100%)	0.15	0 100 100	24, 36, 45, 51	0
14	2S	110/110 (100%)	0.81	12 (10%) 5 3	46, 55, 62, 66	0
15	1T	131/131 (100%)	0.10	2 (1%) 73 68	20, 33, 52, 64	0
15	2T	131/131 (100%)	0.11	4 (3%) 49 39	36, 44, 59, 65	0
16	1U	116/116 (100%)	-0.15	0 100 100	9, 17, 35, 49	0
16	2U	116/116 (100%)	0.47	6 (5%) 27 18	26, 45, 55, 66	0
17	1V	101/101 (100%)	-0.17	1 (0%) 82 77	8, 29, 44, 54	0
17	2V	101/101 (100%)	0.48	5 (4%) 28 19	32, 51, 59, 67	0
18	1W	112/112 (100%)	-0.25	0 100 100	10, 17, 36, 66	0
18	2W	112/112 (100%)	-0.03	2 (1%) 68 61	25, 34, 48, 60	0
19	1X	95/95 (100%)	-0.14	0 100 100	13, 24, 43, 59	0
19	2X	95/95 (100%)	0.08	1 (1%) 80 75	35, 44, 57, 60	0
20	1Y	107/107 (100%)	-0.26	0 100 100	24, 34, 49, 61	0
20	2Y	107/107 (100%)	0.33	5 (4%) 31 22	44, 54, 62, 73	0
21	1Z	203/203 (100%)	0.60	15 (7%) 14 8	28, 47, 62, 78	0
21	2Z	201/203 (99%)	0.81	27 (13%) 3 1	46, 60, 68, 71	0
22	10	77/77 (100%)	0.12	1 (1%) 77 72	17, 23, 37, 41	0
22	20	77/77 (100%)	0.39	3 (3%) 39 29	39, 45, 54, 63	0
23	11	97/97 (100%)	0.29	8 (8%) 11 6	11, 31, 54, 58	0
23	21	97/97 (100%)	0.20	5 (5%) 27 18	28, 40, 58, 64	0
24	12	70/70 (100%)	-0.15	0 100 100	24, 34, 46, 56	0
24	22	70/70 (100%)	0.08	1 (1%) 75 70	42, 53, 63, 64	0
25	13	59/59 (100%)	-0.10	0 100 100	15, 26, 49, 59	0
25	23	59/59 (100%)	0.44	5 (8%) 10 5	37, 46, 57, 63	0
26	14	69/69 (100%)	0.85	10 (14%) 2 1	35, 60, 72, 81	0
26	24	69/69 (100%)	2.05	31 (44%) 0 0	64, 72, 81, 84	0
27	15	59/59 (100%)	-0.19	0 100 100	8, 23, 42, 51	0
27	25	59/59 (100%)	-0.07	2 (3%) 45 35	23, 38, 52, 58	0
28	16	53/53 (100%)	0.15	0 100 100	24, 29, 41, 50	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
28	26	53/53 (100%)	0.47	3 (5%) 23 15	34, 47, 56, 58	0
29	17	48/48 (100%)	0.03	0 100 100	8, 13, 34, 42	0
29	27	48/48 (100%)	0.19	1 (2%) 63 54	21, 28, 44, 58	0
30	18	64/64 (100%)	-0.16	0 100 100	15, 20, 28, 37	0
30	28	64/64 (100%)	0.12	0 100 100	31, 39, 49, 54	0
31	19	37/37 (100%)	0.06	0 100 100	19, 28, 43, 49	0
31	29	37/37 (100%)	0.60	0 100 100	39, 47, 54, 57	0
32	1a	1488/1520 (97%)	0.74	128 (8%) 10 5	20, 53, 76, 91	0
32	2a	1492/1520 (98%)	0.85	148 (9%) 7 4	32, 59, 77, 90	0
33	1b	231/231 (100%)	0.93	35 (15%) 2 1	50, 60, 69, 74	0
33	2b	231/231 (100%)	1.31	65 (28%) 0 0	54, 66, 71, 81	0
34	1c	206/206 (100%)	0.43	13 (6%) 20 12	47, 57, 66, 69	0
34	2c	206/206 (100%)	0.80	34 (16%) 1 1	53, 65, 71, 74	0
35	1d	208/208 (100%)	0.38	9 (4%) 35 25	41, 56, 67, 70	0
35	2d	208/208 (100%)	0.58	20 (9%) 8 4	48, 57, 64, 69	0
36	1e	148/148 (100%)	0.35	6 (4%) 37 27	33, 49, 58, 69	0
36	2e	148/148 (100%)	0.48	6 (4%) 37 27	48, 56, 63, 76	0
37	1f	100/100 (100%)	0.09	2 (2%) 65 56	46, 53, 60, 64	0
37	2f	100/100 (100%)	0.25	4 (4%) 38 28	38, 54, 62, 67	0
38	1g	155/155 (100%)	0.39	14 (9%) 9 5	47, 55, 69, 76	0
38	2g	155/155 (100%)	0.68	20 (12%) 3 2	53, 62, 71, 80	0
39	1h	137/137 (100%)	0.09	2 (1%) 73 68	40, 51, 58, 65	0
39	2h	137/137 (100%)	0.14	6 (4%) 34 24	46, 56, 62, 65	0
40	1i	127/127 (100%)	0.82	16 (12%) 3 2	40, 61, 68, 72	0
40	2i	126/127 (99%)	1.30	33 (26%) 0 0	55, 65, 72, 79	0
41	1j	97/97 (100%)	1.04	16 (16%) 1 1	44, 61, 73, 78	0
41	2j	96/97 (98%)	1.39	24 (25%) 0 0	52, 66, 72, 74	0
42	1k	114/114 (100%)	0.70	11 (9%) 8 4	29, 50, 61, 65	0
42	2k	114/114 (100%)	0.72	12 (10%) 6 3	45, 57, 64, 68	0
43	1l	121/122 (99%)	0.33	9 (7%) 14 8	32, 43, 56, 61	0
43	2l	121/122 (99%)	0.27	4 (3%) 46 36	41, 52, 60, 63	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
44	1m	116/116 (100%)	0.79	14 (12%) 4 2	45, 55, 64, 67	0
44	2m	114/116 (98%)	0.85	12 (10%) 6 3	56, 65, 72, 76	0
45	1n	60/60 (100%)	0.52	4 (6%) 17 10	47, 53, 59, 62	0
45	2n	60/60 (100%)	1.15	12 (20%) 1 0	58, 64, 69, 72	0
46	1o	88/88 (100%)	0.21	1 (1%) 80 75	36, 46, 58, 65	0
46	2o	88/88 (100%)	0.22	1 (1%) 80 75	45, 52, 61, 69	0
47	1p	82/82 (100%)	0.77	6 (7%) 15 8	43, 55, 62, 64	0
47	2p	82/82 (100%)	0.67	7 (8%) 10 5	46, 54, 61, 68	0
48	1q	99/99 (100%)	0.16	1 (1%) 82 77	36, 51, 61, 65	0
48	2q	99/99 (100%)	0.32	1 (1%) 82 77	43, 53, 60, 65	0
49	1r	68/68 (100%)	0.74	8 (11%) 4 2	43, 52, 62, 69	0
49	2r	68/68 (100%)	0.95	11 (16%) 1 1	48, 55, 64, 67	0
50	1s	83/83 (100%)	0.41	2 (2%) 59 49	50, 60, 67, 73	0
50	2s	83/83 (100%)	0.91	16 (19%) 1 0	55, 67, 75, 77	0
51	1t	96/98 (97%)	0.40	2 (2%) 63 54	45, 56, 64, 68	0
51	2t	98/98 (100%)	0.30	4 (4%) 37 27	46, 53, 64, 68	0
52	1u	23/23 (100%)	0.45	0 100 100	48, 52, 57, 58	0
52	2u	23/23 (100%)	1.53	7 (30%) 0 0	58, 62, 67, 68	0
53	1v	3/3 (100%)	0.22	0 100 100	37, 37, 39, 40	0
53	2v	3/3 (100%)	0.49	0 100 100	53, 53, 57, 62	0
54	1x	72/76 (94%)	0.45	2 (2%) 53 43	15, 41, 61, 71	0
54	2x	72/76 (94%)	1.12	17 (23%) 0 0	32, 57, 68, 75	0
55	1y	16/16 (100%)	-0.11	0 100 100	14, 20, 32, 39	0
55	2y	16/16 (100%)	0.06	0 100 100	28, 33, 48, 48	0
All	All	20755/20948 (99%)	0.50	1574 (7%) 13 7	6, 47, 71, 93	0

All (1574) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	1A	1133	G	15.3
1	2A	2128	C	14.8
1	1A	2149	G	13.8
1	1A	2155	G	13.7
1	1A	1135	G	13.2

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Mol	Chain	Res	Type	RSRZ
1	1A	2180	A	12.6
1	2A	2127	G	12.1
1	1A	2139	A	11.6
1	2A	2112	G	10.7
1	1A	2150	C	10.6
1	2A	2119	A	10.5
1	1A	2152	U	10.5
1	2A	2147	G	10.4
1	1A	2154	U	10.2
1	2A	2173	A	10.2
1	2A	2159	G	10.1
1	1A	1149	A	9.9
21	1Z	192	ALA	9.7
21	1Z	193	GLU	9.7
1	2A	2118	U	9.7
1	1A	1113	A	9.5
1	1A	1134	A	9.5
1	1A	2179	G	9.4
1	1A	1137	G	9.3
1	1A	1112	U	9.2
1	2A	2124	G	9.1
1	1A	1132	A	9.1
1	2A	2162	G	9.0
1	2A	2123	G	9.0
1	1A	2151	C	9.0
1	1A	1110	C	9.0
1	2A	2168	G	8.9
1	1A	2178	G	8.8
1	2A	2133	G	8.8
1	1A	1109	G	8.5
1	1A	1123	A	8.4
1	1A	1150	C	8.4
1	2A	2131	G	8.4
1	2A	2129	C	8.3
1	1A	2141	A	8.3
1	2A	2157	G	8.3
32	2a	1030(A)	G	8.2
1	1A	1121	C	8.2
1	1A	2148	A	8.2
1	1A	2146	G	8.2
1	1A	1103	A	8.2
1	1A	2128	G	8.2

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Mol	Chain	Res	Type	RSRZ
1	1A	2153	G	8.1
1	1A	1120	G	8.1
1	1A	2806	G	8.1
1	1A	2145	G	8.1
1	2A	2172	U	8.0
1	2A	2106	G	8.0
1	2A	2158	A	7.9
38	1g	83	ALA	7.9
1	1A	2181	G	7.8
32	2a	1002	G	7.8
1	2A	2125	G	7.7
1	1A	2807	C	7.7
1	1A	1108	G	7.7
1	1A	1122	C	7.7
20	2Y	1	MET	7.6
32	2a	1027	C	7.6
1	2A	2132	U	7.6
1	2A	2110	G	7.6
1	2A	2179	C	7.6
1	2A	2174	C	7.5
1	2A	2105	C	7.5
1	1A	1117	G	7.5
1	1A	2195	A	7.4
1	1A	2142	G	7.4
1	1A	1114	G	7.3
32	2a	1003	G	7.3
1	1A	2147	G	7.2
32	2a	1026	G	7.2
33	1b	232	PRO	7.2
1	2A	2111	C	7.2
1	1A	2156	A	7.2
1	2A	2134	A	7.1
1	1A	1139	G	7.1
1	1A	2134	G	7.1
32	1a	1027	C	7.1
32	1a	1026	G	7.1
32	1a	1030	C	7.0
40	2i	62	TYR	7.0
1	1A	1118	C	7.0
1	2A	2169	A	7.0
21	2Z	193	GLU	6.9
1	2A	2117	A	6.9

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Mol	Chain	Res	Type	RSRZ
1	2A	1067	A	6.9
1	2A	2107	C	6.8
1	2A	2802	G	6.8
38	2g	84	ASN	6.8
1	1A	2169	G	6.8
1	1A	2177	G	6.8
1	1A	1131	A	6.8
21	1Z	191	VAL	6.8
1	2A	1076	C	6.8
1	1A	1124	U	6.8
1	1A	1111	U	6.7
32	1a	1024	G	6.7
1	2A	2164	C	6.7
1	1A	1130	A	6.7
21	1Z	194	PRO	6.7
21	1Z	202	GLU	6.6
1	1A	1101	G	6.6
32	2a	1005	A	6.6
32	2a	1034	G	6.6
1	1A	1148	C	6.6
1	2A	2126	A	6.6
32	1a	91	C	6.6
1	1A	1151	U	6.6
1	1A	2805	G	6.5
1	2A	2155	G	6.5
1	2A	2163	C	6.5
1	1A	2198	A	6.5
1	2A	2130	U	6.5
1	1A	2126	G	6.5
1	1A	2191	A	6.4
1	1A	932	C	6.3
1	1A	2173	G	6.3
1	2A	2152	G	6.3
1	2A	1095	A	6.3
1	1A	2184	G	6.2
1	2A	2156	G	6.2
1	2A	2120	G	6.2
7	2H	95	ARG	6.1
1	1A	2130	C	6.1
33	2b	233	SER	6.1
32	1a	1031	G	6.1
32	1a	1028	C	6.1

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Mol	Chain	Res	Type	RSRZ
1	2A	1056	G	6.1
1	1A	2183	C	6.1
1	2A	2108	C	6.1
33	2b	48	MET	6.0
32	1a	1036	G	6.0
32	2a	1001(A)	G	6.0
1	1A	2140	U	6.0
1	2A	2151	G	6.0
1	2A	2113	U	6.0
41	2j	96	ILE	6.0
38	1g	84	ASN	5.9
1	2A	2793	G	5.9
1	1A	2190	G	5.9
1	1A	1129	U	5.9
44	2m	6	GLY	5.9
33	2b	17	PHE	5.9
1	1A	1119	A	5.8
1	1A	1127	U	5.8
6	2G	149	VAL	5.8
32	1a	1001(A)	G	5.8
32	1a	1030(D)	A	5.8
32	1a	1029	C	5.8
1	1A	2182	G	5.8
32	1a	1034	G	5.8
32	2a	1032	G	5.8
1	1A	2196	C	5.7
1	2A	2154	G	5.7
32	2a	1033	G	5.7
33	1b	228	GLY	5.7
1	1A	1126	C	5.7
1	2A	2148	G	5.7
32	1a	78	G	5.6
1	2A	2805	G	5.6
1	2A	2170	A	5.6
1	1A	2132	G	5.5
21	2Z	192	ALA	5.5
34	1c	192	THR	5.5
1	1A	2170	G	5.5
1	2A	2141	G	5.5
1	2A	888	C	5.5
1	2A	1099	G	5.5
1	1A	2194	U	5.5

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Mol	Chain	Res	Type	RSRZ
1	1A	1555	C	5.5
1	2A	1075	C	5.5
1	1A	1102	G	5.4
1	1A	1104	G	5.4
1	2A	1058	G	5.4
1	1A	2202	U	5.4
1	1A	933	C	5.4
1	1A	2185	C	5.4
1	1A	2816	G	5.4
1	1A	1116	A	5.4
32	1a	1002	G	5.4
26	14	18	CYS	5.4
33	2b	232	PRO	5.4
32	1a	1030(B)	C	5.4
26	24	49	PHE	5.3
32	2a	91	C	5.3
1	2A	1068	G	5.3
38	2g	81	GLY	5.3
32	1a	92	C	5.3
1	1A	1220	U	5.3
1	2A	279	C	5.3
1	2A	2137	C	5.3
7	2H	106	THR	5.3
54	2x	46	G	5.3
1	2A	2153	G	5.2
1	1A	1556	A	5.2
1	1A	2163	G	5.2
1	1A	2133	C	5.2
1	1A	2197	C	5.2
32	2a	1030	C	5.2
32	1a	1030(A)	G	5.2
1	2A	2138	C	5.1
1	1A	2131	U	5.1
1	2A	2792	G	5.1
1	2A	1066	U	5.1
35	2d	11	LEU	5.1
1	2A	889	C	5.1
1	2A	1509	C	5.1
1	2A	2142	C	5.1
26	24	67	TYR	5.1
33	2b	139	LYS	5.1
1	2A	2176	A	5.1

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Mol	Chain	Res	Type	RSRZ
1	1A	2127	C	5.1
1	1A	2171	G	5.1
21	2Z	194	PRO	5.0
38	2g	83	ALA	5.0
7	2H	56	SER	5.0
1	2A	1083	U	5.0
1	1A	1141	A	5.0
32	1a	1032	G	5.0
21	1Z	197	ILE	5.0
1	1A	1138	C	5.0
1	2A	1055	G	5.0
26	24	41	PRO	4.9
1	1A	1128	U	4.9
32	1a	77	G	4.9
32	2a	1020	U	4.9
21	2Z	201	LYS	4.9
1	2A	896	A	4.9
1	1A	2201	C	4.9
1	2A	1064	C	4.9
32	1a	1025	U	4.9
33	2b	190	THR	4.9
32	1a	1023	G	4.9
21	1Z	203	GLU	4.9
1	2A	2150	U	4.9
1	1A	2129	C	4.8
7	2H	128	PRO	4.8
32	1a	93	G	4.8
1	2A	2161	C	4.8
32	2a	1029	C	4.8
1	2A	2803	C	4.8
41	1j	98	ILE	4.8
1	1A	1100	A	4.8
21	1Z	196	VAL	4.8
1	1A	2208	G	4.8
1	2A	2136	C	4.8
32	2a	1036	G	4.8
1	1A	934	A	4.8
32	2a	1030(B)	C	4.8
33	2b	44	LEU	4.8
26	14	52	THR	4.8
33	2b	231	GLU	4.7
1	2A	1054	A	4.7

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Mol	Chain	Res	Type	RSRZ
1	1A	1099	C	4.7
32	1a	1033	G	4.7
1	2A	1057	A	4.7
1	1A	1125	C	4.7
1	1A	2804	C	4.7
32	1a	90	U	4.7
1	2A	2114	A	4.7
1	2A	2801(A)	A	4.7
32	1a	1037	C	4.7
1	2A	2160	G	4.7
1	2A	2171	A	4.7
32	1a	344	A	4.7
33	2b	145	LEU	4.7
1	1A	2815	C	4.7
1	2A	2149	G	4.7
1	1A	1136	U	4.7
33	1b	48	MET	4.7
33	2b	228	GLY	4.7
32	1a	79	G	4.7
8	1I	65	ALA	4.6
1	1A	2159	C	4.6
32	2a	1006	C	4.6
26	24	63	TYR	4.6
34	2c	190	ARG	4.6
40	2i	29	ASN	4.6
22	20	8	GLY	4.6
26	24	27	THR	4.6
1	1A	2187	G	4.6
1	2A	2165	G	4.6
32	1a	70	G	4.6
32	1a	97	G	4.6
32	2a	1024	G	4.6
1	2A	1538	G	4.5
41	1j	72	VAL	4.5
33	2b	49	GLU	4.5
1	1A	1879	A	4.5
1	2A	2167	U	4.5
1	1A	2176	G	4.5
1	2A	2166	G	4.5
16	2U	89	GLU	4.5
26	14	49	PHE	4.5
1	2A	2122	U	4.5

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Mol	Chain	Res	Type	RSRZ
1	1A	2186	C	4.5
1	2A	274	G	4.5
33	1b	188	ALA	4.5
26	24	66	SER	4.5
33	2b	118	LEU	4.5
1	1A	936	C	4.5
1	1A	2210	C	4.5
1	1A	925	A	4.5
32	2a	1007	C	4.5
32	2a	1028	C	4.5
25	23	60	GLU	4.5
41	2j	34	VAL	4.5
41	2j	72	VAL	4.5
21	2Z	197	ILE	4.4
15	1T	38	ASN	4.4
1	1A	1143	U	4.4
1	1A	930	G	4.4
21	2Z	200	GLY	4.4
34	2c	107	GLN	4.4
1	2A	10	G	4.4
32	2a	1021	G	4.4
1	2A	2794	C	4.4
1	1A	2136	A	4.4
1	1A	2189	U	4.4
1	2A	883	G	4.4
32	1a	1003	G	4.4
8	2I	74	ASN	4.4
1	1A	2209	G	4.4
26	14	45	GLY	4.4
26	24	64	GLY	4.4
1	2A	229	A	4.4
32	1a	160	A	4.3
22	10	8	GLY	4.3
1	1A	1140	U	4.3
50	2s	20	LEU	4.3
1	2A	652(B)	A	4.3
21	2Z	191	VAL	4.3
1	1A	2902	G	4.3
40	2i	54	ASP	4.3
33	1b	190	THR	4.3
41	1j	5	ARG	4.3
1	1A	2193	A	4.3

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Mol	Chain	Res	Type	RSRZ
1	2A	1085	A	4.3
1	2A	2178	C	4.3
1	1A	2144	U	4.3
1	2A	2109	U	4.3
32	2a	1004	A	4.3
42	2k	27	ASN	4.2
33	1b	17	PHE	4.2
1	1A	935	C	4.2
38	1g	156	TRP	4.2
1	2A	1914	C	4.2
41	2j	26	ALA	4.2
15	1T	37	GLY	4.2
47	2p	51	VAL	4.2
1	2A	2180	U	4.2
1	1A	2207	C	4.2
21	1Z	200	GLY	4.2
1	1A	2138	G	4.2
1	1A	2199	C	4.2
34	1c	194	GLY	4.2
32	1a	1257	U	4.2
39	1h	117	GLY	4.1
1	2A	2135	A	4.1
33	2b	123	ALA	4.1
32	2a	1531	A	4.1
32	2a	79	G	4.1
1	2A	11	G	4.1
32	2a	1035	A	4.1
44	1m	56	LEU	4.1
1	2A	1450	G	4.1
40	2i	30	GLY	4.1
42	2k	90	GLY	4.1
1	1A	2192	A	4.1
1	2A	1528	A	4.1
32	1a	1035	A	4.1
1	2A	2896	C	4.1
32	1a	1137	C	4.1
1	1A	1218	G	4.1
1	1A	2803	A	4.1
1	2A	1103	A	4.1
1	2A	890	A	4.1
32	2a	77	G	4.1
1	1A	1219	A	4.0

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Mol	Chain	Res	Type	RSRZ
32	1a	1447	A	4.0
1	1A	1905	G	4.0
32	1a	71	C	4.0
34	1c	193	TYR	4.0
1	2A	877	U	4.0
8	2I	63	ALA	4.0
33	1b	233	SER	4.0
1	1A	2206	G	4.0
38	2g	154	TYR	4.0
1	2A	1467	C	4.0
1	2A	2143	C	4.0
1	2A	2175	C	4.0
33	2b	12	GLU	4.0
33	2b	18	GLY	4.0
1	2A	1449	A	4.0
1	1A	2200	C	4.0
44	2m	66	LEU	4.0
32	1a	1140	C	4.0
33	1b	231	GLU	4.0
1	1A	1554	A	4.0
32	1a	1001	A	4.0
1	2A	2145	C	4.0
7	2H	126	PRO	4.0
40	1i	81	ILE	4.0
34	1c	81	GLY	4.0
1	2A	886	C	4.0
1	1A	938	G	4.0
1	1A	2203	G	4.0
1	2A	1087	G	4.0
34	2c	189	ALA	4.0
1	1A	1553	A	3.9
1	2A	894	C	3.9
32	2a	76	C	3.9
54	2x	20	U	3.9
32	1a	1532	U	3.9
1	2A	878	A	3.9
32	1a	152	A	3.9
43	2l	62	SER	3.9
32	1a	76	C	3.9
40	2i	90	PRO	3.9
32	1a	69	G	3.9
32	2a	78	G	3.9

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Mol	Chain	Res	Type	RSRZ
54	2x	21	A	3.9
32	1a	345	C	3.9
39	1h	115	SER	3.9
1	2A	875	G	3.9
42	2k	43	SER	3.9
1	1A	302	A	3.9
1	1A	2172	U	3.9
6	2G	41	GLN	3.9
32	2a	1141	C	3.9
47	2p	48	TRP	3.8
43	2l	64	TYR	3.8
1	1A	1152	G	3.8
1	2A	899	A	3.8
38	1g	79	ARG	3.8
40	1i	82	ALA	3.8
1	2A	1102	C	3.8
6	2G	42	GLY	3.8
21	2Z	114	GLY	3.8
40	2i	99	LEU	3.8
39	2h	56	LYS	3.8
2	2B	4	C	3.8
38	2g	4	ARG	3.8
32	2a	1031	G	3.8
38	2g	82	GLY	3.8
43	1l	63	GLY	3.8
41	2j	23	ILE	3.8
32	2a	1008	C	3.8
52	2u	14	TRP	3.8
1	2A	2181	G	3.8
40	2i	88	TYR	3.8
32	1a	702	A	3.8
49	2r	58	LEU	3.8
14	2S	52	SER	3.8
21	1Z	201	LYS	3.8
6	2G	136	ARG	3.8
1	1A	2812	A	3.8
1	2A	2121	G	3.8
32	1a	161	A	3.8
15	2T	126	ALA	3.8
23	2l	83	GLU	3.8
1	1A	697	C	3.7
1	1A	926	G	3.7

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Mol	Chain	Res	Type	RSRZ
1	2A	271(N)	U	3.7
14	2S	58	LEU	3.7
26	24	32	TYR	3.7
34	2c	71	ALA	3.7
1	2A	1086	A	3.7
1	2A	1508	A	3.7
54	2x	48	C	3.7
1	2A	1859	A	3.7
1	2A	892	G	3.7
52	2u	16	GLY	3.7
7	2H	55	PRO	3.7
1	1A	939	C	3.7
32	2a	90	U	3.7
1	1A	2123	G	3.7
32	1a	1138	G	3.7
40	2i	3	GLN	3.7
44	2m	75	ALA	3.7
32	2a	932	C	3.7
54	2x	49	G	3.7
1	2A	1532	C	3.7
21	1Z	195	GLU	3.7
1	1A	1530	G	3.7
1	2A	2804	C	3.6
52	2u	15	ARG	3.6
32	2a	1025	U	3.6
26	24	46	GLN	3.6
38	1g	81	GLY	3.6
32	2a	1022	G	3.6
6	2G	140	ILE	3.6
51	1t	31	SER	3.6
1	1A	11	G	3.6
32	1a	145	G	3.6
1	1A	1142	A	3.6
33	1b	237	ALA	3.6
26	24	39	CYS	3.6
33	1b	229	VAL	3.6
33	2b	202	PRO	3.6
1	1A	386	U	3.6
1	1A	1936	C	3.6
1	2A	271(J)	C	3.6
1	2A	2139	C	3.6
1	2A	2833	G	3.6

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Mol	Chain	Res	Type	RSRZ
38	2g	116	ALA	3.6
44	1m	2	ALA	3.6
43	1l	29	GLY	3.6
1	1A	943	C	3.6
1	1A	2188	G	3.6
26	24	4	GLY	3.6
1	2A	1053	C	3.5
1	2A	2100	G	3.5
1	2A	1084	A	3.5
39	2h	52	ASP	3.5
42	2k	25	TYR	3.5
34	2c	185	GLY	3.5
7	2H	51	ARG	3.5
1	2A	1106	G	3.5
32	2a	73	G	3.5
32	2a	1023	G	3.5
14	2S	54	LEU	3.5
1	1A	269	G	3.5
32	1a	1531	A	3.5
38	1g	85	TYR	3.5
1	2A	1104	C	3.5
6	2G	60	LEU	3.5
49	1r	56	THR	3.5
1	2A	1445	A	3.5
32	2a	1102	A	3.5
32	2a	1019	C	3.5
50	2s	35	SER	3.5
33	2b	122	PHE	3.5
40	2i	18	PHE	3.5
1	1A	1144	A	3.5
1	1A	1221	G	3.5
32	1a	1007	C	3.5
32	2a	1130	A	3.5
45	2n	10	ALA	3.5
17	2V	26	ASP	3.5
1	1A	931	C	3.5
33	2b	229	VAL	3.5
1	1A	937	A	3.5
1	2A	1541	G	3.5
1	2A	2188	C	3.5
33	2b	31	TYR	3.5
1	1A	2814	C	3.5

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Mol	Chain	Res	Type	RSRZ
32	1a	1021	G	3.5
35	2d	44	GLY	3.4
42	2k	44	SER	3.4
52	2u	2	GLY	3.4
33	2b	16	HIS	3.4
41	2j	6	ILE	3.4
42	2k	29	ILE	3.4
1	2A	645	C	3.4
1	2A	901	A	3.4
1	2A	879	G	3.4
32	1a	144	G	3.4
26	24	40	HIS	3.4
35	2d	38	TYR	3.4
44	1m	51	ALA	3.4
40	2i	26	VAL	3.4
1	1A	940	C	3.4
1	1A	1935	A	3.4
7	2H	94	TYR	3.4
52	2u	10	ARG	3.4
33	2b	92	TYR	3.4
34	1c	80	GLY	3.4
1	2A	1507	A	3.4
35	2d	43	HIS	3.4
33	1b	21	ARG	3.4
34	2c	105	GLU	3.4
8	2I	61	ARG	3.4
26	24	5	ILE	3.4
45	2n	34	TYR	3.4
1	1A	10	G	3.4
32	1a	98	G	3.4
1	2A	2146	C	3.4
2	2B	3	C	3.4
8	2I	57	ARG	3.4
32	2a	1262	C	3.4
40	2i	7	THR	3.4
8	1I	61	ARG	3.4
44	1m	22	ILE	3.4
26	24	36	CYS	3.4
54	2x	59	A	3.3
40	2i	102	LEU	3.3
50	2s	24	ALA	3.3
32	1a	72	C	3.3

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Mol	Chain	Res	Type	RSRZ
1	2A	1082	U	3.3
42	2k	42	TRP	3.3
44	1m	50	GLU	3.3
34	2c	160	ALA	3.3
40	2i	53	VAL	3.3
7	2H	61	HIS	3.3
1	2A	317	G	3.3
7	2H	124	GLU	3.3
34	2c	196	LEU	3.3
43	1l	52	LEU	3.3
1	1A	1938	A	3.3
1	2A	278	A	3.3
26	14	50	VAL	3.3
54	2x	16	C	3.3
32	1a	73	G	3.3
1	1A	941	U	3.3
1	2A	2897	U	3.3
33	2b	42	ILE	3.3
45	2n	55	GLY	3.3
34	2c	72	LYS	3.3
38	1g	4	ARG	3.3
33	1b	19	HIS	3.3
49	2r	46	GLU	3.3
32	2a	1043	C	3.3
1	2A	2115	G	3.3
1	2A	2894	G	3.3
32	2a	97	G	3.3
34	1c	72	LYS	3.3
49	2r	47	THR	3.3
33	1b	230	VAL	3.3
1	2A	1096	A	3.3
32	2a	88	A	3.3
32	2a	1030(C)	G	3.3
1	2A	1046	A	3.3
1	2A	1073	A	3.3
32	2a	1044	A	3.3
7	2H	97	ARG	3.3
1	2A	2189	U	3.3
26	24	43	TYR	3.3
6	2G	150	ASP	3.3
2	2B	117	G	3.3
33	1b	129	GLU	3.2

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Mol	Chain	Res	Type	RSRZ
1	1A	2905	C	3.2
1	2A	652(V)	C	3.2
1	2A	897	C	3.2
45	2n	8	GLU	3.2
1	1A	2903	G	3.2
6	2G	56	ALA	3.2
2	2B	2	C	3.2
32	1a	1004	A	3.2
35	2d	33	MET	3.2
42	1k	57	THR	3.2
34	2c	108	ASN	3.2
1	1A	2174	G	3.2
1	2A	652(T)	C	3.2
32	2a	1261	A	3.2
32	2a	1287	A	3.2
44	1m	4	ILE	3.2
41	2j	27	ALA	3.2
1	1A	1145	G	3.2
1	1A	2162	C	3.2
1	2A	1527	G	3.2
26	24	7	PRO	3.2
32	1a	1030(C)	G	3.2
45	1n	7	ILE	3.2
1	1A	1551	C	3.2
38	2g	5	ARG	3.2
1	1A	2813	G	3.2
40	2i	91	ASP	3.2
32	1a	204	U	3.2
45	2n	25	VAL	3.2
41	1j	97	GLU	3.2
1	1A	1153	G	3.2
32	2a	1001	A	3.2
32	2a	1392	G	3.2
23	11	84	GLY	3.2
40	2i	31	GLN	3.2
41	2j	84	GLN	3.2
1	1A	1147	U	3.2
42	2k	28	THR	3.2
1	2A	1069	A	3.2
23	11	26	ARG	3.2
26	24	10	VAL	3.2
32	1a	1009	G	3.2

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Mol	Chain	Res	Type	RSRZ
32	1a	1493	A	3.2
44	2m	42	ALA	3.2
35	2d	23	GLY	3.2
25	23	2	PRO	3.2
1	1A	696	C	3.2
1	2A	318	C	3.2
26	14	17	GLY	3.1
32	2a	1030(D)	A	3.1
32	2a	1447	A	3.1
34	2c	145	GLY	3.1
1	1A	1217	G	3.1
1	2A	1059	G	3.1
21	1Z	198	LYS	3.1
32	1a	154	C	3.1
40	2i	4	TYR	3.1
33	1b	210	SER	3.1
26	24	55	ARG	3.1
21	1Z	70	LEU	3.1
35	2d	12	CYS	3.1
1	1A	2143	G	3.1
1	2A	652(C)	G	3.1
1	2A	2104	G	3.1
32	2a	1257	U	3.1
38	1g	82	GLY	3.1
42	1k	56	GLY	3.1
45	1n	22	THR	3.1
37	2f	93	SER	3.1
1	2A	900	A	3.1
1	2A	2892	A	3.1
51	2t	100	ILE	3.1
32	1a	1446	U	3.1
54	2x	9	G	3.1
1	2A	885	C	3.1
7	2H	98	LEU	3.1
6	2G	146	TYR	3.1
9	2N	9	VAL	3.1
32	2a	1286	A	3.1
32	1a	841	U	3.1
33	1b	29	ALA	3.1
33	2b	136	VAL	3.1
33	2b	9	GLU	3.1
1	2A	874	G	3.1

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Mol	Chain	Res	Type	RSRZ
1	2A	1093	G	3.1
32	1a	153	C	3.1
32	1a	189(A)	C	3.1
41	2j	87	THR	3.1
26	24	17	GLY	3.1
26	24	35	VAL	3.1
1	1A	2164	C	3.1
1	2A	280	C	3.1
1	2A	1109	C	3.1
32	2a	1249	C	3.1
1	1A	273	G	3.1
1	1A	387	G	3.1
1	2A	275	G	3.1
21	2Z	2	GLU	3.1
41	1j	31	GLY	3.1
40	1i	15	ALA	3.1
40	2i	95	LYS	3.1
1	2A	876	C	3.1
2	1B	3	C	3.1
32	1a	189(B)	C	3.1
5	2F	14	PRO	3.1
33	2b	14	GLY	3.1
45	2n	7	ILE	3.1
33	2b	124	SER	3.0
48	2q	16	GLN	3.1
32	1a	202	U	3.0
29	27	48	LYS	3.0
1	1A	1491	A	3.0
1	1A	2161	C	3.0
1	2A	1531	C	3.0
47	1p	17	TYR	3.0
47	2p	46	PRO	3.0
1	1A	1513	G	3.0
1	2A	2190	G	3.0
7	2H	96	ALA	3.0
14	2S	35	ILE	3.0
39	2h	116	LYS	3.0
7	2H	44	VAL	3.0
45	2n	27	CYS	3.0
1	1A	2175	G	3.0
21	1Z	33	LEU	3.0
23	11	27	GLU	3.0

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Mol	Chain	Res	Type	RSRZ
26	24	57	GLU	3.0
49	2r	62	GLU	3.0
1	1A	2901	A	3.0
17	2V	47	VAL	3.0
44	1m	23	TYR	3.0
7	2H	42	ARG	3.0
26	14	59	PHE	3.0
32	2a	142	G	3.0
44	2m	16	ASP	3.0
33	2b	144	ARG	3.0
38	2g	156	TRP	3.0
1	1A	303	C	3.0
1	2A	1509(A)	A	3.0
1	2A	2860	A	3.0
23	11	54	ALA	3.0
32	1a	1503	A	3.0
1	2A	2893	G	3.0
32	1a	725	G	3.0
32	2a	189	G	3.0
32	2a	1532	U	3.0
1	2A	2629	A	3.0
49	2r	55	ARG	3.0
1	2A	354	G	3.0
6	2G	90	LEU	3.0
26	24	42	PHE	3.0
33	1b	28	PHE	3.0
1	2A	902	C	3.0
32	1a	457	C	3.0
35	2d	158	ILE	3.0
44	1m	25	ILE	3.0
37	2f	95	GLU	3.0
41	1j	18	ALA	3.0
33	1b	227	GLY	3.0
33	2b	47	THR	3.0
1	1A	945	A	3.0
33	2b	41	ILE	3.0
44	2m	51	ALA	2.9
32	1a	1008	C	2.9
36	1e	38	GLN	2.9
21	2Z	96	VAL	2.9
41	1j	34	VAL	2.9
44	1m	24	GLY	2.9

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Mol	Chain	Res	Type	RSRZ
32	1a	1163	C	2.9
32	2a	71	C	2.9
32	2a	532	A	2.9
35	2d	36	ARG	2.9
33	1b	207	ALA	2.9
21	2Z	195	GLU	2.9
24	22	46	GLN	2.9
1	2A	2177	C	2.9
20	2Y	2	ARG	2.9
32	2a	155	C	2.9
33	2b	39	ILE	2.9
43	1l	62	SER	2.9
1	2A	2191	G	2.9
2	2B	118	G	2.9
1	1A	2641	A	2.9
1	1A	924	U	2.9
35	2d	37	PRO	2.9
26	24	65	ASP	2.9
41	1j	73	ASP	2.9
2	1B	2	C	2.9
25	23	59	VAL	2.9
6	2G	139	LEU	2.9
38	1g	57	GLU	2.9
1	1A	2137	G	2.9
1	2A	1090	U	2.9
32	2a	80	G	2.9
35	1d	166	LYS	2.9
47	2p	76	GLN	2.9
34	2c	126	ARG	2.9
32	2a	92	C	2.9
32	2a	1129	C	2.9
40	1i	33	PHE	2.9
1	2A	1465	G	2.9
32	1a	1143	G	2.9
1	2A	1100	C	2.9
1	2A	271(K)	U	2.9
32	2a	202	U	2.9
1	1A	698	G	2.9
21	2Z	196	VAL	2.9
35	2d	6	GLY	2.9
41	2j	25	GLU	2.9
50	2s	43	GLU	2.9

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Mol	Chain	Res	Type	RSRZ
7	2H	103	LEU	2.9
21	2Z	4	ARG	2.9
33	2b	120	ALA	2.9
33	2b	216	SER	2.9
49	1r	53	ARG	2.9
1	1A	2167	C	2.9
1	2A	1166	C	2.9
32	2a	1096	C	2.9
1	2A	1105	U	2.9
1	1A	1898	A	2.9
35	2d	90	GLY	2.9
1	1A	1512	G	2.9
1	2A	2116	G	2.9
6	2G	43	LEU	2.9
32	1a	1144	G	2.9
44	2m	14	ARG	2.9
1	2A	362	U	2.8
1	2A	1866	C	2.8
34	2c	74	GLY	2.8
38	2g	28	ASN	2.8
1	2A	1885	A	2.8
6	2G	69	ALA	2.8
33	2b	121	LEU	2.8
1	1A	691	G	2.8
32	1a	993	G	2.8
40	2i	64	THR	2.8
7	2H	48	GLY	2.8
10	2O	57	VAL	2.8
33	1b	109	SER	2.8
32	1a	651	C	2.8
32	2a	144	G	2.8
32	2a	1131	G	2.8
33	2b	19	HIS	2.8
36	1e	118	ILE	2.8
21	2Z	198	LYS	2.8
1	1A	700	A	2.8
1	2A	1486	A	2.8
1	2A	1876	A	2.8
5	1F	15	SER	2.8
38	2g	3	ARG	2.8
17	2V	42	GLY	2.8
1	1A	385	G	2.8

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Mol	Chain	Res	Type	RSRZ
1	2A	652(E)	G	2.8
1	2A	1719	G	2.8
32	2a	1144	G	2.8
32	2a	1202	G	2.8
41	2j	24	VAL	2.8
38	2g	6	ARG	2.8
1	1A	1466	U	2.8
1	2A	1108	U	2.8
54	2x	47	U	2.8
23	11	55	GLY	2.8
7	2H	123	PHE	2.8
33	2b	37	ASN	2.8
54	2x	64	G	2.8
49	1r	21	LYS	2.8
33	2b	43	ASP	2.8
1	2A	1450(A)	C	2.8
32	2a	1097	C	2.8
35	2d	13	ARG	2.8
1	1A	2122	G	2.8
36	1e	114	GLY	2.8
47	2p	9	PHE	2.8
33	1b	79	ASP	2.8
7	2H	105	LEU	2.8
32	2a	270	A	2.8
32	2a	995	C	2.8
33	2b	45	GLN	2.8
41	1j	27	ALA	2.8
1	1A	272	U	2.8
1	2A	1470	G	2.8
1	2A	2862	G	2.8
32	2a	1084	G	2.8
47	1p	19	ILE	2.8
34	2c	198	VAL	2.8
1	2A	271(M)	G	2.7
18	2W	63	ASP	2.7
21	2Z	175	VAL	2.7
34	2c	49	SER	2.7
40	2i	52	ALA	2.7
49	2r	60	ALA	2.7
32	2a	1038	C	2.7
32	1a	393	A	2.7
49	2r	61	LYS	2.7

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Mol	Chain	Res	Type	RSRZ
33	2b	201	ILE	2.7
49	2r	29	PHE	2.7
1	1A	929	G	2.7
33	2b	133	LYS	2.7
1	2A	1505	C	2.7
32	1a	203	U	2.7
8	2I	58	LEU	2.7
26	14	48	ARG	2.7
52	2u	6	ARG	2.7
1	2A	1107	G	2.7
32	2a	1133	G	2.7
32	2a	1380	U	2.7
32	2a	1390	U	2.7
1	2A	1913	A	2.7
26	24	51	ASP	2.7
40	1i	47	LEU	2.7
44	2m	70	LEU	2.7
1	1A	1896	G	2.7
1	1A	2211	U	2.7
1	2A	652(U)	G	2.7
32	2a	1143	G	2.7
32	1a	1039	C	2.7
32	1a	1043	C	2.7
50	2s	32	LYS	2.7
32	2a	1268	A	2.7
49	2r	22	VAL	2.7
44	1m	26	GLY	2.7
40	1i	62	TYR	2.7
43	1l	64	TYR	2.7
34	2c	124	ILE	2.7
1	1A	1897	C	2.7
1	2A	272(J)	C	2.7
1	2A	1546	C	2.7
1	2A	1098	A	2.7
32	2a	1126	U	2.7
35	1d	25	ARG	2.7
38	2g	78	ARG	2.7
40	2i	63	ILE	2.7
32	1a	1038	C	2.7
41	2j	85	LEU	2.7
1	1A	1531	G	2.7
1	2A	2187	G	2.7

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Mol	Chain	Res	Type	RSRZ
5	1F	16	GLY	2.7
8	2I	53	ALA	2.7
1	2A	887	A	2.7
7	2H	58	GLU	2.7
8	2I	54	GLN	2.7
45	2n	22	THR	2.7
11	1P	143	GLY	2.7
32	1a	932	C	2.7
26	24	68	ARG	2.7
32	2a	540	G	2.7
32	2a	1442	G	2.7
32	2a	1446	U	2.6
6	2G	108	ASN	2.6
33	1b	135	GLN	2.6
34	2c	191	THR	2.6
32	2a	154	C	2.6
32	2a	1037	C	2.6
1	2A	1485	G	2.6
1	2A	271(L)	U	2.6
4	2E	87	GLU	2.6
32	2a	427	U	2.6
32	2a	841	U	2.6
32	2a	1503	A	2.6
34	2c	184	TYR	2.6
15	2T	39	ARG	2.6
38	1g	3	ARG	2.6
1	2A	1893	C	2.6
36	2e	94	ALA	2.6
6	2G	55	LYS	2.6
26	24	59	PHE	2.6
1	2A	1060	U	2.6
32	2a	1170	A	2.6
34	2c	159	GLY	2.6
44	1m	54	VAL	2.6
21	2Z	95	PRO	2.6
21	2Z	176	PRO	2.6
40	2i	27	THR	2.6
38	2g	2	ALA	2.6
42	1k	60	ALA	2.6
32	1a	1006	C	2.6
6	2G	39	ILE	2.6
32	1a	96	U	2.6

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Mol	Chain	Res	Type	RSRZ
1	2A	271(I)	G	2.6
32	2a	145	G	2.6
34	2c	109	PRO	2.6
40	2i	98	PRO	2.6
1	2A	2140	C	2.6
6	2G	58	GLN	2.6
50	2s	29	ARG	2.6
49	2r	51	LEU	2.6
17	2V	22	VAL	2.6
26	14	54	GLY	2.6
49	1r	24	ALA	2.6
1	1A	389	G	2.6
1	1A	1115	A	2.6
1	2A	653	A	2.6
1	1A	1552	C	2.6
1	2A	1584	C	2.6
32	2a	1045	C	2.6
50	2s	28	LYS	2.6
40	1i	8	GLY	2.6
25	23	58	VAL	2.6
26	14	51	ASP	2.6
44	2m	67	GLU	2.6
40	2i	94	ALA	2.6
1	1A	1588	G	2.6
1	2A	882	G	2.6
32	1a	1005	A	2.6
32	2a	1094	G	2.6
23	21	2	SER	2.6
33	1b	105	PHE	2.6
41	1j	29	ARG	2.6
1	1A	942	A	2.6
32	2a	1236	A	2.6
1	2A	893	C	2.6
1	2A	1504	C	2.6
32	2a	1442(A)	G	2.6
33	2b	113	HIS	2.6
45	2n	38	GLY	2.6
54	2x	15	G	2.6
33	2b	165	VAL	2.6
51	2t	6	PRO	2.6
41	2j	98	ILE	2.5
1	1A	1106	U	2.5

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Mol	Chain	Res	Type	RSRZ
34	1c	87	LEU	2.5
47	1p	37	GLY	2.5
1	1A	2125	C	2.5
1	2A	2184	G	2.5
32	2a	485	G	2.5
54	1x	46	G	2.5
34	2c	194	GLY	2.5
41	2j	74	ILE	2.5
11	2P	123	LEU	2.5
1	1A	2135	U	2.5
33	2b	140	HIS	2.5
35	2d	8	VAL	2.5
1	2A	1080	C	2.5
1	2A	361	G	2.5
1	2A	1110	G	2.5
50	2s	50	ALA	2.5
8	1I	131	LYS	2.5
7	2H	101	ARG	2.5
40	2i	20	ARG	2.5
32	1a	189(K)	U	2.5
32	1a	1121	U	2.5
1	1A	1550	C	2.5
1	1A	1591	A	2.5
40	2i	36	TYR	2.5
1	2A	1539	G	2.5
6	2G	40	ASN	2.5
33	2b	152	PHE	2.5
1	2A	1895	C	2.5
32	2a	848	C	2.5
45	1n	8	GLU	2.5
39	2h	29	SER	2.5
41	2j	29	ARG	2.5
6	2G	19	LEU	2.5
41	1j	85	LEU	2.5
32	2a	204	U	2.5
32	2a	1142	G	2.5
33	2b	83	MET	2.5
34	2c	106	VAL	2.5
16	2U	78	THR	2.5
20	2Y	89	PHE	2.5
41	2j	47	PHE	2.5
6	2G	57	ALA	2.5

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Mol	Chain	Res	Type	RSRZ
45	2n	29	ARG	2.5
51	2t	89	ARG	2.5
14	2S	56	LEU	2.5
23	11	85	LEU	2.5
32	2a	141	A	2.5
47	2p	74	LEU	2.5
6	2G	155	MET	2.5
9	1N	140	VAL	2.5
16	2U	90	VAL	2.5
1	1A	1494	G	2.5
1	2A	1089	G	2.5
28	26	50	ARG	2.5
35	2d	159	ARG	2.5
34	2c	100	ALA	2.5
39	2h	55	GLY	2.5
1	2A	652(D)	C	2.5
32	1a	1141	C	2.5
54	2x	65	C	2.5
1	1A	2904	U	2.5
35	1d	170	VAL	2.5
40	2i	28	VAL	2.5
38	2g	79	ARG	2.5
51	2t	93	GLU	2.5
1	2A	1042	G	2.5
1	2A	1525	G	2.5
50	2s	26	GLY	2.5
40	2i	92	TYR	2.5
33	2b	10	LEU	2.5
41	2j	8	LEU	2.5
50	2s	30	LEU	2.5
7	2H	30	LYS	2.5
33	1b	18	GLY	2.5
1	1A	1572	G	2.5
33	2b	115	LEU	2.5
41	2j	38	ILE	2.5
8	1I	19	VAL	2.4
1	1A	1507	A	2.4
33	2b	132	LYS	2.4
33	2b	38	GLY	2.4
26	24	48	ARG	2.4
34	2c	157	ILE	2.4
34	2c	188	LEU	2.4

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Mol	Chain	Res	Type	RSRZ
32	1a	183	G	2.4
32	2a	1088	G	2.4
1	1A	1146	C	2.4
8	2I	47	LEU	2.4
33	2b	138	LEU	2.4
33	2b	142	LEU	2.4
1	1A	274	U	2.4
7	2H	45	VAL	2.4
33	1b	15	VAL	2.4
1	2A	1040	C	2.4
1	2A	2101	G	2.4
26	24	54	GLY	2.4
12	2Q	59	ARG	2.4
22	20	11	ARG	2.4
23	21	78	LYS	2.4
23	11	28	GLY	2.4
32	1a	419	C	2.4
32	1a	68	G	2.4
33	1b	143	GLU	2.4
33	2b	207	ALA	2.4
34	2c	122	GLU	2.4
41	1j	20	ALA	2.4
23	21	82	LEU	2.4
36	2e	109	ILE	2.4
35	2d	10	ARG	2.4
43	1l	112	ASP	2.4
1	2A	1049	C	2.4
15	2T	131	ALA	2.4
34	2c	65	ALA	2.4
43	1l	51	ALA	2.4
45	1n	2	ALA	2.4
1	2A	1466	G	2.4
32	1a	146	G	2.4
21	2Z	177	PRO	2.4
14	2S	22	GLY	2.4
38	1g	78	ARG	2.4
54	2x	17	C	2.4
1	2A	1112	G	2.4
11	2P	121	LYS	2.4
32	1a	1022	G	2.4
32	2a	93	G	2.4
38	2g	14	PRO	2.4

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Mol	Chain	Res	Type	RSRZ
49	1r	22	VAL	2.4
6	2G	64	THR	2.4
2	2B	58	A	2.4
32	2a	994	A	2.4
40	2i	124	GLN	2.4
42	1k	81	ASP	2.4
1	2A	1179	C	2.4
20	2Y	96	ILE	2.4
32	1a	163	C	2.4
36	2e	76	ILE	2.4
33	1b	16	HIS	2.4
1	2A	1529	G	2.4
42	1k	28	THR	2.4
1	2A	1469	A	2.4
1	2A	1848	A	2.4
1	2A	1916	A	2.4
33	2b	24	TRP	2.4
33	2b	235	SER	2.4
50	2s	23	ASN	2.4
33	1b	44	LEU	2.4
2	2B	62	C	2.4
11	2P	119	GLU	2.3
38	1g	55	GLY	2.3
41	2j	97	GLU	2.3
40	2i	123	PRO	2.3
1	1A	271	U	2.3
1	2A	9	U	2.3
47	1p	76	GLN	2.3
1	1A	927	G	2.3
1	1A	1529	G	2.3
1	2A	2859	G	2.3
2	2B	63	G	2.3
32	1a	1120	G	2.3
18	2W	60	ASN	2.3
1	2A	1077	A	2.3
1	2A	1877	A	2.3
32	2a	1442(B)	A	2.3
42	1k	98	LEU	2.3
7	2H	111	HIS	2.3
32	1a	1263	C	2.3
7	2H	50	VAL	2.3
37	2f	90	VAL	2.3

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Mol	Chain	Res	Type	RSRZ
44	1m	15	VAL	2.3
6	2G	49	ASP	2.3
45	2n	11	LYS	2.3
7	2H	129	THR	2.3
33	2b	13	ALA	2.3
41	2j	20	ALA	2.3
11	1P	135	LEU	2.3
14	2S	33	LYS	2.3
40	1i	83	ARG	2.3
50	1s	50	ALA	2.3
21	2Z	70	LEU	2.3
27	25	59	GLU	2.3
35	2d	163	GLU	2.3
37	2f	38	GLU	2.3
32	1a	1142	G	2.3
32	2a	1294	G	2.3
43	1l	43	VAL	2.3
32	2a	962	C	2.3
32	2a	952	U	2.3
41	2j	37	PRO	2.3
33	2b	143	GLU	2.3
40	2i	19	LEU	2.3
1	1A	699	C	2.3
1	2A	1544	A	2.3
1	2A	1884	A	2.3
32	1a	1133	G	2.3
32	2a	460	G	2.3
32	2a	1385	G	2.3
6	2G	2	PRO	2.3
32	1a	921	U	2.3
26	24	28	LYS	2.3
27	25	60	VAL	2.3
1	2A	2895	U	2.3
1	1A	928	G	2.3
1	2A	1062	G	2.3
2	2B	5	C	2.3
35	2d	26	CYS	2.3
8	2I	88	ILE	2.3
40	1i	79	LEU	2.3
45	2n	2	ALA	2.3
11	1P	118	GLY	2.3
50	2s	82	GLY	2.3

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Mol	Chain	Res	Type	RSRZ
50	2s	27	GLU	2.3
14	2S	34	HIS	2.3
32	1a	591	U	2.3
36	1e	117	ASP	2.3
54	2x	50	U	2.3
1	1A	1595	C	2.3
7	2H	54	ARG	2.3
32	1a	188	C	2.3
32	2a	1275	A	2.3
33	2b	33	TYR	2.3
1	2A	355	G	2.3
32	1a	156	G	2.3
32	1a	1274	G	2.3
34	2c	2	GLY	2.3
40	1i	78	LYS	2.3
42	1k	53	SER	2.3
6	2G	29	TRP	2.3
40	2i	16	ARG	2.3
1	1A	270	C	2.3
1	2A	1894	C	2.3
34	1c	78	GLY	2.3
46	2o	80	ALA	2.3
1	2A	654	A	2.3
32	1a	270	A	2.3
32	1a	1046	A	2.3
1	2A	1044	G	2.3
32	2a	1164	G	2.3
36	2e	75	THR	2.2
42	2k	31	THR	2.2
38	2g	115	ARG	2.2
1	1A	1154	U	2.2
42	2k	89	ALA	2.2
1	1A	1514	C	2.2
1	1A	1904	C	2.2
32	1a	417	C	2.2
32	1a	1533	C	2.2
21	1Z	126	VAL	2.2
32	2a	1492	A	2.2
2	2B	107	G	2.2
32	2a	70	G	2.2
5	1F	14	PRO	2.2
8	1I	12	LEU	2.2

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Mol	Chain	Res	Type	RSRZ
11	2P	116	GLY	2.2
21	2Z	125	LEU	2.2
25	23	42	ALA	2.2
1	1A	388	A	2.2
1	1A	1467	G	2.2
21	2Z	155	LEU	2.2
32	1a	1082	G	2.2
32	2a	69	G	2.2
32	2a	216	G	2.2
32	2a	447	G	2.2
32	2a	1258	G	2.2
34	2c	158	GLY	2.2
33	2b	214	ILE	2.2
6	2G	115	ARG	2.2
33	1b	130	ARG	2.2
32	2a	1263	C	2.2
54	2x	61	C	2.2
1	2A	1460	A	2.2
32	2a	640	A	2.2
19	2X	92	LEU	2.2
23	21	79	GLY	2.2
33	1b	126	GLU	2.2
34	1c	196	LEU	2.2
40	1i	50	LEU	2.2
35	2d	4	TYR	2.2
1	1A	304	C	2.2
17	2V	5	VAL	2.2
21	2Z	56	VAL	2.2
32	1a	155	C	2.2
32	2a	1395	C	2.2
1	2A	284	U	2.2
6	2G	147	ASP	2.2
1	2A	1220	A	2.2
36	1e	112	LEU	2.2
41	2j	73	ASP	2.2
15	2T	42	ILE	2.2
32	2a	996	A	2.2
33	1b	214	ILE	2.2
40	1i	52	ALA	2.2
38	1g	53	LYS	2.2
49	2r	21	LYS	2.2
52	2u	23	PRO	2.2

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Mol	Chain	Res	Type	RSRZ
1	2A	281	G	2.2
1	1A	692	C	2.2
23	11	89	GLU	2.2
38	2g	19	GLY	2.2
1	2A	1113	U	2.2
7	2H	102	ALA	2.2
33	2b	28	PHE	2.2
33	2b	127	ILE	2.2
44	2m	49	THR	2.2
32	1a	162	A	2.2
1	2A	271(H)	G	2.2
7	2H	100	GLY	2.2
32	1a	471	G	2.2
32	2a	1173	G	2.2
38	2g	114	ARG	2.2
48	1q	14	LYS	2.2
41	2j	89	ASP	2.2
2	2B	1	U	2.2
17	1V	27	ALA	2.2
34	1c	154	SER	2.2
41	1j	35	SER	2.2
32	2a	1248	A	2.2
6	2G	70	VAL	2.2
20	2Y	93	GLY	2.2
37	1f	36	ARG	2.2
32	2a	1011	G	2.2
32	2a	1085	U	2.2
32	2a	1266	G	2.2
54	2x	60	U	2.2
8	2I	71	ILE	2.2
47	1p	61	SER	2.2
7	2H	130	ARG	2.2
42	1k	92	GLU	2.2
1	1A	1906	A	2.2
1	2A	289	A	2.2
26	24	50	VAL	2.2
35	1d	138	TYR	2.2
38	1g	80	VAL	2.2
44	2m	17	VAL	2.2
47	2p	49	LEU	2.1
1	1A	1511	C	2.1
1	2A	1065	U	2.1

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Mol	Chain	Res	Type	RSRZ
21	2Z	146	ILE	2.1
32	1a	443	C	2.1
32	1a	999	C	2.1
32	2a	89	C	2.1
33	1b	211	ILE	2.1
33	1b	222	ILE	2.1
54	1x	20	U	2.1
1	1A	694	G	2.1
1	2A	1063	G	2.1
34	2c	192	THR	2.1
36	2e	16	THR	2.1
11	2P	24	GLY	2.1
14	2S	108	GLY	2.1
35	1d	4	TYR	2.1
21	2Z	93	ASP	2.1
8	1I	63	ALA	2.1
21	2Z	133	ILE	2.1
32	1a	178	C	2.1
40	1i	128	ARG	2.1
1	1A	391	G	2.1
1	1A	1495	G	2.1
32	2a	1300	G	2.1
7	2H	125	VAL	2.1
33	2b	230	VAL	2.1
43	1l	44	THR	2.1
43	2l	63	GLY	2.1
40	1i	4	TYR	2.1
28	26	37	ARG	2.1
33	2b	111	ARG	2.1
39	2h	28	ALA	2.1
42	2k	92	GLU	2.1
51	1t	75	ASN	2.1
1	1A	923	C	2.1
7	2H	8	PRO	2.1
8	2I	134	PRO	2.1
41	1j	77	PRO	2.1
40	1i	80	GLY	2.1
1	1A	1105	G	2.1
1	2A	1114	G	2.1
1	2A	1170	G	2.1
1	2A	1747(A)	G	2.1
32	1a	540	G	2.1

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Mol	Chain	Res	Type	RSRZ
1	2A	895	U	2.1
8	1I	64	GLU	2.1
32	2a	1091	U	2.1
1	2A	884	C	2.1
32	2a	153	C	2.1
32	2a	840	C	2.1
34	2c	51	GLY	2.1
1	1A	2843	G	2.1
1	2A	1484	G	2.1
32	1a	189	G	2.1
33	2b	141	GLU	2.1
47	1p	54	GLU	2.1
16	2U	88	ILE	2.1
32	2a	1391	U	2.1
21	2Z	199	LYS	2.1
32	1a	472	A	2.1
32	1a	532	A	2.1
49	1r	57	GLY	2.1
50	2s	53	ASN	2.1
33	2b	234	PRO	2.1
35	1d	37	PRO	2.1
1	2A	2879	C	2.1
32	2a	217	C	2.1
32	2a	271	C	2.1
14	2S	75	GLU	2.1
36	1e	43	LEU	2.1
44	1m	19	LEU	2.1
40	2i	125	TYR	2.1
41	1j	17	ASP	2.1
28	26	54	ILE	2.1
32	2a	955	U	2.1
41	1j	75	ILE	2.1
1	1A	1468	G	2.1
1	2A	880	G	2.1
1	2A	1388	G	2.1
1	2A	1526	G	2.1
32	1a	394	G	2.1
32	1a	460	G	2.1
32	2a	630	G	2.1
43	2l	123	LYS	2.1
34	1c	2	GLY	2.1
1	2A	1048	A	2.1

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Mol	Chain	Res	Type	RSRZ
1	2A	1111	A	2.1
1	2A	1490	A	2.1
34	2c	195	VAL	2.1
49	1r	42	ARG	2.1
1	1A	2158	C	2.1
42	1k	42	TRP	2.1
35	2d	89	THR	2.1
32	1a	182	U	2.1
34	2c	187	ALA	2.1
35	1d	41	GLY	2.1
1	1A	693	G	2.1
8	1I	8	PRO	2.1
32	1a	1042	G	2.1
36	2e	105	VAL	2.1
44	2m	7	VAL	2.1
1	2A	6	A	2.1
32	1a	432	A	2.1
32	2a	1018	C	2.1
33	1b	133	LYS	2.1
41	2j	68	HIS	2.1
42	1k	44	SER	2.1
16	2U	76	TYR	2.1
50	2s	80	TYR	2.1
1	2A	1078	U	2.1
49	1r	87	ARG	2.1
35	1d	165	MET	2.1
1	2A	1519	G	2.1
32	1a	1010	G	2.1
32	2a	428	G	2.1
14	2S	73	LEU	2.0
34	1c	43	LEU	2.0
1	1A	944	C	2.0
1	1A	1492	C	2.0
1	2A	272(H)	C	2.0
1	2A	1041	C	2.0
1	2A	1079	C	2.0
32	1a	418	C	2.0
32	2a	590	C	2.0
8	1I	96	ASP	2.0
8	2I	46	ALA	2.0
46	1o	69	TYR	2.0
11	2P	118	GLY	2.0

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Mol	Chain	Res	Type	RSRZ
37	1f	38	GLU	2.0
42	2k	26	ASN	2.0
6	2G	62	LEU	2.0
32	1a	189(L)	G	2.0
32	2a	987	G	2.0
32	2a	998	G	2.0
33	2b	21	ARG	2.0
1	1A	1574	A	2.0
1	1A	1594	C	2.0
1	1A	1899	A	2.0
1	1A	2160	C	2.0
7	2H	110	SER	2.0
1	2A	1542	A	2.0
1	2A	1097	U	2.0
35	1d	32	ALA	2.0
34	1c	82	GLU	2.0
50	2s	52	TYR	2.0
9	2N	140	VAL	2.0
14	2S	49	VAL	2.0
6	2G	142	PRO	2.0
33	2b	101	MET	2.0
40	2i	21	PRO	2.0
22	20	55	ARG	2.0
26	24	6	HIS	2.0
1	1A	1571	G	2.0
1	1A	2165	C	2.0
1	1A	2865	C	2.0
8	2I	34	GLY	2.0
32	1a	219	C	2.0
32	1a	444	C	2.0
32	2a	1136	U	2.0
32	2a	1444	C	2.0
34	2c	112	SER	2.0
42	1k	90	GLY	2.0
1	2A	1088	A	2.0
32	2a	51	A	2.0
7	2H	99	VAL	2.0
8	2I	81	VAL	2.0
21	2Z	128	VAL	2.0
33	1b	221	LEU	2.0
38	2g	41	ARG	2.0
40	1i	90	PRO	2.0

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Mol	Chain	Res	Type	RSRZ
44	1m	55	ARG	2.0
50	1s	30	LEU	2.0
16	2U	80	ILE	2.0
1	1A	12	U	2.0
1	2A	334	C	2.0
32	2a	514	C	2.0
32	2a	1090	U	2.0
32	2a	1260	C	2.0
1	2A	351	G	2.0
1	2A	353	G	2.0
6	2G	160	VAL	2.0
32	1a	933	G	2.0
32	2a	928	G	2.0
54	2x	22	G	2.0
11	2P	122	PRO	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
1	5MU	2A	1915	21/22	0.85	0.42	58,65,81,94	0
32	2MG	2a	1207	24/25	0.87	0.27	58,64,73,77	0
32	PSU	2a	516	20/21	0.88	0.34	58,63,69,71	0
54	PSU	2x	55	20/21	0.88	0.15	54,59,67,69	0
43	0TD	2l	92	10/11	0.89	0.17	50,53,56,61	0
32	2MG	1a	1207	24/25	0.90	0.30	54,58,61,69	0
1	5MU	1A	1937	21/22	0.90	0.45	50,57,72,76	0
54	5MU	2x	54	21/22	0.90	0.19	56,60,63,66	0
1	PSU	1A	1939	20/21	0.90	0.31	34,47,52,52	0
32	M2G	2a	966	25/26	0.91	0.19	48,53,60,61	0
54	4SU	2x	8	20/21	0.91	0.23	51,57,61,61	0
32	5MC	2a	967	21/22	0.91	0.21	52,56,63,69	0
1	PSU	2A	1917	20/21	0.91	0.26	46,58,67,72	0
32	4OC	2a	1402	22/23	0.92	0.24	44,50,53,56	0
32	7MG	2a	527	24/25	0.93	0.17	52,56,62,67	0
32	5MC	1a	1400	21/22	0.93	0.17	39,42,46,48	0
54	PSU	1x	55	20/21	0.93	0.19	37,44,48,52	0
32	PSU	1a	516	20/21	0.93	0.20	39,48,50,50	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
1	OMC	2A	1920	21/22	0.94	0.21	39,46,48,50	0
32	5MC	2a	1404	21/22	0.94	0.18	36,41,44,47	0
32	5MC	2a	1407	21/22	0.94	0.17	35,44,46,47	0
32	M2G	1a	966	25/26	0.94	0.19	34,37,46,48	0
32	5MC	1a	1407	21/22	0.94	0.19	27,31,35,36	0
43	0TD	1l	92	10/11	0.94	0.16	41,43,47,48	0
32	5MC	1a	967	21/22	0.94	0.18	35,43,47,49	0
32	7MG	1a	527	24/25	0.94	0.18	33,38,43,46	0
1	PSU	2A	1911	20/21	0.95	0.25	45,51,57,60	0
32	UR3	2a	1498	21/22	0.95	0.24	39,44,48,51	0
32	MA6	2a	1518	24/25	0.95	0.18	41,45,47,48	0
1	5MC	2A	1962	21/22	0.95	0.19	30,33,36,42	0
54	4SU	1x	8	20/21	0.95	0.15	36,42,44,45	0
1	PSU	2A	2605	20/21	0.95	0.19	22,26,27,27	0
54	5MC	1x	32	21/22	0.95	0.18	36,39,43,49	0
54	5MC	2x	32	21/22	0.95	0.16	46,55,57,59	0
54	5MU	1x	54	21/22	0.95	0.18	43,48,53,60	0
32	5MC	2a	1400	21/22	0.95	0.16	54,59,62,64	0
32	4OC	1a	1402	22/23	0.95	0.20	31,35,37,39	0
32	5MC	1a	1404	21/22	0.95	0.17	27,31,34,45	0
32	MA6	2a	1519	24/25	0.96	0.22	37,43,46,49	0
1	PSU	1A	2617	20/21	0.96	0.19	10,12,14,16	0
1	PSU	1A	1933	20/21	0.96	0.22	31,43,46,49	0
1	5MC	2A	1942	21/22	0.96	0.13	35,37,40,45	0
32	MA6	1a	1518	24/25	0.96	0.19	23,27,28,29	0
1	5MU	1A	1961	21/22	0.97	0.18	12,16,19,21	0
1	5MC	1A	1964	21/22	0.97	0.14	25,29,33,40	0
1	OMG	1A	2263	24/25	0.97	0.18	9,10,12,12	0
1	OMU	1A	2564	21/22	0.97	0.20	14,18,20,21	0
32	UR3	1a	1498	21/22	0.97	0.18	26,29,32,33	0
1	5MU	2A	1939	21/22	0.97	0.15	26,28,30,31	0
1	OMC	1A	1942	21/22	0.97	0.21	26,34,40,42	0
32	MA6	1a	1519	24/25	0.97	0.18	24,28,29,31	0
1	OMG	2A	2251	24/25	0.97	0.18	19,25,27,28	0
1	2MA	2A	2503	23/24	0.97	0.22	18,21,24,27	0
1	OMU	2A	2552	21/22	0.97	0.20	26,27,29,31	0
1	2MA	1A	2515	23/24	0.98	0.18	5,9,11,15	0
1	5MC	1A	1984	21/22	0.98	0.18	19,23,25,30	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(Å ²)	Q<0.9
56	MG	2a	1667	1/1	0.18	0.71	79,79,79,79	0
56	MG	2a	1725	1/1	0.20	0.85	71,71,71,71	0
56	MG	2A	3744	1/1	0.24	0.57	45,45,45,45	0
56	MG	2A	3872	1/1	0.28	0.34	69,69,69,69	0
56	MG	2a	1780	1/1	0.28	0.87	77,77,77,77	0
56	MG	2a	1807	1/1	0.35	0.46	58,58,58,58	0
56	MG	2a	1713	1/1	0.38	0.22	59,59,59,59	0
56	MG	2a	1690	1/1	0.38	0.10	57,57,57,57	0
56	MG	1a	1781	1/1	0.42	0.23	68,68,68,68	0
56	MG	2a	1805	1/1	0.46	0.79	94,94,94,94	0
56	MG	2d	505	1/1	0.47	0.21	73,73,73,73	0
56	MG	2B	3002	1/1	0.49	0.20	60,60,60,60	0
56	MG	2A	3866	1/1	0.49	0.42	84,84,84,84	0
56	MG	2A	3477	1/1	0.49	0.38	62,62,62,62	0
56	MG	1A	8514	1/1	0.51	0.34	48,48,48,48	0
56	MG	2A	3520	1/1	0.52	0.30	74,74,74,74	0
56	MG	2A	3953	1/1	0.52	0.15	37,37,37,37	0
56	MG	2A	3684	1/1	0.52	0.32	68,68,68,68	0
56	MG	2a	1610	1/1	0.52	0.85	63,63,63,63	0
56	MG	2A	3079	1/1	0.52	1.07	61,61,61,61	0
56	MG	1d	506	1/1	0.52	0.17	77,77,77,77	0
56	MG	2a	1716	1/1	0.55	0.32	65,65,65,65	0
56	MG	1A	8628	1/1	0.55	0.22	62,62,62,62	0
56	MG	2x	108	1/1	0.55	0.17	53,53,53,53	0
56	MG	2a	1763	1/1	0.56	0.24	81,81,81,81	0
56	MG	2A	3243	1/1	0.56	0.45	31,31,31,31	0
56	MG	2l	201	1/1	0.56	0.53	65,65,65,65	0
56	MG	2A	3816	1/1	0.56	0.13	62,62,62,62	0
56	MG	2A	3087	1/1	0.57	0.20	54,54,54,54	0
56	MG	2H	8002	1/1	0.57	0.67	79,79,79,79	0
56	MG	1a	1753	1/1	0.57	0.17	54,54,54,54	0
56	MG	2A	3742	1/1	0.57	0.86	35,35,35,35	0
56	MG	1A	8872	1/1	0.57	0.32	59,59,59,59	0
56	MG	2A	3827	1/1	0.58	0.19	66,66,66,66	0
56	MG	2A	3835	1/1	0.58	0.18	40,40,40,40	0
56	MG	2A	3061	1/1	0.59	0.59	68,68,68,68	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
56	MG	2B	3018	1/1	0.59	0.11	57,57,57,57	0
56	MG	2A	3848	1/1	0.60	0.18	63,63,63,63	0
56	MG	2d	504	1/1	0.60	0.35	64,64,64,64	0
56	MG	2A	3720	1/1	0.60	0.31	60,60,60,60	0
56	MG	2B	3024	1/1	0.60	0.21	61,61,61,61	0
56	MG	2a	1722	1/1	0.60	0.08	61,61,61,61	0
56	MG	1a	1639	1/1	0.61	0.20	50,50,50,50	0
56	MG	2A	3252	1/1	0.61	0.34	53,53,53,53	0
56	MG	2A	3317	1/1	0.61	0.18	68,68,68,68	0
56	MG	2A	3201	1/1	0.61	0.29	51,51,51,51	0
56	MG	2P	203	1/1	0.61	0.23	63,63,63,63	0
56	MG	2A	3548	1/1	0.62	0.16	52,52,52,52	0
56	MG	1A	8701	1/1	0.63	0.37	49,49,49,49	0
56	MG	2A	3463	1/1	0.64	0.13	42,42,42,42	0
56	MG	2a	1809	1/1	0.64	0.32	81,81,81,81	0
56	MG	2A	3905	1/1	0.64	0.24	56,56,56,56	0
56	MG	2H	8001	1/1	0.64	0.55	71,71,71,71	0
56	MG	2a	1714	1/1	0.64	0.22	60,60,60,60	0
56	MG	2a	1640	1/1	0.64	0.21	64,64,64,64	0
56	MG	2A	3448	1/1	0.65	0.16	65,65,65,65	0
56	MG	1A	8880	1/1	0.65	0.39	46,46,46,46	0
56	MG	2a	1758	1/1	0.65	0.78	83,83,83,83	0
56	MG	2D	316	1/1	0.65	0.14	47,47,47,47	0
56	MG	2B	3014	1/1	0.65	0.45	66,66,66,66	0
56	MG	2a	1646	1/1	0.65	0.60	48,48,48,48	0
56	MG	1a	1748	1/1	0.66	0.18	65,65,65,65	0
56	MG	1a	1785	1/1	0.66	0.15	74,74,74,74	0
56	MG	2A	3527	1/1	0.66	0.17	42,42,42,42	0
56	MG	2A	3433	1/1	0.66	0.13	43,43,43,43	0
56	MG	2a	1625	1/1	0.66	0.22	63,63,63,63	0
56	MG	2A	3620	1/1	0.66	0.23	61,61,61,61	0
56	MG	2B	3015	1/1	0.66	0.26	59,59,59,59	0
56	MG	1a	1754	1/1	0.66	0.21	59,59,59,59	0
56	MG	2B	3020	1/1	0.66	0.26	54,54,54,54	0
56	MG	2A	3856	1/1	0.66	0.42	53,53,53,53	0
56	MG	1a	1768	1/1	0.66	0.26	53,53,53,53	0
56	MG	2D	317	1/1	0.66	0.36	59,59,59,59	0
56	MG	2A	3833	1/1	0.67	0.24	28,28,28,28	0
56	MG	1P	204	1/1	0.67	0.18	62,62,62,62	0
56	MG	2A	3967	1/1	0.67	0.58	55,55,55,55	0
56	MG	2e	201	1/1	0.67	0.17	56,56,56,56	0
56	MG	2a	1687	1/1	0.67	0.12	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	1a	1707	1/1	0.67	0.14	51,51,51,51	0
56	MG	2a	1635	1/1	0.68	0.69	69,69,69,69	0
56	MG	2B	3019	1/1	0.68	0.09	62,62,62,62	0
56	MG	2A	3536	1/1	0.68	0.13	31,31,31,31	0
56	MG	2A	3699	1/1	0.68	0.43	46,46,46,46	0
56	MG	1A	8317	1/1	0.68	0.09	35,35,35,35	0
56	MG	2a	1740	1/1	0.68	0.15	62,62,62,62	0
56	MG	2a	1742	1/1	0.68	0.22	62,62,62,62	0
56	MG	1A	8468	1/1	0.68	0.14	29,29,29,29	0
56	MG	2a	1701	1/1	0.68	0.20	82,82,82,82	0
56	MG	10	104	1/1	0.69	0.15	41,41,41,41	0
56	MG	2R	201	1/1	0.69	0.27	42,42,42,42	0
56	MG	2A	3885	1/1	0.69	0.17	55,55,55,55	0
56	MG	2a	1676	1/1	0.69	0.17	65,65,65,65	0
56	MG	1a	1729	1/1	0.69	0.18	52,52,52,52	0
56	MG	2a	1783	1/1	0.69	0.11	59,59,59,59	0
56	MG	2A	3425	1/1	0.69	0.19	25,25,25,25	0
56	MG	2a	1786	1/1	0.70	0.14	48,48,48,48	0
56	MG	2a	1734	1/1	0.70	0.11	59,59,59,59	0
56	MG	2A	3849	1/1	0.70	0.22	56,56,56,56	0
56	MG	2A	3685	1/1	0.70	0.15	50,50,50,50	0
56	MG	1a	1789	1/1	0.70	0.30	61,61,61,61	0
56	MG	2a	1759	1/1	0.70	0.36	76,76,76,76	0
56	MG	1A	8413	1/1	0.70	0.17	44,44,44,44	0
56	MG	2A	3434	1/1	0.70	0.13	34,34,34,34	0
56	MG	1A	8370	1/1	0.70	0.17	10,10,10,10	0
56	MG	2A	3326	1/1	0.71	0.21	55,55,55,55	0
56	MG	2a	1767	1/1	0.71	0.37	65,65,65,65	0
56	MG	2a	1769	1/1	0.71	0.30	59,59,59,59	0
56	MG	2a	1677	1/1	0.71	0.12	62,62,62,62	0
56	MG	2G	3002	1/1	0.71	0.16	63,63,63,63	0
56	MG	1P	201	1/1	0.71	0.14	18,18,18,18	0
56	MG	2A	3063	1/1	0.71	0.22	38,38,38,38	0
56	MG	2A	3763	1/1	0.72	0.70	51,51,51,51	0
56	MG	2A	3686	1/1	0.72	0.44	53,53,53,53	0
56	MG	2A	3690	1/1	0.72	0.59	67,67,67,67	0
56	MG	1A	8881	1/1	0.72	0.23	53,53,53,53	0
56	MG	2A	3524	1/1	0.72	0.21	59,59,59,59	0
56	MG	1a	1791	1/1	0.72	0.23	56,56,56,56	0
56	MG	1a	1694	1/1	0.72	0.11	27,27,27,27	0
56	MG	2a	1664	1/1	0.73	0.13	44,44,44,44	0
56	MG	2A	3605	1/1	0.73	0.16	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	8617	1/1	0.73	0.17	43,43,43,43	0
56	MG	2A	3093	1/1	0.73	0.40	61,61,61,61	0
56	MG	2A	3798	1/1	0.73	0.20	59,59,59,59	0
56	MG	2G	3003	1/1	0.73	0.17	59,59,59,59	0
56	MG	2A	3803	1/1	0.73	0.47	71,71,71,71	0
56	MG	2a	1702	1/1	0.73	0.25	54,54,54,54	0
56	MG	2A	3806	1/1	0.73	0.35	65,65,65,65	0
56	MG	2A	3810	1/1	0.73	0.12	53,53,53,53	0
56	MG	2A	3412	1/1	0.73	0.17	21,21,21,21	0
56	MG	1a	1773	1/1	0.73	0.13	44,44,44,44	0
56	MG	2A	3688	1/1	0.73	0.13	47,47,47,47	0
56	MG	1F	301	1/1	0.73	0.25	21,21,21,21	0
56	MG	1a	1800	1/1	0.73	0.11	31,31,31,31	0
56	MG	2A	3285	1/1	0.73	0.14	30,30,30,30	0
56	MG	2A	3786	1/1	0.74	0.26	62,62,62,62	0
56	MG	2B	3017	1/1	0.74	0.42	74,74,74,74	0
56	MG	2A	3098	1/1	0.74	1.62	62,62,62,62	0
56	MG	2a	1706	1/1	0.74	0.15	55,55,55,55	0
56	MG	1A	8922	1/1	0.74	0.26	16,16,16,16	0
56	MG	2A	3373	1/1	0.74	0.12	29,29,29,29	0
56	MG	1a	1803	1/1	0.74	0.17	47,47,47,47	0
56	MG	2A	3614	1/1	0.74	0.12	42,42,42,42	0
56	MG	2A	3923	1/1	0.74	0.24	39,39,39,39	0
56	MG	1A	8631	1/1	0.74	0.09	53,53,53,53	0
56	MG	2A	3658	1/1	0.74	0.11	29,29,29,29	0
56	MG	2A	3660	1/1	0.74	0.27	51,51,51,51	0
56	MG	2a	1680	1/1	0.74	0.63	59,59,59,59	0
56	MG	1A	8679	1/1	0.74	0.19	34,34,34,34	0
56	MG	1A	8508	1/1	0.75	0.09	34,34,34,34	0
56	MG	2B	3021	1/1	0.75	0.24	50,50,50,50	0
56	MG	2A	3327	1/1	0.75	0.33	61,61,61,61	0
56	MG	2A	3332	1/1	0.75	0.15	69,69,69,69	0
56	MG	2A	3799	1/1	0.75	0.16	54,54,54,54	0
56	MG	1A	8888	1/1	0.75	0.47	62,62,62,62	0
56	MG	1A	8058	1/1	0.75	0.15	44,44,44,44	0
56	MG	2A	3535	1/1	0.75	0.21	55,55,55,55	0
56	MG	2A	3814	1/1	0.75	0.10	33,33,33,33	0
56	MG	1A	8687	1/1	0.75	0.16	46,46,46,46	0
56	MG	2a	1794	1/1	0.75	0.30	71,71,71,71	0
56	MG	2A	3074	1/1	0.75	0.45	33,33,33,33	0
56	MG	2U	204	1/1	0.75	0.30	52,52,52,52	0
56	MG	2A	3576	1/1	0.75	0.26	47,47,47,47	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	1a	1660	1/1	0.75	0.41	39,39,39,39	0
56	MG	2A	3613	1/1	0.75	0.09	62,62,62,62	0
56	MG	1N	204	1/1	0.75	0.26	68,68,68,68	0
56	MG	2a	1732	1/1	0.75	0.19	77,77,77,77	0
56	MG	2x	104	1/1	0.75	1.16	68,68,68,68	0
56	MG	2a	1642	1/1	0.75	0.34	51,51,51,51	0
56	MG	1A	8286	1/1	0.76	0.10	11,11,11,11	0
56	MG	2A	3596	1/1	0.76	0.22	35,35,35,35	0
56	MG	2A	3603	1/1	0.76	0.48	53,53,53,53	0
56	MG	2A	3158	1/1	0.76	0.38	40,40,40,40	0
56	MG	1a	1772	1/1	0.76	0.13	53,53,53,53	0
56	MG	2A	3072	1/1	0.76	0.22	36,36,36,36	0
56	MG	1a	1667	1/1	0.76	0.32	59,59,59,59	0
56	MG	2A	3532	1/1	0.76	0.17	54,54,54,54	0
56	MG	1a	1623	1/1	0.76	0.34	47,47,47,47	0
56	MG	2a	1821	1/1	0.76	0.19	71,71,71,71	0
56	MG	2A	3667	1/1	0.76	0.34	58,58,58,58	0
56	MG	1a	1827	1/1	0.76	0.17	62,62,62,62	0
56	MG	2a	1751	1/1	0.76	0.13	50,50,50,50	0
56	MG	2h	3002	1/1	0.76	0.54	64,64,64,64	0
56	MG	1A	8320	1/1	0.76	0.19	7,7,7,7	0
56	MG	2a	1693	1/1	0.76	0.12	47,47,47,47	0
56	MG	2a	1623	1/1	0.76	0.28	41,41,41,41	0
56	MG	2A	3721	1/1	0.77	0.26	47,47,47,47	0
56	MG	2A	3324	1/1	0.77	0.12	33,33,33,33	0
56	MG	1a	1776	1/1	0.77	0.16	35,35,35,35	0
56	MG	1A	8356	1/1	0.77	0.12	9,9,9,9	0
56	MG	2A	3778	1/1	0.77	0.30	46,46,46,46	0
56	MG	1B	3023	1/1	0.77	0.11	46,46,46,46	0
56	MG	2A	3341	1/1	0.77	0.14	43,43,43,43	0
56	MG	2A	3370	1/1	0.77	0.13	21,21,21,21	0
56	MG	1a	1786	1/1	0.77	0.15	56,56,56,56	0
56	MG	2A	3092	1/1	0.77	0.58	48,48,48,48	0
56	MG	1a	1619	1/1	0.77	0.23	45,45,45,45	0
56	MG	1a	1744	1/1	0.77	0.15	59,59,59,59	0
56	MG	1A	8385	1/1	0.77	0.13	15,15,15,15	0
56	MG	2A	3180	1/1	0.77	0.34	46,46,46,46	0
56	MG	2A	3679	1/1	0.77	0.22	60,60,60,60	0
56	MG	1a	1635	1/1	0.77	0.19	38,38,38,38	0
56	MG	2A	3224	1/1	0.77	0.31	48,48,48,48	0
56	MG	1H	202	1/1	0.77	0.12	39,39,39,39	0
56	MG	1a	1659	1/1	0.77	0.20	50,50,50,50	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
56	MG	1A	8484	1/1	0.77	0.37	17,17,17,17	0
56	MG	2a	1715	1/1	0.77	0.21	50,50,50,50	0
56	MG	1A	8498	1/1	0.77	0.12	34,34,34,34	0
56	MG	2a	1719	1/1	0.77	0.40	39,39,39,39	0
56	MG	2v	101	1/1	0.77	0.19	61,61,61,61	0
56	MG	2A	3323	1/1	0.77	0.22	47,47,47,47	0
56	MG	20	105	1/1	0.77	0.35	50,50,50,50	0
56	MG	1D	314	1/1	0.78	0.23	31,31,31,31	0
56	MG	1a	1813	1/1	0.78	0.11	49,49,49,49	0
56	MG	2a	1762	1/1	0.78	0.12	58,58,58,58	0
56	MG	2G	3001	1/1	0.78	0.17	67,67,67,67	0
56	MG	2A	3870	1/1	0.78	0.33	63,63,63,63	0
56	MG	2A	3765	1/1	0.78	0.08	48,48,48,48	0
56	MG	1A	8205	1/1	0.78	0.20	25,25,25,25	0
56	MG	2A	3666	1/1	0.78	0.25	48,48,48,48	0
56	MG	1A	8630	1/1	0.78	0.19	36,36,36,36	0
56	MG	1x	3011	1/1	0.78	0.16	34,34,34,34	0
56	MG	2A	3057	1/1	0.78	0.28	42,42,42,42	0
56	MG	2A	3982	1/1	0.78	0.36	26,26,26,26	0
56	MG	1A	8916	1/1	0.78	0.07	75,75,75,75	0
56	MG	2A	3394	1/1	0.78	0.34	65,65,65,65	0
56	MG	1A	8527	1/1	0.78	0.15	11,11,11,11	0
56	MG	1B	3017	1/1	0.78	0.12	44,44,44,44	0
56	MG	2A	3696	1/1	0.78	0.11	54,54,54,54	0
56	MG	2A	3267	1/1	0.78	0.21	58,58,58,58	0
56	MG	1A	8417	1/1	0.78	0.11	37,37,37,37	0
56	MG	2a	1660	1/1	0.78	0.41	59,59,59,59	0
56	MG	1a	1604	1/1	0.78	0.33	50,50,50,50	0
56	MG	1a	1801	1/1	0.78	0.19	60,60,60,60	0
56	MG	2x	111	1/1	0.78	0.14	67,67,67,67	0
56	MG	2A	3421	1/1	0.79	0.14	49,49,49,49	0
56	MG	2A	3112	1/1	0.79	0.30	29,29,29,29	0
56	MG	2a	1755	1/1	0.79	0.15	52,52,52,52	0
56	MG	2A	3775	1/1	0.79	0.58	51,51,51,51	0
56	MG	1A	8840	1/1	0.79	0.17	9,9,9,9	0
56	MG	2A	3864	1/1	0.79	0.22	39,39,39,39	0
56	MG	1D	307	1/1	0.79	0.29	20,20,20,20	0
56	MG	2D	301	1/1	0.79	0.32	52,52,52,52	0
56	MG	1a	1625	1/1	0.79	0.35	47,47,47,47	0
56	MG	1a	1755	1/1	0.79	0.25	60,60,60,60	0
56	MG	2A	3873	1/1	0.79	0.37	74,74,74,74	0
56	MG	1a	1839	1/1	0.79	0.22	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	2A	3805	1/1	0.79	0.08	40,40,40,40	0
56	MG	2A	3916	1/1	0.79	0.35	86,86,86,86	0
56	MG	1A	8544	1/1	0.79	0.18	27,27,27,27	0
56	MG	2A	3933	1/1	0.79	0.12	51,51,51,51	0
56	MG	1A	8377	1/1	0.79	0.21	20,20,20,20	0
56	MG	2A	3637	1/1	0.79	0.22	48,48,48,48	0
56	MG	2A	3013	1/1	0.79	0.22	29,29,29,29	0
56	MG	2a	1718	1/1	0.79	0.77	72,72,72,72	0
56	MG	2A	3403	1/1	0.79	0.11	40,40,40,40	0
56	MG	2B	3005	1/1	0.79	0.29	55,55,55,55	0
56	MG	2B	3013	1/1	0.79	0.12	51,51,51,51	0
56	MG	2a	1626	1/1	0.79	0.24	63,63,63,63	0
56	MG	2A	3832	1/1	0.79	0.24	31,31,31,31	0
56	MG	1A	8621	1/1	0.79	0.16	24,24,24,24	0
56	MG	2B	3006	1/1	0.80	0.39	48,48,48,48	0
56	MG	2A	3279	1/1	0.80	0.17	49,49,49,49	0
56	MG	2A	3591	1/1	0.80	0.21	51,51,51,51	0
56	MG	2A	3702	1/1	0.80	0.34	55,55,55,55	0
56	MG	2a	1753	1/1	0.80	0.20	57,57,57,57	0
56	MG	1A	8689	1/1	0.80	0.21	33,33,33,33	0
56	MG	2A	3426	1/1	0.80	0.09	55,55,55,55	0
56	MG	2A	3431	1/1	0.80	0.09	39,39,39,39	0
56	MG	1a	1796	1/1	0.80	0.20	58,58,58,58	0
56	MG	2A	3105	1/1	0.80	0.40	46,46,46,46	0
56	MG	1a	1775	1/1	0.80	0.20	41,41,41,41	0
56	MG	2A	3125	1/1	0.80	0.85	39,39,39,39	0
56	MG	2A	3467	1/1	0.80	0.12	52,52,52,52	0
56	MG	1B	3022	1/1	0.80	0.14	41,41,41,41	0
56	MG	2A	3899	1/1	0.80	0.42	62,62,62,62	0
56	MG	1A	8667	1/1	0.80	0.24	40,40,40,40	0
56	MG	2A	3915	1/1	0.80	0.13	42,42,42,42	0
56	MG	1a	1783	1/1	0.80	0.39	60,60,60,60	0
56	MG	2a	1711	1/1	0.80	0.18	64,64,64,64	0
56	MG	2A	3917	1/1	0.80	0.63	49,49,49,49	0
56	MG	2A	3677	1/1	0.80	0.18	60,60,60,60	0
56	MG	1a	1825	1/1	0.80	0.14	43,43,43,43	0
56	MG	2A	3234	1/1	0.80	0.21	42,42,42,42	0
56	MG	1A	8784	1/1	0.80	0.20	38,38,38,38	0
56	MG	25	104	1/1	0.80	0.26	53,53,53,53	0
56	MG	1A	8249	1/1	0.80	0.31	36,36,36,36	0
56	MG	1A	8336	1/1	0.80	0.15	32,32,32,32	0
56	MG	2a	1731	1/1	0.80	0.13	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	2A	3551	1/1	0.80	0.27	34,34,34,34	0
56	MG	1a	1678	1/1	0.81	0.23	43,43,43,43	0
56	MG	2A	3245	1/1	0.81	0.28	46,46,46,46	0
56	MG	2A	3672	1/1	0.81	0.17	46,46,46,46	0
56	MG	2A	3675	1/1	0.81	0.19	44,44,44,44	0
56	MG	1A	8653	1/1	0.81	0.17	47,47,47,47	0
56	MG	2A	3263	1/1	0.81	0.41	46,46,46,46	0
56	MG	1A	8172	1/1	0.81	0.13	53,53,53,53	0
56	MG	2A	3854	1/1	0.81	0.20	32,32,32,32	0
56	MG	1a	1726	1/1	0.81	0.36	56,56,56,56	0
56	MG	1A	8197	1/1	0.81	0.29	42,42,42,42	0
56	MG	2A	3304	1/1	0.81	0.14	47,47,47,47	0
56	MG	2A	3869	1/1	0.81	0.17	38,38,38,38	0
56	MG	1A	8039	1/1	0.81	0.16	12,12,12,12	0
56	MG	1A	8970	1/1	0.81	0.24	29,29,29,29	0
56	MG	1A	8423	1/1	0.81	0.11	28,28,28,28	0
56	MG	1A	8221	1/1	0.81	0.10	43,43,43,43	0
56	MG	2A	3712	1/1	0.81	0.08	29,29,29,29	0
56	MG	1A	8711	1/1	0.81	0.12	27,27,27,27	0
56	MG	1a	1762	1/1	0.81	0.07	54,54,54,54	0
56	MG	1a	1815	1/1	0.81	0.16	57,57,57,57	0
56	MG	2A	3346	1/1	0.81	0.12	29,29,29,29	0
56	MG	2A	3106	1/1	0.81	0.32	31,31,31,31	0
56	MG	1a	1824	1/1	0.81	0.11	54,54,54,54	0
56	MG	1B	3027	1/1	0.81	0.32	66,66,66,66	0
56	MG	2a	1784	1/1	0.81	0.25	64,64,64,64	0
56	MG	2a	1656	1/1	0.81	0.32	65,65,65,65	0
56	MG	2A	3958	1/1	0.81	0.24	51,51,51,51	0
56	MG	2a	1801	1/1	0.81	0.14	61,61,61,61	0
56	MG	2A	3962	1/1	0.81	0.53	54,54,54,54	0
56	MG	1A	8123	1/1	0.81	0.66	22,22,22,22	0
56	MG	2A	3781	1/1	0.81	0.23	51,51,51,51	0
56	MG	2A	3785	1/1	0.81	0.17	29,29,29,29	0
56	MG	2A	3606	1/1	0.81	0.17	42,42,42,42	0
56	MG	2A	3406	1/1	0.81	0.16	51,51,51,51	0
56	MG	1A	8260	1/1	0.81	0.30	28,28,28,28	0
56	MG	2A	3418	1/1	0.81	0.11	57,57,57,57	0
56	MG	2a	1697	1/1	0.81	0.08	54,54,54,54	0
56	MG	1d	505	1/1	0.81	0.05	56,56,56,56	0
56	MG	1A	8279	1/1	0.81	0.10	30,30,30,30	0
56	MG	1A	8636	1/1	0.81	0.20	45,45,45,45	0
56	MG	2A	3662	1/1	0.81	0.11	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	1B	3010	1/1	0.82	0.15	44,44,44,44	0
56	MG	1Q	202	1/1	0.82	0.10	53,53,53,53	0
56	MG	1a	1710	1/1	0.82	0.09	47,47,47,47	0
56	MG	1A	8863	1/1	0.82	0.22	24,24,24,24	0
56	MG	18	101	1/1	0.82	0.28	49,49,49,49	0
56	MG	2A	3076	1/1	0.82	1.03	44,44,44,44	0
56	MG	1a	1731	1/1	0.82	0.40	64,64,64,64	0
56	MG	2A	3729	1/1	0.82	0.38	76,76,76,76	0
56	MG	1a	1795	1/1	0.82	0.09	52,52,52,52	0
56	MG	1a	1733	1/1	0.82	0.33	58,58,58,58	0
56	MG	2a	1601	1/1	0.82	0.18	47,47,47,47	0
56	MG	2a	1743	1/1	0.82	0.39	41,41,41,41	0
56	MG	1A	8866	1/1	0.82	0.09	32,32,32,32	0
56	MG	1A	8110	1/1	0.82	0.34	14,14,14,14	0
56	MG	2A	3772	1/1	0.82	0.25	43,43,43,43	0
56	MG	1A	8082	1/1	0.82	0.24	27,27,27,27	0
56	MG	2A	3350	1/1	0.82	0.24	28,28,28,28	0
56	MG	1a	1804	1/1	0.82	0.14	46,46,46,46	0
56	MG	1A	8145	1/1	0.82	0.23	15,15,15,15	0
56	MG	2A	3114	1/1	0.82	0.16	33,33,33,33	0
56	MG	2a	1649	1/1	0.82	0.68	48,48,48,48	0
56	MG	2a	1770	1/1	0.82	0.14	52,52,52,52	0
56	MG	2a	1775	1/1	0.82	0.48	68,68,68,68	0
56	MG	1A	8884	1/1	0.82	0.19	65,65,65,65	0
56	MG	1a	1759	1/1	0.82	0.11	63,63,63,63	0
56	MG	2a	1661	1/1	0.82	0.38	43,43,43,43	0
56	MG	2A	3165	1/1	0.82	0.30	42,42,42,42	0
56	MG	2a	1788	1/1	0.82	0.11	50,50,50,50	0
56	MG	1A	8747	1/1	0.82	0.09	27,27,27,27	0
56	MG	2a	1797	1/1	0.82	0.12	47,47,47,47	0
56	MG	1a	1642	1/1	0.82	0.20	57,57,57,57	0
56	MG	2A	3202	1/1	0.82	0.70	42,42,42,42	0
56	MG	2A	3813	1/1	0.82	0.19	64,64,64,64	0
56	MG	2A	3223	1/1	0.82	0.19	52,52,52,52	0
56	MG	1G	3002	1/1	0.82	0.10	44,44,44,44	0
56	MG	1A	8098	1/1	0.82	0.38	19,19,19,19	0
56	MG	1A	8608	1/1	0.82	0.23	29,29,29,29	0
56	MG	1x	3006	1/1	0.82	0.20	47,47,47,47	0
56	MG	1A	8855	1/1	0.82	0.20	29,29,29,29	0
56	MG	2a	1703	1/1	0.82	0.09	47,47,47,47	0
56	MG	2n	502	1/1	0.82	0.31	55,55,55,55	0
56	MG	2A	3846	1/1	0.82	0.14	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	3257	1/1	0.82	0.25	44,44,44,44	0
56	MG	1a	1779	1/1	0.82	0.13	50,50,50,50	0
56	MG	2A	3486	1/1	0.82	0.23	47,47,47,47	0
56	MG	1A	8753	1/1	0.83	0.39	13,13,13,13	0
56	MG	2A	3668	1/1	0.83	0.48	57,57,57,57	0
56	MG	2a	1622	1/1	0.83	0.26	59,59,59,59	0
56	MG	2A	3924	1/1	0.83	0.27	26,26,26,26	0
56	MG	1B	3001	1/1	0.83	0.15	37,37,37,37	0
56	MG	1A	8665	1/1	0.83	0.27	63,63,63,63	0
56	MG	2a	1630	1/1	0.83	0.16	50,50,50,50	0
56	MG	1A	8234	1/1	0.83	0.16	32,32,32,32	0
56	MG	1a	1620	1/1	0.83	0.18	46,46,46,46	0
56	MG	2A	3342	1/1	0.83	0.19	25,25,25,25	0
56	MG	2a	1761	1/1	0.83	0.12	42,42,42,42	0
56	MG	1A	8237	1/1	0.83	0.23	41,41,41,41	0
56	MG	2A	3985	1/1	0.83	0.18	39,39,39,39	0
56	MG	1A	8859	1/1	0.83	0.15	37,37,37,37	0
56	MG	1A	8076	1/1	0.83	0.44	22,22,22,22	0
56	MG	2A	3817	1/1	0.83	0.55	52,52,52,52	0
56	MG	2A	3823	1/1	0.83	0.18	43,43,43,43	0
56	MG	2a	1778	1/1	0.83	0.16	42,42,42,42	0
56	MG	1A	8488	1/1	0.83	0.20	46,46,46,46	0
56	MG	2A	3563	1/1	0.83	0.30	51,51,51,51	0
56	MG	1a	1758	1/1	0.83	0.15	38,38,38,38	0
56	MG	2a	1785	1/1	0.83	0.28	70,70,70,70	0
56	MG	1A	8871	1/1	0.83	0.37	38,38,38,38	0
56	MG	1A	8691	1/1	0.83	0.18	14,14,14,14	0
56	MG	2A	3262	1/1	0.83	0.16	38,38,38,38	0
56	MG	1A	8604	1/1	0.83	0.25	29,29,29,29	0
56	MG	2A	3265	1/1	0.83	0.40	56,56,56,56	0
56	MG	2A	3731	1/1	0.83	0.46	63,63,63,63	0
56	MG	1A	8252	1/1	0.83	0.24	24,24,24,24	0
56	MG	1A	8718	1/1	0.83	0.28	27,27,27,27	0
56	MG	2A	3757	1/1	0.83	0.24	32,32,32,32	0
56	MG	2A	3280	1/1	0.83	0.15	35,35,35,35	0
56	MG	2A	3629	1/1	0.83	0.20	25,25,25,25	0
56	MG	2A	3768	1/1	0.83	0.13	42,42,42,42	0
56	MG	1a	1686	1/1	0.83	0.20	46,46,46,46	0
56	MG	2A	3296	1/1	0.83	0.12	49,49,49,49	0
56	MG	2A	3902	1/1	0.83	0.12	39,39,39,39	0
56	MG	1A	8734	1/1	0.83	0.14	22,22,22,22	0
56	MG	1A	8735	1/1	0.83	0.16	15,15,15,15	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	25	103	1/1	0.83	0.30	46,46,46,46	0
56	MG	1A	8610	1/1	0.83	0.29	41,41,41,41	0
56	MG	1a	1749	1/1	0.84	0.14	54,54,54,54	0
56	MG	1A	8849	1/1	0.84	0.13	39,39,39,39	0
56	MG	1A	8853	1/1	0.84	0.21	50,50,50,50	0
56	MG	1A	8328	1/1	0.84	0.26	38,38,38,38	0
56	MG	2a	1662	1/1	0.84	0.16	48,48,48,48	0
56	MG	1A	8549	1/1	0.84	0.19	38,38,38,38	0
56	MG	2A	3664	1/1	0.84	0.20	25,25,25,25	0
56	MG	1A	8552	1/1	0.84	0.19	23,23,23,23	0
56	MG	1A	8864	1/1	0.84	0.15	26,26,26,26	0
56	MG	2a	1679	1/1	0.84	0.15	51,51,51,51	0
56	MG	1A	8676	1/1	0.84	0.06	26,26,26,26	0
56	MG	1A	8554	1/1	0.84	0.30	34,34,34,34	0
56	MG	1a	1605	1/1	0.84	0.15	43,43,43,43	0
56	MG	2a	1691	1/1	0.84	0.10	52,52,52,52	0
56	MG	2A	3903	1/1	0.84	0.30	49,49,49,49	0
56	MG	1a	1774	1/1	0.84	0.25	59,59,59,59	0
56	MG	2a	1700	1/1	0.84	0.17	51,51,51,51	0
56	MG	2A	3374	1/1	0.84	0.12	57,57,57,57	0
56	MG	2A	3385	1/1	0.84	0.17	24,24,24,24	0
56	MG	1A	8578	1/1	0.84	0.17	10,10,10,10	0
56	MG	2a	1705	1/1	0.84	0.26	63,63,63,63	0
56	MG	1A	8594	1/1	0.84	0.15	36,36,36,36	0
56	MG	1a	1777	1/1	0.84	0.41	56,56,56,56	0
56	MG	2A	3689	1/1	0.84	0.14	32,32,32,32	0
56	MG	1A	8277	1/1	0.84	0.30	50,50,50,50	0
56	MG	2A	3413	1/1	0.84	0.20	44,44,44,44	0
56	MG	1A	8247	1/1	0.84	0.17	25,25,25,25	0
56	MG	1A	8367	1/1	0.84	0.13	33,33,33,33	0
56	MG	1a	1636	1/1	0.84	0.13	56,56,56,56	0
56	MG	2A	3719	1/1	0.84	0.49	37,37,37,37	0
56	MG	1A	8900	1/1	0.84	0.14	13,13,13,13	0
56	MG	2a	1726	1/1	0.84	0.10	51,51,51,51	0
56	MG	2A	3143	1/1	0.84	0.15	33,33,33,33	0
56	MG	1A	8909	1/1	0.84	0.22	15,15,15,15	0
56	MG	1A	8030	1/1	0.84	0.31	20,20,20,20	0
56	MG	2A	3446	1/1	0.84	0.27	29,29,29,29	0
56	MG	2a	1741	1/1	0.84	0.09	61,61,61,61	0
56	MG	2A	3743	1/1	0.84	0.35	47,47,47,47	0
56	MG	1A	8730	1/1	0.84	0.13	62,62,62,62	0
56	MG	2A	3752	1/1	0.84	0.41	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	1752	1/1	0.84	0.57	71,71,71,71	0
56	MG	1A	8371	1/1	0.84	0.12	11,11,11,11	0
56	MG	1a	1797	1/1	0.84	0.29	47,47,47,47	0
56	MG	1A	8625	1/1	0.84	0.21	39,39,39,39	0
56	MG	2B	3023	1/1	0.84	0.15	41,41,41,41	0
56	MG	1a	1685	1/1	0.84	0.12	51,51,51,51	0
56	MG	2A	3502	1/1	0.84	0.10	47,47,47,47	0
56	MG	1B	3004	1/1	0.84	0.11	35,35,35,35	0
56	MG	2A	3523	1/1	0.84	0.29	38,38,38,38	0
56	MG	2F	309	1/1	0.84	0.14	58,58,58,58	0
56	MG	2A	3237	1/1	0.84	0.17	45,45,45,45	0
56	MG	1A	8736	1/1	0.84	0.35	38,38,38,38	0
56	MG	1a	1807	1/1	0.84	0.18	51,51,51,51	0
56	MG	1A	8374	1/1	0.84	0.12	41,41,41,41	0
56	MG	1A	8751	1/1	0.84	0.16	44,44,44,44	0
56	MG	2A	3539	1/1	0.84	0.19	47,47,47,47	0
56	MG	1a	1816	1/1	0.84	0.14	49,49,49,49	0
56	MG	2A	3549	1/1	0.84	0.10	39,39,39,39	0
56	MG	1A	8015	1/1	0.84	0.15	28,28,28,28	0
56	MG	2A	3559	1/1	0.84	0.26	25,25,25,25	0
56	MG	1A	8773	1/1	0.84	0.14	29,29,29,29	0
56	MG	29	503	1/1	0.84	0.21	62,62,62,62	0
56	MG	1A	8380	1/1	0.84	0.16	16,16,16,16	0
56	MG	2a	1609	1/1	0.84	0.15	45,45,45,45	0
56	MG	1a	1828	1/1	0.84	0.21	52,52,52,52	0
56	MG	2a	1810	1/1	0.84	0.87	53,53,53,53	0
56	MG	1A	8809	1/1	0.84	0.15	21,21,21,21	0
56	MG	2A	3283	1/1	0.84	0.16	30,30,30,30	0
56	MG	2A	3828	1/1	0.84	0.21	58,58,58,58	0
56	MG	1A	8817	1/1	0.84	0.07	31,31,31,31	0
56	MG	1A	8103	1/1	0.84	0.23	13,13,13,13	0
56	MG	1i	3001	1/1	0.84	0.17	46,46,46,46	0
56	MG	2a	1637	1/1	0.84	0.15	36,36,36,36	0
56	MG	2t	201	1/1	0.84	0.23	46,46,46,46	0
56	MG	1o	101	1/1	0.84	0.37	50,50,50,50	0
56	MG	2A	3320	1/1	0.84	0.19	27,27,27,27	0
56	MG	2A	3623	1/1	0.84	0.35	53,53,53,53	0
56	MG	2a	1647	1/1	0.84	0.17	48,48,48,48	0
56	MG	1A	8187	1/1	0.85	0.24	20,20,20,20	0
56	MG	2W	3001	1/1	0.85	0.11	45,45,45,45	0
56	MG	20	104	1/1	0.85	0.19	55,55,55,55	0
56	MG	1A	8605	1/1	0.85	0.22	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	1647	1/1	0.85	0.10	53,53,53,53	0
56	MG	1A	8674	1/1	0.85	0.26	35,35,35,35	0
56	MG	28	101	1/1	0.85	0.14	54,54,54,54	0
56	MG	1A	8250	1/1	0.85	0.50	50,50,50,50	0
56	MG	1a	1812	1/1	0.85	0.08	35,35,35,35	0
56	MG	2a	1606	1/1	0.85	0.18	35,35,35,35	0
56	MG	1A	8308	1/1	0.85	0.10	41,41,41,41	0
56	MG	2A	3922	1/1	0.85	0.28	65,65,65,65	0
56	MG	2a	1615	1/1	0.85	0.62	50,50,50,50	0
56	MG	1a	1670	1/1	0.85	0.17	44,44,44,44	0
56	MG	2a	1744	1/1	0.85	0.34	43,43,43,43	0
56	MG	1A	8798	1/1	0.85	0.21	24,24,24,24	0
56	MG	2A	3927	1/1	0.85	0.15	30,30,30,30	0
56	MG	1A	8800	1/1	0.85	0.28	44,44,44,44	0
56	MG	1A	8905	1/1	0.85	0.08	42,42,42,42	0
56	MG	2A	3452	1/1	0.85	0.09	34,34,34,34	0
56	MG	2A	3312	1/1	0.85	0.14	25,25,25,25	0
56	MG	1A	8615	1/1	0.85	0.21	13,13,13,13	0
56	MG	2a	1641	1/1	0.85	0.29	59,59,59,59	0
56	MG	1A	8814	1/1	0.85	0.07	62,62,62,62	0
56	MG	2A	3480	1/1	0.85	0.39	63,63,63,63	0
56	MG	2A	3482	1/1	0.85	0.29	43,43,43,43	0
56	MG	1A	8220	1/1	0.85	0.12	52,52,52,52	0
56	MG	2a	1771	1/1	0.85	0.11	55,55,55,55	0
56	MG	2a	1654	1/1	0.85	0.11	62,62,62,62	0
56	MG	2A	3673	1/1	0.85	0.28	41,41,41,41	0
56	MG	2B	3010	1/1	0.85	0.17	38,38,38,38	0
56	MG	1d	502	1/1	0.85	0.21	56,56,56,56	0
56	MG	2A	3509	1/1	0.85	0.35	66,66,66,66	0
56	MG	1d	504	1/1	0.85	0.12	45,45,45,45	0
56	MG	1a	1714	1/1	0.85	0.09	42,42,42,42	0
56	MG	2a	1672	1/1	0.85	0.16	64,64,64,64	0
56	MG	2a	1793	1/1	0.85	0.09	52,52,52,52	0
56	MG	2a	1674	1/1	0.85	0.09	37,37,37,37	0
56	MG	2A	3199	1/1	0.85	0.43	30,30,30,30	0
56	MG	2A	3525	1/1	0.85	0.14	25,25,25,25	0
56	MG	1A	8536	1/1	0.85	0.15	54,54,54,54	0
56	MG	1A	8465	1/1	0.85	0.12	24,24,24,24	0
56	MG	2A	3217	1/1	0.85	0.52	30,30,30,30	0
56	MG	2A	3349	1/1	0.85	0.10	43,43,43,43	0
56	MG	2a	1815	1/1	0.85	0.42	58,58,58,58	0
56	MG	1A	8240	1/1	0.85	0.21	13,13,13,13	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	2A	3545	1/1	0.85	0.12	47,47,47,47	0
56	MG	2A	3706	1/1	0.85	0.20	32,32,32,32	0
56	MG	1a	1788	1/1	0.85	0.22	42,42,42,42	0
56	MG	1A	8471	1/1	0.85	0.21	17,17,17,17	0
56	MG	1A	8473	1/1	0.85	0.24	35,35,35,35	0
56	MG	1A	8263	1/1	0.85	0.15	26,26,26,26	0
56	MG	2o	3001	1/1	0.85	0.15	32,32,32,32	0
56	MG	1A	8646	1/1	0.85	0.12	30,30,30,30	0
56	MG	2A	3248	1/1	0.85	0.32	34,34,34,34	0
56	MG	2N	203	1/1	0.85	0.13	49,49,49,49	0
56	MG	2A	3578	1/1	0.85	0.08	47,47,47,47	0
56	MG	1A	8143	1/1	0.85	0.10	20,20,20,20	0
57	ZN	14	501	1/1	0.85	0.13	75,75,75,75	0
56	MG	2a	1707	1/1	0.86	0.22	61,61,61,61	0
56	MG	2A	3503	1/1	0.86	0.21	47,47,47,47	0
56	MG	2A	3339	1/1	0.86	0.12	35,35,35,35	0
56	MG	2A	3518	1/1	0.86	0.19	24,24,24,24	0
56	MG	1A	8614	1/1	0.86	0.20	41,41,41,41	0
56	MG	1A	8795	1/1	0.86	0.35	21,21,21,21	0
56	MG	1A	8649	1/1	0.86	0.31	18,18,18,18	0
56	MG	2A	3840	1/1	0.86	0.19	42,42,42,42	0
56	MG	2a	1720	1/1	0.86	0.15	43,43,43,43	0
56	MG	1A	8704	1/1	0.86	0.20	34,34,34,34	0
56	MG	2A	3526	1/1	0.86	0.13	46,46,46,46	0
56	MG	1A	8801	1/1	0.86	0.10	25,25,25,25	0
56	MG	2A	3364	1/1	0.86	0.26	42,42,42,42	0
56	MG	1a	1756	1/1	0.86	0.11	51,51,51,51	0
56	MG	2a	1733	1/1	0.86	0.20	69,69,69,69	0
56	MG	1A	8804	1/1	0.86	0.09	31,31,31,31	0
56	MG	1A	8419	1/1	0.86	0.20	31,31,31,31	0
56	MG	1A	8899	1/1	0.86	0.12	37,37,37,37	0
56	MG	2A	3705	1/1	0.86	0.18	48,48,48,48	0
56	MG	2A	3547	1/1	0.86	0.18	43,43,43,43	0
56	MG	2A	3709	1/1	0.86	0.21	40,40,40,40	0
56	MG	2a	1604	1/1	0.86	0.19	44,44,44,44	0
56	MG	2A	3083	1/1	0.86	0.20	25,25,25,25	0
56	MG	2A	3400	1/1	0.86	0.09	41,41,41,41	0
56	MG	1A	8251	1/1	0.86	0.18	33,33,33,33	0
56	MG	2a	1611	1/1	0.86	0.41	61,61,61,61	0
56	MG	1A	8438	1/1	0.86	0.12	34,34,34,34	0
56	MG	2A	3726	1/1	0.86	0.12	50,50,50,50	0
56	MG	2A	3560	1/1	0.86	0.56	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	1680	1/1	0.86	0.26	27,27,27,27	0
56	MG	2A	3733	1/1	0.86	0.08	33,33,33,33	0
56	MG	2A	3734	1/1	0.86	0.08	33,33,33,33	0
56	MG	2A	3564	1/1	0.86	0.26	51,51,51,51	0
56	MG	1A	8835	1/1	0.86	0.10	36,36,36,36	0
56	MG	2a	1638	1/1	0.86	0.34	54,54,54,54	0
56	MG	2A	3273	1/1	0.86	0.27	44,44,44,44	0
56	MG	2A	3747	1/1	0.86	0.27	39,39,39,39	0
56	MG	1A	8670	1/1	0.86	0.45	41,41,41,41	0
56	MG	1U	201	1/1	0.86	0.13	26,26,26,26	0
56	MG	1A	8201	1/1	0.86	0.30	45,45,45,45	0
56	MG	1A	8955	1/1	0.86	0.28	11,11,11,11	0
56	MG	2A	3124	1/1	0.86	0.16	46,46,46,46	0
56	MG	1A	8295	1/1	0.86	0.10	21,21,21,21	0
56	MG	2A	3435	1/1	0.86	0.11	33,33,33,33	0
56	MG	2A	3305	1/1	0.86	0.08	41,41,41,41	0
56	MG	2a	1799	1/1	0.86	0.19	57,57,57,57	0
56	MG	1A	8232	1/1	0.86	0.17	34,34,34,34	0
56	MG	2a	1804	1/1	0.86	0.23	65,65,65,65	0
56	MG	2B	3007	1/1	0.86	0.12	42,42,42,42	0
56	MG	2B	3008	1/1	0.86	0.23	52,52,52,52	0
56	MG	2B	3009	1/1	0.86	0.22	67,67,67,67	0
56	MG	1B	3003	1/1	0.86	0.13	43,43,43,43	0
56	MG	2A	3636	1/1	0.86	0.33	48,48,48,48	0
56	MG	2a	1820	1/1	0.86	0.30	60,60,60,60	0
56	MG	2A	3795	1/1	0.86	0.19	28,28,28,28	0
56	MG	2A	3319	1/1	0.86	0.20	68,68,68,68	0
56	MG	1A	8686	1/1	0.86	0.21	38,38,38,38	0
56	MG	1A	8193	1/1	0.86	0.19	28,28,28,28	0
56	MG	1a	1735	1/1	0.86	0.24	54,54,54,54	0
56	MG	1x	3005	1/1	0.86	0.21	51,51,51,51	0
56	MG	2A	3808	1/1	0.86	0.11	31,31,31,31	0
56	MG	1A	8074	1/1	0.86	0.26	18,18,18,18	0
56	MG	2A	3500	1/1	0.86	0.32	45,45,45,45	0
56	MG	2A	3207	1/1	0.86	0.67	44,44,44,44	0
56	MG	2D	312	1/1	0.86	0.19	39,39,39,39	0
56	MG	2D	314	1/1	0.86	0.24	25,25,25,25	0
56	MG	2A	3670	1/1	0.86	0.19	32,32,32,32	0
56	MG	2A	3671	1/1	0.86	0.31	45,45,45,45	0
56	MG	2a	1696	1/1	0.87	0.19	36,36,36,36	0
56	MG	1A	8045	1/1	0.87	0.53	11,11,11,11	0
56	MG	1a	1723	1/1	0.87	0.10	40,40,40,40	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	1Q	201	1/1	0.87	0.20	17,17,17,17	0
56	MG	2A	3501	1/1	0.87	0.12	41,41,41,41	0
56	MG	1A	8093	1/1	0.87	0.20	20,20,20,20	0
56	MG	2B	3022	1/1	0.87	0.10	59,59,59,59	0
56	MG	1A	8344	1/1	0.87	0.10	26,26,26,26	0
56	MG	2A	3504	1/1	0.87	0.23	45,45,45,45	0
56	MG	2a	1710	1/1	0.87	0.18	55,55,55,55	0
56	MG	1A	8261	1/1	0.87	0.15	55,55,55,55	0
56	MG	2a	1712	1/1	0.87	0.32	64,64,64,64	0
56	MG	2A	3821	1/1	0.87	0.11	48,48,48,48	0
56	MG	2A	3115	1/1	0.87	0.21	41,41,41,41	0
56	MG	2A	3519	1/1	0.87	0.22	31,31,31,31	0
56	MG	1A	8902	1/1	0.87	0.46	51,51,51,51	0
56	MG	1a	1739	1/1	0.87	0.17	50,50,50,50	0
56	MG	1a	1740	1/1	0.87	0.42	54,54,54,54	0
56	MG	1A	8192	1/1	0.87	0.30	22,22,22,22	0
56	MG	1A	8802	1/1	0.87	0.11	26,26,26,26	0
56	MG	2A	3174	1/1	0.87	0.10	40,40,40,40	0
56	MG	2A	3847	1/1	0.87	0.40	53,53,53,53	0
56	MG	1A	8266	1/1	0.87	0.21	13,13,13,13	0
56	MG	2A	3698	1/1	0.87	0.12	35,35,35,35	0
56	MG	1A	8276	1/1	0.87	0.36	15,15,15,15	0
56	MG	2A	3700	1/1	0.87	0.10	42,42,42,42	0
56	MG	2A	3857	1/1	0.87	0.19	40,40,40,40	0
56	MG	2Y	201	1/1	0.87	0.72	85,85,85,85	0
56	MG	2Y	203	1/1	0.87	0.07	47,47,47,47	0
56	MG	2A	3858	1/1	0.87	0.15	46,46,46,46	0
56	MG	2A	3862	1/1	0.87	0.25	32,32,32,32	0
56	MG	23	101	1/1	0.87	0.29	51,51,51,51	0
56	MG	2A	3863	1/1	0.87	0.25	54,54,54,54	0
56	MG	1A	8137	1/1	0.87	0.40	11,11,11,11	0
56	MG	2A	3704	1/1	0.87	0.22	53,53,53,53	0
56	MG	1A	8196	1/1	0.87	0.18	49,49,49,49	0
56	MG	1a	1629	1/1	0.87	0.31	36,36,36,36	0
56	MG	1A	8972	1/1	0.87	0.25	20,20,20,20	0
56	MG	2A	3219	1/1	0.87	0.22	29,29,29,29	0
56	MG	1A	8695	1/1	0.87	0.17	11,11,11,11	0
56	MG	2a	1764	1/1	0.87	0.23	55,55,55,55	0
56	MG	2a	1766	1/1	0.87	0.50	67,67,67,67	0
56	MG	2A	3893	1/1	0.87	0.15	44,44,44,44	0
56	MG	1A	8005	1/1	0.87	0.14	20,20,20,20	0
56	MG	2a	1613	1/1	0.87	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	3552	1/1	0.87	0.31	47,47,47,47	0
56	MG	2a	1621	1/1	0.87	0.20	49,49,49,49	0
56	MG	1A	8080	1/1	0.87	0.24	18,18,18,18	0
56	MG	2A	3402	1/1	0.87	0.09	39,39,39,39	0
56	MG	2A	3908	1/1	0.87	0.77	57,57,57,57	0
56	MG	1A	8542	1/1	0.87	0.26	40,40,40,40	0
56	MG	1a	1657	1/1	0.87	0.12	55,55,55,55	0
56	MG	1A	8299	1/1	0.87	0.08	28,28,28,28	0
56	MG	2a	1787	1/1	0.87	0.08	49,49,49,49	0
56	MG	2A	3736	1/1	0.87	0.29	51,51,51,51	0
56	MG	1A	8857	1/1	0.87	0.17	44,44,44,44	0
56	MG	2A	3588	1/1	0.87	0.24	44,44,44,44	0
56	MG	1a	1661	1/1	0.87	0.20	48,48,48,48	0
56	MG	2a	1798	1/1	0.87	0.18	49,49,49,49	0
56	MG	2A	3931	1/1	0.87	0.14	47,47,47,47	0
56	MG	2a	1800	1/1	0.87	0.14	39,39,39,39	0
56	MG	1A	8169	1/1	0.87	0.63	16,16,16,16	0
56	MG	2A	3424	1/1	0.87	0.30	50,50,50,50	0
56	MG	2A	3755	1/1	0.87	0.27	50,50,50,50	0
56	MG	2a	1650	1/1	0.87	0.21	46,46,46,46	0
56	MG	2A	3040	1/1	0.87	0.07	53,53,53,53	0
56	MG	1A	8644	1/1	0.87	0.24	36,36,36,36	0
56	MG	2A	3977	1/1	0.87	0.26	30,30,30,30	0
56	MG	1a	1671	1/1	0.87	0.16	39,39,39,39	0
56	MG	2A	3983	1/1	0.87	0.10	23,23,23,23	0
56	MG	1a	1782	1/1	0.87	0.10	38,38,38,38	0
56	MG	1A	8313	1/1	0.87	0.13	16,16,16,16	0
56	MG	1A	8210	1/1	0.87	0.22	14,14,14,14	0
56	MG	1A	8215	1/1	0.87	0.25	12,12,12,12	0
56	MG	1A	8657	1/1	0.87	0.21	19,19,19,19	0
56	MG	1A	8879	1/1	0.87	0.14	25,25,25,25	0
56	MG	2A	3650	1/1	0.87	0.18	36,36,36,36	0
56	MG	2A	3286	1/1	0.87	0.14	21,21,21,21	0
56	MG	2a	1684	1/1	0.87	0.31	41,41,41,41	0
56	MG	2B	3011	1/1	0.87	0.08	73,73,73,73	0
56	MG	2A	3290	1/1	0.87	0.15	31,31,31,31	0
56	MG	1A	8662	1/1	0.87	0.19	29,29,29,29	0
56	MG	1A	8585	1/1	0.87	0.14	29,29,29,29	0
57	ZN	2Y	202	1/1	0.87	0.05	66,66,66,66	0
56	MG	2A	3362	1/1	0.88	0.13	61,61,61,61	0
56	MG	1A	8102	1/1	0.88	0.24	16,16,16,16	0
56	MG	1A	8316	1/1	0.88	0.19	14,14,14,14	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	1A	8023	1/1	0.88	0.15	21,21,21,21	0
56	MG	1A	8683	1/1	0.88	0.27	30,30,30,30	0
56	MG	2A	3880	1/1	0.88	0.18	32,32,32,32	0
56	MG	2A	3376	1/1	0.88	0.12	23,23,23,23	0
56	MG	1A	8176	1/1	0.88	0.10	28,28,28,28	0
56	MG	2A	3091	1/1	0.88	0.19	50,50,50,50	0
56	MG	1A	8582	1/1	0.88	0.10	15,15,15,15	0
56	MG	19	104	1/1	0.88	0.19	34,34,34,34	0
56	MG	1A	8437	1/1	0.88	0.16	6,6,6,6	0
56	MG	1A	8865	1/1	0.88	0.21	28,28,28,28	0
56	MG	1A	8324	1/1	0.88	0.12	17,17,17,17	0
56	MG	2A	3678	1/1	0.88	0.31	49,49,49,49	0
56	MG	1A	8602	1/1	0.88	0.11	47,47,47,47	0
56	MG	2A	3683	1/1	0.88	0.23	73,73,73,73	0
56	MG	1A	8442	1/1	0.88	0.15	47,47,47,47	0
56	MG	2A	3419	1/1	0.88	0.08	48,48,48,48	0
56	MG	1A	8449	1/1	0.88	0.08	61,61,61,61	0
56	MG	1A	8464	1/1	0.88	0.21	7,7,7,7	0
56	MG	1A	8716	1/1	0.88	0.11	39,39,39,39	0
56	MG	2A	3945	1/1	0.88	0.13	22,22,22,22	0
56	MG	2A	3947	1/1	0.88	0.30	24,24,24,24	0
56	MG	1a	1780	1/1	0.88	0.13	61,61,61,61	0
56	MG	2A	3957	1/1	0.88	0.34	41,41,41,41	0
56	MG	2A	3427	1/1	0.88	0.19	22,22,22,22	0
56	MG	2A	3149	1/1	0.88	0.20	32,32,32,32	0
56	MG	1A	8010	1/1	0.88	0.21	7,7,7,7	0
56	MG	1A	8722	1/1	0.88	0.10	22,22,22,22	0
56	MG	1A	8724	1/1	0.88	0.12	17,17,17,17	0
56	MG	2A	3437	1/1	0.88	0.07	59,59,59,59	0
56	MG	1a	1784	1/1	0.88	0.20	54,54,54,54	0
56	MG	1A	8727	1/1	0.88	0.10	36,36,36,36	0
56	MG	2A	3200	1/1	0.88	0.23	21,21,21,21	0
56	MG	2A	3711	1/1	0.88	0.12	29,29,29,29	0
56	MG	1a	1652	1/1	0.88	0.16	47,47,47,47	0
56	MG	1a	1656	1/1	0.88	0.15	51,51,51,51	0
56	MG	2A	3205	1/1	0.88	1.05	44,44,44,44	0
56	MG	1A	8612	1/1	0.88	0.14	8,8,8,8	0
56	MG	2A	3213	1/1	0.88	0.22	32,32,32,32	0
56	MG	2A	3728	1/1	0.88	0.11	56,56,56,56	0
56	MG	2a	1727	1/1	0.88	0.23	49,49,49,49	0
56	MG	2A	3485	1/1	0.88	0.07	44,44,44,44	0
56	MG	1A	8904	1/1	0.88	0.10	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	2A	3498	1/1	0.88	0.18	45,45,45,45	0
56	MG	1A	8732	1/1	0.88	0.24	33,33,33,33	0
56	MG	1A	8264	1/1	0.88	0.24	37,37,37,37	0
56	MG	2A	3737	1/1	0.88	0.20	44,44,44,44	0
56	MG	1A	8469	1/1	0.88	0.08	29,29,29,29	0
56	MG	2A	3232	1/1	0.88	0.30	46,46,46,46	0
56	MG	1a	1669	1/1	0.88	0.40	42,42,42,42	0
56	MG	1A	8119	1/1	0.88	0.09	29,29,29,29	0
56	MG	2A	3239	1/1	0.88	0.35	51,51,51,51	0
56	MG	1A	8048	1/1	0.88	0.18	22,22,22,22	0
56	MG	1A	8966	1/1	0.88	0.11	22,22,22,22	0
56	MG	1A	8055	1/1	0.88	0.25	10,10,10,10	0
56	MG	1A	8033	1/1	0.88	0.22	27,27,27,27	0
56	MG	2a	1760	1/1	0.88	0.13	56,56,56,56	0
56	MG	2E	303	1/1	0.88	0.17	64,64,64,64	0
56	MG	2A	3767	1/1	0.88	0.14	52,52,52,52	0
56	MG	1A	8767	1/1	0.88	0.09	33,33,33,33	0
56	MG	2A	3261	1/1	0.88	1.14	42,42,42,42	0
56	MG	1a	1814	1/1	0.88	0.16	40,40,40,40	0
56	MG	2A	3528	1/1	0.88	0.08	40,40,40,40	0
56	MG	2A	3779	1/1	0.88	0.23	34,34,34,34	0
56	MG	2N	201	1/1	0.88	0.21	50,50,50,50	0
56	MG	1A	8144	1/1	0.88	0.16	35,35,35,35	0
56	MG	1a	1697	1/1	0.88	0.08	38,38,38,38	0
56	MG	1a	1700	1/1	0.88	0.21	45,45,45,45	0
56	MG	2A	3792	1/1	0.88	0.10	44,44,44,44	0
56	MG	2U	205	1/1	0.88	0.24	49,49,49,49	0
56	MG	2A	3793	1/1	0.88	0.15	34,34,34,34	0
56	MG	1a	1704	1/1	0.88	0.17	47,47,47,47	0
56	MG	1A	8504	1/1	0.88	0.17	30,30,30,30	0
56	MG	1A	8634	1/1	0.88	0.20	39,39,39,39	0
56	MG	1a	1834	1/1	0.88	0.15	46,46,46,46	0
56	MG	1A	8202	1/1	0.88	0.27	11,11,11,11	0
56	MG	1a	1718	1/1	0.88	0.09	44,44,44,44	0
56	MG	1A	8069	1/1	0.88	0.18	18,18,18,18	0
56	MG	27	102	1/1	0.88	0.12	56,56,56,56	0
56	MG	1A	8519	1/1	0.88	0.22	29,29,29,29	0
56	MG	1A	8206	1/1	0.88	0.31	18,18,18,18	0
56	MG	1a	1730	1/1	0.88	0.25	43,43,43,43	0
56	MG	2a	1803	1/1	0.88	0.10	41,41,41,41	0
56	MG	1l	201	1/1	0.88	0.14	42,42,42,42	0
56	MG	1A	8532	1/1	0.88	0.27	15,15,15,15	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	1x	3002	1/1	0.88	0.19	44,44,44,44	0
56	MG	1A	8534	1/1	0.88	0.15	52,52,52,52	0
56	MG	2A	3590	1/1	0.88	0.14	65,65,65,65	0
56	MG	2a	1811	1/1	0.88	0.10	59,59,59,59	0
56	MG	1A	8383	1/1	0.88	0.09	10,10,10,10	0
56	MG	1A	8312	1/1	0.88	0.10	7,7,7,7	0
56	MG	2A	3602	1/1	0.88	0.12	53,53,53,53	0
56	MG	1H	201	1/1	0.88	0.14	38,38,38,38	0
56	MG	1A	8412	1/1	0.88	0.18	6,6,6,6	0
56	MG	2a	1624	1/1	0.88	0.51	48,48,48,48	0
56	MG	2A	3041	1/1	0.88	0.18	39,39,39,39	0
56	MG	2A	3050	1/1	0.88	0.21	39,39,39,39	0
56	MG	1a	1747	1/1	0.88	0.13	65,65,65,65	0
56	MG	1A	8547	1/1	0.88	0.11	21,21,21,21	0
56	MG	2A	3343	1/1	0.88	0.15	35,35,35,35	0
56	MG	2A	3062	1/1	0.88	0.28	37,37,37,37	0
56	MG	2A	3630	1/1	0.88	0.19	57,57,57,57	0
56	MG	1A	8846	1/1	0.88	0.17	37,37,37,37	0
56	MG	1a	1751	1/1	0.88	0.30	59,59,59,59	0
56	MG	2A	3356	1/1	0.88	0.15	30,30,30,30	0
56	MG	2A	3657	1/1	0.88	0.41	33,33,33,33	0
56	MG	2A	3910	1/1	0.89	0.23	60,60,60,60	0
56	MG	2A	3259	1/1	0.89	0.29	33,33,33,33	0
56	MG	2A	3018	1/1	0.89	0.27	55,55,55,55	0
56	MG	2A	3029	1/1	0.89	1.02	31,31,31,31	0
56	MG	2A	3495	1/1	0.89	0.32	57,57,57,57	0
56	MG	2A	3035	1/1	0.89	0.15	37,37,37,37	0
56	MG	2A	3499	1/1	0.89	0.25	51,51,51,51	0
56	MG	1A	8171	1/1	0.89	0.14	28,28,28,28	0
56	MG	2A	3928	1/1	0.89	0.30	31,31,31,31	0
56	MG	2A	3929	1/1	0.89	0.15	48,48,48,48	0
56	MG	1A	8389	1/1	0.89	0.07	32,32,32,32	0
56	MG	2a	1681	1/1	0.89	0.18	45,45,45,45	0
56	MG	2A	3044	1/1	0.89	0.17	39,39,39,39	0
56	MG	2A	3049	1/1	0.89	0.14	43,43,43,43	0
56	MG	1A	8124	1/1	0.89	0.16	16,16,16,16	0
56	MG	2A	3282	1/1	0.89	0.24	63,63,63,63	0
56	MG	2A	3051	1/1	0.89	0.26	29,29,29,29	0
56	MG	2A	3722	1/1	0.89	0.12	42,42,42,42	0
56	MG	1A	8794	1/1	0.89	0.12	24,24,24,24	0
56	MG	2A	3727	1/1	0.89	0.21	44,44,44,44	0
56	MG	1a	1677	1/1	0.89	0.15	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	8129	1/1	0.89	0.19	19,19,19,19	0
56	MG	1A	8797	1/1	0.89	0.11	20,20,20,20	0
56	MG	2A	3298	1/1	0.89	0.11	29,29,29,29	0
56	MG	2A	3303	1/1	0.89	0.12	30,30,30,30	0
56	MG	1a	1681	1/1	0.89	0.17	52,52,52,52	0
56	MG	1a	1682	1/1	0.89	0.47	45,45,45,45	0
56	MG	1a	1683	1/1	0.89	0.15	39,39,39,39	0
56	MG	2A	3316	1/1	0.89	0.34	34,34,34,34	0
56	MG	1A	8573	1/1	0.89	0.15	18,18,18,18	0
56	MG	1A	8130	1/1	0.89	0.20	20,20,20,20	0
56	MG	2A	3749	1/1	0.89	0.29	50,50,50,50	0
56	MG	2A	3544	1/1	0.89	0.08	38,38,38,38	0
56	MG	1A	8495	1/1	0.89	0.16	14,14,14,14	0
56	MG	2A	3546	1/1	0.89	0.22	54,54,54,54	0
56	MG	1A	8894	1/1	0.89	0.14	8,8,8,8	0
56	MG	1A	8418	1/1	0.89	0.09	22,22,22,22	0
56	MG	1A	8648	1/1	0.89	0.16	27,27,27,27	0
56	MG	1S	201	1/1	0.89	0.13	23,23,23,23	0
56	MG	1A	8348	1/1	0.89	0.14	7,7,7,7	0
56	MG	1a	1713	1/1	0.89	0.11	39,39,39,39	0
56	MG	1A	8013	1/1	0.89	0.14	20,20,20,20	0
56	MG	10	107	1/1	0.89	0.10	36,36,36,36	0
56	MG	15	103	1/1	0.89	0.19	20,20,20,20	0
56	MG	2D	302	1/1	0.89	0.31	44,44,44,44	0
56	MG	2A	3123	1/1	0.89	0.12	41,41,41,41	0
56	MG	1a	1805	1/1	0.89	0.07	55,55,55,55	0
56	MG	2A	3584	1/1	0.89	0.18	30,30,30,30	0
56	MG	15	106	1/1	0.89	0.32	20,20,20,20	0
56	MG	2A	3794	1/1	0.89	0.07	63,63,63,63	0
56	MG	2A	3138	1/1	0.89	0.24	31,31,31,31	0
56	MG	2A	3358	1/1	0.89	0.08	27,27,27,27	0
56	MG	1A	8255	1/1	0.89	0.58	33,33,33,33	0
56	MG	1A	8827	1/1	0.89	0.07	12,12,12,12	0
56	MG	1A	8915	1/1	0.89	0.13	38,38,38,38	0
56	MG	2A	3161	1/1	0.89	0.14	33,33,33,33	0
56	MG	1A	8828	1/1	0.89	0.07	40,40,40,40	0
56	MG	2N	202	1/1	0.89	0.21	49,49,49,49	0
56	MG	2A	3610	1/1	0.89	0.14	57,57,57,57	0
56	MG	1a	1612	1/1	0.89	0.09	52,52,52,52	0
56	MG	1a	1614	1/1	0.89	0.24	52,52,52,52	0
56	MG	2R	202	1/1	0.89	0.21	21,21,21,21	0
56	MG	2A	3617	1/1	0.89	0.09	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	2A	3390	1/1	0.89	0.10	45,45,45,45	0
56	MG	2U	207	1/1	0.89	0.15	29,29,29,29	0
56	MG	2A	3622	1/1	0.89	0.17	44,44,44,44	0
56	MG	2A	3181	1/1	0.89	0.35	31,31,31,31	0
56	MG	2a	1779	1/1	0.89	0.16	48,48,48,48	0
56	MG	2A	3628	1/1	0.89	0.15	59,59,59,59	0
56	MG	2A	3398	1/1	0.89	0.21	39,39,39,39	0
56	MG	2A	3830	1/1	0.89	0.13	42,42,42,42	0
56	MG	2A	3182	1/1	0.89	0.24	34,34,34,34	0
56	MG	2A	3185	1/1	0.89	0.24	45,45,45,45	0
56	MG	2A	3834	1/1	0.89	0.28	55,55,55,55	0
56	MG	1A	8834	1/1	0.89	0.09	18,18,18,18	0
56	MG	2a	1791	1/1	0.89	0.11	51,51,51,51	0
56	MG	2A	3837	1/1	0.89	0.20	21,21,21,21	0
56	MG	1a	1742	1/1	0.89	0.15	32,32,32,32	0
56	MG	1A	8934	1/1	0.89	0.12	48,48,48,48	0
56	MG	1A	8140	1/1	0.89	0.06	52,52,52,52	0
56	MG	1A	8526	1/1	0.89	0.08	42,42,42,42	0
56	MG	2a	1607	1/1	0.89	0.35	55,55,55,55	0
56	MG	1A	8107	1/1	0.89	0.24	18,18,18,18	0
56	MG	2A	3420	1/1	0.89	0.18	54,54,54,54	0
56	MG	1A	8447	1/1	0.89	0.20	13,13,13,13	0
56	MG	1A	8852	1/1	0.89	0.11	27,27,27,27	0
56	MG	1A	8096	1/1	0.89	0.20	10,10,10,10	0
56	MG	2A	3221	1/1	0.89	0.62	29,29,29,29	0
56	MG	1A	8051	1/1	0.89	0.20	10,10,10,10	0
56	MG	1B	3007	1/1	0.89	0.12	37,37,37,37	0
56	MG	1n	101	1/1	0.89	0.31	51,51,51,51	0
56	MG	1A	8738	1/1	0.89	0.08	38,38,38,38	0
56	MG	2A	3235	1/1	0.89	0.33	43,43,43,43	0
56	MG	2a	1629	1/1	0.89	0.53	53,53,53,53	0
56	MG	1A	8026	1/1	0.89	0.32	10,10,10,10	0
56	MG	1B	3018	1/1	0.89	0.13	41,41,41,41	0
56	MG	1B	3020	1/1	0.89	0.14	23,23,23,23	0
56	MG	2A	3881	1/1	0.89	0.26	56,56,56,56	0
56	MG	1A	8270	1/1	0.89	0.24	20,20,20,20	0
56	MG	2A	3889	1/1	0.89	0.30	63,63,63,63	0
56	MG	2A	3892	1/1	0.89	0.15	34,34,34,34	0
56	MG	2A	3461	1/1	0.89	0.13	30,30,30,30	0
56	MG	1A	8685	1/1	0.89	0.10	51,51,51,51	0
56	MG	2A	3015	1/1	0.89	0.19	18,18,18,18	0
56	MG	2x	109	1/1	0.89	0.24	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	3255	1/1	0.89	0.17	45,45,45,45	0
56	MG	2A	3479	1/1	0.89	0.12	26,26,26,26	0
56	MG	2A	3016	1/1	0.89	0.55	34,34,34,34	0
57	ZN	24	501	1/1	0.89	0.14	99,99,99,99	0
56	MG	2A	3438	1/1	0.90	0.16	25,25,25,25	0
56	MG	2A	3442	1/1	0.90	0.19	23,23,23,23	0
56	MG	1a	1757	1/1	0.90	0.13	44,44,44,44	0
56	MG	2A	3250	1/1	0.90	0.71	40,40,40,40	0
56	MG	2A	3891	1/1	0.90	0.23	43,43,43,43	0
56	MG	2A	3034	1/1	0.90	0.19	23,23,23,23	0
56	MG	1A	8613	1/1	0.90	0.10	36,36,36,36	0
56	MG	2a	1652	1/1	0.90	0.17	28,28,28,28	0
56	MG	2A	3036	1/1	0.90	0.14	34,34,34,34	0
56	MG	2a	1655	1/1	0.90	0.18	48,48,48,48	0
56	MG	2A	3037	1/1	0.90	0.18	50,50,50,50	0
56	MG	2A	3468	1/1	0.90	0.19	47,47,47,47	0
56	MG	2A	3475	1/1	0.90	0.09	23,23,23,23	0
56	MG	1A	8958	1/1	0.90	0.22	28,28,28,28	0
56	MG	1A	8214	1/1	0.90	0.27	10,10,10,10	0
56	MG	2A	3914	1/1	0.90	0.16	51,51,51,51	0
56	MG	1A	8443	1/1	0.90	0.17	13,13,13,13	0
56	MG	1A	8971	1/1	0.90	0.21	9,9,9,9	0
56	MG	2A	3484	1/1	0.90	0.23	57,57,57,57	0
56	MG	1A	8616	1/1	0.90	0.26	61,61,61,61	0
56	MG	2A	3703	1/1	0.90	0.15	26,26,26,26	0
56	MG	1A	8829	1/1	0.90	0.33	42,42,42,42	0
56	MG	2A	3055	1/1	0.90	0.54	32,32,32,32	0
56	MG	1A	8001	1/1	0.90	0.14	37,37,37,37	0
56	MG	2a	1686	1/1	0.90	0.06	41,41,41,41	0
56	MG	1A	8618	1/1	0.90	0.29	41,41,41,41	0
56	MG	2a	1689	1/1	0.90	0.16	41,41,41,41	0
56	MG	1A	8839	1/1	0.90	0.30	31,31,31,31	0
56	MG	1A	8157	1/1	0.90	0.20	23,23,23,23	0
56	MG	2A	3937	1/1	0.90	0.27	38,38,38,38	0
56	MG	2A	3944	1/1	0.90	0.48	28,28,28,28	0
56	MG	1B	3011	1/1	0.90	0.08	39,39,39,39	0
56	MG	2A	3287	1/1	0.90	0.20	53,53,53,53	0
56	MG	1A	8457	1/1	0.90	0.11	9,9,9,9	0
56	MG	2A	3955	1/1	0.90	0.38	35,35,35,35	0
56	MG	1a	1668	1/1	0.90	0.28	47,47,47,47	0
56	MG	1A	8847	1/1	0.90	0.25	16,16,16,16	0
56	MG	1A	8461	1/1	0.90	0.12	10,10,10,10	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	1A	8168	1/1	0.90	0.15	23,23,23,23	0
56	MG	1A	8546	1/1	0.90	0.11	21,21,21,21	0
56	MG	2A	3309	1/1	0.90	0.08	38,38,38,38	0
56	MG	1A	8012	1/1	0.90	0.11	18,18,18,18	0
56	MG	2A	3984	1/1	0.90	0.55	37,37,37,37	0
56	MG	2A	3314	1/1	0.90	0.18	22,22,22,22	0
56	MG	1A	8198	1/1	0.90	0.19	8,8,8,8	0
56	MG	1D	312	1/1	0.90	0.13	41,41,41,41	0
56	MG	2A	3739	1/1	0.90	0.28	46,46,46,46	0
56	MG	1A	8550	1/1	0.90	0.17	35,35,35,35	0
56	MG	1E	306	1/1	0.90	0.09	41,41,41,41	0
56	MG	1A	8034	1/1	0.90	0.14	24,24,24,24	0
56	MG	2a	1724	1/1	0.90	0.22	56,56,56,56	0
56	MG	1A	8402	1/1	0.90	0.11	29,29,29,29	0
56	MG	1A	8737	1/1	0.90	0.08	24,24,24,24	0
56	MG	2A	3117	1/1	0.90	0.39	45,45,45,45	0
56	MG	2a	1730	1/1	0.90	0.10	71,71,71,71	0
56	MG	2A	3118	1/1	0.90	0.37	48,48,48,48	0
56	MG	2A	3122	1/1	0.90	0.09	55,55,55,55	0
56	MG	2A	3758	1/1	0.90	0.21	28,28,28,28	0
56	MG	1A	8558	1/1	0.90	0.08	42,42,42,42	0
56	MG	2a	1735	1/1	0.90	0.26	51,51,51,51	0
56	MG	2a	1736	1/1	0.90	0.14	68,68,68,68	0
56	MG	1a	1698	1/1	0.90	0.07	29,29,29,29	0
56	MG	2A	3766	1/1	0.90	0.12	41,41,41,41	0
56	MG	1A	8741	1/1	0.90	0.33	25,25,25,25	0
56	MG	1A	8742	1/1	0.90	0.09	50,50,50,50	0
56	MG	2A	3770	1/1	0.90	0.08	40,40,40,40	0
56	MG	2A	3142	1/1	0.90	0.25	36,36,36,36	0
56	MG	1A	8559	1/1	0.90	0.15	43,43,43,43	0
56	MG	2A	3354	1/1	0.90	0.09	27,27,27,27	0
56	MG	1A	8571	1/1	0.90	0.08	34,34,34,34	0
56	MG	2A	3566	1/1	0.90	0.14	43,43,43,43	0
56	MG	2A	3571	1/1	0.90	0.16	26,26,26,26	0
56	MG	1A	8121	1/1	0.90	0.11	19,19,19,19	0
56	MG	1R	204	1/1	0.90	0.16	26,26,26,26	0
56	MG	1A	8482	1/1	0.90	0.14	31,31,31,31	0
56	MG	2A	3586	1/1	0.90	0.17	33,33,33,33	0
56	MG	2A	3365	1/1	0.90	0.16	47,47,47,47	0
56	MG	2A	3796	1/1	0.90	0.18	29,29,29,29	0
56	MG	2A	3368	1/1	0.90	0.50	54,54,54,54	0
56	MG	2A	3167	1/1	0.90	0.16	26,26,26,26	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	1A	8242	1/1	0.90	0.22	44,44,44,44	0
56	MG	10	101	1/1	0.90	0.22	42,42,42,42	0
56	MG	2a	1774	1/1	0.90	0.14	54,54,54,54	0
56	MG	1A	8244	1/1	0.90	0.19	11,11,11,11	0
56	MG	2P	201	1/1	0.90	0.25	38,38,38,38	0
56	MG	2A	3604	1/1	0.90	0.08	43,43,43,43	0
56	MG	2Q	203	1/1	0.90	0.25	33,33,33,33	0
56	MG	2A	3382	1/1	0.90	0.11	38,38,38,38	0
56	MG	10	106	1/1	0.90	0.08	46,46,46,46	0
56	MG	1A	8672	1/1	0.90	0.13	19,19,19,19	0
56	MG	2A	3195	1/1	0.90	0.29	31,31,31,31	0
56	MG	1A	8246	1/1	0.90	0.14	45,45,45,45	0
56	MG	2A	3399	1/1	0.90	0.27	46,46,46,46	0
56	MG	2a	1789	1/1	0.90	0.05	63,63,63,63	0
56	MG	2X	102	1/1	0.90	0.11	40,40,40,40	0
56	MG	1A	8060	1/1	0.90	0.14	31,31,31,31	0
56	MG	2A	3621	1/1	0.90	0.13	44,44,44,44	0
56	MG	15	107	1/1	0.90	0.19	17,17,17,17	0
56	MG	2A	3829	1/1	0.90	0.25	53,53,53,53	0
56	MG	1A	8177	1/1	0.90	0.52	55,55,55,55	0
56	MG	2A	3624	1/1	0.90	0.15	52,52,52,52	0
56	MG	1A	8425	1/1	0.90	0.16	12,12,12,12	0
56	MG	1a	1743	1/1	0.90	0.16	41,41,41,41	0
56	MG	1A	8907	1/1	0.90	0.34	26,26,26,26	0
56	MG	2A	3414	1/1	0.90	0.07	46,46,46,46	0
56	MG	1l	203	1/1	0.90	0.15	56,56,56,56	0
56	MG	2A	3639	1/1	0.90	0.46	41,41,41,41	0
56	MG	2A	3644	1/1	0.90	0.07	40,40,40,40	0
56	MG	1A	8291	1/1	0.90	0.47	13,13,13,13	0
56	MG	2a	1608	1/1	0.90	0.13	36,36,36,36	0
56	MG	2a	1819	1/1	0.90	0.34	59,59,59,59	0
56	MG	1a	1608	1/1	0.90	0.23	47,47,47,47	0
56	MG	2A	3851	1/1	0.90	0.11	37,37,37,37	0
56	MG	2d	503	1/1	0.90	0.09	54,54,54,54	0
56	MG	1A	8518	1/1	0.90	0.15	35,35,35,35	0
56	MG	2a	1612	1/1	0.90	0.11	43,43,43,43	0
56	MG	1x	3003	1/1	0.90	0.14	31,31,31,31	0
56	MG	2h	3001	1/1	0.90	0.36	30,30,30,30	0
56	MG	2A	3225	1/1	0.90	0.34	42,42,42,42	0
56	MG	2A	3663	1/1	0.90	0.20	61,61,61,61	0
56	MG	1a	1750	1/1	0.90	0.19	56,56,56,56	0
56	MG	1A	8803	1/1	0.90	0.12	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	3428	1/1	0.90	0.13	30,30,30,30	0
56	MG	1a	1752	1/1	0.90	0.14	45,45,45,45	0
56	MG	2A	3868	1/1	0.90	0.15	48,48,48,48	0
56	MG	2a	1627	1/1	0.90	0.08	45,45,45,45	0
56	MG	1A	8921	1/1	0.90	0.14	52,52,52,52	0
56	MG	2x	110	1/1	0.90	0.11	42,42,42,42	0
56	MG	1A	8061	1/1	0.90	0.09	41,41,41,41	0
56	MG	2A	3871	1/1	0.90	0.14	56,56,56,56	0
56	MG	1A	8688	1/1	0.90	0.09	20,20,20,20	0
56	MG	1A	8946	1/1	0.90	0.21	11,11,11,11	0
56	MG	2A	3802	1/1	0.91	0.31	54,54,54,54	0
56	MG	2A	3556	1/1	0.91	0.14	49,49,49,49	0
56	MG	2A	3804	1/1	0.91	0.54	33,33,33,33	0
56	MG	1A	8523	1/1	0.91	0.15	23,23,23,23	0
56	MG	1A	8911	1/1	0.91	0.30	32,32,32,32	0
56	MG	2A	3807	1/1	0.91	0.10	29,29,29,29	0
56	MG	1A	8289	1/1	0.91	0.17	8,8,8,8	0
56	MG	2A	3077	1/1	0.91	0.36	30,30,30,30	0
56	MG	1A	8002	1/1	0.91	0.17	21,21,21,21	0
56	MG	2A	3567	1/1	0.91	0.11	43,43,43,43	0
56	MG	2A	3082	1/1	0.91	0.26	35,35,35,35	0
56	MG	2a	1617	1/1	0.91	0.10	50,50,50,50	0
56	MG	2A	3331	1/1	0.91	0.24	48,48,48,48	0
56	MG	2A	3577	1/1	0.91	0.19	25,25,25,25	0
56	MG	1A	8918	1/1	0.91	0.18	16,16,16,16	0
56	MG	2A	3582	1/1	0.91	0.28	27,27,27,27	0
56	MG	1a	1624	1/1	0.91	0.22	34,34,34,34	0
56	MG	1A	8919	1/1	0.91	0.14	11,11,11,11	0
56	MG	2A	3587	1/1	0.91	0.78	39,39,39,39	0
56	MG	1a	1778	1/1	0.91	0.10	33,33,33,33	0
56	MG	1A	8641	1/1	0.91	0.13	20,20,20,20	0
56	MG	2A	3344	1/1	0.91	0.12	41,41,41,41	0
56	MG	1a	1634	1/1	0.91	0.15	22,22,22,22	0
56	MG	2A	3600	1/1	0.91	0.27	40,40,40,40	0
56	MG	1A	8106	1/1	0.91	0.15	22,22,22,22	0
56	MG	1A	8925	1/1	0.91	0.20	32,32,32,32	0
56	MG	2A	3111	1/1	0.91	0.47	47,47,47,47	0
56	MG	2a	1643	1/1	0.91	0.30	57,57,57,57	0
56	MG	1a	1638	1/1	0.91	0.14	27,27,27,27	0
56	MG	1A	8789	1/1	0.91	0.16	22,22,22,22	0
56	MG	2A	3609	1/1	0.91	0.12	47,47,47,47	0
56	MG	1A	8941	1/1	0.91	0.29	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	2A	3612	1/1	0.91	0.15	40,40,40,40	0
56	MG	2A	3363	1/1	0.91	0.13	26,26,26,26	0
56	MG	1A	8533	1/1	0.91	0.14	28,28,28,28	0
56	MG	2A	3860	1/1	0.91	0.09	46,46,46,46	0
56	MG	1A	8952	1/1	0.91	0.28	17,17,17,17	0
56	MG	2A	3618	1/1	0.91	0.15	43,43,43,43	0
56	MG	1A	8241	1/1	0.91	0.14	10,10,10,10	0
56	MG	2A	3369	1/1	0.91	0.10	25,25,25,25	0
56	MG	2a	1666	1/1	0.91	0.15	55,55,55,55	0
56	MG	1A	8300	1/1	0.91	0.18	23,23,23,23	0
56	MG	2a	1670	1/1	0.91	0.24	53,53,53,53	0
56	MG	1a	1792	1/1	0.91	0.11	41,41,41,41	0
56	MG	1a	1658	1/1	0.91	0.40	29,29,29,29	0
56	MG	2a	1675	1/1	0.91	0.18	42,42,42,42	0
56	MG	2A	3375	1/1	0.91	0.19	24,24,24,24	0
56	MG	2A	3131	1/1	0.91	1.08	33,33,33,33	0
56	MG	2A	3377	1/1	0.91	0.19	32,32,32,32	0
56	MG	2A	3879	1/1	0.91	0.22	36,36,36,36	0
56	MG	2A	3633	1/1	0.91	0.30	44,44,44,44	0
56	MG	2A	3379	1/1	0.91	0.11	36,36,36,36	0
56	MG	2A	3883	1/1	0.91	0.09	60,60,60,60	0
56	MG	1A	8420	1/1	0.91	0.09	28,28,28,28	0
56	MG	2A	3139	1/1	0.91	0.23	45,45,45,45	0
56	MG	2A	3640	1/1	0.91	0.28	26,26,26,26	0
56	MG	2A	3389	1/1	0.91	0.07	45,45,45,45	0
56	MG	2A	3646	1/1	0.91	0.15	51,51,51,51	0
56	MG	2A	3141	1/1	0.91	0.11	27,27,27,27	0
56	MG	1A	8655	1/1	0.91	0.16	22,22,22,22	0
56	MG	1A	8050	1/1	0.91	0.20	23,23,23,23	0
56	MG	1A	8024	1/1	0.91	0.29	8,8,8,8	0
56	MG	2A	3157	1/1	0.91	0.10	40,40,40,40	0
56	MG	1A	8115	1/1	0.91	0.19	13,13,13,13	0
56	MG	2A	3159	1/1	0.91	0.14	36,36,36,36	0
56	MG	1A	8666	1/1	0.91	0.10	18,18,18,18	0
56	MG	2A	3410	1/1	0.91	0.04	45,45,45,45	0
56	MG	1A	8548	1/1	0.91	0.09	27,27,27,27	0
56	MG	2A	3921	1/1	0.91	0.34	19,19,19,19	0
56	MG	1A	8315	1/1	0.91	0.23	28,28,28,28	0
56	MG	1B	3008	1/1	0.91	0.14	35,35,35,35	0
56	MG	2A	3415	1/1	0.91	0.29	34,34,34,34	0
56	MG	2A	3925	1/1	0.91	0.05	42,42,42,42	0
56	MG	2A	3416	1/1	0.91	0.10	28,28,28,28	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	1A	8019	1/1	0.91	0.38	12,12,12,12	0
56	MG	1A	8200	1/1	0.91	0.13	46,46,46,46	0
56	MG	1B	3016	1/1	0.91	0.14	51,51,51,51	0
56	MG	1A	8152	1/1	0.91	0.09	28,28,28,28	0
56	MG	2A	3680	1/1	0.91	0.38	38,38,38,38	0
56	MG	2A	3188	1/1	0.91	0.34	33,33,33,33	0
56	MG	1a	1821	1/1	0.91	0.20	39,39,39,39	0
56	MG	1a	1823	1/1	0.91	0.11	42,42,42,42	0
56	MG	2a	1728	1/1	0.91	0.34	64,64,64,64	0
56	MG	2a	1729	1/1	0.91	0.32	62,62,62,62	0
56	MG	2A	3948	1/1	0.91	0.46	42,42,42,42	0
56	MG	1A	8448	1/1	0.91	0.19	8,8,8,8	0
56	MG	2A	3954	1/1	0.91	0.55	41,41,41,41	0
56	MG	1A	8323	1/1	0.91	0.10	20,20,20,20	0
56	MG	1A	8154	1/1	0.91	0.24	22,22,22,22	0
56	MG	2A	3203	1/1	0.91	0.58	28,28,28,28	0
56	MG	2A	3960	1/1	0.91	0.72	45,45,45,45	0
56	MG	2A	3204	1/1	0.91	0.33	31,31,31,31	0
56	MG	1A	8203	1/1	0.91	0.11	15,15,15,15	0
56	MG	2A	3971	1/1	0.91	0.47	41,41,41,41	0
56	MG	1A	8120	1/1	0.91	0.12	53,53,53,53	0
56	MG	2A	3978	1/1	0.91	0.16	41,41,41,41	0
56	MG	2a	1745	1/1	0.91	0.05	55,55,55,55	0
56	MG	1D	304	1/1	0.91	0.21	14,14,14,14	0
56	MG	1a	1840	1/1	0.91	0.22	55,55,55,55	0
56	MG	1A	8579	1/1	0.91	0.25	27,27,27,27	0
56	MG	2a	1754	1/1	0.91	0.07	42,42,42,42	0
56	MG	1A	8027	1/1	0.91	0.13	38,38,38,38	0
56	MG	2B	3001	1/1	0.91	0.12	59,59,59,59	0
56	MG	1A	8040	1/1	0.91	0.34	32,32,32,32	0
56	MG	2A	3460	1/1	0.91	0.19	25,25,25,25	0
56	MG	1A	8587	1/1	0.91	0.24	21,21,21,21	0
56	MG	1A	8698	1/1	0.91	0.06	30,30,30,30	0
56	MG	1A	8044	1/1	0.91	0.24	7,7,7,7	0
56	MG	2A	3715	1/1	0.91	0.15	28,28,28,28	0
56	MG	1A	8600	1/1	0.91	0.33	26,26,26,26	0
56	MG	2A	3474	1/1	0.91	0.07	37,37,37,37	0
56	MG	1A	8858	1/1	0.91	0.14	28,28,28,28	0
56	MG	1N	203	1/1	0.91	0.14	47,47,47,47	0
56	MG	1o	102	1/1	0.91	0.10	26,26,26,26	0
56	MG	2B	3016	1/1	0.91	0.19	55,55,55,55	0
56	MG	1A	8126	1/1	0.91	0.22	12,12,12,12	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	2a	1777	1/1	0.91	0.20	45,45,45,45	0
56	MG	1A	8175	1/1	0.91	0.19	25,25,25,25	0
56	MG	1A	8478	1/1	0.91	0.42	9,9,9,9	0
56	MG	2A	3730	1/1	0.91	0.22	50,50,50,50	0
56	MG	1A	8719	1/1	0.91	0.13	9,9,9,9	0
56	MG	1A	8269	1/1	0.91	0.12	23,23,23,23	0
56	MG	2A	3490	1/1	0.91	0.17	39,39,39,39	0
56	MG	2A	3006	1/1	0.91	0.21	45,45,45,45	0
56	MG	2A	3010	1/1	0.91	0.34	28,28,28,28	0
56	MG	1A	8128	1/1	0.91	0.24	40,40,40,40	0
56	MG	2A	3740	1/1	0.91	0.40	39,39,39,39	0
56	MG	2a	1790	1/1	0.91	0.15	51,51,51,51	0
56	MG	2A	3014	1/1	0.91	0.23	39,39,39,39	0
56	MG	2D	315	1/1	0.91	0.10	24,24,24,24	0
56	MG	1A	8224	1/1	0.91	0.25	15,15,15,15	0
56	MG	1A	8874	1/1	0.91	0.10	9,9,9,9	0
56	MG	2E	301	1/1	0.91	0.18	37,37,37,37	0
56	MG	2E	302	1/1	0.91	0.11	26,26,26,26	0
56	MG	1A	8491	1/1	0.91	0.15	9,9,9,9	0
56	MG	2F	301	1/1	0.91	0.16	43,43,43,43	0
56	MG	2F	302	1/1	0.91	0.32	28,28,28,28	0
56	MG	1A	8731	1/1	0.91	0.41	40,40,40,40	0
56	MG	2A	3030	1/1	0.91	0.15	47,47,47,47	0
56	MG	2a	1806	1/1	0.91	0.18	65,65,65,65	0
56	MG	2A	3031	1/1	0.91	0.48	27,27,27,27	0
56	MG	10	105	1/1	0.91	0.12	27,27,27,27	0
56	MG	2A	3281	1/1	0.91	0.16	52,52,52,52	0
56	MG	1A	8493	1/1	0.91	0.14	16,16,16,16	0
56	MG	2a	1813	1/1	0.91	0.18	42,42,42,42	0
56	MG	2A	3764	1/1	0.91	0.07	62,62,62,62	0
56	MG	1A	8227	1/1	0.91	0.25	14,14,14,14	0
56	MG	1A	8029	1/1	0.91	0.18	15,15,15,15	0
56	MG	1A	8282	1/1	0.91	0.09	45,45,45,45	0
56	MG	2b	3001	1/1	0.91	0.17	56,56,56,56	0
56	MG	1A	8283	1/1	0.91	0.23	13,13,13,13	0
56	MG	2A	3043	1/1	0.91	0.19	42,42,42,42	0
56	MG	2A	3529	1/1	0.91	0.14	44,44,44,44	0
56	MG	2A	3294	1/1	0.91	0.09	50,50,50,50	0
56	MG	2A	3776	1/1	0.91	0.07	51,51,51,51	0
56	MG	2A	3777	1/1	0.91	0.41	61,61,61,61	0
56	MG	17	102	1/1	0.91	0.14	34,34,34,34	0
56	MG	1A	8390	1/1	0.91	0.11	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	8517	1/1	0.91	0.10	32,32,32,32	0
56	MG	1a	1603	1/1	0.91	0.11	39,39,39,39	0
56	MG	1A	8401	1/1	0.91	0.21	28,28,28,28	0
56	MG	2A	3790	1/1	0.91	0.15	45,45,45,45	0
56	MG	1A	8744	1/1	0.91	0.14	17,17,17,17	0
56	MG	2A	3311	1/1	0.91	0.10	29,29,29,29	0
56	MG	1A	8185	1/1	0.91	0.23	26,26,26,26	0
56	MG	1a	1610	1/1	0.91	0.38	36,36,36,36	0
56	MG	1a	1763	1/1	0.91	0.06	55,55,55,55	0
56	MG	2A	3069	1/1	0.91	0.42	36,36,36,36	0
56	MG	2A	3555	1/1	0.91	0.20	35,35,35,35	0
56	MG	2A	3328	1/1	0.92	0.34	31,31,31,31	0
56	MG	1A	8298	1/1	0.92	0.13	12,12,12,12	0
56	MG	1a	1643	1/1	0.92	0.16	53,53,53,53	0
56	MG	1A	8350	1/1	0.92	0.18	8,8,8,8	0
56	MG	2A	3574	1/1	0.92	0.17	31,31,31,31	0
56	MG	2A	3575	1/1	0.92	0.30	42,42,42,42	0
56	MG	2A	3815	1/1	0.92	0.11	33,33,33,33	0
56	MG	1a	1648	1/1	0.92	0.21	38,38,38,38	0
56	MG	1a	1649	1/1	0.92	0.37	32,32,32,32	0
56	MG	1A	8150	1/1	0.92	0.23	36,36,36,36	0
56	MG	2a	1616	1/1	0.92	0.16	37,37,37,37	0
56	MG	2A	3581	1/1	0.92	0.14	31,31,31,31	0
56	MG	2A	3826	1/1	0.92	0.07	33,33,33,33	0
56	MG	1B	3006	1/1	0.92	0.13	25,25,25,25	0
56	MG	1A	8485	1/1	0.92	0.12	30,30,30,30	0
56	MG	2A	3109	1/1	0.92	0.22	41,41,41,41	0
56	MG	1A	8037	1/1	0.92	0.12	14,14,14,14	0
56	MG	2A	3352	1/1	0.92	0.15	60,60,60,60	0
56	MG	1A	8848	1/1	0.92	0.08	13,13,13,13	0
56	MG	1A	8490	1/1	0.92	0.25	18,18,18,18	0
56	MG	1A	8568	1/1	0.92	0.15	11,11,11,11	0
56	MG	1a	1799	1/1	0.92	0.10	35,35,35,35	0
56	MG	2A	3601	1/1	0.92	0.29	44,44,44,44	0
56	MG	2A	3844	1/1	0.92	0.15	46,46,46,46	0
56	MG	2A	3845	1/1	0.92	0.37	51,51,51,51	0
56	MG	1A	8183	1/1	0.92	0.12	24,24,24,24	0
56	MG	1A	8733	1/1	0.92	0.18	54,54,54,54	0
56	MG	1A	8856	1/1	0.92	0.15	18,18,18,18	0
56	MG	2a	1644	1/1	0.92	0.17	46,46,46,46	0
56	MG	1A	8424	1/1	0.92	0.14	26,26,26,26	0
56	MG	2A	3850	1/1	0.92	0.17	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	8651	1/1	0.92	0.16	23,23,23,23	0
56	MG	1a	1673	1/1	0.92	0.19	35,35,35,35	0
56	MG	1a	1809	1/1	0.92	0.18	51,51,51,51	0
56	MG	1a	1676	1/1	0.92	0.22	30,30,30,30	0
56	MG	2A	3140	1/1	0.92	0.18	25,25,25,25	0
56	MG	1A	8057	1/1	0.92	0.13	12,12,12,12	0
56	MG	2a	1659	1/1	0.92	0.16	46,46,46,46	0
56	MG	1A	8861	1/1	0.92	0.17	39,39,39,39	0
56	MG	1a	1679	1/1	0.92	0.25	36,36,36,36	0
56	MG	1A	8654	1/1	0.92	0.28	32,32,32,32	0
56	MG	2A	3151	1/1	0.92	0.60	32,32,32,32	0
56	MG	2A	3867	1/1	0.92	0.11	42,42,42,42	0
56	MG	1a	1819	1/1	0.92	0.11	37,37,37,37	0
56	MG	1A	8431	1/1	0.92	0.10	17,17,17,17	0
56	MG	1A	8434	1/1	0.92	0.18	16,16,16,16	0
56	MG	2A	3160	1/1	0.92	0.15	28,28,28,28	0
56	MG	1E	303	1/1	0.92	0.13	11,11,11,11	0
56	MG	2A	3162	1/1	0.92	0.17	39,39,39,39	0
56	MG	2A	3401	1/1	0.92	0.16	38,38,38,38	0
56	MG	2a	1678	1/1	0.92	0.12	37,37,37,37	0
56	MG	1A	8505	1/1	0.92	0.15	24,24,24,24	0
56	MG	1A	8868	1/1	0.92	0.11	22,22,22,22	0
56	MG	2A	3882	1/1	0.92	0.05	46,46,46,46	0
56	MG	1F	305	1/1	0.92	0.15	15,15,15,15	0
56	MG	1a	1830	1/1	0.92	0.10	45,45,45,45	0
56	MG	2A	3411	1/1	0.92	0.17	36,36,36,36	0
56	MG	2A	3890	1/1	0.92	0.36	60,60,60,60	0
56	MG	1a	1832	1/1	0.92	0.07	44,44,44,44	0
56	MG	1F	307	1/1	0.92	0.20	13,13,13,13	0
56	MG	1a	1838	1/1	0.92	0.13	46,46,46,46	0
56	MG	2a	1695	1/1	0.92	0.26	53,53,53,53	0
56	MG	1A	8586	1/1	0.92	0.23	27,27,27,27	0
56	MG	2A	3659	1/1	0.92	0.14	30,30,30,30	0
56	MG	1A	8745	1/1	0.92	0.18	17,17,17,17	0
56	MG	2A	3196	1/1	0.92	0.30	31,31,31,31	0
56	MG	1A	8155	1/1	0.92	0.21	24,24,24,24	0
56	MG	1A	8877	1/1	0.92	0.10	38,38,38,38	0
56	MG	2A	3665	1/1	0.92	0.21	29,29,29,29	0
56	MG	1A	8038	1/1	0.92	0.09	40,40,40,40	0
56	MG	1A	8668	1/1	0.92	0.24	32,32,32,32	0
56	MG	1f	8001	1/1	0.92	0.15	36,36,36,36	0
56	MG	1A	8763	1/1	0.92	0.37	28,28,28,28	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	1A	8882	1/1	0.92	0.15	38,38,38,38	0
56	MG	1a	1722	1/1	0.92	0.08	32,32,32,32	0
56	MG	2A	3429	1/1	0.92	0.12	37,37,37,37	0
56	MG	2A	3211	1/1	0.92	0.28	35,35,35,35	0
56	MG	1A	8159	1/1	0.92	0.14	21,21,21,21	0
56	MG	1R	201	1/1	0.92	0.16	18,18,18,18	0
56	MG	1A	8772	1/1	0.92	0.06	27,27,27,27	0
56	MG	2A	3930	1/1	0.92	0.39	48,48,48,48	0
56	MG	1A	8138	1/1	0.92	0.13	14,14,14,14	0
56	MG	1A	8776	1/1	0.92	0.25	35,35,35,35	0
56	MG	2A	3934	1/1	0.92	0.34	32,32,32,32	0
56	MG	1A	8780	1/1	0.92	0.24	10,10,10,10	0
56	MG	2A	3444	1/1	0.92	0.12	32,32,32,32	0
56	MG	1A	8781	1/1	0.92	0.16	14,14,14,14	0
56	MG	2A	3687	1/1	0.92	0.10	30,30,30,30	0
56	MG	2A	3226	1/1	0.92	0.23	27,27,27,27	0
56	MG	2A	3228	1/1	0.92	0.39	34,34,34,34	0
56	MG	2A	3456	1/1	0.92	0.12	23,23,23,23	0
56	MG	2A	3458	1/1	0.92	0.13	37,37,37,37	0
56	MG	2A	3230	1/1	0.92	0.26	33,33,33,33	0
56	MG	1x	3007	1/1	0.92	0.13	37,37,37,37	0
56	MG	2A	3462	1/1	0.92	0.21	26,26,26,26	0
56	MG	1a	1736	1/1	0.92	0.07	40,40,40,40	0
56	MG	1A	8384	1/1	0.92	0.28	36,36,36,36	0
56	MG	2A	3968	1/1	0.92	0.22	38,38,38,38	0
56	MG	2A	3007	1/1	0.92	0.15	38,38,38,38	0
56	MG	2A	3469	1/1	0.92	0.24	31,31,31,31	0
56	MG	2A	3472	1/1	0.92	0.22	29,29,29,29	0
56	MG	2a	1746	1/1	0.92	0.20	59,59,59,59	0
56	MG	2a	1750	1/1	0.92	0.14	67,67,67,67	0
56	MG	2A	3980	1/1	0.92	0.17	51,51,51,51	0
56	MG	2A	3008	1/1	0.92	0.12	27,27,27,27	0
56	MG	2A	3710	1/1	0.92	0.17	39,39,39,39	0
56	MG	1A	8787	1/1	0.92	0.12	8,8,8,8	0
56	MG	1a	1741	1/1	0.92	0.18	47,47,47,47	0
56	MG	2a	1757	1/1	0.92	0.24	55,55,55,55	0
56	MG	2A	3713	1/1	0.92	0.12	24,24,24,24	0
56	MG	1A	8059	1/1	0.92	0.18	7,7,7,7	0
56	MG	2B	3004	1/1	0.92	0.17	63,63,63,63	0
56	MG	2A	3717	1/1	0.92	0.25	24,24,24,24	0
56	MG	2A	3249	1/1	0.92	0.21	31,31,31,31	0
56	MG	1A	8790	1/1	0.92	0.11	20,20,20,20	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	1A	8525	1/1	0.92	0.20	10,10,10,10	0
56	MG	2a	1765	1/1	0.92	0.39	47,47,47,47	0
56	MG	1A	8387	1/1	0.92	0.20	28,28,28,28	0
56	MG	2A	3724	1/1	0.92	0.55	50,50,50,50	0
56	MG	2a	1768	1/1	0.92	0.23	57,57,57,57	0
56	MG	2A	3020	1/1	0.92	0.21	26,26,26,26	0
56	MG	2A	3488	1/1	0.92	0.20	30,30,30,30	0
56	MG	2A	3025	1/1	0.92	0.13	33,33,33,33	0
56	MG	2A	3027	1/1	0.92	0.18	31,31,31,31	0
56	MG	2A	3496	1/1	0.92	0.11	36,36,36,36	0
56	MG	2A	3028	1/1	0.92	0.41	34,34,34,34	0
56	MG	1A	8222	1/1	0.92	0.24	18,18,18,18	0
56	MG	1A	8917	1/1	0.92	0.45	21,21,21,21	0
56	MG	1A	8032	1/1	0.92	0.20	6,6,6,6	0
56	MG	2a	1782	1/1	0.92	0.48	61,61,61,61	0
56	MG	2A	3032	1/1	0.92	0.27	43,43,43,43	0
56	MG	2A	3276	1/1	0.92	0.13	42,42,42,42	0
56	MG	1A	8398	1/1	0.92	0.19	41,41,41,41	0
56	MG	1A	8199	1/1	0.92	0.17	14,14,14,14	0
56	MG	2B	3025	1/1	0.92	0.39	52,52,52,52	0
56	MG	2A	3512	1/1	0.92	0.05	53,53,53,53	0
56	MG	2A	3513	1/1	0.92	0.19	38,38,38,38	0
56	MG	1A	8466	1/1	0.92	0.10	25,25,25,25	0
56	MG	2D	313	1/1	0.92	0.21	32,32,32,32	0
56	MG	2a	1792	1/1	0.92	0.19	55,55,55,55	0
56	MG	1A	8054	1/1	0.92	0.16	9,9,9,9	0
56	MG	2A	3750	1/1	0.92	0.06	24,24,24,24	0
56	MG	2a	1795	1/1	0.92	0.23	65,65,65,65	0
56	MG	1A	8931	1/1	0.92	0.15	18,18,18,18	0
56	MG	2A	3521	1/1	0.92	0.21	34,34,34,34	0
56	MG	2A	3522	1/1	0.92	0.33	51,51,51,51	0
56	MG	1A	8410	1/1	0.92	0.07	35,35,35,35	0
56	MG	2A	3759	1/1	0.92	0.12	52,52,52,52	0
56	MG	2a	1802	1/1	0.92	0.12	60,60,60,60	0
56	MG	2E	305	1/1	0.92	0.29	60,60,60,60	0
56	MG	2A	3761	1/1	0.92	0.40	43,43,43,43	0
56	MG	1A	8696	1/1	0.92	0.14	20,20,20,20	0
56	MG	1a	1617	1/1	0.92	0.14	53,53,53,53	0
56	MG	2A	3048	1/1	0.92	0.39	40,40,40,40	0
56	MG	1a	1618	1/1	0.92	0.20	57,57,57,57	0
56	MG	1A	8470	1/1	0.92	0.22	39,39,39,39	0
56	MG	1A	8948	1/1	0.92	0.17	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	2a	1812	1/1	0.92	0.14	64,64,64,64	0
56	MG	2A	3769	1/1	0.92	0.08	31,31,31,31	0
56	MG	2A	3530	1/1	0.92	0.58	45,45,45,45	0
56	MG	2a	1818	1/1	0.92	0.08	61,61,61,61	0
56	MG	2A	3300	1/1	0.92	0.22	30,30,30,30	0
56	MG	2A	3302	1/1	0.92	0.20	48,48,48,48	0
56	MG	2A	3053	1/1	0.92	0.41	27,27,27,27	0
56	MG	2A	3537	1/1	0.92	0.16	33,33,33,33	0
56	MG	1A	8623	1/1	0.92	0.57	18,18,18,18	0
56	MG	2A	3540	1/1	0.92	0.16	48,48,48,48	0
56	MG	2A	3541	1/1	0.92	0.15	24,24,24,24	0
56	MG	1a	1769	1/1	0.92	0.18	46,46,46,46	0
56	MG	1A	8341	1/1	0.92	0.14	17,17,17,17	0
56	MG	2A	3787	1/1	0.92	0.27	41,41,41,41	0
56	MG	1A	8063	1/1	0.92	0.13	22,22,22,22	0
56	MG	1a	1628	1/1	0.92	0.12	39,39,39,39	0
56	MG	2A	3064	1/1	0.92	0.16	34,34,34,34	0
56	MG	2A	3066	1/1	0.92	0.18	26,26,26,26	0
56	MG	1A	8959	1/1	0.92	0.17	27,27,27,27	0
56	MG	1A	8629	1/1	0.92	0.17	45,45,45,45	0
56	MG	2A	3553	1/1	0.92	0.10	52,52,52,52	0
56	MG	1A	8967	1/1	0.92	0.36	27,27,27,27	0
56	MG	2A	3800	1/1	0.92	0.14	34,34,34,34	0
56	MG	1A	8831	1/1	0.92	0.13	41,41,41,41	0
56	MG	1A	8833	1/1	0.92	0.14	12,12,12,12	0
56	MG	1A	8717	1/1	0.92	0.14	16,16,16,16	0
56	MG	1a	1641	1/1	0.92	0.21	33,33,33,33	0
56	MG	1A	8703	1/1	0.93	0.19	28,28,28,28	0
56	MG	1A	8597	1/1	0.93	0.27	14,14,14,14	0
56	MG	1A	8599	1/1	0.93	0.16	24,24,24,24	0
56	MG	2a	1620	1/1	0.93	0.28	69,69,69,69	0
56	MG	1a	1692	1/1	0.93	0.20	40,40,40,40	0
56	MG	1A	8014	1/1	0.93	0.19	5,5,5,5	0
56	MG	2A	3176	1/1	0.93	0.24	42,42,42,42	0
56	MG	2A	3177	1/1	0.93	0.52	56,56,56,56	0
56	MG	1E	304	1/1	0.93	0.10	27,27,27,27	0
56	MG	2A	3855	1/1	0.93	0.15	32,32,32,32	0
56	MG	1d	503	1/1	0.93	0.28	38,38,38,38	0
56	MG	1A	8497	1/1	0.93	0.12	20,20,20,20	0
56	MG	2A	3183	1/1	0.93	0.18	36,36,36,36	0
56	MG	1A	8603	1/1	0.93	0.13	24,24,24,24	0
56	MG	2a	1636	1/1	0.93	0.25	33,33,33,33	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	1a	1703	1/1	0.93	0.12	48,48,48,48	0
56	MG	2A	3191	1/1	0.93	0.26	35,35,35,35	0
56	MG	2A	3192	1/1	0.93	0.21	29,29,29,29	0
56	MG	2A	3865	1/1	0.93	0.15	48,48,48,48	0
56	MG	1A	8148	1/1	0.93	0.13	7,7,7,7	0
56	MG	2A	3417	1/1	0.93	0.17	51,51,51,51	0
56	MG	1A	8097	1/1	0.93	0.13	18,18,18,18	0
56	MG	1A	8122	1/1	0.93	0.10	18,18,18,18	0
56	MG	1A	8609	1/1	0.93	0.13	18,18,18,18	0
56	MG	2a	1648	1/1	0.93	0.27	33,33,33,33	0
56	MG	1A	8507	1/1	0.93	0.19	33,33,33,33	0
56	MG	1A	8041	1/1	0.93	0.23	24,24,24,24	0
56	MG	1a	1721	1/1	0.93	0.11	49,49,49,49	0
56	MG	2A	3874	1/1	0.93	0.18	32,32,32,32	0
56	MG	1A	8228	1/1	0.93	0.36	13,13,13,13	0
56	MG	1A	8430	1/1	0.93	0.09	13,13,13,13	0
56	MG	2a	1657	1/1	0.93	0.40	38,38,38,38	0
56	MG	1a	1724	1/1	0.93	0.13	50,50,50,50	0
56	MG	2A	3210	1/1	0.93	0.15	34,34,34,34	0
56	MG	1A	8025	1/1	0.93	0.57	23,23,23,23	0
56	MG	2A	3884	1/1	0.93	0.18	37,37,37,37	0
56	MG	1a	1727	1/1	0.93	0.09	32,32,32,32	0
56	MG	2A	3888	1/1	0.93	0.15	41,41,41,41	0
56	MG	1a	1728	1/1	0.93	0.10	38,38,38,38	0
56	MG	1x	3013	1/1	0.93	0.13	53,53,53,53	0
56	MG	2A	3003	1/1	0.93	0.13	42,42,42,42	0
56	MG	1A	8433	1/1	0.93	0.12	14,14,14,14	0
56	MG	1A	8876	1/1	0.93	0.15	10,10,10,10	0
56	MG	2A	3895	1/1	0.93	0.11	27,27,27,27	0
56	MG	1Q	205	1/1	0.93	0.15	26,26,26,26	0
56	MG	2A	3900	1/1	0.93	0.11	41,41,41,41	0
56	MG	1A	8522	1/1	0.93	0.14	34,34,34,34	0
56	MG	2A	3227	1/1	0.93	0.26	34,34,34,34	0
56	MG	1A	8271	1/1	0.93	0.21	21,21,21,21	0
56	MG	2a	1683	1/1	0.93	0.17	61,61,61,61	0
56	MG	1A	8524	1/1	0.93	0.20	31,31,31,31	0
56	MG	2A	3457	1/1	0.93	0.12	50,50,50,50	0
56	MG	2A	3912	1/1	0.93	0.78	49,49,49,49	0
56	MG	1A	8436	1/1	0.93	0.15	7,7,7,7	0
56	MG	2A	3233	1/1	0.93	0.45	28,28,28,28	0
56	MG	1V	202	1/1	0.93	0.17	26,26,26,26	0
56	MG	2A	3017	1/1	0.93	0.23	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	3920	1/1	0.93	0.18	43,43,43,43	0
56	MG	2A	3236	1/1	0.93	0.41	46,46,46,46	0
56	MG	1A	8273	1/1	0.93	0.11	32,32,32,32	0
56	MG	1A	8274	1/1	0.93	0.11	23,23,23,23	0
56	MG	2A	3697	1/1	0.93	0.35	35,35,35,35	0
56	MG	1A	8233	1/1	0.93	0.28	21,21,21,21	0
56	MG	1A	8065	1/1	0.93	0.16	11,11,11,11	0
56	MG	1a	1746	1/1	0.93	0.31	44,44,44,44	0
56	MG	2A	3701	1/1	0.93	0.23	42,42,42,42	0
56	MG	1A	8895	1/1	0.93	0.09	12,12,12,12	0
56	MG	1A	8896	1/1	0.93	0.10	35,35,35,35	0
56	MG	2A	3932	1/1	0.93	0.18	31,31,31,31	0
56	MG	2A	3478	1/1	0.93	0.15	38,38,38,38	0
56	MG	1A	8897	1/1	0.93	0.11	48,48,48,48	0
56	MG	1A	8105	1/1	0.93	0.34	12,12,12,12	0
56	MG	2A	3939	1/1	0.93	0.26	43,43,43,43	0
56	MG	2A	3707	1/1	0.93	0.06	31,31,31,31	0
56	MG	2a	1717	1/1	0.93	0.13	54,54,54,54	0
56	MG	1A	8161	1/1	0.93	0.41	10,10,10,10	0
56	MG	2A	3946	1/1	0.93	0.69	29,29,29,29	0
56	MG	2A	3258	1/1	0.93	0.16	36,36,36,36	0
56	MG	1A	8759	1/1	0.93	0.26	15,15,15,15	0
56	MG	2A	3951	1/1	0.93	0.29	30,30,30,30	0
56	MG	2A	3260	1/1	0.93	0.18	26,26,26,26	0
56	MG	1A	8760	1/1	0.93	0.10	12,12,12,12	0
56	MG	2A	3714	1/1	0.93	0.11	39,39,39,39	0
56	MG	1A	8539	1/1	0.93	0.17	26,26,26,26	0
56	MG	2A	3716	1/1	0.93	0.38	37,37,37,37	0
56	MG	2A	3493	1/1	0.93	0.12	32,32,32,32	0
56	MG	1A	8906	1/1	0.93	0.13	13,13,13,13	0
56	MG	2A	3963	1/1	0.93	0.31	53,53,53,53	0
56	MG	1A	8764	1/1	0.93	0.11	27,27,27,27	0
56	MG	2A	3042	1/1	0.93	0.14	38,38,38,38	0
56	MG	1a	1606	1/1	0.93	0.18	36,36,36,36	0
56	MG	1a	1607	1/1	0.93	0.10	49,49,49,49	0
56	MG	2a	1737	1/1	0.93	0.08	53,53,53,53	0
56	MG	2A	3277	1/1	0.93	0.44	59,59,59,59	0
56	MG	2A	3979	1/1	0.93	0.15	57,57,57,57	0
56	MG	2A	3278	1/1	0.93	0.11	30,30,30,30	0
56	MG	1A	8540	1/1	0.93	0.10	21,21,21,21	0
56	MG	1A	8541	1/1	0.93	0.17	31,31,31,31	0
56	MG	2A	3505	1/1	0.93	0.30	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	2A	3508	1/1	0.93	0.13	44,44,44,44	0
56	MG	1A	8083	1/1	0.93	0.12	15,15,15,15	0
56	MG	1a	1765	1/1	0.93	0.13	44,44,44,44	0
56	MG	2A	3735	1/1	0.93	0.08	46,46,46,46	0
56	MG	1a	1767	1/1	0.93	0.14	55,55,55,55	0
56	MG	2A	3517	1/1	0.93	0.21	47,47,47,47	0
56	MG	1a	1613	1/1	0.93	0.27	15,15,15,15	0
56	MG	1A	8373	1/1	0.93	0.13	13,13,13,13	0
56	MG	2A	3741	1/1	0.93	0.21	69,69,69,69	0
56	MG	2A	3058	1/1	0.93	0.09	42,42,42,42	0
56	MG	1A	8285	1/1	0.93	0.14	10,10,10,10	0
56	MG	1A	8088	1/1	0.93	0.15	16,16,16,16	0
56	MG	1A	8091	1/1	0.93	0.26	16,16,16,16	0
56	MG	1A	8290	1/1	0.93	0.10	19,19,19,19	0
56	MG	1a	1622	1/1	0.93	0.18	32,32,32,32	0
56	MG	1A	8114	1/1	0.93	0.18	20,20,20,20	0
56	MG	2A	3754	1/1	0.93	0.27	36,36,36,36	0
56	MG	1A	8174	1/1	0.93	0.14	28,28,28,28	0
56	MG	1A	8930	1/1	0.93	0.17	23,23,23,23	0
56	MG	1a	1626	1/1	0.93	0.17	38,38,38,38	0
56	MG	1A	8793	1/1	0.93	0.12	27,27,27,27	0
56	MG	2A	3310	1/1	0.93	0.18	25,25,25,25	0
56	MG	2a	1772	1/1	0.93	0.33	57,57,57,57	0
56	MG	1A	8661	1/1	0.93	0.11	7,7,7,7	0
56	MG	1A	8936	1/1	0.93	0.23	11,11,11,11	0
56	MG	1A	8031	1/1	0.93	0.19	12,12,12,12	0
56	MG	1A	8556	1/1	0.93	0.28	17,17,17,17	0
56	MG	2D	304	1/1	0.93	0.22	41,41,41,41	0
56	MG	2A	3090	1/1	0.93	0.28	39,39,39,39	0
56	MG	1A	8116	1/1	0.93	0.20	25,25,25,25	0
56	MG	1A	8094	1/1	0.93	0.19	12,12,12,12	0
56	MG	1A	8392	1/1	0.93	0.14	37,37,37,37	0
56	MG	2A	3097	1/1	0.93	0.43	38,38,38,38	0
56	MG	1A	8569	1/1	0.93	0.15	16,16,16,16	0
56	MG	2A	3101	1/1	0.93	0.37	48,48,48,48	0
56	MG	2A	3103	1/1	0.93	0.21	30,30,30,30	0
56	MG	1A	8570	1/1	0.93	0.19	34,34,34,34	0
56	MG	1A	8303	1/1	0.93	0.08	11,11,11,11	0
56	MG	2E	306	1/1	0.93	0.07	44,44,44,44	0
56	MG	2A	3780	1/1	0.93	0.30	44,44,44,44	0
56	MG	2A	3336	1/1	0.93	0.08	44,44,44,44	0
56	MG	2A	3554	1/1	0.93	0.41	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	2A	3107	1/1	0.93	0.22	34,34,34,34	0
56	MG	1A	8805	1/1	0.93	0.10	34,34,34,34	0
56	MG	1A	8572	1/1	0.93	0.14	5,5,5,5	0
56	MG	1A	8677	1/1	0.93	0.14	24,24,24,24	0
56	MG	1A	8483	1/1	0.93	0.14	30,30,30,30	0
56	MG	1A	8818	1/1	0.93	0.38	33,33,33,33	0
56	MG	1A	8824	1/1	0.93	0.14	37,37,37,37	0
56	MG	1A	8577	1/1	0.93	0.12	21,21,21,21	0
56	MG	2A	3569	1/1	0.93	0.07	43,43,43,43	0
56	MG	2A	3119	1/1	0.93	0.14	35,35,35,35	0
56	MG	2A	3353	1/1	0.93	0.17	27,27,27,27	0
56	MG	2A	3121	1/1	0.93	0.05	42,42,42,42	0
56	MG	1A	8307	1/1	0.93	0.05	18,18,18,18	0
56	MG	1A	8179	1/1	0.93	0.39	16,16,16,16	0
56	MG	1a	1666	1/1	0.93	0.30	31,31,31,31	0
56	MG	2U	206	1/1	0.93	0.24	38,38,38,38	0
56	MG	1A	8487	1/1	0.93	0.14	31,31,31,31	0
56	MG	1A	8311	1/1	0.93	0.15	11,11,11,11	0
56	MG	1A	8218	1/1	0.93	0.13	11,11,11,11	0
56	MG	2A	3367	1/1	0.93	0.36	55,55,55,55	0
56	MG	1A	8258	1/1	0.93	0.41	24,24,24,24	0
56	MG	20	103	1/1	0.93	0.10	62,62,62,62	0
56	MG	1A	8836	1/1	0.93	0.08	17,17,17,17	0
56	MG	1A	8591	1/1	0.93	0.27	10,10,10,10	0
56	MG	2A	3371	1/1	0.93	0.13	18,18,18,18	0
56	MG	2A	3593	1/1	0.93	0.27	24,24,24,24	0
56	MG	1A	8592	1/1	0.93	0.16	24,24,24,24	0
56	MG	1A	8697	1/1	0.93	0.13	32,32,32,32	0
56	MG	1A	8593	1/1	0.93	0.26	16,16,16,16	0
56	MG	2j	201	1/1	0.93	0.17	65,65,65,65	0
56	MG	29	502	1/1	0.93	0.24	53,53,53,53	0
56	MG	1A	8700	1/1	0.93	0.15	27,27,27,27	0
56	MG	2A	3156	1/1	0.93	0.18	33,33,33,33	0
56	MG	2A	3378	1/1	0.93	0.14	41,41,41,41	0
56	MG	1D	301	1/1	0.93	0.14	21,21,21,21	0
56	MG	2A	3380	1/1	0.93	0.17	25,25,25,25	0
56	MG	2A	3607	1/1	0.93	0.15	37,37,37,37	0
56	MG	1A	8259	1/1	0.93	0.14	28,28,28,28	0
56	MG	2A	3383	1/1	0.93	0.18	27,27,27,27	0
56	MG	2A	3384	1/1	0.93	0.16	40,40,40,40	0
56	MG	1a	1829	1/1	0.93	0.12	36,36,36,36	0
56	MG	1D	305	1/1	0.93	0.18	18,18,18,18	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	2a	1614	1/1	0.93	0.13	49,49,49,49	0
59	K	1x	3001	1/1	0.93	0.15	46,46,46,46	0
59	K	2A	3001	1/1	0.93	0.16	65,65,65,65	0
56	MG	1A	8156	1/1	0.94	0.41	25,25,25,25	0
56	MG	2A	3253	1/1	0.94	0.37	39,39,39,39	0
56	MG	2A	3254	1/1	0.94	0.23	38,38,38,38	0
56	MG	1A	8878	1/1	0.94	0.10	16,16,16,16	0
56	MG	2A	3507	1/1	0.94	0.14	43,43,43,43	0
56	MG	2U	201	1/1	0.94	0.13	42,42,42,42	0
56	MG	2U	202	1/1	0.94	0.37	50,50,50,50	0
56	MG	1A	8626	1/1	0.94	0.19	22,22,22,22	0
56	MG	1V	201	1/1	0.94	0.22	28,28,28,28	0
56	MG	1A	8627	1/1	0.94	0.24	48,48,48,48	0
56	MG	1A	8372	1/1	0.94	0.07	51,51,51,51	0
56	MG	2V	201	1/1	0.94	0.08	32,32,32,32	0
56	MG	2A	3773	1/1	0.94	0.08	24,24,24,24	0
56	MG	2A	3514	1/1	0.94	0.10	36,36,36,36	0
56	MG	2A	3516	1/1	0.94	0.10	48,48,48,48	0
56	MG	10	103	1/1	0.94	0.21	21,21,21,21	0
56	MG	20	102	1/1	0.94	0.06	43,43,43,43	0
56	MG	2A	3039	1/1	0.94	0.20	38,38,38,38	0
56	MG	1A	8052	1/1	0.94	0.17	12,12,12,12	0
56	MG	1A	8463	1/1	0.94	0.19	7,7,7,7	0
56	MG	2A	3266	1/1	0.94	0.14	25,25,25,25	0
56	MG	23	102	1/1	0.94	0.25	41,41,41,41	0
56	MG	1A	8885	1/1	0.94	0.11	31,31,31,31	0
56	MG	2A	3271	1/1	0.94	0.43	42,42,42,42	0
56	MG	1A	8306	1/1	0.94	0.15	14,14,14,14	0
56	MG	1A	8890	1/1	0.94	0.13	23,23,23,23	0
56	MG	1A	8268	1/1	0.94	0.26	15,15,15,15	0
56	MG	1A	8178	1/1	0.94	0.24	14,14,14,14	0
56	MG	1A	8757	1/1	0.94	0.27	42,42,42,42	0
56	MG	2a	1603	1/1	0.94	0.17	45,45,45,45	0
56	MG	1A	8638	1/1	0.94	0.07	18,18,18,18	0
56	MG	1A	8239	1/1	0.94	0.18	13,13,13,13	0
56	MG	2A	3797	1/1	0.94	0.18	38,38,38,38	0
56	MG	2A	3054	1/1	0.94	0.12	22,22,22,22	0
56	MG	1A	8762	1/1	0.94	0.08	34,34,34,34	0
56	MG	1A	8643	1/1	0.94	0.29	28,28,28,28	0
56	MG	1a	1760	1/1	0.94	0.16	56,56,56,56	0
56	MG	2A	3538	1/1	0.94	0.09	32,32,32,32	0
56	MG	1A	8077	1/1	0.94	0.16	15,15,15,15	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	1A	8160	1/1	0.94	0.11	20,20,20,20	0
56	MG	2A	3292	1/1	0.94	0.16	51,51,51,51	0
56	MG	2A	3542	1/1	0.94	0.16	23,23,23,23	0
56	MG	1a	1764	1/1	0.94	0.22	54,54,54,54	0
56	MG	2a	1618	1/1	0.94	0.14	38,38,38,38	0
56	MG	2A	3295	1/1	0.94	0.23	43,43,43,43	0
56	MG	2A	3811	1/1	0.94	0.07	47,47,47,47	0
56	MG	2A	3812	1/1	0.94	0.11	22,22,22,22	0
56	MG	1A	8108	1/1	0.94	0.39	18,18,18,18	0
56	MG	1A	8555	1/1	0.94	0.10	37,37,37,37	0
56	MG	2A	3067	1/1	0.94	0.20	20,20,20,20	0
56	MG	1A	8774	1/1	0.94	0.12	25,25,25,25	0
56	MG	2A	3550	1/1	0.94	0.33	50,50,50,50	0
56	MG	2A	3820	1/1	0.94	0.07	29,29,29,29	0
56	MG	1A	8650	1/1	0.94	0.20	39,39,39,39	0
56	MG	2a	1632	1/1	0.94	0.21	51,51,51,51	0
56	MG	1A	8914	1/1	0.94	0.12	46,46,46,46	0
56	MG	2A	3825	1/1	0.94	0.08	27,27,27,27	0
56	MG	2A	3075	1/1	0.94	0.15	35,35,35,35	0
56	MG	1A	8777	1/1	0.94	0.19	31,31,31,31	0
56	MG	1a	1615	1/1	0.94	0.12	51,51,51,51	0
56	MG	2A	3078	1/1	0.94	0.32	24,24,24,24	0
56	MG	2A	3558	1/1	0.94	0.45	32,32,32,32	0
56	MG	1a	1616	1/1	0.94	0.21	45,45,45,45	0
56	MG	2A	3080	1/1	0.94	0.30	31,31,31,31	0
56	MG	2A	3562	1/1	0.94	0.21	33,33,33,33	0
56	MG	1A	8186	1/1	0.94	0.11	26,26,26,26	0
56	MG	1A	8477	1/1	0.94	0.09	14,14,14,14	0
56	MG	2A	3838	1/1	0.94	0.39	44,44,44,44	0
56	MG	2A	3565	1/1	0.94	0.18	32,32,32,32	0
56	MG	2a	1651	1/1	0.94	0.14	48,48,48,48	0
56	MG	2A	3841	1/1	0.94	0.12	40,40,40,40	0
56	MG	2a	1653	1/1	0.94	0.25	40,40,40,40	0
56	MG	1A	8782	1/1	0.94	0.14	24,24,24,24	0
56	MG	2A	3088	1/1	0.94	0.32	33,33,33,33	0
56	MG	2A	3568	1/1	0.94	0.23	22,22,22,22	0
56	MG	2A	3322	1/1	0.94	0.09	37,37,37,37	0
56	MG	2a	1658	1/1	0.94	0.17	63,63,63,63	0
56	MG	2A	3089	1/1	0.94	0.27	34,34,34,34	0
56	MG	1A	8164	1/1	0.94	0.10	31,31,31,31	0
56	MG	1A	8785	1/1	0.94	0.07	23,23,23,23	0
56	MG	1A	8786	1/1	0.94	0.08	15,15,15,15	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	2a	1663	1/1	0.94	0.18	43,43,43,43	0
56	MG	2A	3853	1/1	0.94	0.14	54,54,54,54	0
56	MG	1A	8560	1/1	0.94	0.19	18,18,18,18	0
56	MG	1A	8929	1/1	0.94	0.18	17,17,17,17	0
56	MG	2a	1669	1/1	0.94	0.13	40,40,40,40	0
56	MG	1A	8656	1/1	0.94	0.08	22,22,22,22	0
56	MG	2A	3099	1/1	0.94	0.19	34,34,34,34	0
56	MG	2A	3337	1/1	0.94	0.15	28,28,28,28	0
56	MG	2A	3859	1/1	0.94	0.09	41,41,41,41	0
56	MG	2A	3585	1/1	0.94	0.34	33,33,33,33	0
56	MG	1A	8565	1/1	0.94	0.27	17,17,17,17	0
56	MG	1A	8566	1/1	0.94	0.16	22,22,22,22	0
56	MG	1a	1631	1/1	0.94	0.14	34,34,34,34	0
56	MG	1A	8479	1/1	0.94	0.23	38,38,38,38	0
56	MG	1a	1790	1/1	0.94	0.12	46,46,46,46	0
56	MG	1A	8939	1/1	0.94	0.17	12,12,12,12	0
56	MG	2A	3348	1/1	0.94	0.25	19,19,19,19	0
56	MG	2a	1685	1/1	0.94	0.08	41,41,41,41	0
56	MG	2A	3598	1/1	0.94	0.10	50,50,50,50	0
56	MG	1A	8480	1/1	0.94	0.11	34,34,34,34	0
56	MG	1a	1793	1/1	0.94	0.13	45,45,45,45	0
56	MG	2A	3351	1/1	0.94	0.10	40,40,40,40	0
56	MG	1A	8190	1/1	0.94	0.07	15,15,15,15	0
56	MG	1A	8393	1/1	0.94	0.15	20,20,20,20	0
56	MG	2A	3875	1/1	0.94	0.15	23,23,23,23	0
56	MG	2A	3878	1/1	0.94	0.10	45,45,45,45	0
56	MG	1A	8949	1/1	0.94	0.37	16,16,16,16	0
56	MG	2a	1699	1/1	0.94	0.12	68,68,68,68	0
56	MG	1A	8322	1/1	0.94	0.15	45,45,45,45	0
56	MG	1A	8009	1/1	0.94	0.25	20,20,20,20	0
56	MG	2A	3120	1/1	0.94	0.15	28,28,28,28	0
56	MG	1A	8957	1/1	0.94	0.19	26,26,26,26	0
56	MG	2a	1704	1/1	0.94	0.48	38,38,38,38	0
56	MG	1A	8574	1/1	0.94	0.08	15,15,15,15	0
56	MG	1A	8151	1/1	0.94	0.14	10,10,10,10	0
56	MG	1a	1650	1/1	0.94	0.18	42,42,42,42	0
56	MG	1A	8403	1/1	0.94	0.17	13,13,13,13	0
56	MG	2A	3126	1/1	0.94	0.16	32,32,32,32	0
56	MG	1A	8408	1/1	0.94	0.08	19,19,19,19	0
56	MG	1A	8807	1/1	0.94	0.08	18,18,18,18	0
56	MG	2A	3372	1/1	0.94	0.13	48,48,48,48	0
56	MG	2A	3894	1/1	0.94	0.09	36,36,36,36	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	1A	8327	1/1	0.94	0.17	32,32,32,32	0
56	MG	2A	3897	1/1	0.94	0.15	59,59,59,59	0
56	MG	1A	8812	1/1	0.94	0.11	31,31,31,31	0
56	MG	2A	3625	1/1	0.94	0.15	51,51,51,51	0
56	MG	2A	3626	1/1	0.94	0.15	60,60,60,60	0
56	MG	1A	8680	1/1	0.94	0.12	19,19,19,19	0
56	MG	1A	8816	1/1	0.94	0.10	12,12,12,12	0
56	MG	2A	3906	1/1	0.94	0.10	39,39,39,39	0
56	MG	2A	3907	1/1	0.94	0.14	23,23,23,23	0
56	MG	1a	1817	1/1	0.94	0.36	52,52,52,52	0
56	MG	2A	3631	1/1	0.94	0.10	48,48,48,48	0
56	MG	2A	3144	1/1	0.94	0.09	63,63,63,63	0
56	MG	2A	3148	1/1	0.94	0.14	50,50,50,50	0
56	MG	1a	1663	1/1	0.94	0.15	51,51,51,51	0
56	MG	1a	1664	1/1	0.94	0.19	38,38,38,38	0
56	MG	2A	3152	1/1	0.94	0.14	32,32,32,32	0
56	MG	2A	3643	1/1	0.94	0.27	27,27,27,27	0
56	MG	2A	3153	1/1	0.94	0.21	39,39,39,39	0
56	MG	1A	8284	1/1	0.94	0.20	50,50,50,50	0
56	MG	2A	3386	1/1	0.94	0.18	29,29,29,29	0
56	MG	2a	1739	1/1	0.94	0.15	48,48,48,48	0
56	MG	2A	3652	1/1	0.94	0.07	43,43,43,43	0
56	MG	2A	3654	1/1	0.94	0.43	41,41,41,41	0
56	MG	1A	8331	1/1	0.94	0.17	19,19,19,19	0
56	MG	1A	8333	1/1	0.94	0.17	39,39,39,39	0
56	MG	2A	3391	1/1	0.94	0.28	20,20,20,20	0
56	MG	1a	1826	1/1	0.94	0.15	65,65,65,65	0
56	MG	1A	8590	1/1	0.94	0.19	29,29,29,29	0
56	MG	1A	8028	1/1	0.94	0.17	11,11,11,11	0
56	MG	1A	8500	1/1	0.94	0.18	45,45,45,45	0
56	MG	1A	8339	1/1	0.94	0.07	32,32,32,32	0
56	MG	2A	3936	1/1	0.94	0.12	20,20,20,20	0
56	MG	2A	3166	1/1	0.94	0.09	42,42,42,42	0
56	MG	1A	8692	1/1	0.94	0.13	19,19,19,19	0
56	MG	2a	1756	1/1	0.94	0.14	38,38,38,38	0
56	MG	2A	3942	1/1	0.94	0.12	43,43,43,43	0
56	MG	2A	3168	1/1	0.94	0.17	24,24,24,24	0
56	MG	2A	3407	1/1	0.94	0.10	29,29,29,29	0
56	MG	2A	3408	1/1	0.94	0.09	38,38,38,38	0
56	MG	2A	3169	1/1	0.94	0.49	31,31,31,31	0
56	MG	2A	3172	1/1	0.94	0.26	25,25,25,25	0
56	MG	2A	3950	1/1	0.94	0.12	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	2A	3173	1/1	0.94	0.16	37,37,37,37	0
56	MG	1a	1833	1/1	0.94	0.32	39,39,39,39	0
56	MG	1A	8340	1/1	0.94	0.12	19,19,19,19	0
56	MG	1A	8595	1/1	0.94	0.14	35,35,35,35	0
56	MG	2A	3178	1/1	0.94	0.27	31,31,31,31	0
56	MG	1A	8153	1/1	0.94	0.16	12,12,12,12	0
56	MG	1A	8226	1/1	0.94	0.19	17,17,17,17	0
56	MG	1B	3025	1/1	0.94	0.13	26,26,26,26	0
56	MG	1B	3026	1/1	0.94	0.28	35,35,35,35	0
56	MG	2a	1773	1/1	0.94	0.06	52,52,52,52	0
56	MG	2A	3966	1/1	0.94	0.23	50,50,50,50	0
56	MG	1A	8345	1/1	0.94	0.09	30,30,30,30	0
56	MG	1A	8601	1/1	0.94	0.11	36,36,36,36	0
56	MG	2A	3190	1/1	0.94	0.35	32,32,32,32	0
56	MG	1A	8426	1/1	0.94	0.06	31,31,31,31	0
56	MG	1A	8428	1/1	0.94	0.11	14,14,14,14	0
56	MG	2a	1781	1/1	0.94	0.17	61,61,61,61	0
56	MG	1h	8001	1/1	0.94	0.07	52,52,52,52	0
56	MG	1D	306	1/1	0.94	0.14	21,21,21,21	0
56	MG	2A	3430	1/1	0.94	0.10	30,30,30,30	0
56	MG	2A	3197	1/1	0.94	0.08	37,37,37,37	0
56	MG	1A	8173	1/1	0.94	0.28	15,15,15,15	0
56	MG	1l	202	1/1	0.94	0.05	38,38,38,38	0
56	MG	1A	8850	1/1	0.94	0.32	34,34,34,34	0
56	MG	2A	3436	1/1	0.94	0.15	29,29,29,29	0
56	MG	1a	1699	1/1	0.94	0.10	26,26,26,26	0
56	MG	1A	8712	1/1	0.94	0.13	24,24,24,24	0
56	MG	2A	3439	1/1	0.94	0.06	25,25,25,25	0
56	MG	1E	301	1/1	0.94	0.07	22,22,22,22	0
56	MG	1q	201	1/1	0.94	0.10	37,37,37,37	0
56	MG	1A	8715	1/1	0.94	0.12	17,17,17,17	0
56	MG	2a	1796	1/1	0.94	0.14	53,53,53,53	0
56	MG	2A	3208	1/1	0.94	0.42	31,31,31,31	0
56	MG	1A	8520	1/1	0.94	0.23	9,9,9,9	0
56	MG	2B	3012	1/1	0.94	0.14	52,52,52,52	0
56	MG	1x	3004	1/1	0.94	0.10	47,47,47,47	0
56	MG	1A	8607	1/1	0.94	0.13	18,18,18,18	0
56	MG	2A	3214	1/1	0.94	0.17	32,32,32,32	0
56	MG	1a	1711	1/1	0.94	0.08	45,45,45,45	0
56	MG	2A	3218	1/1	0.94	0.34	37,37,37,37	0
56	MG	1E	307	1/1	0.94	0.08	28,28,28,28	0
56	MG	1A	8104	1/1	0.94	0.27	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	3465	1/1	0.94	0.18	23,23,23,23	0
56	MG	2A	3222	1/1	0.94	0.05	48,48,48,48	0
56	MG	1x	3012	1/1	0.94	0.13	38,38,38,38	0
56	MG	1a	1716	1/1	0.94	0.18	52,52,52,52	0
56	MG	1F	303	1/1	0.94	0.21	19,19,19,19	0
56	MG	1A	8354	1/1	0.94	0.10	9,9,9,9	0
56	MG	1A	8355	1/1	0.94	0.17	7,7,7,7	0
56	MG	1F	308	1/1	0.94	0.19	18,18,18,18	0
56	MG	2A	3229	1/1	0.94	0.14	30,30,30,30	0
56	MG	2D	306	1/1	0.94	0.14	34,34,34,34	0
56	MG	1A	8860	1/1	0.94	0.06	22,22,22,22	0
56	MG	2A	3231	1/1	0.94	0.41	32,32,32,32	0
56	MG	2A	3481	1/1	0.94	0.14	39,39,39,39	0
56	MG	1A	8230	1/1	0.94	0.37	13,13,13,13	0
56	MG	2A	3483	1/1	0.94	0.18	48,48,48,48	0
56	MG	1A	8726	1/1	0.94	0.27	17,17,17,17	0
56	MG	1A	8357	1/1	0.94	0.09	6,6,6,6	0
56	MG	1A	8358	1/1	0.94	0.08	7,7,7,7	0
56	MG	2A	3487	1/1	0.94	0.22	26,26,26,26	0
56	MG	1A	8366	1/1	0.94	0.07	14,14,14,14	0
56	MG	2A	3489	1/1	0.94	0.12	27,27,27,27	0
56	MG	1A	8231	1/1	0.94	0.12	25,25,25,25	0
56	MG	1A	8445	1/1	0.94	0.09	18,18,18,18	0
56	MG	2F	305	1/1	0.94	0.16	26,26,26,26	0
56	MG	2x	101	1/1	0.94	0.22	48,48,48,48	0
56	MG	2x	102	1/1	0.94	0.27	51,51,51,51	0
56	MG	2F	307	1/1	0.94	0.60	37,37,37,37	0
56	MG	2x	105	1/1	0.94	0.21	59,59,59,59	0
56	MG	2x	106	1/1	0.94	0.16	52,52,52,52	0
56	MG	2x	107	1/1	0.94	0.15	52,52,52,52	0
56	MG	2A	3751	1/1	0.94	0.20	32,32,32,32	0
56	MG	2A	3494	1/1	0.94	0.20	30,30,30,30	0
56	MG	2A	3241	1/1	0.94	0.22	49,49,49,49	0
56	MG	2A	3021	1/1	0.94	0.18	30,30,30,30	0
56	MG	1a	1734	1/1	0.94	0.11	42,42,42,42	0
56	MG	1A	8368	1/1	0.94	0.18	14,14,14,14	0
56	MG	1A	8537	1/1	0.94	0.11	21,21,21,21	0
56	MG	1A	8075	1/1	0.94	0.16	20,20,20,20	0
56	MG	2A	3762	1/1	0.94	0.15	44,44,44,44	0
56	MG	1g	3001	1/1	0.95	0.13	38,38,38,38	0
56	MG	1A	8928	1/1	0.95	0.36	16,16,16,16	0
56	MG	1A	8134	1/1	0.95	0.14	12,12,12,12	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	2A	3760	1/1	0.95	0.13	47,47,47,47	0
56	MG	1A	8207	1/1	0.95	0.24	11,11,11,11	0
56	MG	2S	201	1/1	0.95	0.15	27,27,27,27	0
56	MG	1A	8208	1/1	0.95	0.19	11,11,11,11	0
56	MG	1A	8659	1/1	0.95	0.15	23,23,23,23	0
56	MG	1A	8788	1/1	0.95	0.17	34,34,34,34	0
56	MG	1A	8248	1/1	0.95	0.27	17,17,17,17	0
56	MG	1A	8467	1/1	0.95	0.19	9,9,9,9	0
56	MG	1A	8791	1/1	0.95	0.10	39,39,39,39	0
56	MG	1A	8947	1/1	0.95	0.09	19,19,19,19	0
56	MG	1A	8663	1/1	0.95	0.17	21,21,21,21	0
56	MG	1a	1662	1/1	0.95	0.13	44,44,44,44	0
56	MG	1A	8209	1/1	0.95	0.15	15,15,15,15	0
56	MG	1A	8181	1/1	0.95	0.14	18,18,18,18	0
56	MG	20	101	1/1	0.95	0.22	46,46,46,46	0
56	MG	1A	8953	1/1	0.95	0.19	13,13,13,13	0
56	MG	1x	3009	1/1	0.95	0.23	41,41,41,41	0
56	MG	1x	3010	1/1	0.95	0.14	34,34,34,34	0
56	MG	1A	8211	1/1	0.95	0.38	15,15,15,15	0
56	MG	1A	8213	1/1	0.95	0.17	14,14,14,14	0
56	MG	2A	3238	1/1	0.95	0.13	24,24,24,24	0
56	MG	1A	8669	1/1	0.95	0.20	27,27,27,27	0
56	MG	2A	3782	1/1	0.95	0.32	60,60,60,60	0
56	MG	2A	3784	1/1	0.95	0.17	45,45,45,45	0
56	MG	1x	3014	1/1	0.95	0.16	29,29,29,29	0
56	MG	1A	8472	1/1	0.95	0.12	11,11,11,11	0
56	MG	2A	3515	1/1	0.95	0.10	48,48,48,48	0
56	MG	2A	3788	1/1	0.95	0.10	36,36,36,36	0
56	MG	2A	3789	1/1	0.95	0.08	48,48,48,48	0
56	MG	2A	3004	1/1	0.95	0.12	39,39,39,39	0
56	MG	2a	1605	1/1	0.95	0.14	40,40,40,40	0
56	MG	2A	3791	1/1	0.95	0.11	52,52,52,52	0
56	MG	1A	8960	1/1	0.95	0.11	20,20,20,20	0
56	MG	1a	1672	1/1	0.95	0.20	38,38,38,38	0
56	MG	1A	8961	1/1	0.95	0.13	20,20,20,20	0
56	MG	2A	3009	1/1	0.95	0.13	42,42,42,42	0
56	MG	1A	8963	1/1	0.95	0.35	14,14,14,14	0
56	MG	2A	3011	1/1	0.95	0.17	29,29,29,29	0
56	MG	1A	8253	1/1	0.95	0.28	23,23,23,23	0
56	MG	1A	8254	1/1	0.95	0.15	15,15,15,15	0
56	MG	1A	8968	1/1	0.95	0.10	34,34,34,34	0
56	MG	2A	3801	1/1	0.95	0.07	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	8182	1/1	0.95	0.10	12,12,12,12	0
56	MG	1A	8256	1/1	0.95	0.25	14,14,14,14	0
56	MG	1A	8806	1/1	0.95	0.45	16,16,16,16	0
56	MG	1A	8973	1/1	0.95	0.25	12,12,12,12	0
56	MG	1A	8257	1/1	0.95	0.13	11,11,11,11	0
56	MG	2A	3022	1/1	0.95	0.31	29,29,29,29	0
56	MG	2A	3023	1/1	0.95	0.13	43,43,43,43	0
56	MG	2A	3024	1/1	0.95	0.39	30,30,30,30	0
56	MG	2A	3270	1/1	0.95	0.12	20,20,20,20	0
56	MG	1B	3002	1/1	0.95	0.10	33,33,33,33	0
56	MG	2a	1628	1/1	0.95	0.72	58,58,58,58	0
56	MG	1a	1689	1/1	0.95	0.12	41,41,41,41	0
56	MG	2A	3275	1/1	0.95	0.17	42,42,42,42	0
56	MG	1A	8808	1/1	0.95	0.10	17,17,17,17	0
56	MG	2a	1634	1/1	0.95	0.39	54,54,54,54	0
56	MG	1A	8386	1/1	0.95	0.09	16,16,16,16	0
56	MG	1B	3005	1/1	0.95	0.27	34,34,34,34	0
56	MG	1A	8810	1/1	0.95	0.12	8,8,8,8	0
56	MG	1A	8085	1/1	0.95	0.19	15,15,15,15	0
56	MG	1A	8813	1/1	0.95	0.10	11,11,11,11	0
56	MG	1a	1701	1/1	0.95	0.16	44,44,44,44	0
56	MG	1a	1702	1/1	0.95	0.13	48,48,48,48	0
56	MG	1A	8583	1/1	0.95	0.18	8,8,8,8	0
56	MG	1A	8217	1/1	0.95	0.22	11,11,11,11	0
56	MG	1a	1706	1/1	0.95	0.09	27,27,27,27	0
56	MG	1B	3013	1/1	0.95	0.10	24,24,24,24	0
56	MG	2A	3291	1/1	0.95	0.35	19,19,19,19	0
56	MG	1A	8158	1/1	0.95	0.18	27,27,27,27	0
56	MG	1A	8486	1/1	0.95	0.17	26,26,26,26	0
56	MG	1A	8819	1/1	0.95	0.22	20,20,20,20	0
56	MG	1B	3019	1/1	0.95	0.07	23,23,23,23	0
56	MG	1A	8822	1/1	0.95	0.04	44,44,44,44	0
56	MG	2A	3561	1/1	0.95	0.29	32,32,32,32	0
56	MG	1A	8823	1/1	0.95	0.09	23,23,23,23	0
56	MG	2A	3843	1/1	0.95	0.17	43,43,43,43	0
56	MG	1A	8391	1/1	0.95	0.14	6,6,6,6	0
56	MG	1A	8825	1/1	0.95	0.12	35,35,35,35	0
56	MG	1A	8690	1/1	0.95	0.12	20,20,20,20	0
56	MG	1A	8117	1/1	0.95	0.26	27,27,27,27	0
56	MG	2A	3306	1/1	0.95	0.10	29,29,29,29	0
56	MG	1A	8319	1/1	0.95	0.09	27,27,27,27	0
56	MG	1D	303	1/1	0.95	0.09	17,17,17,17	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	2A	3059	1/1	0.95	0.12	21,21,21,21	0
56	MG	2a	1665	1/1	0.95	0.13	53,53,53,53	0
56	MG	1A	8394	1/1	0.95	0.09	37,37,37,37	0
56	MG	1A	8396	1/1	0.95	0.07	14,14,14,14	0
56	MG	2A	3315	1/1	0.95	0.15	44,44,44,44	0
56	MG	1A	8397	1/1	0.95	0.14	18,18,18,18	0
56	MG	1A	8087	1/1	0.95	0.12	45,45,45,45	0
56	MG	2A	3580	1/1	0.95	0.12	49,49,49,49	0
56	MG	2A	3318	1/1	0.95	0.10	30,30,30,30	0
56	MG	2A	3065	1/1	0.95	0.49	43,43,43,43	0
56	MG	2A	3861	1/1	0.95	0.06	50,50,50,50	0
56	MG	2A	3583	1/1	0.95	0.12	25,25,25,25	0
56	MG	1A	8188	1/1	0.95	0.44	16,16,16,16	0
56	MG	2A	3321	1/1	0.95	0.14	18,18,18,18	0
56	MG	1A	8265	1/1	0.95	0.17	18,18,18,18	0
56	MG	2a	1682	1/1	0.95	0.11	53,53,53,53	0
56	MG	1A	8142	1/1	0.95	0.36	11,11,11,11	0
56	MG	2A	3070	1/1	0.95	0.43	39,39,39,39	0
56	MG	2A	3325	1/1	0.95	0.24	35,35,35,35	0
56	MG	1A	8843	1/1	0.95	0.13	33,33,33,33	0
56	MG	2A	3073	1/1	0.95	0.15	32,32,32,32	0
56	MG	2A	3594	1/1	0.95	0.10	44,44,44,44	0
56	MG	2A	3595	1/1	0.95	0.12	32,32,32,32	0
56	MG	1A	8325	1/1	0.95	0.20	21,21,21,21	0
56	MG	2a	1692	1/1	0.95	0.24	44,44,44,44	0
56	MG	1E	305	1/1	0.95	0.31	12,12,12,12	0
56	MG	2a	1694	1/1	0.95	0.13	28,28,28,28	0
56	MG	2A	3599	1/1	0.95	0.10	48,48,48,48	0
56	MG	2A	3876	1/1	0.95	0.53	30,30,30,30	0
56	MG	1A	8708	1/1	0.95	0.18	17,17,17,17	0
56	MG	2A	3335	1/1	0.95	0.14	37,37,37,37	0
56	MG	1A	8191	1/1	0.95	0.20	17,17,17,17	0
56	MG	1A	8035	1/1	0.95	0.19	30,30,30,30	0
56	MG	2A	3338	1/1	0.95	0.21	40,40,40,40	0
56	MG	1F	302	1/1	0.95	0.22	16,16,16,16	0
56	MG	1A	8713	1/1	0.95	0.08	9,9,9,9	0
56	MG	2A	3081	1/1	0.95	0.16	27,27,27,27	0
56	MG	1A	8714	1/1	0.95	0.12	9,9,9,9	0
56	MG	1A	8511	1/1	0.95	0.15	32,32,32,32	0
56	MG	2A	3086	1/1	0.95	0.56	40,40,40,40	0
56	MG	1A	8854	1/1	0.95	0.09	22,22,22,22	0
56	MG	1G	3001	1/1	0.95	0.11	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	3615	1/1	0.95	0.35	36,36,36,36	0
56	MG	1A	8606	1/1	0.95	0.08	26,26,26,26	0
56	MG	1A	8513	1/1	0.95	0.06	27,27,27,27	0
56	MG	2A	3896	1/1	0.95	0.04	28,28,28,28	0
56	MG	1A	8016	1/1	0.95	0.12	18,18,18,18	0
56	MG	1A	8515	1/1	0.95	0.11	28,28,28,28	0
56	MG	1A	8516	1/1	0.95	0.13	34,34,34,34	0
56	MG	1A	8414	1/1	0.95	0.06	35,35,35,35	0
56	MG	2a	1721	1/1	0.95	0.15	47,47,47,47	0
56	MG	1A	8725	1/1	0.95	0.13	18,18,18,18	0
56	MG	2a	1723	1/1	0.95	0.14	50,50,50,50	0
56	MG	1A	8862	1/1	0.95	0.07	42,42,42,42	0
56	MG	2A	3100	1/1	0.95	0.18	37,37,37,37	0
56	MG	2A	3627	1/1	0.95	0.19	55,55,55,55	0
56	MG	1A	8332	1/1	0.95	0.11	48,48,48,48	0
56	MG	2A	3102	1/1	0.95	0.20	29,29,29,29	0
56	MG	1A	8195	1/1	0.95	0.22	8,8,8,8	0
56	MG	1Q	206	1/1	0.95	0.12	17,17,17,17	0
56	MG	2A	3632	1/1	0.95	0.12	38,38,38,38	0
56	MG	1A	8729	1/1	0.95	0.15	43,43,43,43	0
56	MG	2A	3635	1/1	0.95	0.11	36,36,36,36	0
56	MG	1R	202	1/1	0.95	0.22	26,26,26,26	0
56	MG	1A	8335	1/1	0.95	0.24	38,38,38,38	0
56	MG	2A	3638	1/1	0.95	0.10	32,32,32,32	0
56	MG	1A	8867	1/1	0.95	0.12	55,55,55,55	0
56	MG	1T	201	1/1	0.95	0.09	37,37,37,37	0
56	MG	1A	8079	1/1	0.95	0.27	16,16,16,16	0
56	MG	1U	202	1/1	0.95	0.14	17,17,17,17	0
56	MG	2A	3645	1/1	0.95	0.31	29,29,29,29	0
56	MG	1A	8338	1/1	0.95	0.16	13,13,13,13	0
56	MG	2A	3648	1/1	0.95	0.09	34,34,34,34	0
56	MG	1A	8147	1/1	0.95	0.33	18,18,18,18	0
56	MG	1W	3001	1/1	0.95	0.13	21,21,21,21	0
56	MG	2a	1747	1/1	0.95	0.22	39,39,39,39	0
56	MG	2a	1749	1/1	0.95	0.19	57,57,57,57	0
56	MG	1A	8620	1/1	0.95	0.16	25,25,25,25	0
56	MG	1A	8275	1/1	0.95	0.22	10,10,10,10	0
56	MG	2A	3935	1/1	0.95	0.11	68,68,68,68	0
56	MG	1A	8070	1/1	0.95	0.22	16,16,16,16	0
56	MG	1A	8343	1/1	0.95	0.12	12,12,12,12	0
56	MG	1A	8007	1/1	0.95	0.15	8,8,8,8	0
56	MG	2A	3940	1/1	0.95	0.34	8,8,8,8	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	1A	8278	1/1	0.95	0.12	8,8,8,8	0
56	MG	11	102	1/1	0.95	0.14	23,23,23,23	0
56	MG	2A	3388	1/1	0.95	0.17	23,23,23,23	0
56	MG	2A	3127	1/1	0.95	0.47	27,27,27,27	0
56	MG	2A	3130	1/1	0.95	0.13	27,27,27,27	0
56	MG	15	101	1/1	0.95	0.10	32,32,32,32	0
56	MG	2A	3393	1/1	0.95	0.17	27,27,27,27	0
56	MG	2A	3132	1/1	0.95	0.12	32,32,32,32	0
56	MG	2A	3397	1/1	0.95	0.20	21,21,21,21	0
56	MG	2A	3135	1/1	0.95	0.09	24,24,24,24	0
56	MG	1A	8346	1/1	0.95	0.18	14,14,14,14	0
56	MG	2A	3956	1/1	0.95	0.49	35,35,35,35	0
56	MG	15	104	1/1	0.95	0.23	16,16,16,16	0
56	MG	2A	3676	1/1	0.95	0.15	31,31,31,31	0
56	MG	15	105	1/1	0.95	0.23	12,12,12,12	0
56	MG	1a	1787	1/1	0.95	0.45	47,47,47,47	0
56	MG	1A	8236	1/1	0.95	0.26	22,22,22,22	0
56	MG	1A	8883	1/1	0.95	0.08	30,30,30,30	0
56	MG	15	108	1/1	0.95	0.16	28,28,28,28	0
56	MG	2A	3147	1/1	0.95	0.11	36,36,36,36	0
56	MG	2A	3969	1/1	0.95	0.21	55,55,55,55	0
56	MG	2A	3409	1/1	0.95	0.24	31,31,31,31	0
56	MG	2A	3972	1/1	0.95	0.11	31,31,31,31	0
56	MG	2A	3974	1/1	0.95	0.21	27,27,27,27	0
56	MG	1A	8349	1/1	0.95	0.11	13,13,13,13	0
56	MG	1A	8746	1/1	0.95	0.19	22,22,22,22	0
56	MG	19	101	1/1	0.95	0.57	24,24,24,24	0
56	MG	1a	1794	1/1	0.95	0.43	43,43,43,43	0
56	MG	19	103	1/1	0.95	0.25	23,23,23,23	0
56	MG	1A	8281	1/1	0.95	0.09	28,28,28,28	0
56	MG	1A	8632	1/1	0.95	0.09	55,55,55,55	0
56	MG	1a	1798	1/1	0.95	0.13	48,48,48,48	0
56	MG	2A	3987	1/1	0.95	0.28	28,28,28,28	0
56	MG	1A	8891	1/1	0.95	0.09	15,15,15,15	0
56	MG	1A	8892	1/1	0.95	0.11	28,28,28,28	0
56	MG	2B	3003	1/1	0.95	0.08	37,37,37,37	0
56	MG	1A	8353	1/1	0.95	0.16	7,7,7,7	0
56	MG	1A	8756	1/1	0.95	0.25	14,14,14,14	0
56	MG	1A	8635	1/1	0.95	0.20	34,34,34,34	0
56	MG	1a	1609	1/1	0.95	0.22	43,43,43,43	0
56	MG	1A	8440	1/1	0.95	0.17	5,5,5,5	0
56	MG	1A	8898	1/1	0.95	0.15	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	1811	1/1	0.95	0.07	58,58,58,58	0
56	MG	2A	3708	1/1	0.95	0.09	30,30,30,30	0
56	MG	1A	8020	1/1	0.95	0.23	8,8,8,8	0
56	MG	1A	8639	1/1	0.95	0.11	24,24,24,24	0
56	MG	1A	8901	1/1	0.95	0.17	34,34,34,34	0
56	MG	2A	3175	1/1	0.95	0.15	35,35,35,35	0
56	MG	1A	8113	1/1	0.95	0.15	16,16,16,16	0
56	MG	1A	8084	1/1	0.95	0.21	23,23,23,23	0
56	MG	1A	8100	1/1	0.95	0.23	28,28,28,28	0
56	MG	1A	8769	1/1	0.95	0.11	20,20,20,20	0
56	MG	1A	8770	1/1	0.95	0.14	21,21,21,21	0
56	MG	1a	1621	1/1	0.95	0.27	26,26,26,26	0
56	MG	1A	8908	1/1	0.95	0.16	9,9,9,9	0
56	MG	2a	1814	1/1	0.95	0.26	40,40,40,40	0
56	MG	1A	8771	1/1	0.95	0.08	24,24,24,24	0
56	MG	2a	1816	1/1	0.95	0.17	56,56,56,56	0
56	MG	2A	3187	1/1	0.95	0.28	42,42,42,42	0
56	MG	1A	8645	1/1	0.95	0.17	11,11,11,11	0
56	MG	2A	3725	1/1	0.95	0.11	29,29,29,29	0
56	MG	1A	8912	1/1	0.95	0.14	15,15,15,15	0
56	MG	1A	8913	1/1	0.95	0.14	48,48,48,48	0
56	MG	1a	1627	1/1	0.95	0.44	37,37,37,37	0
56	MG	2D	311	1/1	0.95	0.14	29,29,29,29	0
56	MG	1A	8131	1/1	0.95	0.24	12,12,12,12	0
56	MG	1A	8362	1/1	0.95	0.06	52,52,52,52	0
56	MG	2f	8001	1/1	0.95	0.14	43,43,43,43	0
56	MG	1A	8775	1/1	0.95	0.06	9,9,9,9	0
56	MG	2A	3732	1/1	0.95	0.20	62,62,62,62	0
56	MG	2i	3001	1/1	0.95	0.14	36,36,36,36	0
56	MG	2A	3198	1/1	0.95	0.06	36,36,36,36	0
56	MG	1A	8452	1/1	0.95	0.06	26,26,26,26	0
56	MG	1a	1835	1/1	0.95	0.14	43,43,43,43	0
56	MG	1a	1836	1/1	0.95	0.35	36,36,36,36	0
56	MG	1a	1837	1/1	0.95	0.15	39,39,39,39	0
56	MG	2A	3738	1/1	0.95	0.10	43,43,43,43	0
56	MG	1A	8551	1/1	0.95	0.04	32,32,32,32	0
56	MG	1A	8779	1/1	0.95	0.08	29,29,29,29	0
56	MG	2x	103	1/1	0.95	0.14	49,49,49,49	0
56	MG	1A	8920	1/1	0.95	0.23	6,6,6,6	0
56	MG	2A	3206	1/1	0.95	0.21	48,48,48,48	0
56	MG	2F	306	1/1	0.95	0.14	30,30,30,30	0
56	MG	2A	3476	1/1	0.95	0.09	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	8455	1/1	0.95	0.09	22,22,22,22	0
56	MG	1A	8363	1/1	0.95	0.24	15,15,15,15	0
56	MG	2A	3209	1/1	0.95	0.28	37,37,37,37	0
56	MG	1A	8364	1/1	0.95	0.13	26,26,26,26	0
56	MG	1A	8927	1/1	0.95	0.30	8,8,8,8	0
56	MG	2A	3212	1/1	0.95	0.32	27,27,27,27	0
56	MG	2A	3753	1/1	0.95	0.29	27,27,27,27	0
57	ZN	2n	501	1/1	0.95	0.08	64,64,64,64	0
56	MG	1a	1644	1/1	0.95	0.22	38,38,38,38	0
56	MG	1a	1645	1/1	0.95	0.21	34,34,34,34	0
56	MG	2A	3898	1/1	0.96	0.19	46,46,46,46	0
56	MG	2A	3150	1/1	0.96	0.30	35,35,35,35	0
56	MG	1a	1745	1/1	0.96	0.11	41,41,41,41	0
56	MG	2A	3510	1/1	0.96	0.14	54,54,54,54	0
56	MG	1A	8310	1/1	0.96	0.09	8,8,8,8	0
56	MG	2a	1645	1/1	0.96	0.12	53,53,53,53	0
56	MG	1A	8067	1/1	0.96	0.20	10,10,10,10	0
56	MG	2A	3154	1/1	0.96	0.16	31,31,31,31	0
56	MG	1A	8416	1/1	0.96	0.08	36,36,36,36	0
56	MG	2A	3005	1/1	0.96	0.31	32,32,32,32	0
56	MG	2A	3909	1/1	0.96	0.22	29,29,29,29	0
56	MG	1B	3012	1/1	0.96	0.11	25,25,25,25	0
56	MG	1A	8342	1/1	0.96	0.12	9,9,9,9	0
56	MG	1A	8068	1/1	0.96	0.20	16,16,16,16	0
56	MG	2A	3329	1/1	0.96	0.12	30,30,30,30	0
56	MG	1A	8376	1/1	0.96	0.07	14,14,14,14	0
56	MG	1A	8647	1/1	0.96	0.42	14,14,14,14	0
56	MG	2A	3334	1/1	0.96	0.14	23,23,23,23	0
56	MG	2A	3718	1/1	0.96	0.14	30,30,30,30	0
56	MG	2A	3164	1/1	0.96	0.17	29,29,29,29	0
56	MG	1A	8799	1/1	0.96	0.22	23,23,23,23	0
56	MG	2A	3012	1/1	0.96	0.16	41,41,41,41	0
56	MG	1A	8589	1/1	0.96	0.31	13,13,13,13	0
56	MG	2A	3926	1/1	0.96	0.28	36,36,36,36	0
56	MG	1B	3021	1/1	0.96	0.10	28,28,28,28	0
56	MG	1A	8204	1/1	0.96	0.36	20,20,20,20	0
56	MG	1A	8721	1/1	0.96	0.13	11,11,11,11	0
56	MG	2A	3531	1/1	0.96	0.18	36,36,36,36	0
56	MG	1A	8421	1/1	0.96	0.07	26,26,26,26	0
56	MG	1A	8378	1/1	0.96	0.14	24,24,24,24	0
56	MG	2a	1671	1/1	0.96	0.11	34,34,34,34	0
56	MG	1A	8118	1/1	0.96	0.18	10,10,10,10	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	2A	3347	1/1	0.96	0.15	34,34,34,34	0
56	MG	1A	8381	1/1	0.96	0.15	10,10,10,10	0
56	MG	1A	8538	1/1	0.96	0.11	14,14,14,14	0
56	MG	1a	1630	1/1	0.96	0.28	17,17,17,17	0
56	MG	2A	3179	1/1	0.96	0.11	35,35,35,35	0
56	MG	1A	8262	1/1	0.96	0.28	58,58,58,58	0
56	MG	1A	8427	1/1	0.96	0.17	7,7,7,7	0
56	MG	2A	3943	1/1	0.96	0.23	40,40,40,40	0
56	MG	1A	8036	1/1	0.96	0.12	17,17,17,17	0
56	MG	2A	3355	1/1	0.96	0.12	20,20,20,20	0
56	MG	1A	8660	1/1	0.96	0.11	16,16,16,16	0
56	MG	2A	3357	1/1	0.96	0.15	20,20,20,20	0
56	MG	1a	1637	1/1	0.96	0.42	38,38,38,38	0
56	MG	2A	3361	1/1	0.96	0.07	42,42,42,42	0
56	MG	1D	310	1/1	0.96	0.12	12,12,12,12	0
56	MG	1D	311	1/1	0.96	0.10	31,31,31,31	0
56	MG	1A	8225	1/1	0.96	0.20	10,10,10,10	0
56	MG	2A	3033	1/1	0.96	0.28	28,28,28,28	0
56	MG	2A	3366	1/1	0.96	0.12	29,29,29,29	0
56	MG	1D	313	1/1	0.96	0.19	33,33,33,33	0
56	MG	2A	3194	1/1	0.96	0.14	24,24,24,24	0
56	MG	1A	8903	1/1	0.96	0.15	19,19,19,19	0
56	MG	1A	8543	1/1	0.96	0.09	20,20,20,20	0
56	MG	2a	1698	1/1	0.96	0.29	40,40,40,40	0
56	MG	2A	3756	1/1	0.96	0.10	28,28,28,28	0
56	MG	2A	3964	1/1	0.96	0.35	37,37,37,37	0
56	MG	1E	302	1/1	0.96	0.15	9,9,9,9	0
56	MG	2A	3038	1/1	0.96	0.27	30,30,30,30	0
56	MG	1A	8003	1/1	0.96	0.15	29,29,29,29	0
56	MG	1A	8664	1/1	0.96	0.12	26,26,26,26	0
56	MG	1A	8545	1/1	0.96	0.11	33,33,33,33	0
56	MG	1A	8352	1/1	0.96	0.08	21,21,21,21	0
56	MG	2A	3973	1/1	0.96	0.17	35,35,35,35	0
56	MG	1A	8820	1/1	0.96	0.11	24,24,24,24	0
56	MG	2A	3976	1/1	0.96	0.29	28,28,28,28	0
56	MG	1a	1653	1/1	0.96	0.23	32,32,32,32	0
56	MG	2A	3046	1/1	0.96	0.22	26,26,26,26	0
56	MG	1a	1654	1/1	0.96	0.19	43,43,43,43	0
56	MG	2A	3572	1/1	0.96	0.22	56,56,56,56	0
56	MG	2A	3573	1/1	0.96	0.11	41,41,41,41	0
56	MG	1A	8821	1/1	0.96	0.07	9,9,9,9	0
56	MG	1A	8739	1/1	0.96	0.18	28,28,28,28	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	1A	8194	1/1	0.96	0.31	17,17,17,17	0
56	MG	2A	3986	1/1	0.96	0.19	37,37,37,37	0
56	MG	2A	3052	1/1	0.96	0.32	37,37,37,37	0
56	MG	2A	3774	1/1	0.96	0.50	56,56,56,56	0
56	MG	1A	8163	1/1	0.96	0.24	17,17,17,17	0
56	MG	1A	8743	1/1	0.96	0.27	14,14,14,14	0
56	MG	1A	8004	1/1	0.96	0.17	18,18,18,18	0
56	MG	1A	8294	1/1	0.96	0.06	29,29,29,29	0
56	MG	1A	8042	1/1	0.96	0.11	33,33,33,33	0
56	MG	1A	8830	1/1	0.96	0.09	27,27,27,27	0
56	MG	1A	8139	1/1	0.96	0.18	15,15,15,15	0
56	MG	1A	8675	1/1	0.96	0.17	17,17,17,17	0
56	MG	2A	3783	1/1	0.96	0.13	55,55,55,55	0
56	MG	1A	8395	1/1	0.96	0.16	34,34,34,34	0
56	MG	1A	8924	1/1	0.96	0.14	12,12,12,12	0
56	MG	1P	203	1/1	0.96	0.12	8,8,8,8	0
56	MG	1A	8754	1/1	0.96	0.20	18,18,18,18	0
56	MG	1A	8499	1/1	0.96	0.16	18,18,18,18	0
56	MG	2A	3068	1/1	0.96	0.21	34,34,34,34	0
56	MG	2A	3404	1/1	0.96	0.09	25,25,25,25	0
56	MG	1A	8837	1/1	0.96	0.07	18,18,18,18	0
56	MG	1a	1806	1/1	0.96	0.11	49,49,49,49	0
56	MG	2A	3071	1/1	0.96	0.11	25,25,25,25	0
56	MG	1A	8444	1/1	0.96	0.12	12,12,12,12	0
56	MG	1a	1808	1/1	0.96	0.07	35,35,35,35	0
56	MG	1A	8359	1/1	0.96	0.08	24,24,24,24	0
56	MG	1a	1810	1/1	0.96	0.07	52,52,52,52	0
56	MG	1A	8841	1/1	0.96	0.09	34,34,34,34	0
56	MG	1A	8932	1/1	0.96	0.22	21,21,21,21	0
56	MG	1A	8681	1/1	0.96	0.16	32,32,32,32	0
56	MG	1A	8361	1/1	0.96	0.09	26,26,26,26	0
56	MG	2A	3608	1/1	0.96	0.18	21,21,21,21	0
56	MG	2D	309	1/1	0.96	0.14	37,37,37,37	0
56	MG	1A	8272	1/1	0.96	0.17	27,27,27,27	0
56	MG	1A	8563	1/1	0.96	0.13	11,11,11,11	0
56	MG	2A	3611	1/1	0.96	0.55	34,34,34,34	0
56	MG	1a	1684	1/1	0.96	0.17	35,35,35,35	0
56	MG	2A	3244	1/1	0.96	0.43	30,30,30,30	0
56	MG	1a	1818	1/1	0.96	0.11	41,41,41,41	0
56	MG	2A	3809	1/1	0.96	0.13	20,20,20,20	0
56	MG	2A	3423	1/1	0.96	0.11	37,37,37,37	0
56	MG	2A	3616	1/1	0.96	0.15	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	3246	1/1	0.96	0.08	26,26,26,26	0
56	MG	2A	3085	1/1	0.96	0.35	28,28,28,28	0
56	MG	2A	3619	1/1	0.96	0.23	36,36,36,36	0
56	MG	1A	8942	1/1	0.96	0.14	11,11,11,11	0
56	MG	1U	203	1/1	0.96	0.17	13,13,13,13	0
56	MG	2F	303	1/1	0.96	0.14	29,29,29,29	0
56	MG	2F	304	1/1	0.96	0.09	44,44,44,44	0
56	MG	1a	1822	1/1	0.96	0.05	25,25,25,25	0
56	MG	1A	8944	1/1	0.96	0.14	24,24,24,24	0
56	MG	1A	8765	1/1	0.96	0.08	23,23,23,23	0
56	MG	2A	3822	1/1	0.96	0.04	46,46,46,46	0
56	MG	1V	203	1/1	0.96	0.10	40,40,40,40	0
56	MG	2A	3824	1/1	0.96	0.08	42,42,42,42	0
56	MG	2A	3432	1/1	0.96	0.09	45,45,45,45	0
56	MG	1A	8766	1/1	0.96	0.05	37,37,37,37	0
56	MG	1W	3002	1/1	0.96	0.30	28,28,28,28	0
56	MG	2A	3096	1/1	0.96	0.33	21,21,21,21	0
56	MG	1W	3003	1/1	0.96	0.12	12,12,12,12	0
56	MG	1X	101	1/1	0.96	0.07	20,20,20,20	0
56	MG	2A	3831	1/1	0.96	0.28	35,35,35,35	0
56	MG	1A	8851	1/1	0.96	0.08	33,33,33,33	0
56	MG	1A	8564	1/1	0.96	0.24	11,11,11,11	0
56	MG	2Q	204	1/1	0.96	0.14	42,42,42,42	0
56	MG	1A	8951	1/1	0.96	0.10	20,20,20,20	0
56	MG	1A	8768	1/1	0.96	0.15	12,12,12,12	0
56	MG	2A	3836	1/1	0.96	0.16	32,32,32,32	0
56	MG	1a	1705	1/1	0.96	0.15	25,25,25,25	0
56	MG	2A	3447	1/1	0.96	0.18	22,22,22,22	0
56	MG	2A	3839	1/1	0.96	0.10	27,27,27,27	0
56	MG	2A	3269	1/1	0.96	0.40	44,44,44,44	0
56	MG	2A	3104	1/1	0.96	0.24	25,25,25,25	0
56	MG	2A	3453	1/1	0.96	0.15	44,44,44,44	0
56	MG	1A	8064	1/1	0.96	0.14	23,23,23,23	0
56	MG	2A	3272	1/1	0.96	0.18	30,30,30,30	0
56	MG	2X	101	1/1	0.96	0.13	33,33,33,33	0
56	MG	1A	8510	1/1	0.96	0.16	29,29,29,29	0
56	MG	1a	1708	1/1	0.96	0.25	43,43,43,43	0
56	MG	10	108	1/1	0.96	0.13	35,35,35,35	0
56	MG	11	101	1/1	0.96	0.15	26,26,26,26	0
56	MG	2A	3653	1/1	0.96	0.10	41,41,41,41	0
56	MG	1b	3001	1/1	0.96	0.12	50,50,50,50	0
56	MG	2A	3655	1/1	0.96	0.19	25,25,25,25	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
56	MG	2A	3656	1/1	0.96	0.32	24,24,24,24	0
56	MG	1a	1712	1/1	0.96	0.04	39,39,39,39	0
56	MG	1A	8043	1/1	0.96	0.16	24,24,24,24	0
56	MG	25	101	1/1	0.96	0.12	27,27,27,27	0
56	MG	13	102	1/1	0.96	0.20	20,20,20,20	0
56	MG	1A	8305	1/1	0.96	0.12	29,29,29,29	0
56	MG	27	101	1/1	0.96	0.34	39,39,39,39	0
56	MG	2A	3661	1/1	0.96	0.20	36,36,36,36	0
56	MG	1A	8456	1/1	0.96	0.07	25,25,25,25	0
56	MG	2A	3473	1/1	0.96	0.28	51,51,51,51	0
56	MG	2A	3284	1/1	0.96	0.10	41,41,41,41	0
56	MG	1e	201	1/1	0.96	0.11	28,28,28,28	0
56	MG	1A	8405	1/1	0.96	0.12	16,16,16,16	0
56	MG	1A	8407	1/1	0.96	0.11	20,20,20,20	0
56	MG	1A	8216	1/1	0.96	0.37	15,15,15,15	0
56	MG	2A	3669	1/1	0.96	0.09	34,34,34,34	0
56	MG	1A	8965	1/1	0.96	0.25	14,14,14,14	0
56	MG	1A	8409	1/1	0.96	0.10	35,35,35,35	0
56	MG	2A	3293	1/1	0.96	0.14	24,24,24,24	0
56	MG	1A	8699	1/1	0.96	0.12	17,17,17,17	0
56	MG	2A	3674	1/1	0.96	0.06	32,32,32,32	0
56	MG	1A	8633	1/1	0.96	0.09	10,10,10,10	0
56	MG	1A	8575	1/1	0.96	0.15	14,14,14,14	0
56	MG	2A	3297	1/1	0.96	0.10	31,31,31,31	0
56	MG	1A	8576	1/1	0.96	0.06	29,29,29,29	0
56	MG	2l	202	1/1	0.96	0.09	50,50,50,50	0
56	MG	2A	3299	1/1	0.96	0.04	41,41,41,41	0
56	MG	1A	8783	1/1	0.96	0.14	15,15,15,15	0
56	MG	2A	3133	1/1	0.96	0.49	39,39,39,39	0
56	MG	1a	1601	1/1	0.96	0.07	43,43,43,43	0
56	MG	2A	3136	1/1	0.96	0.17	34,34,34,34	0
56	MG	1A	8090	1/1	0.96	0.08	36,36,36,36	0
56	MG	1A	8705	1/1	0.96	0.10	10,10,10,10	0
56	MG	2A	3308	1/1	0.96	0.17	47,47,47,47	0
56	MG	2A	3886	1/1	0.96	0.13	43,43,43,43	0
56	MG	2A	3887	1/1	0.96	0.12	41,41,41,41	0
56	MG	1A	8707	1/1	0.96	0.06	45,45,45,45	0
56	MG	1a	1737	1/1	0.96	0.12	40,40,40,40	0
56	MG	2A	3693	1/1	0.96	0.21	34,34,34,34	0
56	MG	1A	8873	1/1	0.96	0.13	10,10,10,10	0
56	MG	2a	1631	1/1	0.96	0.23	42,42,42,42	0
56	MG	1A	8238	1/1	0.96	0.15	19,19,19,19	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	ZN	1n	102	1/1	0.96	0.10	55,55,55,55	0
56	MG	1A	8875	1/1	0.96	0.28	10,10,10,10	0
56	MG	2A	3145	1/1	0.96	0.15	32,32,32,32	0
56	MG	1A	8709	1/1	0.96	0.11	23,23,23,23	0
56	MG	1A	8710	1/1	0.96	0.10	16,16,16,16	0
56	MG	1a	1611	1/1	0.96	0.09	38,38,38,38	0
56	MG	2A	3695	1/1	0.97	0.07	33,33,33,33	0
56	MG	1a	1719	1/1	0.97	0.22	35,35,35,35	0
56	MG	1a	1720	1/1	0.97	0.17	49,49,49,49	0
56	MG	1A	8280	1/1	0.97	0.08	18,18,18,18	0
56	MG	1A	8066	1/1	0.97	0.17	25,25,25,25	0
56	MG	1A	8453	1/1	0.97	0.08	24,24,24,24	0
56	MG	1A	8329	1/1	0.97	0.08	24,24,24,24	0
56	MG	1A	8056	1/1	0.97	0.08	12,12,12,12	0
56	MG	2A	3313	1/1	0.97	0.13	31,31,31,31	0
56	MG	2a	1639	1/1	0.97	0.10	27,27,27,27	0
56	MG	2A	3904	1/1	0.97	0.28	47,47,47,47	0
56	MG	2A	3146	1/1	0.97	0.33	28,28,28,28	0
56	MG	1A	8162	1/1	0.97	0.15	10,10,10,10	0
56	MG	1A	8460	1/1	0.97	0.13	33,33,33,33	0
56	MG	1A	8388	1/1	0.97	0.09	11,11,11,11	0
56	MG	1A	8462	1/1	0.97	0.13	8,8,8,8	0
56	MG	1A	8219	1/1	0.97	0.38	12,12,12,12	0
56	MG	2A	3911	1/1	0.97	0.08	53,53,53,53	0
56	MG	1A	8099	1/1	0.97	0.18	12,12,12,12	0
56	MG	2A	3913	1/1	0.97	0.40	34,34,34,34	0
56	MG	1A	8844	1/1	0.97	0.22	15,15,15,15	0
56	MG	1A	8845	1/1	0.97	0.17	28,28,28,28	0
56	MG	2A	3155	1/1	0.97	0.11	24,24,24,24	0
56	MG	2A	3002	1/1	0.97	0.18	28,28,28,28	0
56	MG	2A	3918	1/1	0.97	0.06	43,43,43,43	0
56	MG	1A	8962	1/1	0.97	0.17	11,11,11,11	0
56	MG	1A	8047	1/1	0.97	0.31	6,6,6,6	0
56	MG	1a	1738	1/1	0.97	0.12	43,43,43,43	0
56	MG	1A	8964	1/1	0.97	0.15	12,12,12,12	0
56	MG	1A	8337	1/1	0.97	0.16	34,34,34,34	0
56	MG	2A	3330	1/1	0.97	0.22	23,23,23,23	0
56	MG	1A	8740	1/1	0.97	0.14	27,27,27,27	0
56	MG	2A	3163	1/1	0.97	0.14	23,23,23,23	0
56	MG	2A	3723	1/1	0.97	0.08	45,45,45,45	0
56	MG	2A	3333	1/1	0.97	0.15	39,39,39,39	0
56	MG	1a	1602	1/1	0.97	0.13	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	8642	1/1	0.97	0.10	18,18,18,18	0
56	MG	1A	8287	1/1	0.97	0.18	23,23,23,23	0
56	MG	2a	1668	1/1	0.97	0.21	46,46,46,46	0
56	MG	1A	8969	1/1	0.97	0.23	12,12,12,12	0
56	MG	1A	8553	1/1	0.97	0.14	18,18,18,18	0
56	MG	1A	8288	1/1	0.97	0.16	8,8,8,8	0
56	MG	2A	3170	1/1	0.97	0.15	39,39,39,39	0
56	MG	2a	1673	1/1	0.97	0.06	33,33,33,33	0
56	MG	1A	8167	1/1	0.97	0.39	17,17,17,17	0
56	MG	2A	3938	1/1	0.97	0.47	38,38,38,38	0
56	MG	1A	8223	1/1	0.97	0.45	18,18,18,18	0
56	MG	1A	8557	1/1	0.97	0.27	16,16,16,16	0
56	MG	2A	3345	1/1	0.97	0.07	39,39,39,39	0
56	MG	1A	8749	1/1	0.97	0.13	22,22,22,22	0
56	MG	1A	8141	1/1	0.97	0.20	22,22,22,22	0
56	MG	1A	8752	1/1	0.97	0.10	12,12,12,12	0
56	MG	1A	8292	1/1	0.97	0.09	26,26,26,26	0
56	MG	1A	8399	1/1	0.97	0.04	34,34,34,34	0
56	MG	2A	3543	1/1	0.97	0.04	50,50,50,50	0
56	MG	2A	3949	1/1	0.97	0.23	26,26,26,26	0
56	MG	1A	8561	1/1	0.97	0.21	17,17,17,17	0
56	MG	1A	8562	1/1	0.97	0.14	9,9,9,9	0
56	MG	1B	3009	1/1	0.97	0.31	37,37,37,37	0
56	MG	2A	3746	1/1	0.97	0.21	27,27,27,27	0
56	MG	1A	8474	1/1	0.97	0.16	13,13,13,13	0
56	MG	2A	3748	1/1	0.97	0.18	47,47,47,47	0
56	MG	2A	3184	1/1	0.97	0.23	25,25,25,25	0
56	MG	1A	8475	1/1	0.97	0.16	28,28,28,28	0
56	MG	1a	1761	1/1	0.97	0.14	44,44,44,44	0
56	MG	2A	3961	1/1	0.97	0.45	35,35,35,35	0
56	MG	1A	8400	1/1	0.97	0.25	42,42,42,42	0
56	MG	2A	3360	1/1	0.97	0.12	33,33,33,33	0
56	MG	1A	8658	1/1	0.97	0.27	9,9,9,9	0
56	MG	1B	3014	1/1	0.97	0.10	31,31,31,31	0
56	MG	1B	3015	1/1	0.97	0.14	18,18,18,18	0
56	MG	2A	3193	1/1	0.97	0.14	27,27,27,27	0
56	MG	2A	3557	1/1	0.97	0.53	33,33,33,33	0
56	MG	2A	3970	1/1	0.97	0.42	53,53,53,53	0
56	MG	1a	1766	1/1	0.97	0.15	34,34,34,34	0
56	MG	1A	8006	1/1	0.97	0.13	14,14,14,14	0
56	MG	1A	8567	1/1	0.97	0.12	31,31,31,31	0
56	MG	2a	1708	1/1	0.97	0.08	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	1A	8170	1/1	0.97	0.28	23,23,23,23	0
56	MG	2A	3975	1/1	0.97	0.13	22,22,22,22	0
56	MG	1a	1770	1/1	0.97	0.22	47,47,47,47	0
56	MG	1a	1771	1/1	0.97	0.11	46,46,46,46	0
56	MG	1A	8296	1/1	0.97	0.11	21,21,21,21	0
56	MG	1A	8347	1/1	0.97	0.22	13,13,13,13	0
56	MG	1A	8406	1/1	0.97	0.16	42,42,42,42	0
56	MG	2A	3981	1/1	0.97	0.63	41,41,41,41	0
56	MG	1A	8297	1/1	0.97	0.09	13,13,13,13	0
56	MG	2A	3045	1/1	0.97	0.34	20,20,20,20	0
56	MG	1a	1632	1/1	0.97	0.47	41,41,41,41	0
56	MG	1A	8021	1/1	0.97	0.30	12,12,12,12	0
56	MG	1B	3024	1/1	0.97	0.15	18,18,18,18	0
56	MG	1A	8017	1/1	0.97	0.11	13,13,13,13	0
56	MG	1A	8351	1/1	0.97	0.11	16,16,16,16	0
56	MG	2A	3381	1/1	0.97	0.09	31,31,31,31	0
56	MG	1A	8089	1/1	0.97	0.19	20,20,20,20	0
56	MG	1A	8301	1/1	0.97	0.13	27,27,27,27	0
56	MG	1a	1640	1/1	0.97	0.13	47,47,47,47	0
56	MG	1A	8671	1/1	0.97	0.12	17,17,17,17	0
56	MG	2A	3056	1/1	0.97	0.10	29,29,29,29	0
56	MG	2A	3216	1/1	0.97	0.25	28,28,28,28	0
56	MG	1A	8146	1/1	0.97	0.19	13,13,13,13	0
56	MG	1A	8492	1/1	0.97	0.08	18,18,18,18	0
56	MG	1A	8415	1/1	0.97	0.08	16,16,16,16	0
56	MG	2A	3392	1/1	0.97	0.07	35,35,35,35	0
56	MG	2A	3220	1/1	0.97	0.31	29,29,29,29	0
56	MG	2A	3060	1/1	0.97	0.16	51,51,51,51	0
56	MG	2A	3589	1/1	0.97	0.38	30,30,30,30	0
56	MG	2A	3395	1/1	0.97	0.08	38,38,38,38	0
56	MG	1A	8304	1/1	0.97	0.10	17,17,17,17	0
56	MG	2A	3592	1/1	0.97	0.20	42,42,42,42	0
56	MG	1a	1646	1/1	0.97	0.36	34,34,34,34	0
56	MG	1D	308	1/1	0.97	0.13	8,8,8,8	0
56	MG	1A	8886	1/1	0.97	0.13	24,24,24,24	0
56	MG	1A	8496	1/1	0.97	0.12	21,21,21,21	0
56	MG	1A	8018	1/1	0.97	0.17	10,10,10,10	0
56	MG	2a	1748	1/1	0.97	0.14	50,50,50,50	0
56	MG	1a	1651	1/1	0.97	0.14	26,26,26,26	0
56	MG	1A	8062	1/1	0.97	0.19	13,13,13,13	0
56	MG	2A	3405	1/1	0.97	0.24	28,28,28,28	0
56	MG	1A	8125	1/1	0.97	0.18	30,30,30,30	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	0.97	0.18	25,25,25,25	0
56	MG	1A	8235	1/1	0.97	0.20	9,9,9,9	0
56	MG	1A	8502	1/1	0.97	0.17	18,18,18,18	0
56	MG	2D	307	1/1	0.97	0.13	33,33,33,33	0
56	MG	2D	308	1/1	0.97	0.08	33,33,33,33	0
56	MG	1A	8360	1/1	0.97	0.07	25,25,25,25	0
56	MG	1A	8309	1/1	0.97	0.10	19,19,19,19	0
56	MG	1A	8267	1/1	0.97	0.09	15,15,15,15	0
56	MG	1A	8092	1/1	0.97	0.54	17,17,17,17	0
56	MG	1A	8596	1/1	0.97	0.09	17,17,17,17	0
56	MG	1A	8509	1/1	0.97	0.16	42,42,42,42	0
56	MG	1A	8598	1/1	0.97	0.13	43,43,43,43	0
56	MG	1A	8796	1/1	0.97	0.04	35,35,35,35	0
56	MG	2A	3242	1/1	0.97	0.24	30,30,30,30	0
56	MG	1a	1665	1/1	0.97	0.24	51,51,51,51	0
56	MG	1A	8694	1/1	0.97	0.05	30,30,30,30	0
56	MG	2E	304	1/1	0.97	0.21	21,21,21,21	0
56	MG	1F	306	1/1	0.97	0.14	7,7,7,7	0
56	MG	1A	8127	1/1	0.97	0.18	11,11,11,11	0
56	MG	2A	3422	1/1	0.97	0.09	45,45,45,45	0
56	MG	2A	3818	1/1	0.97	0.25	44,44,44,44	0
56	MG	2A	3819	1/1	0.97	0.07	32,32,32,32	0
56	MG	2A	3084	1/1	0.97	0.30	21,21,21,21	0
56	MG	2a	1776	1/1	0.97	0.07	51,51,51,51	0
56	MG	1A	8365	1/1	0.97	0.23	24,24,24,24	0
56	MG	1F	310	1/1	0.97	0.10	29,29,29,29	0
56	MG	2A	3251	1/1	0.97	0.11	43,43,43,43	0
56	MG	1A	8512	1/1	0.97	0.11	28,28,28,28	0
56	MG	1A	8109	1/1	0.97	0.10	12,12,12,12	0
56	MG	1A	8429	1/1	0.97	0.13	12,12,12,12	0
56	MG	1a	1675	1/1	0.97	0.12	19,19,19,19	0
56	MG	1A	8314	1/1	0.97	0.12	12,12,12,12	0
56	MG	1N	201	1/1	0.97	0.11	24,24,24,24	0
56	MG	1a	1820	1/1	0.97	0.05	51,51,51,51	0
56	MG	2A	3094	1/1	0.97	0.14	38,38,38,38	0
56	MG	2A	3095	1/1	0.97	0.15	29,29,29,29	0
56	MG	1A	8053	1/1	0.97	0.07	11,11,11,11	0
56	MG	2P	202	1/1	0.97	0.23	37,37,37,37	0
56	MG	1A	8702	1/1	0.97	0.07	30,30,30,30	0
56	MG	2Q	201	1/1	0.97	0.16	38,38,38,38	0
56	MG	2A	3264	1/1	0.97	0.67	65,65,65,65	0
56	MG	1A	8432	1/1	0.97	0.08	26,26,26,26	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	2A	3440	1/1	0.97	0.09	30,30,30,30	0
56	MG	2A	3441	1/1	0.97	0.09	38,38,38,38	0
56	MG	1A	8369	1/1	0.97	0.12	11,11,11,11	0
56	MG	1A	8111	1/1	0.97	0.25	12,12,12,12	0
56	MG	2A	3445	1/1	0.97	0.10	42,42,42,42	0
56	MG	2U	203	1/1	0.97	0.18	35,35,35,35	0
56	MG	2A	3842	1/1	0.97	0.08	48,48,48,48	0
56	MG	2A	3268	1/1	0.97	0.21	42,42,42,42	0
56	MG	1A	8706	1/1	0.97	0.06	39,39,39,39	0
56	MG	1A	8435	1/1	0.97	0.12	16,16,16,16	0
56	MG	2A	3450	1/1	0.97	0.11	27,27,27,27	0
56	MG	2A	3649	1/1	0.97	0.05	42,42,42,42	0
56	MG	1Q	203	1/1	0.97	0.12	19,19,19,19	0
56	MG	2A	3651	1/1	0.97	0.21	35,35,35,35	0
56	MG	1Q	204	1/1	0.97	0.07	20,20,20,20	0
56	MG	2A	3454	1/1	0.97	0.10	28,28,28,28	0
56	MG	2A	3852	1/1	0.97	0.22	40,40,40,40	0
56	MG	2A	3455	1/1	0.97	0.08	40,40,40,40	0
56	MG	1a	1687	1/1	0.97	0.15	39,39,39,39	0
56	MG	2A	3274	1/1	0.97	0.16	42,42,42,42	0
56	MG	1a	1831	1/1	0.97	0.39	14,14,14,14	0
56	MG	2a	1817	1/1	0.97	0.10	49,49,49,49	0
56	MG	2A	3459	1/1	0.97	0.21	33,33,33,33	0
56	MG	1A	8008	1/1	0.97	0.26	23,23,23,23	0
56	MG	2A	3108	1/1	0.97	0.30	27,27,27,27	0
56	MG	1A	8611	1/1	0.97	0.11	17,17,17,17	0
56	MG	1a	1693	1/1	0.97	0.10	29,29,29,29	0
56	MG	1A	8318	1/1	0.97	0.18	6,6,6,6	0
56	MG	1a	1696	1/1	0.97	0.06	54,54,54,54	0
56	MG	1A	8815	1/1	0.97	0.19	21,21,21,21	0
56	MG	1A	8923	1/1	0.97	0.17	17,17,17,17	0
56	MG	2A	3470	1/1	0.97	0.09	24,24,24,24	0
56	MG	2g	3001	1/1	0.97	0.13	52,52,52,52	0
56	MG	1A	8212	1/1	0.97	0.32	33,33,33,33	0
56	MG	2a	1602	1/1	0.97	0.12	48,48,48,48	0
56	MG	1A	8439	1/1	0.97	0.12	6,6,6,6	0
56	MG	1A	8926	1/1	0.97	0.10	35,35,35,35	0
56	MG	1A	8243	1/1	0.97	0.17	17,17,17,17	0
56	MG	2A	3288	1/1	0.97	0.12	25,25,25,25	0
56	MG	2A	3289	1/1	0.97	0.13	22,22,22,22	0
56	MG	1A	8132	1/1	0.97	0.23	19,19,19,19	0
56	MG	1A	8528	1/1	0.97	0.21	18,18,18,18	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	1A	8245	1/1	0.97	0.13	8,8,8,8	0
56	MG	1A	8046	1/1	0.97	0.15	12,12,12,12	0
56	MG	1A	8379	1/1	0.97	0.14	19,19,19,19	0
56	MG	1A	8622	1/1	0.97	0.12	26,26,26,26	0
56	MG	2A	3129	1/1	0.97	0.14	28,28,28,28	0
56	MG	2A	3682	1/1	0.97	0.08	40,40,40,40	0
56	MG	1A	8446	1/1	0.97	0.11	26,26,26,26	0
56	MG	1A	8826	1/1	0.97	0.08	14,14,14,14	0
56	MG	1A	8940	1/1	0.97	0.17	6,6,6,6	0
56	MG	2a	1619	1/1	0.97	0.46	50,50,50,50	0
56	MG	1A	8624	1/1	0.97	0.07	34,34,34,34	0
56	MG	1A	8136	1/1	0.97	0.14	10,10,10,10	0
56	MG	1A	8326	1/1	0.97	0.22	20,20,20,20	0
56	MG	2A	3491	1/1	0.97	0.20	27,27,27,27	0
56	MG	2A	3492	1/1	0.97	0.21	35,35,35,35	0
56	MG	2A	3691	1/1	0.97	0.16	29,29,29,29	0
56	MG	2A	3692	1/1	0.97	0.09	33,33,33,33	0
58	SF4	1d	501	8/8	0.97	0.08	48,49,54,54	0
58	SF4	2d	501	8/8	0.97	0.08	47,53,59,65	0
56	MG	1A	8945	1/1	0.97	0.12	8,8,8,8	0
56	MG	2A	3694	1/1	0.97	0.12	35,35,35,35	0
56	MG	2A	3047	1/1	0.98	0.16	18,18,18,18	0
56	MG	1A	8133	1/1	0.98	0.14	15,15,15,15	0
56	MG	2A	3941	1/1	0.98	0.12	35,35,35,35	0
56	MG	1A	8792	1/1	0.98	0.10	15,15,15,15	0
56	MG	2A	3570	1/1	0.98	0.05	35,35,35,35	0
56	MG	1A	8073	1/1	0.98	0.15	17,17,17,17	0
56	MG	1A	8682	1/1	0.98	0.08	23,23,23,23	0
56	MG	2A	3247	1/1	0.98	0.12	25,25,25,25	0
56	MG	1A	8476	1/1	0.98	0.08	17,17,17,17	0
56	MG	1a	1655	1/1	0.98	0.16	28,28,28,28	0
56	MG	1A	8684	1/1	0.98	0.08	35,35,35,35	0
56	MG	10	102	1/1	0.98	0.11	19,19,19,19	0
56	MG	1A	8422	1/1	0.98	0.05	33,33,33,33	0
56	MG	2A	3952	1/1	0.98	0.14	36,36,36,36	0
56	MG	2A	3579	1/1	0.98	0.10	25,25,25,25	0
56	MG	2A	3464	1/1	0.98	0.28	40,40,40,40	0
56	MG	1A	8637	1/1	0.98	0.12	11,11,11,11	0
56	MG	2A	3466	1/1	0.98	0.08	46,46,46,46	0
56	MG	2a	1738	1/1	0.98	0.10	43,43,43,43	0
56	MG	1A	8135	1/1	0.98	0.11	26,26,26,26	0
56	MG	1A	8011	1/1	0.98	0.18	27,27,27,27	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
56	MG	2A	3959	1/1	0.98	0.34	38,38,38,38	0
56	MG	2A	3359	1/1	0.98	0.13	30,30,30,30	0
56	MG	2A	3256	1/1	0.98	0.19	33,33,33,33	0
56	MG	2A	3471	1/1	0.98	0.12	35,35,35,35	0
56	MG	1A	8640	1/1	0.98	0.15	40,40,40,40	0
56	MG	1A	8450	1/1	0.98	0.10	14,14,14,14	0
56	MG	2A	3965	1/1	0.98	0.16	32,32,32,32	0
56	MG	1A	8481	1/1	0.98	0.06	20,20,20,20	0
56	MG	1A	8451	1/1	0.98	0.06	19,19,19,19	0
56	MG	1A	8693	1/1	0.98	0.07	28,28,28,28	0
56	MG	1A	8189	1/1	0.98	0.21	11,11,11,11	0
56	MG	1A	8748	1/1	0.98	0.16	18,18,18,18	0
56	MG	1A	8081	1/1	0.98	0.14	16,16,16,16	0
56	MG	1A	8933	1/1	0.98	0.30	20,20,20,20	0
56	MG	2A	3597	1/1	0.98	0.27	44,44,44,44	0
56	MG	1A	8869	1/1	0.98	0.09	20,20,20,20	0
56	MG	1A	8935	1/1	0.98	0.32	5,5,5,5	0
56	MG	1A	8870	1/1	0.98	0.09	20,20,20,20	0
56	MG	1a	1674	1/1	0.98	0.15	40,40,40,40	0
56	MG	17	101	1/1	0.98	0.13	21,21,21,21	0
56	MG	1A	8937	1/1	0.98	0.12	11,11,11,11	0
56	MG	2A	3171	1/1	0.98	0.18	33,33,33,33	0
56	MG	1D	309	1/1	0.98	0.17	26,26,26,26	0
56	MG	1A	8750	1/1	0.98	0.05	31,31,31,31	0
56	MG	1A	8521	1/1	0.98	0.14	12,12,12,12	0
56	MG	1A	8454	1/1	0.98	0.09	16,16,16,16	0
56	MG	1A	8382	1/1	0.98	0.14	8,8,8,8	0
56	MG	1A	8943	1/1	0.98	0.34	19,19,19,19	0
56	MG	1A	8404	1/1	0.98	0.14	8,8,8,8	0
56	MG	1A	8302	1/1	0.98	0.17	21,21,21,21	0
56	MG	2a	1633	1/1	0.98	0.14	41,41,41,41	0
56	MG	1A	8458	1/1	0.98	0.18	53,53,53,53	0
56	MG	2A	3497	1/1	0.98	0.07	28,28,28,28	0
56	MG	1A	8652	1/1	0.98	0.14	24,24,24,24	0
56	MG	1A	8459	1/1	0.98	0.09	24,24,24,24	0
56	MG	1A	8321	1/1	0.98	0.14	5,5,5,5	0
56	MG	1a	1690	1/1	0.98	0.25	36,36,36,36	0
56	MG	1a	1691	1/1	0.98	0.10	30,30,30,30	0
56	MG	2A	3186	1/1	0.98	0.26	39,39,39,39	0
56	MG	1A	8950	1/1	0.98	0.10	26,26,26,26	0
56	MG	1A	8530	1/1	0.98	0.14	27,27,27,27	0
56	MG	2A	3745	1/1	0.98	0.08	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	3506	1/1	0.98	0.06	33,33,33,33	0
56	MG	2A	3189	1/1	0.98	0.25	32,32,32,32	0
56	MG	1A	8149	1/1	0.98	0.12	11,11,11,11	0
56	MG	1a	1695	1/1	0.98	0.11	27,27,27,27	0
56	MG	1A	8494	1/1	0.98	0.30	17,17,17,17	0
56	MG	2A	3511	1/1	0.98	0.14	39,39,39,39	0
56	MG	1F	304	1/1	0.98	0.07	9,9,9,9	0
56	MG	2A	3877	1/1	0.98	0.13	20,20,20,20	0
56	MG	1A	8954	1/1	0.98	0.16	13,13,13,13	0
56	MG	1A	8022	1/1	0.98	0.22	12,12,12,12	0
56	MG	1A	8956	1/1	0.98	0.12	11,11,11,11	0
56	MG	1A	8049	1/1	0.98	0.21	12,12,12,12	0
56	MG	2A	3634	1/1	0.98	0.03	43,43,43,43	0
56	MG	1F	309	1/1	0.98	0.12	14,14,14,14	0
56	MG	1A	8101	1/1	0.98	0.28	11,11,11,11	0
56	MG	2A	3301	1/1	0.98	0.13	52,52,52,52	0
56	MG	1A	8887	1/1	0.98	0.33	24,24,24,24	0
56	MG	2D	305	1/1	0.98	0.11	33,33,33,33	0
56	MG	1A	8411	1/1	0.98	0.11	12,12,12,12	0
56	MG	1A	8165	1/1	0.98	0.12	10,10,10,10	0
56	MG	2A	3641	1/1	0.98	0.27	35,35,35,35	0
56	MG	2A	3642	1/1	0.98	0.12	37,37,37,37	0
56	MG	2D	310	1/1	0.98	0.15	37,37,37,37	0
56	MG	1A	8180	1/1	0.98	0.13	17,17,17,17	0
56	MG	1A	8619	1/1	0.98	0.32	20,20,20,20	0
56	MG	2a	1808	1/1	0.98	0.12	53,53,53,53	0
56	MG	1N	202	1/1	0.98	0.10	28,28,28,28	0
56	MG	1A	8501	1/1	0.98	0.12	29,29,29,29	0
56	MG	2A	3647	1/1	0.98	0.10	28,28,28,28	0
56	MG	1A	8071	1/1	0.98	0.14	10,10,10,10	0
56	MG	2A	3019	1/1	0.98	0.28	33,33,33,33	0
56	MG	2A	3110	1/1	0.98	0.26	35,35,35,35	0
56	MG	1A	8832	1/1	0.98	0.23	12,12,12,12	0
56	MG	1P	202	1/1	0.98	0.12	39,39,39,39	0
56	MG	2A	3901	1/1	0.98	0.08	29,29,29,29	0
56	MG	1a	1715	1/1	0.98	0.07	32,32,32,32	0
56	MG	2A	3533	1/1	0.98	0.08	50,50,50,50	0
56	MG	2A	3534	1/1	0.98	0.10	35,35,35,35	0
56	MG	1A	8580	1/1	0.98	0.06	27,27,27,27	0
56	MG	2A	3116	1/1	0.98	0.23	36,36,36,36	0
56	MG	2d	502	1/1	0.98	0.08	53,53,53,53	0
56	MG	1a	1717	1/1	0.98	0.11	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	8581	1/1	0.98	0.15	15,15,15,15	0
56	MG	2A	3026	1/1	0.98	0.33	28,28,28,28	0
56	MG	1A	8503	1/1	0.98	0.04	23,23,23,23	0
56	MG	2a	1688	1/1	0.98	0.24	53,53,53,53	0
56	MG	2F	308	1/1	0.98	0.38	46,46,46,46	0
56	MG	1a	1633	1/1	0.98	0.10	27,27,27,27	0
56	MG	1A	8778	1/1	0.98	0.06	21,21,21,21	0
56	MG	1A	8720	1/1	0.98	0.14	27,27,27,27	0
56	MG	1A	8838	1/1	0.98	0.13	7,7,7,7	0
56	MG	1A	8078	1/1	0.98	0.17	9,9,9,9	0
56	MG	1a	1725	1/1	0.98	0.10	35,35,35,35	0
56	MG	1A	8584	1/1	0.98	0.20	35,35,35,35	0
56	MG	2A	3128	1/1	0.98	0.09	48,48,48,48	0
56	MG	2A	3919	1/1	0.98	0.14	32,32,32,32	0
56	MG	1A	8330	1/1	0.98	0.08	13,13,13,13	0
56	MG	1A	8673	1/1	0.98	0.22	32,32,32,32	0
56	MG	1R	203	1/1	0.98	0.26	16,16,16,16	0
56	MG	1A	8506	1/1	0.98	0.14	30,30,30,30	0
56	MG	2Q	202	1/1	0.98	0.16	23,23,23,23	0
56	MG	1A	8293	1/1	0.98	0.15	12,12,12,12	0
56	MG	2A	3134	1/1	0.98	0.15	24,24,24,24	0
56	MG	1a	1732	1/1	0.98	0.07	38,38,38,38	0
56	MG	1A	8728	1/1	0.98	0.11	24,24,24,24	0
56	MG	2A	3443	1/1	0.98	0.15	31,31,31,31	0
56	MG	2a	1709	1/1	0.98	0.07	33,33,33,33	0
56	MG	1A	8910	1/1	0.98	0.08	19,19,19,19	0
56	MG	2x	112	1/1	0.98	0.16	39,39,39,39	0
57	ZN	1Y	501	1/1	0.98	0.07	47,47,47,47	0
56	MG	1A	8588	1/1	0.98	0.13	11,11,11,11	0
56	MG	2A	3681	1/1	0.98	0.19	57,57,57,57	0
56	MG	2A	3340	1/1	0.98	0.10	32,32,32,32	0
56	MG	1A	8229	1/1	0.98	0.13	21,21,21,21	0
57	ZN	25	102	1/1	0.98	0.05	53,53,53,53	0
57	ZN	26	101	1/1	0.98	0.06	42,42,42,42	0
56	MG	1A	8678	1/1	0.98	0.13	21,21,21,21	0
56	MG	2A	3449	1/1	0.98	0.21	25,25,25,25	0
56	MG	2A	3240	1/1	0.98	0.08	57,57,57,57	0
56	MG	2A	3451	1/1	0.98	0.15	46,46,46,46	0
56	MG	1A	8086	1/1	0.98	0.16	18,18,18,18	0
56	MG	1x	3008	1/1	0.99	0.17	36,36,36,36	0
56	MG	2A	3137	1/1	0.99	0.11	26,26,26,26	0
56	MG	2A	3387	1/1	0.99	0.15	47,47,47,47	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	1A	8938	1/1	0.99	0.14	12,12,12,12	0
56	MG	1a	1688	1/1	0.99	0.12	43,43,43,43	0
56	MG	1A	8375	1/1	0.99	0.13	11,11,11,11	0
56	MG	1A	8112	1/1	0.99	0.17	13,13,13,13	0
56	MG	1A	8535	1/1	0.99	0.07	31,31,31,31	0
56	MG	2A	3113	1/1	0.99	0.25	29,29,29,29	0
56	MG	1D	302	1/1	0.99	0.17	11,11,11,11	0
56	MG	1A	8755	1/1	0.99	0.27	16,16,16,16	0
56	MG	2A	3396	1/1	0.99	0.08	25,25,25,25	0
56	MG	2A	3771	1/1	0.99	0.21	41,41,41,41	0
56	MG	1A	8334	1/1	0.99	0.12	13,13,13,13	0
56	MG	1A	8489	1/1	0.99	0.20	9,9,9,9	0
56	MG	1A	8758	1/1	0.99	0.10	11,11,11,11	0
56	MG	1A	8441	1/1	0.99	0.05	16,16,16,16	0
56	MG	1A	8889	1/1	0.99	0.16	17,17,17,17	0
56	MG	1A	8184	1/1	0.99	0.24	17,17,17,17	0
56	MG	1A	8072	1/1	0.99	0.19	11,11,11,11	0
56	MG	1A	8529	1/1	0.99	0.12	21,21,21,21	0
56	MG	2A	3307	1/1	0.99	0.16	43,43,43,43	0
56	MG	1a	1802	1/1	0.99	0.14	30,30,30,30	0
56	MG	2A	3215	1/1	0.99	0.12	26,26,26,26	0
56	MG	13	101	1/1	0.99	0.12	17,17,17,17	0
57	ZN	15	102	1/1	0.99	0.08	31,31,31,31	0
57	ZN	16	101	1/1	0.99	0.09	24,24,24,24	0
57	ZN	19	102	1/1	0.99	0.12	27,27,27,27	0
56	MG	1A	8893	1/1	0.99	0.11	21,21,21,21	0
56	MG	1G	3003	1/1	0.99	0.10	31,31,31,31	0
56	MG	1A	8095	1/1	0.99	0.21	6,6,6,6	0
56	MG	1t	3001	1/1	0.99	0.22	37,37,37,37	0
56	MG	1A	8842	1/1	0.99	0.05	11,11,11,11	0
57	ZN	29	501	1/1	0.99	0.07	52,52,52,52	0
56	MG	1A	8723	1/1	0.99	0.15	20,20,20,20	0
56	MG	1A	8811	1/1	0.99	0.16	35,35,35,35	0
56	MG	1a	1709	1/1	0.99	0.09	30,30,30,30	0
56	MG	1A	8531	1/1	0.99	0.11	26,26,26,26	0
56	MG	1A	8166	1/1	0.99	0.11	14,14,14,14	0
56	MG	1A	8761	1/1	1.00	0.13	7,7,7,7	0

6.5 Other polymers i

There are no such residues in this entry.