



# Full wwPDB X-ray Structure Validation Report ⓘ

Jan 3, 2024 – 12:07 am GMT

PDB ID : 4ZER  
Title : Crystal structure of the Onc112 antimicrobial peptide bound to the *Thermus thermophilus* 70S ribosome  
Authors : Seefeldt, A.C.; Nguyen, F.; Antunes, S.; Perebaskine, N.; Graf, M.; Arenz, S.; Inampudi, K.K.; Douat, C.; Guichard, G.; Wilson, D.N.; Innis, C.A.  
Deposited on : 2015-04-20  
Resolution : 3.10 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity : 4.02b-467  
Mogul : 1.8.4, 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

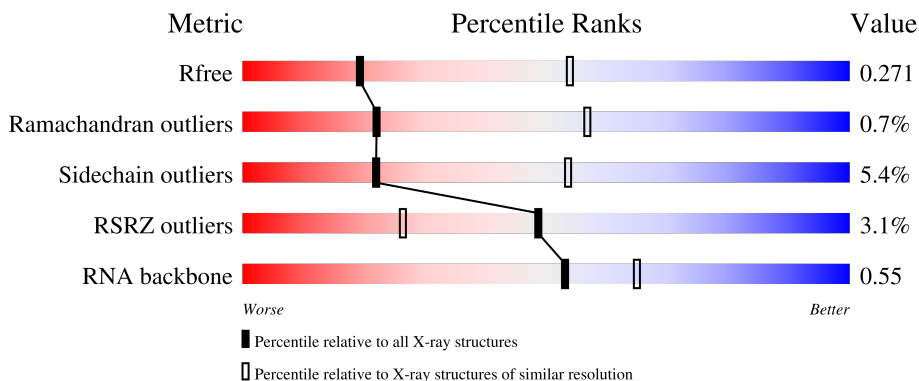
# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.10 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.



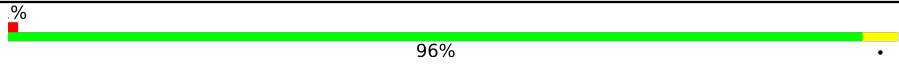
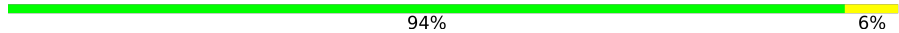
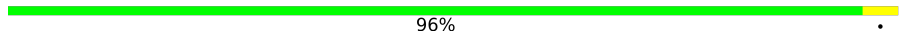


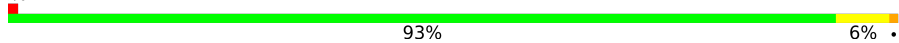

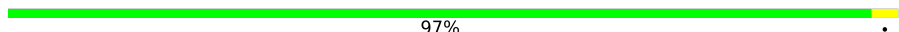
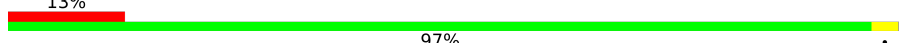



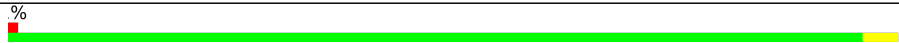



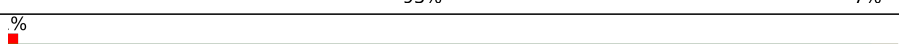

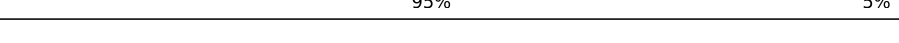

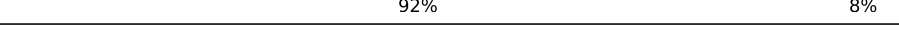

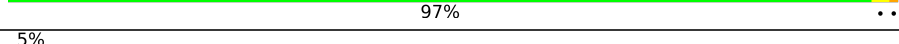
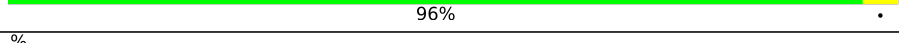
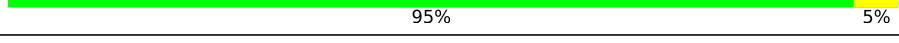
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	130704	1094 (3.10-3.10)
Ramachandran outliers	138981	1141 (3.10-3.10)
Sidechain outliers	138945	1141 (3.10-3.10)
RSRZ outliers	127900	1067 (3.10-3.10)
RNA backbone	3102	1116 (3.40-2.80)

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

Mol	Chain	Length	Quality of chain
1	1A	2915	 3% 81% 15%
1	2A	2915	 4% 81% 17%
2	1B	120	 88% 11%
2	2B	120	 90% 10%
3	1D	275	 96%

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Mol	Chain	Length	Quality of chain
3	2D	275	 96%
4	1E	204	 94% 6%
4	2E	204	 96%
5	1F	203	 94% 6%
5	2F	203	 93% 7%
6	1G	181	 93% 6%
6	2G	181	 93% 7%
7	1H	174	 97%
7	2H	174	 13% 97%
8	1I	147	 90% 10%
8	2I	147	 94% 5%
9	1N	140	 94% 6%
9	2N	140	 96%
10	1O	122	 97%
10	2O	122	 97%
11	1P	149	 93% 7%
11	2P	149	 97%
12	1Q	141	 95% 5%
12	2Q	141	 95% 5%
13	1R	118	 92% 8%
13	2R	118	 89% 11%
14	1S	110	 97%
14	2S	110	 5% 96%
15	1T	131	 95% 5%
15	2T	131	 98%

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Mol	Chain	Length	Quality of chain
16	1U	116	95% 5%
16	2U	116	95% 5%
17	1V	101	92% 7%
17	2V	101	92% 7%
18	1W	112	94% 6%
18	2W	112	96%
19	1X	95	98%
19	2X	95	96%
20	1Y	107	96%
20	2Y	107	8% 97%
21	1Z	203	6% 94% 6%
21	2Z	203	8% 94% 5%
22	10	77	96%
22	20	77	13% 97%
23	11	97	2% 98%
23	21	97	96%
24	12	70	99%
24	22	70	97%
25	13	59	93% 7%
25	23	59	3% 95% 5%
26	14	69	7% 90% 9%
26	24	69	9% 90% 10%
27	15	59	97%
27	25	59	2% 98%
28	16	53	94% 6%

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Mol	Chain	Length	Quality of chain
28	26	53	2% 94% 6%
29	17	48	4% 92% 8%
29	27	48	4% 100%
30	18	64	94% 6%
30	28	64	95% 5%
31	19	37	5% 100%
31	29	37	5% 100%
32	1a	1521	2% 80% 18% ..
32	2a	1521	3% 81% 17% ..
33	1b	231	4% 87% 13%
33	2b	231	4% 90% 10%
34	1c	206	5% 97% .
34	2c	206	6% 94% 6%
35	1d	208	2% 95% 5%
35	2d	208	97% .
36	1e	148	1% 98% .
36	2e	148	1% 97% .
37	1f	100	1% 99% .
37	2f	100	1% 100%
38	1g	155	6% 98% .
38	2g	155	12% 95% 5% .
39	1h	137	1% 96% .
39	2h	137	3% 95% 5%
40	1i	127	10% 94% 6%
40	2i	127	21% 91% 8% .

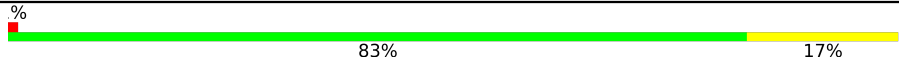




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Mol	Chain	Length	Quality of chain
41	1j	97	16% 94% 6%
41	2j	97	23% 96% ..
42	1k	114	97% .
42	2k	114	2% 97% .
43	1l	122	2% 96% .
43	2l	122	2% 96% .
44	1m	116	5% 94% 6%
44	2m	116	12% 90% 9% .
45	1n	60	5% 95% 5%
45	2n	60	23% 98% .
46	1o	88	% 97% .
46	2o	88	% 93% 7%
47	1p	82	9% 93% 7%
47	2p	82	2% 93% 7%
48	1q	99	98% .
48	2q	99	% 98% .
49	1r	68	% 99% .
49	2r	68	3% 99% .
50	1s	83	13% 95% 5%
50	2s	83	24% 94% 6%
51	1t	98	3% 94% ... .
51	2t	98	2% 96% .
52	1u	23	9% 100%
52	2u	23	48% 96% .
53	1x	76	87% 12% .

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Mol	Chain	Length	Quality of chain
53	2x	76	
54	1y	19	
54	2y	19	
55	A	27	
55	B	27	

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	3084	-	-	-	X
56	MG	1A	3089	-	-	-	X
56	MG	1A	3116	-	-	-	X
56	MG	1A	3123	-	-	-	X
56	MG	1A	3149	-	-	-	X
56	MG	1A	3185	-	-	-	X
56	MG	1A	3226	-	-	-	X
56	MG	1A	3229	-	-	-	X
56	MG	1A	3277	-	-	-	X
56	MG	1A	3507	-	-	-	X
56	MG	1A	3545	-	-	-	X
56	MG	1A	3645	-	-	-	X
56	MG	1A	3713	-	-	-	X
56	MG	1A	3764	-	-	-	X
56	MG	1A	3795	-	-	-	X
56	MG	1A	3922	-	-	-	X
56	MG	1B	215	-	-	-	X
56	MG	1D	309	-	-	-	X
56	MG	1a	1611	-	-	-	X
56	MG	1a	1624	-	-	-	X
56	MG	1a	1653	-	-	-	X
56	MG	1a	1665	-	-	-	X
56	MG	1a	1667	-	-	-	X
56	MG	1a	1668	-	-	-	X
56	MG	1a	1682	-	-	-	X
56	MG	1a	1706	-	-	-	X
56	MG	1a	1728	-	-	-	X
56	MG	1a	1732	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
56	MG	1a	1760	-	-	-	X
56	MG	1a	1773	-	-	-	X
56	MG	1a	1823	-	-	-	X
56	MG	1e	201	-	-	-	X
56	MG	1o	101	-	-	-	X
56	MG	2A	3005	-	-	-	X
56	MG	2A	3006	-	-	-	X
56	MG	2A	3009	-	-	-	X
56	MG	2A	3070	-	-	-	X
56	MG	2A	3077	-	-	-	X
56	MG	2A	3081	-	-	-	X
56	MG	2A	3089	-	-	-	X
56	MG	2A	3110	-	-	-	X
56	MG	2A	3139	-	-	-	X
56	MG	2A	3148	-	-	-	X
56	MG	2A	3176	-	-	-	X
56	MG	2A	3177	-	-	-	X
56	MG	2A	3178	-	-	-	X
56	MG	2A	3182	-	-	-	X
56	MG	2A	3183	-	-	-	X
56	MG	2A	3187	-	-	-	X
56	MG	2A	3190	-	-	-	X
56	MG	2A	3191	-	-	-	X
56	MG	2A	3220	-	-	-	X
56	MG	2A	3233	-	-	-	X
56	MG	2A	3237	-	-	-	X
56	MG	2A	3299	-	-	-	X
56	MG	2A	3328	-	-	-	X
56	MG	2A	3399	-	-	-	X
56	MG	2A	3410	-	-	-	X
56	MG	2A	3437	-	-	-	X
56	MG	2A	3568	-	-	-	X
56	MG	2A	3600	-	-	-	X
56	MG	2A	3661	-	-	-	X
56	MG	2D	302	-	-	-	X
56	MG	2U	202	-	-	-	X
56	MG	2a	1602	-	-	-	X
56	MG	2a	1606	-	-	-	X
56	MG	2a	1608	-	-	-	X
56	MG	2a	1622	-	-	-	X
56	MG	2a	1630	-	-	-	X
56	MG	2a	1658	-	-	-	X

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<b>Mol</b>	<b>Type</b>	<b>Chain</b>	<b>Res</b>	<b>Chirality</b>	<b>Geometry</b>	<b>Clashes</b>	<b>Electron density</b>
56	MG	2a	1668	-	-	-	X
56	MG	2a	1683	-	-	-	X
56	MG	2a	1696	-	-	-	X
56	MG	2t	3001	-	-	-	X
56	MG	2x	108	-	-	-	X

## 2 Entry composition [i](#)

There are 63 unique types of molecules in this entry. The entry contains 293672 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	2824	Total	C	N	O	P	0	0	0
			60842	27081	11388	19550	2823			
1	2A	2869	Total	C	N	O	P	0	0	0
			61801	27510	11560	19864	2867			

- Molecule 2 is a RNA chain called 5s ribosomal RNA.

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

- 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
42	2k	114	Total	C	N	O	S	0	0	0
			833	519	156	155	3			

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

- Molecule 53 is a RNA chain called tRNA met.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
53	1x	76	Total	C	N	O	P	S	0	0	0
			1625	725	294	529	76	1			
53	2x	76	Total	C	N	O	P	S	0	0	0
			1625	725	294	529	76	1			

- Molecule 54 is a protein called Onc112.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
54	1y	12	Total	C	N	O	0	0	0
			101	67	19	15			
54	2y	12	Total	C	N	O	0	0	0
			101	67	19	15			

- Molecule 55 is a RNA chain called mRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
55	A	3	Total	C	N	O	P	0	0	0
			65	29	12	21	3			
55	B	3	Total	C	N	O	P	0	0	0
			65	29	12	21	3			

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
56	1A	946	Total	Mg	0	0
			946	946		
56	1B	29	Total	Mg	0	0
			29	29		
56	1D	21	Total	Mg	0	0
			21	21		
56	1E	6	Total	Mg	0	0
			6	6		
56	1F	9	Total	Mg	0	0
			9	9		
56	1G	4	Total	Mg	0	0
			4	4		
56	1H	2	Total	Mg	0	0
			2	2		
56	1N	3	Total	Mg	0	0
			3	3		
56	1O	1	Total	Mg	0	0
			1	1		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
56	1P	2	Total 2	Mg 2	0	0
56	1Q	4	Total 4	Mg 4	0	0
56	1R	4	Total 4	Mg 4	0	0
56	1T	2	Total 2	Mg 2	0	0
56	1U	5	Total 5	Mg 5	0	0
56	1V	3	Total 3	Mg 3	0	0
56	1W	3	Total 3	Mg 3	0	0
56	1X	1	Total 1	Mg 1	0	0
56	1Y	1	Total 1	Mg 1	0	0
56	1Z	1	Total 1	Mg 1	0	0
56	10	7	Total 7	Mg 7	0	0
56	11	3	Total 3	Mg 3	0	0
56	13	3	Total 3	Mg 3	0	0
56	15	3	Total 3	Mg 3	0	0
56	17	2	Total 2	Mg 2	0	0
56	18	1	Total 1	Mg 1	0	0
56	19	2	Total 2	Mg 2	0	0
56	1a	261	Total 261	Mg 261	0	0
56	1b	1	Total 1	Mg 1	0	0
56	1d	4	Total 4	Mg 4	0	0
56	1e	4	Total 4	Mg 4	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
56	1f	1	Total Mg 1 1	0	0
56	1g	1	Total Mg 1 1	0	0
56	1i	1	Total Mg 1 1	0	0
56	1l	1	Total Mg 1 1	0	0
56	1n	1	Total Mg 1 1	0	0
56	1o	2	Total Mg 2 2	0	0
56	1r	1	Total Mg 1 1	0	0
56	1t	1	Total Mg 1 1	0	0
56	1x	12	Total Mg 12 12	0	0
56	2A	679	Total Mg 679 679	0	0
56	2B	17	Total Mg 17 17	0	0
56	2D	8	Total Mg 8 8	0	0
56	2E	7	Total Mg 7 7	0	0
56	2F	3	Total Mg 3 3	0	0
56	2G	2	Total Mg 2 2	0	0
56	2I	1	Total Mg 1 1	0	0
56	2N	1	Total Mg 1 1	0	0
56	2O	2	Total Mg 2 2	0	0
56	2P	1	Total Mg 1 1	0	0
56	2Q	2	Total Mg 2 2	0	0
56	2R	1	Total Mg 1 1	0	0

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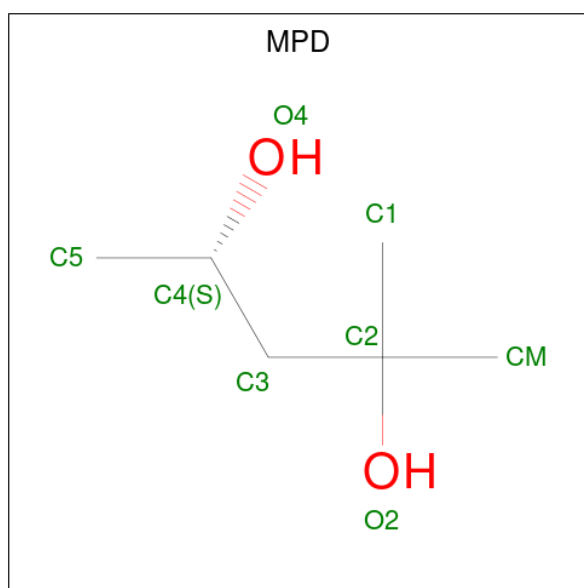
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
56	2T	4	Total 4	Mg 4	0	0
56	2U	2	Total 2	Mg 2	0	0
56	2V	3	Total 3	Mg 3	0	0
56	2W	1	Total 1	Mg 1	0	0
56	2X	1	Total 1	Mg 1	0	0
56	2Y	1	Total 1	Mg 1	0	0
56	20	1	Total 1	Mg 1	0	0
56	21	1	Total 1	Mg 1	0	0
56	23	1	Total 1	Mg 1	0	0
56	28	2	Total 2	Mg 2	0	0
56	2a	183	Total 183	Mg 183	0	0
56	2e	1	Total 1	Mg 1	0	0
56	2f	1	Total 1	Mg 1	0	0
56	2j	1	Total 1	Mg 1	0	0
56	2k	1	Total 1	Mg 1	0	0
56	2l	1	Total 1	Mg 1	0	0
56	2n	1	Total 1	Mg 1	0	0
56	2p	1	Total 1	Mg 1	0	0
56	2q	1	Total 1	Mg 1	0	0
56	2t	1	Total 1	Mg 1	0	0
56	2x	10	Total 10	Mg 10	0	0

- Molecule 57 is UNKNOWN ATOM OR ION (three-letter code: UNX) (formula: X).

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

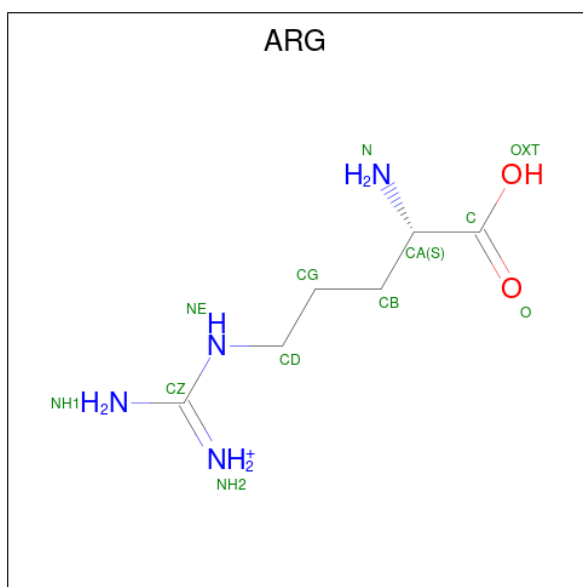
- Molecule 58 is (4S)-2-METHYL-2,4-PENTANEDIOL (three-letter code: MPD) (formula: C<sub>6</sub>H<sub>14</sub>O<sub>2</sub>).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
58	1A	1	Total C O 8 6 2	0	0
58	1a	1	Total C O 8 6 2	0	0

- Molecule 59 is ARGinine (three-letter code: ARG) (formula: C<sub>6</sub>H<sub>15</sub>N<sub>4</sub>O<sub>2</sub>).





Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
59	1B	1	Total	C	N	O	0	0
			12	6	4	2		

- Molecule 60 is ZINC ION (three-letter code: ZN) (formula: Zn).

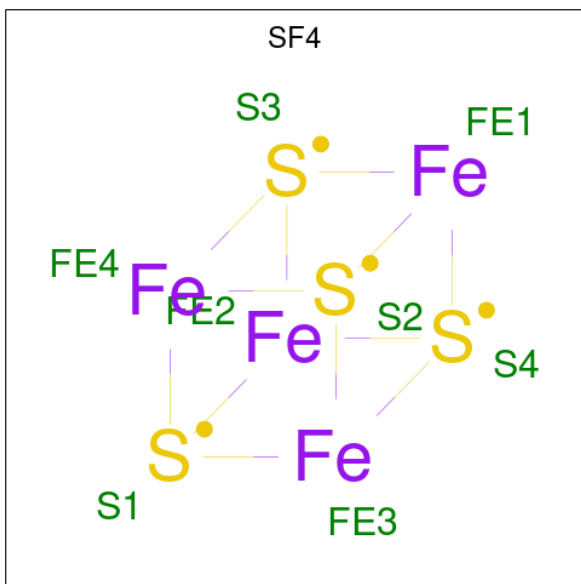
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
60	1Y	1	Total	Zn	0	0
			1	1		
60	14	1	Total	Zn	0	0
			1	1		
60	15	1	Total	Zn	0	0
			1	1		
60	16	1	Total	Zn	0	0
			1	1		
60	19	1	Total	Zn	0	0
			1	1		
60	1n	1	Total	Zn	0	0
			1	1		
60	2Y	1	Total	Zn	0	0
			1	1		
60	24	1	Total	Zn	0	0
			1	1		
60	25	1	Total	Zn	0	0
			1	1		
60	26	1	Total	Zn	0	0
			1	1		
60	29	1	Total	Zn	0	0
			1	1		

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
60	2n	1	Total Zn 1 1	0	0

- Molecule 61 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe<sub>4</sub>S<sub>4</sub>).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
61	1d	1	Total Fe S 8 4 4	0	0
61	2d	1	Total Fe S 8 4 4	0	0

- Molecule 62 is POTASSIUM ION (three-letter code: K) (formula: K).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
62	2A	1	Total K 1 1	0	0

- Molecule 63 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
63	1A	1632	Total O 1632 1632	0	0
63	1B	50	Total O 50 50	0	0
63	1D	20	Total O 20 20	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
63	1E	17	Total 17	O 17	0	0
63	1F	14	Total 14	O 14	0	0
63	1G	5	Total 5	O 5	0	0
63	1H	4	Total 4	O 4	0	0
63	1N	7	Total 7	O 7	0	0
63	1O	2	Total 2	O 2	0	0
63	1P	18	Total 18	O 18	0	0
63	1Q	5	Total 5	O 5	0	0
63	1R	7	Total 7	O 7	0	0
63	1T	4	Total 4	O 4	0	0
63	1U	3	Total 3	O 3	0	0
63	1V	3	Total 3	O 3	0	0
63	1X	6	Total 6	O 6	0	0
63	1Y	2	Total 2	O 2	0	0
63	10	4	Total 4	O 4	0	0
63	11	3	Total 3	O 3	0	0
63	13	6	Total 6	O 6	0	0
63	15	2	Total 2	O 2	0	0
63	16	3	Total 3	O 3	0	0
63	18	7	Total 7	O 7	0	0
63	19	3	Total 3	O 3	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
63	1a	369	Total 369	O 369	0	0
63	1c	1	Total 1	O 1	0	0
63	1d	6	Total 6	O 6	0	0
63	1e	3	Total 3	O 3	0	0
63	1f	1	Total 1	O 1	0	0
63	1h	1	Total 1	O 1	0	0
63	1l	3	Total 3	O 3	0	0
63	1m	1	Total 1	O 1	0	0
63	1n	1	Total 1	O 1	0	0
63	1o	2	Total 2	O 2	0	0
63	1p	1	Total 1	O 1	0	0
63	1t	1	Total 1	O 1	0	0
63	1x	2	Total 2	O 2	0	0
63	2A	1221	Total 1221	O 1221	0	0
63	2B	33	Total 33	O 33	0	0
63	2D	13	Total 13	O 13	0	0
63	2E	12	Total 12	O 12	0	0
63	2F	4	Total 4	O 4	0	0
63	2N	2	Total 2	O 2	0	0
63	2O	4	Total 4	O 4	0	0
63	2P	7	Total 7	O 7	0	0

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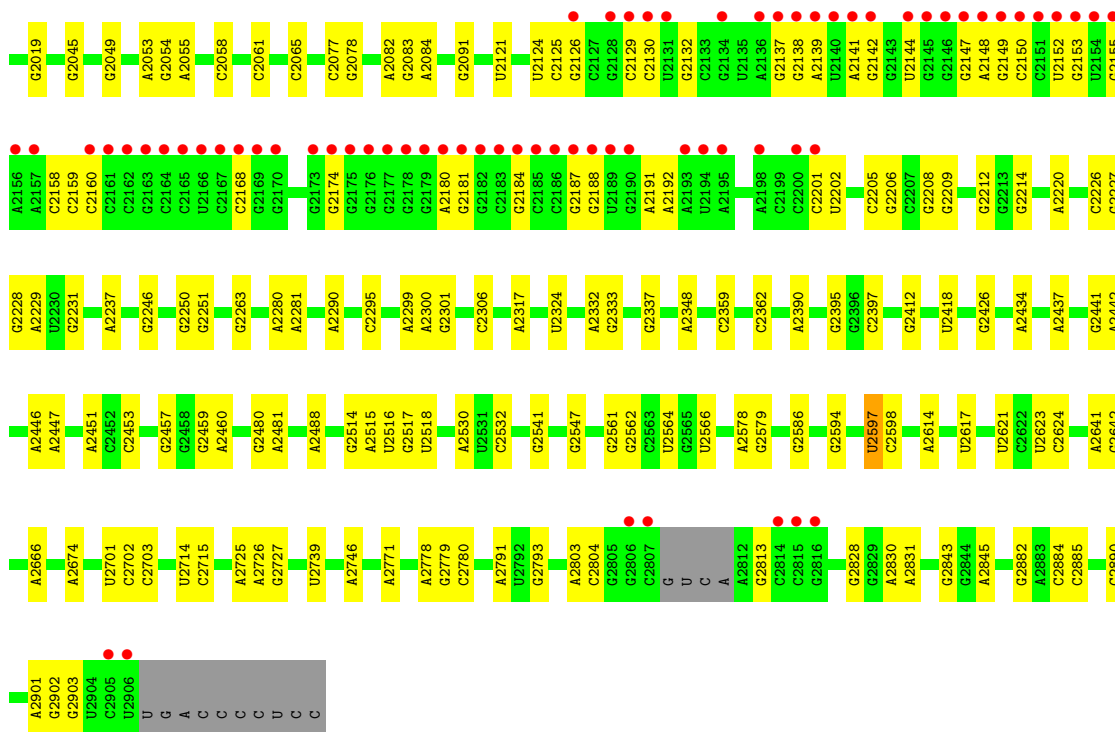
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
63	2Q	5	Total 5	O 5	0	0
63	2R	2	Total 2	O 2	0	0
63	2T	2	Total 2	O 2	0	0
63	2U	3	Total 3	O 3	0	0
63	2X	4	Total 4	O 4	0	0
63	2Y	1	Total 1	O 1	0	0
63	20	2	Total 2	O 2	0	0
63	21	2	Total 2	O 2	0	0
63	23	2	Total 2	O 2	0	0
63	25	1	Total 1	O 1	0	0
63	26	2	Total 2	O 2	0	0
63	28	5	Total 5	O 5	0	0
63	2a	305	Total 305	O 305	0	0
63	2d	3	Total 3	O 3	0	0
63	2e	1	Total 1	O 1	0	0
63	2j	2	Total 2	O 2	0	0
63	2l	1	Total 1	O 1	0	0
63	2n	1	Total 1	O 1	0	0
63	2p	1	Total 1	O 1	0	0
63	2r	1	Total 1	O 1	0	0
63	2t	1	Total 1	O 1	0	0

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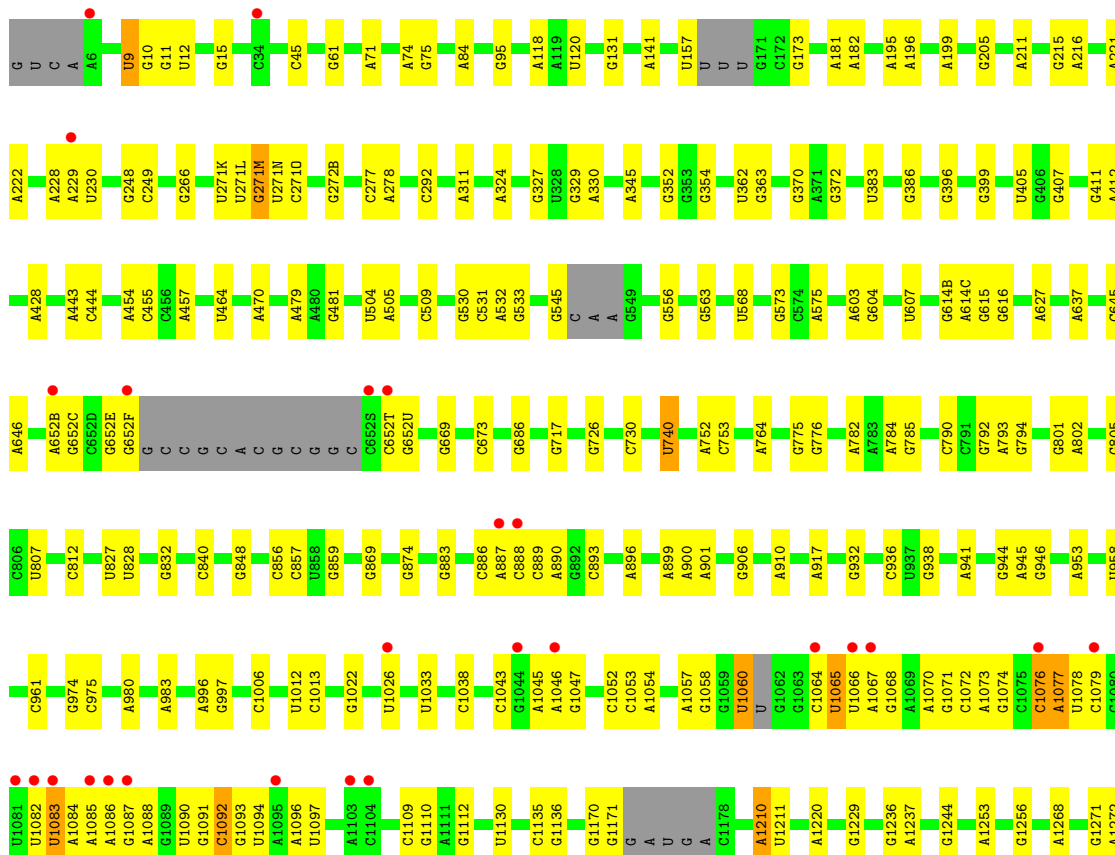
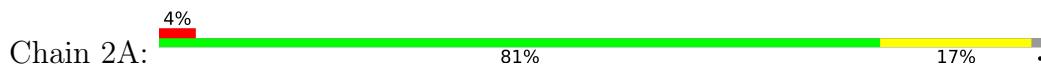
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<b>Mol</b>	<b>Chain</b>	<b>Residues</b>	<b>Atoms</b>	<b>ZeroOcc</b>	<b>AltConf</b>
63	2x	2	Total O 2 2	0	0
63	A	1	Total O 1 1	0	0

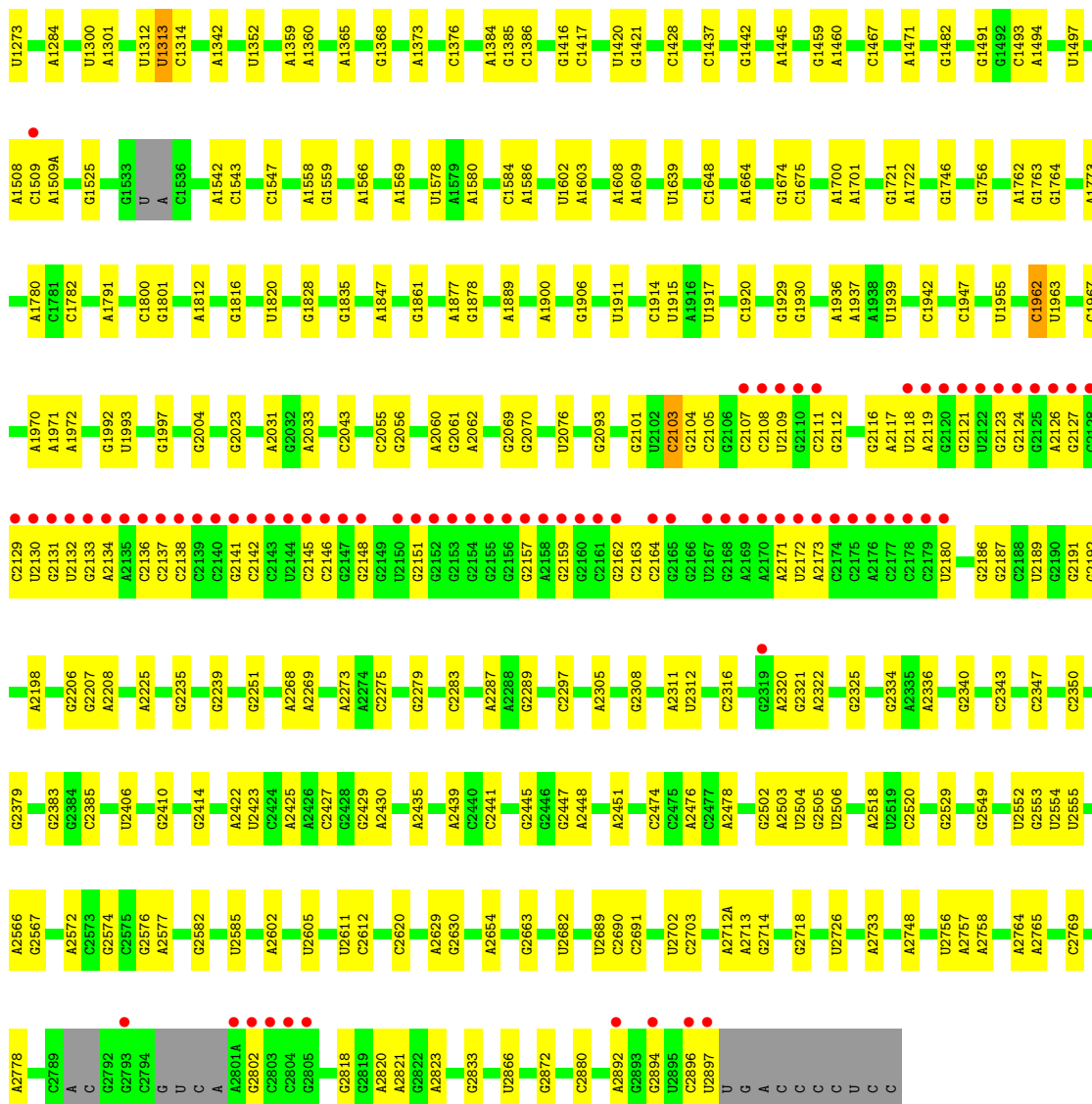




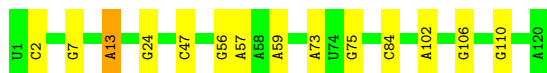
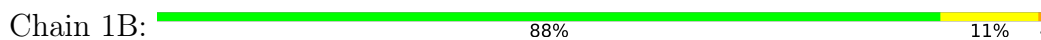
• Molecule 1: 23s ribosomal RNA







• Molecule 2: 5s ribosomal RNA



• Molecule 2: 5s ribosomal RNA



• Molecule 3: 50S ribosomal protein L2





- Molecule 3: 50S ribosomal protein L2



- Molecule 4: 50S ribosomal protein L3



- Molecule 4: 50S ribosomal protein L3



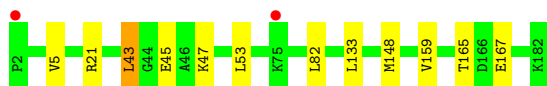
- Molecule 5: 50S ribosomal protein L4



- Molecule 5: 50S ribosomal protein L4



- Molecule 6: 50S ribosomal protein L5



- Molecule 6: 50S ribosomal protein L5

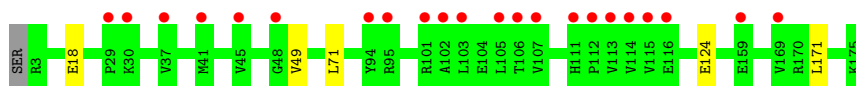




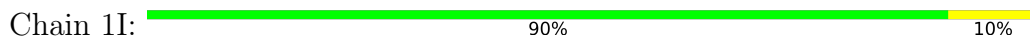
- Molecule 7: 50S ribosomal protein L6



- Molecule 7: 50S ribosomal protein L6



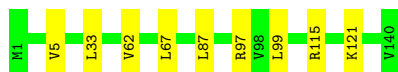
- Molecule 8: 50S ribosomal protein L9



- Molecule 8: 50S ribosomal protein L9



- Molecule 9: 50S ribosomal protein L13

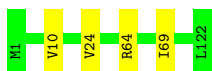


- Molecule 9: 50S ribosomal protein L13



- Molecule 10: 50S ribosomal protein L14





- Molecule 10: 50S ribosomal protein L14



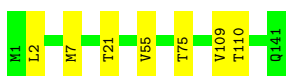
- Molecule 11: 50S ribosomal protein L15



- Molecule 11: 50S ribosomal protein L15



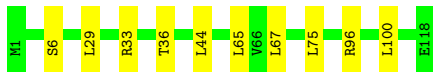
- Molecule 12: 50S ribosomal protein L16



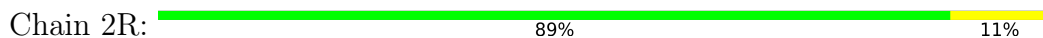
- Molecule 12: 50S ribosomal protein L16



- Molecule 13: 50S ribosomal protein L17



- Molecule 13: 50S ribosomal protein L17





- Molecule 14: 50S ribosomal protein L18



- Molecule 14: 50S ribosomal protein L18



- Molecule 15: 50S ribosomal protein L19



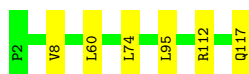
- Molecule 15: 50S ribosomal protein L19



- Molecule 16: 50S ribosomal protein L20



- Molecule 16: 50S ribosomal protein L20



- Molecule 17: 50S ribosomal protein L21





- Molecule 17: 50S ribosomal protein L21



- Molecule 18: 50S ribosomal protein L22



- Molecule 18: 50S ribosomal protein L22



- Molecule 19: 50S ribosomal protein L23



- Molecule 19: 50S ribosomal protein L23



- Molecule 20: 50S ribosomal protein L24



- Molecule 20: 50S ribosomal protein L24

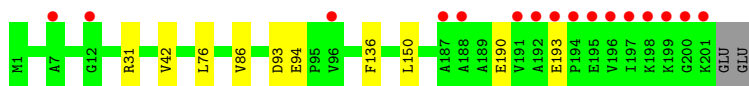




- Molecule 21: 50S ribosomal protein L25



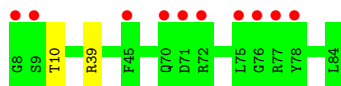
- Molecule 21: 50S ribosomal protein L25



- Molecule 22: 50S ribosomal protein L27



- Molecule 22: 50S ribosomal protein L27



- Molecule 23: 50S ribosomal protein L28



- Molecule 23: 50S ribosomal protein L28



- Molecule 24: 50S ribosomal protein L29

Chain 12:  99%



- Molecule 24: 50S ribosomal protein L29

Chain 22:  97%



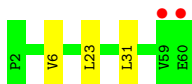
- Molecule 25: 50S ribosomal protein L30

Chain 13:  93%




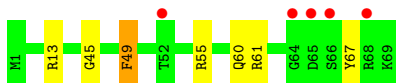
- Molecule 25: 50S ribosomal protein L30

Chain 23:  95%

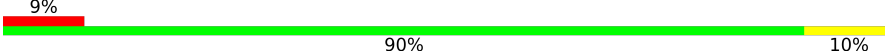


- Molecule 26: 50S ribosomal protein L31

Chain 14:  90%



- Molecule 26: 50S ribosomal protein L31

Chain 24:  90%



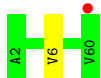
- Molecule 27: 50S ribosomal protein L32

Chain 15:  97%

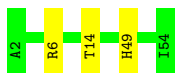


- Molecule 27: 50S ribosomal protein L32





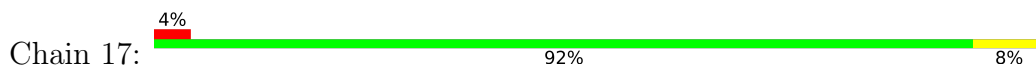
- Molecule 28: 50S ribosomal protein L33



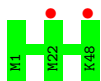
- Molecule 28: 50S ribosomal protein L33



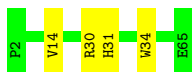
- Molecule 29: 50S ribosomal protein L34



- Molecule 29: 50S ribosomal protein L34



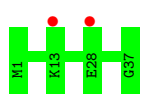
- Molecule 30: 50S ribosomal protein L35



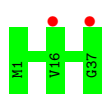
- Molecule 30: 50S ribosomal protein L35



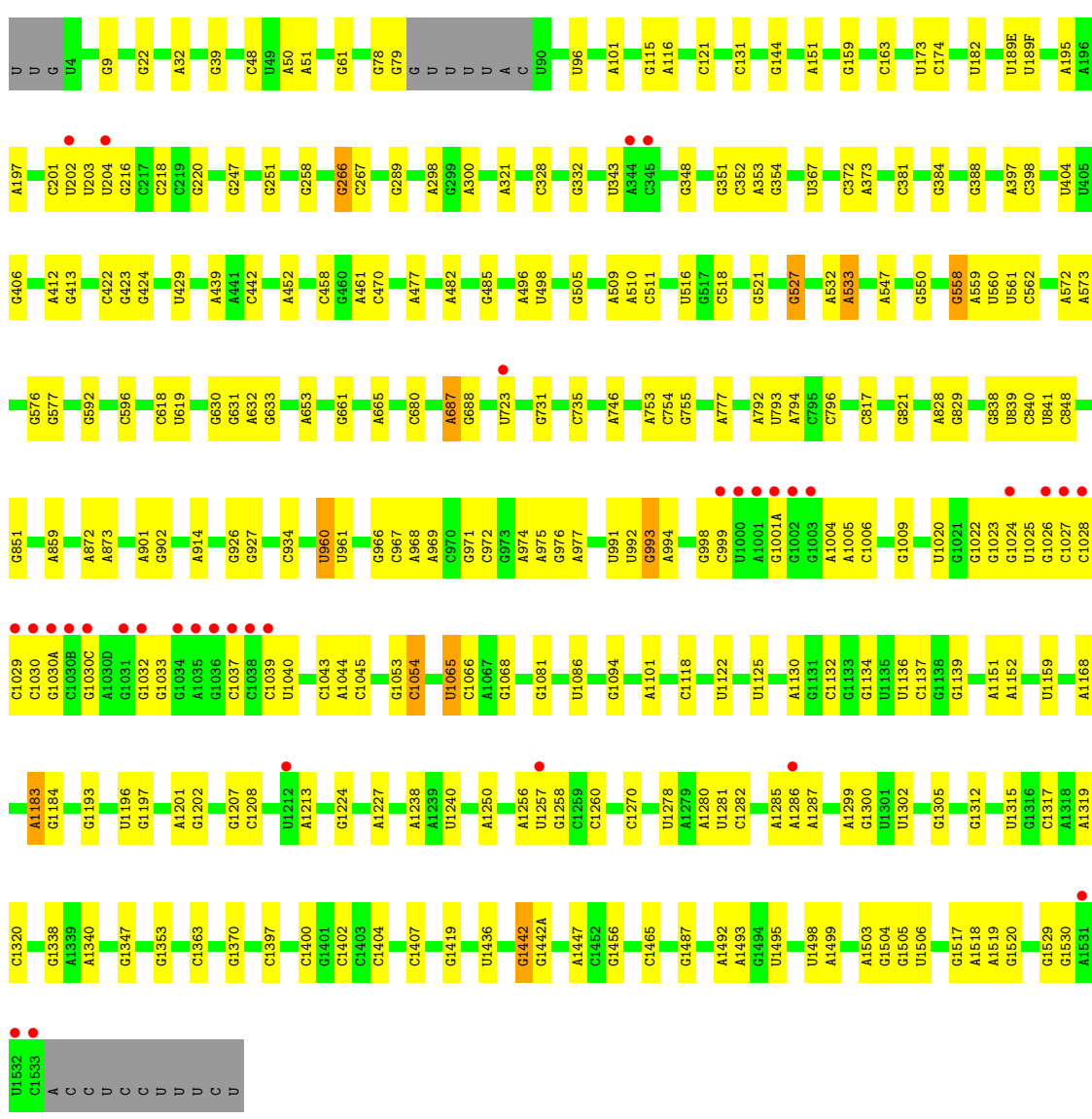
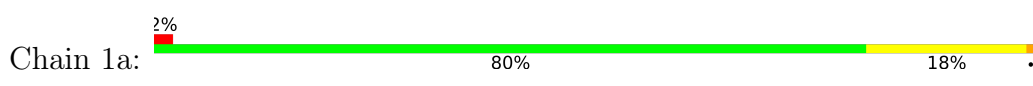
- Molecule 31: 50S ribosomal protein L36



• Molecule 31: 50S ribosomal protein L36



• Molecule 32: 16s ribosomal RNA



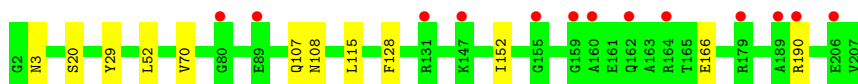




- Molecule 34: 30S ribosomal protein S3



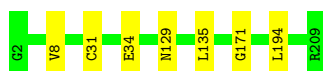
- Molecule 34: 30S ribosomal protein S3



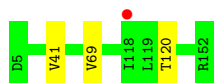
- Molecule 35: 30S ribosomal protein S4



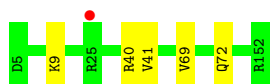
- Molecule 35: 30S ribosomal protein S4



- Molecule 36: 30S ribosomal protein S5



- Molecule 36: 30S ribosomal protein S5



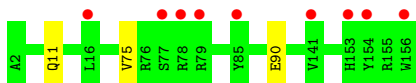
- Molecule 37: 30S ribosomal protein S6



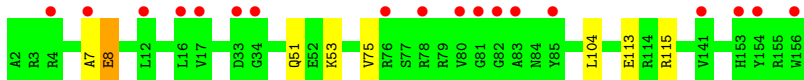
- Molecule 37: 30S ribosomal protein S6



- Molecule 38: 30S ribosomal protein S7



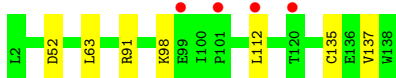
- Molecule 38: 30S ribosomal protein S7



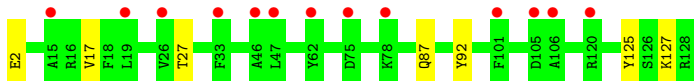
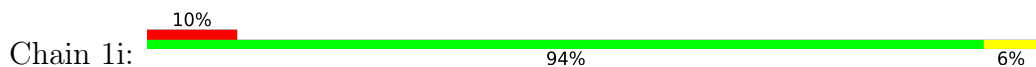
- Molecule 39: 30S ribosomal protein S8



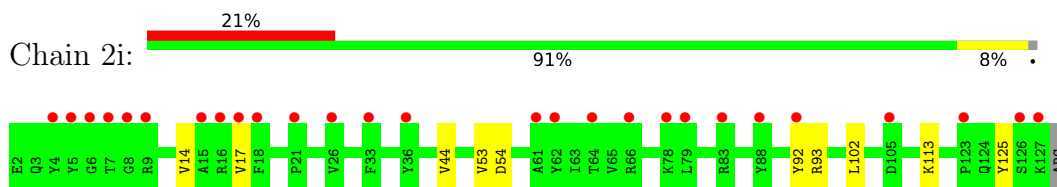
- Molecule 39: 30S ribosomal protein S8



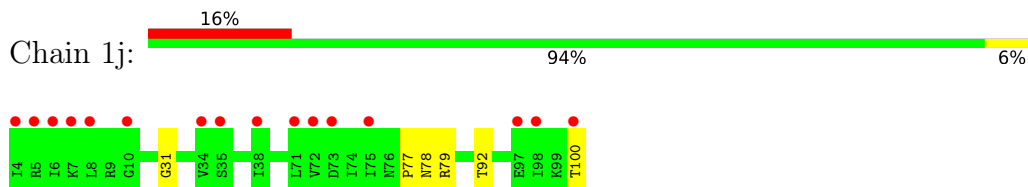
- Molecule 40: 30S ribosomal protein S9



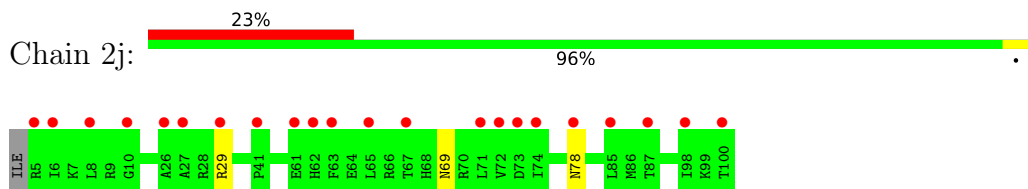
- Molecule 40: 30S ribosomal protein S9



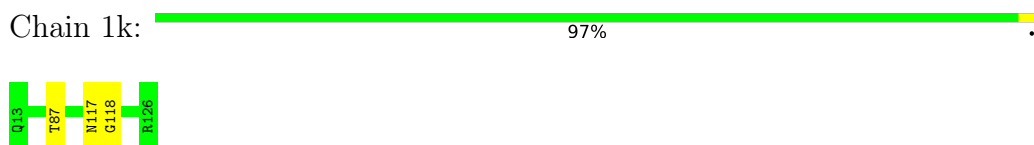
- Molecule 41: 30S ribosomal protein S10



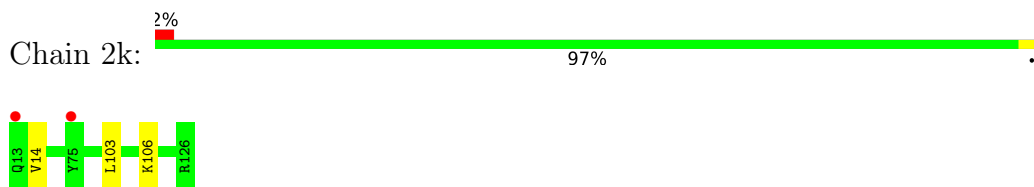
- Molecule 41: 30S ribosomal protein S10



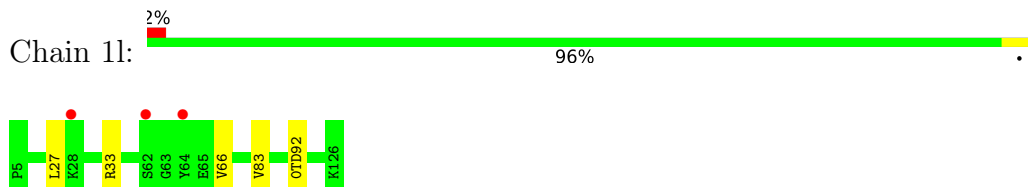
- Molecule 42: 30S ribosomal protein S11



- Molecule 42: 30S ribosomal protein S11

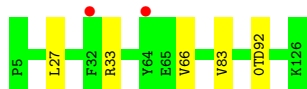


- Molecule 43: 30S ribosomal protein S12

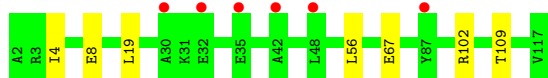


- Molecule 43: 30S ribosomal protein S12





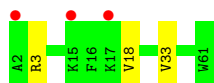
- Molecule 44: 30S ribosomal protein S13



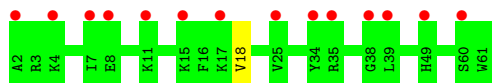
- Molecule 44: 30S ribosomal protein S13



- Molecule 45: 30S ribosomal protein S14 type Z



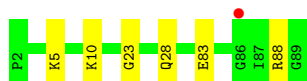
- Molecule 45: 30S ribosomal protein S14 type Z



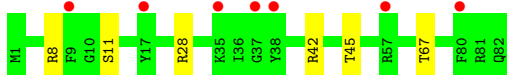
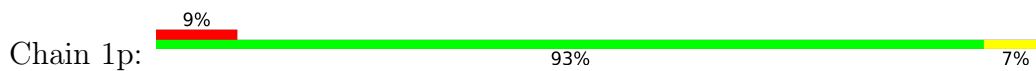
- Molecule 46: 30S ribosomal protein S15



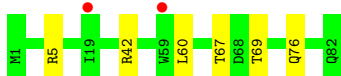
- Molecule 46: 30S ribosomal protein S15



- Molecule 47: 30S ribosomal protein S16



- Molecule 47: 30S ribosomal protein S16



- Molecule 48: 30S ribosomal protein S17



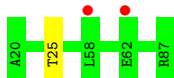
- Molecule 48: 30S ribosomal protein S17



- Molecule 49: 30S ribosomal protein S18



- Molecule 49: 30S ribosomal protein S18

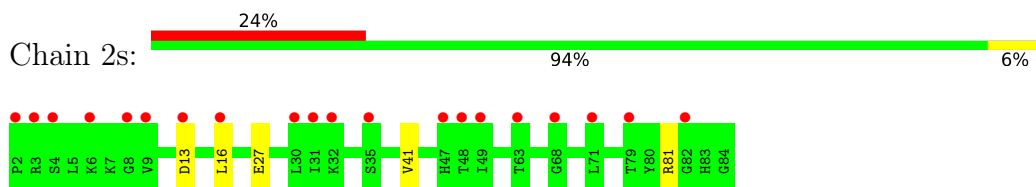


- Molecule 50: 30S ribosomal protein S19

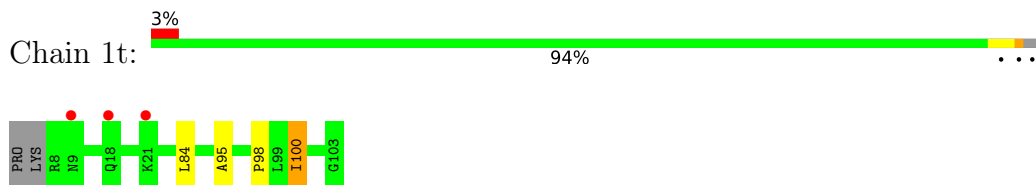




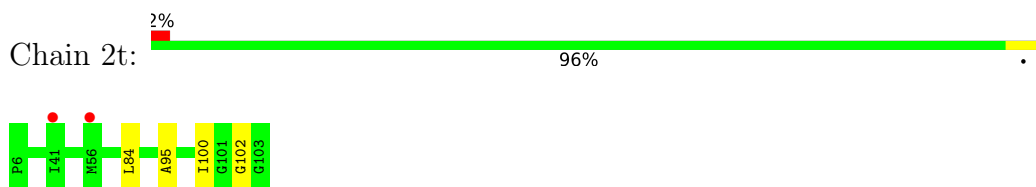
- Molecule 50: 30S ribosomal protein S19



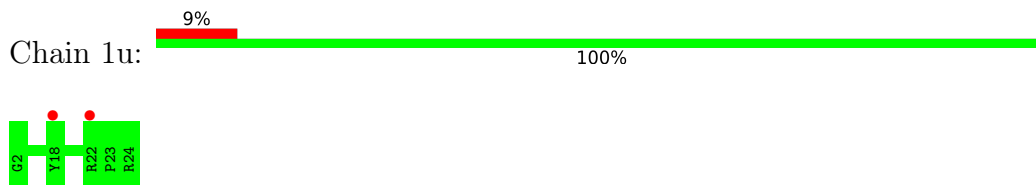
- Molecule 51: 30S ribosomal protein S20



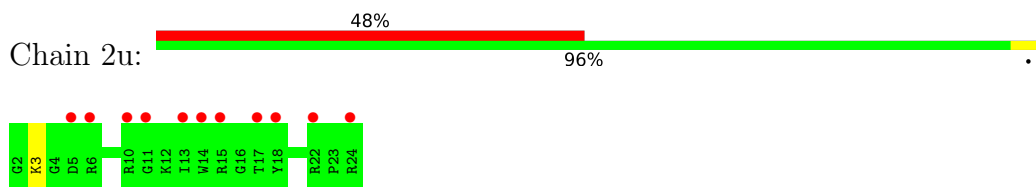
- Molecule 51: 30S ribosomal protein S20



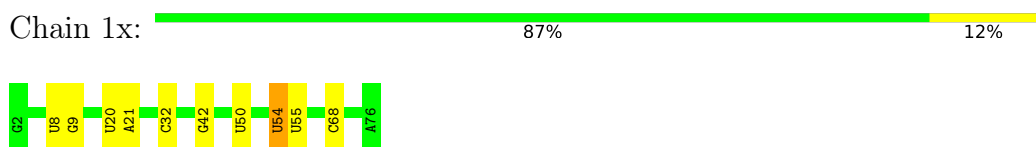
- Molecule 52: 30S ribosomal protein Thx



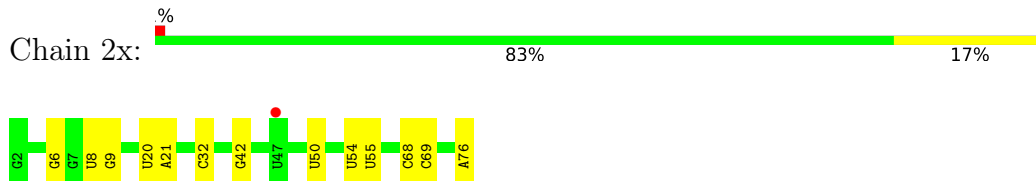
- Molecule 52: 30S ribosomal protein Thx



- Molecule 53: tRNA met

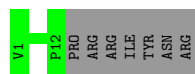


- Molecule 53: tRNA met



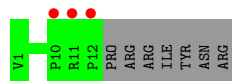
- Molecule 54: Onc112

Chain 1y:  63% 37%



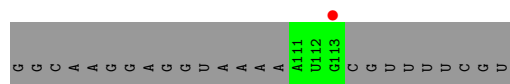
- Molecule 54: Onc112

Chain 2y:  16% 63% 37%



- Molecule 55: mRNA

Chain A:  4% 11% 89%



- Molecule 55: mRNA

Chain B:  4% 11% 89%



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	209.30Å 452.29Å 625.12Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.72 – 3.10 49.72 – 3.10	Depositor EDS
% Data completeness (in resolution range)	99.1 (49.72-3.10) 99.1 (49.72-3.10)	Depositor EDS
$R_{merge}$	0.22	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.30 (at 3.12Å)	Xtrriage
Refinement program	PHENIX	Depositor
R, $R_{free}$	0.231 , 0.271 0.231 , 0.271	Depositor DCC
$R_{free}$ test set	52535 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	71.9	Xtrriage
Anisotropy	0.244	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.26 , 41.4	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.44$ , $\langle L^2 \rangle = 0.26$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.92	EDS
Total number of atoms	293672	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	61.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.57% of the height of the origin peak. No significant pseudotranslation is detected.*

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

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

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: K, 0TD, OMC, UR3, PSU, MPD, 4SU, 5MU, M2G, OMG, MG, UNX, 2MG, SF4, G7M, MA6, 5MC, ZN, 4OC, 2MA, 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	0.45	0/67879	0.88	48/105953 (0.0%)
1	2A	0.35	0/68951	0.85	38/107627 (0.0%)
2	1B	0.42	0/2876	1.00	8/4486 (0.2%)
2	2B	0.34	0/2878	0.84	0/4490
3	1D	0.31	0/2181	0.51	0/2940
3	2D	0.28	0/2186	0.50	0/2944
4	1E	0.32	0/1592	0.52	0/2149
4	2E	0.27	0/1592	0.52	0/2149
5	1F	0.31	0/1619	0.50	0/2193
5	2F	0.28	0/1615	0.49	0/2188
6	1G	0.26	0/1451	0.51	0/1961
6	2G	0.27	0/1449	0.49	0/1957
7	1H	0.29	0/1356	0.49	0/1834
7	2H	0.26	0/1350	0.49	0/1826
8	1I	0.27	0/1109	0.53	0/1512
8	2I	0.26	0/1091	0.50	0/1490
9	1N	0.29	0/1148	0.48	0/1547
9	2N	0.25	0/1144	0.46	0/1543
10	1O	0.35	0/943	0.51	0/1269
10	2O	0.31	0/943	0.49	0/1269
11	1P	0.32	0/1152	0.51	0/1533
11	2P	0.26	0/1152	0.48	0/1533
12	1Q	0.32	0/1143	0.48	0/1527
12	2Q	0.27	0/1143	0.44	0/1527
13	1R	0.30	0/982	0.52	0/1312
13	2R	0.26	0/982	0.46	0/1312
14	1S	0.27	0/887	0.52	0/1180
14	2S	0.26	0/880	0.48	0/1172
15	1T	0.32	0/1105	0.52	0/1477
15	2T	0.27	0/1097	0.48	0/1468
16	1U	0.34	0/977	0.47	0/1301

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
16	2U	0.28	0/977	0.45	0/1301
17	1V	0.32	0/786	0.49	0/1053
17	2V	0.28	0/782	0.50	0/1049
18	1W	0.34	0/897	0.49	0/1205
18	2W	0.27	0/897	0.45	0/1205
19	1X	0.34	0/764	0.52	0/1025
19	2X	0.28	0/764	0.51	0/1025
20	1Y	0.32	0/823	0.51	0/1099
20	2Y	0.27	0/823	0.50	0/1100
21	1Z	0.27	0/1620	0.47	0/2200
21	2Z	0.26	0/1590	0.47	0/2162
22	10	0.31	0/616	0.49	0/821
22	20	0.27	0/616	0.48	0/821
23	11	0.30	0/761	0.49	0/1013
23	21	0.28	0/766	0.46	0/1018
24	12	0.29	0/590	0.48	0/781
24	22	0.27	0/594	0.43	0/785
25	13	0.29	0/474	0.46	0/635
25	23	0.24	0/469	0.43	0/630
26	14	0.29	0/559	0.57	0/754
26	24	0.34	0/549	0.57	0/741
27	15	0.32	0/473	0.49	0/639
27	25	0.27	0/469	0.48	0/635
28	16	0.30	0/460	0.45	0/613
28	26	0.26	0/456	0.44	0/608
29	17	0.34	0/426	0.53	0/561
29	27	0.27	0/426	0.48	0/561
30	18	0.32	0/525	0.48	0/691
30	28	0.28	0/525	0.47	0/691
31	19	0.32	0/310	0.51	0/407
31	29	0.28	0/310	0.48	0/407
32	1a	0.35	0/35795	0.85	32/55864 (0.1%)
32	2a	0.34	0/35890	0.86	40/56012 (0.1%)
33	1b	0.27	0/1876	0.52	0/2533
33	2b	0.29	0/1860	0.49	0/2518
34	1c	0.26	0/1582	0.44	0/2137
34	2c	0.28	0/1566	0.45	0/2119
35	1d	0.27	0/1695	0.48	0/2274
35	2d	0.26	0/1698	0.47	0/2277
36	1e	0.26	0/1149	0.49	0/1548
36	2e	0.26	0/1149	0.49	0/1548
37	1f	0.26	0/827	0.44	0/1120
37	2f	0.27	0/829	0.47	0/1123

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
38	1g	0.24	0/1254	0.44	0/1683
38	2g	0.25	0/1248	0.44	0/1676
39	1h	0.24	0/1118	0.48	0/1506
39	2h	0.25	0/1108	0.47	0/1494
40	1i	0.27	0/1005	0.48	0/1351
40	2i	0.30	0/985	0.50	0/1329
41	1j	0.28	0/732	0.51	0/993
41	2j	0.29	0/723	0.51	0/984
42	1k	0.27	0/849	0.47	0/1150
42	2k	0.27	0/848	0.49	0/1149
43	1l	0.27	0/937	0.48	0/1260
43	2l	0.27	0/937	0.55	0/1260
44	1m	0.25	0/924	0.49	0/1242
44	2m	0.27	0/905	0.49	0/1217
45	1n	0.25	0/501	0.45	0/664
45	2n	0.28	0/501	0.41	0/664
46	1o	0.26	0/739	0.46	0/985
46	2o	0.26	0/739	0.45	0/985
47	1p	0.26	0/697	0.47	0/939
47	2p	0.26	0/693	0.49	0/935
48	1q	0.27	0/836	0.50	0/1117
48	2q	0.26	0/836	0.47	0/1117
49	1r	0.27	0/560	0.47	0/746
49	2r	0.26	0/560	0.45	0/746
50	1s	0.26	0/663	0.49	0/895
50	2s	0.27	0/660	0.54	0/893
51	1t	0.26	0/734	0.48	0/969
51	2t	0.25	0/736	0.44	0/976
52	1u	0.24	0/203	0.46	0/266
52	2u	0.27	0/203	0.47	0/266
53	1x	0.41	0/1725	0.95	0/2689
53	2x	0.40	0/1725	0.93	1/2689 (0.0%)
54	1y	0.33	0/106	0.63	0/146
54	2y	0.27	0/106	0.55	0/146
55	A	0.58	0/72	1.13	0/110
55	B	0.53	0/72	1.09	0/110
All	All	0.35	0/311106	0.78	167/465325 (0.0%)

There are no bond length outliers.

All (167) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1A	1100	A	OP1-P-OP2	16.92	144.98	119.60
1	1A	1100	A	O5'-P-OP1	-14.97	92.23	105.70
1	1A	1099	C	OP1-P-O3'	-14.88	72.47	105.20
1	1A	1099	C	OP2-P-O3'	-13.42	75.67	105.20
1	1A	720	C	C2-N3-C4	-9.29	115.26	119.90
1	2A	1092	C	N1-C2-O2	8.72	124.13	118.90
1	1A	854	U	C2-N3-C4	-8.62	121.83	127.00
1	2A	1092	C	C2-N1-C1'	8.18	127.79	118.80
2	1B	75	G	C6-N1-C2	-8.15	120.21	125.10
32	2a	1397	C	C2-N1-C1'	8.09	127.69	118.80
1	2A	1097	U	C2-N1-C1'	8.04	127.35	117.70
32	1a	1495	U	N1-C2-O2	7.98	128.38	122.80
1	2A	673	C	C2-N3-C4	-7.85	115.97	119.90
1	1A	848	G	O5'-P-OP2	-7.77	98.71	105.70
2	1B	102	A	C6-N1-C2	-7.74	113.96	118.60
32	2a	343	U	C2-N1-C1'	-7.69	108.47	117.70
1	1A	2058	C	O5'-P-OP1	-7.67	98.79	105.70
32	2a	343	U	N3-C4-O4	-7.56	114.11	119.40
32	2a	343	U	C5-C4-O4	7.56	130.43	125.90
32	1a	839	U	P-O3'-C3'	7.37	128.55	119.70
1	1A	952	G	C5-C6-O6	7.36	133.01	128.60
32	2a	1397	C	N1-C2-O2	7.32	123.29	118.90
32	2a	1465	C	C2-N3-C4	-7.28	116.26	119.90
32	2a	1158	C	N1-C2-O2	7.28	123.27	118.90
32	2a	1158	C	C2-N1-C1'	7.25	126.77	118.80
32	2a	1495	U	N1-C2-O2	7.24	127.86	122.80
32	1a	1465	C	C2-N3-C4	-7.23	116.29	119.90
1	1A	1045	U	O5'-P-OP2	-7.22	99.20	105.70
1	2A	1060	U	C2-N1-C1'	7.20	126.33	117.70
1	2A	906	G	C5-C6-O6	6.96	132.77	128.60
1	2A	807	U	C2-N3-C4	-6.87	122.88	127.00
1	1A	1358	U	C5-C4-O4	6.83	130.00	125.90
1	1A	1099	C	N1-C2-O2	6.83	123.00	118.90
1	1A	2459	G	C6-N1-C2	-6.82	121.01	125.10
1	2A	1092	C	N3-C2-O2	-6.65	117.25	121.90
32	1a	1436	U	C2-N3-C4	-6.63	123.02	127.00
32	1a	343	U	C2-N1-C1'	-6.52	109.88	117.70
1	2A	2103	C	C2-N1-C1'	6.46	125.90	118.80
32	2a	266	G	P-O3'-C3'	6.39	127.37	119.70
32	1a	266	G	P-O3'-C3'	6.38	127.35	119.70
32	2a	1183	A	P-O3'-C3'	6.37	127.34	119.70
1	2A	1076	C	OP1-P-O3'	6.33	119.13	105.20
1	1A	410	U	N1-C2-O2	6.33	127.23	122.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1A	101	A	C4-C5-C6	6.29	120.15	117.00
32	2a	1003	G	N3-C4-C5	-6.29	125.45	128.60
1	1A	1386	U	C2-N3-C4	-6.24	123.26	127.00
1	2A	1077	A	O5'-P-OP1	-6.22	100.10	105.70
1	1A	537	G	O4'-C1'-N9	6.20	113.16	108.20
1	1A	1985	U	C2-N1-C1'	6.19	125.12	117.70
53	2x	6	G	O5'-P-OP2	-6.17	100.15	105.70
32	2a	960	U	C2-N1-C1'	6.14	125.07	117.70
1	1A	31	C	O5'-P-OP1	-6.13	100.18	105.70
1	1A	2390	A	N1-C6-N6	6.13	122.28	118.60
32	1a	1285	A	P-O3'-C3'	6.12	127.04	119.70
1	1A	720	C	N3-C4-C5	6.11	124.34	121.90
32	2a	1054	C	C2-N1-C1'	6.11	125.52	118.80
32	2a	346	G	C6-N1-C2	-6.11	121.44	125.10
1	2A	2103	C	N1-C2-O2	6.08	122.55	118.90
32	2a	1003	G	C2-N3-C4	6.07	114.93	111.90
32	1a	404	U	N1-C2-O2	6.01	127.01	122.80
1	1A	1162	C	C5-C6-N1	6.00	124.00	121.00
1	1A	82	G	N9-C4-C5	-6.00	103.00	105.40
32	1a	1495	U	N3-C2-O2	-5.99	118.00	122.20
32	2a	343	U	C6-N1-C1'	5.97	129.55	121.20
32	1a	558	G	O5'-P-OP1	-5.95	100.34	105.70
1	1A	82	G	C2-N3-C4	-5.90	108.95	111.90
1	2A	1092	C	C6-N1-C2	-5.88	117.95	120.30
1	2A	2103	C	C6-N1-C2	-5.87	117.95	120.30
32	2a	754	C	C2-N1-C1'	5.87	125.25	118.80
1	2A	9	U	C5-C6-N1	5.85	125.63	122.70
32	1a	901	A	N1-C6-N6	5.84	122.11	118.60
1	2A	1097	U	N1-C2-O2	5.82	126.87	122.80
32	1a	1465	C	C5-C4-N4	-5.81	116.13	120.20
32	2a	1397	C	C6-N1-C1'	-5.75	113.90	120.80
1	1A	1162	C	C2-N1-C1'	5.73	125.10	118.80
1	2A	383	U	N1-C2-O2	5.72	126.80	122.80
32	2a	1436	U	C2-N3-C4	-5.72	123.57	127.00
32	2a	346	G	N3-C4-C5	-5.71	125.75	128.60
1	2A	1313	U	C2-N1-C1'	5.70	124.54	117.70
1	1A	720	C	C5-C4-N4	-5.66	116.24	120.20
32	1a	960	U	C2-N1-C1'	5.65	124.48	117.70
1	2A	2447	G	C6-N1-C2	-5.65	121.71	125.10
32	1a	839	U	OP1-P-O3'	5.64	117.62	105.20
32	2a	404	U	N1-C2-O2	5.64	126.75	122.80
1	1A	1346	U	P-O3'-C3'	5.63	126.45	119.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	2a	1158	C	N3-C2-O2	-5.62	117.97	121.90
1	1A	1359	U	C2-N1-C1'	5.60	124.42	117.70
1	1A	1418	U	C5-C4-O4	-5.55	122.57	125.90
32	2a	1281	U	C2-N1-C1'	5.54	124.35	117.70
32	2a	1397	C	N3-C2-O2	-5.53	118.03	121.90
32	2a	1024	G	C2-N3-C4	5.53	114.66	111.90
32	2a	1495	U	C2-N1-C1'	5.52	124.33	117.70
1	1A	1222	A	O5'-P-OP1	-5.52	100.73	105.70
32	1a	1065	U	P-O3'-C3'	5.51	126.32	119.70
2	1B	75	G	C5-C6-N1	5.50	114.25	111.50
32	2a	1028	C	C6-N1-C2	-5.49	118.10	120.30
32	1a	1201	A	P-O3'-C3'	5.48	126.28	119.70
1	2A	271(M)	G	P-O3'-C3'	5.48	126.28	119.70
1	2A	1097	U	C6-N1-C1'	-5.47	113.54	121.20
1	1A	1462	G	O4'-C1'-N9	5.47	112.58	108.20
1	2A	1092	C	C6-N1-C1'	-5.47	114.24	120.80
1	2A	271(M)	G	OP1-P-O3'	5.46	117.22	105.20
32	2a	1491	G	P-O3'-C3'	5.45	126.23	119.70
32	1a	1183	A	P-O3'-C3'	5.43	126.22	119.70
1	1A	1539	C	C2-N1-C1'	5.43	124.77	118.80
32	1a	533	A	N1-C6-N6	5.43	121.86	118.60
1	2A	1083	U	C2-N1-C1'	5.42	124.21	117.70
1	2A	807	U	C5-C4-O4	-5.41	122.65	125.90
32	1a	343	U	O4'-C1'-N1	5.40	112.52	108.20
1	1A	952	G	N1-C6-O6	-5.38	116.67	119.90
1	2A	740	U	O5'-P-OP2	-5.37	100.86	105.70
1	2A	1092	C	C5-C6-N1	5.35	123.68	121.00
1	1A	854	U	N1-C2-N3	5.35	118.11	114.90
32	2a	1054	C	N1-C2-O2	5.32	122.09	118.90
1	1A	1221	G	OP1-P-O3'	5.30	116.86	105.20
1	2A	2451	A	C5-N7-C8	-5.30	101.25	103.90
1	2A	673	C	N3-C4-C5	5.29	124.02	121.90
32	1a	754	C	C2-N1-C1'	5.29	124.61	118.80
1	1A	2597	U	OP1-P-O3'	5.28	116.82	105.20
1	2A	1097	U	C5-C6-N1	5.27	125.33	122.70
32	1a	1183	A	OP1-P-O3'	5.25	116.76	105.20
32	2a	1491	G	OP2-P-O3'	5.25	116.76	105.20
32	1a	533	A	C5-C6-N6	-5.24	119.50	123.70
1	1A	101	A	N1-C6-N6	5.24	121.75	118.60
32	2a	343	U	O4'-C1'-N1	5.24	112.39	108.20
32	1a	1442	G	N3-C4-C5	-5.23	125.98	128.60
32	1a	115	G	P-O3'-C3'	5.22	125.97	119.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	1B	24	G	C4-N9-C1'	5.22	133.29	126.50
1	2A	1312	U	C5-C4-O4	5.22	129.03	125.90
1	1A	1700	G	P-O3'-C3'	5.21	125.95	119.70
32	2a	993	G	N3-C4-N9	5.21	129.13	126.00
32	1a	300	A	N1-C6-N6	5.20	121.72	118.60
1	2A	801	G	O5'-P-OP2	-5.20	101.02	105.70
32	1a	687	A	P-O3'-C3'	5.19	125.92	119.70
32	1a	991	U	P-O3'-C3'	5.18	125.92	119.70
2	1B	24	G	N3-C4-C5	-5.17	126.02	128.60
32	2a	1065	U	P-O3'-C3'	5.17	125.90	119.70
32	2a	1465	C	C5-C4-N4	-5.16	116.58	120.20
1	1A	847	A	N1-C6-N6	-5.16	115.50	118.60
1	2A	2103	C	N3-C2-O2	-5.16	118.29	121.90
1	2A	1060	U	C6-N1-C1'	-5.15	113.99	121.20
1	1A	952	G	N3-C4-N9	-5.14	122.92	126.00
32	2a	992	U	P-O3'-C3'	5.13	125.85	119.70
32	2a	687	A	P-O3'-C3'	5.11	125.84	119.70
1	1A	1099	C	N3-C2-O2	-5.11	118.32	121.90
1	2A	1210	A	P-O3'-C3'	5.10	125.82	119.70
32	1a	1465	C	N3-C4-C5	5.10	123.94	121.90
2	1B	13	A	O5'-P-OP2	-5.09	101.12	105.70
1	1A	410	U	N3-C2-O2	-5.09	118.64	122.20
32	1a	343	U	C5-C4-O4	5.09	128.95	125.90
1	1A	1085	G	N9-C4-C5	-5.06	103.38	105.40
32	1a	993	G	N3-C4-N9	5.06	129.03	126.00
1	1A	952	G	N9-C4-C5	5.06	107.42	105.40
32	1a	1442	G	P-O3'-C3'	5.06	125.77	119.70
1	2A	1065	U	P-O3'-C3'	5.06	125.77	119.70
2	1B	59	A	C6-N1-C2	-5.05	115.57	118.60
32	2a	533	A	N1-C6-N6	5.05	121.63	118.60
32	1a	1054	C	N1-C2-O2	5.05	121.93	118.90
1	1A	1220	U	P-O3'-C3'	5.04	125.75	119.70
1	1A	1359	U	O4'-C1'-N1	5.03	112.23	108.20
32	2a	1067	A	P-O3'-C3'	5.03	125.74	119.70
1	2A	2157	G	C8-N9-C4	-5.03	104.39	106.40
1	2A	906	G	N9-C4-C5	5.03	107.41	105.40
32	2a	991	U	P-O3'-C3'	5.02	125.72	119.70
2	1B	102	A	N1-C2-N3	5.02	131.81	129.30
1	1A	2201	C	N1-C2-O2	5.01	121.91	118.90
1	1A	952	G	C6-C5-N7	5.01	133.40	130.40

There are no chirality outliers.

There are no planarity outliers.

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

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

## 5.3 Torsion angles [i](#)

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

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	1D	273/275 (99%)	259 (95%)	14 (5%)	0	100	100
3	2D	273/275 (99%)	259 (95%)	14 (5%)	0	100	100
4	1E	202/204 (99%)	195 (96%)	6 (3%)	1 (0%)	29	64
4	2E	202/204 (99%)	193 (96%)	8 (4%)	1 (0%)	29	64
5	1F	201/203 (99%)	193 (96%)	7 (4%)	1 (0%)	29	64
5	2F	201/203 (99%)	195 (97%)	4 (2%)	2 (1%)	15	49
6	1G	179/181 (99%)	167 (93%)	10 (6%)	2 (1%)	14	46
6	2G	179/181 (99%)	163 (91%)	13 (7%)	3 (2%)	9	36
7	1H	172/174 (99%)	162 (94%)	10 (6%)	0	100	100
7	2H	171/174 (98%)	162 (95%)	9 (5%)	0	100	100
8	1I	145/147 (99%)	132 (91%)	9 (6%)	4 (3%)	5	25
8	2I	144/147 (98%)	134 (93%)	9 (6%)	1 (1%)	22	57
9	1N	138/140 (99%)	135 (98%)	3 (2%)	0	100	100
9	2N	138/140 (99%)	135 (98%)	3 (2%)	0	100	100
10	1O	120/122 (98%)	114 (95%)	6 (5%)	0	100	100
10	2O	120/122 (98%)	114 (95%)	6 (5%)	0	100	100
11	1P	147/149 (99%)	138 (94%)	8 (5%)	1 (1%)	22	57
11	2P	147/149 (99%)	139 (95%)	7 (5%)	1 (1%)	22	57
12	1Q	139/141 (99%)	130 (94%)	9 (6%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
12	2Q	139/141 (99%)	130 (94%)	9 (6%)	0	100	100
13	1R	116/118 (98%)	109 (94%)	7 (6%)	0	100	100
13	2R	116/118 (98%)	109 (94%)	7 (6%)	0	100	100
14	1S	108/110 (98%)	100 (93%)	7 (6%)	1 (1%)	17	52
14	2S	108/110 (98%)	102 (94%)	6 (6%)	0	100	100
15	1T	129/131 (98%)	123 (95%)	6 (5%)	0	100	100
15	2T	129/131 (98%)	126 (98%)	3 (2%)	0	100	100
16	1U	114/116 (98%)	114 (100%)	0	0	100	100
16	2U	114/116 (98%)	114 (100%)	0	0	100	100
17	1V	99/101 (98%)	93 (94%)	5 (5%)	1 (1%)	15	49
17	2V	99/101 (98%)	93 (94%)	5 (5%)	1 (1%)	15	49
18	1W	110/112 (98%)	107 (97%)	3 (3%)	0	100	100
18	2W	110/112 (98%)	107 (97%)	3 (3%)	0	100	100
19	1X	93/95 (98%)	91 (98%)	1 (1%)	1 (1%)	14	46
19	2X	93/95 (98%)	90 (97%)	2 (2%)	1 (1%)	14	46
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%)	187 (93%)	14 (7%)	0	100	100
21	2Z	199/203 (98%)	183 (92%)	16 (8%)	0	100	100
22	10	75/77 (97%)	73 (97%)	2 (3%)	0	100	100
22	20	75/77 (97%)	72 (96%)	3 (4%)	0	100	100
23	11	95/97 (98%)	94 (99%)	1 (1%)	0	100	100
23	21	95/97 (98%)	92 (97%)	3 (3%)	0	100	100
24	12	68/70 (97%)	67 (98%)	1 (2%)	0	100	100
24	22	68/70 (97%)	67 (98%)	1 (2%)	0	100	100
25	13	57/59 (97%)	56 (98%)	1 (2%)	0	100	100
25	23	57/59 (97%)	55 (96%)	2 (4%)	0	100	100
26	14	67/69 (97%)	52 (78%)	12 (18%)	3 (4%)	2	15
26	24	67/69 (97%)	51 (76%)	12 (18%)	4 (6%)	1	9
27	15	57/59 (97%)	55 (96%)	2 (4%)	0	100	100
27	25	57/59 (97%)	54 (95%)	3 (5%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
28	16	51/53 (96%)	48 (94%)	3 (6%)	0	100	100
28	26	51/53 (96%)	48 (94%)	3 (6%)	0	100	100
29	17	46/48 (96%)	44 (96%)	2 (4%)	0	100	100
29	27	46/48 (96%)	45 (98%)	1 (2%)	0	100	100
30	18	62/64 (97%)	60 (97%)	2 (3%)	0	100	100
30	28	62/64 (97%)	61 (98%)	1 (2%)	0	100	100
31	19	35/37 (95%)	35 (100%)	0	0	100	100
31	29	35/37 (95%)	35 (100%)	0	0	100	100
33	1b	229/231 (99%)	199 (87%)	21 (9%)	9 (4%)	3	18
33	2b	229/231 (99%)	200 (87%)	23 (10%)	6 (3%)	5	26
34	1c	204/206 (99%)	194 (95%)	10 (5%)	0	100	100
34	2c	204/206 (99%)	191 (94%)	11 (5%)	2 (1%)	15	49
35	1d	206/208 (99%)	193 (94%)	11 (5%)	2 (1%)	15	49
35	2d	206/208 (99%)	196 (95%)	8 (4%)	2 (1%)	15	49
36	1e	146/148 (99%)	141 (97%)	5 (3%)	0	100	100
36	2e	146/148 (99%)	141 (97%)	5 (3%)	0	100	100
37	1f	98/100 (98%)	95 (97%)	3 (3%)	0	100	100
37	2f	98/100 (98%)	94 (96%)	4 (4%)	0	100	100
38	1g	153/155 (99%)	146 (95%)	7 (5%)	0	100	100
38	2g	153/155 (99%)	143 (94%)	8 (5%)	2 (1%)	12	42
39	1h	135/137 (98%)	129 (96%)	6 (4%)	0	100	100
39	2h	135/137 (98%)	130 (96%)	5 (4%)	0	100	100
40	1i	125/127 (98%)	115 (92%)	9 (7%)	1 (1%)	19	54
40	2i	124/127 (98%)	111 (90%)	11 (9%)	2 (2%)	9	37
41	1j	95/97 (98%)	82 (86%)	9 (10%)	4 (4%)	3	16
41	2j	94/97 (97%)	84 (89%)	9 (10%)	1 (1%)	14	46
42	1k	112/114 (98%)	105 (94%)	6 (5%)	1 (1%)	17	52
42	2k	112/114 (98%)	107 (96%)	5 (4%)	0	100	100
43	1l	119/122 (98%)	112 (94%)	7 (6%)	0	100	100
43	2l	119/122 (98%)	110 (92%)	9 (8%)	0	100	100
44	1m	114/116 (98%)	106 (93%)	7 (6%)	1 (1%)	17	52

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
44	2m	112/116 (97%)	105 (94%)	5 (4%)	2 (2%)	8	34
45	1n	58/60 (97%)	56 (97%)	2 (3%)	0	100	100
45	2n	58/60 (97%)	55 (95%)	3 (5%)	0	100	100
46	1o	86/88 (98%)	84 (98%)	1 (1%)	1 (1%)	13	44
46	2o	86/88 (98%)	81 (94%)	3 (4%)	2 (2%)	6	28
47	1p	80/82 (98%)	75 (94%)	5 (6%)	0	100	100
47	2p	80/82 (98%)	74 (92%)	6 (8%)	0	100	100
48	1q	97/99 (98%)	92 (95%)	4 (4%)	1 (1%)	15	49
48	2q	97/99 (98%)	93 (96%)	4 (4%)	0	100	100
49	1r	66/68 (97%)	65 (98%)	1 (2%)	0	100	100
49	2r	66/68 (97%)	65 (98%)	1 (2%)	0	100	100
50	1s	81/83 (98%)	75 (93%)	6 (7%)	0	100	100
50	2s	81/83 (98%)	75 (93%)	6 (7%)	0	100	100
51	1t	94/98 (96%)	90 (96%)	1 (1%)	3 (3%)	4	22
51	2t	96/98 (98%)	90 (94%)	3 (3%)	3 (3%)	4	23
52	1u	21/23 (91%)	19 (90%)	2 (10%)	0	100	100
52	2u	21/23 (91%)	19 (90%)	1 (5%)	1 (5%)	2	14
54	1y	10/19 (53%)	9 (90%)	1 (10%)	0	100	100
54	2y	10/19 (53%)	9 (90%)	1 (10%)	0	100	100
All	All	11460/11686 (98%)	10814 (94%)	571 (5%)	75 (1%)	22	57

All (75) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
5	1F	130	ALA
8	1I	105	HIS
26	14	49	PHE
35	1d	171	GLY
40	1i	127	LYS
41	1j	77	PRO
41	1j	79	ARG
44	1m	67	GLU
48	1q	68	ARG
5	2F	21	ALA
5	2F	130	ALA

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
6	2G	50	ALA
19	2X	94	GLY
26	24	49	PHE
33	2b	8	LYS
33	2b	16	HIS
33	2b	17	PHE
38	2g	8	GLU
40	2i	44	VAL
40	2i	54	ASP
44	2m	67	GLU
8	1I	11	ASN
19	1X	94	GLY
26	14	45	GLY
33	1b	17	PHE
33	1b	126	GLU
42	1k	118	GLY
4	2E	51	PHE
6	2G	43	LEU
34	2c	107	GLN
35	2d	171	GLY
38	2g	7	ALA
6	1G	43	LEU
8	1I	73	GLU
14	1S	59	LYS
33	1b	20	GLU
35	1d	129	ASN
41	1j	78	ASN
26	24	47	GLN
26	24	60	GLN
46	2o	88	ARG
51	2t	100	ILE
51	2t	102	GLY
4	1E	52	LEU
8	1I	85	GLU
33	1b	8	LYS
51	1t	95	ALA
8	2I	85	GLU
33	2b	125	PRO
34	2c	108	ASN
35	2d	129	ASN
41	2j	78	ASN
46	2o	23	GLY

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Mol	Chain	Res	Type
51	2t	95	ALA
11	1P	122	PRO
33	1b	125	PRO
11	2P	122	PRO
17	2V	79	VAL
33	2b	123	ALA
52	2u	3	LYS
6	1G	47	LYS
26	14	55	ARG
33	1b	21	ARG
46	1o	23	GLY
6	2G	47	LYS
44	2m	5	ALA
41	1j	31	GLY
17	1V	79	VAL
33	1b	124	SER
33	1b	127	ILE
26	24	45	GLY
33	2b	232	PRO
51	1t	100	ILE
33	1b	232	PRO
51	1t	98	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%)	202 (94%)	12 (6%)	21	52
3	2D	215/217 (99%)	204 (95%)	11 (5%)	24	56
4	1E	164/165 (99%)	152 (93%)	12 (7%)	14	43
4	2E	164/165 (99%)	156 (95%)	8 (5%)	25	57
5	1F	160/161 (99%)	149 (93%)	11 (7%)	15	45
5	2F	159/161 (99%)	147 (92%)	12 (8%)	13	42
6	1G	144/155 (93%)	133 (92%)	11 (8%)	13	41

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
6	2G	142/155 (92%)	133 (94%)	9 (6%)	18	48
7	1H	144/145 (99%)	139 (96%)	5 (4%)	36	68
7	2H	143/145 (99%)	138 (96%)	5 (4%)	36	68
8	1I	111/123 (90%)	100 (90%)	11 (10%)	8	29
8	2I	108/123 (88%)	101 (94%)	7 (6%)	17	47
9	1N	119/119 (100%)	110 (92%)	9 (8%)	13	41
9	2N	118/119 (99%)	112 (95%)	6 (5%)	24	56
10	1O	100/100 (100%)	96 (96%)	4 (4%)	31	65
10	2O	100/100 (100%)	96 (96%)	4 (4%)	31	65
11	1P	115/116 (99%)	106 (92%)	9 (8%)	12	40
11	2P	115/116 (99%)	111 (96%)	4 (4%)	36	68
12	1Q	111/111 (100%)	104 (94%)	7 (6%)	18	48
12	2Q	111/111 (100%)	104 (94%)	7 (6%)	18	48
13	1R	101/101 (100%)	91 (90%)	10 (10%)	8	29
13	2R	101/101 (100%)	88 (87%)	13 (13%)	4	18
14	1S	87/87 (100%)	84 (97%)	3 (3%)	37	69
14	2S	85/87 (98%)	81 (95%)	4 (5%)	26	59
15	1T	115/115 (100%)	109 (95%)	6 (5%)	23	55
15	2T	113/115 (98%)	110 (97%)	3 (3%)	44	74
16	1U	93/93 (100%)	87 (94%)	6 (6%)	17	47
16	2U	93/93 (100%)	87 (94%)	6 (6%)	17	47
17	1V	81/82 (99%)	73 (90%)	8 (10%)	8	29
17	2V	80/82 (98%)	72 (90%)	8 (10%)	7	28
18	1W	90/91 (99%)	83 (92%)	7 (8%)	12	40
18	2W	90/91 (99%)	86 (96%)	4 (4%)	28	61
19	1X	77/77 (100%)	76 (99%)	1 (1%)	69	87
19	2X	77/77 (100%)	74 (96%)	3 (4%)	32	65
20	1Y	86/88 (98%)	82 (95%)	4 (5%)	26	59
20	2Y	86/88 (98%)	83 (96%)	3 (4%)	36	68
21	1Z	169/176 (96%)	156 (92%)	13 (8%)	13	41
21	2Z	165/176 (94%)	155 (94%)	10 (6%)	18	49

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
22	10	61/62 (98%)	58 (95%)	3 (5%)	25	57
22	20	61/62 (98%)	59 (97%)	2 (3%)	38	69
23	11	79/82 (96%)	77 (98%)	2 (2%)	47	75
23	21	81/82 (99%)	77 (95%)	4 (5%)	25	57
24	12	65/66 (98%)	64 (98%)	1 (2%)	65	85
24	22	66/66 (100%)	64 (97%)	2 (3%)	41	71
25	13	51/51 (100%)	47 (92%)	4 (8%)	12	40
25	23	50/51 (98%)	47 (94%)	3 (6%)	19	49
26	14	58/62 (94%)	53 (91%)	5 (9%)	10	37
26	24	54/62 (87%)	51 (94%)	3 (6%)	21	52
27	15	51/51 (100%)	49 (96%)	2 (4%)	32	65
27	25	50/51 (98%)	49 (98%)	1 (2%)	55	80
28	16	51/51 (100%)	48 (94%)	3 (6%)	19	50
28	26	50/51 (98%)	47 (94%)	3 (6%)	19	49
29	17	41/41 (100%)	37 (90%)	4 (10%)	8	29
29	27	41/41 (100%)	41 (100%)	0	100	100
30	18	54/54 (100%)	50 (93%)	4 (7%)	13	42
30	28	54/54 (100%)	51 (94%)	3 (6%)	21	52
31	19	34/34 (100%)	34 (100%)	0	100	100
31	29	34/34 (100%)	34 (100%)	0	100	100
33	1b	191/199 (96%)	169 (88%)	22 (12%)	5	22
33	2b	187/199 (94%)	171 (91%)	16 (9%)	10	37
34	1c	144/160 (90%)	138 (96%)	6 (4%)	30	62
34	2c	140/160 (88%)	130 (93%)	10 (7%)	14	44
35	1d	171/180 (95%)	163 (95%)	8 (5%)	26	59
35	2d	172/180 (96%)	167 (97%)	5 (3%)	42	72
36	1e	114/114 (100%)	111 (97%)	3 (3%)	46	74
36	2e	114/114 (100%)	109 (96%)	5 (4%)	28	61
37	1f	85/90 (94%)	84 (99%)	1 (1%)	71	88
37	2f	85/90 (94%)	85 (100%)	0	100	100
38	1g	120/126 (95%)	117 (98%)	3 (2%)	47	75

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
38	2g	119/126 (94%)	112 (94%)	7 (6%)	19	50
39	1h	116/118 (98%)	111 (96%)	5 (4%)	29	62
39	2h	114/118 (97%)	107 (94%)	7 (6%)	18	49
40	1i	91/98 (93%)	85 (93%)	6 (7%)	16	47
40	2i	88/98 (90%)	80 (91%)	8 (9%)	9	33
41	1j	68/87 (78%)	66 (97%)	2 (3%)	42	72
41	2j	68/87 (78%)	66 (97%)	2 (3%)	42	72
42	1k	83/86 (96%)	81 (98%)	2 (2%)	49	76
42	2k	83/86 (96%)	80 (96%)	3 (4%)	35	67
43	1l	96/102 (94%)	92 (96%)	4 (4%)	30	62
43	2l	96/102 (94%)	92 (96%)	4 (4%)	30	62
44	1m	90/94 (96%)	84 (93%)	6 (7%)	16	46
44	2m	87/94 (93%)	79 (91%)	8 (9%)	9	33
45	1n	49/49 (100%)	46 (94%)	3 (6%)	18	49
45	2n	49/49 (100%)	48 (98%)	1 (2%)	55	80
46	1o	78/79 (99%)	76 (97%)	2 (3%)	46	74
46	2o	78/79 (99%)	74 (95%)	4 (5%)	24	56
47	1p	69/71 (97%)	63 (91%)	6 (9%)	10	36
47	2p	68/71 (96%)	62 (91%)	6 (9%)	10	36
48	1q	94/94 (100%)	93 (99%)	1 (1%)	73	89
48	2q	94/94 (100%)	92 (98%)	2 (2%)	53	79
49	1r	59/59 (100%)	58 (98%)	1 (2%)	60	83
49	2r	59/59 (100%)	58 (98%)	1 (2%)	60	83
50	1s	68/72 (94%)	64 (94%)	4 (6%)	19	50
50	2s	67/72 (93%)	62 (92%)	5 (8%)	13	42
51	1t	71/76 (93%)	69 (97%)	2 (3%)	43	73
51	2t	70/76 (92%)	69 (99%)	1 (1%)	67	86
52	1u	18/18 (100%)	18 (100%)	0	100	100
52	2u	18/18 (100%)	18 (100%)	0	100	100
54	1y	12/19 (63%)	12 (100%)	0	100	100
54	2y	12/19 (63%)	12 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	9387/9734 (96%)	8880 (95%)	507 (5%)	22 53

All (507) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	1D	61	LEU
3	1D	69	ARG
3	1D	94	LEU
3	1D	103	ARG
3	1D	106	ILE
3	1D	111	LEU
3	1D	141	VAL
3	1D	193	VAL
3	1D	211	ARG
3	1D	217	ARG
3	1D	229	VAL
3	1D	242	ARG
4	1E	7	VAL
4	1E	21	VAL
4	1E	33	VAL
4	1E	49	LEU
4	1E	73	GLU
4	1E	78	LEU
4	1E	116	VAL
4	1E	119	ARG
4	1E	144	ARG
4	1E	154	LYS
4	1E	175	VAL
4	1E	178	GLU
5	1F	12	LEU
5	1F	18	ARG
5	1F	32	LEU
5	1F	33	LEU
5	1F	57	VAL
5	1F	74	ARG
5	1F	95	ARG
5	1F	110	LEU
5	1F	170	LEU
5	1F	192	LEU
5	1F	197	ASP
6	1G	5	VAL
6	1G	21	ARG

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
6	1G	43	LEU
6	1G	45	GLU
6	1G	53	LEU
6	1G	82	LEU
6	1G	133	LEU
6	1G	148	MET
6	1G	159	VAL
6	1G	165	THR
6	1G	167	GLU
7	1H	13	LYS
7	1H	15	VAL
7	1H	45	VAL
7	1H	71	LEU
7	1H	84	SER
8	1I	5	LEU
8	1I	10	GLU
8	1I	12	LEU
8	1I	38	LEU
8	1I	44	LEU
8	1I	64	GLU
8	1I	75	LEU
8	1I	78	THR
8	1I	92	VAL
8	1I	109	ILE
8	1I	140	LEU
9	1N	5	VAL
9	1N	33	LEU
9	1N	62	VAL
9	1N	67	LEU
9	1N	87	LEU
9	1N	97	ARG
9	1N	99	LEU
9	1N	115	ARG
9	1N	121	LYS
10	1O	10	VAL
10	1O	24	VAL
10	1O	64	ARG
10	1O	69	ILE
11	1P	2	LYS
11	1P	3	LEU
11	1P	59	LEU
11	1P	83	VAL

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
11	1P	98	GLU
11	1P	99	LEU
11	1P	112	LEU
11	1P	125	VAL
11	1P	147	LEU
12	1Q	2	LEU
12	1Q	7	MET
12	1Q	21	THR
12	1Q	55	VAL
12	1Q	75	THR
12	1Q	109	VAL
12	1Q	110	THR
13	1R	6	SER
13	1R	29	LEU
13	1R	33	ARG
13	1R	36	THR
13	1R	44	LEU
13	1R	65	LEU
13	1R	67	LEU
13	1R	75	LEU
13	1R	96	ARG
13	1R	100	LEU
14	1S	36	TYR
14	1S	59	LYS
14	1S	69	VAL
15	1T	13	ARG
15	1T	17	THR
15	1T	34	VAL
15	1T	59	THR
15	1T	89	VAL
15	1T	108	ARG
16	1U	8	VAL
16	1U	36	ARG
16	1U	52	ARG
16	1U	74	LEU
16	1U	83	LEU
16	1U	104	GLN
17	1V	46	VAL
17	1V	52	VAL
17	1V	61	VAL
17	1V	62	LEU
17	1V	72	VAL

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
17	1V	79	VAL
17	1V	82	ARG
17	1V	85	LYS
18	1W	11	ARG
18	1W	15	ARG
18	1W	17	VAL
18	1W	19	LEU
18	1W	23	LEU
18	1W	60	ASN
18	1W	107	LEU
19	1X	66	LEU
20	1Y	43	ASN
20	1Y	85	VAL
20	1Y	90	LEU
20	1Y	99	CYS
21	1Z	11	GLU
21	1Z	18	LEU
21	1Z	31	ARG
21	1Z	42	VAL
21	1Z	46	LYS
21	1Z	72	ARG
21	1Z	86	VAL
21	1Z	91	LEU
21	1Z	135	GLU
21	1Z	150	LEU
21	1Z	182	LYS
21	1Z	202	GLU
21	1Z	203	GLU
22	10	10	THR
22	10	11	ARG
22	10	39	ARG
23	11	23	LYS
23	11	95	LEU
24	12	3	LEU
25	13	6	VAL
25	13	8	LEU
25	13	54	VAL
25	13	55	ARG
26	14	13	ARG
26	14	49	PHE
26	14	60	GLN
26	14	61	ARG

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
26	14	67	TYR
27	15	29	THR
27	15	35	GLU
28	16	6	ARG
28	16	14	THR
28	16	49	HIS
29	17	1	MET
29	17	10	ARG
29	17	43	THR
29	17	47	ARG
30	18	14	VAL
30	18	30	ARG
30	18	31	HIS
30	18	34	TRP
33	1b	15	VAL
33	1b	19	HIS
33	1b	21	ARG
33	1b	24	TRP
33	1b	45	GLN
33	1b	67	THR
33	1b	68	ILE
33	1b	73	THR
33	1b	81	VAL
33	1b	106	LYS
33	1b	111	ARG
33	1b	112	VAL
33	1b	114	ARG
33	1b	122	PHE
33	1b	128	GLU
33	1b	158	LEU
33	1b	160	ASP
33	1b	172	ILE
33	1b	178	ARG
33	1b	200	ILE
33	1b	221	LEU
33	1b	224	GLN
34	1c	3	ASN
34	1c	15	THR
34	1c	29	TYR
34	1c	36	ASP
34	1c	64	VAL
34	1c	161	GLU

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
35	1d	8	VAL
35	1d	127	THR
35	1d	135	LEU
35	1d	158	ILE
35	1d	178	VAL
35	1d	188	LEU
35	1d	194	LEU
35	1d	196	LEU
36	1e	41	VAL
36	1e	69	VAL
36	1e	120	THR
37	1f	92	LYS
38	1g	11	GLN
38	1g	75	VAL
38	1g	90	GLU
39	1h	26	VAL
39	1h	51	VAL
39	1h	52	ASP
39	1h	63	LEU
39	1h	95	VAL
40	1i	2	GLU
40	1i	17	VAL
40	1i	27	THR
40	1i	87	GLN
40	1i	92	TYR
40	1i	125	TYR
41	1j	92	THR
41	1j	100	THR
42	1k	87	THR
42	1k	117	ASN
43	1l	27	LEU
43	1l	33	ARG
43	1l	66	VAL
43	1l	83	VAL
44	1m	4	ILE
44	1m	8	GLU
44	1m	19	LEU
44	1m	56	LEU
44	1m	102	ARG
44	1m	109	THR
45	1n	3	ARG
45	1n	18	VAL

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
45	1n	33	VAL
46	1o	3	ILE
46	1o	39	LEU
47	1p	8	ARG
47	1p	11	SER
47	1p	28	ARG
47	1p	42	ARG
47	1p	45	THR
47	1p	67	THR
48	1q	93	GLN
49	1r	76	LEU
50	1s	4	SER
50	1s	5	LEU
50	1s	37	ARG
50	1s	41	VAL
51	1t	84	LEU
51	1t	100	ILE
3	2D	61	LEU
3	2D	69	ARG
3	2D	94	LEU
3	2D	103	ARG
3	2D	111	LEU
3	2D	138	VAL
3	2D	141	VAL
3	2D	193	VAL
3	2D	211	ARG
3	2D	229	VAL
3	2D	242	ARG
4	2E	21	VAL
4	2E	33	VAL
4	2E	89	ASP
4	2E	116	VAL
4	2E	144	ARG
4	2E	154	LYS
4	2E	175	VAL
4	2E	184	VAL
5	2F	18	ARG
5	2F	27	GLU
5	2F	33	LEU
5	2F	53	THR
5	2F	57	VAL
5	2F	74	ARG

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
5	2F	88	VAL
5	2F	158	THR
5	2F	170	LEU
5	2F	183	VAL
5	2F	192	LEU
5	2F	197	ASP
6	2G	3	LEU
6	2G	5	VAL
6	2G	49	ASP
6	2G	53	LEU
6	2G	91	ARG
6	2G	108	ASN
6	2G	133	LEU
6	2G	159	VAL
6	2G	165	THR
7	2H	18	GLU
7	2H	49	VAL
7	2H	71	LEU
7	2H	124	GLU
7	2H	171	LEU
8	2I	5	LEU
8	2I	47	LEU
8	2I	66	GLU
8	2I	75	LEU
8	2I	123	LEU
8	2I	140	LEU
8	2I	144	VAL
9	2N	12	ARG
9	2N	28	THR
9	2N	33	LEU
9	2N	34	LEU
9	2N	87	LEU
9	2N	99	LEU
10	2O	10	VAL
10	2O	24	VAL
10	2O	53	LYS
10	2O	69	ILE
11	2P	59	LEU
11	2P	83	VAL
11	2P	112	LEU
11	2P	125	VAL
12	2Q	16	ARG

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
12	2Q	21	THR
12	2Q	55	VAL
12	2Q	60	ARG
12	2Q	75	THR
12	2Q	109	VAL
12	2Q	110	THR
13	2R	6	SER
13	2R	18	LEU
13	2R	24	GLN
13	2R	44	LEU
13	2R	65	LEU
13	2R	67	LEU
13	2R	71	GLN
13	2R	75	LEU
13	2R	79	LEU
13	2R	86	ARG
13	2R	96	ARG
13	2R	100	LEU
13	2R	111	LEU
14	2S	13	ARG
14	2S	14	VAL
14	2S	25	ARG
14	2S	75	GLU
15	2T	16	ARG
15	2T	74	ARG
15	2T	89	VAL
16	2U	8	VAL
16	2U	60	LEU
16	2U	74	LEU
16	2U	95	LEU
16	2U	112	ARG
16	2U	117	GLN
17	2V	7	THR
17	2V	18	LEU
17	2V	52	VAL
17	2V	57	VAL
17	2V	62	LEU
17	2V	72	VAL
17	2V	79	VAL
17	2V	82	ARG
18	2W	11	ARG
18	2W	15	ARG

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
18	2W	17	VAL
18	2W	107	LEU
19	2X	8	ILE
19	2X	57	LEU
19	2X	66	LEU
20	2Y	72	VAL
20	2Y	85	VAL
20	2Y	99	CYS
21	2Z	31	ARG
21	2Z	42	VAL
21	2Z	76	LEU
21	2Z	86	VAL
21	2Z	93	ASP
21	2Z	94	GLU
21	2Z	136	PHE
21	2Z	150	LEU
21	2Z	190	GLU
21	2Z	193	GLU
22	20	10	THR
22	20	39	ARG
23	21	52	ARG
23	21	75	GLU
23	21	85	LEU
23	21	95	LEU
24	22	32	LEU
24	22	70	GLN
25	23	6	VAL
25	23	23	LEU
25	23	31	LEU
26	24	50	VAL
26	24	53	GLU
26	24	67	TYR
27	25	6	VAL
28	26	6	ARG
28	26	14	THR
28	26	49	HIS
30	28	14	VAL
30	28	31	HIS
30	28	34	TRP
33	2b	24	TRP
33	2b	67	THR
33	2b	68	ILE

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
33	2b	73	THR
33	2b	128	GLU
33	2b	135	GLN
33	2b	136	VAL
33	2b	139	LYS
33	2b	154	LEU
33	2b	160	ASP
33	2b	185	ILE
33	2b	191	ASP
33	2b	196	LEU
33	2b	217	ARG
33	2b	224	GLN
33	2b	230	VAL
34	2c	3	ASN
34	2c	20	SER
34	2c	29	TYR
34	2c	52	LEU
34	2c	70	VAL
34	2c	115	LEU
34	2c	128	PHE
34	2c	152	ILE
34	2c	166	GLU
34	2c	190	ARG
35	2d	8	VAL
35	2d	31	CYS
35	2d	34	GLU
35	2d	135	LEU
35	2d	194	LEU
36	2e	9	LYS
36	2e	40	ARG
36	2e	41	VAL
36	2e	69	VAL
36	2e	72	GLN
38	2g	8	GLU
38	2g	51	GLN
38	2g	53	LYS
38	2g	75	VAL
38	2g	104	LEU
38	2g	113	GLU
38	2g	115	ARG
39	2h	52	ASP
39	2h	63	LEU

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
39	2h	91	ARG
39	2h	98	LYS
39	2h	112	LEU
39	2h	135	CYS
39	2h	137	VAL
40	2i	14	VAL
40	2i	17	VAL
40	2i	53	VAL
40	2i	92	TYR
40	2i	93	ARG
40	2i	102	LEU
40	2i	113	LYS
40	2i	125	TYR
41	2j	29	ARG
41	2j	69	ASN
42	2k	14	VAL
42	2k	103	LEU
42	2k	106	LYS
43	2l	27	LEU
43	2l	33	ARG
43	2l	66	VAL
43	2l	83	VAL
44	2m	4	ILE
44	2m	8	GLU
44	2m	19	LEU
44	2m	60	VAL
44	2m	65	LYS
44	2m	94	ARG
44	2m	102	ARG
44	2m	109	THR
45	2n	18	VAL
46	2o	5	LYS
46	2o	10	LYS
46	2o	28	GLN
46	2o	83	GLU
47	2p	5	ARG
47	2p	42	ARG
47	2p	60	LEU
47	2p	67	THR
47	2p	69	THR
47	2p	76	GLN
48	2q	50	LYS

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Mol	Chain	Res	Type
48	2q	74	LEU
49	2r	25	THR
50	2s	13	ASP
50	2s	16	LEU
50	2s	27	GLU
50	2s	41	VAL
50	2s	81	ARG
51	2t	84	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (83) such sidechains are listed below:

Mol	Chain	Res	Type
3	1D	116	GLN
3	1D	143	HIS
3	1D	253	GLN
4	1E	48	GLN
5	1F	8	GLN
5	1F	75	HIS
5	1F	203	GLN
6	1G	79	ASN
8	1I	54	GLN
8	1I	105	HIS
9	1N	8	GLN
10	1O	3	GLN
10	1O	5	GLN
12	1Q	123	HIS
14	1S	68	GLN
14	1S	95	HIS
15	1T	58	ASN
16	1U	104	GLN
19	1X	31	HIS
20	1Y	6	HIS
20	1Y	92	ASN
21	1Z	32	HIS
21	1Z	73	GLN
30	18	35	GLN
34	1c	6	HIS
34	1c	181	ASN
35	1d	119	GLN
35	1d	123	HIS
35	1d	129	ASN
37	1f	100	ASN

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
38	1g	13	GLN
38	1g	28	ASN
38	1g	109	ASN
40	1i	3	GLN
41	1j	56	HIS
41	1j	62	HIS
46	1o	28	GLN
48	1q	26	GLN
50	1s	47	HIS
50	1s	56	GLN
3	2D	116	GLN
3	2D	253	GLN
5	2F	69	HIS
5	2F	203	GLN
10	2O	5	GLN
12	2Q	12	GLN
12	2Q	123	HIS
13	2R	13	HIS
14	2S	95	HIS
15	2T	58	ASN
18	2W	61	ASN
19	2X	31	HIS
21	2Z	54	HIS
21	2Z	73	GLN
21	2Z	151	HIS
22	20	50	ASN
22	20	70	GLN
26	24	46	GLN
31	29	20	HIS
33	2b	40	HIS
34	2c	6	HIS
34	2c	176	HIS
34	2c	181	ASN
35	2d	116	GLN
35	2d	119	GLN
35	2d	123	HIS
35	2d	129	ASN
36	2e	78	HIS
37	2f	94	GLN
38	2g	11	GLN
38	2g	86	GLN
40	2i	3	GLN

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Mol	Chain	Res	Type
40	2i	124	GLN
41	2j	13	HIS
41	2j	69	ASN
44	2m	92	HIS
46	2o	62	GLN
47	2p	76	GLN
48	2q	16	GLN
48	2q	26	GLN
50	2s	23	ASN
50	2s	57	HIS
50	2s	69	HIS

### 5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	1A	2814/2915 (96%)	427 (15%)	31 (1%)
1	2A	2859/2915 (98%)	486 (16%)	28 (0%)
2	1B	119/120 (99%)	10 (8%)	0
2	2B	119/120 (99%)	12 (10%)	0
32	1a	1494/1521 (98%)	255 (17%)	0
32	2a	1498/1521 (98%)	249 (16%)	0
53	1x	75/76 (98%)	7 (9%)	0
53	2x	75/76 (98%)	8 (10%)	0
55	A	2/27 (7%)	0	0
55	B	2/27 (7%)	0	0
All	All	9057/9318 (97%)	1454 (16%)	59 (0%)

All (1454) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	1A	12	U
1	1A	15	G
1	1A	34	C
1	1A	45	C
1	1A	54	G
1	1A	60	G
1	1A	63	A
1	1A	70	A
1	1A	73	A
1	1A	74	G
1	1A	116	A

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	1A	117	A
1	1A	118	U
1	1A	121	G
1	1A	123	G
1	1A	170	A
1	1A	171	A
1	1A	185	A
1	1A	188	A
1	1A	194	G
1	1A	203	G
1	1A	204	G
1	1A	205	A
1	1A	206	G
1	1A	211	A
1	1A	218	A
1	1A	222	A
1	1A	237	G
1	1A	269	G
1	1A	271	U
1	1A	272	U
1	1A	273	G
1	1A	274	U
1	1A	275	C
1	1A	288	U
1	1A	289	G
1	1A	296	U
1	1A	299	G
1	1A	303	C
1	1A	335	A
1	1A	348	A
1	1A	354	A
1	1A	376	G
1	1A	387	G
1	1A	397	G
1	1A	398	A
1	1A	399	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

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	1A	455	A
1	1A	474	U
1	1A	480	A
1	1A	481	C
1	1A	483	A
1	1A	507	G
1	1A	510	C
1	1A	530	A
1	1A	534	C
1	1A	554	A
1	1A	555	G
1	1A	556	C
1	1A	557	A
1	1A	558	G
1	1A	569	G
1	1A	573	G
1	1A	586	G
1	1A	596	G
1	1A	598	A
1	1A	626	A
1	1A	627	G
1	1A	630	U
1	1A	638	U
1	1A	639	G
1	1A	641	G
1	1A	642	G
1	1A	652	A
1	1A	662	A
1	1A	670	C
1	1A	692	C
1	1A	693	G
1	1A	694	G
1	1A	697	C
1	1A	698	G
1	1A	716	G
1	1A	733	G
1	1A	764	G
1	1A	777	C
1	1A	787	U
1	1A	800	C
1	1A	809	U
1	1A	812	G

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	1A	822	G
1	1A	823	G
1	1A	829	A
1	1A	831	A
1	1A	832	G
1	1A	837	C
1	1A	839	G
1	1A	847	A
1	1A	852	G
1	1A	858	U
1	1A	859	C
1	1A	874	U
1	1A	875	U
1	1A	906	G
1	1A	913	A
1	1A	926	G
1	1A	927	G
1	1A	931	C
1	1A	932	C
1	1A	933	C
1	1A	935	C
1	1A	936	C
1	1A	937	A
1	1A	938	G
1	1A	942	A
1	1A	956	A
1	1A	977	G
1	1A	990	A
1	1A	991	G
1	1A	998	A
1	1A	1003	U
1	1A	1004	A
1	1A	1006	C
1	1A	1019	G
1	1A	1020	C
1	1A	1029	A
1	1A	1036	A
1	1A	1042	A
1	1A	1051	C
1	1A	1058	U
1	1A	1059	C
1	1A	1067	A

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	1A	1072	U
1	1A	1079	U
1	1A	1088	G
1	1A	1092	A
1	1A	1093	G
1	1A	1094	A
1	1A	1098	C
1	1A	1099	C
1	1A	1100	A
1	1A	1155	C
1	1A	1156	G
1	1A	1158	G
1	1A	1162	C
1	1A	1174	A
1	1A	1175	A
1	1A	1176	U
1	1A	1180	C
1	1A	1181	G
1	1A	1184	G
1	1A	1186	U
1	1A	1195	G
1	1A	1201	A
1	1A	1202	A
1	1A	1217	G
1	1A	1218	G
1	1A	1219	A
1	1A	1220	U
1	1A	1221	G
1	1A	1222	A
1	1A	1223	C
1	1A	1234	A
1	1A	1255	A
1	1A	1256	U
1	1A	1263	C
1	1A	1290	G
1	1A	1299	A
1	1A	1302	G
1	1A	1314	A
1	1A	1317	G
1	1A	1318	A
1	1A	1321	A
1	1A	1335	C

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	1A	1346	U
1	1A	1347	A
1	1A	1359	U
1	1A	1367	A
1	1A	1378	G
1	1A	1391	C
1	1A	1398	U
1	1A	1405	A
1	1A	1406	A
1	1A	1411	A
1	1A	1414	G
1	1A	1416	C
1	1A	1425	A
1	1A	1430	A
1	1A	1431	G
1	1A	1432	C
1	1A	1441	A
1	1A	1462	G
1	1A	1463	C
1	1A	1466	U
1	1A	1467	G
1	1A	1474	C
1	1A	1483	C
1	1A	1491	A
1	1A	1492	C
1	1A	1497	G
1	1A	1500	A
1	1A	1506	G
1	1A	1514	C
1	1A	1518	A
1	1A	1529	G
1	1A	1539	C
1	1A	1542	A
1	1A	1554	A
1	1A	1555	C
1	1A	1556	A
1	1A	1589	A
1	1A	1605	A
1	1A	1613	A
1	1A	1616	A
1	1A	1625	U
1	1A	1626	A

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	1A	1631	C
1	1A	1632	A
1	1A	1654	A
1	1A	1655	A
1	1A	1656	A
1	1A	1662	A
1	1A	1686	U
1	1A	1695	C
1	1A	1701	A
1	1A	1711	A
1	1A	1721	G
1	1A	1743	G
1	1A	1747	A
1	1A	1748	A
1	1A	1766	G
1	1A	1767	A
1	1A	1768	U
1	1A	1769	G
1	1A	1787	G
1	1A	1794	G
1	1A	1795	G
1	1A	1804	A
1	1A	1805	C
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	1859	G
1	1A	1870	G
1	1A	1878	A
1	1A	1879	A
1	1A	1896	G
1	1A	1899	A
1	1A	1900	G
1	1A	1911	A
1	1A	1922	A
1	1A	1928	G
1	1A	1935	A
1	1A	1936	C
1	1A	1937	5MU

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	1A	1942	OMC
1	1A	1951	G
1	1A	1952	G
1	1A	1959	A
1	1A	1960	A
1	1A	1977	U
1	1A	1985	U
1	1A	1989	C
1	1A	1992	A
1	1A	1993	A
1	1A	1994	A
1	1A	2014	G
1	1A	2015	U
1	1A	2019	G
1	1A	2045	G
1	1A	2049	G
1	1A	2053	A
1	1A	2054	G
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	2121	U
1	1A	2124	U
1	1A	2125	C
1	1A	2126	G
1	1A	2129	C
1	1A	2130	C
1	1A	2132	G
1	1A	2137	G
1	1A	2138	G
1	1A	2139	A
1	1A	2141	A
1	1A	2142	G
1	1A	2144	U
1	1A	2147	G
1	1A	2148	A

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	1A	2149	G
1	1A	2150	C
1	1A	2152	U
1	1A	2153	G
1	1A	2155	G
1	1A	2158	C
1	1A	2159	C
1	1A	2160	C
1	1A	2168	C
1	1A	2174	G
1	1A	2180	A
1	1A	2181	G
1	1A	2184	G
1	1A	2187	G
1	1A	2188	G
1	1A	2191	A
1	1A	2192	A
1	1A	2202	U
1	1A	2205	C
1	1A	2206	G
1	1A	2208	G
1	1A	2209	G
1	1A	2212	G
1	1A	2214	G
1	1A	2220	A
1	1A	2226	C
1	1A	2227	G
1	1A	2228	G
1	1A	2229	A
1	1A	2231	G
1	1A	2237	A
1	1A	2246	G
1	1A	2250	G
1	1A	2251	G
1	1A	2280	A
1	1A	2281	A
1	1A	2290	A
1	1A	2295	C
1	1A	2299	A
1	1A	2301	G
1	1A	2306	C
1	1A	2317	A

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	1A	2324	U
1	1A	2332	A
1	1A	2333	G
1	1A	2337	G
1	1A	2348	A
1	1A	2359	C
1	1A	2362	C
1	1A	2395	G
1	1A	2397	C
1	1A	2412	G
1	1A	2418	U
1	1A	2426	G
1	1A	2434	A
1	1A	2437	A
1	1A	2441	G
1	1A	2442	A
1	1A	2446	A
1	1A	2447	A
1	1A	2451	A
1	1A	2453	C
1	1A	2457	G
1	1A	2460	A
1	1A	2480	G
1	1A	2481	A
1	1A	2488	A
1	1A	2514	G
1	1A	2516	U
1	1A	2517	G
1	1A	2518	U
1	1A	2530	A
1	1A	2532	C
1	1A	2541	G
1	1A	2547	G
1	1A	2561	G
1	1A	2562	G
1	1A	2566	U
1	1A	2578	A
1	1A	2579	G
1	1A	2586	G
1	1A	2594	G
1	1A	2597	U
1	1A	2598	C

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	1A	2614	A
1	1A	2621	U
1	1A	2623	U
1	1A	2624	C
1	1A	2641	A
1	1A	2642	G
1	1A	2666	A
1	1A	2674	A
1	1A	2701	U
1	1A	2702	C
1	1A	2703	C
1	1A	2714	U
1	1A	2715	C
1	1A	2725	A
1	1A	2726	A
1	1A	2727	G
1	1A	2739	U
1	1A	2746	A
1	1A	2771	A
1	1A	2778	A
1	1A	2779	G
1	1A	2780	C
1	1A	2791	A
1	1A	2793	G
1	1A	2803	A
1	1A	2804	C
1	1A	2813	G
1	1A	2828	G
1	1A	2830	A
1	1A	2831	A
1	1A	2843	G
1	1A	2845	A
1	1A	2882	G
1	1A	2884	C
1	1A	2885	C
1	1A	2890	C
1	1A	2901	A
1	1A	2903	G
2	1B	2	C
2	1B	7	G
2	1B	13	A
2	1B	47	C

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
2	1B	56	G
2	1B	57	A
2	1B	73	A
2	1B	84	C
2	1B	106	G
2	1B	110	G
32	1a	9	G
32	1a	22	G
32	1a	32	A
32	1a	39	G
32	1a	48	C
32	1a	50	A
32	1a	51	A
32	1a	61	G
32	1a	78	G
32	1a	79	G
32	1a	96	U
32	1a	101	A
32	1a	116	A
32	1a	121	C
32	1a	131	C
32	1a	144	G
32	1a	151	A
32	1a	159	G
32	1a	163	C
32	1a	173	U
32	1a	174	C
32	1a	182	U
32	1a	189(E)	U
32	1a	189(F)	U
32	1a	195	A
32	1a	197	A
32	1a	201	C
32	1a	202	U
32	1a	203	U
32	1a	204	U
32	1a	216	G
32	1a	218	C
32	1a	220	G
32	1a	247	G
32	1a	251	G
32	1a	258	G

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
32	1a	266	G
32	1a	267	C
32	1a	289	G
32	1a	298	A
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	381	C
32	1a	384	G
32	1a	388	G
32	1a	397	A
32	1a	398	C
32	1a	406	G
32	1a	412	A
32	1a	413	G
32	1a	422	C
32	1a	423	G
32	1a	424	G
32	1a	429	U
32	1a	439	A
32	1a	442	C
32	1a	452	A
32	1a	458	C
32	1a	461	A
32	1a	470	C
32	1a	477	A
32	1a	482	A
32	1a	485	G
32	1a	496	A
32	1a	498	U
32	1a	505	G
32	1a	509	A
32	1a	510	A
32	1a	511	C

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
32	1a	518	C
32	1a	521	G
32	1a	527	G7M
32	1a	532	A
32	1a	533	A
32	1a	547	A
32	1a	550	G
32	1a	558	G
32	1a	559	A
32	1a	560	U
32	1a	561	U
32	1a	562	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	618	C
32	1a	619	U
32	1a	630	G
32	1a	631	G
32	1a	632	A
32	1a	633	G
32	1a	653	A
32	1a	661	G
32	1a	665	A
32	1a	680	C
32	1a	687	A
32	1a	688	G
32	1a	723	U
32	1a	731	G
32	1a	735	C
32	1a	746	A
32	1a	753	A
32	1a	755	G
32	1a	777	A
32	1a	792	A
32	1a	793	U
32	1a	794	A
32	1a	796	C
32	1a	817	C

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
32	1a	821	G
32	1a	828	A
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	872	A
32	1a	873	A
32	1a	902	G
32	1a	914	A
32	1a	926	G
32	1a	927	G
32	1a	934	C
32	1a	960	U
32	1a	961	U
32	1a	968	A
32	1a	969	A
32	1a	971	G
32	1a	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	998	G
32	1a	999	C
32	1a	1001(A)	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

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
32	1a	1027	C
32	1a	1028	C
32	1a	1029	C
32	1a	1030	C
32	1a	1030(A)	G
32	1a	1030(C)	G
32	1a	1032	G
32	1a	1033	G
32	1a	1037	C
32	1a	1039	C
32	1a	1040	U
32	1a	1043	C
32	1a	1044	A
32	1a	1045	C
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	1086	U
32	1a	1094	G
32	1a	1101	A
32	1a	1118	C
32	1a	1122	U
32	1a	1125	U
32	1a	1130	A
32	1a	1132	C
32	1a	1134	G
32	1a	1136	U
32	1a	1137	C
32	1a	1139	G
32	1a	1151	A
32	1a	1152	A
32	1a	1159	U
32	1a	1168	A
32	1a	1183	A
32	1a	1184	G
32	1a	1193	G
32	1a	1196	U
32	1a	1197	G
32	1a	1202	G

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
32	1a	1208	C
32	1a	1213	A
32	1a	1224	G
32	1a	1227	A
32	1a	1238	A
32	1a	1240	U
32	1a	1250	A
32	1a	1256	A
32	1a	1257	U
32	1a	1258	G
32	1a	1260	C
32	1a	1270	C
32	1a	1278	U
32	1a	1280	A
32	1a	1281	U
32	1a	1282	C
32	1a	1286	A
32	1a	1287	A
32	1a	1299	A
32	1a	1300	G
32	1a	1302	U
32	1a	1305	G
32	1a	1312	G
32	1a	1315	U
32	1a	1317	C
32	1a	1319	A
32	1a	1320	C
32	1a	1338	G
32	1a	1340	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	1447	A
32	1a	1456	G
32	1a	1487	G
32	1a	1492	A
32	1a	1493	A

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
32	1a	1499	A
32	1a	1503	A
32	1a	1504	G
32	1a	1505	G
32	1a	1506	U
32	1a	1517	G
32	1a	1520	G
32	1a	1529	G
32	1a	1530	G
53	1x	9	G
53	1x	20	U
53	1x	21	A
53	1x	42	G
53	1x	50	U
53	1x	54	5MU
53	1x	68	C
1	2A	10	G
1	2A	11	G
1	2A	12	U
1	2A	15	G
1	2A	45	C
1	2A	61	G
1	2A	71	A
1	2A	74	A
1	2A	75	G
1	2A	84	A
1	2A	95	G
1	2A	118	A
1	2A	120	U
1	2A	131	G
1	2A	141	A
1	2A	157	U
1	2A	173	G
1	2A	181	A
1	2A	182	A
1	2A	196	A
1	2A	199	A
1	2A	205	G
1	2A	211	A
1	2A	215	G
1	2A	216	A
1	2A	221	A

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	2A	222	A
1	2A	228	A
1	2A	229	A
1	2A	230	U
1	2A	248	G
1	2A	249	C
1	2A	271(K)	U
1	2A	271(L)	U
1	2A	271(M)	G
1	2A	271(N)	U
1	2A	271(O)	C
1	2A	272(B)	G
1	2A	277	C
1	2A	278	A
1	2A	292	C
1	2A	311	A
1	2A	324	A
1	2A	327	G
1	2A	329	G
1	2A	330	A
1	2A	345	A
1	2A	352	G
1	2A	354	G
1	2A	362	U
1	2A	363	G
1	2A	370	G
1	2A	372	G
1	2A	386	G
1	2A	396	G
1	2A	399	G
1	2A	405	U
1	2A	407	G
1	2A	411	G
1	2A	412	A
1	2A	428	A
1	2A	443	A
1	2A	444	C
1	2A	454	A
1	2A	455	C
1	2A	457	A
1	2A	464	U
1	2A	470	A

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	2A	479	A
1	2A	481	G
1	2A	504	U
1	2A	505	A
1	2A	509	C
1	2A	530	G
1	2A	531	C
1	2A	532	A
1	2A	533	G
1	2A	545	G
1	2A	556	G
1	2A	563	G
1	2A	568	U
1	2A	573	G
1	2A	575	A
1	2A	603	A
1	2A	604	G
1	2A	607	U
1	2A	614(B)	G
1	2A	614(C)	A
1	2A	615	G
1	2A	616	G
1	2A	627	A
1	2A	637	A
1	2A	645	C
1	2A	646	A
1	2A	652(B)	A
1	2A	652(C)	G
1	2A	652(F)	G
1	2A	652(T)	C
1	2A	652(U)	G
1	2A	669	G
1	2A	686	G
1	2A	717	G
1	2A	726	G
1	2A	730	C
1	2A	740	U
1	2A	753	C
1	2A	764	A
1	2A	775	G
1	2A	776	G
1	2A	782	A

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	2A	784	A
1	2A	785	G
1	2A	790	C
1	2A	792	G
1	2A	793	A
1	2A	794	G
1	2A	802	A
1	2A	805	G
1	2A	812	C
1	2A	827	U
1	2A	828	U
1	2A	832	G
1	2A	848	G
1	2A	857	C
1	2A	859	G
1	2A	869	G
1	2A	874	G
1	2A	883	G
1	2A	886	C
1	2A	887	A
1	2A	888	C
1	2A	889	C
1	2A	890	A
1	2A	893	C
1	2A	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	936	C
1	2A	938	G
1	2A	941	A
1	2A	944	G
1	2A	945	A
1	2A	946	G
1	2A	953	A
1	2A	958	U
1	2A	961	C
1	2A	974	G
1	2A	975	C

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	2A	980	A
1	2A	983	A
1	2A	996	A
1	2A	997	G
1	2A	1006	C
1	2A	1012	U
1	2A	1013	C
1	2A	1022	G
1	2A	1026	U
1	2A	1033	U
1	2A	1038	C
1	2A	1043	C
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	1058	G
1	2A	1060	U
1	2A	1064	C
1	2A	1065	U
1	2A	1066	U
1	2A	1067	A
1	2A	1068	G
1	2A	1070	A
1	2A	1071	G
1	2A	1072	C
1	2A	1073	A
1	2A	1074	G
1	2A	1076	C
1	2A	1077	A
1	2A	1078	U
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	1087	G
1	2A	1088	A
1	2A	1090	U

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	2A	1091	G
1	2A	1092	C
1	2A	1093	G
1	2A	1094	U
1	2A	1096	A
1	2A	1109	C
1	2A	1110	G
1	2A	1112	G
1	2A	1130	U
1	2A	1135	C
1	2A	1136	G
1	2A	1170	G
1	2A	1171	G
1	2A	1211	U
1	2A	1220	A
1	2A	1229	G
1	2A	1236	G
1	2A	1237	A
1	2A	1244	G
1	2A	1253	A
1	2A	1256	G
1	2A	1268	A
1	2A	1271	G
1	2A	1272	A
1	2A	1273	U
1	2A	1284	A
1	2A	1300	U
1	2A	1301	A
1	2A	1313	U
1	2A	1314	C
1	2A	1342	A
1	2A	1352	U
1	2A	1359	A
1	2A	1360	A
1	2A	1365	A
1	2A	1368	G
1	2A	1373	A
1	2A	1376	C
1	2A	1384	A
1	2A	1385	G
1	2A	1386	C
1	2A	1416	G

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	2A	1417	C
1	2A	1420	U
1	2A	1421	G
1	2A	1428	C
1	2A	1437	C
1	2A	1445	A
1	2A	1459	G
1	2A	1460	A
1	2A	1467	C
1	2A	1471	A
1	2A	1482	G
1	2A	1493	C
1	2A	1494	A
1	2A	1497	U
1	2A	1508	A
1	2A	1509	C
1	2A	1509(A)	A
1	2A	1525	G
1	2A	1542	A
1	2A	1543	C
1	2A	1547	C
1	2A	1558	A
1	2A	1559	G
1	2A	1566	A
1	2A	1569	A
1	2A	1578	U
1	2A	1580	A
1	2A	1584	C
1	2A	1586	A
1	2A	1602	U
1	2A	1603	A
1	2A	1608	A
1	2A	1609	A
1	2A	1639	U
1	2A	1648	C
1	2A	1664	A
1	2A	1674	G
1	2A	1675	C
1	2A	1700	A
1	2A	1701	A
1	2A	1721	G
1	2A	1722	A

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	2A	1746	G
1	2A	1756	G
1	2A	1762	A
1	2A	1763	G
1	2A	1764	G
1	2A	1773	A
1	2A	1780	A
1	2A	1782	C
1	2A	1791	A
1	2A	1800	C
1	2A	1801	G
1	2A	1812	A
1	2A	1816	G
1	2A	1820	U
1	2A	1828	G
1	2A	1835	G
1	2A	1847	A
1	2A	1861	G
1	2A	1877	A
1	2A	1878	G
1	2A	1889	A
1	2A	1900	A
1	2A	1906	G
1	2A	1914	C
1	2A	1929	G
1	2A	1930	G
1	2A	1936	A
1	2A	1937	A
1	2A	1947	C
1	2A	1955	U
1	2A	1962	5MC
1	2A	1963	U
1	2A	1967	C
1	2A	1970	A
1	2A	1971	A
1	2A	1972	A
1	2A	1992	G
1	2A	1993	U
1	2A	1997	G
1	2A	2004	G
1	2A	2023	G
1	2A	2031	A

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	2A	2033	A
1	2A	2043	C
1	2A	2055	C
1	2A	2056	G
1	2A	2060	A
1	2A	2061	G
1	2A	2062	A
1	2A	2069	G
1	2A	2070	G
1	2A	2076	U
1	2A	2093	G
1	2A	2101	G
1	2A	2103	C
1	2A	2104	G
1	2A	2105	C
1	2A	2107	C
1	2A	2108	C
1	2A	2109	U
1	2A	2111	C
1	2A	2112	G
1	2A	2116	G
1	2A	2117	A
1	2A	2118	U
1	2A	2119	A
1	2A	2121	G
1	2A	2123	G
1	2A	2124	G
1	2A	2126	A
1	2A	2127	G
1	2A	2129	C
1	2A	2130	U
1	2A	2131	G
1	2A	2132	U
1	2A	2133	G
1	2A	2134	A
1	2A	2136	C
1	2A	2137	C
1	2A	2138	C
1	2A	2141	G
1	2A	2142	C
1	2A	2145	C
1	2A	2146	C

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	2A	2148	G
1	2A	2151	G
1	2A	2159	G
1	2A	2162	G
1	2A	2163	C
1	2A	2164	C
1	2A	2172	U
1	2A	2173	A
1	2A	2180	U
1	2A	2186	G
1	2A	2187	G
1	2A	2189	U
1	2A	2191	G
1	2A	2192	G
1	2A	2198	A
1	2A	2206	G
1	2A	2207	G
1	2A	2208	A
1	2A	2225	A
1	2A	2235	G
1	2A	2239	G
1	2A	2268	A
1	2A	2269	A
1	2A	2273	A
1	2A	2275	C
1	2A	2279	G
1	2A	2283	C
1	2A	2287	A
1	2A	2289	G
1	2A	2297	C
1	2A	2305	A
1	2A	2308	G
1	2A	2311	A
1	2A	2312	U
1	2A	2316	C
1	2A	2320	A
1	2A	2321	G
1	2A	2322	A
1	2A	2325	G
1	2A	2334	G
1	2A	2336	A
1	2A	2340	G

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	2A	2343	C
1	2A	2347	C
1	2A	2350	C
1	2A	2379	G
1	2A	2383	G
1	2A	2385	C
1	2A	2406	U
1	2A	2410	G
1	2A	2414	G
1	2A	2422	A
1	2A	2423	U
1	2A	2425	A
1	2A	2427	C
1	2A	2429	G
1	2A	2430	A
1	2A	2435	A
1	2A	2439	A
1	2A	2441	C
1	2A	2445	G
1	2A	2448	A
1	2A	2474	C
1	2A	2476	A
1	2A	2478	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	2529	G
1	2A	2549	G
1	2A	2553	G
1	2A	2554	U
1	2A	2555	U
1	2A	2566	A
1	2A	2567	G
1	2A	2572	A
1	2A	2574	G
1	2A	2576	G
1	2A	2577	A
1	2A	2582	G
1	2A	2585	U

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	2A	2602	A
1	2A	2611	U
1	2A	2612	C
1	2A	2620	C
1	2A	2629	A
1	2A	2630	G
1	2A	2654	A
1	2A	2663	G
1	2A	2682	U
1	2A	2689	U
1	2A	2690	C
1	2A	2691	C
1	2A	2702	U
1	2A	2703	C
1	2A	2712(A)	A
1	2A	2713	A
1	2A	2714	G
1	2A	2718	G
1	2A	2726	U
1	2A	2733	A
1	2A	2748	A
1	2A	2757	A
1	2A	2758	A
1	2A	2764	A
1	2A	2765	A
1	2A	2769	C
1	2A	2778	A
1	2A	2802	G
1	2A	2818	G
1	2A	2820	A
1	2A	2821	A
1	2A	2823	A
1	2A	2833	G
1	2A	2866	U
1	2A	2872	G
1	2A	2880	C
1	2A	2892	A
1	2A	2894	G
1	2A	2896	C
1	2A	2897	U
2	2B	2	C
2	2B	7	G

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
2	2B	8	U
2	2B	13	A
2	2B	15	A
2	2B	33	G
2	2B	42	C
2	2B	56	G
2	2B	73	A
2	2B	84	C
2	2B	106	G
2	2B	110	G
32	2a	5	U
32	2a	9	G
32	2a	10	A
32	2a	22	G
32	2a	32	A
32	2a	39	G
32	2a	48	C
32	2a	50	A
32	2a	51	A
32	2a	66	G
32	2a	89	C
32	2a	96	U
32	2a	101	A
32	2a	116	A
32	2a	121	C
32	2a	131	C
32	2a	144	G
32	2a	151	A
32	2a	163	C
32	2a	173	U
32	2a	174	C
32	2a	182	U
32	2a	189(E)	U
32	2a	189(F)	U
32	2a	195	A
32	2a	197	A
32	2a	201	C
32	2a	202	U
32	2a	203	U
32	2a	204	U
32	2a	216	G
32	2a	218	C

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
32	2a	220	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	298	A
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
32	2a	372	C
32	2a	373	A
32	2a	381	C
32	2a	384	G
32	2a	388	G
32	2a	397	A
32	2a	398	C
32	2a	406	G
32	2a	412	A
32	2a	413	G
32	2a	422	C
32	2a	423	G
32	2a	424	G
32	2a	429	U
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	477	A
32	2a	482	A
32	2a	485	G
32	2a	496	A
32	2a	498	U

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
32	2a	505	G
32	2a	509	A
32	2a	510	A
32	2a	511	C
32	2a	518	C
32	2a	521	G
32	2a	527	G7M
32	2a	532	A
32	2a	533	A
32	2a	547	A
32	2a	550	G
32	2a	558	G
32	2a	559	A
32	2a	560	U
32	2a	561	U
32	2a	562	C
32	2a	572	A
32	2a	573	A
32	2a	576	G
32	2a	592	G
32	2a	596	C
32	2a	618	C
32	2a	619	U
32	2a	630	G
32	2a	631	G
32	2a	632	A
32	2a	633	G
32	2a	653	A
32	2a	661	G
32	2a	665	A
32	2a	687	A
32	2a	688	G
32	2a	723	U
32	2a	731	G
32	2a	746	A
32	2a	753	A
32	2a	755	G
32	2a	766	A
32	2a	777	A
32	2a	792	A
32	2a	793	U
32	2a	794	A

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
32	2a	796	C
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	872	A
32	2a	873	A
32	2a	902	G
32	2a	914	A
32	2a	926	G
32	2a	927	G
32	2a	934	C
32	2a	960	U
32	2a	961	U
32	2a	968	A
32	2a	969	A
32	2a	971	G
32	2a	972	C
32	2a	974	A
32	2a	975	A
32	2a	976	G
32	2a	977	A
32	2a	982	U
32	2a	992	U
32	2a	993	G
32	2a	994	A
32	2a	1005	A
32	2a	1009	G
32	2a	1022	G
32	2a	1023	G
32	2a	1024	G
32	2a	1025	U
32	2a	1026	G
32	2a	1027	C
32	2a	1028	C
32	2a	1030(A)	G

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
32	2a	1030(B)	C
32	2a	1030(C)	G
32	2a	1032	G
32	2a	1033	G
32	2a	1034	G
32	2a	1039	C
32	2a	1040	U
32	2a	1044	A
32	2a	1045	C
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	1086	U
32	2a	1094	G
32	2a	1095	U
32	2a	1101	A
32	2a	1117	G
32	2a	1118	C
32	2a	1122	U
32	2a	1125	U
32	2a	1129	C
32	2a	1130	A
32	2a	1132	C
32	2a	1136	U
32	2a	1137	C
32	2a	1138	G
32	2a	1139	G
32	2a	1140	C
32	2a	1147	C
32	2a	1151	A
32	2a	1152	A
32	2a	1158	C
32	2a	1159	U
32	2a	1168	A
32	2a	1183	A
32	2a	1184	G
32	2a	1193	G
32	2a	1196	U
32	2a	1197	G

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
32	2a	1211	U
32	2a	1212	U
32	2a	1213	A
32	2a	1224	G
32	2a	1227	A
32	2a	1238	A
32	2a	1240	U
32	2a	1250	A
32	2a	1256	A
32	2a	1257	U
32	2a	1258	G
32	2a	1260	C
32	2a	1270	C
32	2a	1278	U
32	2a	1279	A
32	2a	1280	A
32	2a	1286	A
32	2a	1287	A
32	2a	1299	A
32	2a	1300	G
32	2a	1305	G
32	2a	1312	G
32	2a	1315	U
32	2a	1317	C
32	2a	1319	A
32	2a	1320	C
32	2a	1340	A
32	2a	1347	G
32	2a	1353	G
32	2a	1363	C
32	2a	1370	G
32	2a	1397	C
32	2a	1419	G
32	2a	1442	G
32	2a	1442(A)	G
32	2a	1447	A
32	2a	1456	G
32	2a	1487	G
32	2a	1492	A
32	2a	1493	A
32	2a	1499	A
32	2a	1503	A

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
32	2a	1504	G
32	2a	1505	G
32	2a	1506	U
32	2a	1517	G
32	2a	1520	G
32	2a	1529	G
32	2a	1530	G
53	2x	9	G
53	2x	20	U
53	2x	21	A
53	2x	42	G
53	2x	50	U
53	2x	68	C
53	2x	69	C
53	2x	76	A

All (59) RNA pucker outliers are listed below:

<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	1A	78	G
1	1A	115	G
1	1A	185	A
1	1A	302	A
1	1A	509	A
1	1A	532	A
1	1A	831	A
1	1A	874	U
1	1A	913	A
1	1A	941	U
1	1A	1003	U
1	1A	1065	U
1	1A	1067	A
1	1A	1093	G
1	1A	1097	G
1	1A	1099	C
1	1A	1201	A
1	1A	1219	A
1	1A	1220	U
1	1A	1221	G
1	1A	1255	A
1	1A	1299	A
1	1A	1346	U

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Mol	Chain	Res	Type
1	1A	1700	G
1	1A	1710	C
1	1A	2300	A
1	1A	2434	A
1	1A	2442	A
1	1A	2597	U
1	1A	2701	U
1	1A	2902	G
1	2A	9	U
1	2A	195	A
1	2A	266	G
1	2A	271(M)	G
1	2A	277	C
1	2A	532	A
1	2A	652(E)	G
1	2A	752	A
1	2A	840	C
1	2A	856	C
1	2A	900	A
1	2A	1053	C
1	2A	1057	A
1	2A	1065	U
1	2A	1067	A
1	2A	1073	A
1	2A	1076	C
1	2A	1210	A
1	2A	1420	U
1	2A	1442	G
1	2A	1491	G
1	2A	1992	G
1	2A	2126	A
1	2A	2171	A
1	2A	2172	U
1	2A	2321	G
1	2A	2689	U
1	2A	2756	U

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

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
32	M2G	1a	966	32	20,27,28	3.16	7 (35%)	22,40,43	1.39	5 (22%)
32	5MC	1a	1404	32	18,22,23	0.94	0	26,32,35	1.21	5 (19%)
32	2MG	2a	1207	32	18,26,27	1.86	4 (22%)	16,38,41	1.26	2 (12%)
32	5MC	2a	1400	32	18,22,23	1.00	1 (5%)	26,32,35	1.32	4 (15%)
32	5MC	1a	1400	32	18,22,23	1.07	1 (5%)	26,32,35	1.32	3 (11%)
1	5MU	2A	1939	1	19,22,23	0.81	1 (5%)	28,32,35	1.16	2 (7%)
1	5MC	1A	1964	1	18,22,23	0.90	0	26,32,35	1.31	4 (15%)
1	5MC	2A	1942	1	18,22,23	1.01	1 (5%)	26,32,35	1.23	4 (15%)
32	PSU	1a	516	32	18,21,22	1.38	3 (16%)	22,30,33	1.96	5 (22%)
1	OMG	2A	2251	56,1,53	18,26,27	1.81	4 (22%)	19,38,41	1.51	4 (21%)
32	5MC	1a	1407	32	18,22,23	1.07	1 (5%)	26,32,35	1.18	5 (19%)
32	G7M	2a	527	56,32	20,26,27	3.14	8 (40%)	17,39,42	1.03	3 (17%)
32	M2G	2a	966	32	20,27,28	3.25	7 (35%)	22,40,43	1.36	5 (22%)
32	5MC	2a	1404	32	18,22,23	0.99	1 (5%)	26,32,35	1.21	5 (19%)
32	5MC	2a	1407	32	18,22,23	0.98	2 (11%)	26,32,35	1.23	4 (15%)
1	OMC	2A	1920	1	19,22,23	2.51	7 (36%)	26,31,34	0.87	1 (3%)
53	PSU	2x	55	53	18,21,22	1.54	3 (16%)	22,30,33	1.69	5 (22%)
1	OMG	1A	2263	56,1,53	18,26,27	1.87	5 (27%)	19,38,41	1.56	4 (21%)
32	PSU	2a	516	32	18,21,22	1.37	2 (11%)	22,30,33	2.09	6 (27%)
32	4OC	1a	1402	32	20,23,24	2.63	8 (40%)	26,32,35	0.84	0
32	MA6	1a	1519	32	19,26,27	1.04	2 (10%)	18,38,41	5.06	3 (16%)
1	5MU	1A	1961	1	19,22,23	0.80	1 (5%)	28,32,35	1.20	3 (10%)
53	5MU	1x	54	53	19,22,23	1.10	2 (10%)	28,32,35	1.12	2 (7%)
1	2MA	2A	2503	56,1	17,25,26	1.85	3 (17%)	17,37,40	1.30	3 (17%)
32	MA6	1a	1518	32	19,26,27	1.01	2 (10%)	18,38,41	4.86	3 (16%)
1	2MA	1A	2515	56,1	17,25,26	1.81	4 (23%)	17,37,40	1.37	3 (17%)
32	2MG	1a	1207	56,32	18,26,27	1.95	5 (27%)	16,38,41	1.61	4 (25%)
1	5MU	1A	1937	1	19,22,23	1.31	2 (10%)	28,32,35	1.47	5 (17%)
53	5MU	2x	54	53	19,22,23	0.97	2 (10%)	28,32,35	1.10	2 (7%)
43	0TD	1l	92	43	7,9,10	2.47	2 (28%)	6,11,13	3.01	4 (66%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
53	4SU	1x	8	53	18,21,22	1.16	2 (11%)	26,30,33	0.80	1 (3%)
1	OMC	1A	1942	56,1	19,22,23	2.46	7 (36%)	26,31,34	0.90	1 (3%)
32	5MC	2a	967	32	18,22,23	0.98	1 (5%)	26,32,35	1.29	4 (15%)
32	MA6	2a	1518	32	19,26,27	1.01	2 (10%)	18,38,41	5.28	3 (16%)
32	5MC	1a	967	32	18,22,23	1.06	2 (11%)	26,32,35	1.21	3 (11%)
53	4SU	2x	8	56,53	18,21,22	1.18	2 (11%)	26,30,33	0.85	2 (7%)
1	PSU	2A	1917	1	18,21,22	1.30	3 (16%)	22,30,33	1.62	5 (22%)
32	UR3	2a	1498	32	19,22,23	1.97	3 (15%)	26,32,35	1.36	2 (7%)
53	5MC	1x	32	53	18,22,23	1.08	3 (16%)	26,32,35	1.25	5 (19%)
32	UR3	1a	1498	32	19,22,23	1.99	3 (15%)	26,32,35	1.33	3 (11%)
1	OMU	2A	2552	56,1	19,22,23	6.69	10 (52%)	26,31,34	2.40	7 (26%)
53	PSU	1x	55	53	18,21,22	1.44	3 (16%)	22,30,33	1.59	3 (13%)
1	PSU	2A	1911	1	18,21,22	1.34	3 (16%)	22,30,33	1.59	5 (22%)
1	PSU	2A	2605	1	18,21,22	1.39	3 (16%)	22,30,33	1.67	2 (9%)
53	5MC	2x	32	53	18,22,23	1.08	2 (11%)	26,32,35	1.30	4 (15%)
43	0TD	2l	92	43	7,9,10	2.04	1 (14%)	6,11,13	2.43	3 (50%)
1	5MU	2A	1915	1	19,22,23	1.21	2 (10%)	28,32,35	1.30	3 (10%)
1	5MC	1A	1984	1	18,22,23	0.95	1 (5%)	26,32,35	1.33	4 (15%)
1	PSU	1A	1939	56,1	18,21,22	1.18	3 (16%)	22,30,33	1.48	5 (22%)
32	4OC	2a	1402	32	20,23,24	2.65	8 (40%)	26,32,35	0.97	1 (3%)
32	G7M	1a	527	56,32	20,26,27	3.15	8 (40%)	17,39,42	0.98	1 (5%)
1	PSU	1A	1933	1	18,21,22	1.33	3 (16%)	22,30,33	1.51	4 (18%)
32	MA6	2a	1519	32	19,26,27	1.05	2 (10%)	18,38,41	5.02	3 (16%)
1	5MC	2A	1962	56,1	18,22,23	0.98	1 (5%)	26,32,35	1.33	4 (15%)
1	PSU	1A	2617	1	18,21,22	1.18	3 (16%)	22,30,33	1.61	2 (9%)
1	OMU	1A	2564	1	19,22,23	6.69	10 (52%)	26,31,34	2.58	8 (30%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
32	M2G	1a	966	32	-	0/7/29/30	0/3/3/3
32	5MC	1a	1404	32	-	0/7/25/26	0/2/2/2
32	2MG	2a	1207	32	-	0/5/27/28	0/3/3/3
32	5MC	2a	1400	32	-	1/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
32	5MC	1a	1400	32	-	2/7/25/26	0/2/2/2
1	5MU	2A	1939	1	-	0/7/25/26	0/2/2/2
1	5MC	1A	1964	1	-	0/7/25/26	0/2/2/2
1	5MC	2A	1942	1	-	0/7/25/26	0/2/2/2
32	PSU	1a	516	32	-	1/7/25/26	0/2/2/2
1	OMG	2A	2251	56,1,53	-	0/5/27/28	0/3/3/3
32	5MC	1a	1407	32	-	0/7/25/26	0/2/2/2
32	G7M	2a	527	56,32	-	2/3/25/26	0/3/3/3
32	M2G	2a	966	32	-	0/7/29/30	0/3/3/3
32	5MC	2a	1404	32	-	0/7/25/26	0/2/2/2
32	5MC	2a	1407	32	-	0/7/25/26	0/2/2/2
1	OMC	2A	1920	1	-	1/9/27/28	0/2/2/2
53	PSU	2x	55	53	-	0/7/25/26	0/2/2/2
1	OMG	1A	2263	56,1,53	-	1/5/27/28	0/3/3/3
32	PSU	2a	516	32	-	1/7/25/26	0/2/2/2
32	4OC	1a	1402	32	-	2/9/29/30	0/2/2/2
32	MA6	1a	1519	32	-	4/7/29/30	0/3/3/3
1	5MU	1A	1961	1	-	0/7/25/26	0/2/2/2
53	5MU	1x	54	53	-	2/7/25/26	0/2/2/2
1	2MA	2A	2503	56,1	-	3/3/25/26	0/3/3/3
32	MA6	1a	1518	32	-	0/7/29/30	0/3/3/3
1	2MA	1A	2515	56,1	-	2/3/25/26	0/3/3/3
32	2MG	1a	1207	56,32	-	2/5/27/28	0/3/3/3
1	5MU	1A	1937	1	-	4/7/25/26	0/2/2/2
53	5MU	2x	54	53	-	0/7/25/26	0/2/2/2
43	0TD	1l	92	43	-	2/7/12/14	-
53	4SU	1x	8	53	-	0/7/25/26	0/2/2/2
1	OMC	1A	1942	56,1	-	3/9/27/28	0/2/2/2
32	5MC	2a	967	32	-	0/7/25/26	0/2/2/2
32	MA6	2a	1518	32	-	0/7/29/30	0/3/3/3
32	5MC	1a	967	32	-	1/7/25/26	0/2/2/2
53	4SU	2x	8	56,53	-	0/7/25/26	0/2/2/2
1	PSU	2A	1917	1	-	0/7/25/26	0/2/2/2
32	UR3	2a	1498	32	-	0/7/25/26	0/2/2/2
53	5MC	1x	32	53	-	0/7/25/26	0/2/2/2
32	UR3	1a	1498	32	-	1/7/25/26	0/2/2/2
1	OMU	2A	2552	56,1	-	0/9/27/28	0/2/2/2
53	PSU	1x	55	53	-	0/7/25/26	0/2/2/2
1	PSU	2A	1911	1	-	0/7/25/26	0/2/2/2
1	PSU	2A	2605	1	-	0/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
53	5MC	2x	32	53	-	0/7/25/26	0/2/2/2
43	0TD	2l	92	43	-	2/7/12/14	-
1	5MU	2A	1915	1	-	2/7/25/26	0/2/2/2
1	5MC	1A	1984	1	-	0/7/25/26	0/2/2/2
1	PSU	1A	1939	56,1	-	0/7/25/26	0/2/2/2
32	4OC	2a	1402	32	-	5/9/29/30	0/2/2/2
32	G7M	1a	527	56,32	-	3/3/25/26	0/3/3/3
1	PSU	1A	1933	1	-	0/7/25/26	0/2/2/2
32	MA6	2a	1519	32	-	4/7/29/30	0/3/3/3
1	5MC	2A	1962	56,1	-	2/7/25/26	0/2/2/2
1	PSU	1A	2617	1	-	0/7/25/26	0/2/2/2
1	OMU	1A	2564	1	-	1/9/27/28	0/2/2/2

All (182) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	1A	2564	OMU	C5-C4	15.72	1.78	1.43
1	2A	2552	OMU	C5-C4	15.66	1.78	1.43
1	1A	2564	OMU	C4-N3	-14.82	1.12	1.38
1	2A	2552	OMU	C4-N3	-14.53	1.12	1.38
32	2a	966	M2G	C2-N3	11.72	1.45	1.30
32	1a	966	M2G	C2-N3	11.38	1.44	1.30
1	1A	2564	OMU	C6-C5	-10.14	1.11	1.35
1	2A	2552	OMU	C6-C5	-10.10	1.11	1.35
1	1A	2564	OMU	C3'-C2'	-8.93	1.33	1.52
1	2A	2552	OMU	C6-N1	8.71	1.59	1.38
1	2A	2552	OMU	C3'-C2'	-8.64	1.33	1.52
32	1a	527	G7M	C8-N9	8.46	1.48	1.33
32	2a	527	G7M	C8-N9	8.41	1.48	1.33
1	1A	2564	OMU	C6-N1	8.39	1.58	1.38
32	2a	527	G7M	C8-N7	8.03	1.47	1.33
32	1a	527	G7M	C8-N7	7.86	1.47	1.33
1	2A	2552	OMU	O4'-C1'	6.50	1.57	1.42
1	1A	2564	OMU	O4'-C1'	6.33	1.57	1.42
1	2A	2552	OMU	O4'-C4'	-6.27	1.31	1.45
1	2A	1920	OMC	C4-N4	5.89	1.47	1.33
1	1A	1942	OMC	C4-N4	5.81	1.47	1.33
1	1A	2564	OMU	O4'-C4'	-5.77	1.32	1.45
32	1a	1402	4OC	C4-N4	5.75	1.47	1.35
32	2a	1402	4OC	C4-N4	5.71	1.47	1.35
1	2A	2503	2MA	C2-N3	5.63	1.43	1.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	1A	2515	2MA	C2-N3	5.37	1.42	1.31
1	1A	2564	OMU	C1'-N1	-5.33	1.32	1.47
43	1l	92	0TD	CB-SB	-5.32	1.76	1.82
1	2A	2552	OMU	C1'-N1	-5.15	1.32	1.47
32	2a	1498	UR3	C6-C5	5.14	1.47	1.35
32	1a	1498	UR3	C6-C5	5.11	1.46	1.35
32	2a	966	M2G	C2-N2	5.06	1.44	1.35
32	1a	1207	2MG	C2-N1	5.00	1.44	1.36
32	1a	966	M2G	C2-N2	4.89	1.44	1.35
1	2A	1920	OMC	C6-C5	4.80	1.46	1.35
32	2a	1402	4OC	C6-C5	4.79	1.46	1.35
32	1a	1498	UR3	C2-N1	4.72	1.45	1.38
32	1a	527	G7M	C2-N3	4.71	1.44	1.33
32	1a	1402	4OC	C6-C5	4.67	1.45	1.35
32	2a	1207	2MG	C2-N1	4.62	1.44	1.36
1	1A	1942	OMC	C2-N3	4.59	1.45	1.36
1	1A	1937	5MU	C2-N1	4.58	1.45	1.38
1	1A	2263	OMG	C2-N3	4.54	1.44	1.33
32	1a	1402	4OC	C2-N3	4.52	1.45	1.36
1	1A	1942	OMC	C6-C5	4.51	1.45	1.35
32	1a	1402	4OC	C4-N3	4.51	1.40	1.32
1	2A	1920	OMC	C2-N3	4.50	1.45	1.36
32	2a	527	G7M	C2-N3	4.48	1.44	1.33
1	2A	2251	OMG	C2-N3	4.41	1.43	1.33
32	2a	1498	UR3	C2-N1	4.40	1.44	1.38
32	2a	1402	4OC	C2-N3	4.36	1.45	1.36
53	2x	55	PSU	C2-N1	4.28	1.42	1.36
32	1a	1207	2MG	C2-N2	4.26	1.42	1.33
32	2a	1207	2MG	C2-N2	4.15	1.42	1.33
1	1A	2564	OMU	C3'-C4'	4.12	1.63	1.53
53	1x	55	PSU	C2-N1	4.10	1.42	1.36
1	2A	2552	OMU	C3'-C4'	4.09	1.63	1.53
43	2l	92	0TD	CB-SB	-4.03	1.78	1.82
32	2a	1498	UR3	C2-N3	3.97	1.46	1.39
32	2a	1402	4OC	C5-C4	3.97	1.49	1.40
32	2a	1402	4OC	C4-N3	3.96	1.39	1.32
32	2a	966	M2G	C4-N3	3.96	1.47	1.37
32	2a	516	PSU	C2-N1	3.95	1.42	1.36
32	1a	1402	4OC	C5-C4	3.89	1.49	1.40
32	1a	1498	UR3	C2-N3	3.84	1.46	1.39
1	2A	1915	5MU	C2-N1	3.84	1.44	1.38
32	1a	516	PSU	C2-N1	3.84	1.41	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
53	1x	8	4SU	C4-S4	-3.77	1.61	1.68
1	2A	1917	PSU	C2-N1	3.77	1.41	1.36
1	1A	1942	OMC	C2-N1	3.72	1.48	1.40
1	2A	1920	OMC	C2-N1	3.70	1.48	1.40
1	2A	1911	PSU	C2-N1	3.69	1.41	1.36
32	1a	966	M2G	C4-N3	3.65	1.46	1.37
1	2A	2605	PSU	C2-N1	3.57	1.41	1.36
32	2a	1402	4OC	C2-N1	3.54	1.47	1.40
1	2A	2251	OMG	C4-N3	3.48	1.45	1.37
1	1A	2263	OMG	C4-N3	3.39	1.45	1.37
32	1a	527	G7M	C4-N3	3.38	1.45	1.37
32	2a	527	G7M	C4-N3	3.31	1.45	1.37
1	1A	1933	PSU	C2-N1	3.30	1.41	1.36
32	2a	527	G7M	C2-N2	3.21	1.41	1.34
32	1a	527	G7M	C2-N2	3.20	1.41	1.34
32	1a	1402	4OC	C2-N1	3.16	1.46	1.40
53	2x	55	PSU	C4-N3	3.14	1.44	1.38
1	1A	2515	2MA	C5-C4	-3.07	1.35	1.43
32	2a	1402	4OC	O2-C2	-3.04	1.18	1.23
32	1a	1207	2MG	C4-N3	3.02	1.44	1.37
1	2A	2503	2MA	C5-C4	-3.02	1.35	1.43
32	1a	1400	5MC	C2-N1	3.00	1.46	1.40
53	2x	32	5MC	C2-N1	3.00	1.46	1.40
32	2a	1207	2MG	C4-N3	2.99	1.44	1.37
53	1x	54	5MU	C2-N1	2.97	1.43	1.38
1	1A	1942	OMC	C4-N3	2.97	1.40	1.34
32	1a	1402	4OC	O2-C2	-2.95	1.18	1.23
1	2A	2605	PSU	C4-N3	2.95	1.44	1.38
1	1A	2515	2MA	C4-N3	2.93	1.44	1.37
1	2A	1920	OMC	O2-C2	-2.92	1.18	1.23
32	1a	966	M2G	C2-N1	2.91	1.43	1.36
32	2a	1402	4OC	CM4-N4	-2.88	1.40	1.45
1	2A	2251	OMG	C5-C4	-2.87	1.35	1.43
53	2x	8	4SU	C2-N3	2.86	1.43	1.38
1	1A	1933	PSU	C4-N3	2.85	1.44	1.38
32	2a	966	M2G	C2-N1	2.84	1.43	1.36
1	2A	2503	2MA	C4-N3	2.84	1.44	1.37
1	1A	2263	OMG	C5-C4	-2.83	1.35	1.43
1	2A	1920	OMC	C4-N3	2.83	1.40	1.34
1	2A	1920	OMC	C5-C4	2.82	1.49	1.42
1	1A	1942	OMC	O2-C2	-2.79	1.18	1.23
1	1A	1939	PSU	C2-N1	2.78	1.40	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	1a	1407	5MC	C2-N1	2.78	1.46	1.40
32	2a	1519	MA6	C2-N3	2.77	1.36	1.32
32	1a	1519	MA6	C2-N3	2.76	1.36	1.32
32	2a	516	PSU	O4'-C1'	-2.75	1.40	1.43
32	2a	966	M2G	C5-C4	-2.71	1.36	1.43
32	1a	967	5MC	C2-N1	2.71	1.45	1.40
32	2a	527	G7M	C2-N1	2.70	1.44	1.37
32	1a	527	G7M	C2-N1	2.68	1.44	1.37
32	2a	1518	MA6	C2-N3	2.67	1.36	1.32
53	1x	55	PSU	C4-N3	2.66	1.43	1.38
32	1a	966	M2G	C5-C4	-2.66	1.36	1.43
32	2a	1400	5MC	C2-N1	2.62	1.45	1.40
53	2x	55	PSU	C6-N1	2.61	1.40	1.36
32	1a	516	PSU	O4'-C1'	-2.60	1.40	1.43
1	1A	2617	PSU	C2-N1	2.57	1.40	1.36
1	2A	2552	OMU	O2'-C2'	2.56	1.49	1.42
53	1x	55	PSU	C6-N1	2.56	1.40	1.36
53	2x	54	5MU	C2-N1	2.55	1.42	1.38
32	1a	1518	MA6	C2-N3	2.55	1.36	1.32
1	2A	1915	5MU	C2-N3	2.53	1.42	1.38
1	1A	1942	OMC	C5-C4	2.52	1.48	1.42
1	2A	2605	PSU	C6-N1	2.50	1.40	1.36
53	2x	8	4SU	C4-S4	-2.50	1.63	1.68
32	1a	1402	4OC	CM4-N4	-2.49	1.41	1.45
53	1x	54	5MU	C2-N3	2.44	1.42	1.38
1	1A	1939	PSU	C4-N3	2.44	1.43	1.38
32	1a	966	M2G	C5-C6	2.42	1.52	1.47
53	1x	8	4SU	C2-N3	2.38	1.42	1.38
1	2A	1911	PSU	C4-N3	2.35	1.43	1.38
32	2a	967	5MC	C2-N1	2.35	1.45	1.40
1	1A	1937	5MU	C2-N3	2.34	1.42	1.38
32	2a	966	M2G	C6-N1	2.33	1.41	1.37
32	1a	527	G7M	C5-C6	2.32	1.51	1.45
32	1a	516	PSU	C6-N1	2.31	1.40	1.36
1	2A	1911	PSU	C6-N1	2.31	1.40	1.36
1	1A	2564	OMU	O2'-C2'	2.30	1.48	1.42
1	1A	2617	PSU	C4-N3	2.30	1.43	1.38
32	2a	966	M2G	C5-C6	2.28	1.52	1.47
53	2x	54	5MU	C2-N3	2.27	1.42	1.38
1	1A	2263	OMG	C2-N2	2.26	1.39	1.34
32	2a	527	G7M	C5-C6	2.26	1.51	1.45
53	1x	32	5MC	C2-N1	2.26	1.44	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	2a	1207	2MG	CM2-N2	-2.26	1.41	1.45
1	1A	1933	PSU	C6-N1	2.25	1.40	1.36
1	2A	1917	PSU	C6-N1	2.25	1.40	1.36
1	2A	1942	5MC	C2-N1	2.24	1.44	1.40
1	1A	2617	PSU	C6-N1	2.24	1.39	1.36
53	1x	32	5MC	C6-C5	2.24	1.38	1.34
1	2A	1917	PSU	C4-N3	2.22	1.43	1.38
1	2A	1962	5MC	C2-N1	2.20	1.44	1.40
32	1a	1518	MA6	C5-C4	-2.19	1.35	1.40
1	1A	1939	PSU	C6-N1	2.14	1.39	1.36
1	2A	2251	OMG	C6-N1	2.13	1.41	1.37
1	1A	1984	5MC	C2-N1	2.12	1.44	1.40
1	1A	2263	OMG	C6-N1	2.12	1.41	1.37
32	2a	527	G7M	C6-N1	2.12	1.41	1.37
32	1a	1207	2MG	CM2-N2	-2.12	1.41	1.45
1	2A	1939	5MU	C2-N3	2.11	1.41	1.38
32	1a	966	M2G	C6-N1	2.11	1.41	1.37
32	1a	1519	MA6	C5-C4	-2.10	1.35	1.40
53	1x	32	5MC	C2-N3	2.09	1.40	1.36
43	1l	92	0TD	CA-N	-2.07	1.41	1.47
32	2a	1407	5MC	C6-C5	2.07	1.38	1.34
32	2a	1519	MA6	C5-C4	-2.06	1.35	1.40
32	2a	1407	5MC	C2-N1	2.06	1.44	1.40
32	1a	967	5MC	C2-N3	2.06	1.40	1.36
53	2x	32	5MC	C6-C5	2.05	1.38	1.34
32	2a	1518	MA6	C5-C4	-2.05	1.35	1.40
1	1A	1961	5MU	C2-N3	2.03	1.41	1.38
32	1a	527	G7M	C6-N1	2.03	1.40	1.37
1	1A	2515	2MA	C2-N1	2.01	1.42	1.36
32	1a	1207	2MG	C5-C4	-2.00	1.38	1.43
32	2a	1404	5MC	C2-N1	2.00	1.44	1.40

All (196) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	2a	1518	MA6	N1-C6-N6	-20.73	95.24	117.06
32	1a	1519	MA6	N1-C6-N6	-19.98	96.03	117.06
32	2a	1519	MA6	N1-C6-N6	-19.76	96.26	117.06
32	1a	1518	MA6	N1-C6-N6	-18.94	97.12	117.06
1	2A	2552	OMU	C5-C4-N3	7.44	125.97	114.84
1	1A	2564	OMU	C5-C4-N3	7.27	125.71	114.84
32	2a	516	PSU	C6-C5-C4	6.96	123.06	118.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	1a	516	PSU	C6-C5-C4	6.44	122.70	118.20
1	1A	2564	OMU	C4-N3-C2	-6.28	118.30	126.58
32	2a	1518	MA6	C1'-N9-C4	-6.19	115.77	126.64
32	1a	1518	MA6	C1'-N9-C4	-5.91	116.26	126.64
1	2A	2552	OMU	C4-N3-C2	-5.76	118.99	126.58
1	2A	2605	PSU	C6-C5-C4	5.62	122.13	118.20
32	2a	1519	MA6	C1'-N9-C4	-5.51	116.97	126.64
32	1a	1519	MA6	C1'-N9-C4	-5.39	117.17	126.64
32	2a	1518	MA6	N3-C2-N1	-5.37	120.29	128.68
32	2a	1519	MA6	N3-C2-N1	-5.34	120.34	128.68
32	1a	1519	MA6	N3-C2-N1	-5.31	120.38	128.68
53	2x	55	PSU	C6-C5-C4	5.25	121.87	118.20
32	1a	1518	MA6	N3-C2-N1	-5.17	120.59	128.68
53	1x	55	PSU	C6-C5-C4	5.14	121.79	118.20
1	1A	2617	PSU	C6-C5-C4	5.11	121.77	118.20
1	2A	1917	PSU	C6-C5-C4	4.96	121.66	118.20
32	2a	1498	UR3	C4-N3-C2	-4.93	119.92	124.56
1	1A	2564	OMU	N3-C2-N1	4.70	121.12	114.89
1	2A	1911	PSU	C6-C5-C4	4.61	121.42	118.20
32	1a	1498	UR3	C4-N3-C2	-4.61	120.22	124.56
43	2l	92	0TD	CSB-SB-CB	4.25	110.13	102.44
43	1l	92	0TD	OD2-CG-CB	4.15	122.10	113.15
1	1A	1933	PSU	C6-C5-C4	4.09	121.06	118.20
43	1l	92	0TD	CSB-SB-CB	4.04	109.75	102.44
1	2A	2552	OMU	N3-C2-N1	3.71	119.82	114.89
1	1A	1939	PSU	C6-C5-C4	3.68	120.77	118.20
32	2a	1400	5MC	C5-C4-N3	3.64	125.61	121.67
32	1a	1400	5MC	C5-C4-N3	3.62	125.58	121.67
1	1A	1964	5MC	C5-C4-N3	3.62	125.58	121.67
1	1A	2263	OMG	C5-C6-N1	3.60	120.32	113.95
1	2A	1962	5MC	C5-C6-N1	-3.56	119.68	123.34
1	1A	1984	5MC	C5-C4-N3	3.56	125.51	121.67
53	2x	32	5MC	C5-C4-N3	3.56	125.51	121.67
1	1A	2515	2MA	C5-C6-N1	3.44	119.96	114.02
32	2a	967	5MC	C5-C4-N3	3.42	125.36	121.67
1	1A	1964	5MC	C5-C6-N1	-3.40	119.84	123.34
32	2a	1400	5MC	C5-C6-N1	-3.39	119.85	123.34
1	1A	1984	5MC	C5-C6-N1	-3.38	119.86	123.34
53	2x	32	5MC	C5-C6-N1	-3.37	119.87	123.34
32	2a	966	M2G	C5-C6-N1	3.37	119.90	113.95
1	2A	1962	5MC	C5-C4-N3	3.36	125.30	121.67
32	1a	967	5MC	C5-C4-N3	3.36	125.30	121.67

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	2A	2552	OMU	O4-C4-C5	-3.35	119.27	125.16
1	2A	2251	OMG	C5-C6-N1	3.34	119.84	113.95
53	1x	32	5MC	C5-C6-N1	-3.33	119.91	123.34
1	2A	2503	2MA	C5-C6-N1	3.33	119.76	114.02
1	2A	1942	5MC	C5-C6-N1	-3.30	119.94	123.34
1	1A	1961	5MU	C6-C5-C4	3.30	120.79	118.03
1	1A	1961	5MU	C4-N3-C2	-3.30	123.08	127.35
32	2a	516	PSU	N1-C2-N3	3.29	118.86	115.13
53	1x	54	5MU	C6-C5-C4	3.25	120.75	118.03
43	1l	92	0TD	CB-CA-N	-3.23	102.22	109.10
32	2a	967	5MC	C5-C6-N1	-3.21	120.04	123.34
1	1A	2564	OMU	O4-C4-C5	-3.20	119.53	125.16
1	1A	1937	5MU	C4-N3-C2	-3.20	123.21	127.35
1	2A	1915	5MU	C6-C5-C4	3.20	120.70	118.03
32	1a	516	PSU	N1-C2-N3	3.17	118.73	115.13
32	2a	1407	5MC	C5-C6-N1	-3.17	120.08	123.34
32	1a	966	M2G	C5-C6-N1	3.17	119.54	113.95
1	2A	1939	5MU	C6-C5-C4	3.15	120.67	118.03
1	1A	2263	OMG	C2-N1-C6	-3.14	119.32	125.10
32	2a	1407	5MC	C5-C4-N3	3.13	125.05	121.67
1	2A	2251	OMG	C2-N1-C6	-3.12	119.36	125.10
1	2A	1939	5MU	C4-N3-C2	-3.11	123.33	127.35
32	1a	1407	5MC	C5-C4-N3	3.10	125.02	121.67
1	2A	2552	OMU	O4-C4-N3	-3.10	114.76	119.31
1	1A	2564	OMU	O4-C4-N3	-3.09	114.76	119.31
32	1a	1207	2MG	C5-C6-N1	3.09	119.41	113.95
32	1a	1400	5MC	C5-C6-N1	-3.08	120.17	123.34
1	2A	1942	5MC	C5-C4-N3	3.08	125.00	121.67
32	1a	1404	5MC	C5-C6-N1	-3.08	120.17	123.34
1	2A	1915	5MU	C4-N3-C2	-3.06	123.39	127.35
32	2a	1404	5MC	C5-C6-N1	-3.01	120.24	123.34
32	1a	966	M2G	N1-C2-N2	3.00	120.60	118.04
32	2a	1207	2MG	C5-C6-N1	3.00	119.25	113.95
32	1a	967	5MC	C5-C6-N1	-3.00	120.25	123.34
1	1A	1937	5MU	C6-C5-C4	3.00	120.54	118.03
1	2A	1962	5MC	C4-N3-C2	-2.99	116.65	120.69
53	2x	54	5MU	C4-N3-C2	-2.97	123.50	127.35
1	1A	2564	OMU	O2-C2-N1	-2.94	118.88	122.79
53	1x	32	5MC	C5-C4-N3	2.93	124.84	121.67
32	2a	1404	5MC	C5-C4-N3	2.93	124.84	121.67
43	2l	92	0TD	OD2-CG-CB	2.91	119.45	113.15
53	1x	8	4SU	C4-N3-C2	-2.91	124.51	127.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1A	1984	5MC	C4-N3-C2	-2.91	116.75	120.69
32	1a	1404	5MC	C5-C4-N3	2.91	124.81	121.67
53	2x	54	5MU	C6-C5-C4	2.89	120.44	118.03
1	1A	1937	5MU	C1'-N1-C2	2.88	122.79	117.57
1	2A	2251	OMG	C8-N7-C5	2.85	108.43	102.99
1	1A	1964	5MC	C4-N3-C2	-2.83	116.86	120.69
1	2A	2552	OMU	C6-C5-C4	-2.83	115.64	119.52
1	1A	2263	OMG	C8-N7-C5	2.83	108.39	102.99
32	1a	1207	2MG	C8-N7-C5	2.81	108.35	102.99
32	2a	967	5MC	C4-N3-C2	-2.81	116.89	120.69
53	1x	32	5MC	C4-N3-C2	-2.81	116.89	120.69
1	2A	2503	2MA	C8-N7-C5	2.80	108.33	102.99
53	1x	54	5MU	C4-N3-C2	-2.79	123.75	127.35
1	1A	1933	PSU	O2-C2-N1	-2.78	119.72	122.79
1	1A	1939	PSU	O2-C2-N1	-2.74	119.78	122.79
32	1a	1404	5MC	C4-N3-C2	-2.73	116.99	120.69
1	1A	2515	2MA	CM2-C2-N1	2.72	122.28	116.23
32	2a	1400	5MC	C4-N3-C2	-2.68	117.06	120.69
1	2A	1942	5MC	C4-N3-C2	-2.68	117.06	120.69
32	2a	1207	2MG	C8-N7-C5	2.68	108.09	102.99
32	2a	1404	5MC	C4-N3-C2	-2.65	117.11	120.69
32	2a	966	M2G	C8-N7-C5	2.63	108.00	102.99
32	1a	1400	5MC	C4-N3-C2	-2.63	117.14	120.69
32	1a	966	M2G	C8-N7-C5	2.62	107.97	102.99
32	2a	1402	4OC	O2-C2-N3	-2.61	118.08	122.33
53	2x	8	4SU	C6-C5-C4	2.60	122.21	119.95
53	2x	32	5MC	C4-N3-C2	-2.60	117.18	120.69
1	1A	2515	2MA	C8-N7-C5	2.59	107.93	102.99
1	2A	2552	OMU	O2-C2-N1	-2.59	119.35	122.79
53	2x	8	4SU	C4-N3-C2	-2.58	124.84	127.34
32	2a	966	M2G	C2-N1-C6	-2.57	119.44	123.71
32	1a	966	M2G	C2-N1-C6	-2.57	119.44	123.71
32	1a	1407	5MC	C5-C6-N1	-2.56	120.70	123.34
1	1A	2564	OMU	C6-C5-C4	-2.52	116.07	119.52
1	2A	1911	PSU	O2-C2-N1	-2.52	120.01	122.79
1	1A	1937	5MU	C1'-N1-C6	-2.52	116.93	121.12
32	1a	967	5MC	C4-N3-C2	-2.52	117.29	120.69
43	1l	92	0TD	OD2-CG-OD1	-2.51	118.39	124.09
1	2A	1917	PSU	O2-C2-N1	-2.49	120.05	122.79
32	2a	1407	5MC	C4-N3-C2	-2.46	117.37	120.69
32	2a	516	PSU	C6-N1-C2	-2.43	120.19	122.68
53	2x	55	PSU	O2-C2-N1	-2.43	120.12	122.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
53	2x	32	5MC	N4-C4-N3	-2.40	114.10	118.48
1	2A	2251	OMG	O6-C6-C5	-2.37	119.74	124.37
1	1A	1939	PSU	O4-C4-N3	-2.37	115.57	120.12
1	1A	2617	PSU	O2-C2-N1	-2.37	120.18	122.79
32	1a	527	G7M	C2-N1-C6	-2.34	120.80	125.10
1	2A	2605	PSU	O2-C2-N1	-2.33	120.22	122.79
32	2a	966	M2G	O6-C6-C5	-2.33	119.82	124.37
53	1x	55	PSU	O2-C2-N1	-2.33	120.23	122.79
32	1a	516	PSU	C4-N3-C2	-2.32	122.99	126.34
32	2a	967	5MC	N4-C4-N3	-2.30	114.28	118.48
32	1a	1498	UR3	C6-N1-C2	-2.30	119.73	121.79
32	1a	1407	5MC	C4-N3-C2	-2.29	117.59	120.69
32	1a	1407	5MC	N4-C4-N3	-2.29	114.31	118.48
1	1A	2564	OMU	C2'-C1'-N1	-2.27	109.81	114.22
1	2A	1911	PSU	O4-C4-N3	-2.27	115.77	120.12
32	2a	516	PSU	C4-N3-C2	-2.26	123.08	126.34
1	2A	1920	OMC	O2-C2-N3	-2.25	118.67	122.33
1	1A	1933	PSU	N1-C2-N3	2.23	117.66	115.13
32	2a	966	M2G	N1-C2-N2	2.22	119.93	118.04
32	1a	1207	2MG	O3'-C3'-C2'	2.22	118.99	111.82
1	1A	2263	OMG	O6-C6-C5	-2.21	120.06	124.37
1	2A	1917	PSU	O4-C4-N3	-2.20	115.90	120.12
32	1a	1498	UR3	C1'-N1-C2	2.19	120.69	116.99
32	2a	516	PSU	O4'-C1'-C2'	2.18	108.22	105.14
1	2A	2503	2MA	CM2-C2-N1	2.18	121.08	116.23
53	1x	32	5MC	N4-C4-N3	-2.18	114.51	118.48
1	2A	1911	PSU	N1-C2-N3	2.17	117.59	115.13
32	1a	1207	2MG	CM2-N2-C2	-2.17	119.07	123.86
32	2a	1498	UR3	C1'-N1-C2	2.17	120.65	116.99
32	2a	1400	5MC	N4-C4-N3	-2.16	114.53	118.48
32	2a	1404	5MC	N4-C4-N3	-2.15	114.55	118.48
32	2a	1404	5MC	CM5-C5-C6	-2.15	119.98	122.85
32	2a	1407	5MC	N4-C4-N3	-2.14	114.57	118.48
32	1a	1404	5MC	N4-C4-N3	-2.14	114.57	118.48
1	1A	1961	5MU	C5-C6-N1	-2.14	121.14	123.34
1	1A	1933	PSU	O4-C4-N3	-2.14	116.02	120.12
32	2a	527	G7M	C2-N1-C6	-2.13	121.18	125.10
1	2A	1917	PSU	N1-C2-N3	2.12	117.53	115.13
32	2a	527	G7M	N2-C2-N1	2.11	121.20	116.71
1	1A	1964	5MC	N4-C4-N3	-2.10	114.64	118.48
32	1a	516	PSU	C6-N1-C2	-2.10	120.54	122.68
32	2a	516	PSU	O4-C4-N3	-2.08	116.12	120.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
53	2x	55	PSU	O4-C4-N3	-2.08	116.13	120.12
53	2x	55	PSU	C4-N3-C2	-2.08	123.34	126.34
1	1A	1942	OMC	O2-C2-N3	-2.07	118.96	122.33
32	1a	966	M2G	O6-C6-C5	-2.06	120.34	124.37
32	2a	527	G7M	N1-C2-N3	-2.06	119.46	123.32
53	2x	55	PSU	N1-C2-N3	2.06	117.46	115.13
1	2A	1915	5MU	C1'-N1-C2	2.05	121.29	117.57
1	2A	1962	5MC	N4-C4-N3	-2.05	114.74	118.48
32	1a	516	PSU	O2-C2-N1	-2.04	120.54	122.79
43	2l	92	0TD	OD2-CG-OD1	-2.04	119.45	124.09
1	2A	1942	5MC	N4-C4-N3	-2.04	114.76	118.48
1	1A	1939	PSU	O4-C4-C5	2.03	129.37	124.05
1	1A	1937	5MU	C5M-C5-C6	-2.03	120.13	122.85
1	1A	1939	PSU	N1-C2-N3	2.03	117.43	115.13
1	1A	1984	5MC	N4-C4-N3	-2.03	114.78	118.48
53	1x	55	PSU	C4-N3-C2	-2.02	123.42	126.34
32	1a	1404	5MC	CM5-C5-C6	-2.02	120.15	122.85
53	1x	32	5MC	CM5-C5-C6	-2.02	120.16	122.85
1	2A	1917	PSU	C4-N3-C2	-2.01	123.44	126.34
1	2A	1911	PSU	O4-C4-C5	2.01	129.32	124.05
32	1a	1407	5MC	CM5-C5-C6	-2.01	120.16	122.85

There are no chirality outliers.

All (54) 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	1937	5MU	O4'-C4'-C5'-O5'
1	1A	2263	OMG	C1'-C2'-O2'-CM2
32	1a	1402	4OC	O4'-C4'-C5'-O5'
32	1a	1402	4OC	C3'-C4'-C5'-O5'
32	1a	1519	MA6	O4'-C4'-C5'-O5'
53	1x	54	5MU	C3'-C4'-C5'-O5'
53	1x	54	5MU	O4'-C4'-C5'-O5'
1	2A	1915	5MU	O4'-C1'-N1-C2
1	2A	1915	5MU	O4'-C1'-N1-C6
1	2A	1962	5MC	O4'-C4'-C5'-O5'
32	2a	1402	4OC	O4'-C4'-C5'-O5'
32	2a	1402	4OC	C3'-C4'-C5'-O5'
32	2a	1519	MA6	O4'-C4'-C5'-O5'
1	1A	1937	5MU	C3'-C4'-C5'-O5'

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Mol	Chain	Res	Type	Atoms
32	1a	1519	MA6	C3'-C4'-C5'-O5'
1	2A	1962	5MC	C3'-C4'-C5'-O5'
1	2A	2503	2MA	O4'-C4'-C5'-O5'
32	2a	527	G7M	C3'-C4'-C5'-O5'
32	2a	1519	MA6	C3'-C4'-C5'-O5'
32	1a	1400	5MC	O4'-C4'-C5'-O5'
32	1a	527	G7M	C3'-C4'-C5'-O5'
32	1a	1400	5MC	C3'-C4'-C5'-O5'
1	2A	2503	2MA	C3'-C4'-C5'-O5'
32	2a	527	G7M	O4'-C4'-C5'-O5'
32	1a	1519	MA6	C5-C6-N6-C9
32	2a	1519	MA6	C5-C6-N6-C10
1	1A	2515	2MA	O4'-C4'-C5'-O5'
32	1a	527	G7M	O4'-C4'-C5'-O5'
32	1a	1207	2MG	O4'-C4'-C5'-O5'
43	1l	92	0TD	CG-CB-SB-CSB
43	2l	92	0TD	CG-CB-SB-CSB
1	1A	1942	OMC	O4'-C4'-C5'-O5'
32	2a	1402	4OC	C3'-C2'-O2'-CM2
32	1a	1207	2MG	C3'-C4'-C5'-O5'
32	1a	527	G7M	C4'-C5'-O5'-P
1	2A	2503	2MA	C4'-C5'-O5'-P
1	1A	1942	OMC	C3'-C4'-C5'-O5'
32	2a	1519	MA6	C4'-C5'-O5'-P
1	1A	2564	OMU	C3'-C2'-O2'-CM2
32	2a	1402	4OC	C2'-C1'-N1-C6
32	1a	516	PSU	O4'-C4'-C5'-O5'
32	2a	1400	5MC	O4'-C4'-C5'-O5'
43	1l	92	0TD	SB-CB-CG-OD2
32	2a	1402	4OC	C2'-C1'-N1-C2
1	1A	2515	2MA	C3'-C4'-C5'-O5'
32	1a	967	5MC	O4'-C4'-C5'-O5'
1	1A	1942	OMC	C2'-C1'-N1-C2
32	2a	516	PSU	O4'-C4'-C5'-O5'
43	2l	92	0TD	SB-CB-CG-OD1
32	1a	1498	UR3	O4'-C4'-C5'-O5'
1	2A	1920	OMC	C2'-C1'-N1-C2
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 2322 ligands modelled in this entry, 2315 are monoatomic and 2 are unknown - leaving 5 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
59	ARG	1B	229	-	10,11,11	0.72	1 (10%)	11,13,13	1.15	2 (18%)
58	MPD	1A	3907	-	7,7,7	0.34	0	9,10,10	0.27	0
61	SF4	1d	501	35	0,12,12	-	-	-	-	-
58	MPD	1a	1860	-	7,7,7	0.38	0	9,10,10	0.35	0
61	SF4	2d	501	35	0,12,12	-	-	-	-	-

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
59	ARG	1B	229	-	-	2/11/11/11	-
58	MPD	1A	3907	-	-	0/5/5/5	-
61	SF4	1d	501	35	-	-	0/6/5/5
58	MPD	1a	1860	-	-	2/5/5/5	-
61	SF4	2d	501	35	-	-	0/6/5/5

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
59	1B	229	ARG	OXT-C	-2.03	1.23	1.30

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
59	1B	229	ARG	OXT-C-O	-2.91	117.49	124.09
59	1B	229	ARG	OXT-C-CA	2.31	121.25	113.38

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
58	1a	1860	MPD	C2-C3-C4-O4
59	1B	229	ARG	NE-CD-CG-CB
58	1a	1860	MPD	C1-C2-C3-C4
59	1B	229	ARG	CG-CD-NE-CZ

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](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	1A	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	1A	1151:U	O3'	1152:G	P	3.02

## 6 Fit of model and data i

### 6.1 Protein, DNA and RNA chains i

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	1A	2813/2915 (96%)	-0.11	76 (2%) 54 31	23, 42, 82, 95	0
1	2A	2858/2915 (98%)	-0.12	103 (3%) 42 22	40, 59, 86, 96	0
2	1B	120/120 (100%)	-0.51	0 100 100	38, 57, 63, 76	0
2	2B	120/120 (100%)	-0.19	0 100 100	62, 75, 81, 82	0
3	1D	275/275 (100%)	-0.27	0 100 100	30, 44, 54, 67	0
3	2D	275/275 (100%)	-0.19	2 (0%) 87 75	43, 55, 62, 69	0
4	1E	204/204 (100%)	-0.26	0 100 100	28, 47, 60, 69	0
4	2E	204/204 (100%)	-0.14	1 (0%) 91 81	43, 59, 67, 75	0
5	1F	203/203 (100%)	-0.29	0 100 100	26, 48, 66, 73	0
5	2F	203/203 (100%)	-0.19	0 100 100	44, 65, 72, 79	0
6	1G	181/181 (100%)	-0.39	2 (1%) 80 64	55, 64, 72, 80	0
6	2G	181/181 (100%)	0.23	3 (1%) 70 49	71, 75, 79, 85	0
7	1H	174/174 (100%)	-0.28	0 100 100	43, 54, 62, 65	0
7	2H	173/174 (99%)	0.63	22 (12%) 3 1	66, 75, 79, 85	0
8	1I	147/147 (100%)	-0.22	0 100 100	51, 67, 74, 76	0
8	2I	146/147 (99%)	0.15	2 (1%) 75 56	59, 75, 79, 82	0
9	1N	140/140 (100%)	-0.19	0 100 100	35, 45, 61, 67	0
9	2N	140/140 (100%)	0.01	2 (1%) 75 56	52, 63, 71, 78	0
10	1O	122/122 (100%)	-0.14	0 100 100	38, 47, 58, 62	0
10	2O	122/122 (100%)	-0.27	0 100 100	50, 57, 64, 69	0
11	1P	149/149 (100%)	-0.23	0 100 100	28, 50, 61, 73	0
11	2P	149/149 (100%)	0.07	2 (1%) 77 59	46, 67, 75, 78	0
12	1Q	141/141 (100%)	-0.21	0 100 100	36, 49, 56, 63	0
12	2Q	141/141 (100%)	-0.30	0 100 100	51, 64, 69, 75	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
13	1R	118/118 (100%)	-0.20	0 100 100	35, 42, 53, 65	0
13	2R	118/118 (100%)	-0.12	0 100 100	48, 56, 62, 69	0
14	1S	110/110 (100%)	-0.12	0 100 100	45, 53, 60, 64	0
14	2S	110/110 (100%)	0.45	5 (4%) 33 16	65, 71, 74, 76	0
15	1T	131/131 (100%)	-0.27	1 (0%) 86 72	42, 51, 67, 74	0
15	2T	131/131 (100%)	-0.20	0 100 100	55, 60, 70, 75	0
16	1U	116/116 (100%)	-0.28	0 100 100	30, 40, 52, 58	0
16	2U	116/116 (100%)	-0.16	0 100 100	50, 60, 69, 74	0
17	1V	101/101 (100%)	-0.23	0 100 100	27, 49, 59, 64	0
17	2V	101/101 (100%)	-0.04	0 100 100	48, 67, 73, 76	0
18	1W	112/112 (100%)	-0.29	0 100 100	31, 38, 54, 71	0
18	2W	112/112 (100%)	-0.07	0 100 100	46, 54, 64, 71	0
19	1X	95/95 (100%)	-0.11	0 100 100	34, 44, 60, 67	0
19	2X	95/95 (100%)	-0.01	0 100 100	53, 61, 68, 69	0
20	1Y	107/107 (100%)	-0.16	1 (0%) 84 69	46, 53, 65, 68	0
20	2Y	107/107 (100%)	0.71	9 (8%) 11 4	62, 68, 73, 83	0
21	1Z	203/203 (100%)	0.03	13 (6%) 19 8	50, 61, 72, 81	0
21	2Z	201/203 (99%)	0.43	16 (7%) 12 5	66, 73, 79, 82	0
22	10	77/77 (100%)	-0.20	1 (1%) 77 59	37, 45, 53, 57	0
22	20	77/77 (100%)	0.75	10 (12%) 3 1	57, 63, 68, 70	0
23	11	97/97 (100%)	0.04	2 (2%) 63 43	32, 48, 65, 71	0
23	21	97/97 (100%)	0.29	1 (1%) 82 67	47, 59, 70, 74	0
24	12	70/70 (100%)	-0.19	0 100 100	44, 52, 58, 71	0
24	22	70/70 (100%)	0.11	1 (1%) 75 56	61, 67, 72, 74	0
25	13	59/59 (100%)	-0.15	0 100 100	36, 45, 62, 70	0
25	23	59/59 (100%)	0.65	2 (3%) 45 24	57, 62, 69, 72	0
26	14	69/69 (100%)	0.29	5 (7%) 15 6	62, 73, 82, 84	0
26	24	69/69 (100%)	0.72	6 (8%) 10 4	75, 80, 84, 85	0
27	15	59/59 (100%)	-0.23	0 100 100	28, 45, 57, 63	0
27	25	59/59 (100%)	-0.25	1 (1%) 70 49	46, 57, 68, 73	0
28	16	53/53 (100%)	-0.21	0 100 100	45, 50, 58, 60	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
28	26	53/53 (100%)	0.35	1 (1%) 66 46	59, 63, 67, 72	0
29	17	48/48 (100%)	0.01	2 (4%) 36 18	30, 33, 52, 56	0
29	27	48/48 (100%)	0.14	2 (4%) 36 18	43, 48, 61, 69	0
30	18	64/64 (100%)	-0.09	0 100 100	35, 41, 46, 48	0
30	28	64/64 (100%)	0.13	0 100 100	52, 57, 62, 64	0
31	19	37/37 (100%)	0.31	2 (5%) 25 12	40, 48, 58, 62	0
31	29	37/37 (100%)	0.59	2 (5%) 25 12	62, 66, 70, 71	0
32	1a	1488/1521 (97%)	-0.11	34 (2%) 60 39	45, 72, 87, 97	0
32	2a	1492/1521 (98%)	-0.10	40 (2%) 54 31	52, 73, 88, 95	0
33	1b	231/231 (100%)	0.10	10 (4%) 35 17	69, 75, 81, 84	0
33	2b	231/231 (100%)	0.27	9 (3%) 39 20	72, 77, 82, 84	0
34	1c	206/206 (100%)	0.39	10 (4%) 29 14	70, 76, 79, 81	0
34	2c	206/206 (100%)	0.32	13 (6%) 20 8	73, 78, 81, 84	0
35	1d	208/208 (100%)	0.12	4 (1%) 66 46	65, 74, 78, 81	0
35	2d	208/208 (100%)	0.02	0 100 100	64, 70, 75, 78	0
36	1e	148/148 (100%)	-0.02	1 (0%) 87 75	61, 68, 73, 82	0
36	2e	148/148 (100%)	0.01	1 (0%) 87 75	65, 71, 76, 83	0
37	1f	100/100 (100%)	-0.17	1 (1%) 82 67	63, 70, 73, 76	0
37	2f	100/100 (100%)	-0.26	1 (1%) 82 67	67, 71, 75, 77	0
38	1g	155/155 (100%)	0.23	9 (5%) 23 10	67, 72, 80, 85	0
38	2g	155/155 (100%)	0.57	18 (11%) 4 2	74, 77, 80, 86	0
39	1h	137/137 (100%)	-0.02	1 (0%) 87 75	64, 68, 72, 76	0
39	2h	137/137 (100%)	0.20	4 (2%) 51 28	67, 71, 74, 75	0
40	1i	127/127 (100%)	0.76	13 (10%) 6 2	69, 78, 81, 83	0
40	2i	126/127 (99%)	1.27	27 (21%) 0 0	72, 80, 83, 85	0
41	1j	97/97 (100%)	1.13	16 (16%) 1 1	71, 78, 80, 83	0
41	2j	96/97 (98%)	1.12	22 (22%) 0 0	74, 80, 83, 85	0
42	1k	114/114 (100%)	-0.23	0 100 100	56, 68, 72, 74	0
42	2k	114/114 (100%)	-0.04	2 (1%) 68 47	63, 72, 75, 79	0
43	1l	121/122 (99%)	0.22	3 (2%) 57 34	58, 66, 70, 74	0
43	2l	121/122 (99%)	0.06	2 (1%) 70 49	60, 65, 70, 74	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
44	1m	116/116 (100%)	0.33	6 (5%) 27 12	64, 74, 78, 80	0
44	2m	114/116 (98%)	0.66	14 (12%) 4 1	73, 79, 82, 82	0
45	1n	60/60 (100%)	0.37	3 (5%) 28 13	71, 74, 77, 79	0
45	2n	60/60 (100%)	1.03	14 (23%) 0 0	74, 78, 81, 82	0
46	1o	88/88 (100%)	-0.05	1 (1%) 80 64	57, 66, 73, 76	0
46	2o	88/88 (100%)	0.10	1 (1%) 80 64	63, 69, 74, 76	0
47	1p	82/82 (100%)	0.70	7 (8%) 10 4	67, 73, 77, 79	0
47	2p	82/82 (100%)	0.26	2 (2%) 59 37	63, 69, 74, 76	0
48	1q	99/99 (100%)	0.08	0 100 100	62, 66, 72, 73	0
48	2q	99/99 (100%)	0.22	1 (1%) 82 67	63, 69, 73, 75	0
49	1r	68/68 (100%)	0.20	1 (1%) 73 54	64, 69, 75, 77	0
49	2r	68/68 (100%)	0.35	2 (2%) 51 28	68, 71, 76, 77	0
50	1s	83/83 (100%)	0.88	11 (13%) 3 1	70, 76, 79, 81	0
50	2s	83/83 (100%)	1.40	20 (24%) 0 0	71, 80, 82, 83	0
51	1t	96/98 (97%)	0.38	3 (3%) 49 26	65, 70, 75, 78	0
51	2t	98/98 (100%)	0.27	2 (2%) 65 44	62, 68, 75, 75	0
52	1u	23/23 (100%)	0.87	2 (8%) 10 4	70, 73, 76, 77	0
52	2u	23/23 (100%)	1.66	11 (47%) 0 0	76, 77, 79, 80	0
53	1x	72/76 (94%)	-0.18	0 100 100	41, 66, 76, 80	0
53	2x	72/76 (94%)	0.11	1 (1%) 75 56	56, 73, 81, 90	0
54	1y	12/19 (63%)	0.39	0 100 100	37, 48, 57, 59	0
54	2y	12/19 (63%)	1.01	3 (25%) 0 0	52, 59, 62, 69	0
55	A	3/27 (11%)	2.13	1 (33%) 0 0	70, 70, 71, 74	0
55	B	3/27 (11%)	0.59	1 (33%) 0 0	64, 64, 65, 69	0
All	All	20701/21004 (98%)	0.01	646 (3%) 49 26	23, 65, 82, 97	0

All (646) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
21	1Z	192	ALA	8.1
21	1Z	198	LYS	8.0
21	1Z	200	GLY	8.0
21	1Z	193	GLU	8.0
32	2a	1030(B)	C	7.4

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
21	1Z	203	GLU	7.4
32	2a	1030(A)	G	6.9
21	2Z	193	GLU	6.8
1	2A	2125	G	6.7
21	1Z	197	ILE	6.5
38	1g	156	TRP	6.2
32	1a	1036	G	6.2
41	1j	98	ILE	6.1
22	20	8	GLY	6.0
40	2i	6	GLY	5.8
32	2a	1036	G	5.8
1	2A	2173	A	5.7
21	2Z	191	VAL	5.7
21	2Z	200	GLY	5.6
44	2m	7	VAL	5.6
1	2A	2148	G	5.5
32	1a	1034	G	5.5
23	2l	2	SER	5.4
1	2A	2162	G	5.4
22	10	8	GLY	5.4
41	1j	10	GLY	5.3
21	1Z	194	PRO	5.3
40	2i	7	THR	5.3
41	1j	35	SER	5.2
38	2g	156	TRP	5.1
1	2A	2146	C	5.1
21	1Z	196	VAL	5.1
21	2Z	194	PRO	5.1
1	2A	2147	G	5.1
32	2a	1034	G	5.0
1	2A	2110	G	4.9
32	2a	1026	G	4.9
34	1c	206	GLU	4.9
50	1s	39	THR	4.9
1	1A	2145	G	4.9
55	A	113	G	4.8
21	1Z	202	GLU	4.8
21	1Z	201	LYS	4.8
1	1A	1555	C	4.8
1	2A	2109	U	4.7
50	2s	31	ILE	4.7
50	1s	4	SER	4.7

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Mol	Chain	Res	Type	RSRZ
26	24	68	ARG	4.6
1	2A	2124	G	4.6
1	1A	2154	U	4.5
1	2A	2174	C	4.5
1	2A	2802	G	4.5
32	1a	1030(B)	C	4.5
1	2A	2133	G	4.5
21	2Z	196	VAL	4.5
6	2G	2	PRO	4.5
21	2Z	197	ILE	4.5
21	1Z	195	GLU	4.4
21	2Z	198	LYS	4.4
38	2g	16	LEU	4.3
21	2Z	192	ALA	4.3
40	2i	62	TYR	4.3
40	1i	106	ALA	4.3
1	1A	2139	A	4.3
41	2j	6	ILE	4.3
1	2A	1082	U	4.3
32	1a	1037	C	4.3
28	26	54	ILE	4.3
40	2i	15	ALA	4.3
45	1n	2	ALA	4.3
32	1a	1035	A	4.2
1	1A	2165	C	4.2
21	1Z	199	LYS	4.2
1	1A	2169	G	4.2
1	2A	2154	G	4.2
1	2A	229	A	4.2
1	2A	1085	A	4.2
1	2A	2169	A	4.2
1	2A	2897	U	4.2
1	2A	2143	C	4.1
32	1a	1286	A	4.1
32	2a	1030	C	4.1
40	2i	5	TYR	4.1
1	1A	2183	C	4.1
7	2H	112	PRO	4.1
29	17	48	LYS	4.1
52	2u	11	GLY	4.1
1	2A	2134	A	4.0
32	2a	1030(C)	G	4.0

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
41	1j	72	VAL	4.0
22	20	9	SER	4.0
1	1A	2166	U	4.0
1	2A	2159	G	4.0
1	1A	2163	G	4.0
31	29	37	GLY	4.0
45	2n	39	LEU	4.0
32	2a	1035	A	4.0
1	2A	2139	C	3.9
21	2Z	195	GLU	3.9
45	2n	2	ALA	3.9
26	24	69	LYS	3.9
33	1b	130	ARG	3.9
32	1a	1001	A	3.9
32	1a	1026	G	3.9
32	1a	1030(C)	G	3.9
44	2m	92	HIS	3.9
1	2A	2801(A)	A	3.9
1	2A	2176	A	3.8
1	2A	2803	C	3.8
1	2A	2896	C	3.8
32	2a	1027	C	3.8
1	1A	2180	A	3.8
1	2A	2108	C	3.8
1	2A	2155	G	3.8
7	2H	105	LEU	3.8
1	2A	1067	A	3.8
51	1t	18	GLN	3.8
1	1A	2175	G	3.8
41	1j	97	GLU	3.7
1	2A	2144	U	3.7
20	1Y	1	MET	3.7
32	1a	202	U	3.7
32	1a	1030	C	3.7
1	2A	1509	C	3.7
38	2g	82	GLY	3.7
38	2g	154	TYR	3.7
32	1a	1028	C	3.7
1	2A	2123	G	3.7
43	1l	28	LYS	3.7
7	2H	113	VAL	3.7
1	1A	2138	G	3.7

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Mol	Chain	Res	Type	RSRZ
1	2A	652(F)	G	3.6
1	2A	2127	G	3.6
32	2a	1001(A)	G	3.6
1	2A	2179	C	3.6
41	1j	8	LEU	3.6
1	1A	2164	C	3.6
1	2A	1076	C	3.6
21	2Z	201	LYS	3.6
40	2i	33	PHE	3.6
23	11	2	SER	3.6
41	2j	85	LEU	3.6
1	2A	652(B)	A	3.6
40	2i	26	VAL	3.6
50	2s	49	ILE	3.6
1	1A	2187	G	3.6
1	2A	2132	U	3.6
32	1a	1533	C	3.6
20	2Y	60	PHE	3.6
1	2A	2153	G	3.5
1	2A	1046	A	3.5
20	2Y	1	MET	3.5
1	1A	2182	G	3.5
50	1s	40	ILE	3.5
33	2b	101	MET	3.5
47	1p	35	LYS	3.5
20	2Y	5	MET	3.5
1	2A	1083	U	3.5
32	1a	1000	U	3.5
41	1j	5	ARG	3.4
43	1l	64	TYR	3.4
1	1A	2173	G	3.4
1	1A	2181	G	3.4
40	2i	8	GLY	3.4
45	2n	34	TYR	3.4
50	2s	4	SER	3.4
1	1A	1221	G	3.4
52	2u	5	ASP	3.4
1	2A	2130	U	3.4
45	1n	17	LYS	3.4
32	2a	1286	A	3.4
1	2A	2128	C	3.4
26	14	64	GLY	3.3

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	2A	2178	C	3.3
32	1a	1030(A)	G	3.3
34	1c	192	THR	3.3
38	2g	17	VAL	3.3
1	2A	2137	C	3.3
32	1a	1027	C	3.3
47	2p	19	ILE	3.3
34	2c	155	GLY	3.3
1	2A	1087	G	3.3
1	2A	2152	G	3.3
1	1A	2906	U	3.3
1	2A	2120	G	3.3
43	1l	62	SER	3.3
41	2j	10	GLY	3.3
1	2A	2138	C	3.3
1	2A	2118	U	3.3
1	2A	2160	G	3.3
32	1a	1002	G	3.3
52	2u	6	ARG	3.3
32	1a	344	A	3.3
45	2n	25	VAL	3.3
44	2m	75	ALA	3.3
50	1s	50	ALA	3.3
1	1A	2129	C	3.3
1	1A	2193	A	3.3
1	2A	2126	A	3.3
1	2A	2172	U	3.3
1	1A	2195	A	3.2
7	2H	103	LEU	3.2
50	2s	30	LEU	3.2
1	2A	2131	G	3.2
1	2A	1103	A	3.2
40	2i	18	PHE	3.2
50	1s	56	GLN	3.2
38	1g	79	ARG	3.2
50	2s	79	THR	3.2
22	20	76	GLY	3.2
1	2A	1064	C	3.2
1	1A	2189	U	3.2
52	1u	18	TYR	3.2
1	2A	887	A	3.2
32	1a	1257	U	3.2

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Mol	Chain	Res	Type	RSRZ
41	2j	74	ILE	3.2
50	2s	71	LEU	3.2
6	1G	2	PRO	3.1
40	2i	127	LYS	3.1
7	2H	159	GLU	3.1
40	2i	79	LEU	3.1
32	2a	1001	A	3.1
1	1A	2186	C	3.1
32	2a	1257	U	3.1
1	2A	1095	A	3.1
41	2j	72	VAL	3.1
1	2A	2175	C	3.1
1	1A	2188	G	3.1
32	2a	1531	A	3.1
34	2c	189	ALA	3.1
21	1Z	191	VAL	3.1
44	2m	6	GLY	3.1
7	2H	114	VAL	3.1
1	2A	2161	C	3.1
1	1A	2134	G	3.1
1	2A	1026	U	3.1
41	2j	65	LEU	3.1
50	2s	16	LEU	3.1
34	2c	190	ARG	3.1
36	1e	118	ILE	3.0
44	2m	95	GLY	3.0
1	1A	2152	U	3.0
38	2g	80	VAL	3.0
1	1A	2816	G	3.0
7	2H	111	HIS	3.0
51	1t	9	ASN	3.0
26	14	66	SER	3.0
40	1i	75	ASP	3.0
1	1A	2190	G	3.0
1	2A	2121	G	3.0
35	1d	3	ARG	3.0
44	1m	87	TYR	3.0
44	2m	4	ILE	3.0
38	1g	16	LEU	3.0
1	1A	2137	G	3.0
1	2A	2168	G	3.0
1	2A	2164	C	3.0

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
32	1a	1001(A)	G	3.0
32	2a	1002	G	3.0
26	24	46	GLN	3.0
32	2a	1028	C	3.0
34	1c	193	TYR	2.9
50	2s	35	SER	2.9
33	1b	131	PRO	2.9
6	2G	34	LEU	2.9
40	2i	36	TYR	2.9
32	2a	1042	G	2.9
1	2A	1104	C	2.9
33	2b	70	PHE	2.9
22	20	77	ARG	2.9
38	1g	78	ARG	2.9
1	2A	2165	G	2.9
32	2a	80	G	2.9
41	1j	75	ILE	2.9
41	2j	41	PRO	2.9
50	2s	3	ARG	2.9
32	1a	1029	C	2.9
50	2s	32	LYS	2.9
7	2H	115	VAL	2.9
14	2S	5	THR	2.9
1	1A	2194	U	2.9
22	20	45	PHE	2.9
1	1A	935	C	2.9
45	2n	35	ARG	2.9
40	2i	78	LYS	2.9
7	2H	94	TYR	2.9
26	24	67	TYR	2.9
37	1f	55	ASP	2.9
41	2j	73	ASP	2.8
40	1i	47	LEU	2.8
41	2j	63	PHE	2.8
1	2A	888	C	2.8
22	20	72	ARG	2.8
38	1g	153	HIS	2.8
43	2l	64	TYR	2.8
1	2A	2145	C	2.8
40	1i	33	PHE	2.8
33	1b	123	ALA	2.8
1	2A	2111	C	2.8

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
7	2H	102	ALA	2.8
32	1a	1038	C	2.8
32	1a	204	U	2.8
1	2A	2129	C	2.8
40	2i	21	PRO	2.8
1	2A	2157	G	2.8
45	2n	8	GLU	2.8
7	2H	169	VAL	2.8
1	1A	2128	G	2.8
1	1A	2149	G	2.8
1	1A	2153	G	2.8
38	2g	34	GLY	2.8
22	20	71	ASP	2.7
34	2c	206	GLU	2.7
1	2A	2151	G	2.7
1	1A	2156	A	2.7
34	2c	164	ARG	2.7
26	14	52	THR	2.7
50	1s	19	VAL	2.7
41	2j	62	HIS	2.7
50	2s	2	PRO	2.7
50	2s	47	HIS	2.7
1	1A	2126	G	2.7
1	2A	2107	C	2.7
14	2S	111	GLU	2.7
38	2g	78	ARG	2.7
44	2m	111	LYS	2.7
29	27	48	LYS	2.7
40	1i	15	ALA	2.7
47	1p	37	GLY	2.7
32	2a	1030(D)	A	2.7
32	1a	723	U	2.7
32	2a	1031	G	2.7
47	1p	17	TYR	2.6
34	2c	159	GLY	2.6
1	2A	2136	C	2.6
40	1i	46	ALA	2.6
33	1b	133	LYS	2.6
34	1c	170	GLN	2.6
1	1A	2141	A	2.6
52	2u	10	ARG	2.6
32	2a	1037	C	2.6

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
34	2c	147	LYS	2.6
38	2g	85	TYR	2.6
1	2A	2158	A	2.6
1	2A	2140	C	2.6
26	14	68	ARG	2.6
40	2i	66	ARG	2.6
44	2m	94	ARG	2.6
7	2H	29	PRO	2.6
32	2a	90	U	2.6
45	2n	15	LYS	2.6
1	1A	2815	C	2.6
50	1s	48	THR	2.6
11	2P	109	GLY	2.6
33	1b	201	ILE	2.6
9	2N	10	GLU	2.6
40	1i	26	VAL	2.6
7	2H	30	LYS	2.6
45	1n	15	LYS	2.6
34	1c	160	ALA	2.6
31	29	16	VAL	2.6
45	2n	38	GLY	2.6
14	2S	58	LEU	2.6
41	1j	73	ASP	2.6
1	1A	2814	C	2.6
41	1j	71	LEU	2.6
41	2j	87	THR	2.6
50	1s	30	LEU	2.6
32	2a	1041	A	2.6
1	2A	2142	C	2.6
33	2b	161	ALA	2.5
1	2A	2119	A	2.5
1	1A	1099	C	2.5
1	1A	2177	G	2.5
32	2a	1032	G	2.5
41	2j	29	ARG	2.5
52	2u	15	ARG	2.5
33	1b	232	PRO	2.5
7	2H	116	GLU	2.5
32	1a	1003	G	2.5
32	1a	1031	G	2.5
33	1b	122	PHE	2.5
32	2a	1533	C	2.5

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
38	2g	153	HIS	2.5
1	1A	2155	G	2.5
20	2Y	91	GLU	2.5
25	23	59	VAL	2.5
34	1c	201	TYR	2.5
33	1b	129	GLU	2.5
1	2A	1044	G	2.5
32	2a	1023	G	2.5
50	2s	8	GLY	2.5
35	1d	135	LEU	2.5
38	1g	154	TYR	2.5
1	2A	6	A	2.5
54	2y	10	PRO	2.5
1	2A	2150	U	2.5
41	2j	100	THR	2.5
52	2u	22	ARG	2.5
34	1c	200	ALA	2.5
41	1j	34	VAL	2.5
53	2x	47	U	2.5
1	1A	2142	G	2.5
1	1A	2184	G	2.5
1	1A	2130	C	2.4
1	1A	2185	C	2.4
1	2A	2793	G	2.4
1	2A	2894	G	2.4
40	2i	92	TYR	2.4
39	2h	99	GLU	2.4
41	1j	6	ILE	2.4
51	2t	56	MET	2.4
40	2i	88	TYR	2.4
32	1a	999	C	2.4
29	27	22	MET	2.4
41	2j	98	ILE	2.4
4	2E	1	MET	2.4
32	2a	1006	C	2.4
1	1A	2147	G	2.4
40	1i	62	TYR	2.4
35	1d	168	ARG	2.4
41	2j	71	LEU	2.4
20	2Y	59	GLY	2.4
1	1A	2905	C	2.4
32	1a	1531	A	2.4

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
38	2g	7	ALA	2.4
34	1c	101	LEU	2.4
1	1A	2140	U	2.4
32	1a	1212	U	2.4
7	2H	101	ARG	2.4
33	1b	135	GLN	2.4
33	2b	187	LEU	2.4
32	2a	1117	G	2.4
41	2j	5	ARG	2.4
1	1A	2151	C	2.4
32	1a	345	C	2.4
39	2h	112	LEU	2.4
44	1m	42	ALA	2.4
41	1j	4	ILE	2.4
50	2s	6	LYS	2.4
27	25	60	VAL	2.4
1	1A	2161	C	2.4
25	23	60	GLU	2.4
1	1A	2198	A	2.4
1	2A	1066	U	2.4
1	2A	2805	G	2.4
40	2i	9	ARG	2.4
21	2Z	188	ALA	2.4
21	2Z	199	LYS	2.4
52	2u	14	TRP	2.3
7	2H	48	GLY	2.3
41	2j	26	ALA	2.3
1	1A	696	C	2.3
29	17	47	ARG	2.3
32	2a	91	C	2.3
46	2o	86	GLY	2.3
1	2A	2319	G	2.3
47	1p	9	PHE	2.3
50	2s	82	GLY	2.3
37	2f	89	MET	2.3
38	2g	33	ASP	2.3
1	1A	2136	A	2.3
1	2A	2122	U	2.3
32	2a	1532	U	2.3
45	2n	4	LYS	2.3
44	2m	110	ARG	2.3
3	2D	153	ALA	2.3

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
35	1d	4	TYR	2.3
41	2j	27	ALA	2.3
22	20	70	GLN	2.3
41	2j	8	LEU	2.3
1	1A	2170	G	2.3
1	1A	2178	G	2.3
1	2A	2167	U	2.3
36	2e	25	ARG	2.3
46	1o	6	GLU	2.3
41	1j	7	LYS	2.3
11	2P	110	TYR	2.3
31	19	28	GLU	2.3
50	2s	63	THR	2.3
1	2A	652(T)	C	2.3
1	2A	1079	C	2.3
20	2Y	57	GLN	2.3
42	2k	13	GLN	2.3
7	2H	106	THR	2.3
38	1g	141	VAL	2.3
40	2i	16	ARG	2.3
51	1t	21	LYS	2.3
54	2y	12	PRO	2.3
1	1A	2200	C	2.3
32	2a	204	U	2.3
40	2i	64	THR	2.3
49	2r	58	LEU	2.3
40	2i	83	ARG	2.3
54	2y	11	ARG	2.3
7	2H	37	VAL	2.3
1	2A	2804	C	2.3
50	1s	59	PRO	2.3
31	19	13	LYS	2.3
33	1b	214	ILE	2.3
8	2I	92	VAL	2.3
1	1A	2176	G	2.2
34	2c	89	GLU	2.2
52	2u	24	ARG	2.2
1	1A	2807	C	2.2
1	2A	34	C	2.2
39	2h	101	PRO	2.2
45	2n	17	LYS	2.2
1	2A	2171	A	2.2

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	1A	2174	G	2.2
24	22	1	MET	2.2
40	1i	19	LEU	2.2
41	1j	100	THR	2.2
50	2s	13	ASP	2.2
52	2u	13	ILE	2.2
1	1A	2150	C	2.2
47	1p	38	TYR	2.2
21	2Z	96	VAL	2.2
1	1A	2806	G	2.2
1	2A	2156	G	2.2
40	1i	105	ASP	2.2
40	2i	61	ALA	2.2
40	2i	123	PRO	2.2
44	1m	48	LEU	2.2
45	2n	49	HIS	2.2
1	2A	2141	G	2.2
1	1A	933	C	2.2
1	2A	2177	C	2.2
44	1m	32	GLU	2.2
6	2G	3	LEU	2.2
40	1i	78	LYS	2.2
40	2i	126	SER	2.2
1	1A	2160	C	2.2
1	1A	2179	G	2.2
38	2g	4	ARG	2.2
32	2a	1248	A	2.2
32	2a	89	C	2.2
32	2a	1029	C	2.2
34	2c	162	GLN	2.2
50	2s	48	THR	2.2
55	B	116	G	2.2
1	1A	2148	A	2.2
15	1T	126	ALA	2.2
22	20	78	TYR	2.2
7	2H	41	MET	2.2
32	1a	1039	C	2.2
1	2A	1081	U	2.2
38	1g	77	SER	2.2
1	2A	1086	A	2.2
1	1A	2162	C	2.2
50	2s	68	GLY	2.2

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
22	20	75	LEU	2.2
44	2m	5	ALA	2.2
9	2N	8	GLN	2.2
47	1p	80	PHE	2.2
48	2q	60	ILE	2.2
1	2A	2170	A	2.2
34	2c	179	ARG	2.2
1	1A	2131	U	2.1
1	2A	2180	U	2.1
41	2j	78	ASN	2.1
21	2Z	7	ALA	2.1
33	2b	163	PHE	2.1
7	2H	95	ARG	2.1
41	2j	61	GLU	2.1
44	2m	56	LEU	2.1
34	1c	100	ALA	2.1
38	2g	83	ALA	2.1
33	2b	114	ARG	2.1
45	2n	7	ILE	2.1
50	1s	49	ILE	2.1
21	2Z	12	GLY	2.1
34	2c	80	GLY	2.1
44	2m	97	PRO	2.1
40	1i	120	ARG	2.1
44	1m	30	ALA	2.1
45	2n	11	LYS	2.1
52	1u	22	ARG	2.1
44	2m	60	VAL	2.1
1	2A	2892	A	2.1
26	14	65	ASP	2.1
34	2c	131	ARG	2.1
38	1g	85	TYR	2.1
7	2H	45	VAL	2.1
39	2h	120	THR	2.1
41	1j	38	ILE	2.1
14	2S	26	LEU	2.1
26	24	45	GLY	2.1
32	2a	1044	A	2.1
1	1A	2144	U	2.1
44	1m	35	GLU	2.1
51	2t	41	ILE	2.1
40	2i	4	TYR	2.1

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
52	2u	18	TYR	2.1
1	1A	2168	C	2.1
44	2m	64	TRP	2.1
52	2u	17	THR	2.1
32	1a	1032	G	2.1
32	2a	1024	G	2.1
20	2Y	88	LYS	2.1
33	2b	165	VAL	2.1
45	2n	60	SER	2.1
39	1h	4	ASP	2.1
33	2b	95	GLN	2.1
26	24	63	TYR	2.1
8	2l	3	VAL	2.1
20	2Y	42	VAL	2.1
3	2D	38	LYS	2.1
32	1a	1532	U	2.1
38	2g	76	ARG	2.1
42	2k	75	TYR	2.1
40	2i	17	VAL	2.1
38	2g	81	GLY	2.1
1	1A	2167	C	2.1
1	2A	652(S)	C	2.1
32	2a	1270	C	2.1
33	2b	105	PHE	2.0
40	2i	105	ASP	2.1
50	2s	9	VAL	2.0
1	2A	2135	A	2.0
47	1p	57	ARG	2.0
50	1s	38	SER	2.0
47	2p	59	TRP	2.0
32	2a	1043	C	2.0
32	1a	1024	G	2.0
1	1A	2157	A	2.0
7	2H	107	VAL	2.0
1	1A	2201	C	2.0
21	2Z	187	ALA	2.0
34	1c	189	ALA	2.0
34	2c	160	ALA	2.0
38	2g	141	VAL	2.0
6	1G	75	LYS	2.0
14	2S	35	ILE	2.0
32	2a	723	U	2.0

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Mol	Chain	Res	Type	RSRZ
32	2a	1131	G	2.0
1	1A	697	C	2.0
43	2l	32	PHE	2.0
41	2j	67	THR	2.0
1	1A	2146	G	2.0
40	1i	101	PHE	2.0
49	2r	62	GLU	2.0
20	2Y	90	LEU	2.0
23	11	98	LEU	2.0
38	2g	12	LEU	2.0
49	1r	78	LEU	2.0

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

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
53	PSU	2x	55	20/21	0.85	0.18	74,74,76,76	0
32	PSU	1a	516	20/21	0.86	0.17	69,72,73,73	0
32	PSU	2a	516	20/21	0.88	0.17	73,74,78,78	0
43	0TD	1l	92	10/11	0.90	0.26	66,66,67,69	0
1	5MU	1A	1937	21/22	0.91	0.21	69,72,80,81	0
53	5MC	1x	32	21/22	0.92	0.20	65,66,69,69	0
1	5MU	2A	1915	21/22	0.92	0.18	78,80,84,87	0
32	2MG	1a	1207	24/25	0.92	0.13	72,75,78,79	0
32	G7M	2a	527	24/25	0.92	0.20	69,70,71,72	0
43	0TD	2l	92	10/11	0.92	0.18	65,65,66,67	0
53	4SU	2x	8	20/21	0.92	0.16	72,75,76,77	0
1	PSU	1A	1939	20/21	0.92	0.15	62,65,68,69	0
32	2MG	2a	1207	24/25	0.93	0.20	75,77,78,79	0
32	4OC	2a	1402	22/23	0.93	0.20	64,66,67,69	0
1	2MA	2A	2503	23/24	0.93	0.26	41,43,46,48	0
53	PSU	1x	55	20/21	0.93	0.16	66,67,69,69	0
53	5MU	2x	54	21/22	0.93	0.17	73,74,76,77	0
53	4SU	1x	8	20/21	0.93	0.14	66,68,68,69	0
32	5MC	2a	1407	21/22	0.94	0.19	58,63,64,65	0
1	OMU	1A	2564	21/22	0.94	0.20	35,37,38,39	0
32	M2G	2a	966	25/26	0.94	0.21	68,70,72,73	0
53	5MC	2x	32	21/22	0.94	0.16	70,71,72,73	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
32	5MC	1a	1400	21/22	0.94	0.19	62,64,65,65	0
32	M2G	1a	966	25/26	0.94	0.20	66,67,69,70	0
32	5MC	2a	967	21/22	0.95	0.16	70,71,74,77	0
32	5MC	1a	967	21/22	0.95	0.17	67,68,69,70	0
32	5MC	2a	1400	21/22	0.95	0.21	67,69,71,71	0
1	PSU	2A	1917	20/21	0.95	0.10	67,70,73,74	0
32	5MC	1a	1407	21/22	0.95	0.18	52,56,59,60	0
1	PSU	2A	2605	20/21	0.96	0.19	42,45,45,45	0
32	MA6	1a	1518	24/25	0.96	0.21	53,54,56,57	0
32	MA6	1a	1519	24/25	0.96	0.22	51,55,55,56	0
1	5MC	1A	1984	21/22	0.96	0.16	42,43,46,49	0
1	PSU	1A	1933	20/21	0.96	0.14	58,61,63,64	0
1	PSU	1A	2617	20/21	0.96	0.23	36,37,38,39	0
53	5MU	1x	54	21/22	0.96	0.16	67,69,72,75	0
1	OMC	1A	1942	21/22	0.96	0.20	54,57,58,59	0
32	5MC	2a	1404	21/22	0.96	0.16	59,60,62,62	0
1	PSU	2A	1911	20/21	0.96	0.09	67,68,69,69	0
32	UR3	2a	1498	21/22	0.96	0.16	60,61,63,64	0
32	MA6	2a	1518	24/25	0.96	0.18	60,61,62,62	0
32	MA6	2a	1519	24/25	0.96	0.19	58,59,60,60	0
32	4OC	1a	1402	22/23	0.96	0.22	60,61,62,62	0
32	5MC	1a	1404	21/22	0.96	0.17	57,59,61,61	0
1	OMC	2A	1920	21/22	0.96	0.18	62,64,66,66	0
1	5MU	2A	1939	21/22	0.96	0.18	46,49,50,50	0
32	G7M	1a	527	24/25	0.96	0.16	66,67,68,68	0
1	OMG	2A	2251	24/25	0.97	0.20	45,46,50,51	0
1	2MA	1A	2515	23/24	0.97	0.21	24,26,28,30	0
1	OMU	2A	2552	21/22	0.97	0.15	45,46,48,48	0
1	5MC	1A	1964	21/22	0.97	0.12	40,43,44,45	0
1	5MU	1A	1961	21/22	0.97	0.21	37,39,40,40	0
32	UR3	1a	1498	21/22	0.97	0.16	56,57,60,61	0
1	5MC	2A	1942	21/22	0.97	0.15	55,56,57,57	0
1	5MC	2A	1962	21/22	0.98	0.15	53,54,57,58	0
1	OMG	1A	2263	24/25	0.98	0.18	31,33,36,36	0

### 6.3 Carbohydrates [\(i\)](#)

There are no monosaccharides in this entry.

## 6.4 Ligands i

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
56	MG	2A	3475	1/1	0.22	0.27	48,48,48,48	0
56	MG	2A	3437	1/1	0.25	0.53	62,62,62,62	0
56	MG	1d	505	1/1	0.35	0.16	77,77,77,77	0
56	MG	2A	3650	1/1	0.36	0.19	70,70,70,70	0
56	MG	1B	215	1/1	0.40	0.63	71,71,71,71	0
56	MG	1a	1786	1/1	0.41	0.40	65,65,65,65	0
56	MG	2a	1724	1/1	0.43	0.13	74,74,74,74	0
56	MG	1a	1761	1/1	0.44	0.37	68,68,68,68	0
56	MG	1A	3658	1/1	0.49	0.38	50,50,50,50	0
56	MG	1A	3123	1/1	0.51	0.44	41,41,41,41	0
56	MG	1A	3791	1/1	0.52	0.12	60,60,60,60	0
56	MG	2a	1668	1/1	0.53	0.60	60,60,60,60	0
56	MG	2A	3349	1/1	0.53	0.20	55,55,55,55	0
56	MG	1a	1764	1/1	0.54	0.13	70,70,70,70	0
56	MG	1a	1773	1/1	0.55	0.62	82,82,82,82	0
56	MG	2A	3183	1/1	0.55	0.52	54,54,54,54	0
56	MG	2A	3078	1/1	0.56	0.19	67,67,67,67	0
56	MG	2a	1606	1/1	0.56	0.66	59,59,59,59	0
56	MG	1D	309	1/1	0.56	0.94	42,42,42,42	0
56	MG	2A	3220	1/1	0.56	0.45	51,51,51,51	0
56	MG	2A	3311	1/1	0.57	0.20	45,45,45,45	0
56	MG	2D	302	1/1	0.57	1.20	48,48,48,48	0
56	MG	2A	3156	1/1	0.57	0.28	58,58,58,58	0
56	MG	1A	3175	1/1	0.57	0.19	57,57,57,57	0
56	MG	1A	3275	1/1	0.57	0.18	70,70,70,70	0
56	MG	2A	3379	1/1	0.60	0.14	55,55,55,55	0
56	MG	1a	1760	1/1	0.60	0.69	65,65,65,65	0
56	MG	1a	1706	1/1	0.60	0.62	66,66,66,66	0
56	MG	1a	1723	1/1	0.60	0.11	69,69,69,69	0
56	MG	2j	8001	1/1	0.60	0.17	79,79,79,79	0
56	MG	1A	3258	1/1	0.61	0.15	71,71,71,71	0
56	MG	1a	1823	1/1	0.61	0.83	54,54,54,54	0
56	MG	1a	1732	1/1	0.61	0.74	74,74,74,74	0
56	MG	2A	3410	1/1	0.61	0.41	63,63,63,63	0
56	MG	2A	3201	1/1	0.61	0.30	53,53,53,53	0
56	MG	1x	111	1/1	0.61	0.18	72,72,72,72	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	1A	3870	1/1	0.62	0.16	35,35,35,35	0
56	MG	1a	1624	1/1	0.62	0.49	51,51,51,51	0
56	MG	2A	3097	1/1	0.62	0.39	62,62,62,62	0
56	MG	2a	1608	1/1	0.62	1.49	69,69,69,69	0
56	MG	2A	3299	1/1	0.62	0.92	66,66,66,66	0
56	MG	1A	3639	1/1	0.62	0.28	45,45,45,45	0
56	MG	2a	1754	1/1	0.62	0.23	69,69,69,69	0
56	MG	2A	3568	1/1	0.62	0.76	56,56,56,56	0
56	MG	2a	1669	1/1	0.63	0.23	63,63,63,63	0
56	MG	1a	1682	1/1	0.63	0.47	55,55,55,55	0
56	MG	1A	3764	1/1	0.63	0.48	47,47,47,47	0
56	MG	2A	3184	1/1	0.63	0.34	59,59,59,59	0
56	MG	1A	3779	1/1	0.64	0.13	46,46,46,46	0
56	MG	1a	1657	1/1	0.64	0.16	71,71,71,71	0
56	MG	2a	1658	1/1	0.64	0.68	58,58,58,58	0
56	MG	2A	3532	1/1	0.64	0.16	50,50,50,50	0
56	MG	2a	1661	1/1	0.65	0.27	65,65,65,65	0
56	MG	1A	3545	1/1	0.65	0.44	54,54,54,54	0
56	MG	1o	101	1/1	0.65	0.43	66,66,66,66	0
56	MG	1A	3146	1/1	0.65	0.32	52,52,52,52	0
56	MG	2A	3055	1/1	0.65	0.26	62,62,62,62	0
56	MG	1A	3279	1/1	0.65	0.12	49,49,49,49	0
56	MG	2A	3110	1/1	0.66	0.57	53,53,53,53	0
56	MG	2A	3570	1/1	0.66	0.23	43,43,43,43	0
56	MG	2a	1632	1/1	0.66	0.39	60,60,60,60	0
56	MG	1a	1698	1/1	0.66	0.26	72,72,72,72	0
56	MG	2A	3559	1/1	0.66	0.19	47,47,47,47	0
56	MG	2A	3318	1/1	0.67	0.19	50,50,50,50	0
56	MG	2a	1696	1/1	0.67	0.57	63,63,63,63	0
56	MG	2A	3431	1/1	0.67	0.25	61,61,61,61	0
56	MG	1a	1801	1/1	0.67	0.13	85,85,85,85	0
56	MG	1a	1640	1/1	0.67	0.33	71,71,71,71	0
56	MG	2a	1684	1/1	0.68	0.16	66,66,66,66	0
56	MG	1A	3616	1/1	0.68	0.11	67,67,67,67	0
56	MG	1A	3752	1/1	0.68	0.10	50,50,50,50	0
56	MG	1a	1604	1/1	0.68	0.36	72,72,72,72	0
56	MG	1A	3613	1/1	0.68	0.21	68,68,68,68	0
56	MG	2x	103	1/1	0.68	0.34	73,73,73,73	0
56	MG	1A	3277	1/1	0.69	0.66	70,70,70,70	0
56	MG	2A	3081	1/1	0.69	1.11	62,62,62,62	0
56	MG	2A	3190	1/1	0.69	0.45	52,52,52,52	0
56	MG	1Z	8001	1/1	0.69	0.38	60,60,60,60	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	2A	3005	1/1	0.69	0.50	53,53,53,53	0
56	MG	2A	3127	1/1	0.69	0.33	61,61,61,61	0
56	MG	1a	1639	1/1	0.69	0.38	61,61,61,61	0
56	MG	2a	1738	1/1	0.69	0.10	58,58,58,58	0
56	MG	2a	1618	1/1	0.69	0.15	80,80,80,80	0
56	MG	2a	1763	1/1	0.69	0.22	82,82,82,82	0
56	MG	2a	1621	1/1	0.69	0.22	60,60,60,60	0
56	MG	2A	3312	1/1	0.69	0.13	69,69,69,69	0
56	MG	1A	3285	1/1	0.70	0.19	37,37,37,37	0
56	MG	2A	3191	1/1	0.70	0.43	50,50,50,50	0
56	MG	1a	1858	1/1	0.70	0.24	62,62,62,62	0
56	MG	2a	1727	1/1	0.70	0.11	64,64,64,64	0
56	MG	2A	3148	1/1	0.70	0.42	66,66,66,66	0
56	MG	2a	1751	1/1	0.70	0.19	77,77,77,77	0
56	MG	2A	3606	1/1	0.70	0.11	47,47,47,47	0
56	MG	1A	3717	1/1	0.70	0.20	57,57,57,57	0
56	MG	1a	1653	1/1	0.70	0.43	56,56,56,56	0
56	MG	1a	1802	1/1	0.70	0.12	71,71,71,71	0
56	MG	2E	307	1/1	0.71	0.19	52,52,52,52	0
56	MG	2V	203	1/1	0.71	0.29	61,61,61,61	0
56	MG	2A	3196	1/1	0.71	0.35	52,52,52,52	0
56	MG	1i	3001	1/1	0.71	0.22	68,68,68,68	0
56	MG	2A	3204	1/1	0.71	0.18	56,56,56,56	0
56	MG	1A	3535	1/1	0.71	0.23	34,34,34,34	0
56	MG	2a	1630	1/1	0.71	1.09	76,76,76,76	0
56	MG	2A	3187	1/1	0.71	0.71	57,57,57,57	0
56	MG	1A	3832	1/1	0.71	0.16	45,45,45,45	0
56	MG	2A	3661	1/1	0.71	0.63	62,62,62,62	0
56	MG	1A	3660	1/1	0.71	0.14	38,38,38,38	0
56	MG	1a	1790	1/1	0.72	0.11	59,59,59,59	0
56	MG	2A	3009	1/1	0.72	0.54	59,59,59,59	0
56	MG	1A	3457	1/1	0.72	0.15	28,28,28,28	0
56	MG	2A	3348	1/1	0.72	0.21	41,41,41,41	0
56	MG	2A	3063	1/1	0.72	0.18	53,53,53,53	0
56	MG	1A	3751	1/1	0.72	0.25	43,43,43,43	0
56	MG	2A	3399	1/1	0.72	0.55	53,53,53,53	0
56	MG	2A	3404	1/1	0.72	0.36	55,55,55,55	0
56	MG	1A	3246	1/1	0.72	0.24	59,59,59,59	0
56	MG	2B	3012	1/1	0.72	0.10	64,64,64,64	0
56	MG	1a	1854	1/1	0.72	0.14	72,72,72,72	0
56	MG	1a	1629	1/1	0.73	0.33	54,54,54,54	0
56	MG	2A	3077	1/1	0.73	0.74	56,56,56,56	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	1A	3795	1/1	0.73	0.46	39,39,39,39	0
56	MG	1a	1799	1/1	0.73	0.24	66,66,66,66	0
56	MG	2A	3328	1/1	0.73	0.46	71,71,71,71	0
56	MG	1a	1665	1/1	0.73	0.53	55,55,55,55	0
56	MG	1A	3645	1/1	0.73	0.60	37,37,37,37	0
56	MG	2a	1764	1/1	0.73	0.15	66,66,66,66	0
56	MG	2A	3233	1/1	0.73	0.51	49,49,49,49	0
56	MG	2A	3292	1/1	0.73	0.30	60,60,60,60	0
56	MG	1A	3185	1/1	0.74	0.58	42,42,42,42	0
56	MG	1A	3817	1/1	0.74	0.14	32,32,32,32	0
56	MG	1A	3345	1/1	0.74	0.14	45,45,45,45	0
56	MG	1a	1813	1/1	0.74	0.11	72,72,72,72	0
56	MG	2B	3011	1/1	0.74	0.17	78,78,78,78	0
56	MG	1a	1652	1/1	0.74	0.31	55,55,55,55	0
56	MG	1A	3371	1/1	0.74	0.24	30,30,30,30	0
56	MG	2A	3158	1/1	0.74	0.08	78,78,78,78	0
56	MG	2A	3177	1/1	0.74	0.41	54,54,54,54	0
56	MG	2A	3178	1/1	0.74	0.41	49,49,49,49	0
56	MG	1a	1787	1/1	0.74	0.13	65,65,65,65	0
56	MG	2A	3495	1/1	0.74	0.09	65,65,65,65	0
56	MG	1A	3927	1/1	0.74	0.38	50,50,50,50	0
56	MG	2A	3317	1/1	0.74	0.13	54,54,54,54	0
56	MG	1e	201	1/1	0.74	0.55	68,68,68,68	0
56	MG	1A	3905	1/1	0.75	0.21	54,54,54,54	0
56	MG	2A	3116	1/1	0.75	0.18	73,73,73,73	0
56	MG	2A	3518	1/1	0.75	0.14	63,63,63,63	0
56	MG	2A	3522	1/1	0.75	0.19	50,50,50,50	0
56	MG	1A	3320	1/1	0.75	0.20	26,26,26,26	0
56	MG	1A	3084	1/1	0.75	0.40	49,49,49,49	0
56	MG	1A	3116	1/1	0.75	0.67	40,40,40,40	0
56	MG	1A	3598	1/1	0.75	0.36	55,55,55,55	0
56	MG	2A	3021	1/1	0.75	0.19	67,67,67,67	0
56	MG	2A	3614	1/1	0.75	0.13	64,64,64,64	0
56	MG	2A	3108	1/1	0.75	0.21	72,72,72,72	0
56	MG	2a	1774	1/1	0.75	0.35	68,68,68,68	0
56	MG	2A	3322	1/1	0.75	0.11	71,71,71,71	0
56	MG	2A	3672	1/1	0.75	0.35	64,64,64,64	0
56	MG	2x	108	1/1	0.75	0.64	57,57,57,57	0
56	MG	1A	3713	1/1	0.76	0.56	59,59,59,59	0
56	MG	1a	1609	1/1	0.76	0.25	68,68,68,68	0
56	MG	2A	3362	1/1	0.76	0.21	46,46,46,46	0
56	MG	2A	3240	1/1	0.76	0.32	60,60,60,60	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	1A	3607	1/1	0.76	0.24	45,45,45,45	0
56	MG	1a	1831	1/1	0.76	0.22	69,69,69,69	0
56	MG	2A	3006	1/1	0.76	0.47	52,52,52,52	0
56	MG	1A	3619	1/1	0.76	0.25	32,32,32,32	0
56	MG	2a	1760	1/1	0.76	0.11	65,65,65,65	0
56	MG	1a	1795	1/1	0.76	0.21	76,76,76,76	0
56	MG	2a	1649	1/1	0.76	0.25	68,68,68,68	0
56	MG	1d	502	1/1	0.76	0.28	68,68,68,68	0
56	MG	2a	1776	1/1	0.76	0.32	65,65,65,65	0
56	MG	1A	3429	1/1	0.76	0.18	34,34,34,34	0
56	MG	2a	1663	1/1	0.76	0.31	65,65,65,65	0
56	MG	15	104	1/1	0.76	0.36	63,63,63,63	0
56	MG	2a	1699	1/1	0.77	0.13	59,59,59,59	0
56	MG	2A	3176	1/1	0.77	0.41	52,52,52,52	0
56	MG	1H	8001	1/1	0.77	0.26	61,61,61,61	0
56	MG	2a	1633	1/1	0.77	0.28	54,54,54,54	0
56	MG	2a	1641	1/1	0.77	0.36	76,76,76,76	0
56	MG	1A	3781	1/1	0.77	0.09	66,66,66,66	0
56	MG	2a	1656	1/1	0.77	0.26	68,68,68,68	0
56	MG	2A	3448	1/1	0.77	0.15	47,47,47,47	0
56	MG	2U	202	1/1	0.77	0.62	59,59,59,59	0
56	MG	2A	3083	1/1	0.77	0.14	76,76,76,76	0
56	MG	2A	3086	1/1	0.77	0.29	58,58,58,58	0
56	MG	2A	3511	1/1	0.77	0.09	64,64,64,64	0
56	MG	1A	3623	1/1	0.77	0.38	53,53,53,53	0
56	MG	1r	3001	1/1	0.77	0.20	70,70,70,70	0
58	MPD	1a	1860	8/8	0.77	0.31	65,70,76,77	0
56	MG	1A	3501	1/1	0.78	0.10	43,43,43,43	0
56	MG	1A	3872	1/1	0.78	0.21	58,58,58,58	0
56	MG	2A	3100	1/1	0.78	0.29	60,60,60,60	0
56	MG	2a	1622	1/1	0.78	0.60	56,56,56,56	0
56	MG	2a	1628	1/1	0.78	0.30	58,58,58,58	0
56	MG	1a	1711	1/1	0.78	0.16	77,77,77,77	0
56	MG	2A	3453	1/1	0.78	0.10	47,47,47,47	0
56	MG	2A	3206	1/1	0.78	0.32	57,57,57,57	0
56	MG	1A	3229	1/1	0.78	0.48	32,32,32,32	0
56	MG	2A	3496	1/1	0.78	0.14	45,45,45,45	0
56	MG	2A	3503	1/1	0.78	0.13	62,62,62,62	0
56	MG	1A	3922	1/1	0.78	0.86	31,31,31,31	0
56	MG	1a	1816	1/1	0.78	0.19	57,57,57,57	0
56	MG	2A	3243	1/1	0.78	0.29	50,50,50,50	0
56	MG	2A	3139	1/1	0.78	0.92	57,57,57,57	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	1A	3089	1/1	0.78	0.56	41,41,41,41	0
56	MG	2a	1683	1/1	0.78	0.56	71,71,71,71	0
56	MG	1a	1659	1/1	0.78	0.39	64,64,64,64	0
56	MG	2A	3030	1/1	0.78	0.31	51,51,51,51	0
56	MG	2A	3584	1/1	0.78	0.19	64,64,64,64	0
56	MG	2A	3315	1/1	0.78	0.18	48,48,48,48	0
56	MG	2A	3160	1/1	0.78	0.22	63,63,63,63	0
56	MG	2A	3641	1/1	0.78	0.11	61,61,61,61	0
56	MG	2A	3174	1/1	0.78	0.33	55,55,55,55	0
56	MG	1A	3149	1/1	0.78	0.63	35,35,35,35	0
56	MG	1a	1667	1/1	0.78	0.45	83,83,83,83	0
56	MG	2A	3070	1/1	0.78	0.64	49,49,49,49	0
56	MG	2A	3180	1/1	0.78	0.10	65,65,65,65	0
56	MG	2A	3351	1/1	0.78	0.18	53,53,53,53	0
56	MG	1a	1668	1/1	0.78	0.40	70,70,70,70	0
56	MG	1a	1670	1/1	0.78	0.14	59,59,59,59	0
56	MG	2t	3001	1/1	0.78	0.53	66,66,66,66	0
56	MG	1A	3602	1/1	0.78	0.12	48,48,48,48	0
56	MG	2a	1602	1/1	0.78	0.55	64,64,64,64	0
56	MG	1e	202	1/1	0.78	0.17	64,64,64,64	0
56	MG	2A	3294	1/1	0.79	0.14	50,50,50,50	0
56	MG	1A	3435	1/1	0.79	0.23	35,35,35,35	0
56	MG	1A	3583	1/1	0.79	0.13	65,65,65,65	0
56	MG	2A	3563	1/1	0.79	0.34	45,45,45,45	0
56	MG	1a	1611	1/1	0.79	0.54	49,49,49,49	0
56	MG	2A	3169	1/1	0.79	0.14	50,50,50,50	0
56	MG	1A	3597	1/1	0.79	0.20	34,34,34,34	0
56	MG	1A	3226	1/1	0.79	0.76	36,36,36,36	0
56	MG	1A	3025	1/1	0.79	0.26	55,55,55,55	0
56	MG	2a	1673	1/1	0.79	0.26	65,65,65,65	0
56	MG	1a	1726	1/1	0.79	0.10	60,60,60,60	0
56	MG	1a	1728	1/1	0.79	0.45	75,75,75,75	0
56	MG	1A	3507	1/1	0.79	0.56	52,52,52,52	0
56	MG	1a	1651	1/1	0.79	0.28	52,52,52,52	0
56	MG	2A	3185	1/1	0.79	0.31	56,56,56,56	0
56	MG	1d	503	1/1	0.79	0.24	70,70,70,70	0
56	MG	1B	205	1/1	0.79	0.23	57,57,57,57	0
56	MG	2A	3089	1/1	0.79	0.45	69,69,69,69	0
56	MG	1A	3224	1/1	0.79	0.29	46,46,46,46	0
56	MG	1B	216	1/1	0.79	0.25	49,49,49,49	0
56	MG	1f	8001	1/1	0.79	0.14	63,63,63,63	0
56	MG	1A	3675	1/1	0.79	0.23	36,36,36,36	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	2a	1768	1/1	0.79	0.13	69,69,69,69	0
56	MG	1A	3693	1/1	0.79	0.15	34,34,34,34	0
56	MG	1A	3815	1/1	0.79	0.13	27,27,27,27	0
56	MG	2A	3237	1/1	0.79	0.57	58,58,58,58	0
56	MG	1a	1792	1/1	0.79	0.21	68,68,68,68	0
56	MG	2A	3143	1/1	0.79	0.27	56,56,56,56	0
56	MG	2A	3272	1/1	0.79	0.23	54,54,54,54	0
56	MG	1A	3696	1/1	0.79	0.09	40,40,40,40	0
56	MG	2A	3478	1/1	0.80	0.15	50,50,50,50	0
56	MG	1A	3786	1/1	0.80	0.16	38,38,38,38	0
56	MG	2A	3114	1/1	0.80	0.38	50,50,50,50	0
56	MG	1A	3600	1/1	0.80	0.26	38,38,38,38	0
56	MG	2A	3032	1/1	0.80	0.19	63,63,63,63	0
56	MG	1A	3524	1/1	0.80	0.13	55,55,55,55	0
56	MG	2a	1701	1/1	0.80	0.23	61,61,61,61	0
56	MG	2a	1703	1/1	0.80	0.38	77,77,77,77	0
56	MG	2a	1715	1/1	0.80	0.15	75,75,75,75	0
56	MG	2a	1719	1/1	0.80	0.17	63,63,63,63	0
56	MG	1a	1800	1/1	0.80	0.08	66,66,66,66	0
56	MG	1a	1736	1/1	0.80	0.32	73,73,73,73	0
56	MG	2A	3149	1/1	0.80	0.35	44,44,44,44	0
56	MG	1A	3719	1/1	0.80	0.10	42,42,42,42	0
56	MG	2A	3565	1/1	0.80	0.23	48,48,48,48	0
56	MG	1a	1804	1/1	0.80	0.52	67,67,67,67	0
56	MG	2a	1761	1/1	0.80	0.28	63,63,63,63	0
56	MG	1A	3437	1/1	0.80	0.26	26,26,26,26	0
56	MG	1A	3375	1/1	0.80	0.14	56,56,56,56	0
56	MG	2A	3600	1/1	0.80	0.42	80,80,80,80	0
56	MG	2a	1769	1/1	0.80	0.11	73,73,73,73	0
56	MG	2a	1770	1/1	0.80	0.13	68,68,68,68	0
56	MG	1x	104	1/1	0.80	0.14	69,69,69,69	0
56	MG	1A	3496	1/1	0.80	0.18	40,40,40,40	0
56	MG	1A	3286	1/1	0.80	0.15	27,27,27,27	0
56	MG	2A	3099	1/1	0.80	0.31	57,57,57,57	0
56	MG	1A	3096	1/1	0.80	0.70	33,33,33,33	0
56	MG	2A	3182	1/1	0.80	0.41	57,57,57,57	0
56	MG	1A	3914	1/1	0.80	0.41	57,57,57,57	0
56	MG	1a	1688	1/1	0.81	0.47	58,58,58,58	0
56	MG	1a	1788	1/1	0.81	0.10	67,67,67,67	0
56	MG	1a	1689	1/1	0.81	0.44	69,69,69,69	0
56	MG	1A	3692	1/1	0.81	0.12	58,58,58,58	0
56	MG	2B	3004	1/1	0.81	0.29	64,64,64,64	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	2A	3264	1/1	0.81	0.23	49,49,49,49	0
56	MG	1A	3098	1/1	0.81	0.23	51,51,51,51	0
56	MG	1A	3380	1/1	0.81	0.12	44,44,44,44	0
56	MG	1A	3712	1/1	0.81	0.26	48,48,48,48	0
56	MG	2I	3001	1/1	0.81	0.18	74,74,74,74	0
56	MG	2a	1713	1/1	0.81	0.12	67,67,67,67	0
56	MG	1A	3386	1/1	0.81	0.22	32,32,32,32	0
56	MG	1A	3464	1/1	0.81	0.17	26,26,26,26	0
56	MG	2X	101	1/1	0.81	0.13	61,61,61,61	0
56	MG	1A	3470	1/1	0.81	0.10	37,37,37,37	0
56	MG	2a	1730	1/1	0.81	0.10	66,66,66,66	0
56	MG	1A	3181	1/1	0.81	0.29	45,45,45,45	0
56	MG	1a	1625	1/1	0.81	0.20	71,71,71,71	0
56	MG	2a	1752	1/1	0.81	0.19	64,64,64,64	0
56	MG	1A	3593	1/1	0.81	0.42	52,52,52,52	0
56	MG	1a	1827	1/1	0.81	0.34	77,77,77,77	0
56	MG	1a	1828	1/1	0.81	0.28	60,60,60,60	0
56	MG	2A	3331	1/1	0.81	0.23	57,57,57,57	0
56	MG	2A	3125	1/1	0.81	0.71	68,68,68,68	0
56	MG	1a	1674	1/1	0.81	0.38	74,74,74,74	0
56	MG	1B	224	1/1	0.81	0.16	54,54,54,54	0
56	MG	2a	1636	1/1	0.81	0.09	81,81,81,81	0
56	MG	2A	3038	1/1	0.81	0.76	49,49,49,49	0
56	MG	1a	1684	1/1	0.81	0.63	56,56,56,56	0
56	MG	2a	1652	1/1	0.81	0.53	58,58,58,58	0
56	MG	2A	3398	1/1	0.81	0.24	64,64,64,64	0
56	MG	2A	3057	1/1	0.81	0.75	53,53,53,53	0
56	MG	2A	3623	1/1	0.81	0.12	51,51,51,51	0
56	MG	2a	1662	1/1	0.81	1.13	77,77,77,77	0
56	MG	1A	3790	1/1	0.82	0.13	32,32,32,32	0
56	MG	1A	3088	1/1	0.82	0.68	32,32,32,32	0
56	MG	1A	3594	1/1	0.82	0.43	48,48,48,48	0
56	MG	1D	304	1/1	0.82	0.76	49,49,49,49	0
56	MG	2A	3599	1/1	0.82	0.12	59,59,59,59	0
56	MG	1A	3100	1/1	0.82	0.55	28,28,28,28	0
56	MG	1A	3038	1/1	0.82	0.41	39,39,39,39	0
56	MG	2A	3608	1/1	0.82	0.21	62,62,62,62	0
56	MG	2a	1675	1/1	0.82	0.78	69,69,69,69	0
56	MG	1A	3821	1/1	0.82	0.71	37,37,37,37	0
56	MG	2A	3352	1/1	0.82	0.20	49,49,49,49	0
56	MG	1A	3825	1/1	0.82	0.07	46,46,46,46	0
56	MG	1a	1836	1/1	0.82	0.10	61,61,61,61	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	2A	3383	1/1	0.82	0.40	57,57,57,57	0
56	MG	2A	3211	1/1	0.82	0.54	60,60,60,60	0
56	MG	2a	1712	1/1	0.82	0.24	66,66,66,66	0
56	MG	2A	3046	1/1	0.82	0.27	61,61,61,61	0
56	MG	2a	1714	1/1	0.82	0.33	62,62,62,62	0
56	MG	2A	3222	1/1	0.82	0.27	57,57,57,57	0
56	MG	2a	1717	1/1	0.82	0.28	67,67,67,67	0
56	MG	2A	3047	1/1	0.82	0.25	56,56,56,56	0
56	MG	2B	3013	1/1	0.82	0.14	72,72,72,72	0
56	MG	2A	3411	1/1	0.82	0.40	58,58,58,58	0
56	MG	2A	3051	1/1	0.82	0.77	49,49,49,49	0
56	MG	1a	1768	1/1	0.82	0.12	68,68,68,68	0
56	MG	2a	1744	1/1	0.82	0.15	62,62,62,62	0
56	MG	1A	3244	1/1	0.82	0.24	31,31,31,31	0
56	MG	2A	3250	1/1	0.82	0.20	48,48,48,48	0
56	MG	1A	3005	1/1	0.82	0.18	40,40,40,40	0
56	MG	2a	1759	1/1	0.82	0.13	78,78,78,78	0
56	MG	1A	3755	1/1	0.82	0.10	45,45,45,45	0
56	MG	1A	3759	1/1	0.82	0.58	53,53,53,53	0
56	MG	1A	3606	1/1	0.82	0.49	40,40,40,40	0
56	MG	1A	3133	1/1	0.82	0.32	35,35,35,35	0
56	MG	2a	1766	1/1	0.82	0.20	70,70,70,70	0
56	MG	2A	3301	1/1	0.82	0.12	52,52,52,52	0
56	MG	2A	3514	1/1	0.82	0.08	63,63,63,63	0
56	MG	2A	3303	1/1	0.82	0.17	44,44,44,44	0
56	MG	2A	3520	1/1	0.82	0.23	46,46,46,46	0
56	MG	2A	3521	1/1	0.82	0.19	49,49,49,49	0
56	MG	1A	3357	1/1	0.82	0.19	29,29,29,29	0
56	MG	2A	3530	1/1	0.82	0.13	56,56,56,56	0
56	MG	2x	102	1/1	0.82	0.08	73,73,73,73	0
56	MG	1A	3194	1/1	0.82	0.16	40,40,40,40	0
56	MG	1a	1647	1/1	0.82	0.43	66,66,66,66	0
56	MG	1a	1713	1/1	0.82	0.37	72,72,72,72	0
56	MG	2A	3298	1/1	0.83	0.13	46,46,46,46	0
56	MG	2A	3519	1/1	0.83	0.25	44,44,44,44	0
56	MG	1a	1646	1/1	0.83	0.13	72,72,72,72	0
56	MG	1a	1814	1/1	0.83	0.19	64,64,64,64	0
56	MG	2A	3167	1/1	0.83	0.17	66,66,66,66	0
56	MG	2a	1643	1/1	0.83	0.30	67,67,67,67	0
56	MG	2A	3526	1/1	0.83	0.18	60,60,60,60	0
56	MG	1A	3171	1/1	0.83	0.85	42,42,42,42	0
56	MG	1a	1724	1/1	0.83	0.40	78,78,78,78	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	2A	3541	1/1	0.83	0.15	49,49,49,49	0
56	MG	2A	3558	1/1	0.83	0.26	50,50,50,50	0
56	MG	1A	3234	1/1	0.83	0.33	41,41,41,41	0
56	MG	1B	217	1/1	0.83	0.11	59,59,59,59	0
56	MG	2A	3564	1/1	0.83	0.09	68,68,68,68	0
56	MG	1A	3241	1/1	0.83	0.50	30,30,30,30	0
56	MG	2a	1670	1/1	0.83	0.28	58,58,58,58	0
56	MG	1A	3183	1/1	0.83	0.45	42,42,42,42	0
56	MG	1a	1750	1/1	0.83	0.39	63,63,63,63	0
56	MG	1A	3142	1/1	0.83	0.19	34,34,34,34	0
56	MG	1A	3484	1/1	0.83	0.18	43,43,43,43	0
56	MG	1A	3873	1/1	0.83	0.26	55,55,55,55	0
56	MG	2A	3603	1/1	0.83	0.17	46,46,46,46	0
56	MG	2A	3604	1/1	0.83	0.12	49,49,49,49	0
56	MG	1A	3876	1/1	0.83	0.22	32,32,32,32	0
56	MG	2A	3087	1/1	0.83	0.43	51,51,51,51	0
56	MG	2A	3088	1/1	0.83	0.27	60,60,60,60	0
56	MG	1A	3881	1/1	0.83	0.27	53,53,53,53	0
56	MG	2A	3628	1/1	0.83	0.24	58,58,58,58	0
56	MG	1a	1779	1/1	0.83	0.10	66,66,66,66	0
56	MG	2A	3391	1/1	0.83	0.17	48,48,48,48	0
56	MG	1A	3257	1/1	0.83	0.20	55,55,55,55	0
56	MG	2A	3663	1/1	0.83	0.51	55,55,55,55	0
56	MG	1a	1675	1/1	0.83	0.26	46,46,46,46	0
56	MG	2B	3003	1/1	0.83	0.28	68,68,68,68	0
56	MG	1a	1678	1/1	0.83	0.29	74,74,74,74	0
56	MG	2a	1747	1/1	0.83	0.15	66,66,66,66	0
56	MG	2a	1750	1/1	0.83	0.08	76,76,76,76	0
56	MG	1A	3296	1/1	0.83	0.10	45,45,45,45	0
56	MG	1A	3309	1/1	0.83	0.11	36,36,36,36	0
56	MG	1x	110	1/1	0.83	0.11	58,58,58,58	0
56	MG	2A	3117	1/1	0.83	0.15	55,55,55,55	0
56	MG	1A	3722	1/1	0.83	0.07	36,36,36,36	0
56	MG	2A	3451	1/1	0.83	0.12	53,53,53,53	0
56	MG	2T	3001	1/1	0.83	0.31	54,54,54,54	0
56	MG	1A	3944	1/1	0.83	0.14	31,31,31,31	0
56	MG	2A	3466	1/1	0.83	0.21	57,57,57,57	0
56	MG	2A	3470	1/1	0.83	0.22	57,57,57,57	0
56	MG	2A	3248	1/1	0.83	0.20	51,51,51,51	0
56	MG	2a	1603	1/1	0.83	0.63	60,60,60,60	0
56	MG	1A	3601	1/1	0.83	0.23	31,31,31,31	0
56	MG	1B	209	1/1	0.83	0.39	61,61,61,61	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	2a	1609	1/1	0.83	0.25	67,67,67,67	0
56	MG	2l	201	1/1	0.83	0.18	71,71,71,71	0
56	MG	2a	1614	1/1	0.83	0.13	65,65,65,65	0
56	MG	2A	3266	1/1	0.83	0.15	50,50,50,50	0
56	MG	1a	1708	1/1	0.83	0.28	64,64,64,64	0
56	MG	2x	105	1/1	0.83	0.21	75,75,75,75	0
56	MG	1a	1641	1/1	0.83	0.35	75,75,75,75	0
56	MG	1a	1805	1/1	0.83	0.12	70,70,70,70	0
56	MG	1a	1862	1/1	0.84	0.59	70,70,70,70	0
56	MG	1D	306	1/1	0.84	0.29	35,35,35,35	0
56	MG	1D	307	1/1	0.84	0.24	45,45,45,45	0
56	MG	1A	3631	1/1	0.84	0.43	43,43,43,43	0
56	MG	1a	1771	1/1	0.84	0.14	71,71,71,71	0
56	MG	1A	3482	1/1	0.84	0.36	28,28,28,28	0
56	MG	1T	201	1/1	0.84	0.23	52,52,52,52	0
56	MG	2A	3617	1/1	0.84	0.15	49,49,49,49	0
56	MG	1g	3001	1/1	0.84	0.18	62,62,62,62	0
56	MG	1A	3391	1/1	0.84	0.10	50,50,50,50	0
56	MG	2A	3418	1/1	0.84	0.24	65,65,65,65	0
56	MG	2A	3649	1/1	0.84	0.38	57,57,57,57	0
56	MG	2a	1685	1/1	0.84	0.07	68,68,68,68	0
56	MG	1A	3651	1/1	0.84	0.17	74,74,74,74	0
56	MG	2A	3658	1/1	0.84	0.22	49,49,49,49	0
56	MG	1A	3495	1/1	0.84	0.26	37,37,37,37	0
56	MG	2A	3662	1/1	0.84	0.83	63,63,63,63	0
56	MG	1A	3890	1/1	0.84	0.46	32,32,32,32	0
56	MG	2A	3124	1/1	0.84	0.58	63,63,63,63	0
56	MG	1A	3426	1/1	0.84	0.25	32,32,32,32	0
56	MG	2A	3247	1/1	0.84	0.12	52,52,52,52	0
56	MG	1a	1619	1/1	0.84	0.48	74,74,74,74	0
56	MG	2A	3136	1/1	0.84	0.23	54,54,54,54	0
56	MG	2a	1720	1/1	0.84	0.16	57,57,57,57	0
56	MG	1A	3663	1/1	0.84	0.09	48,48,48,48	0
56	MG	1A	3209	1/1	0.84	0.54	40,40,40,40	0
56	MG	2A	3269	1/1	0.84	0.29	43,43,43,43	0
56	MG	2A	3499	1/1	0.84	0.21	41,41,41,41	0
56	MG	1A	3506	1/1	0.84	0.10	44,44,44,44	0
56	MG	2A	3289	1/1	0.84	0.27	55,55,55,55	0
56	MG	1A	3940	1/1	0.84	0.09	42,42,42,42	0
56	MG	1a	1803	1/1	0.84	0.50	63,63,63,63	0
56	MG	23	101	1/1	0.84	0.68	58,58,58,58	0
56	MG	2A	3157	1/1	0.84	0.18	47,47,47,47	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	2a	1758	1/1	0.84	0.14	66,66,66,66	0
56	MG	1A	3212	1/1	0.84	0.69	30,30,30,30	0
56	MG	1a	1722	1/1	0.84	0.23	67,67,67,67	0
56	MG	1A	3945	1/1	0.84	0.57	38,38,38,38	0
56	MG	1A	3008	1/1	0.84	0.33	47,47,47,47	0
56	MG	2A	3170	1/1	0.84	0.35	52,52,52,52	0
56	MG	2A	3173	1/1	0.84	0.15	56,56,56,56	0
56	MG	2a	1619	1/1	0.84	0.14	65,65,65,65	0
56	MG	1a	1815	1/1	0.84	0.13	57,57,57,57	0
56	MG	2A	3557	1/1	0.84	0.18	51,51,51,51	0
56	MG	2a	1625	1/1	0.84	0.59	72,72,72,72	0
56	MG	1A	3377	1/1	0.84	0.13	34,34,34,34	0
56	MG	1A	3078	1/1	0.84	0.30	45,45,45,45	0
56	MG	2k	201	1/1	0.84	0.23	64,64,64,64	0
56	MG	1A	3564	1/1	0.84	0.16	35,35,35,35	0
56	MG	1A	3570	1/1	0.84	0.20	42,42,42,42	0
56	MG	1a	1737	1/1	0.84	0.10	74,74,74,74	0
56	MG	1A	3158	1/1	0.84	0.32	42,42,42,42	0
56	MG	1a	1759	1/1	0.84	0.32	69,69,69,69	0
56	MG	2x	107	1/1	0.84	0.18	69,69,69,69	0
56	MG	1A	3848	1/1	0.84	0.12	54,54,54,54	0
56	MG	2A	3595	1/1	0.84	0.10	66,66,66,66	0
56	MG	2A	3482	1/1	0.85	0.10	74,74,74,74	0
56	MG	1A	3787	1/1	0.85	0.12	31,31,31,31	0
56	MG	2A	3217	1/1	0.85	0.34	53,53,53,53	0
56	MG	1A	3313	1/1	0.85	0.18	35,35,35,35	0
56	MG	2A	3500	1/1	0.85	0.18	51,51,51,51	0
56	MG	2A	3501	1/1	0.85	0.12	60,60,60,60	0
56	MG	2A	3084	1/1	0.85	0.37	42,42,42,42	0
56	MG	2A	3223	1/1	0.85	0.58	60,60,60,60	0
56	MG	1A	3632	1/1	0.85	0.31	34,34,34,34	0
56	MG	1A	3317	1/1	0.85	0.17	45,45,45,45	0
56	MG	1a	1817	1/1	0.85	0.28	72,72,72,72	0
56	MG	1G	3001	1/1	0.85	0.12	69,69,69,69	0
56	MG	1A	3551	1/1	0.85	0.45	54,54,54,54	0
56	MG	2a	1654	1/1	0.85	0.48	62,62,62,62	0
56	MG	1R	203	1/1	0.85	0.30	39,39,39,39	0
56	MG	1A	3557	1/1	0.85	0.27	42,42,42,42	0
56	MG	2A	3254	1/1	0.85	0.36	42,42,42,42	0
56	MG	2A	3107	1/1	0.85	0.16	66,66,66,66	0
56	MG	1A	3656	1/1	0.85	0.14	41,41,41,41	0
56	MG	1a	1839	1/1	0.85	0.19	63,63,63,63	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	1A	3822	1/1	0.85	0.26	37,37,37,37	0
56	MG	1A	3260	1/1	0.85	0.19	42,42,42,42	0
56	MG	2A	3291	1/1	0.85	0.12	52,52,52,52	0
56	MG	1A	3569	1/1	0.85	0.25	30,30,30,30	0
56	MG	2a	1679	1/1	0.85	0.43	62,62,62,62	0
56	MG	1A	3439	1/1	0.85	0.19	31,31,31,31	0
56	MG	2A	3296	1/1	0.85	0.30	42,42,42,42	0
56	MG	1A	3269	1/1	0.85	0.32	41,41,41,41	0
56	MG	2A	3126	1/1	0.85	0.34	57,57,57,57	0
56	MG	1A	3591	1/1	0.85	0.24	54,54,54,54	0
56	MG	1A	3355	1/1	0.85	0.15	31,31,31,31	0
56	MG	2A	3308	1/1	0.85	0.16	51,51,51,51	0
56	MG	1a	1628	1/1	0.85	0.33	63,63,63,63	0
56	MG	1A	3107	1/1	0.85	0.33	32,32,32,32	0
56	MG	1a	1632	1/1	0.85	0.15	63,63,63,63	0
56	MG	1A	3033	1/1	0.85	0.20	45,45,45,45	0
56	MG	1A	3278	1/1	0.85	0.12	28,28,28,28	0
56	MG	1a	1766	1/1	0.85	0.25	72,72,72,72	0
56	MG	1A	3900	1/1	0.85	0.26	33,33,33,33	0
56	MG	2A	3159	1/1	0.85	0.35	53,53,53,53	0
56	MG	1A	3491	1/1	0.85	0.15	35,35,35,35	0
56	MG	2A	3165	1/1	0.85	0.42	47,47,47,47	0
56	MG	1A	3198	1/1	0.85	0.14	60,60,60,60	0
56	MG	2A	3001	1/1	0.85	0.29	60,60,60,60	0
56	MG	2A	3357	1/1	0.85	0.17	51,51,51,51	0
56	MG	1A	3915	1/1	0.85	0.19	29,29,29,29	0
56	MG	2A	3368	1/1	0.85	0.27	55,55,55,55	0
56	MG	1A	3093	1/1	0.85	0.28	50,50,50,50	0
56	MG	1A	3744	1/1	0.85	0.16	46,46,46,46	0
56	MG	2A	3384	1/1	0.85	0.30	48,48,48,48	0
56	MG	2B	3010	1/1	0.85	0.21	69,69,69,69	0
56	MG	2A	3175	1/1	0.85	0.26	58,58,58,58	0
56	MG	1A	3604	1/1	0.85	0.07	54,54,54,54	0
56	MG	1A	3500	1/1	0.85	0.34	39,39,39,39	0
56	MG	1A	3383	1/1	0.85	0.10	33,33,33,33	0
56	MG	2A	3037	1/1	0.85	0.15	66,66,66,66	0
56	MG	1a	1793	1/1	0.85	0.25	71,71,71,71	0
56	MG	2O	202	1/1	0.85	0.13	63,63,63,63	0
56	MG	1A	3608	1/1	0.85	0.10	36,36,36,36	0
56	MG	1A	3080	1/1	0.85	1.21	33,33,33,33	0
56	MG	1B	213	1/1	0.85	0.09	49,49,49,49	0
56	MG	2A	3441	1/1	0.85	0.14	65,65,65,65	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	2A	3447	1/1	0.85	0.34	42,42,42,42	0
56	MG	1a	1672	1/1	0.85	0.53	61,61,61,61	0
56	MG	2p	101	1/1	0.85	0.44	58,58,58,58	0
56	MG	1A	3776	1/1	0.85	0.22	40,40,40,40	0
56	MG	2a	1604	1/1	0.85	0.43	72,72,72,72	0
56	MG	1A	3059	1/1	0.85	0.23	60,60,60,60	0
56	MG	2A	3067	1/1	0.85	0.66	42,42,42,42	0
56	MG	1A	3513	1/1	0.85	0.13	49,49,49,49	0
56	MG	1A	3072	1/1	0.85	0.21	43,43,43,43	0
56	MG	2x	110	1/1	0.85	0.11	70,70,70,70	0
56	MG	1a	1809	1/1	0.85	0.20	62,62,62,62	0
60	ZN	24	501	1/1	0.85	0.23	94,94,94,94	0
62	K	2A	3665	1/1	0.85	0.48	60,60,60,60	0
56	MG	2A	3238	1/1	0.86	0.30	55,55,55,55	0
56	MG	1A	3705	1/1	0.86	0.16	45,45,45,45	0
56	MG	1A	3711	1/1	0.86	0.16	45,45,45,45	0
56	MG	1A	3849	1/1	0.86	0.21	60,60,60,60	0
56	MG	1a	1843	1/1	0.86	0.60	62,62,62,62	0
56	MG	19	101	1/1	0.86	0.29	48,48,48,48	0
56	MG	2A	3253	1/1	0.86	0.10	53,53,53,53	0
56	MG	1A	3868	1/1	0.86	0.31	56,56,56,56	0
56	MG	1a	1605	1/1	0.86	0.41	67,67,67,67	0
56	MG	1A	3428	1/1	0.86	0.20	24,24,24,24	0
56	MG	1A	3165	1/1	0.86	0.29	36,36,36,36	0
56	MG	1A	3522	1/1	0.86	0.25	39,39,39,39	0
56	MG	2A	3279	1/1	0.86	0.24	60,60,60,60	0
56	MG	1a	1746	1/1	0.86	0.17	69,69,69,69	0
56	MG	1A	3092	1/1	0.86	0.32	33,33,33,33	0
56	MG	1A	3525	1/1	0.86	0.23	31,31,31,31	0
56	MG	1A	3350	1/1	0.86	0.21	32,32,32,32	0
56	MG	1A	3745	1/1	0.86	0.23	49,49,49,49	0
56	MG	1A	3538	1/1	0.86	0.31	56,56,56,56	0
56	MG	2A	3539	1/1	0.86	0.22	57,57,57,57	0
56	MG	1A	3002	1/1	0.86	0.36	44,44,44,44	0
56	MG	2A	3544	1/1	0.86	0.10	61,61,61,61	0
56	MG	2A	3553	1/1	0.86	0.13	63,63,63,63	0
56	MG	2a	1666	1/1	0.86	0.29	84,84,84,84	0
56	MG	2A	3555	1/1	0.86	0.12	59,59,59,59	0
56	MG	1A	3550	1/1	0.86	0.15	51,51,51,51	0
56	MG	1a	1770	1/1	0.86	0.56	65,65,65,65	0
56	MG	1A	3126	1/1	0.86	0.37	32,32,32,32	0
56	MG	1A	3153	1/1	0.86	0.47	49,49,49,49	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	2a	1678	1/1	0.86	0.51	64,64,64,64	0
56	MG	1A	3930	1/1	0.86	0.88	32,32,32,32	0
56	MG	2a	1681	1/1	0.86	0.15	69,69,69,69	0
56	MG	1A	3768	1/1	0.86	0.22	27,27,27,27	0
56	MG	2A	3567	1/1	0.86	0.12	69,69,69,69	0
56	MG	1A	3036	1/1	0.86	0.07	58,58,58,58	0
56	MG	2a	1692	1/1	0.86	0.07	62,62,62,62	0
56	MG	1A	3566	1/1	0.86	0.26	41,41,41,41	0
56	MG	2A	3319	1/1	0.86	0.12	51,51,51,51	0
56	MG	1A	3947	1/1	0.86	0.22	56,56,56,56	0
56	MG	2A	3172	1/1	0.86	0.13	68,68,68,68	0
56	MG	1A	3644	1/1	0.86	0.35	38,38,38,38	0
56	MG	2A	3335	1/1	0.86	0.19	63,63,63,63	0
56	MG	2A	3336	1/1	0.86	0.14	78,78,78,78	0
56	MG	1A	3376	1/1	0.86	0.17	29,29,29,29	0
56	MG	1A	3291	1/1	0.86	0.30	26,26,26,26	0
56	MG	1A	3579	1/1	0.86	0.49	37,37,37,37	0
56	MG	1A	3488	1/1	0.86	0.12	46,46,46,46	0
56	MG	2a	1723	1/1	0.86	0.13	62,62,62,62	0
56	MG	2A	3621	1/1	0.86	0.08	76,76,76,76	0
56	MG	2A	3353	1/1	0.86	0.41	53,53,53,53	0
56	MG	2A	3626	1/1	0.86	0.16	49,49,49,49	0
56	MG	2a	1733	1/1	0.86	0.13	75,75,75,75	0
56	MG	2A	3050	1/1	0.86	0.14	56,56,56,56	0
56	MG	2A	3358	1/1	0.86	0.18	43,43,43,43	0
56	MG	2a	1745	1/1	0.86	0.14	71,71,71,71	0
56	MG	1A	3228	1/1	0.86	0.58	40,40,40,40	0
56	MG	1A	3807	1/1	0.86	0.14	60,60,60,60	0
56	MG	1B	227	1/1	0.86	0.09	51,51,51,51	0
56	MG	1A	3267	1/1	0.86	0.36	52,52,52,52	0
56	MG	1A	3268	1/1	0.86	0.29	40,40,40,40	0
56	MG	2A	3069	1/1	0.86	0.30	41,41,41,41	0
56	MG	1a	1808	1/1	0.86	0.26	66,66,66,66	0
56	MG	2A	3674	1/1	0.86	0.84	50,50,50,50	0
56	MG	2A	3071	1/1	0.86	0.19	65,65,65,65	0
56	MG	2A	3072	1/1	0.86	0.49	54,54,54,54	0
56	MG	1A	3818	1/1	0.86	0.34	29,29,29,29	0
56	MG	1a	1810	1/1	0.86	0.23	74,74,74,74	0
56	MG	1a	1687	1/1	0.86	0.21	71,71,71,71	0
56	MG	2A	3207	1/1	0.86	0.27	68,68,68,68	0
56	MG	2B	3015	1/1	0.86	0.09	76,76,76,76	0
56	MG	2a	1771	1/1	0.86	0.15	79,79,79,79	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	2B	3017	1/1	0.86	0.09	66,66,66,66	0
56	MG	1A	3316	1/1	0.86	0.30	45,45,45,45	0
56	MG	2D	308	1/1	0.86	0.19	47,47,47,47	0
56	MG	2A	3439	1/1	0.86	0.47	70,70,70,70	0
56	MG	1D	311	1/1	0.86	0.26	47,47,47,47	0
56	MG	2A	3442	1/1	0.86	0.14	64,64,64,64	0
56	MG	1a	1690	1/1	0.86	0.18	55,55,55,55	0
56	MG	1A	3418	1/1	0.86	0.08	52,52,52,52	0
56	MG	2A	3450	1/1	0.86	0.06	50,50,50,50	0
56	MG	2W	201	1/1	0.86	0.29	62,62,62,62	0
56	MG	1A	3191	1/1	0.86	0.29	40,40,40,40	0
56	MG	2A	3227	1/1	0.86	0.17	58,58,58,58	0
56	MG	2A	3457	1/1	0.86	0.25	63,63,63,63	0
56	MG	2A	3459	1/1	0.86	0.15	56,56,56,56	0
56	MG	1R	201	1/1	0.86	0.42	35,35,35,35	0
56	MG	1A	3831	1/1	0.86	0.10	58,58,58,58	0
56	MG	1A	3124	1/1	0.87	0.20	40,40,40,40	0
56	MG	13	103	1/1	0.87	0.78	42,42,42,42	0
56	MG	1A	3681	1/1	0.87	0.09	47,47,47,47	0
56	MG	1A	3769	1/1	0.87	0.17	67,67,67,67	0
56	MG	1A	3886	1/1	0.87	0.38	38,38,38,38	0
56	MG	2a	1664	1/1	0.87	0.71	65,65,65,65	0
56	MG	2A	3366	1/1	0.87	0.18	44,44,44,44	0
56	MG	1A	3517	1/1	0.87	0.19	33,33,33,33	0
56	MG	1A	3778	1/1	0.87	0.21	53,53,53,53	0
56	MG	2A	3381	1/1	0.87	0.38	53,53,53,53	0
56	MG	1A	3252	1/1	0.87	0.54	41,41,41,41	0
56	MG	2A	3074	1/1	0.87	0.30	48,48,48,48	0
56	MG	1a	1614	1/1	0.87	0.11	51,51,51,51	0
56	MG	1A	3299	1/1	0.87	0.18	47,47,47,47	0
56	MG	2A	3080	1/1	0.87	0.13	61,61,61,61	0
56	MG	2A	3402	1/1	0.87	0.06	52,52,52,52	0
56	MG	1A	3699	1/1	0.87	0.20	32,32,32,32	0
56	MG	1a	1733	1/1	0.87	0.13	65,65,65,65	0
56	MG	2A	3644	1/1	0.87	0.23	56,56,56,56	0
56	MG	2A	3213	1/1	0.87	0.43	53,53,53,53	0
56	MG	2a	1698	1/1	0.87	0.14	77,77,77,77	0
56	MG	1a	1838	1/1	0.87	0.08	69,69,69,69	0
56	MG	1A	3702	1/1	0.87	0.14	37,37,37,37	0
56	MG	1A	3423	1/1	0.87	0.10	57,57,57,57	0
56	MG	1a	1851	1/1	0.87	0.21	78,78,78,78	0
56	MG	1A	3708	1/1	0.87	0.12	35,35,35,35	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	2A	3091	1/1	0.87	0.22	54,54,54,54	0
56	MG	1A	3792	1/1	0.87	0.18	34,34,34,34	0
56	MG	1a	1754	1/1	0.87	0.51	68,68,68,68	0
56	MG	1a	1756	1/1	0.87	0.18	58,58,58,58	0
56	MG	1A	3793	1/1	0.87	0.17	37,37,37,37	0
56	MG	1d	504	1/1	0.87	0.10	82,82,82,82	0
56	MG	1A	3630	1/1	0.87	0.32	37,37,37,37	0
56	MG	1A	3303	1/1	0.87	0.16	32,32,32,32	0
56	MG	2A	3463	1/1	0.87	0.33	52,52,52,52	0
56	MG	1B	202	1/1	0.87	0.20	61,61,61,61	0
56	MG	1A	3813	1/1	0.87	0.12	35,35,35,35	0
56	MG	1B	206	1/1	0.87	0.16	49,49,49,49	0
56	MG	2E	305	1/1	0.87	0.35	45,45,45,45	0
56	MG	1A	3004	1/1	0.87	0.19	37,37,37,37	0
56	MG	1A	3633	1/1	0.87	0.59	31,31,31,31	0
56	MG	1A	3718	1/1	0.87	0.07	72,72,72,72	0
56	MG	2A	3133	1/1	0.87	0.28	52,52,52,52	0
56	MG	1A	3820	1/1	0.87	0.48	33,33,33,33	0
56	MG	1A	3207	1/1	0.87	0.78	35,35,35,35	0
56	MG	1A	3432	1/1	0.87	0.23	34,34,34,34	0
56	MG	2A	3147	1/1	0.87	0.14	54,54,54,54	0
56	MG	1A	3730	1/1	0.87	0.86	40,40,40,40	0
56	MG	1B	228	1/1	0.87	0.20	67,67,67,67	0
56	MG	1A	3741	1/1	0.87	0.17	31,31,31,31	0
56	MG	1A	3186	1/1	0.87	0.23	34,34,34,34	0
56	MG	1A	3837	1/1	0.87	0.10	46,46,46,46	0
56	MG	2A	3022	1/1	0.87	0.23	59,59,59,59	0
56	MG	2A	3025	1/1	0.87	0.19	56,56,56,56	0
56	MG	2A	3161	1/1	0.87	0.31	47,47,47,47	0
56	MG	2A	3028	1/1	0.87	0.30	51,51,51,51	0
56	MG	2A	3316	1/1	0.87	0.30	67,67,67,67	0
56	MG	1A	3847	1/1	0.87	0.12	46,46,46,46	0
56	MG	2A	3168	1/1	0.87	0.22	52,52,52,52	0
56	MG	1A	3553	1/1	0.87	0.16	58,58,58,58	0
56	MG	2A	3550	1/1	0.87	0.10	43,43,43,43	0
56	MG	1A	3555	1/1	0.87	0.60	38,38,38,38	0
56	MG	1a	1685	1/1	0.87	0.54	67,67,67,67	0
56	MG	2A	3039	1/1	0.87	0.24	56,56,56,56	0
56	MG	2A	3041	1/1	0.87	0.22	63,63,63,63	0
56	MG	1A	3861	1/1	0.87	0.07	50,50,50,50	0
56	MG	2A	3339	1/1	0.87	0.09	65,65,65,65	0
56	MG	2x	109	1/1	0.87	0.15	69,69,69,69	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	1A	3189	1/1	0.87	0.84	43,43,43,43	0
56	MG	2a	1650	1/1	0.87	0.41	61,61,61,61	0
56	MG	1A	3319	1/1	0.87	0.09	43,43,43,43	0
56	MG	1A	3006	1/1	0.87	0.26	34,34,34,34	0
56	MG	2A	3566	1/1	0.88	0.16	62,62,62,62	0
56	MG	1A	3816	1/1	0.88	0.48	42,42,42,42	0
56	MG	1a	1627	1/1	0.88	0.20	57,57,57,57	0
56	MG	1A	3478	1/1	0.88	0.12	41,41,41,41	0
56	MG	1A	3624	1/1	0.88	0.15	62,62,62,62	0
56	MG	1A	3556	1/1	0.88	0.69	39,39,39,39	0
56	MG	1a	1755	1/1	0.88	0.33	68,68,68,68	0
56	MG	1A	3215	1/1	0.88	0.23	48,48,48,48	0
56	MG	1A	3220	1/1	0.88	0.31	28,28,28,28	0
56	MG	2A	3098	1/1	0.88	0.26	59,59,59,59	0
56	MG	1A	3823	1/1	0.88	0.14	59,59,59,59	0
56	MG	1A	3381	1/1	0.88	0.23	38,38,38,38	0
56	MG	1a	1763	1/1	0.88	0.15	82,82,82,82	0
56	MG	1A	3490	1/1	0.88	0.29	44,44,44,44	0
56	MG	2a	1671	1/1	0.88	0.41	71,71,71,71	0
56	MG	1a	1765	1/1	0.88	0.17	80,80,80,80	0
56	MG	2a	1674	1/1	0.88	0.37	64,64,64,64	0
56	MG	2A	3229	1/1	0.88	0.46	45,45,45,45	0
56	MG	2a	1677	1/1	0.88	0.48	76,76,76,76	0
56	MG	2A	3113	1/1	0.88	0.09	59,59,59,59	0
56	MG	1A	3259	1/1	0.88	0.10	71,71,71,71	0
56	MG	1A	3576	1/1	0.88	0.22	43,43,43,43	0
56	MG	1A	3646	1/1	0.88	0.12	37,37,37,37	0
56	MG	2A	3646	1/1	0.88	0.15	66,66,66,66	0
56	MG	2A	3118	1/1	0.88	0.36	47,47,47,47	0
56	MG	2A	3445	1/1	0.88	0.27	61,61,61,61	0
56	MG	2A	3120	1/1	0.88	0.14	60,60,60,60	0
56	MG	2A	3121	1/1	0.88	0.15	68,68,68,68	0
56	MG	1B	226	1/1	0.88	0.18	48,48,48,48	0
56	MG	1A	3188	1/1	0.88	0.30	42,42,42,42	0
56	MG	2A	3666	1/1	0.88	0.19	54,54,54,54	0
56	MG	2A	3668	1/1	0.88	0.10	62,62,62,62	0
56	MG	1a	1778	1/1	0.88	0.20	63,63,63,63	0
56	MG	1A	3022	1/1	0.88	0.27	43,43,43,43	0
56	MG	2A	3679	1/1	0.88	0.38	53,53,53,53	0
56	MG	1a	1781	1/1	0.88	0.35	58,58,58,58	0
56	MG	1a	1785	1/1	0.88	0.27	71,71,71,71	0
56	MG	1A	3851	1/1	0.88	0.10	63,63,63,63	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	2A	3468	1/1	0.88	0.07	69,69,69,69	0
56	MG	2A	3142	1/1	0.88	0.26	61,61,61,61	0
56	MG	1A	3855	1/1	0.88	0.54	42,42,42,42	0
56	MG	1A	3393	1/1	0.88	0.17	31,31,31,31	0
56	MG	1A	3051	1/1	0.88	0.72	32,32,32,32	0
56	MG	2A	3493	1/1	0.88	0.19	61,61,61,61	0
56	MG	2A	3293	1/1	0.88	0.14	63,63,63,63	0
56	MG	1A	3177	1/1	0.88	0.47	35,35,35,35	0
56	MG	2A	3155	1/1	0.88	0.31	46,46,46,46	0
56	MG	2F	302	1/1	0.88	0.19	47,47,47,47	0
56	MG	2G	201	1/1	0.88	0.16	72,72,72,72	0
56	MG	1E	303	1/1	0.88	0.72	33,33,33,33	0
56	MG	1a	1794	1/1	0.88	0.44	69,69,69,69	0
56	MG	1F	309	1/1	0.88	0.33	43,43,43,43	0
56	MG	2A	3504	1/1	0.88	0.14	64,64,64,64	0
56	MG	2A	3507	1/1	0.88	0.19	72,72,72,72	0
56	MG	1a	1680	1/1	0.88	0.59	45,45,45,45	0
56	MG	1A	3871	1/1	0.88	0.16	43,43,43,43	0
56	MG	1A	3272	1/1	0.88	0.15	52,52,52,52	0
56	MG	1A	3676	1/1	0.88	0.34	34,34,34,34	0
56	MG	1A	3122	1/1	0.88	0.10	37,37,37,37	0
56	MG	1A	3053	1/1	0.88	0.81	34,34,34,34	0
56	MG	1A	3143	1/1	0.88	0.08	63,63,63,63	0
56	MG	10	105	1/1	0.88	0.09	49,49,49,49	0
56	MG	2A	3171	1/1	0.88	0.19	69,69,69,69	0
56	MG	1A	3211	1/1	0.88	0.82	30,30,30,30	0
56	MG	2a	1616	1/1	0.88	0.15	57,57,57,57	0
56	MG	1A	3282	1/1	0.88	0.08	67,67,67,67	0
56	MG	1A	3358	1/1	0.88	0.15	30,30,30,30	0
56	MG	1a	1601	1/1	0.88	0.45	50,50,50,50	0
56	MG	1A	3456	1/1	0.88	0.14	36,36,36,36	0
56	MG	1A	3170	1/1	0.88	0.22	42,42,42,42	0
56	MG	1A	3253	1/1	0.88	0.28	40,40,40,40	0
56	MG	2x	104	1/1	0.88	0.10	72,72,72,72	0
56	MG	1A	3465	1/1	0.88	0.10	50,50,50,50	0
56	MG	1a	1725	1/1	0.88	0.35	59,59,59,59	0
56	MG	1a	1612	1/1	0.88	0.30	56,56,56,56	0
56	MG	2a	1634	1/1	0.88	0.26	69,69,69,69	0
56	MG	1A	3255	1/1	0.88	0.59	30,30,30,30	0
56	MG	2a	1637	1/1	0.88	0.21	60,60,60,60	0
56	MG	1A	3936	1/1	0.88	0.52	32,32,32,32	0
56	MG	1A	3714	1/1	0.88	0.43	52,52,52,52	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	1Q	201	1/1	0.89	0.21	41,41,41,41	0
56	MG	1a	1691	1/1	0.89	0.08	67,67,67,67	0
56	MG	1Q	202	1/1	0.89	0.17	35,35,35,35	0
56	MG	1A	3546	1/1	0.89	0.08	41,41,41,41	0
56	MG	1A	3182	1/1	0.89	0.20	60,60,60,60	0
56	MG	2A	3263	1/1	0.89	0.22	52,52,52,52	0
56	MG	2A	3109	1/1	0.89	0.17	54,54,54,54	0
56	MG	1A	3760	1/1	0.89	0.18	58,58,58,58	0
56	MG	1A	3763	1/1	0.89	0.18	33,33,33,33	0
56	MG	1A	3108	1/1	0.89	0.60	40,40,40,40	0
56	MG	2A	3510	1/1	0.89	0.16	67,67,67,67	0
56	MG	2A	3276	1/1	0.89	0.19	47,47,47,47	0
56	MG	10	107	1/1	0.89	0.10	54,54,54,54	0
56	MG	2A	3283	1/1	0.89	0.10	56,56,56,56	0
56	MG	1A	3883	1/1	0.89	0.23	47,47,47,47	0
56	MG	1a	1856	1/1	0.89	0.27	62,62,62,62	0
56	MG	2a	1640	1/1	0.89	0.51	71,71,71,71	0
56	MG	1A	3012	1/1	0.89	0.21	35,35,35,35	0
56	MG	1A	3463	1/1	0.89	0.14	31,31,31,31	0
56	MG	2a	1645	1/1	0.89	0.20	68,68,68,68	0
56	MG	19	103	1/1	0.89	0.15	51,51,51,51	0
56	MG	1A	3893	1/1	0.89	1.39	39,39,39,39	0
56	MG	1a	1602	1/1	0.89	0.08	82,82,82,82	0
56	MG	2a	1653	1/1	0.89	0.39	67,67,67,67	0
56	MG	1A	3898	1/1	0.89	0.29	43,43,43,43	0
56	MG	2A	3132	1/1	0.89	0.29	49,49,49,49	0
56	MG	2A	3302	1/1	0.89	0.20	51,51,51,51	0
56	MG	2A	3548	1/1	0.89	0.16	46,46,46,46	0
56	MG	1A	3056	1/1	0.89	0.17	55,55,55,55	0
56	MG	1a	1742	1/1	0.89	0.13	71,71,71,71	0
56	MG	1a	1606	1/1	0.89	0.26	62,62,62,62	0
56	MG	1a	1747	1/1	0.89	0.18	56,56,56,56	0
56	MG	1A	3902	1/1	0.89	0.57	35,35,35,35	0
56	MG	1A	3300	1/1	0.89	0.20	45,45,45,45	0
56	MG	2A	3561	1/1	0.89	0.08	58,58,58,58	0
56	MG	1A	3467	1/1	0.89	0.14	48,48,48,48	0
56	MG	1t	3001	1/1	0.89	0.24	69,69,69,69	0
56	MG	2A	3151	1/1	0.89	0.21	41,41,41,41	0
56	MG	1a	1613	1/1	0.89	0.14	75,75,75,75	0
56	MG	1A	3469	1/1	0.89	0.29	39,39,39,39	0
56	MG	1a	1615	1/1	0.89	0.31	71,71,71,71	0
56	MG	1a	1616	1/1	0.89	0.14	73,73,73,73	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	2A	3571	1/1	0.89	0.16	57,57,57,57	0
56	MG	1A	3379	1/1	0.89	0.16	43,43,43,43	0
56	MG	1a	1622	1/1	0.89	0.23	65,65,65,65	0
56	MG	1A	3661	1/1	0.89	0.30	40,40,40,40	0
56	MG	2A	3014	1/1	0.89	0.38	76,76,76,76	0
56	MG	2A	3020	1/1	0.89	0.64	49,49,49,49	0
56	MG	1A	3150	1/1	0.89	0.89	32,32,32,32	0
56	MG	1A	3043	1/1	0.89	0.61	29,29,29,29	0
56	MG	2A	3355	1/1	0.89	0.39	53,53,53,53	0
56	MG	2A	3356	1/1	0.89	0.27	55,55,55,55	0
56	MG	1A	3085	1/1	0.89	0.50	42,42,42,42	0
56	MG	1A	3270	1/1	0.89	0.18	49,49,49,49	0
56	MG	1A	3029	1/1	0.89	0.19	30,30,30,30	0
56	MG	1a	1635	1/1	0.89	0.41	75,75,75,75	0
56	MG	1A	3318	1/1	0.89	0.12	25,25,25,25	0
56	MG	1A	3399	1/1	0.89	0.13	49,49,49,49	0
56	MG	1a	1783	1/1	0.89	0.41	63,63,63,63	0
56	MG	2a	1721	1/1	0.89	0.21	71,71,71,71	0
56	MG	1A	3400	1/1	0.89	0.07	61,61,61,61	0
56	MG	1a	1643	1/1	0.89	0.14	65,65,65,65	0
56	MG	1A	3499	1/1	0.89	0.34	43,43,43,43	0
56	MG	2A	3655	1/1	0.89	0.12	46,46,46,46	0
56	MG	2a	1731	1/1	0.89	0.08	69,69,69,69	0
56	MG	2A	3396	1/1	0.89	0.23	58,58,58,58	0
56	MG	1A	3412	1/1	0.89	0.23	28,28,28,28	0
56	MG	1B	210	1/1	0.89	0.08	57,57,57,57	0
56	MG	2A	3400	1/1	0.89	0.19	54,54,54,54	0
56	MG	2A	3052	1/1	0.89	0.18	62,62,62,62	0
56	MG	1A	3127	1/1	0.89	0.53	28,28,28,28	0
56	MG	2A	3671	1/1	0.89	0.18	44,44,44,44	0
56	MG	2A	3407	1/1	0.89	0.06	59,59,59,59	0
56	MG	2A	3409	1/1	0.89	0.18	56,56,56,56	0
56	MG	2a	1755	1/1	0.89	0.10	72,72,72,72	0
56	MG	1A	3710	1/1	0.89	0.16	30,30,30,30	0
56	MG	2A	3062	1/1	0.89	0.50	44,44,44,44	0
56	MG	2A	3417	1/1	0.89	0.18	62,62,62,62	0
56	MG	1A	3421	1/1	0.89	0.06	55,55,55,55	0
56	MG	2A	3424	1/1	0.89	0.12	63,63,63,63	0
56	MG	2A	3427	1/1	0.89	0.08	63,63,63,63	0
56	MG	1A	3128	1/1	0.89	0.33	43,43,43,43	0
56	MG	2A	3434	1/1	0.89	0.22	58,58,58,58	0
56	MG	1A	3508	1/1	0.89	0.10	53,53,53,53	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	1A	3340	1/1	0.89	0.22	53,53,53,53	0
56	MG	1A	3247	1/1	0.89	0.25	36,36,36,36	0
56	MG	1A	3612	1/1	0.89	0.19	65,65,65,65	0
56	MG	1A	3347	1/1	0.89	0.12	30,30,30,30	0
56	MG	2a	1778	1/1	0.89	0.17	77,77,77,77	0
56	MG	1A	3614	1/1	0.89	0.27	42,42,42,42	0
56	MG	1A	3431	1/1	0.89	0.18	29,29,29,29	0
56	MG	2G	202	1/1	0.89	0.10	74,74,74,74	0
56	MG	1A	3738	1/1	0.89	0.52	36,36,36,36	0
56	MG	1A	3101	1/1	0.89	0.64	32,32,32,32	0
56	MG	1D	318	1/1	0.89	0.58	51,51,51,51	0
56	MG	2U	201	1/1	0.89	0.12	52,52,52,52	0
56	MG	2A	3455	1/1	0.89	0.13	53,53,53,53	0
56	MG	2A	3224	1/1	0.89	0.34	46,46,46,46	0
56	MG	1A	3527	1/1	0.89	0.23	49,49,49,49	0
56	MG	1F	308	1/1	0.89	0.59	56,56,56,56	0
56	MG	1A	3138	1/1	0.89	0.15	50,50,50,50	0
56	MG	1A	3436	1/1	0.89	0.15	33,33,33,33	0
56	MG	1A	3076	1/1	0.89	0.87	37,37,37,37	0
56	MG	1a	1818	1/1	0.89	0.23	73,73,73,73	0
56	MG	1a	1819	1/1	0.89	0.24	69,69,69,69	0
56	MG	2A	3321	1/1	0.90	0.20	48,48,48,48	0
56	MG	1A	3806	1/1	0.90	0.14	60,60,60,60	0
56	MG	2a	1620	1/1	0.90	0.62	56,56,56,56	0
56	MG	10	102	1/1	0.90	0.19	43,43,43,43	0
56	MG	2A	3536	1/1	0.90	0.11	57,57,57,57	0
56	MG	1A	3487	1/1	0.90	0.33	51,51,51,51	0
56	MG	2a	1626	1/1	0.90	0.28	61,61,61,61	0
56	MG	2A	3540	1/1	0.90	0.12	47,47,47,47	0
56	MG	2A	3333	1/1	0.90	0.33	58,58,58,58	0
56	MG	1A	3917	1/1	0.90	0.24	40,40,40,40	0
56	MG	1A	3811	1/1	0.90	0.21	30,30,30,30	0
56	MG	15	101	1/1	0.90	0.58	32,32,32,32	0
56	MG	1A	3926	1/1	0.90	0.55	45,45,45,45	0
56	MG	1A	3422	1/1	0.90	0.06	40,40,40,40	0
56	MG	1A	3620	1/1	0.90	0.07	48,48,48,48	0
56	MG	1a	1694	1/1	0.90	0.20	64,64,64,64	0
56	MG	2A	3056	1/1	0.90	0.34	41,41,41,41	0
56	MG	1A	3160	1/1	0.90	0.20	40,40,40,40	0
56	MG	2a	1646	1/1	0.90	0.52	66,66,66,66	0
56	MG	2A	3061	1/1	0.90	0.90	61,61,61,61	0
56	MG	1a	1699	1/1	0.90	0.11	68,68,68,68	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	1A	3294	1/1	0.90	0.14	42,42,42,42	0
56	MG	1A	3562	1/1	0.90	0.07	45,45,45,45	0
56	MG	2A	3363	1/1	0.90	0.12	44,44,44,44	0
56	MG	1A	3203	1/1	0.90	0.12	65,65,65,65	0
56	MG	2A	3188	1/1	0.90	0.56	55,55,55,55	0
56	MG	1A	3261	1/1	0.90	0.26	52,52,52,52	0
56	MG	2A	3575	1/1	0.90	0.14	65,65,65,65	0
56	MG	1a	1608	1/1	0.90	0.10	78,78,78,78	0
56	MG	1A	3430	1/1	0.90	0.13	32,32,32,32	0
56	MG	1A	3736	1/1	0.90	0.11	37,37,37,37	0
56	MG	2A	3387	1/1	0.90	0.08	69,69,69,69	0
56	MG	2A	3601	1/1	0.90	0.24	54,54,54,54	0
56	MG	2A	3602	1/1	0.90	0.26	47,47,47,47	0
56	MG	1A	3636	1/1	0.90	0.14	42,42,42,42	0
56	MG	1A	3827	1/1	0.90	0.07	47,47,47,47	0
56	MG	1A	3372	1/1	0.90	0.13	28,28,28,28	0
56	MG	1A	3204	1/1	0.90	0.13	45,45,45,45	0
56	MG	2A	3212	1/1	0.90	0.36	53,53,53,53	0
56	MG	1A	3095	1/1	0.90	0.67	44,44,44,44	0
56	MG	1A	3243	1/1	0.90	0.24	55,55,55,55	0
56	MG	1a	1620	1/1	0.90	0.24	60,60,60,60	0
56	MG	2A	3625	1/1	0.90	0.10	65,65,65,65	0
56	MG	1A	3585	1/1	0.90	0.27	39,39,39,39	0
56	MG	1a	1846	1/1	0.90	0.10	48,48,48,48	0
56	MG	2a	1689	1/1	0.90	0.14	75,75,75,75	0
56	MG	2a	1690	1/1	0.90	0.29	65,65,65,65	0
56	MG	2A	3636	1/1	0.90	0.15	52,52,52,52	0
56	MG	1a	1849	1/1	0.90	0.22	62,62,62,62	0
56	MG	1a	1744	1/1	0.90	0.13	62,62,62,62	0
56	MG	1B	218	1/1	0.90	0.08	39,39,39,39	0
56	MG	2A	3423	1/1	0.90	0.08	56,56,56,56	0
56	MG	2A	3230	1/1	0.90	0.26	55,55,55,55	0
56	MG	2a	1704	1/1	0.90	0.13	70,70,70,70	0
56	MG	2A	3652	1/1	0.90	0.37	41,41,41,41	0
56	MG	1a	1855	1/1	0.90	0.61	52,52,52,52	0
56	MG	1A	3208	1/1	0.90	0.23	45,45,45,45	0
56	MG	1B	225	1/1	0.90	0.30	55,55,55,55	0
56	MG	1a	1859	1/1	0.90	0.21	62,62,62,62	0
56	MG	1A	3245	1/1	0.90	0.28	44,44,44,44	0
56	MG	2A	3664	1/1	0.90	0.30	55,55,55,55	0
56	MG	1A	3147	1/1	0.90	0.54	36,36,36,36	0
56	MG	1A	3382	1/1	0.90	0.15	30,30,30,30	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	1a	1758	1/1	0.90	0.18	70,70,70,70	0
56	MG	1a	1634	1/1	0.90	0.15	63,63,63,63	0
56	MG	1A	3105	1/1	0.90	0.49	42,42,42,42	0
56	MG	2A	3677	1/1	0.90	0.20	57,57,57,57	0
56	MG	2A	3258	1/1	0.90	0.28	58,58,58,58	0
56	MG	2a	1737	1/1	0.90	0.07	74,74,74,74	0
56	MG	2A	3261	1/1	0.90	0.13	52,52,52,52	0
56	MG	1A	3767	1/1	0.90	0.52	43,43,43,43	0
56	MG	2B	3005	1/1	0.90	0.49	77,77,77,77	0
56	MG	1A	3674	1/1	0.90	0.16	39,39,39,39	0
56	MG	1A	3174	1/1	0.90	0.22	56,56,56,56	0
56	MG	1A	3060	1/1	0.90	0.18	33,33,33,33	0
56	MG	1A	3531	1/1	0.90	0.13	52,52,52,52	0
56	MG	1a	1767	1/1	0.90	0.13	72,72,72,72	0
56	MG	1D	319	1/1	0.90	0.14	66,66,66,66	0
56	MG	1A	3683	1/1	0.90	0.09	46,46,46,46	0
56	MG	2D	303	1/1	0.90	0.20	58,58,58,58	0
56	MG	2D	307	1/1	0.90	0.38	46,46,46,46	0
56	MG	2A	3471	1/1	0.90	0.22	48,48,48,48	0
56	MG	1x	108	1/1	0.90	0.11	65,65,65,65	0
56	MG	1F	304	1/1	0.90	0.68	32,32,32,32	0
56	MG	1A	3324	1/1	0.90	0.14	34,34,34,34	0
56	MG	2A	3488	1/1	0.90	0.14	74,74,74,74	0
56	MG	1A	3605	1/1	0.90	0.12	47,47,47,47	0
56	MG	2A	3494	1/1	0.90	0.20	60,60,60,60	0
56	MG	1A	3035	1/1	0.90	0.16	33,33,33,33	0
56	MG	1G	3004	1/1	0.90	0.11	59,59,59,59	0
56	MG	2A	3007	1/1	0.90	0.20	51,51,51,51	0
56	MG	1A	3341	1/1	0.90	0.16	35,35,35,35	0
56	MG	1A	3283	1/1	0.90	0.15	32,32,32,32	0
56	MG	1a	1669	1/1	0.90	0.35	57,57,57,57	0
56	MG	1A	3075	1/1	0.90	0.22	37,37,37,37	0
56	MG	1A	3195	1/1	0.90	0.45	41,41,41,41	0
56	MG	2a	1601	1/1	0.90	0.44	58,58,58,58	0
56	MG	2A	3024	1/1	0.90	0.23	45,45,45,45	0
56	MG	1A	3904	1/1	0.90	0.18	53,53,53,53	0
56	MG	2A	3314	1/1	0.90	0.05	65,65,65,65	0
56	MG	2a	1605	1/1	0.90	0.08	73,73,73,73	0
56	MG	2A	3026	1/1	0.90	0.19	41,41,41,41	0
56	MG	1a	1791	1/1	0.90	0.24	74,74,74,74	0
56	MG	1A	3552	1/1	0.90	0.26	32,32,32,32	0
56	MG	2a	1610	1/1	0.90	0.48	72,72,72,72	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	1U	205	1/1	0.90	0.40	40,40,40,40	0
60	ZN	14	501	1/1	0.90	0.14	89,89,89,89	0
56	MG	2a	1615	1/1	0.90	0.13	63,63,63,63	0
56	MG	2A	3035	1/1	0.90	0.21	70,70,70,70	0
56	MG	2A	3491	1/1	0.91	0.66	58,58,58,58	0
56	MG	1A	3010	1/1	0.91	0.30	45,45,45,45	0
56	MG	1a	1821	1/1	0.91	0.10	76,76,76,76	0
56	MG	2A	3249	1/1	0.91	0.14	76,76,76,76	0
56	MG	1a	1822	1/1	0.91	0.07	60,60,60,60	0
56	MG	1a	1705	1/1	0.91	0.18	51,51,51,51	0
56	MG	1A	3563	1/1	0.91	0.34	23,23,23,23	0
56	MG	1A	3942	1/1	0.91	0.42	55,55,55,55	0
56	MG	1A	3301	1/1	0.91	0.12	40,40,40,40	0
56	MG	2a	1617	1/1	0.91	0.16	51,51,51,51	0
56	MG	1A	3746	1/1	0.91	0.19	40,40,40,40	0
56	MG	1a	1717	1/1	0.91	0.21	67,67,67,67	0
56	MG	1A	3749	1/1	0.91	0.10	45,45,45,45	0
56	MG	1a	1840	1/1	0.91	0.20	67,67,67,67	0
56	MG	1a	1842	1/1	0.91	0.23	62,62,62,62	0
56	MG	2a	1623	1/1	0.91	0.51	49,49,49,49	0
56	MG	1A	3948	1/1	0.91	0.41	44,44,44,44	0
56	MG	2A	3102	1/1	0.91	0.15	48,48,48,48	0
56	MG	2A	3280	1/1	0.91	0.21	42,42,42,42	0
56	MG	1A	3274	1/1	0.91	0.41	41,41,41,41	0
56	MG	1a	1607	1/1	0.91	0.26	60,60,60,60	0
56	MG	1B	203	1/1	0.91	0.14	55,55,55,55	0
56	MG	1A	3037	1/1	0.91	0.35	38,38,38,38	0
56	MG	1A	3222	1/1	0.91	0.15	62,62,62,62	0
56	MG	1A	3835	1/1	0.91	0.08	59,59,59,59	0
56	MG	2A	3537	1/1	0.91	0.08	60,60,60,60	0
56	MG	1a	1857	1/1	0.91	0.09	64,64,64,64	0
56	MG	1A	3690	1/1	0.91	0.23	42,42,42,42	0
56	MG	1A	3573	1/1	0.91	0.22	35,35,35,35	0
56	MG	1a	1739	1/1	0.91	0.57	65,65,65,65	0
56	MG	2a	1648	1/1	0.91	0.14	70,70,70,70	0
56	MG	1A	3574	1/1	0.91	0.14	32,32,32,32	0
56	MG	2A	3123	1/1	0.91	0.30	69,69,69,69	0
56	MG	1A	3024	1/1	0.91	0.62	34,34,34,34	0
56	MG	1A	3850	1/1	0.91	0.19	44,44,44,44	0
56	MG	1A	3003	1/1	0.91	0.18	40,40,40,40	0
56	MG	1A	3854	1/1	0.91	0.57	59,59,59,59	0
56	MG	1a	1623	1/1	0.91	0.23	65,65,65,65	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	1A	3629	1/1	0.91	0.09	64,64,64,64	0
56	MG	2A	3134	1/1	0.91	0.11	68,68,68,68	0
56	MG	1A	3479	1/1	0.91	0.15	33,33,33,33	0
56	MG	1A	3770	1/1	0.91	0.07	50,50,50,50	0
56	MG	1l	201	1/1	0.91	0.19	63,63,63,63	0
56	MG	1A	3707	1/1	0.91	0.18	52,52,52,52	0
56	MG	1o	102	1/1	0.91	0.22	49,49,49,49	0
56	MG	1D	303	1/1	0.91	0.41	41,41,41,41	0
56	MG	1A	3176	1/1	0.91	1.02	33,33,33,33	0
56	MG	2a	1672	1/1	0.91	0.46	52,52,52,52	0
56	MG	2A	3574	1/1	0.91	0.12	60,60,60,60	0
56	MG	2A	3150	1/1	0.91	0.42	46,46,46,46	0
56	MG	1x	103	1/1	0.91	0.21	63,63,63,63	0
56	MG	2A	3153	1/1	0.91	0.42	51,51,51,51	0
56	MG	2A	3598	1/1	0.91	0.10	54,54,54,54	0
56	MG	1A	3709	1/1	0.91	0.18	37,37,37,37	0
56	MG	1A	3586	1/1	0.91	0.39	36,36,36,36	0
56	MG	1x	109	1/1	0.91	0.18	63,63,63,63	0
56	MG	1a	1636	1/1	0.91	1.08	60,60,60,60	0
56	MG	1A	3045	1/1	0.91	0.34	40,40,40,40	0
56	MG	2a	1688	1/1	0.91	0.06	58,58,58,58	0
56	MG	1A	3083	1/1	0.91	0.26	34,34,34,34	0
56	MG	1D	313	1/1	0.91	0.30	41,41,41,41	0
56	MG	2A	3164	1/1	0.91	0.25	46,46,46,46	0
56	MG	1D	317	1/1	0.91	0.66	35,35,35,35	0
56	MG	2A	3360	1/1	0.91	0.14	62,62,62,62	0
56	MG	1a	1644	1/1	0.91	0.25	62,62,62,62	0
56	MG	2A	3008	1/1	0.91	0.18	45,45,45,45	0
56	MG	1A	3061	1/1	0.91	0.18	43,43,43,43	0
56	MG	1a	1777	1/1	0.91	0.15	74,74,74,74	0
56	MG	2a	1711	1/1	0.91	0.63	77,77,77,77	0
56	MG	2A	3374	1/1	0.91	0.17	74,74,74,74	0
56	MG	1A	3326	1/1	0.91	0.19	48,48,48,48	0
56	MG	1A	3888	1/1	0.91	1.05	32,32,32,32	0
56	MG	1a	1780	1/1	0.91	0.14	71,71,71,71	0
56	MG	2A	3023	1/1	0.91	0.18	53,53,53,53	0
56	MG	1F	303	1/1	0.91	0.69	38,38,38,38	0
56	MG	2A	3390	1/1	0.91	0.23	49,49,49,49	0
56	MG	2A	3651	1/1	0.91	0.16	65,65,65,65	0
56	MG	2a	1722	1/1	0.91	0.08	66,66,66,66	0
56	MG	1A	3064	1/1	0.91	0.32	46,46,46,46	0
56	MG	1A	3086	1/1	0.91	0.24	52,52,52,52	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	2A	3397	1/1	0.91	0.20	48,48,48,48	0
56	MG	2A	3659	1/1	0.91	0.11	60,60,60,60	0
56	MG	1A	3794	1/1	0.91	0.06	44,44,44,44	0
56	MG	2A	3179	1/1	0.91	0.60	52,52,52,52	0
56	MG	2a	1734	1/1	0.91	0.22	69,69,69,69	0
56	MG	2A	3029	1/1	0.91	0.17	50,50,50,50	0
56	MG	2A	3401	1/1	0.91	0.07	56,56,56,56	0
56	MG	2a	1741	1/1	0.91	0.18	68,68,68,68	0
56	MG	2a	1743	1/1	0.91	0.20	60,60,60,60	0
56	MG	1a	1664	1/1	0.91	0.34	71,71,71,71	0
56	MG	1A	3342	1/1	0.91	0.26	33,33,33,33	0
56	MG	1a	1789	1/1	0.91	0.25	74,74,74,74	0
56	MG	1A	3721	1/1	0.91	0.14	53,53,53,53	0
56	MG	1A	3344	1/1	0.91	0.10	31,31,31,31	0
56	MG	2A	3676	1/1	0.91	0.20	54,54,54,54	0
56	MG	1N	203	1/1	0.91	0.11	59,59,59,59	0
56	MG	1A	3809	1/1	0.91	0.09	40,40,40,40	0
56	MG	2A	3042	1/1	0.91	0.11	57,57,57,57	0
56	MG	2A	3043	1/1	0.91	0.36	61,61,61,61	0
56	MG	2A	3200	1/1	0.91	0.19	52,52,52,52	0
56	MG	1a	1671	1/1	0.91	0.15	57,57,57,57	0
56	MG	1A	3910	1/1	0.91	0.34	39,39,39,39	0
56	MG	2A	3432	1/1	0.91	0.16	49,49,49,49	0
56	MG	2A	3205	1/1	0.91	0.29	51,51,51,51	0
56	MG	2A	3049	1/1	0.91	0.15	62,62,62,62	0
56	MG	1a	1797	1/1	0.91	0.21	76,76,76,76	0
56	MG	2A	3209	1/1	0.91	0.62	61,61,61,61	0
56	MG	1A	3725	1/1	0.91	0.11	46,46,46,46	0
56	MG	2D	305	1/1	0.91	0.32	46,46,46,46	0
56	MG	1A	3441	1/1	0.91	0.09	40,40,40,40	0
56	MG	1a	1676	1/1	0.91	0.24	54,54,54,54	0
56	MG	2a	1779	1/1	0.91	0.21	67,67,67,67	0
56	MG	2e	201	1/1	0.91	0.28	57,57,57,57	0
56	MG	1A	3814	1/1	0.91	0.08	42,42,42,42	0
56	MG	2A	3218	1/1	0.91	0.57	55,55,55,55	0
56	MG	1U	201	1/1	0.91	0.28	37,37,37,37	0
56	MG	1U	204	1/1	0.91	0.75	35,35,35,35	0
56	MG	1A	3920	1/1	0.91	0.21	47,47,47,47	0
56	MG	2x	101	1/1	0.91	0.08	70,70,70,70	0
56	MG	1V	203	1/1	0.91	0.28	62,62,62,62	0
56	MG	1A	3732	1/1	0.91	0.10	46,46,46,46	0
56	MG	2A	3228	1/1	0.91	0.38	46,46,46,46	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	1A	3070	1/1	0.91	0.29	31,31,31,31	0
56	MG	1A	3168	1/1	0.91	0.27	39,39,39,39	0
56	MG	1A	3929	1/1	0.91	0.57	31,31,31,31	0
56	MG	2A	3234	1/1	0.91	0.20	55,55,55,55	0
56	MG	11	103	1/1	0.91	0.26	41,41,41,41	0
56	MG	2A	3476	1/1	0.91	0.17	57,57,57,57	0
56	MG	1A	3739	1/1	0.91	0.24	28,28,28,28	0
56	MG	1a	1697	1/1	0.91	0.10	55,55,55,55	0
56	MG	1A	3935	1/1	0.91	0.81	38,38,38,38	0
56	MG	1A	3518	1/1	0.92	0.18	37,37,37,37	0
56	MG	2A	3304	1/1	0.92	0.10	53,53,53,53	0
56	MG	1A	3679	1/1	0.92	0.15	32,32,32,32	0
56	MG	1A	3877	1/1	0.92	0.10	35,35,35,35	0
56	MG	1A	3878	1/1	0.92	0.33	51,51,51,51	0
56	MG	2A	3524	1/1	0.92	0.09	42,42,42,42	0
56	MG	1E	304	1/1	0.92	0.15	50,50,50,50	0
56	MG	1E	305	1/1	0.92	0.26	31,31,31,31	0
56	MG	2A	3531	1/1	0.92	0.36	65,65,65,65	0
56	MG	2A	3011	1/1	0.92	0.21	59,59,59,59	0
56	MG	1A	3449	1/1	0.92	0.08	53,53,53,53	0
56	MG	1a	1784	1/1	0.92	0.14	60,60,60,60	0
56	MG	1A	3451	1/1	0.92	0.13	38,38,38,38	0
56	MG	2A	3320	1/1	0.92	0.09	56,56,56,56	0
56	MG	1A	3684	1/1	0.92	0.17	50,50,50,50	0
56	MG	2A	3542	1/1	0.92	0.05	56,56,56,56	0
56	MG	2a	1635	1/1	0.92	0.47	73,73,73,73	0
56	MG	1A	3685	1/1	0.92	0.14	42,42,42,42	0
56	MG	2A	3547	1/1	0.92	0.07	55,55,55,55	0
56	MG	2a	1639	1/1	0.92	0.51	68,68,68,68	0
56	MG	2A	3162	1/1	0.92	0.54	57,57,57,57	0
56	MG	1A	3773	1/1	0.92	0.09	44,44,44,44	0
56	MG	2A	3551	1/1	0.92	0.16	48,48,48,48	0
56	MG	1A	3227	1/1	0.92	0.20	39,39,39,39	0
56	MG	2A	3334	1/1	0.92	0.12	61,61,61,61	0
56	MG	2a	1647	1/1	0.92	0.12	73,73,73,73	0
56	MG	1A	3897	1/1	0.92	0.48	34,34,34,34	0
56	MG	2A	3027	1/1	0.92	0.42	42,42,42,42	0
56	MG	1N	202	1/1	0.92	0.44	46,46,46,46	0
56	MG	2A	3343	1/1	0.92	0.11	58,58,58,58	0
56	MG	1A	3201	1/1	0.92	0.23	25,25,25,25	0
56	MG	1A	3460	1/1	0.92	0.18	44,44,44,44	0
56	MG	1A	3533	1/1	0.92	0.32	51,51,51,51	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	1A	3782	1/1	0.92	0.19	44,44,44,44	0
56	MG	2a	1659	1/1	0.92	0.39	77,77,77,77	0
56	MG	1A	3157	1/1	0.92	0.11	33,33,33,33	0
56	MG	1R	204	1/1	0.92	0.20	39,39,39,39	0
56	MG	1A	3908	1/1	0.92	0.18	41,41,41,41	0
56	MG	1A	3141	1/1	0.92	0.14	43,43,43,43	0
56	MG	1U	203	1/1	0.92	0.49	36,36,36,36	0
56	MG	2a	1667	1/1	0.92	0.13	66,66,66,66	0
56	MG	1A	3703	1/1	0.92	0.59	43,43,43,43	0
56	MG	2A	3581	1/1	0.92	0.19	67,67,67,67	0
56	MG	1A	3388	1/1	0.92	0.09	42,42,42,42	0
56	MG	2A	3592	1/1	0.92	0.11	47,47,47,47	0
56	MG	1A	3262	1/1	0.92	0.24	42,42,42,42	0
56	MG	2A	3596	1/1	0.92	0.11	56,56,56,56	0
56	MG	1A	3919	1/1	0.92	0.46	41,41,41,41	0
56	MG	1A	3343	1/1	0.92	0.17	25,25,25,25	0
56	MG	2A	3373	1/1	0.92	0.16	45,45,45,45	0
56	MG	1A	3159	1/1	0.92	0.68	38,38,38,38	0
56	MG	2A	3376	1/1	0.92	0.14	50,50,50,50	0
56	MG	1a	1692	1/1	0.92	0.15	70,70,70,70	0
56	MG	2a	1682	1/1	0.92	0.28	58,58,58,58	0
56	MG	1a	1693	1/1	0.92	0.17	75,75,75,75	0
56	MG	2A	3605	1/1	0.92	0.14	49,49,49,49	0
56	MG	1A	3474	1/1	0.92	0.15	56,56,56,56	0
56	MG	1a	1695	1/1	0.92	0.22	67,67,67,67	0
56	MG	2A	3386	1/1	0.92	0.30	48,48,48,48	0
56	MG	1A	3094	1/1	0.92	0.25	36,36,36,36	0
56	MG	2A	3198	1/1	0.92	0.43	59,59,59,59	0
56	MG	1A	3163	1/1	0.92	0.17	33,33,33,33	0
56	MG	1A	3808	1/1	0.92	0.16	55,55,55,55	0
56	MG	1a	1702	1/1	0.92	0.12	51,51,51,51	0
56	MG	2A	3068	1/1	0.92	0.54	51,51,51,51	0
56	MG	2a	1702	1/1	0.92	0.16	62,62,62,62	0
56	MG	2A	3631	1/1	0.92	0.09	57,57,57,57	0
56	MG	1A	3932	1/1	0.92	0.26	51,51,51,51	0
56	MG	2A	3638	1/1	0.92	0.09	58,58,58,58	0
56	MG	1A	3026	1/1	0.92	0.76	32,32,32,32	0
56	MG	2A	3208	1/1	0.92	0.24	50,50,50,50	0
56	MG	1A	3102	1/1	0.92	0.32	31,31,31,31	0
56	MG	2A	3648	1/1	0.92	0.13	64,64,64,64	0
56	MG	1A	3716	1/1	0.92	0.15	60,60,60,60	0
56	MG	1A	3485	1/1	0.92	0.09	47,47,47,47	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	2A	3075	1/1	0.92	0.35	42,42,42,42	0
56	MG	1A	3273	1/1	0.92	0.42	41,41,41,41	0
56	MG	1a	1718	1/1	0.92	0.14	73,73,73,73	0
56	MG	1A	3130	1/1	0.92	0.70	31,31,31,31	0
56	MG	1A	3359	1/1	0.92	0.09	34,34,34,34	0
56	MG	2a	1726	1/1	0.92	0.10	70,70,70,70	0
56	MG	2A	3420	1/1	0.92	0.10	64,64,64,64	0
56	MG	1A	3360	1/1	0.92	0.22	44,44,44,44	0
56	MG	1A	3363	1/1	0.92	0.08	54,54,54,54	0
56	MG	2A	3425	1/1	0.92	0.16	48,48,48,48	0
56	MG	2A	3426	1/1	0.92	0.37	60,60,60,60	0
56	MG	2a	1735	1/1	0.92	0.16	74,74,74,74	0
56	MG	2A	3226	1/1	0.92	0.34	56,56,56,56	0
56	MG	1A	3727	1/1	0.92	0.22	67,67,67,67	0
56	MG	1a	1848	1/1	0.92	0.10	69,69,69,69	0
56	MG	2a	1742	1/1	0.92	0.15	70,70,70,70	0
56	MG	1A	3728	1/1	0.92	0.15	38,38,38,38	0
56	MG	1A	3729	1/1	0.92	0.33	32,32,32,32	0
56	MG	2A	3232	1/1	0.92	0.40	50,50,50,50	0
56	MG	2A	3090	1/1	0.92	0.08	58,58,58,58	0
56	MG	1B	208	1/1	0.92	0.22	54,54,54,54	0
56	MG	1a	1734	1/1	0.92	0.12	54,54,54,54	0
56	MG	2A	3446	1/1	0.92	0.10	60,60,60,60	0
56	MG	2a	1753	1/1	0.92	0.14	58,58,58,58	0
56	MG	1a	1735	1/1	0.92	0.06	62,62,62,62	0
56	MG	1A	3572	1/1	0.92	0.15	35,35,35,35	0
56	MG	2A	3242	1/1	0.92	0.23	55,55,55,55	0
56	MG	1A	3368	1/1	0.92	0.18	58,58,58,58	0
56	MG	1A	3829	1/1	0.92	0.07	40,40,40,40	0
56	MG	2A	3105	1/1	0.92	0.14	42,42,42,42	0
56	MG	2a	1762	1/1	0.92	0.07	79,79,79,79	0
56	MG	1a	1740	1/1	0.92	0.16	70,70,70,70	0
56	MG	1b	3001	1/1	0.92	0.19	73,73,73,73	0
56	MG	2A	3252	1/1	0.92	0.15	41,41,41,41	0
56	MG	1a	1618	1/1	0.92	0.16	73,73,73,73	0
56	MG	1A	3735	1/1	0.92	0.13	55,55,55,55	0
56	MG	1A	3641	1/1	0.92	0.15	40,40,40,40	0
56	MG	1A	3249	1/1	0.92	0.19	48,48,48,48	0
56	MG	2A	3115	1/1	0.92	0.23	46,46,46,46	0
56	MG	1A	3041	1/1	0.92	0.19	46,46,46,46	0
56	MG	1B	219	1/1	0.92	0.08	42,42,42,42	0
56	MG	2A	3479	1/1	0.92	0.25	49,49,49,49	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	1e	204	1/1	0.92	0.07	63,63,63,63	0
56	MG	1A	3740	1/1	0.92	0.13	47,47,47,47	0
56	MG	2A	3489	1/1	0.92	0.35	55,55,55,55	0
56	MG	1a	1626	1/1	0.92	0.11	60,60,60,60	0
56	MG	1A	3433	1/1	0.92	0.16	48,48,48,48	0
56	MG	1A	3580	1/1	0.92	0.19	48,48,48,48	0
56	MG	1A	3581	1/1	0.92	0.35	29,29,29,29	0
56	MG	1a	1631	1/1	0.92	1.46	72,72,72,72	0
56	MG	28	102	1/1	0.92	0.21	49,49,49,49	0
56	MG	2A	3497	1/1	0.92	0.19	51,51,51,51	0
56	MG	1A	3582	1/1	0.92	0.41	39,39,39,39	0
56	MG	1A	3136	1/1	0.92	0.32	33,33,33,33	0
56	MG	1A	3750	1/1	0.92	0.11	44,44,44,44	0
56	MG	1A	3079	1/1	0.92	0.22	39,39,39,39	0
56	MG	1x	105	1/1	0.92	0.17	64,64,64,64	0
56	MG	1A	3662	1/1	0.92	0.09	39,39,39,39	0
56	MG	1A	3156	1/1	0.92	0.21	41,41,41,41	0
56	MG	1A	3321	1/1	0.92	0.21	26,26,26,26	0
56	MG	1A	3322	1/1	0.92	0.08	68,68,68,68	0
56	MG	2l	101	1/1	0.93	0.15	54,54,54,54	0
56	MG	1A	3065	1/1	0.93	0.27	37,37,37,37	0
56	MG	1A	3647	1/1	0.93	0.11	28,28,28,28	0
56	MG	1A	3504	1/1	0.93	0.17	44,44,44,44	0
56	MG	1A	3737	1/1	0.93	0.24	31,31,31,31	0
56	MG	1A	3842	1/1	0.93	0.29	47,47,47,47	0
56	MG	1A	3111	1/1	0.93	0.47	30,30,30,30	0
56	MG	1A	3657	1/1	0.93	0.35	41,41,41,41	0
56	MG	2A	3273	1/1	0.93	0.29	61,61,61,61	0
56	MG	1a	1748	1/1	0.93	0.10	74,74,74,74	0
56	MG	1e	203	1/1	0.93	0.36	63,63,63,63	0
56	MG	2A	3119	1/1	0.93	0.22	49,49,49,49	0
56	MG	1A	3166	1/1	0.93	0.78	36,36,36,36	0
56	MG	1A	3659	1/1	0.93	0.35	38,38,38,38	0
56	MG	1A	3040	1/1	0.93	0.21	49,49,49,49	0
56	MG	1A	3510	1/1	0.93	0.10	52,52,52,52	0
56	MG	1A	3238	1/1	0.93	0.08	65,65,65,65	0
56	MG	1n	101	1/1	0.93	0.33	71,71,71,71	0
56	MG	1A	3587	1/1	0.93	0.23	45,45,45,45	0
56	MG	2A	3129	1/1	0.93	0.23	49,49,49,49	0
56	MG	2A	3517	1/1	0.93	0.12	60,60,60,60	0
56	MG	1A	3667	1/1	0.93	0.23	37,37,37,37	0
56	MG	2a	1624	1/1	0.93	0.47	64,64,64,64	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
56	MG	1A	3672	1/1	0.93	0.09	45,45,45,45	0
56	MG	1D	310	1/1	0.93	0.20	36,36,36,36	0
56	MG	2A	3135	1/1	0.93	0.55	43,43,43,43	0
56	MG	1A	3119	1/1	0.93	0.33	30,30,30,30	0
56	MG	2A	3523	1/1	0.93	0.08	57,57,57,57	0
56	MG	2A	3307	1/1	0.93	0.10	48,48,48,48	0
56	MG	1D	312	1/1	0.93	0.69	48,48,48,48	0
56	MG	2A	3528	1/1	0.93	0.55	51,51,51,51	0
56	MG	2A	3140	1/1	0.93	0.34	65,65,65,65	0
56	MG	1A	3753	1/1	0.93	0.18	51,51,51,51	0
56	MG	1x	106	1/1	0.93	0.22	62,62,62,62	0
56	MG	2A	3533	1/1	0.93	0.07	60,60,60,60	0
56	MG	1A	3592	1/1	0.93	0.07	43,43,43,43	0
56	MG	1A	3121	1/1	0.93	0.25	68,68,68,68	0
56	MG	2a	1644	1/1	0.93	0.69	69,69,69,69	0
56	MG	2A	3538	1/1	0.93	0.08	56,56,56,56	0
56	MG	1A	3521	1/1	0.93	0.11	44,44,44,44	0
56	MG	1a	1649	1/1	0.93	0.18	70,70,70,70	0
56	MG	1A	3071	1/1	0.93	0.56	32,32,32,32	0
56	MG	1A	3880	1/1	0.93	0.24	35,35,35,35	0
56	MG	2A	3154	1/1	0.93	0.37	48,48,48,48	0
56	MG	1A	3205	1/1	0.93	0.19	30,30,30,30	0
56	MG	1A	3766	1/1	0.93	0.28	42,42,42,42	0
56	MG	1A	3461	1/1	0.93	0.13	30,30,30,30	0
56	MG	1a	1663	1/1	0.93	0.15	74,74,74,74	0
56	MG	2a	1657	1/1	0.93	0.19	69,69,69,69	0
56	MG	1a	1782	1/1	0.93	0.39	58,58,58,58	0
56	MG	1A	3030	1/1	0.93	0.12	28,28,28,28	0
56	MG	1A	3889	1/1	0.93	0.18	35,35,35,35	0
56	MG	1A	3688	1/1	0.93	0.17	40,40,40,40	0
56	MG	1A	3892	1/1	0.93	0.34	31,31,31,31	0
56	MG	2A	3345	1/1	0.93	0.13	64,64,64,64	0
56	MG	2A	3347	1/1	0.93	0.17	42,42,42,42	0
56	MG	1A	3689	1/1	0.93	0.14	37,37,37,37	0
56	MG	1H	8002	1/1	0.93	0.23	44,44,44,44	0
56	MG	1A	3895	1/1	0.93	0.19	35,35,35,35	0
56	MG	1A	3772	1/1	0.93	0.09	45,45,45,45	0
56	MG	1A	3032	1/1	0.93	0.50	35,35,35,35	0
56	MG	1A	3691	1/1	0.93	0.11	48,48,48,48	0
56	MG	1Q	203	1/1	0.93	0.30	47,47,47,47	0
56	MG	1Q	204	1/1	0.93	0.16	44,44,44,44	0
56	MG	1A	3009	1/1	0.93	0.23	27,27,27,27	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	2A	3579	1/1	0.93	0.36	50,50,50,50	0
56	MG	2A	3359	1/1	0.93	0.10	47,47,47,47	0
56	MG	2A	3583	1/1	0.93	0.13	68,68,68,68	0
56	MG	2a	1680	1/1	0.93	0.66	58,58,58,58	0
56	MG	2A	3033	1/1	0.93	0.10	58,58,58,58	0
56	MG	1a	1681	1/1	0.93	0.21	56,56,56,56	0
56	MG	1a	1798	1/1	0.93	0.15	71,71,71,71	0
56	MG	1A	3077	1/1	0.93	0.53	41,41,41,41	0
56	MG	1a	1683	1/1	0.93	0.22	67,67,67,67	0
56	MG	1A	3694	1/1	0.93	0.07	39,39,39,39	0
56	MG	1A	3695	1/1	0.93	0.08	38,38,38,38	0
56	MG	1A	3155	1/1	0.93	0.40	32,32,32,32	0
56	MG	2a	1691	1/1	0.93	0.10	60,60,60,60	0
56	MG	2A	3377	1/1	0.93	0.10	49,49,49,49	0
56	MG	2A	3045	1/1	0.93	0.18	56,56,56,56	0
56	MG	1A	3911	1/1	0.93	0.23	28,28,28,28	0
56	MG	2A	3186	1/1	0.93	0.25	59,59,59,59	0
56	MG	1A	3346	1/1	0.93	0.14	43,43,43,43	0
56	MG	2A	3048	1/1	0.93	0.31	51,51,51,51	0
56	MG	2A	3612	1/1	0.93	0.09	51,51,51,51	0
56	MG	1A	3700	1/1	0.93	0.19	35,35,35,35	0
56	MG	2a	1708	1/1	0.93	0.15	56,56,56,56	0
56	MG	1A	3473	1/1	0.93	0.20	39,39,39,39	0
56	MG	1A	3611	1/1	0.93	0.14	50,50,50,50	0
56	MG	2A	3392	1/1	0.93	0.19	52,52,52,52	0
56	MG	2A	3394	1/1	0.93	0.20	62,62,62,62	0
56	MG	1a	1811	1/1	0.93	0.07	73,73,73,73	0
56	MG	2a	1716	1/1	0.93	0.17	72,72,72,72	0
56	MG	2A	3199	1/1	0.93	0.23	56,56,56,56	0
56	MG	1A	3704	1/1	0.93	0.34	36,36,36,36	0
56	MG	1A	3547	1/1	0.93	0.09	38,38,38,38	0
56	MG	2A	3203	1/1	0.93	0.08	71,71,71,71	0
56	MG	1A	3413	1/1	0.93	0.24	24,24,24,24	0
56	MG	1a	1696	1/1	0.93	0.37	58,58,58,58	0
56	MG	1A	3796	1/1	0.93	0.41	37,37,37,37	0
56	MG	1A	3928	1/1	0.93	0.88	35,35,35,35	0
56	MG	2A	3065	1/1	0.93	0.23	47,47,47,47	0
56	MG	1A	3477	1/1	0.93	0.13	49,49,49,49	0
56	MG	15	103	1/1	0.93	0.10	39,39,39,39	0
56	MG	2a	1732	1/1	0.93	0.09	74,74,74,74	0
56	MG	2A	3414	1/1	0.93	0.14	53,53,53,53	0
56	MG	2A	3653	1/1	0.93	0.72	52,52,52,52	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	2A	3654	1/1	0.93	0.86	50,50,50,50	0
56	MG	1a	1704	1/1	0.93	0.06	63,63,63,63	0
56	MG	1A	3104	1/1	0.93	1.00	32,32,32,32	0
56	MG	1a	1825	1/1	0.93	0.07	66,66,66,66	0
56	MG	2A	3422	1/1	0.93	0.12	54,54,54,54	0
56	MG	1A	3256	1/1	0.93	1.31	48,48,48,48	0
56	MG	2A	3219	1/1	0.93	0.25	45,45,45,45	0
56	MG	1A	3218	1/1	0.93	0.55	35,35,35,35	0
56	MG	1a	1829	1/1	0.93	0.11	55,55,55,55	0
56	MG	1A	3622	1/1	0.93	0.12	56,56,56,56	0
56	MG	2A	3430	1/1	0.93	0.07	56,56,56,56	0
56	MG	1a	1832	1/1	0.93	0.05	73,73,73,73	0
56	MG	1a	1712	1/1	0.93	0.20	70,70,70,70	0
56	MG	1A	3219	1/1	0.93	0.17	34,34,34,34	0
56	MG	2A	3435	1/1	0.93	0.10	54,54,54,54	0
56	MG	2a	1756	1/1	0.93	0.27	73,73,73,73	0
56	MG	2A	3082	1/1	0.93	0.14	47,47,47,47	0
56	MG	2B	3002	1/1	0.93	0.22	72,72,72,72	0
56	MG	1A	3129	1/1	0.93	0.65	30,30,30,30	0
56	MG	1A	3049	1/1	0.93	0.23	28,28,28,28	0
56	MG	2A	3231	1/1	0.93	0.09	64,64,64,64	0
56	MG	2B	3009	1/1	0.93	0.10	66,66,66,66	0
56	MG	2A	3085	1/1	0.93	0.30	62,62,62,62	0
56	MG	1A	3223	1/1	0.93	0.16	46,46,46,46	0
56	MG	1A	3489	1/1	0.93	0.12	32,32,32,32	0
56	MG	1a	1844	1/1	0.93	0.07	68,68,68,68	0
56	MG	1A	3034	1/1	0.93	0.36	45,45,45,45	0
56	MG	1A	3265	1/1	0.93	0.33	32,32,32,32	0
56	MG	1A	3314	1/1	0.93	0.17	32,32,32,32	0
56	MG	2A	3454	1/1	0.93	0.12	60,60,60,60	0
56	MG	1A	3134	1/1	0.93	0.32	38,38,38,38	0
56	MG	2A	3456	1/1	0.93	0.20	63,63,63,63	0
56	MG	2a	1780	1/1	0.93	0.17	70,70,70,70	0
56	MG	2A	3244	1/1	0.93	0.06	58,58,58,58	0
56	MG	2E	302	1/1	0.93	0.18	52,52,52,52	0
56	MG	1a	1731	1/1	0.93	0.21	63,63,63,63	0
56	MG	2A	3462	1/1	0.93	0.24	66,66,66,66	0
56	MG	2F	301	1/1	0.93	0.28	45,45,45,45	0
56	MG	1A	3640	1/1	0.93	0.41	43,43,43,43	0
56	MG	2F	303	1/1	0.93	0.36	50,50,50,50	0
56	MG	2A	3464	1/1	0.93	0.13	65,65,65,65	0
56	MG	1A	3497	1/1	0.93	0.23	45,45,45,45	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	2A	3101	1/1	0.93	0.44	47,47,47,47	0
56	MG	1A	3826	1/1	0.93	0.09	47,47,47,47	0
56	MG	1A	3434	1/1	0.93	0.14	38,38,38,38	0
56	MG	2T	3003	1/1	0.93	0.32	56,56,56,56	0
56	MG	2A	3472	1/1	0.93	0.14	68,68,68,68	0
56	MG	1A	3374	1/1	0.93	0.09	31,31,31,31	0
58	MPD	1A	3907	8/8	0.93	0.21	51,53,55,56	0
56	MG	2V	202	1/1	0.93	0.46	53,53,53,53	0
59	ARG	1B	229	12/12	0.93	0.31	41,46,51,52	0
56	MG	2A	3255	1/1	0.93	0.10	69,69,69,69	0
60	ZN	1n	102	1/1	0.93	0.09	76,76,76,76	0
56	MG	2A	3477	1/1	0.93	0.21	50,50,50,50	0
56	MG	2A	3257	1/1	0.93	0.11	46,46,46,46	0
56	MG	2B	3007	1/1	0.94	0.23	63,63,63,63	0
56	MG	1A	3475	1/1	0.94	0.07	32,32,32,32	0
56	MG	1a	1730	1/1	0.94	0.07	55,55,55,55	0
56	MG	1V	201	1/1	0.94	0.38	45,45,45,45	0
56	MG	1A	3761	1/1	0.94	0.07	45,45,45,45	0
56	MG	2A	3408	1/1	0.94	0.06	66,66,66,66	0
56	MG	2B	3014	1/1	0.94	0.05	64,64,64,64	0
56	MG	1W	3002	1/1	0.94	0.21	41,41,41,41	0
56	MG	1x	112	1/1	0.94	0.37	65,65,65,65	0
56	MG	1X	101	1/1	0.94	0.12	39,39,39,39	0
56	MG	2A	3412	1/1	0.94	0.06	47,47,47,47	0
56	MG	1A	3894	1/1	0.94	0.08	53,53,53,53	0
56	MG	2D	306	1/1	0.94	0.41	54,54,54,54	0
56	MG	2A	3181	1/1	0.94	0.38	57,57,57,57	0
56	MG	1A	3762	1/1	0.94	0.11	45,45,45,45	0
56	MG	2E	301	1/1	0.94	0.36	45,45,45,45	0
56	MG	1A	3392	1/1	0.94	0.09	57,57,57,57	0
56	MG	10	106	1/1	0.94	0.09	46,46,46,46	0
56	MG	2E	306	1/1	0.94	0.08	46,46,46,46	0
56	MG	1A	3058	1/1	0.94	0.12	52,52,52,52	0
56	MG	2A	3010	1/1	0.94	0.28	43,43,43,43	0
56	MG	1A	3567	1/1	0.94	0.15	52,52,52,52	0
56	MG	1a	1743	1/1	0.94	0.26	73,73,73,73	0
56	MG	2A	3189	1/1	0.94	0.15	49,49,49,49	0
56	MG	2A	3428	1/1	0.94	0.09	57,57,57,57	0
56	MG	2A	3015	1/1	0.94	0.20	51,51,51,51	0
56	MG	2O	201	1/1	0.94	0.13	54,54,54,54	0
56	MG	1A	3664	1/1	0.94	0.13	44,44,44,44	0
56	MG	2A	3192	1/1	0.94	0.50	50,50,50,50	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	1A	3665	1/1	0.94	0.07	46,46,46,46	0
56	MG	2T	3004	1/1	0.94	0.17	50,50,50,50	0
56	MG	1A	3139	1/1	0.94	0.17	33,33,33,33	0
56	MG	2A	3436	1/1	0.94	0.18	41,41,41,41	0
56	MG	1A	3480	1/1	0.94	0.08	35,35,35,35	0
56	MG	17	101	1/1	0.94	0.08	36,36,36,36	0
56	MG	2A	3440	1/1	0.94	0.06	55,55,55,55	0
56	MG	18	101	1/1	0.94	0.11	49,49,49,49	0
56	MG	20	8001	1/1	0.94	0.10	60,60,60,60	0
56	MG	2A	3202	1/1	0.94	0.64	52,52,52,52	0
56	MG	1A	3290	1/1	0.94	0.11	34,34,34,34	0
56	MG	28	101	1/1	0.94	0.15	62,62,62,62	0
56	MG	1A	3408	1/1	0.94	0.25	42,42,42,42	0
56	MG	1A	3775	1/1	0.94	0.14	36,36,36,36	0
56	MG	1A	3021	1/1	0.94	0.47	36,36,36,36	0
56	MG	1a	1603	1/1	0.94	0.36	64,64,64,64	0
56	MG	2A	3031	1/1	0.94	0.28	56,56,56,56	0
56	MG	2A	3452	1/1	0.94	0.18	66,66,66,66	0
56	MG	1A	3777	1/1	0.94	0.34	39,39,39,39	0
56	MG	2A	3210	1/1	0.94	0.26	42,42,42,42	0
56	MG	1a	1762	1/1	0.94	0.15	71,71,71,71	0
56	MG	1A	3486	1/1	0.94	0.19	46,46,46,46	0
56	MG	2a	1612	1/1	0.94	0.26	66,66,66,66	0
56	MG	1A	3202	1/1	0.94	0.19	29,29,29,29	0
56	MG	2A	3458	1/1	0.94	0.26	42,42,42,42	0
56	MG	2A	3214	1/1	0.94	0.49	49,49,49,49	0
56	MG	1A	3921	1/1	0.94	0.09	55,55,55,55	0
56	MG	1A	3780	1/1	0.94	0.10	44,44,44,44	0
56	MG	1A	3924	1/1	0.94	0.20	51,51,51,51	0
56	MG	1A	3925	1/1	0.94	0.42	42,42,42,42	0
56	MG	1A	3178	1/1	0.94	0.33	37,37,37,37	0
56	MG	2A	3044	1/1	0.94	0.17	61,61,61,61	0
56	MG	1A	3420	1/1	0.94	0.11	43,43,43,43	0
56	MG	1A	3048	1/1	0.94	0.57	40,40,40,40	0
56	MG	1A	3687	1/1	0.94	0.11	46,46,46,46	0
56	MG	1A	3011	1/1	0.94	0.11	37,37,37,37	0
56	MG	1A	3931	1/1	0.94	0.41	42,42,42,42	0
56	MG	1A	3492	1/1	0.94	0.16	45,45,45,45	0
56	MG	2a	1631	1/1	0.94	0.62	64,64,64,64	0
56	MG	1A	3934	1/1	0.94	0.09	44,44,44,44	0
56	MG	2A	3480	1/1	0.94	0.20	49,49,49,49	0
56	MG	1a	1621	1/1	0.94	0.22	71,71,71,71	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	2A	3054	1/1	0.94	0.73	66,66,66,66	0
56	MG	1A	3352	1/1	0.94	0.08	40,40,40,40	0
56	MG	1A	3424	1/1	0.94	0.19	51,51,51,51	0
56	MG	2a	1638	1/1	0.94	0.23	71,71,71,71	0
56	MG	1A	3588	1/1	0.94	0.12	33,33,33,33	0
56	MG	2A	3239	1/1	0.94	0.17	63,63,63,63	0
56	MG	1A	3941	1/1	0.94	0.13	49,49,49,49	0
56	MG	2A	3241	1/1	0.94	0.32	45,45,45,45	0
56	MG	1A	3206	1/1	0.94	0.19	35,35,35,35	0
56	MG	1A	3356	1/1	0.94	0.15	26,26,26,26	0
56	MG	1A	3797	1/1	0.94	0.21	45,45,45,45	0
56	MG	1A	3946	1/1	0.94	0.37	29,29,29,29	0
56	MG	1A	3802	1/1	0.94	0.12	54,54,54,54	0
56	MG	1A	3230	1/1	0.94	0.42	36,36,36,36	0
56	MG	1A	3145	1/1	0.94	0.17	38,38,38,38	0
56	MG	2A	3509	1/1	0.94	0.12	59,59,59,59	0
56	MG	1A	3310	1/1	0.94	0.11	30,30,30,30	0
56	MG	1A	3311	1/1	0.94	0.12	28,28,28,28	0
56	MG	2a	1655	1/1	0.94	0.15	68,68,68,68	0
56	MG	2A	3073	1/1	0.94	0.34	50,50,50,50	0
56	MG	1A	3362	1/1	0.94	0.15	41,41,41,41	0
56	MG	1B	207	1/1	0.94	0.23	45,45,45,45	0
56	MG	2A	3076	1/1	0.94	0.78	49,49,49,49	0
56	MG	2a	1660	1/1	0.94	0.33	81,81,81,81	0
56	MG	1A	3236	1/1	0.94	0.69	47,47,47,47	0
56	MG	1A	3364	1/1	0.94	0.10	39,39,39,39	0
56	MG	2A	3079	1/1	0.94	0.24	51,51,51,51	0
56	MG	1A	3512	1/1	0.94	0.09	54,54,54,54	0
56	MG	1a	1645	1/1	0.94	0.67	59,59,59,59	0
56	MG	2A	3525	1/1	0.94	0.13	55,55,55,55	0
56	MG	1A	3112	1/1	0.94	0.45	37,37,37,37	0
56	MG	1A	3370	1/1	0.94	0.18	35,35,35,35	0
56	MG	2A	3274	1/1	0.94	0.13	54,54,54,54	0
56	MG	1A	3063	1/1	0.94	0.21	37,37,37,37	0
56	MG	1a	1807	1/1	0.94	0.15	56,56,56,56	0
56	MG	1A	3520	1/1	0.94	0.22	40,40,40,40	0
56	MG	1A	3027	1/1	0.94	0.70	39,39,39,39	0
56	MG	2A	3285	1/1	0.94	0.24	49,49,49,49	0
56	MG	2a	1676	1/1	0.94	0.10	68,68,68,68	0
56	MG	2A	3288	1/1	0.94	0.21	41,41,41,41	0
56	MG	1A	3442	1/1	0.94	0.06	61,61,61,61	0
56	MG	1A	3523	1/1	0.94	0.16	57,57,57,57	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	1a	1812	1/1	0.94	0.26	67,67,67,67	0
56	MG	1A	3443	1/1	0.94	0.11	35,35,35,35	0
56	MG	2A	3092	1/1	0.94	0.66	61,61,61,61	0
56	MG	2A	3546	1/1	0.94	0.05	56,56,56,56	0
56	MG	1a	1661	1/1	0.94	0.49	66,66,66,66	0
56	MG	2A	3297	1/1	0.94	0.20	43,43,43,43	0
56	MG	1a	1662	1/1	0.94	0.26	70,70,70,70	0
56	MG	1A	3444	1/1	0.94	0.20	31,31,31,31	0
56	MG	1A	3526	1/1	0.94	0.17	36,36,36,36	0
56	MG	2A	3554	1/1	0.94	0.08	63,63,63,63	0
56	MG	1A	3120	1/1	0.94	0.06	55,55,55,55	0
56	MG	1B	230	1/1	0.94	0.09	55,55,55,55	0
56	MG	1A	3214	1/1	0.94	0.31	30,30,30,30	0
56	MG	2A	3306	1/1	0.94	0.28	59,59,59,59	0
56	MG	2A	3106	1/1	0.94	0.23	49,49,49,49	0
56	MG	1A	3453	1/1	0.94	0.15	46,46,46,46	0
56	MG	2A	3309	1/1	0.94	0.34	61,61,61,61	0
56	MG	2A	3310	1/1	0.94	0.15	48,48,48,48	0
56	MG	1A	3834	1/1	0.94	0.07	47,47,47,47	0
56	MG	1A	3534	1/1	0.94	0.14	36,36,36,36	0
56	MG	2A	3313	1/1	0.94	0.09	44,44,44,44	0
56	MG	1A	3190	1/1	0.94	0.28	44,44,44,44	0
56	MG	1a	1673	1/1	0.94	0.17	53,53,53,53	0
56	MG	1A	3216	1/1	0.94	0.76	34,34,34,34	0
56	MG	1A	3843	1/1	0.94	0.12	29,29,29,29	0
56	MG	2A	3576	1/1	0.94	0.11	70,70,70,70	0
56	MG	2A	3577	1/1	0.94	0.09	48,48,48,48	0
56	MG	1A	3846	1/1	0.94	0.18	31,31,31,31	0
56	MG	1a	1833	1/1	0.94	0.09	73,73,73,73	0
56	MG	1A	3539	1/1	0.94	0.20	53,53,53,53	0
56	MG	1a	1837	1/1	0.94	0.16	57,57,57,57	0
56	MG	1D	316	1/1	0.94	0.33	34,34,34,34	0
56	MG	2A	3594	1/1	0.94	0.19	82,82,82,82	0
56	MG	2A	3323	1/1	0.94	0.18	50,50,50,50	0
56	MG	1A	3540	1/1	0.94	0.12	42,42,42,42	0
56	MG	1A	3541	1/1	0.94	0.23	35,35,35,35	0
56	MG	2A	3332	1/1	0.94	0.27	43,43,43,43	0
56	MG	1a	1841	1/1	0.94	0.26	67,67,67,67	0
56	MG	1A	3635	1/1	0.94	0.09	35,35,35,35	0
56	MG	1A	3544	1/1	0.94	0.15	59,59,59,59	0
56	MG	1A	3637	1/1	0.94	0.25	33,33,33,33	0
56	MG	2A	3337	1/1	0.94	0.07	60,60,60,60	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	2A	3338	1/1	0.94	0.31	40,40,40,40	0
56	MG	2A	3128	1/1	0.94	0.19	51,51,51,51	0
56	MG	1A	3217	1/1	0.94	0.73	33,33,33,33	0
56	MG	2A	3131	1/1	0.94	0.34	63,63,63,63	0
56	MG	1a	1847	1/1	0.94	0.06	72,72,72,72	0
56	MG	2a	1746	1/1	0.94	0.09	71,71,71,71	0
56	MG	2A	3615	1/1	0.94	0.07	63,63,63,63	0
56	MG	2A	3616	1/1	0.94	0.18	73,73,73,73	0
56	MG	1A	3323	1/1	0.94	0.07	42,42,42,42	0
56	MG	1A	3866	1/1	0.94	0.28	36,36,36,36	0
56	MG	1F	305	1/1	0.94	0.44	28,28,28,28	0
56	MG	1F	307	1/1	0.94	0.20	36,36,36,36	0
56	MG	1A	3250	1/1	0.94	0.33	48,48,48,48	0
56	MG	1A	3325	1/1	0.94	0.19	42,42,42,42	0
56	MG	2A	3630	1/1	0.94	0.23	50,50,50,50	0
56	MG	1A	3023	1/1	0.94	0.21	35,35,35,35	0
56	MG	1G	3003	1/1	0.94	0.31	60,60,60,60	0
56	MG	2A	3145	1/1	0.94	0.44	53,53,53,53	0
56	MG	2A	3639	1/1	0.94	0.16	57,57,57,57	0
56	MG	2A	3146	1/1	0.94	0.57	55,55,55,55	0
56	MG	1A	3742	1/1	0.94	0.22	33,33,33,33	0
56	MG	1A	3743	1/1	0.94	0.11	41,41,41,41	0
56	MG	1A	3874	1/1	0.94	0.18	47,47,47,47	0
56	MG	2A	3364	1/1	0.94	0.13	58,58,58,58	0
56	MG	1N	201	1/1	0.94	0.72	41,41,41,41	0
56	MG	1a	1701	1/1	0.94	0.08	53,53,53,53	0
56	MG	2a	1772	1/1	0.94	0.34	62,62,62,62	0
56	MG	2a	1773	1/1	0.94	0.07	63,63,63,63	0
56	MG	2A	3370	1/1	0.94	0.27	62,62,62,62	0
56	MG	2a	1775	1/1	0.94	0.07	65,65,65,65	0
56	MG	2A	3372	1/1	0.94	0.11	58,58,58,58	0
56	MG	1A	3466	1/1	0.94	0.31	29,29,29,29	0
56	MG	1A	3328	1/1	0.94	0.18	49,49,49,49	0
56	MG	2A	3656	1/1	0.94	0.39	50,50,50,50	0
56	MG	2a	1783	1/1	0.94	0.14	67,67,67,67	0
56	MG	2A	3657	1/1	0.94	0.32	49,49,49,49	0
56	MG	1A	3649	1/1	0.94	0.15	36,36,36,36	0
56	MG	1A	3879	1/1	0.94	0.07	66,66,66,66	0
56	MG	1A	3650	1/1	0.94	0.07	40,40,40,40	0
56	MG	1a	1709	1/1	0.94	0.19	56,56,56,56	0
56	MG	1A	3387	1/1	0.94	0.11	34,34,34,34	0
56	MG	1A	3653	1/1	0.94	0.12	47,47,47,47	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	1A	3335	1/1	0.94	0.13	44,44,44,44	0
56	MG	1a	1714	1/1	0.94	0.09	53,53,53,53	0
56	MG	2A	3670	1/1	0.94	0.46	50,50,50,50	0
56	MG	2A	3389	1/1	0.94	0.28	49,49,49,49	0
56	MG	1A	3887	1/1	0.94	0.21	36,36,36,36	0
56	MG	1A	3389	1/1	0.94	0.10	44,44,44,44	0
56	MG	2A	3166	1/1	0.94	0.33	49,49,49,49	0
56	MG	1T	202	1/1	0.94	0.18	51,51,51,51	0
57	UNX	1A	3906	1/1	0.94	0.27	38,38,38,38	0
56	MG	1A	3560	1/1	0.94	0.28	35,35,35,35	0
56	MG	2A	3681	1/1	0.94	0.16	54,54,54,54	0
56	MG	1U	202	1/1	0.94	0.43	42,42,42,42	0
56	MG	1A	3015	1/1	0.94	0.31	37,37,37,37	0
56	MG	1A	3891	1/1	0.94	0.43	38,38,38,38	0
56	MG	1a	1727	1/1	0.94	0.12	51,51,51,51	0
60	ZN	29	501	1/1	0.94	0.08	67,67,67,67	0
56	MG	2B	3006	1/1	0.94	0.45	69,69,69,69	0
56	MG	1A	3599	1/1	0.95	0.07	35,35,35,35	0
56	MG	1A	3734	1/1	0.95	0.08	49,49,49,49	0
56	MG	1A	3494	1/1	0.95	0.10	42,42,42,42	0
56	MG	1A	3369	1/1	0.95	0.07	43,43,43,43	0
56	MG	1A	3549	1/1	0.95	0.29	32,32,32,32	0
56	MG	1A	3603	1/1	0.95	0.12	48,48,48,48	0
56	MG	2A	3194	1/1	0.95	0.14	54,54,54,54	0
56	MG	1A	3315	1/1	0.95	0.11	48,48,48,48	0
56	MG	2A	3556	1/1	0.95	0.23	47,47,47,47	0
56	MG	2A	3059	1/1	0.95	0.33	46,46,46,46	0
56	MG	2a	1629	1/1	0.95	0.10	78,78,78,78	0
56	MG	2A	3060	1/1	0.95	0.20	48,48,48,48	0
56	MG	1A	3670	1/1	0.95	0.29	46,46,46,46	0
56	MG	1A	3671	1/1	0.95	0.06	62,62,62,62	0
56	MG	2A	3562	1/1	0.95	0.10	43,43,43,43	0
56	MG	1A	3824	1/1	0.95	0.24	51,51,51,51	0
56	MG	1A	3148	1/1	0.95	0.25	32,32,32,32	0
56	MG	1A	3416	1/1	0.95	0.27	44,44,44,44	0
56	MG	1A	3458	1/1	0.95	0.11	69,69,69,69	0
56	MG	1a	1820	1/1	0.95	0.32	63,63,63,63	0
56	MG	1W	3003	1/1	0.95	0.74	33,33,33,33	0
56	MG	2A	3382	1/1	0.95	0.23	56,56,56,56	0
56	MG	1A	3173	1/1	0.95	0.14	40,40,40,40	0
56	MG	2A	3572	1/1	0.95	0.26	61,61,61,61	0
56	MG	1A	3678	1/1	0.95	0.09	44,44,44,44	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	10	101	1/1	0.95	0.18	48,48,48,48	0
56	MG	1A	3609	1/1	0.95	0.11	43,43,43,43	0
56	MG	10	103	1/1	0.95	0.21	42,42,42,42	0
56	MG	1A	3833	1/1	0.95	0.19	59,59,59,59	0
56	MG	1A	3939	1/1	0.95	0.43	32,32,32,32	0
56	MG	2A	3216	1/1	0.95	0.13	52,52,52,52	0
56	MG	1a	1703	1/1	0.95	0.06	72,72,72,72	0
56	MG	2A	3587	1/1	0.95	0.06	70,70,70,70	0
56	MG	2A	3395	1/1	0.95	0.17	58,58,58,58	0
56	MG	1A	3187	1/1	0.95	0.30	41,41,41,41	0
56	MG	1a	1834	1/1	0.95	0.12	57,57,57,57	0
56	MG	1A	3295	1/1	0.95	0.15	50,50,50,50	0
56	MG	13	102	1/1	0.95	0.45	53,53,53,53	0
56	MG	1a	1707	1/1	0.95	0.08	47,47,47,47	0
56	MG	1A	3836	1/1	0.95	0.13	42,42,42,42	0
56	MG	2A	3225	1/1	0.95	0.17	57,57,57,57	0
56	MG	1A	3943	1/1	0.95	0.22	47,47,47,47	0
56	MG	2A	3405	1/1	0.95	0.09	66,66,66,66	0
56	MG	1A	3558	1/1	0.95	0.60	31,31,31,31	0
56	MG	2a	1665	1/1	0.95	0.17	81,81,81,81	0
56	MG	1A	3841	1/1	0.95	0.14	45,45,45,45	0
56	MG	1A	3113	1/1	0.95	0.37	35,35,35,35	0
56	MG	2A	3607	1/1	0.95	0.08	66,66,66,66	0
56	MG	17	102	1/1	0.95	0.21	35,35,35,35	0
56	MG	2A	3609	1/1	0.95	0.14	58,58,58,58	0
56	MG	2A	3610	1/1	0.95	0.06	62,62,62,62	0
56	MG	1a	1845	1/1	0.95	0.15	61,61,61,61	0
56	MG	2A	3613	1/1	0.95	0.05	56,56,56,56	0
56	MG	1A	3099	1/1	0.95	1.09	34,34,34,34	0
56	MG	2A	3413	1/1	0.95	0.29	62,62,62,62	0
56	MG	1A	3844	1/1	0.95	0.21	32,32,32,32	0
56	MG	2A	3093	1/1	0.95	0.21	61,61,61,61	0
56	MG	1B	201	1/1	0.95	0.25	53,53,53,53	0
56	MG	1A	3845	1/1	0.95	0.21	32,32,32,32	0
56	MG	2A	3421	1/1	0.95	0.26	61,61,61,61	0
56	MG	1A	3756	1/1	0.95	0.11	39,39,39,39	0
56	MG	1a	1852	1/1	0.95	0.23	63,63,63,63	0
56	MG	1a	1853	1/1	0.95	0.09	66,66,66,66	0
56	MG	1B	204	1/1	0.95	0.09	56,56,56,56	0
56	MG	1A	3757	1/1	0.95	0.12	38,38,38,38	0
56	MG	2a	1687	1/1	0.95	0.17	62,62,62,62	0
56	MG	1A	3618	1/1	0.95	0.34	30,30,30,30	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	2A	3246	1/1	0.95	0.26	54,54,54,54	0
56	MG	1A	3378	1/1	0.95	0.15	40,40,40,40	0
56	MG	1a	1729	1/1	0.95	0.14	52,52,52,52	0
56	MG	1A	3161	1/1	0.95	0.12	35,35,35,35	0
56	MG	2a	1693	1/1	0.95	0.55	63,63,63,63	0
56	MG	2a	1695	1/1	0.95	0.20	58,58,58,58	0
56	MG	1A	3427	1/1	0.95	0.05	53,53,53,53	0
56	MG	2A	3111	1/1	0.95	0.46	48,48,48,48	0
56	MG	1A	3515	1/1	0.95	0.10	46,46,46,46	0
56	MG	1A	3354	1/1	0.95	0.21	31,31,31,31	0
56	MG	2A	3438	1/1	0.95	0.05	56,56,56,56	0
56	MG	1A	3859	1/1	0.95	0.09	35,35,35,35	0
56	MG	1A	3860	1/1	0.95	0.22	35,35,35,35	0
56	MG	2a	1705	1/1	0.95	0.08	62,62,62,62	0
56	MG	1A	3765	1/1	0.95	0.17	54,54,54,54	0
56	MG	2a	1709	1/1	0.95	0.16	63,63,63,63	0
56	MG	2A	3259	1/1	0.95	0.17	59,59,59,59	0
56	MG	1A	3864	1/1	0.95	0.28	42,42,42,42	0
56	MG	1A	3865	1/1	0.95	0.07	44,44,44,44	0
56	MG	1B	220	1/1	0.95	0.11	44,44,44,44	0
56	MG	2A	3265	1/1	0.95	0.07	60,60,60,60	0
56	MG	2A	3449	1/1	0.95	0.13	42,42,42,42	0
56	MG	1B	222	1/1	0.95	0.08	49,49,49,49	0
56	MG	2a	1718	1/1	0.95	0.20	62,62,62,62	0
56	MG	1A	3627	1/1	0.95	0.07	40,40,40,40	0
56	MG	2A	3270	1/1	0.95	0.20	50,50,50,50	0
56	MG	1A	3867	1/1	0.95	0.12	52,52,52,52	0
56	MG	2A	3669	1/1	0.95	0.14	47,47,47,47	0
56	MG	1a	1745	1/1	0.95	0.08	54,54,54,54	0
56	MG	1A	3628	1/1	0.95	0.14	43,43,43,43	0
56	MG	1A	3869	1/1	0.95	0.05	46,46,46,46	0
56	MG	1A	3472	1/1	0.95	0.18	42,42,42,42	0
56	MG	2a	1728	1/1	0.95	0.09	70,70,70,70	0
56	MG	2a	1729	1/1	0.95	0.21	64,64,64,64	0
56	MG	1A	3697	1/1	0.95	0.35	37,37,37,37	0
56	MG	2A	3130	1/1	0.95	0.16	62,62,62,62	0
56	MG	2A	3460	1/1	0.95	0.07	46,46,46,46	0
56	MG	2A	3461	1/1	0.95	0.08	53,53,53,53	0
56	MG	2B	3001	1/1	0.95	0.17	71,71,71,71	0
56	MG	1A	3074	1/1	0.95	0.20	32,32,32,32	0
56	MG	1A	3154	1/1	0.95	0.20	45,45,45,45	0
56	MG	1A	3701	1/1	0.95	0.17	47,47,47,47	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	2a	1740	1/1	0.95	0.07	73,73,73,73	0
56	MG	2A	3465	1/1	0.95	0.14	57,57,57,57	0
56	MG	2A	3290	1/1	0.95	0.04	55,55,55,55	0
56	MG	1a	1757	1/1	0.95	0.16	55,55,55,55	0
56	MG	1A	3304	1/1	0.95	0.13	47,47,47,47	0
56	MG	1a	1630	1/1	0.95	0.17	64,64,64,64	0
56	MG	2A	3138	1/1	0.95	0.23	42,42,42,42	0
56	MG	1A	3385	1/1	0.95	0.14	53,53,53,53	0
56	MG	2a	1749	1/1	0.95	0.12	59,59,59,59	0
56	MG	1A	3578	1/1	0.95	0.21	36,36,36,36	0
56	MG	1a	1633	1/1	0.95	0.28	51,51,51,51	0
56	MG	1A	3090	1/1	0.95	0.56	29,29,29,29	0
56	MG	1A	3706	1/1	0.95	0.13	36,36,36,36	0
56	MG	1A	3263	1/1	0.95	0.27	36,36,36,36	0
56	MG	2A	3004	1/1	0.95	0.12	52,52,52,52	0
56	MG	2A	3487	1/1	0.95	0.06	56,56,56,56	0
56	MG	1D	315	1/1	0.95	0.19	49,49,49,49	0
56	MG	1A	3333	1/1	0.95	0.17	45,45,45,45	0
56	MG	1A	3069	1/1	0.95	0.74	30,30,30,30	0
56	MG	1A	3483	1/1	0.95	0.11	39,39,39,39	0
56	MG	1A	3643	1/1	0.95	0.18	37,37,37,37	0
56	MG	2E	304	1/1	0.95	0.19	47,47,47,47	0
56	MG	1E	302	1/1	0.95	0.68	30,30,30,30	0
56	MG	1a	1775	1/1	0.95	0.24	66,66,66,66	0
56	MG	1a	1776	1/1	0.95	0.08	80,80,80,80	0
56	MG	1A	3584	1/1	0.95	0.27	61,61,61,61	0
56	MG	2A	3017	1/1	0.95	0.82	48,48,48,48	0
56	MG	1A	3339	1/1	0.95	0.10	43,43,43,43	0
56	MG	1a	1648	1/1	0.95	0.38	57,57,57,57	0
56	MG	1A	3050	1/1	0.95	0.43	36,36,36,36	0
56	MG	2A	3506	1/1	0.95	0.31	61,61,61,61	0
56	MG	1F	301	1/1	0.95	0.10	44,44,44,44	0
56	MG	2A	3508	1/1	0.95	0.21	50,50,50,50	0
56	MG	2A	3163	1/1	0.95	0.36	48,48,48,48	0
56	MG	1A	3365	1/1	0.95	0.16	43,43,43,43	0
56	MG	1A	3537	1/1	0.95	0.13	32,32,32,32	0
56	MG	1A	3589	1/1	0.95	0.09	46,46,46,46	0
56	MG	1a	1658	1/1	0.95	0.34	67,67,67,67	0
56	MG	2A	3324	1/1	0.95	0.13	51,51,51,51	0
56	MG	1F	306	1/1	0.95	0.45	31,31,31,31	0
56	MG	1a	1660	1/1	0.95	0.26	68,68,68,68	0
56	MG	1A	3395	1/1	0.95	0.07	43,43,43,43	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	1A	3652	1/1	0.95	0.25	40,40,40,40	0
56	MG	1A	3798	1/1	0.95	0.11	37,37,37,37	0
56	MG	1A	3899	1/1	0.95	0.19	41,41,41,41	0
56	MG	1A	3800	1/1	0.95	0.07	51,51,51,51	0
56	MG	1a	1666	1/1	0.95	0.27	65,65,65,65	0
56	MG	1A	3366	1/1	0.95	0.30	44,44,44,44	0
56	MG	2x	106	1/1	0.95	0.10	63,63,63,63	0
56	MG	1A	3903	1/1	0.95	0.14	53,53,53,53	0
56	MG	2A	3342	1/1	0.95	0.23	61,61,61,61	0
56	MG	1A	3184	1/1	0.95	0.13	37,37,37,37	0
56	MG	1A	3726	1/1	0.95	0.08	51,51,51,51	0
56	MG	1A	3445	1/1	0.95	0.16	42,42,42,42	0
56	MG	1A	3909	1/1	0.95	0.56	43,43,43,43	0
56	MG	1P	202	1/1	0.95	0.10	55,55,55,55	0
56	MG	2A	3350	1/1	0.95	0.20	65,65,65,65	0
56	MG	1A	3595	1/1	0.95	0.26	49,49,49,49	0
56	MG	1A	3401	1/1	0.95	0.12	56,56,56,56	0
56	MG	1A	3812	1/1	0.95	0.17	37,37,37,37	0
56	MG	1A	3450	1/1	0.95	0.08	35,35,35,35	0
60	ZN	2n	102	1/1	0.95	0.06	84,84,84,84	0
56	MG	2A	3545	1/1	0.95	0.09	57,57,57,57	0
56	MG	2A	3195	1/1	0.96	0.42	43,43,43,43	0
56	MG	2a	1611	1/1	0.96	0.12	59,59,59,59	0
56	MG	2A	3534	1/1	0.96	0.45	50,50,50,50	0
56	MG	2A	3354	1/1	0.96	0.12	59,59,59,59	0
56	MG	1A	3172	1/1	0.96	0.25	37,37,37,37	0
56	MG	2A	3197	1/1	0.96	0.31	50,50,50,50	0
56	MG	1B	211	1/1	0.96	0.14	41,41,41,41	0
56	MG	2A	3064	1/1	0.96	0.27	46,46,46,46	0
56	MG	1B	212	1/1	0.96	0.05	40,40,40,40	0
56	MG	1A	3351	1/1	0.96	0.15	29,29,29,29	0
56	MG	2A	3361	1/1	0.96	0.18	60,60,60,60	0
56	MG	1a	1830	1/1	0.96	0.29	68,68,68,68	0
56	MG	1A	3196	1/1	0.96	0.19	41,41,41,41	0
56	MG	1A	3468	1/1	0.96	0.06	47,47,47,47	0
56	MG	2A	3365	1/1	0.96	0.15	48,48,48,48	0
56	MG	2A	3549	1/1	0.96	0.14	53,53,53,53	0
56	MG	1A	3353	1/1	0.96	0.10	43,43,43,43	0
56	MG	1A	3403	1/1	0.96	0.15	35,35,35,35	0
56	MG	1a	1835	1/1	0.96	0.05	64,64,64,64	0
56	MG	1A	3405	1/1	0.96	0.15	26,26,26,26	0
56	MG	1A	3542	1/1	0.96	0.15	49,49,49,49	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	1A	3115	1/1	0.96	0.29	41,41,41,41	0
56	MG	2A	3375	1/1	0.96	0.17	50,50,50,50	0
56	MG	1a	1721	1/1	0.96	0.09	55,55,55,55	0
56	MG	1B	223	1/1	0.96	0.17	43,43,43,43	0
56	MG	2A	3378	1/1	0.96	0.14	50,50,50,50	0
56	MG	1A	3410	1/1	0.96	0.09	50,50,50,50	0
56	MG	2A	3380	1/1	0.96	0.17	59,59,59,59	0
56	MG	1a	1610	1/1	0.96	0.10	71,71,71,71	0
56	MG	1A	3411	1/1	0.96	0.09	62,62,62,62	0
56	MG	2a	1642	1/1	0.96	0.34	75,75,75,75	0
56	MG	1A	3615	1/1	0.96	0.12	59,59,59,59	0
56	MG	1A	3225	1/1	0.96	1.07	38,38,38,38	0
56	MG	2A	3385	1/1	0.96	0.27	53,53,53,53	0
56	MG	1A	3698	1/1	0.96	0.10	30,30,30,30	0
56	MG	1A	3548	1/1	0.96	0.18	47,47,47,47	0
56	MG	1A	3882	1/1	0.96	0.12	57,57,57,57	0
56	MG	1A	3306	1/1	0.96	0.21	40,40,40,40	0
56	MG	1A	3884	1/1	0.96	0.11	44,44,44,44	0
56	MG	2a	1651	1/1	0.96	0.59	62,62,62,62	0
56	MG	1A	3885	1/1	0.96	0.31	30,30,30,30	0
56	MG	1D	308	1/1	0.96	0.20	42,42,42,42	0
56	MG	1A	3415	1/1	0.96	0.05	55,55,55,55	0
56	MG	1A	3307	1/1	0.96	0.11	34,34,34,34	0
56	MG	1A	3308	1/1	0.96	0.15	58,58,58,58	0
56	MG	2A	3095	1/1	0.96	0.24	47,47,47,47	0
56	MG	1a	1738	1/1	0.96	0.09	57,57,57,57	0
56	MG	1A	3199	1/1	0.96	0.35	37,37,37,37	0
56	MG	2A	3593	1/1	0.96	0.06	48,48,48,48	0
56	MG	1A	3200	1/1	0.96	0.08	46,46,46,46	0
56	MG	1a	1861	1/1	0.96	0.11	72,72,72,72	0
56	MG	2A	3235	1/1	0.96	0.43	49,49,49,49	0
56	MG	2A	3236	1/1	0.96	0.21	50,50,50,50	0
56	MG	1A	3361	1/1	0.96	0.25	47,47,47,47	0
56	MG	1A	3020	1/1	0.96	0.20	36,36,36,36	0
56	MG	2A	3104	1/1	0.96	0.37	48,48,48,48	0
56	MG	1A	3118	1/1	0.96	0.42	39,39,39,39	0
56	MG	1A	3054	1/1	0.96	0.18	30,30,30,30	0
56	MG	1A	3561	1/1	0.96	0.12	54,54,54,54	0
56	MG	1A	3896	1/1	0.96	0.17	31,31,31,31	0
56	MG	1A	3232	1/1	0.96	0.10	56,56,56,56	0
56	MG	1a	1749	1/1	0.96	0.06	59,59,59,59	0
56	MG	1A	3233	1/1	0.96	0.38	50,50,50,50	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	2A	3419	1/1	0.96	0.58	44,44,44,44	0
56	MG	1a	1751	1/1	0.96	0.16	69,69,69,69	0
56	MG	2A	3611	1/1	0.96	0.07	57,57,57,57	0
56	MG	1A	3367	1/1	0.96	0.14	33,33,33,33	0
56	MG	1E	306	1/1	0.96	0.10	47,47,47,47	0
56	MG	2A	3251	1/1	0.96	0.26	53,53,53,53	0
56	MG	1a	1637	1/1	0.96	0.39	52,52,52,52	0
56	MG	1A	3565	1/1	0.96	0.14	31,31,31,31	0
56	MG	1F	302	1/1	0.96	0.50	31,31,31,31	0
56	MG	2A	3619	1/1	0.96	0.06	55,55,55,55	0
56	MG	1A	3715	1/1	0.96	0.17	69,69,69,69	0
56	MG	2a	1686	1/1	0.96	0.07	69,69,69,69	0
56	MG	1a	1642	1/1	0.96	0.42	68,68,68,68	0
56	MG	2A	3624	1/1	0.96	0.09	48,48,48,48	0
56	MG	2A	3429	1/1	0.96	0.21	58,58,58,58	0
56	MG	1A	3271	1/1	0.96	0.33	42,42,42,42	0
56	MG	1A	3493	1/1	0.96	0.08	29,29,29,29	0
56	MG	2A	3629	1/1	0.96	0.08	57,57,57,57	0
56	MG	1x	101	1/1	0.96	0.07	69,69,69,69	0
56	MG	2A	3262	1/1	0.96	0.24	49,49,49,49	0
56	MG	2A	3635	1/1	0.96	0.15	48,48,48,48	0
56	MG	2a	1697	1/1	0.96	0.14	65,65,65,65	0
56	MG	1x	102	1/1	0.96	0.15	64,64,64,64	0
56	MG	1A	3047	1/1	0.96	0.67	44,44,44,44	0
56	MG	1A	3642	1/1	0.96	0.09	32,32,32,32	0
56	MG	1A	3057	1/1	0.96	0.33	32,32,32,32	0
56	MG	2A	3642	1/1	0.96	0.46	51,51,51,51	0
56	MG	1A	3571	1/1	0.96	0.10	45,45,45,45	0
56	MG	1x	107	1/1	0.96	0.14	56,56,56,56	0
56	MG	2a	1707	1/1	0.96	0.17	68,68,68,68	0
56	MG	1A	3723	1/1	0.96	0.08	51,51,51,51	0
56	MG	1a	1650	1/1	0.96	0.70	51,51,51,51	0
56	MG	2A	3443	1/1	0.96	0.27	53,53,53,53	0
56	MG	1a	1769	1/1	0.96	0.17	68,68,68,68	0
56	MG	2A	3275	1/1	0.96	0.22	55,55,55,55	0
56	MG	1G	3002	1/1	0.96	0.08	57,57,57,57	0
56	MG	2A	3278	1/1	0.96	0.14	61,61,61,61	0
56	MG	1A	3913	1/1	0.96	0.11	32,32,32,32	0
56	MG	1A	3180	1/1	0.96	0.16	51,51,51,51	0
56	MG	2A	3282	1/1	0.96	0.14	49,49,49,49	0
56	MG	2A	3137	1/1	0.96	0.32	49,49,49,49	0
56	MG	2A	3002	1/1	0.96	0.23	59,59,59,59	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	2A	3286	1/1	0.96	0.18	51,51,51,51	0
56	MG	2A	3287	1/1	0.96	0.13	60,60,60,60	0
56	MG	2A	3003	1/1	0.96	0.12	54,54,54,54	0
56	MG	1a	1654	1/1	0.96	0.29	71,71,71,71	0
56	MG	1a	1655	1/1	0.96	0.36	51,51,51,51	0
56	MG	1a	1656	1/1	0.96	0.14	73,73,73,73	0
56	MG	1A	3014	1/1	0.96	0.09	41,41,41,41	0
56	MG	1A	3819	1/1	0.96	0.24	53,53,53,53	0
56	MG	1A	3106	1/1	0.96	0.12	39,39,39,39	0
56	MG	1A	3648	1/1	0.96	0.12	37,37,37,37	0
56	MG	2A	3673	1/1	0.96	0.17	51,51,51,51	0
56	MG	1A	3575	1/1	0.96	0.10	55,55,55,55	0
56	MG	1P	201	1/1	0.96	0.09	34,34,34,34	0
56	MG	1A	3081	1/1	0.96	0.75	39,39,39,39	0
56	MG	2A	3678	1/1	0.96	0.19	53,53,53,53	0
56	MG	2A	3152	1/1	0.96	0.48	51,51,51,51	0
56	MG	2a	1739	1/1	0.96	0.09	57,57,57,57	0
56	MG	1A	3001	1/1	0.96	0.23	42,42,42,42	0
56	MG	2A	3019	1/1	0.96	0.12	51,51,51,51	0
56	MG	1A	3733	1/1	0.96	0.17	29,29,29,29	0
56	MG	2A	3473	1/1	0.96	0.10	57,57,57,57	0
56	MG	2A	3474	1/1	0.96	0.14	47,47,47,47	0
56	MG	1A	3164	1/1	0.96	0.64	29,29,29,29	0
56	MG	1A	3440	1/1	0.96	0.16	23,23,23,23	0
56	MG	1A	3654	1/1	0.96	0.15	49,49,49,49	0
56	MG	1A	3830	1/1	0.96	0.11	33,33,33,33	0
56	MG	1A	3655	1/1	0.96	0.05	49,49,49,49	0
56	MG	1A	3213	1/1	0.96	0.90	37,37,37,37	0
56	MG	2A	3481	1/1	0.96	0.13	59,59,59,59	0
56	MG	1A	3016	1/1	0.96	0.70	30,30,30,30	0
56	MG	2A	3483	1/1	0.96	0.31	51,51,51,51	0
56	MG	2A	3484	1/1	0.96	0.10	53,53,53,53	0
56	MG	2A	3486	1/1	0.96	0.14	54,54,54,54	0
56	MG	2D	301	1/1	0.96	0.23	49,49,49,49	0
56	MG	1A	3019	1/1	0.96	0.77	27,27,27,27	0
56	MG	1A	3287	1/1	0.96	0.33	41,41,41,41	0
56	MG	1A	3288	1/1	0.96	0.16	25,25,25,25	0
56	MG	1A	3937	1/1	0.96	0.48	32,32,32,32	0
56	MG	1A	3938	1/1	0.96	0.55	33,33,33,33	0
56	MG	1A	3448	1/1	0.96	0.21	30,30,30,30	0
56	MG	1A	3289	1/1	0.96	0.18	32,32,32,32	0
56	MG	2A	3036	1/1	0.96	0.15	65,65,65,65	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
56	MG	1W	3001	1/1	0.96	0.21	38,38,38,38	0
56	MG	2A	3498	1/1	0.96	0.10	42,42,42,42	0
56	MG	1A	3384	1/1	0.96	0.12	30,30,30,30	0
56	MG	1A	3519	1/1	0.96	0.06	56,56,56,56	0
56	MG	1A	3167	1/1	0.96	0.15	50,50,50,50	0
56	MG	2A	3502	1/1	0.96	0.09	70,70,70,70	0
56	MG	2A	3326	1/1	0.96	0.07	55,55,55,55	0
56	MG	1a	1806	1/1	0.96	0.29	68,68,68,68	0
56	MG	2A	3505	1/1	0.96	0.09	59,59,59,59	0
56	MG	1Y	502	1/1	0.96	0.12	56,56,56,56	0
56	MG	1A	3062	1/1	0.96	0.31	41,41,41,41	0
56	MG	1A	3668	1/1	0.96	0.19	51,51,51,51	0
56	MG	2Q	201	1/1	0.96	0.26	59,59,59,59	0
56	MG	2R	8001	1/1	0.96	0.18	50,50,50,50	0
56	MG	1A	3669	1/1	0.96	0.11	64,64,64,64	0
56	MG	2T	3002	1/1	0.96	0.28	58,58,58,58	0
56	MG	1A	3292	1/1	0.96	0.10	45,45,45,45	0
56	MG	10	104	1/1	0.96	0.15	47,47,47,47	0
56	MG	2A	3512	1/1	0.96	0.21	45,45,45,45	0
56	MG	2A	3513	1/1	0.96	0.18	52,52,52,52	0
56	MG	1A	3254	1/1	0.96	0.15	52,52,52,52	0
56	MG	1A	3169	1/1	0.96	0.48	37,37,37,37	0
56	MG	1A	3596	1/1	0.96	0.13	41,41,41,41	0
56	MG	2A	3340	1/1	0.96	0.10	50,50,50,50	0
56	MG	2Y	201	1/1	0.96	0.10	60,60,60,60	0
56	MG	2A	3341	1/1	0.96	0.18	55,55,55,55	0
56	MG	1A	3459	1/1	0.96	0.16	46,46,46,46	0
56	MG	2A	3053	1/1	0.96	0.45	58,58,58,58	0
56	MG	13	101	1/1	0.96	0.10	38,38,38,38	0
56	MG	2A	3346	1/1	0.96	0.25	60,60,60,60	0
56	MG	1A	3390	1/1	0.96	0.15	35,35,35,35	0
56	MG	1A	3114	1/1	0.96	0.35	34,34,34,34	0
56	MG	2A	3527	1/1	0.96	0.16	60,60,60,60	0
56	MG	1A	3152	1/1	0.96	0.75	36,36,36,36	0
56	MG	2A	3529	1/1	0.96	0.18	59,59,59,59	0
56	MG	1A	3532	1/1	0.96	0.14	40,40,40,40	0
56	MG	1A	3682	1/1	0.96	0.12	41,41,41,41	0
61	SF4	1d	501	8/8	0.96	0.15	72,75,79,82	0
56	MG	1A	3349	1/1	0.96	0.13	26,26,26,26	0
56	MG	2A	3515	1/1	0.97	0.10	62,62,62,62	0
56	MG	2A	3516	1/1	0.97	0.29	57,57,57,57	0
56	MG	1A	3634	1/1	0.97	0.06	34,34,34,34	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
56	MG	2A	3660	1/1	0.97	0.56	47,47,47,47	0
56	MG	1A	3828	1/1	0.97	0.20	43,43,43,43	0
56	MG	1A	3754	1/1	0.97	0.13	41,41,41,41	0
56	MG	1A	3239	1/1	0.97	0.09	41,41,41,41	0
56	MG	1A	3068	1/1	0.97	0.20	40,40,40,40	0
56	MG	1A	3912	1/1	0.97	0.07	54,54,54,54	0
56	MG	1D	320	1/1	0.97	0.23	46,46,46,46	0
56	MG	1D	321	1/1	0.97	0.59	46,46,46,46	0
56	MG	2A	3406	1/1	0.97	0.09	56,56,56,56	0
56	MG	1a	1700	1/1	0.97	0.09	50,50,50,50	0
56	MG	1E	301	1/1	0.97	0.15	34,34,34,34	0
56	MG	2A	3295	1/1	0.97	0.13	52,52,52,52	0
56	MG	1a	1796	1/1	0.97	0.22	68,68,68,68	0
56	MG	1A	3481	1/1	0.97	0.18	54,54,54,54	0
56	MG	1A	3638	1/1	0.97	0.07	44,44,44,44	0
56	MG	1a	1617	1/1	0.97	0.27	69,69,69,69	0
56	MG	2A	3300	1/1	0.97	0.28	42,42,42,42	0
56	MG	2A	3415	1/1	0.97	0.12	52,52,52,52	0
56	MG	2A	3535	1/1	0.97	0.05	52,52,52,52	0
56	MG	2A	3416	1/1	0.97	0.11	62,62,62,62	0
56	MG	2A	3096	1/1	0.97	0.22	62,62,62,62	0
56	MG	2A	3193	1/1	0.97	0.28	66,66,66,66	0
56	MG	1A	3242	1/1	0.97	0.24	29,29,29,29	0
56	MG	1A	3536	1/1	0.97	0.15	35,35,35,35	0
56	MG	2A	3305	1/1	0.97	0.14	57,57,57,57	0
56	MG	1A	3918	1/1	0.97	0.15	27,27,27,27	0
56	MG	1A	3438	1/1	0.97	0.07	46,46,46,46	0
56	MG	1A	3042	1/1	0.97	0.47	21,21,21,21	0
56	MG	1A	3840	1/1	0.97	0.07	39,39,39,39	0
56	MG	2a	1694	1/1	0.97	0.06	63,63,63,63	0
56	MG	1A	3293	1/1	0.97	0.11	35,35,35,35	0
56	MG	1A	3221	1/1	0.97	0.76	29,29,29,29	0
56	MG	1A	3590	1/1	0.97	0.19	47,47,47,47	0
56	MG	2B	3016	1/1	0.97	0.10	71,71,71,71	0
56	MG	1A	3398	1/1	0.97	0.05	33,33,33,33	0
56	MG	2a	1700	1/1	0.97	0.08	65,65,65,65	0
56	MG	1A	3125	1/1	0.97	0.09	29,29,29,29	0
56	MG	1A	3007	1/1	0.97	0.12	50,50,50,50	0
56	MG	1A	3298	1/1	0.97	0.16	28,28,28,28	0
56	MG	1A	3446	1/1	0.97	0.07	46,46,46,46	0
56	MG	2A	3112	1/1	0.97	0.47	56,56,56,56	0
56	MG	1A	3330	1/1	0.97	0.21	33,33,33,33	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	1A	3331	1/1	0.97	0.05	40,40,40,40	0
56	MG	1A	3332	1/1	0.97	0.10	48,48,48,48	0
56	MG	2a	1710	1/1	0.97	0.04	73,73,73,73	0
56	MG	2A	3560	1/1	0.97	0.06	54,54,54,54	0
56	MG	2E	303	1/1	0.97	0.17	51,51,51,51	0
56	MG	1A	3144	1/1	0.97	0.33	36,36,36,36	0
56	MG	1A	3452	1/1	0.97	0.05	40,40,40,40	0
56	MG	1A	3857	1/1	0.97	0.27	44,44,44,44	0
56	MG	1A	3858	1/1	0.97	0.16	38,38,38,38	0
56	MG	2A	3327	1/1	0.97	0.15	58,58,58,58	0
56	MG	1O	8001	1/1	0.97	0.09	44,44,44,44	0
56	MG	2A	3329	1/1	0.97	0.07	50,50,50,50	0
56	MG	1A	3013	1/1	0.97	0.24	29,29,29,29	0
56	MG	2A	3569	1/1	0.97	0.25	66,66,66,66	0
56	MG	2A	3122	1/1	0.97	0.32	44,44,44,44	0
56	MG	1A	3455	1/1	0.97	0.19	37,37,37,37	0
56	MG	1a	1824	1/1	0.97	0.25	54,54,54,54	0
56	MG	1A	3554	1/1	0.97	0.10	45,45,45,45	0
56	MG	1A	3862	1/1	0.97	0.13	31,31,31,31	0
56	MG	1A	3863	1/1	0.97	0.11	29,29,29,29	0
56	MG	1A	3337	1/1	0.97	0.21	36,36,36,36	0
56	MG	2A	3578	1/1	0.97	0.24	51,51,51,51	0
56	MG	1A	3046	1/1	0.97	0.26	37,37,37,37	0
56	MG	2A	3580	1/1	0.97	0.35	52,52,52,52	0
56	MG	1A	3414	1/1	0.97	0.07	63,63,63,63	0
56	MG	2A	3582	1/1	0.97	0.10	60,60,60,60	0
56	MG	2A	3034	1/1	0.97	0.21	49,49,49,49	0
56	MG	2a	1736	1/1	0.97	0.10	66,66,66,66	0
56	MG	1A	3789	1/1	0.97	0.06	41,41,41,41	0
56	MG	2A	3585	1/1	0.97	0.17	59,59,59,59	0
56	MG	2A	3586	1/1	0.97	0.07	68,68,68,68	0
56	MG	1A	3251	1/1	0.97	0.16	47,47,47,47	0
56	MG	2A	3589	1/1	0.97	0.09	47,47,47,47	0
56	MG	2A	3590	1/1	0.97	0.09	47,47,47,47	0
56	MG	2A	3591	1/1	0.97	0.16	68,68,68,68	0
56	MG	1A	3559	1/1	0.97	0.14	39,39,39,39	0
56	MG	1A	3373	1/1	0.97	0.10	60,60,60,60	0
56	MG	1A	3724	1/1	0.97	0.35	44,44,44,44	0
56	MG	1A	3610	1/1	0.97	0.11	45,45,45,45	0
56	MG	2a	1748	1/1	0.97	0.04	60,60,60,60	0
56	MG	1A	3666	1/1	0.97	0.13	37,37,37,37	0
56	MG	2A	3597	1/1	0.97	0.07	52,52,52,52	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	1A	3210	1/1	0.97	0.13	33,33,33,33	0
56	MG	1A	3875	1/1	0.97	0.15	28,28,28,28	0
56	MG	2A	3467	1/1	0.97	0.24	62,62,62,62	0
56	MG	2A	3141	1/1	0.97	0.30	57,57,57,57	0
56	MG	1A	3276	1/1	0.97	0.13	49,49,49,49	0
56	MG	1A	3511	1/1	0.97	0.21	47,47,47,47	0
56	MG	2a	1757	1/1	0.97	0.10	69,69,69,69	0
56	MG	2a	1613	1/1	0.97	0.40	61,61,61,61	0
56	MG	2A	3144	1/1	0.97	0.11	49,49,49,49	0
56	MG	1a	1753	1/1	0.97	0.17	50,50,50,50	0
56	MG	1A	3799	1/1	0.97	0.05	32,32,32,32	0
56	MG	2A	3245	1/1	0.97	0.11	56,56,56,56	0
56	MG	1A	3073	1/1	0.97	0.34	32,32,32,32	0
56	MG	1A	3801	1/1	0.97	0.06	51,51,51,51	0
56	MG	1A	3039	1/1	0.97	0.24	53,53,53,53	0
56	MG	2a	1767	1/1	0.97	0.15	63,63,63,63	0
56	MG	1A	3805	1/1	0.97	0.04	31,31,31,31	0
56	MG	1A	3179	1/1	0.97	0.12	57,57,57,57	0
56	MG	1A	3673	1/1	0.97	0.24	44,44,44,44	0
56	MG	1A	3280	1/1	0.97	0.14	35,35,35,35	0
56	MG	1A	3281	1/1	0.97	0.09	35,35,35,35	0
56	MG	1A	3810	1/1	0.97	0.30	28,28,28,28	0
56	MG	2A	3485	1/1	0.97	0.07	53,53,53,53	0
56	MG	2A	3369	1/1	0.97	0.16	45,45,45,45	0
56	MG	2A	3620	1/1	0.97	0.11	44,44,44,44	0
56	MG	2a	1777	1/1	0.97	0.12	66,66,66,66	0
56	MG	2A	3058	1/1	0.97	0.17	31,31,31,31	0
56	MG	2A	3371	1/1	0.97	0.08	50,50,50,50	0
56	MG	2A	3256	1/1	0.97	0.15	56,56,56,56	0
56	MG	2a	1781	1/1	0.97	0.45	50,50,50,50	0
56	MG	2a	1782	1/1	0.97	0.15	63,63,63,63	0
56	MG	1A	3348	1/1	0.97	0.10	32,32,32,32	0
56	MG	1A	3312	1/1	0.97	0.21	27,27,27,27	0
56	MG	2A	3627	1/1	0.97	0.10	46,46,46,46	0
56	MG	1A	3471	1/1	0.97	0.12	33,33,33,33	0
56	MG	1A	3680	1/1	0.97	0.15	30,30,30,30	0
56	MG	2n	101	1/1	0.97	0.37	77,77,77,77	0
56	MG	1A	3231	1/1	0.97	0.16	36,36,36,36	0
56	MG	2q	201	1/1	0.97	0.28	62,62,62,62	0
56	MG	1A	3625	1/1	0.97	0.23	36,36,36,36	0
56	MG	2A	3632	1/1	0.97	0.05	55,55,55,55	0
56	MG	2A	3633	1/1	0.97	0.06	48,48,48,48	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	2A	3634	1/1	0.97	0.14	48,48,48,48	0
56	MG	1A	3626	1/1	0.97	0.06	51,51,51,51	0
56	MG	1A	3131	1/1	0.97	0.26	35,35,35,35	0
56	MG	2A	3637	1/1	0.97	0.10	60,60,60,60	0
56	MG	1a	1772	1/1	0.97	0.14	68,68,68,68	0
56	MG	2A	3267	1/1	0.97	0.13	49,49,49,49	0
56	MG	1D	301	1/1	0.97	0.17	35,35,35,35	0
56	MG	1D	302	1/1	0.97	0.70	34,34,34,34	0
56	MG	1A	3031	1/1	0.97	0.28	32,32,32,32	0
57	UNX	2A	3667	1/1	0.97	0.38	45,45,45,45	0
56	MG	1A	3028	1/1	0.97	0.15	39,39,39,39	0
56	MG	1A	3747	1/1	0.97	0.10	40,40,40,40	0
56	MG	2A	3388	1/1	0.97	0.16	48,48,48,48	0
60	ZN	1Y	501	1/1	0.97	0.07	63,63,63,63	0
56	MG	1A	3748	1/1	0.97	0.06	49,49,49,49	0
56	MG	1a	1686	1/1	0.97	0.13	67,67,67,67	0
60	ZN	2Y	202	1/1	0.97	0.04	77,77,77,77	0
56	MG	1A	3577	1/1	0.97	0.20	28,28,28,28	0
56	MG	1A	3901	1/1	0.97	0.25	51,51,51,51	0
56	MG	1A	3476	1/1	0.97	0.05	38,38,38,38	0
56	MG	1A	3109	1/1	0.97	0.42	40,40,40,40	0
56	MG	1A	3110	1/1	0.97	0.12	35,35,35,35	0
56	MG	1A	3117	1/1	0.98	0.30	45,45,45,45	0
56	MG	1A	3067	1/1	0.98	0.22	35,35,35,35	0
56	MG	1A	3137	1/1	0.98	0.49	32,32,32,32	0
56	MG	2A	3325	1/1	0.98	0.07	50,50,50,50	0
56	MG	2A	3618	1/1	0.98	0.04	42,42,42,42	0
56	MG	2V	201	1/1	0.98	0.13	64,64,64,64	0
56	MG	1A	3406	1/1	0.98	0.08	34,34,34,34	0
56	MG	2a	1706	1/1	0.98	0.10	56,56,56,56	0
56	MG	1A	3407	1/1	0.98	0.07	47,47,47,47	0
56	MG	1A	3528	1/1	0.98	0.18	45,45,45,45	0
56	MG	2A	3622	1/1	0.98	0.12	67,67,67,67	0
56	MG	1A	3774	1/1	0.98	0.04	45,45,45,45	0
56	MG	2A	3330	1/1	0.98	0.12	48,48,48,48	0
56	MG	1A	3529	1/1	0.98	0.12	44,44,44,44	0
56	MG	1A	3686	1/1	0.98	0.07	49,49,49,49	0
56	MG	1A	3530	1/1	0.98	0.11	43,43,43,43	0
56	MG	1A	3731	1/1	0.98	0.12	32,32,32,32	0
56	MG	1A	3568	1/1	0.98	0.14	44,44,44,44	0
56	MG	1A	3017	1/1	0.98	0.27	25,25,25,25	0
56	MG	1A	3305	1/1	0.98	0.28	47,47,47,47	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	1A	3193	1/1	0.98	0.20	33,33,33,33	0
56	MG	1a	1741	1/1	0.98	0.08	63,63,63,63	0
56	MG	2A	3433	1/1	0.98	0.09	52,52,52,52	0
56	MG	2a	1607	1/1	0.98	0.07	70,70,70,70	0
56	MG	1A	3783	1/1	0.98	0.05	51,51,51,51	0
56	MG	1A	3785	1/1	0.98	0.05	36,36,36,36	0
56	MG	2a	1725	1/1	0.98	0.06	63,63,63,63	0
56	MG	1A	3055	1/1	0.98	0.38	37,37,37,37	0
56	MG	1A	3838	1/1	0.98	0.29	45,45,45,45	0
56	MG	2A	3344	1/1	0.98	0.33	61,61,61,61	0
56	MG	2A	3640	1/1	0.98	0.43	59,59,59,59	0
56	MG	1A	3052	1/1	0.98	0.12	28,28,28,28	0
56	MG	1A	3788	1/1	0.98	0.08	55,55,55,55	0
56	MG	2A	3643	1/1	0.98	0.10	54,54,54,54	0
56	MG	1A	3498	1/1	0.98	0.06	56,56,56,56	0
56	MG	2A	3645	1/1	0.98	0.10	50,50,50,50	0
56	MG	1a	1677	1/1	0.98	0.13	49,49,49,49	0
56	MG	2A	3647	1/1	0.98	0.15	60,60,60,60	0
56	MG	1A	3151	1/1	0.98	0.42	31,31,31,31	0
56	MG	2A	3444	1/1	0.98	0.07	46,46,46,46	0
56	MG	2A	3543	1/1	0.98	0.11	45,45,45,45	0
56	MG	1a	1679	1/1	0.98	0.10	81,81,81,81	0
56	MG	1a	1826	1/1	0.98	0.24	68,68,68,68	0
56	MG	2A	3260	1/1	0.98	0.13	63,63,63,63	0
56	MG	2a	1627	1/1	0.98	0.14	58,58,58,58	0
56	MG	2A	3094	1/1	0.98	0.28	55,55,55,55	0
56	MG	2A	3012	1/1	0.98	0.17	45,45,45,45	0
56	MG	2A	3013	1/1	0.98	0.17	57,57,57,57	0
56	MG	1a	1752	1/1	0.98	0.17	67,67,67,67	0
56	MG	1A	3162	1/1	0.98	0.14	36,36,36,36	0
56	MG	2A	3552	1/1	0.98	0.08	47,47,47,47	0
56	MG	1A	3327	1/1	0.98	0.05	46,46,46,46	0
56	MG	1A	3502	1/1	0.98	0.12	43,43,43,43	0
56	MG	2A	3268	1/1	0.98	0.10	45,45,45,45	0
56	MG	1B	214	1/1	0.98	0.14	44,44,44,44	0
56	MG	1A	3617	1/1	0.98	0.05	60,60,60,60	0
56	MG	2A	3271	1/1	0.98	0.08	60,60,60,60	0
56	MG	2A	3103	1/1	0.98	0.11	63,63,63,63	0
56	MG	1A	3503	1/1	0.98	0.09	38,38,38,38	0
56	MG	1A	3417	1/1	0.98	0.12	34,34,34,34	0
56	MG	2A	3367	1/1	0.98	0.14	59,59,59,59	0
56	MG	1A	3543	1/1	0.98	0.05	36,36,36,36	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	1A	3621	1/1	0.98	0.10	53,53,53,53	0
56	MG	1A	3852	1/1	0.98	0.03	47,47,47,47	0
56	MG	2A	3675	1/1	0.98	0.17	59,59,59,59	0
56	MG	1B	221	1/1	0.98	0.22	51,51,51,51	0
56	MG	1R	202	1/1	0.98	0.08	38,38,38,38	0
56	MG	2A	3281	1/1	0.98	0.10	52,52,52,52	0
56	MG	2A	3469	1/1	0.98	0.17	51,51,51,51	0
56	MG	2A	3680	1/1	0.98	0.05	65,65,65,65	0
56	MG	1A	3853	1/1	0.98	0.08	43,43,43,43	0
56	MG	1A	3235	1/1	0.98	0.21	32,32,32,32	0
56	MG	1A	3329	1/1	0.98	0.07	49,49,49,49	0
56	MG	1A	3856	1/1	0.98	0.15	46,46,46,46	0
56	MG	1A	3447	1/1	0.98	0.11	34,34,34,34	0
56	MG	1A	3509	1/1	0.98	0.15	39,39,39,39	0
56	MG	1A	3916	1/1	0.98	0.16	42,42,42,42	0
56	MG	1A	3803	1/1	0.98	0.06	53,53,53,53	0
56	MG	2B	3008	1/1	0.98	0.27	64,64,64,64	0
56	MG	1A	3804	1/1	0.98	0.04	37,37,37,37	0
56	MG	1a	1774	1/1	0.98	0.15	70,70,70,70	0
56	MG	1a	1850	1/1	0.98	0.12	72,72,72,72	0
56	MG	2A	3040	1/1	0.98	0.49	42,42,42,42	0
56	MG	1A	3266	1/1	0.98	0.24	31,31,31,31	0
56	MG	1V	202	1/1	0.98	0.11	46,46,46,46	0
56	MG	2f	3001	1/1	0.98	0.21	67,67,67,67	0
56	MG	1A	3091	1/1	0.98	0.38	23,23,23,23	0
56	MG	1a	1638	1/1	0.98	0.12	68,68,68,68	0
56	MG	1A	3297	1/1	0.98	0.28	37,37,37,37	0
56	MG	1D	305	1/1	0.98	0.15	34,34,34,34	0
56	MG	1A	3394	1/1	0.98	0.09	33,33,33,33	0
56	MG	2A	3393	1/1	0.98	0.38	54,54,54,54	0
56	MG	2D	304	1/1	0.98	0.72	44,44,44,44	0
56	MG	2A	3490	1/1	0.98	0.18	42,42,42,42	0
56	MG	1A	3425	1/1	0.98	0.11	44,44,44,44	0
56	MG	1A	3516	1/1	0.98	0.08	38,38,38,38	0
56	MG	1a	1710	1/1	0.98	0.33	58,58,58,58	0
56	MG	1A	3758	1/1	0.98	0.05	31,31,31,31	0
56	MG	1A	3044	1/1	0.98	0.07	26,26,26,26	0
56	MG	1A	3454	1/1	0.98	0.10	36,36,36,36	0
56	MG	1A	3396	1/1	0.98	0.12	41,41,41,41	0
56	MG	1a	1715	1/1	0.98	0.19	59,59,59,59	0
56	MG	2A	3221	1/1	0.98	0.28	51,51,51,51	0
56	MG	2A	3403	1/1	0.98	0.43	60,60,60,60	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	1a	1716	1/1	0.98	0.08	49,49,49,49	0
56	MG	1A	3334	1/1	0.98	0.23	33,33,33,33	0
56	MG	1A	3066	1/1	0.98	0.28	13,13,13,13	0
56	MG	1a	1719	1/1	0.98	0.14	71,71,71,71	0
56	MG	1a	1720	1/1	0.98	0.09	52,52,52,52	0
56	MG	1A	3677	1/1	0.98	0.09	40,40,40,40	0
60	ZN	15	102	1/1	0.98	0.11	54,54,54,54	0
60	ZN	16	101	1/1	0.98	0.12	49,49,49,49	0
56	MG	1A	3933	1/1	0.98	0.38	49,49,49,49	0
56	MG	11	101	1/1	0.98	0.12	34,34,34,34	0
56	MG	2P	3401	1/1	0.98	0.17	55,55,55,55	0
60	ZN	26	101	1/1	0.98	0.06	67,67,67,67	0
56	MG	1A	3720	1/1	0.98	0.08	34,34,34,34	0
56	MG	2Q	202	1/1	0.98	0.22	61,61,61,61	0
56	MG	1A	3336	1/1	0.98	0.10	41,41,41,41	0
61	SF4	2d	501	8/8	0.98	0.14	70,73,77,79	0
56	MG	2A	3066	1/1	0.98	0.47	59,59,59,59	0
56	MG	11	102	1/1	0.99	0.05	41,41,41,41	0
56	MG	1A	3302	1/1	0.99	0.10	36,36,36,36	0
56	MG	1A	3771	1/1	0.99	0.10	33,33,33,33	0
56	MG	2A	3492	1/1	0.99	0.26	45,45,45,45	0
56	MG	1A	3082	1/1	0.99	0.10	59,59,59,59	0
56	MG	2A	3277	1/1	0.99	0.15	67,67,67,67	0
56	MG	1A	3087	1/1	0.99	0.30	38,38,38,38	0
56	MG	1A	3097	1/1	0.99	0.49	34,34,34,34	0
56	MG	1A	3409	1/1	0.99	0.06	38,38,38,38	0
56	MG	1A	3338	1/1	0.99	0.21	31,31,31,31	0
56	MG	2A	3573	1/1	0.99	0.21	59,59,59,59	0
56	MG	1A	3248	1/1	0.99	0.15	37,37,37,37	0
56	MG	2A	3016	1/1	0.99	0.15	50,50,50,50	0
56	MG	2A	3284	1/1	0.99	0.15	44,44,44,44	0
56	MG	2A	3215	1/1	0.99	0.10	47,47,47,47	0
56	MG	1A	3132	1/1	0.99	0.25	39,39,39,39	0
56	MG	2A	3018	1/1	0.99	0.11	48,48,48,48	0
56	MG	1A	3237	1/1	0.99	0.30	38,38,38,38	0
56	MG	1A	3264	1/1	0.99	0.17	34,34,34,34	0
56	MG	1A	3505	1/1	0.99	0.07	50,50,50,50	0
56	MG	1A	3197	1/1	0.99	0.11	29,29,29,29	0
56	MG	1A	3923	1/1	0.99	0.24	36,36,36,36	0
56	MG	1A	3140	1/1	0.99	0.11	31,31,31,31	0
56	MG	1A	3784	1/1	0.99	0.05	39,39,39,39	0
56	MG	1A	3839	1/1	0.99	0.19	41,41,41,41	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	2A	3588	1/1	0.99	0.13	47,47,47,47	0
56	MG	2a	1765	1/1	0.99	0.12	66,66,66,66	0
56	MG	1A	3240	1/1	0.99	0.12	41,41,41,41	0
56	MG	1A	3462	1/1	0.99	0.14	30,30,30,30	0
56	MG	1A	3397	1/1	0.99	0.07	34,34,34,34	0
56	MG	1A	3419	1/1	0.99	0.09	42,42,42,42	0
56	MG	1A	3018	1/1	0.99	0.15	33,33,33,33	0
60	ZN	19	102	1/1	0.99	0.11	52,52,52,52	0
56	MG	1A	3103	1/1	0.99	0.15	48,48,48,48	0
56	MG	1D	314	1/1	0.99	0.10	33,33,33,33	0
56	MG	1A	3514	1/1	0.99	0.06	42,42,42,42	0
60	ZN	25	101	1/1	0.99	0.09	65,65,65,65	0
56	MG	1A	3284	1/1	0.99	0.11	39,39,39,39	0
56	MG	1A	3135	1/1	0.99	0.19	33,33,33,33	0
56	MG	1A	3402	1/1	0.99	0.05	36,36,36,36	0
56	MG	1A	3192	1/1	0.99	0.15	32,32,32,32	0
56	MG	2N	8001	1/1	0.99	0.08	55,55,55,55	0
56	MG	1A	3404	1/1	0.99	0.09	32,32,32,32	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.