



# Full wwPDB X-ray Structure Validation Report ⓘ

Apr 20, 2024 – 01:28 pm BST

PDB ID : 5VP2  
Title : Crystal structure of the *Thermus thermophilus* 70S ribosome in complex with madumycin II and bound to mRNA and A-, P- and E-site tRNAs at 2.8Å resolution  
Authors : Osterman, I.A.; Khabibullina, N.F.; Komarova, E.S.; Kasatsky, P.; Kartsev, V.G.; Bogdanov, A.A.; Dontsova, O.A.; Konevega, A.L.; Sergiev, P.V.; Polikanov, Y.S.  
Deposited on : 2017-05-04  
Resolution : 2.80 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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 : 2.36.2  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)

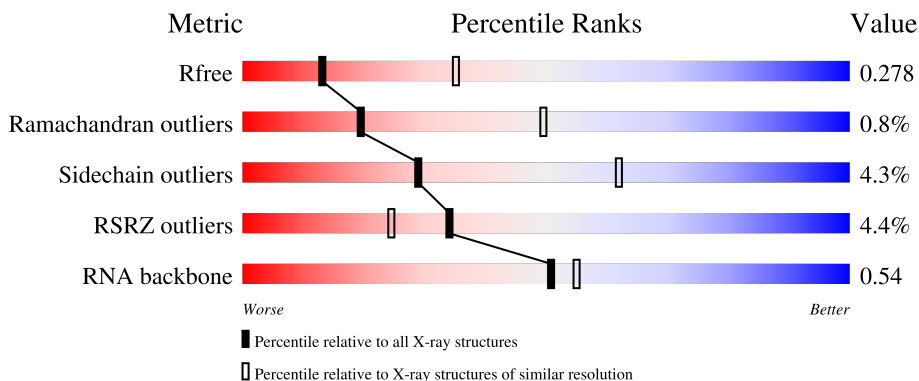
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*


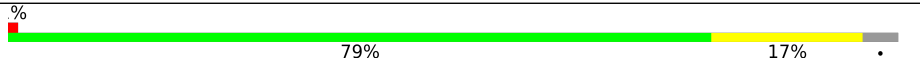
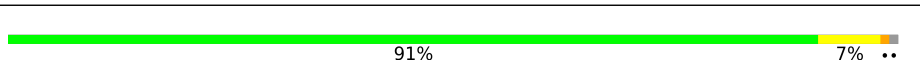
The reported resolution of this entry is 2.80 Å.

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



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

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments 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	
1	2A	2915	
2	1B	121	

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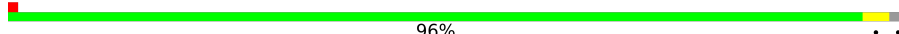
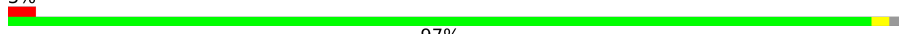


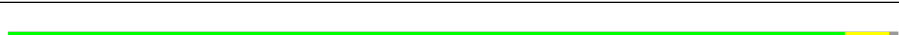
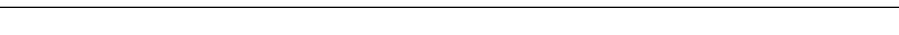
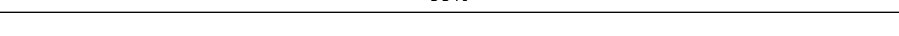
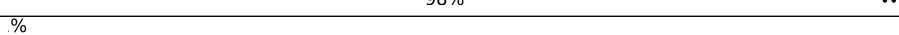
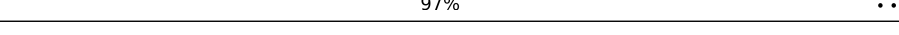
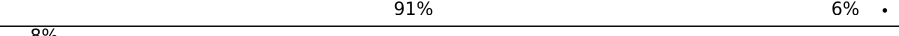



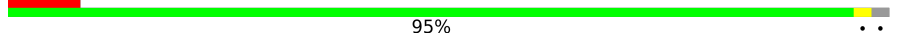
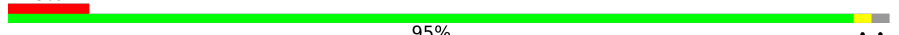
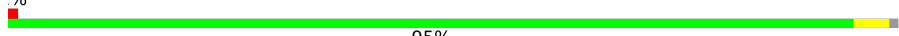





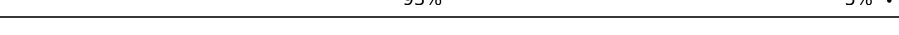

Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.36.2

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Mol	Chain	Length	Quality of chain
2	2B	121	74% 25%
3	1D	276	96%
3	2D	276	96%
4	1E	206	93% 6%
4	2E	206	93% 6%
5	1F	210	91% 6%
5	2F	210	93%
6	1G	182	95%
6	2G	182	93% 6%
7	1H	180	93%
7	2H	180	93%
8	1I	148	91% 7%
8	2I	148	94% 5%
9	1N	140	96%
9	2N	140	92% 8%
10	1O	122	96%
10	2O	122	99%
11	1P	150	95%
11	2P	150	97%
12	1Q	141	97%
12	2Q	141	96%
13	1R	118	92% 8%
13	2R	118	95% 5%
14	1S	112	96%
14	2S	112	96%

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Mol	Chain	Length	Quality of chain
15	1T	146	 86% 10%
15	2T	146	 88% 10%
16	1U	118	 96%
16	2U	118	 97%
17	1V	101	 94% 5%
17	2V	101	 93% 6%
18	1W	113	 94% 5%
18	2W	113	 99%
19	1X	96	 98%
19	2X	96	 97%
20	1Y	110	 91% 6%
20	2Y	110	 91% 6%
21	1Z	206	 69% 5% 25%
21	2Z	206	 74% 22%
22	10	85	 95%
22	20	85	 95%
23	11	98	 95%
23	21	98	 96%
24	12	72	 94%
24	22	72	 94%
25	13	60	 93% 5%
25	23	60	 93% 5%
26	14	71	 86% 10%
26	24	71	 86% 10%
27	15	60	 93% 5%

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Mol	Chain	Length	Quality of chain
27	25	60	92% 7%
28	16	54	94%
28	26	54	9% 96%
29	17	49	6% 92% 6%
29	27	49	12% 94%
30	18	65	3% 92% 6%
30	28	65	9% 92% 6%
31	19	37	97%
31	29	37	27% 97%
32	1a	1521	% 82% 17%
32	2a	1521	3% 79% 20%
33	1b	256	5% 86% 10%
33	2b	256	16% 84% 6% 10%
34	1c	239	3% 85% 14%
34	2c	239	16% 84% 14%
35	1d	209	10% 96%
35	2d	209	10% 97%
36	1e	162	2% 86% 6% 9%
36	2e	162	17% 89% 9%
37	1f	101	98%
37	2f	101	2% 96%
38	1g	156	7% 96%
38	2g	156	16% 96%
39	1h	138	2% 96%
39	2h	138	13% 94% 5%

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Mol	Chain	Length	Quality of chain
40	1i	128	9% 96%
40	2i	128	40% 95%
41	1j	105	12% 87% 6% 8%
41	2j	105	33% 85% 7% 9%
42	1k	129	87% 12%
42	2k	129	8% 84% 5% 12%
43	1l	132	2% 89% 8%
43	2l	132	11% 89% 8%
44	1m	126	3% 94%
44	2m	126	22% 96%
45	1n	61	8% 89% 10%
45	2n	61	59% 90% 8%
46	1o	89	6% 98%
46	2o	89	11% 98%
47	1p	88	11% 89% 5% 7%
47	2p	88	7% 85% 8% 7%
48	1q	105	6% 93% 6%
48	2q	105	21% 90% 6%
49	1r	88	% 76% 23%
49	2r	88	% 74% 23%
50	1s	93	% 84% 5% 11%
50	2s	93	26% 86% 11%
51	1t	106	5% 88% 9%
51	2t	106	9% 87% 9%
52	1u	27	33% 81% 15%

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Mol	Chain	Length	Quality of chain
52	2u	27	
53	1v	24	
53	2v	24	
54	1w	76	
54	1y	76	
54	2w	76	
54	2y	76	
55	1x	77	
55	2x	77	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
56	MG	1A	3372	-	-	-	X
56	MG	1A	3475	-	-	-	X
56	MG	1A	3492	-	-	-	X
56	MG	1A	3891	-	-	-	X
56	MG	1A	4042	-	-	-	X
56	MG	1O	3001	-	-	-	X
56	MG	1v	3001	-	-	-	X
56	MG	1w	108	-	-	-	X
56	MG	2A	3187	-	-	-	X
56	MG	2A	3339	-	-	-	X
56	MG	2A	3432	-	-	-	X
56	MG	2A	3675	-	-	-	X
56	MG	2A	3741	-	-	-	X
56	MG	2A	3873	-	-	-	X
56	MG	2F	301	-	-	-	X
56	MG	2U	202	-	-	-	X
56	MG	2V	201	-	-	-	X
56	MG	2a	3024	-	-	-	X
56	MG	2a	3113	-	-	-	X

## 2 Entry composition [i](#)

There are 61 unique types of molecules in this entry. The entry contains 300935 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
1	1A	2871	Total	C	N	O	P	0	0	0
			61852	27531	11572	19878	2871			
1	2A	2800	Total	C	N	O	P	0	0	0
			60322	26848	11284	19390	2800			

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

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

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

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

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

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

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



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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
6	1G	181	Total 1423	C 913	N 253	O 253	S 4	0	0	0
6	2G	181	Total 1428	C 913	N 258	O 253	S 4	0	0	0

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
8	1I	146	Total 1097	C 701	N 191	O 204	S 1	0	0	0
8	2I	146	Total 1064	C 681	N 186	O 196	S 1	0	0	0

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

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

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

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

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
14	1S	110	873	550	174	149	0	0	0
14	2S	110	870	549	173	148	0	0	0

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
17	1V	101	Total 771	C 495	N 140	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 806	C 517	N 152	O 131	S 6	0	0	0
20	2Y	107	Total 806	C 517	N 152	O 131	S 6	0	0	0

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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



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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
50	1s	83	Total	C	N	O	S	0	0	0
			652	417	120	113	2			
50	2s	83	Total	C	N	O	S	0	0	0
			646	412	119	113	2			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
51	1t	96	Total	C	N	O	S	0	0	0
			728	446	156	124	2			
51	2t	96	Total	C	N	O	S	0	0	0
			727	446	155	124	2			

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

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

- Molecule 53 is a RNA chain called mRNA.

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

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

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
54	1w	72	Total	C	N	O	P	S	0	0	0
			1550	694	277	505	72	2			
54	1y	74	Total	C	N	O	P	S	0	0	0
			1585	707	285	518	74	1			
54	2w	69	Total	C	N	O	P	S	0	0	0
			1482	662	267	482	69	2			
54	2y	73	Total	C	N	O	P	S	0	0	0
			1565	698	283	510	73	1			

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

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

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
56	1A	1143	Total	Mg	0	0
			1143	1143		
56	1B	36	Total	Mg	0	0
			36	36		
56	1D	14	Total	Mg	0	0
			14	14		
56	1E	12	Total	Mg	0	0
			12	12		
56	1F	8	Total	Mg	0	0
			8	8		
56	1G	5	Total	Mg	0	0
			5	5		
56	1I	1	Total	Mg	0	0
			1	1		
56	1N	6	Total	Mg	0	0
			6	6		

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

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
56	1a	235	Total Mg 235 235	0	0
56	1b	2	Total Mg 2 2	0	0
56	1d	1	Total Mg 1 1	0	0
56	1e	1	Total Mg 1 1	0	0
56	1f	2	Total Mg 2 2	0	0
56	1l	3	Total Mg 3 3	0	0
56	1m	1	Total Mg 1 1	0	0
56	1n	2	Total Mg 2 2	0	0
56	1p	1	Total Mg 1 1	0	0
56	1s	1	Total Mg 1 1	0	0
56	1t	1	Total Mg 1 1	0	0
56	1v	1	Total Mg 1 1	0	0
56	1w	11	Total Mg 11 11	0	0
56	1x	15	Total Mg 15 15	0	0
56	1y	5	Total Mg 5 5	0	0
56	2A	876	Total Mg 876 876	0	0
56	2B	21	Total Mg 21 21	0	0
56	2D	7	Total Mg 7 7	0	0
56	2E	7	Total Mg 7 7	0	0
56	2F	4	Total Mg 4 4	0	0
56	2G	1	Total Mg 1 1	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
56	2O	1	Total Mg 1 1	0	0
56	2Q	4	Total Mg 4 4	0	0
56	2R	2	Total Mg 2 2	0	0
56	2T	3	Total Mg 3 3	0	0
56	2U	6	Total Mg 6 6	0	0
56	2V	1	Total Mg 1 1	0	0
56	2W	2	Total Mg 2 2	0	0
56	2X	2	Total Mg 2 2	0	0
56	2Z	1	Total Mg 1 1	0	0
56	20	2	Total Mg 2 2	0	0
56	23	1	Total Mg 1 1	0	0
56	25	4	Total Mg 4 4	0	0
56	26	1	Total Mg 1 1	0	0
56	27	1	Total Mg 1 1	0	0
56	28	1	Total Mg 1 1	0	0
56	2a	230	Total Mg 230 230	0	0
56	2d	2	Total Mg 2 2	0	0
56	2e	1	Total Mg 1 1	0	0
56	2f	1	Total Mg 1 1	0	0
56	2g	1	Total Mg 1 1	0	0
56	2j	2	Total Mg 2 2	0	0

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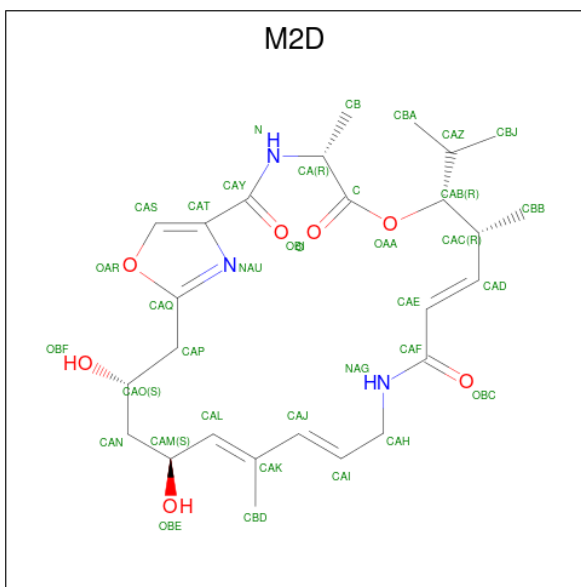
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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
56	2l	2	Total Mg 2 2	0	0
56	2p	1	Total Mg 1 1	0	0
56	2q	3	Total Mg 3 3	0	0
56	2r	2	Total Mg 2 2	0	0
56	2t	1	Total Mg 1 1	0	0
56	2v	3	Total Mg 3 3	0	0
56	2w	7	Total Mg 7 7	0	0
56	2x	6	Total Mg 6 6	0	0
56	2y	6	Total Mg 6 6	0	0

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

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

- Molecule 58 is Madumycin II (three-letter code: M2D) (formula: C<sub>26</sub>H<sub>37</sub>N<sub>3</sub>O<sub>7</sub>).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
58	1A	1	36	26	3	7	0	0
58	2A	1	36	26	3	7	0	0

- Molecule 59 is ZINC ION (three-letter code: ZN) (formula: Zn).

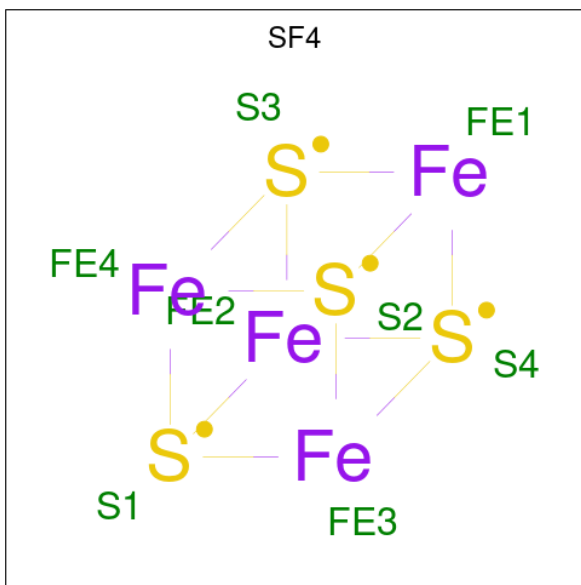
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Zn		
59	1Y	1	1	1	0	0
59	14	1	1	1	0	0
59	15	1	1	1	0	0
59	16	1	1	1	0	0
59	19	1	1	1	0	0
59	1n	1	1	1	0	0
59	2Y	1	1	1	0	0
59	24	1	1	1	0	0
59	25	1	1	1	0	0
59	26	1	1	1	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
59	29	1	Total Zn 1 1	0	0
59	2n	1	Total Zn 1 1	0	0

- Molecule 60 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe<sub>4</sub>S<sub>4</sub>).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
60	1d	1	Total Fe S 8 4 4	0	0
60	2d	1	Total Fe S 8 4 4	0	0

- Molecule 61 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
61	1A	2255	Total O 2255 2255	0	0
61	1B	68	Total O 68 68	0	0
61	1D	30	Total O 30 30	0	0
61	1E	28	Total O 28 28	0	0
61	1F	21	Total O 21 21	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
61	1G	5	Total 5	O 5	0	0
61	1H	1	Total 1	O 1	0	0
61	1I	2	Total 2	O 2	0	0
61	1N	8	Total 8	O 8	0	0
61	1O	11	Total 11	O 11	0	0
61	1P	25	Total 25	O 25	0	0
61	1Q	13	Total 13	O 13	0	0
61	1R	15	Total 15	O 15	0	0
61	1S	4	Total 4	O 4	0	0
61	1T	5	Total 5	O 5	0	0
61	1U	13	Total 13	O 13	0	0
61	1V	10	Total 10	O 10	0	0
61	1W	9	Total 9	O 9	0	0
61	1X	6	Total 6	O 6	0	0
61	1Y	5	Total 5	O 5	0	0
61	1Z	1	Total 1	O 1	0	0
61	10	8	Total 8	O 8	0	0
61	11	14	Total 14	O 14	0	0
61	12	4	Total 4	O 4	0	0
61	13	4	Total 4	O 4	0	0
61	14	1	Total 1	O 1	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
61	15	7	Total O 7 7	0	0
61	16	4	Total O 4 4	0	0
61	17	7	Total O 7 7	0	0
61	18	13	Total O 13 13	0	0
61	19	3	Total O 3 3	0	0
61	1a	454	Total O 454 454	0	0
61	1b	1	Total O 1 1	0	0
61	1f	1	Total O 1 1	0	0
61	1l	7	Total O 7 7	0	0
61	1m	2	Total O 2 2	0	0
61	1o	1	Total O 1 1	0	0
61	1q	3	Total O 3 3	0	0
61	1r	1	Total O 1 1	0	0
61	1u	1	Total O 1 1	0	0
61	1v	6	Total O 6 6	0	0
61	1w	18	Total O 18 18	0	0
61	1x	16	Total O 16 16	0	0
61	1y	3	Total O 3 3	0	0
61	2A	1418	Total O 1418 1418	0	0
61	2B	26	Total O 26 26	0	0
61	2D	29	Total O 29 29	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
61	2E	14	Total O 14 14	0	0
61	2F	15	Total O 15 15	0	0
61	2I	4	Total O 4 4	0	0
61	2N	2	Total O 2 2	0	0
61	2O	1	Total O 1 1	0	0
61	2P	13	Total O 13 13	0	0
61	2Q	2	Total O 2 2	0	0
61	2R	2	Total O 2 2	0	0
61	2T	4	Total O 4 4	0	0
61	2U	2	Total O 2 2	0	0
61	2V	1	Total O 1 1	0	0
61	2W	3	Total O 3 3	0	0
61	2X	5	Total O 5 5	0	0
61	2Y	1	Total O 1 1	0	0
61	2Z	2	Total O 2 2	0	0
61	20	5	Total O 5 5	0	0
61	21	14	Total O 14 14	0	0
61	22	1	Total O 1 1	0	0
61	23	2	Total O 2 2	0	0
61	25	5	Total O 5 5	0	0
61	26	1	Total O 1 1	0	0

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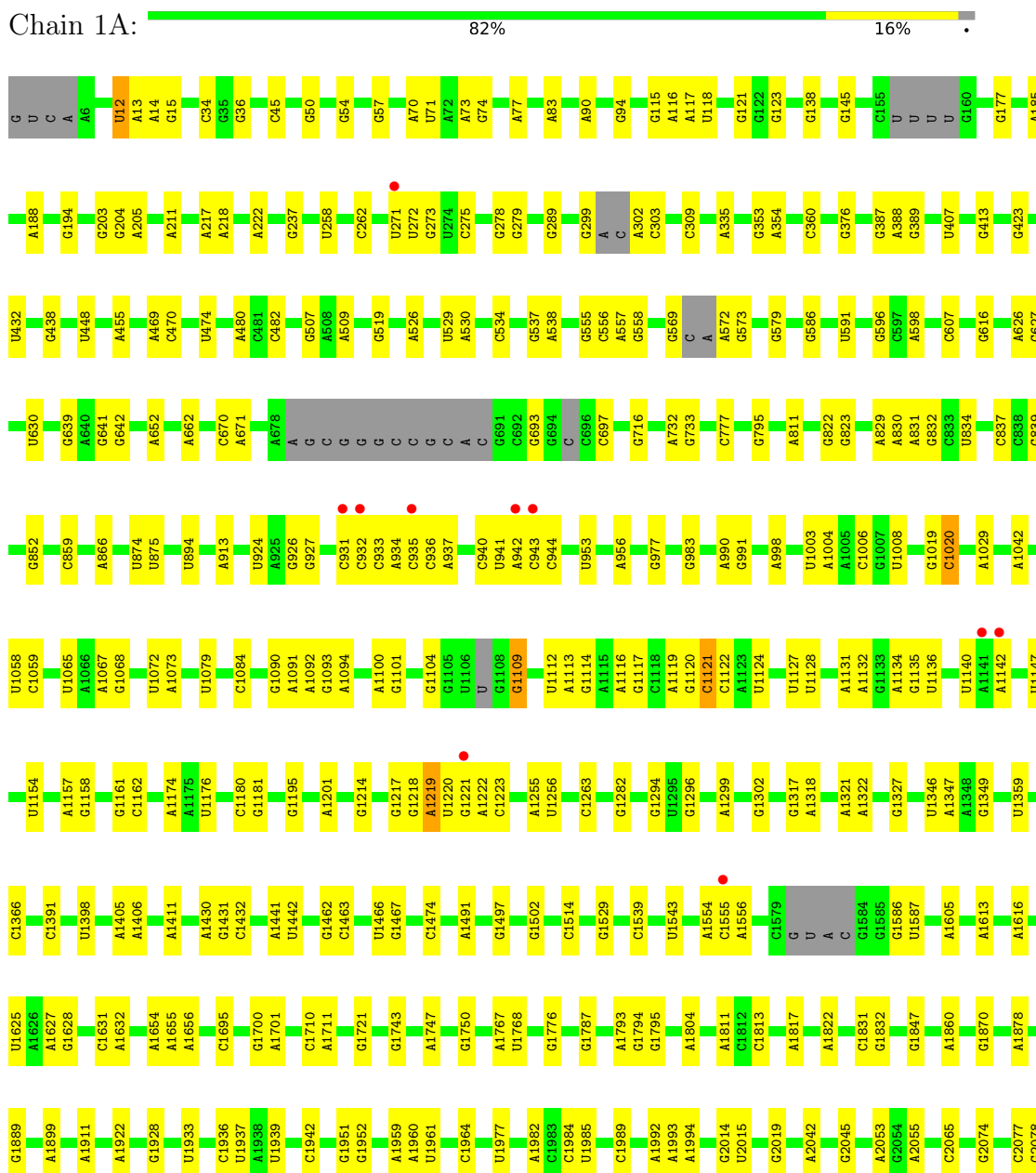
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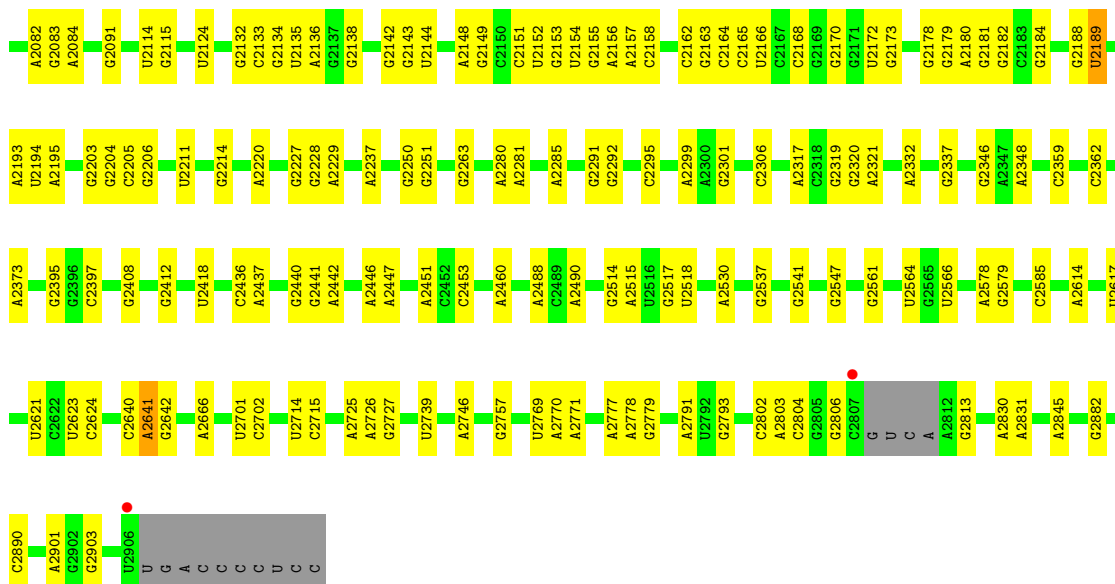
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
61	27	3	Total O 3 3	0	0
61	28	5	Total O 5 5	0	0
61	29	1	Total O 1 1	0	0
61	2a	392	Total O 392 392	0	0
61	2c	2	Total O 2 2	0	0
61	2d	4	Total O 4 4	0	0
61	2e	2	Total O 2 2	0	0
61	2g	1	Total O 1 1	0	0
61	2j	4	Total O 4 4	0	0
61	2k	1	Total O 1 1	0	0
61	2l	6	Total O 6 6	0	0
61	2o	4	Total O 4 4	0	0
61	2p	2	Total O 2 2	0	0
61	2q	1	Total O 1 1	0	0
61	2r	1	Total O 1 1	0	0
61	2t	3	Total O 3 3	0	0
61	2u	1	Total O 1 1	0	0
61	2v	4	Total O 4 4	0	0
61	2w	1	Total O 1 1	0	0
61	2x	6	Total O 6 6	0	0
61	2y	19	Total O 19 19	0	0

### 3 Residue-property plots

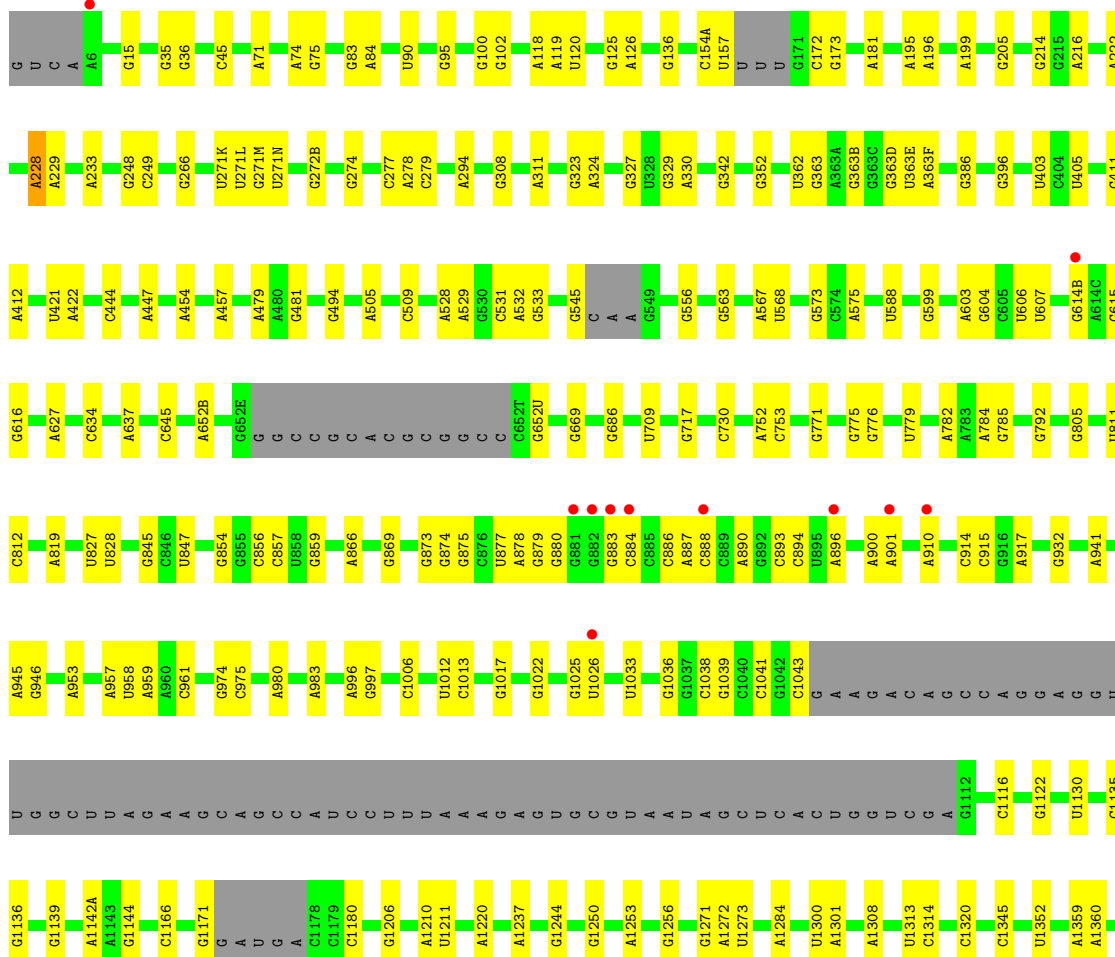
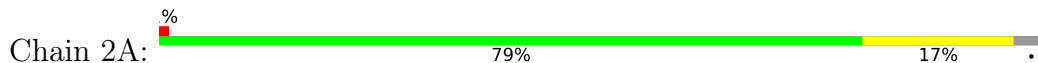
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

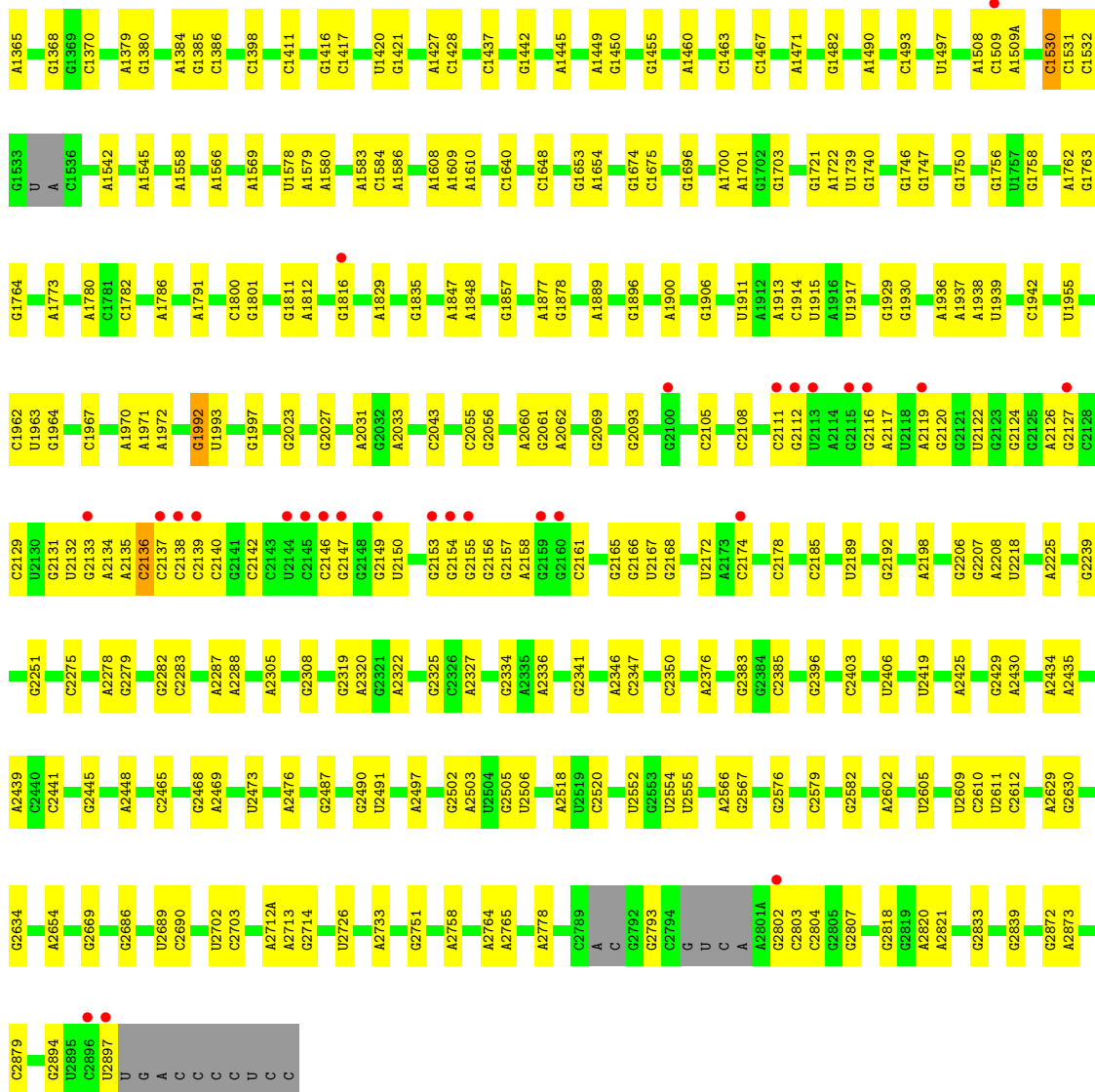
- Molecule 1: 23S Ribosomal RNA





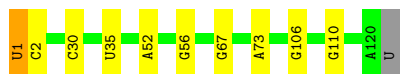
● Molecule 1: 23S Ribosomal RNA





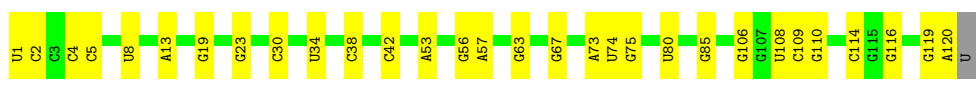
• Molecule 2: 5S ribosomal RNA

Chain 1B:  91%  7% ..



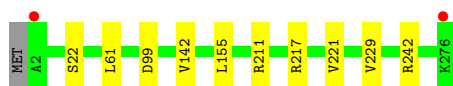
• Molecule 2: 5S ribosomal RNA

Chain 2B:  74%  25% .



• Molecule 3: 50S ribosomal protein L2

Chain 1D:  96%  .



- Molecule 3: 50S ribosomal protein L2



- Molecule 4: 50S ribosomal protein L3



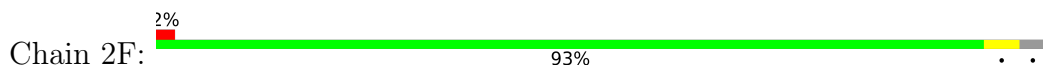
- Molecule 4: 50S ribosomal protein L3



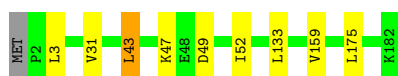
- Molecule 5: 50S ribosomal protein L4



- Molecule 5: 50S ribosomal protein L4



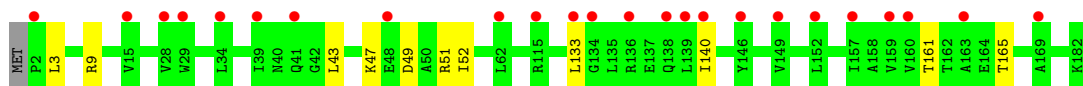
- Molecule 6: 50S ribosomal protein L5



- Molecule 6: 50S ribosomal protein L5



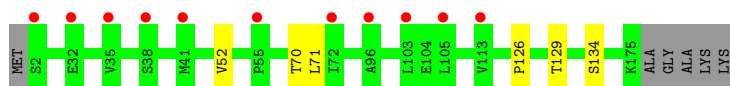




- Molecule 7: 50S ribosomal protein L6



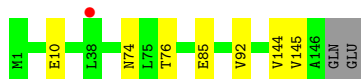
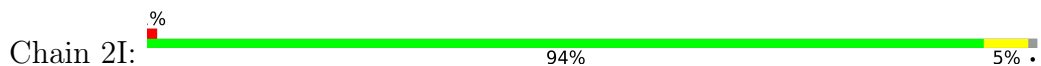
- Molecule 7: 50S ribosomal protein L6



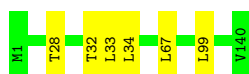
- Molecule 8: 50S ribosomal protein L9



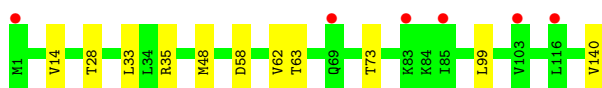
- Molecule 8: 50S ribosomal protein L9



- Molecule 9: 50S ribosomal protein L13



- Molecule 9: 50S ribosomal protein L13



- Molecule 10: 50S ribosomal protein L14





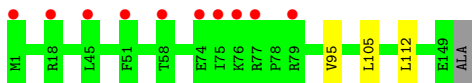
- Molecule 10: 50S ribosomal protein L14



- Molecule 11: 50S ribosomal protein L15



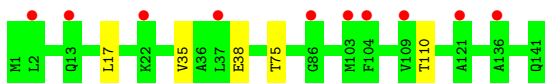
- Molecule 11: 50S ribosomal protein L15



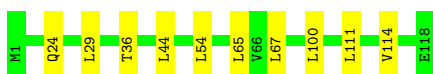
- Molecule 12: 50S ribosomal protein L16



- Molecule 12: 50S ribosomal protein L16

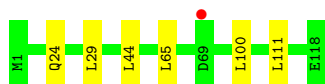


- Molecule 13: 50S ribosomal protein L17

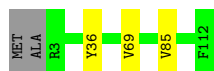


- Molecule 13: 50S ribosomal protein L17

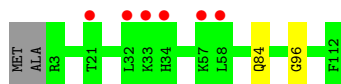




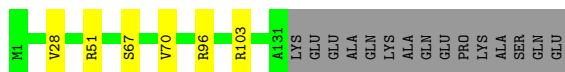
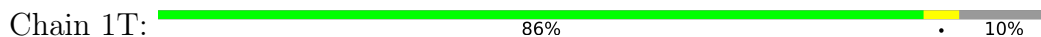
- Molecule 14: 50S ribosomal protein L18



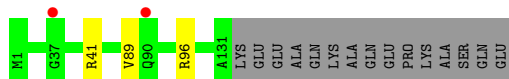
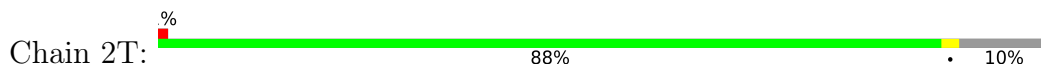
- Molecule 14: 50S ribosomal protein L18



- Molecule 15: 50S ribosomal protein L19



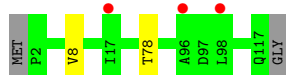
- Molecule 15: 50S ribosomal protein L19



- Molecule 16: 50S ribosomal protein L20



- Molecule 16: 50S ribosomal protein L20



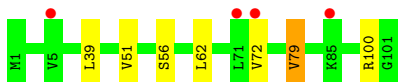
- Molecule 17: 50S ribosomal protein L21

Chain 1V:  94% 5%



- Molecule 17: 50S ribosomal protein L21

Chain 2V:  4% 93% 6%



- Molecule 18: 50S ribosomal protein L22

Chain 1W:  94% 5%



- Molecule 18: 50S ribosomal protein L22

Chain 2W:  99%



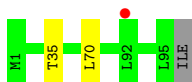
- Molecule 19: 50S ribosomal protein L23

Chain 1X:  98%



- Molecule 19: 50S ribosomal protein L23

Chain 2X:  % 97%

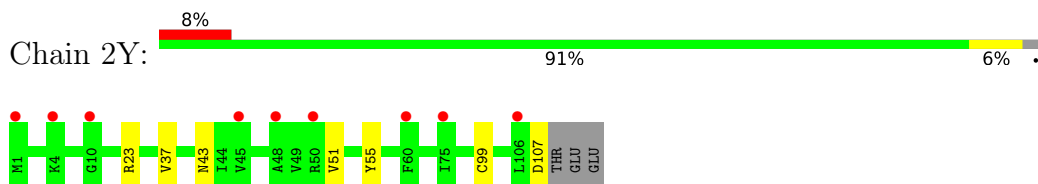


- Molecule 20: 50S ribosomal protein L24

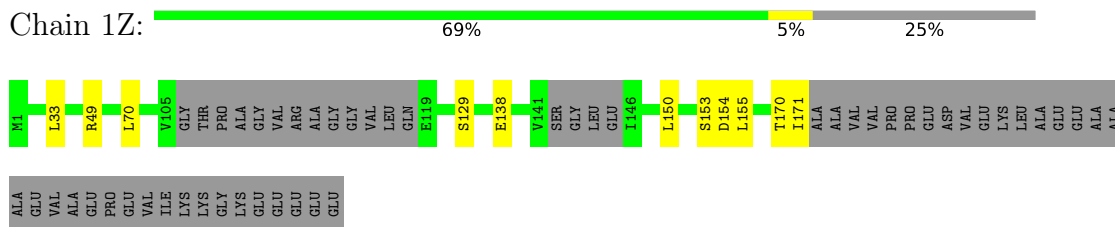
Chain 1Y:  91% 6%



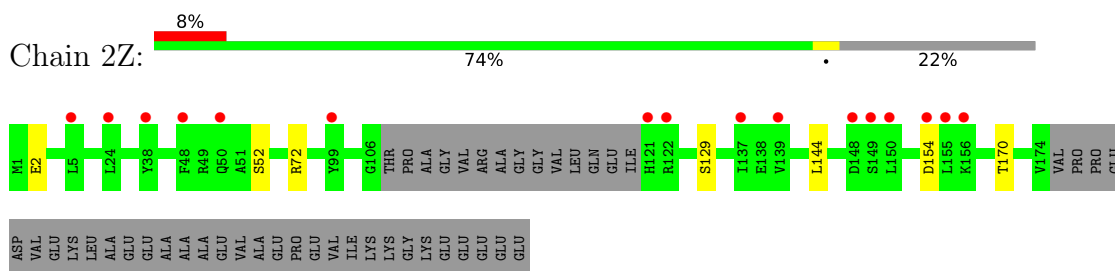
- Molecule 20: 50S ribosomal protein L24



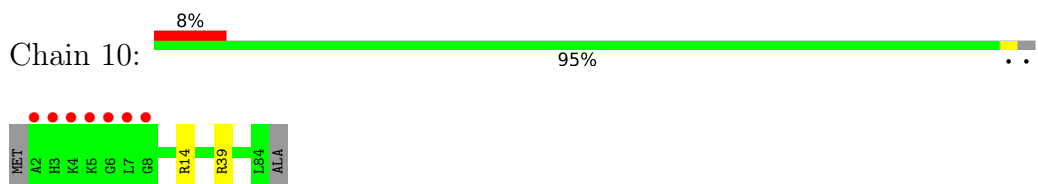
• Molecule 21: 50S ribosomal protein L25



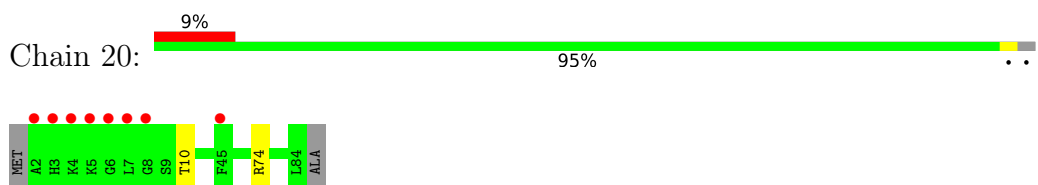
• Molecule 21: 50S ribosomal protein L25



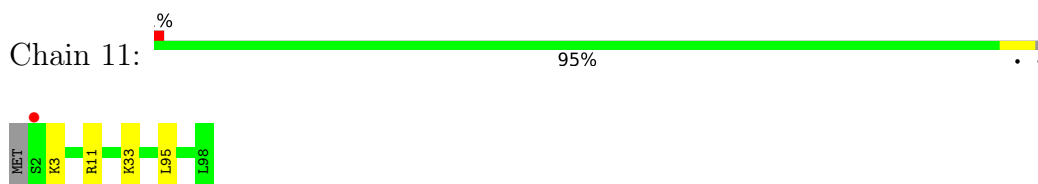
• Molecule 22: 50S ribosomal protein L27



• Molecule 22: 50S ribosomal protein L27

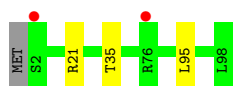


• Molecule 23: 50S ribosomal protein L28

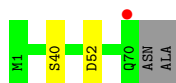


• Molecule 23: 50S ribosomal protein L28





- Molecule 24: 50S ribosomal protein L29



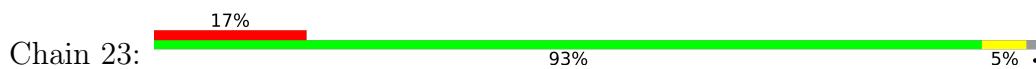
- Molecule 24: 50S ribosomal protein L29



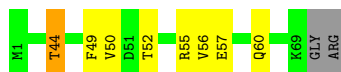
- Molecule 25: 50S ribosomal protein L30



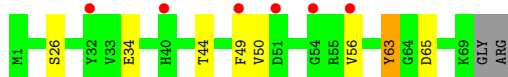
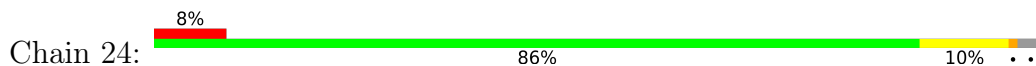
- Molecule 25: 50S ribosomal protein L30



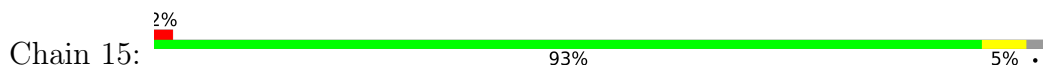
- Molecule 26: 50S ribosomal protein L31



- Molecule 26: 50S ribosomal protein L31



- Molecule 27: 50S ribosomal protein L32



- Molecule 27: 50S ribosomal protein L32



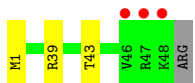
- Molecule 28: 50S ribosomal protein L33



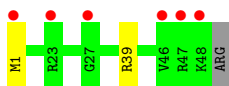
- Molecule 28: 50S ribosomal protein L33



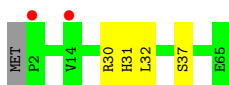
- Molecule 29: 50S ribosomal protein L34



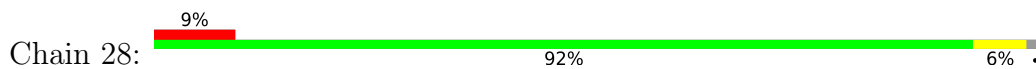
- Molecule 29: 50S ribosomal protein L34



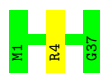
- Molecule 30: 50S ribosomal protein L35



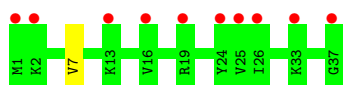
- Molecule 30: 50S ribosomal protein L35



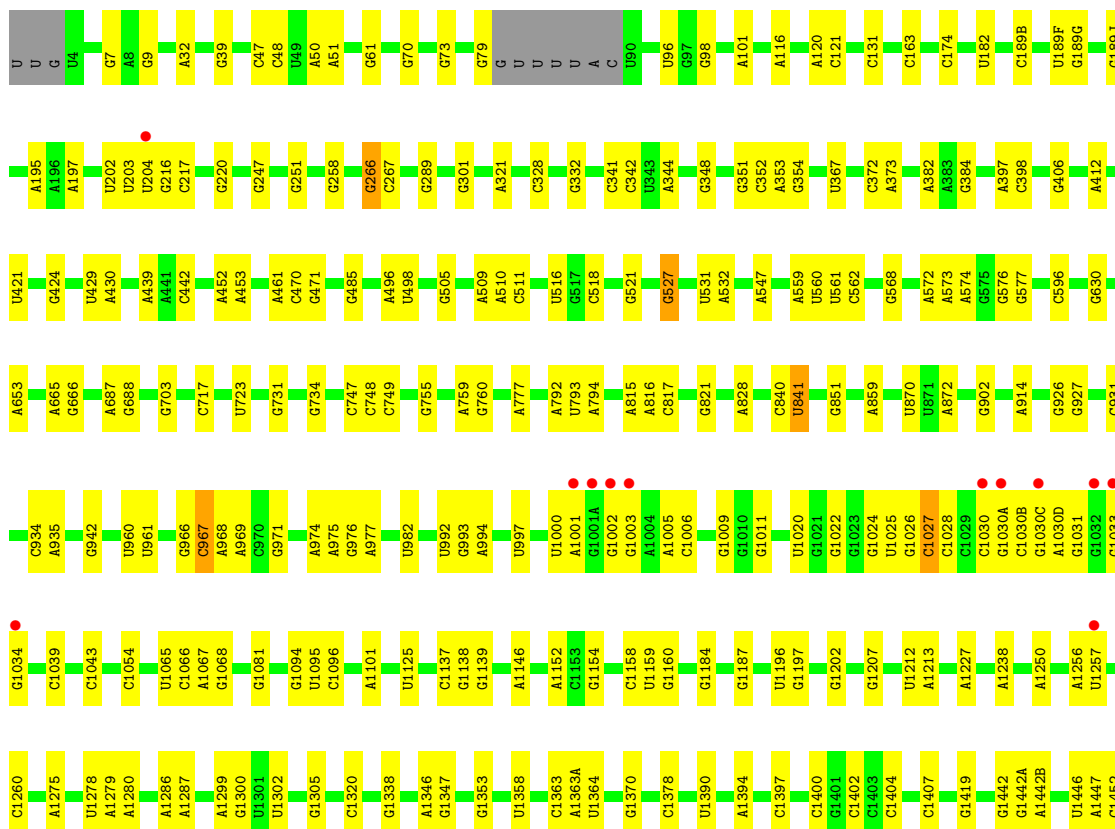
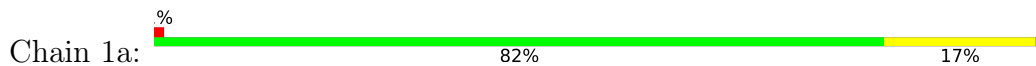
- Molecule 31: 50S ribosomal protein L36



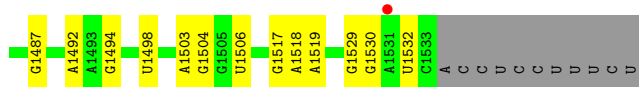
- Molecule 31: 50S ribosomal protein L36



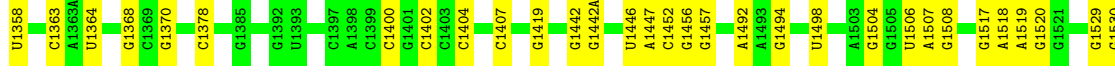
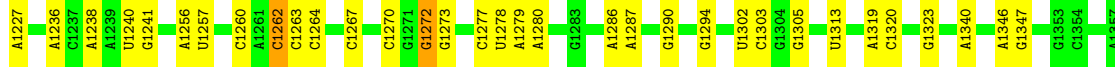
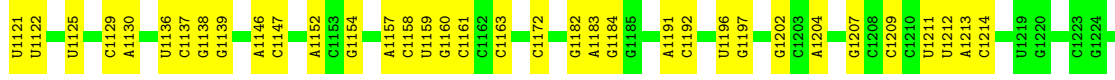
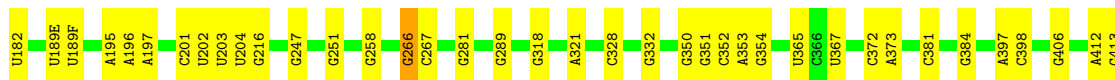
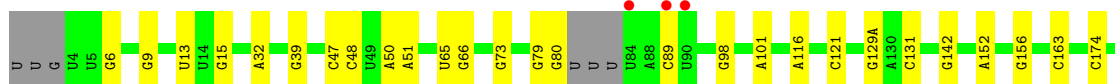
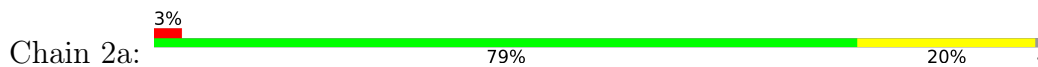
- Molecule 32: 16S ribosomal RNA



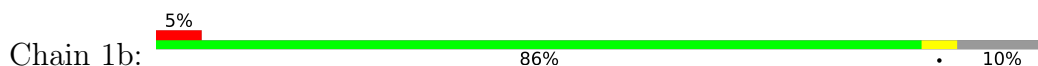


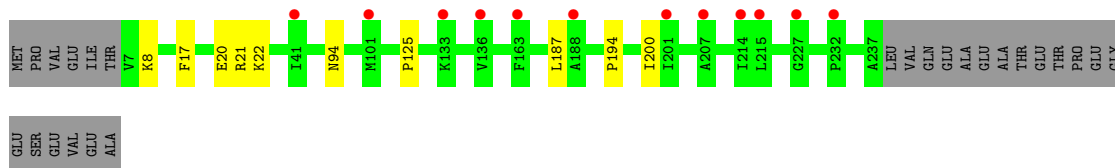


• Molecule 32: 16S ribosomal RNA

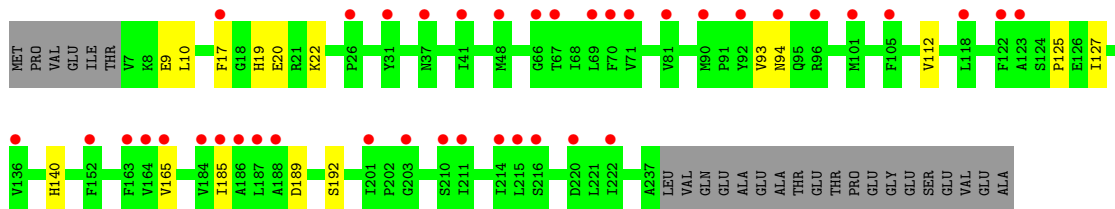
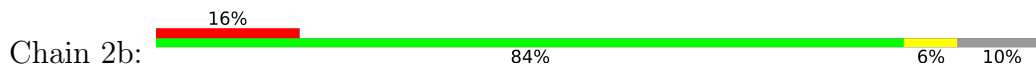


• Molecule 33: 30S ribosomal protein S2

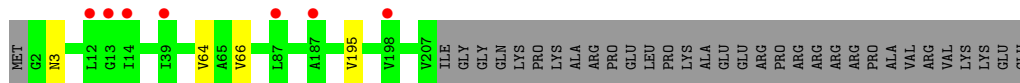
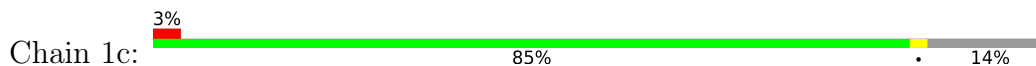




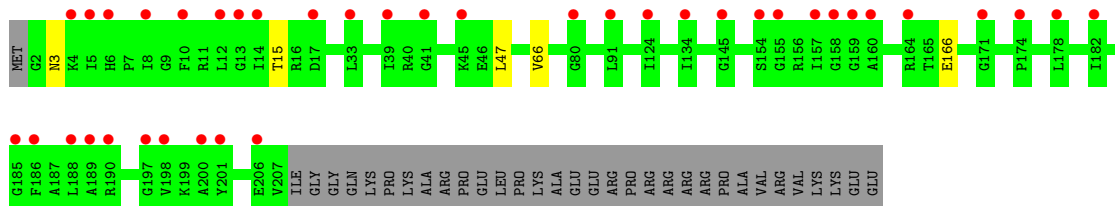
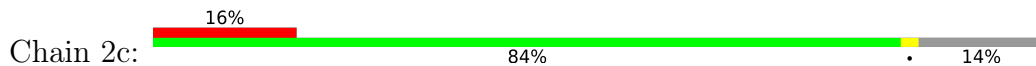
- Molecule 33: 30S ribosomal protein S2



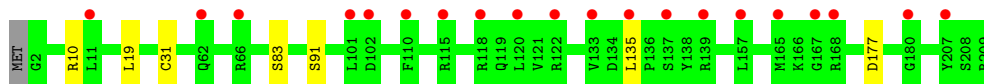
- Molecule 34: 30S ribosomal protein S3



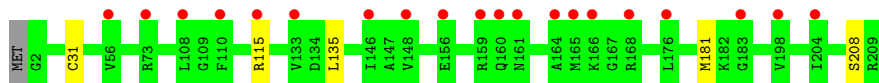
- Molecule 34: 30S ribosomal protein S3



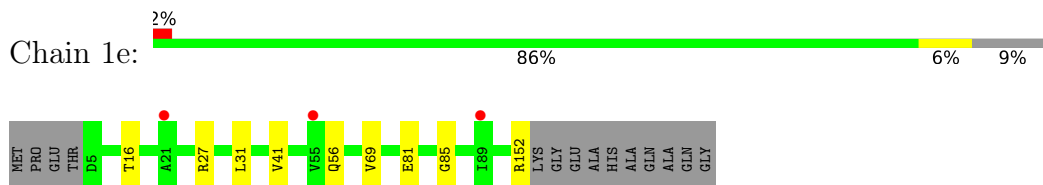
- Molecule 35: 30S ribosomal protein S4



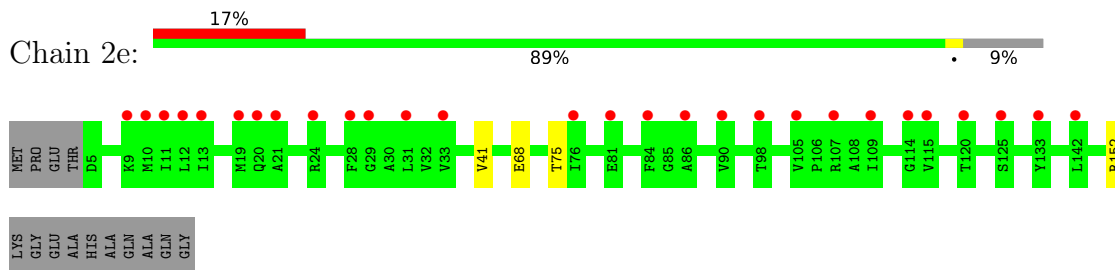
- Molecule 35: 30S ribosomal protein S4



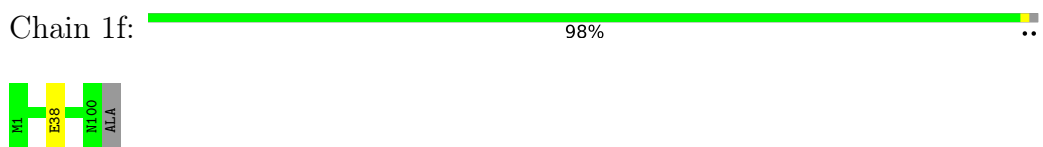
- Molecule 36: 30S ribosomal protein S5



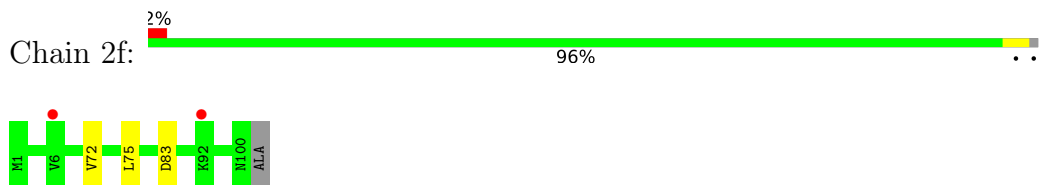
- Molecule 36: 30S ribosomal protein S5



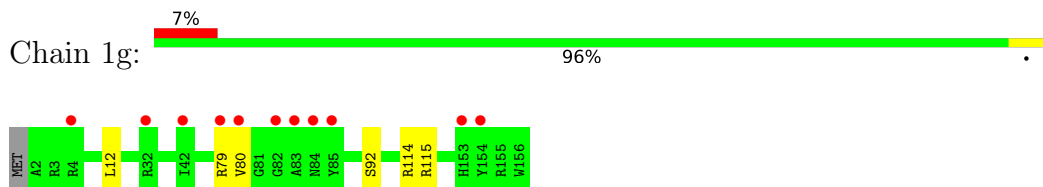
- Molecule 37: 30S ribosomal protein S6



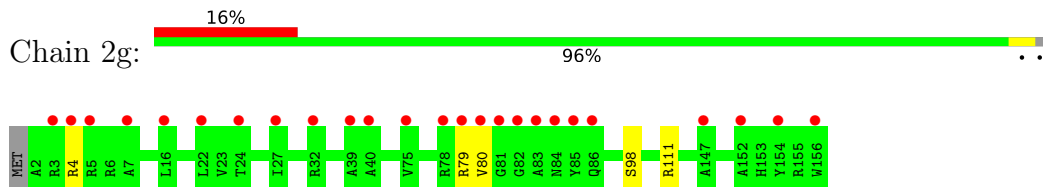
- Molecule 37: 30S ribosomal protein S6



- Molecule 38: 30S ribosomal protein S7

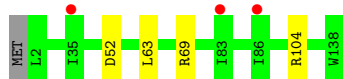


- Molecule 38: 30S ribosomal protein S7

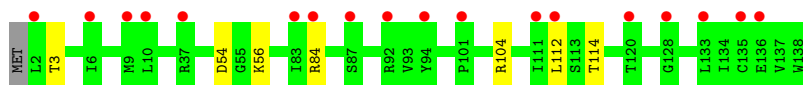


- Molecule 39: 30S ribosomal protein S8





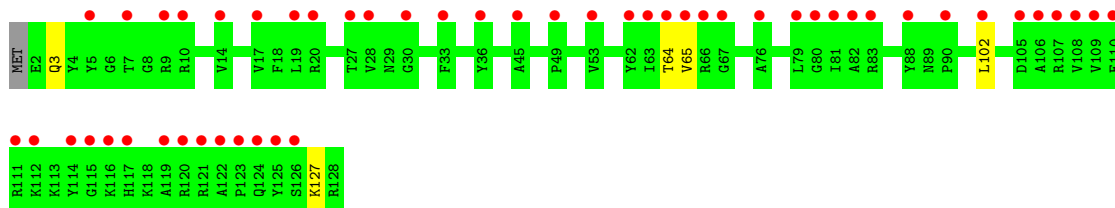
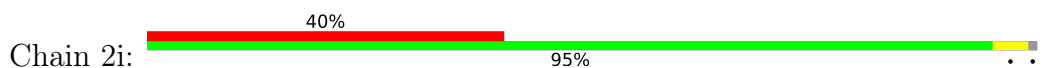
- Molecule 39: 30S ribosomal protein S8



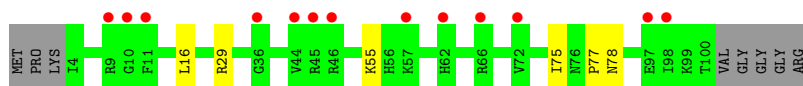
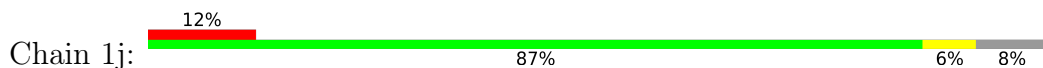
- Molecule 40: 30S ribosomal protein S9



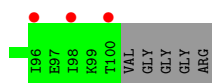
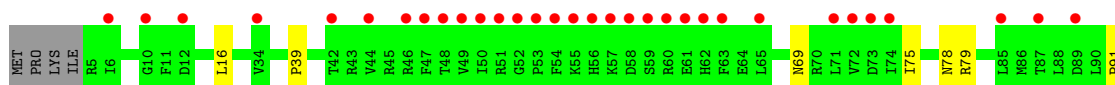
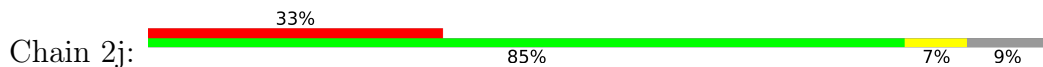
- Molecule 40: 30S ribosomal protein S9




- Molecule 41: 30S ribosomal protein S10

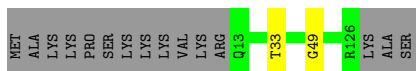


- Molecule 41: 30S ribosomal protein S10




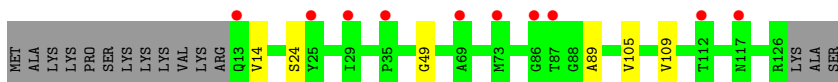
- Molecule 42: 30S ribosomal protein S11

Chain 1k:  87% 12%




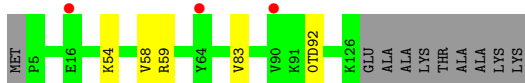
- Molecule 42: 30S ribosomal protein S11

Chain 2k:  84% 5% 12% 8%




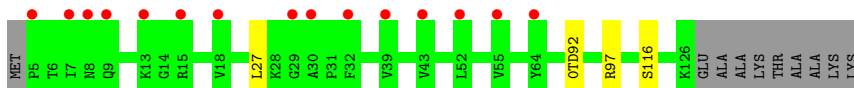
- Molecule 43: 30S ribosomal protein S12

Chain 1l:  89% 8% 2%



- Molecule 43: 30S ribosomal protein S12

Chain 2l:  89% 8% 11%



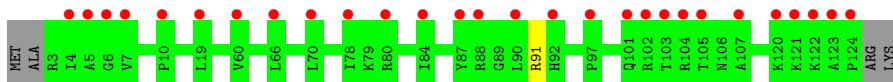
- Molecule 44: 30S ribosomal protein S13

Chain 1m:  94% 3% 3%




- Molecule 44: 30S ribosomal protein S13

Chain 2m:  96% 22% 2%

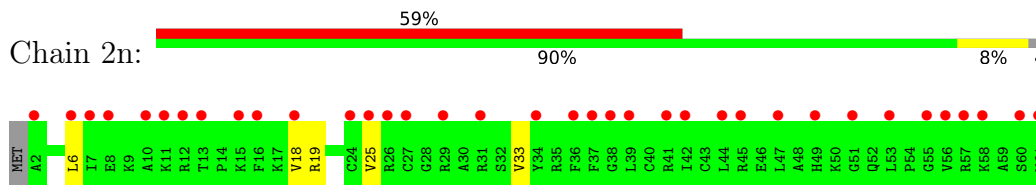


- Molecule 45: 30S ribosomal protein S14 type Z

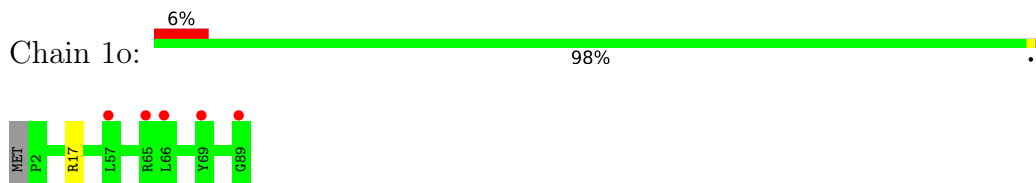
Chain 1n:  89% 10% 8%



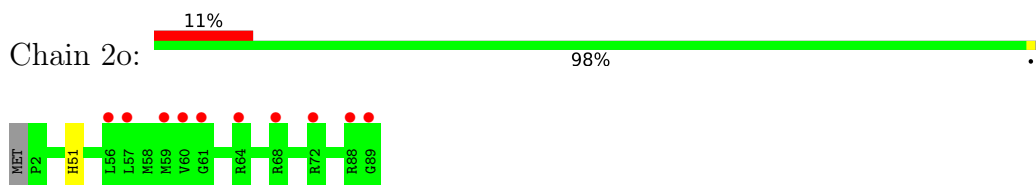
- Molecule 45: 30S ribosomal protein S14 type Z



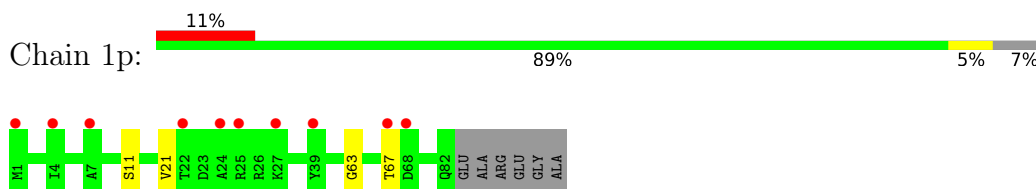
- Molecule 46: 30S ribosomal protein S15



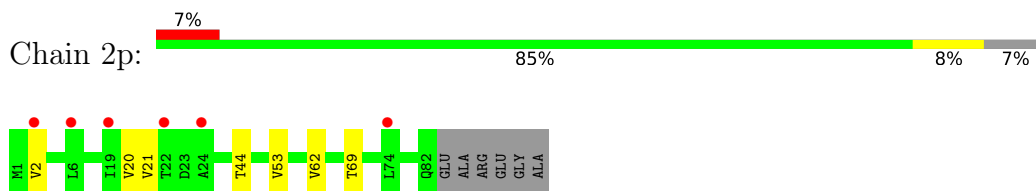
- Molecule 46: 30S ribosomal protein S15



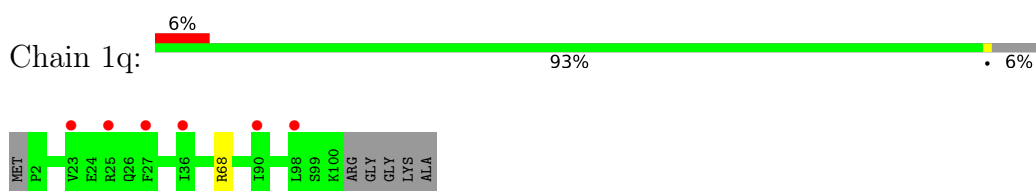
- Molecule 47: 30S ribosomal protein S16



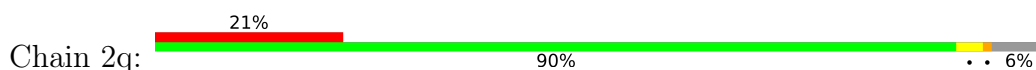
- Molecule 47: 30S ribosomal protein S16



- Molecule 48: 30S ribosomal protein S17

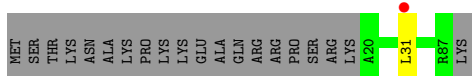
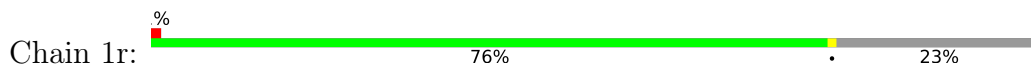


- Molecule 48: 30S ribosomal protein S17

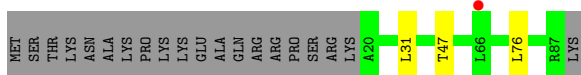
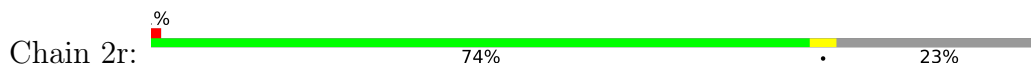




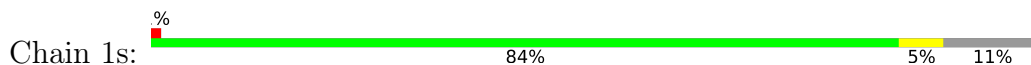
- Molecule 49: 30S ribosomal protein S18



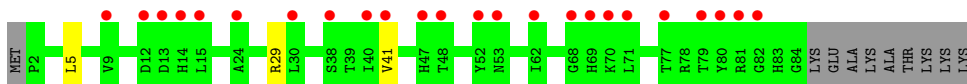
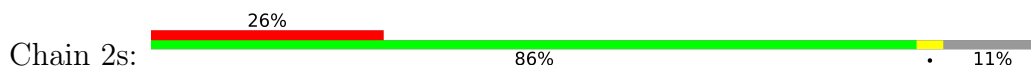
- Molecule 49: 30S ribosomal protein S18



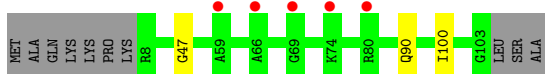
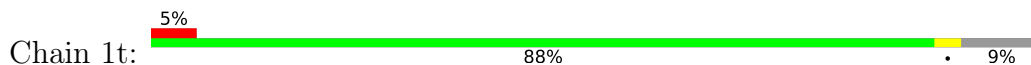
- Molecule 50: 30S ribosomal protein S19



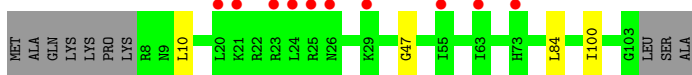
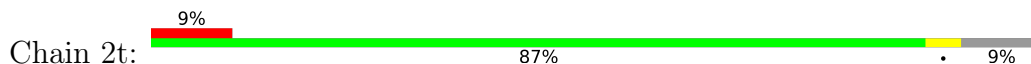
- Molecule 50: 30S ribosomal protein S19



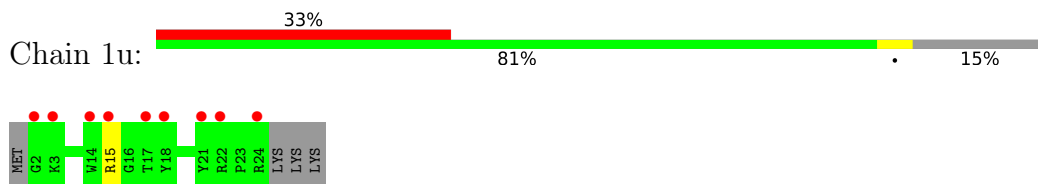
- Molecule 51: 30S ribosomal protein S20



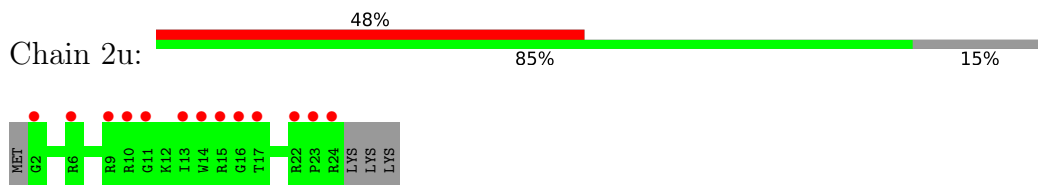
- Molecule 51: 30S ribosomal protein S20



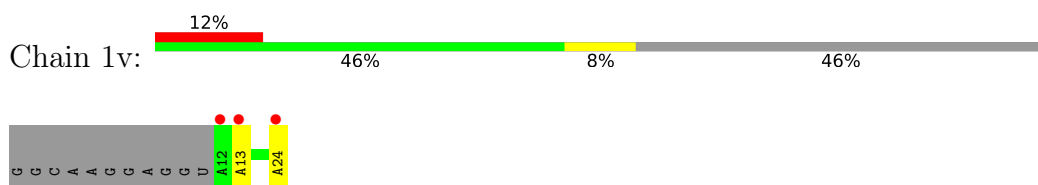
- Molecule 52: 30S ribosomal protein Thx



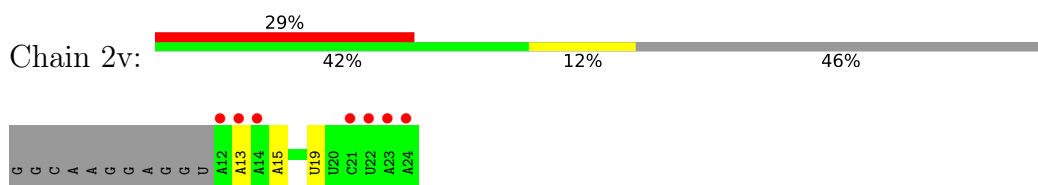
• Molecule 52: 30S ribosomal protein Thx



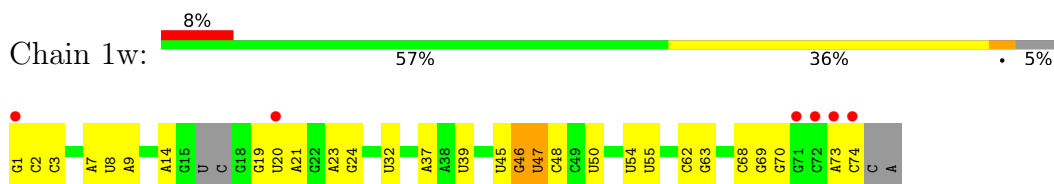
• Molecule 53: mRNA



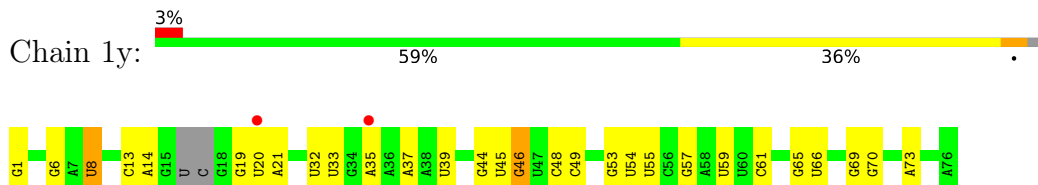
• Molecule 53: mRNA



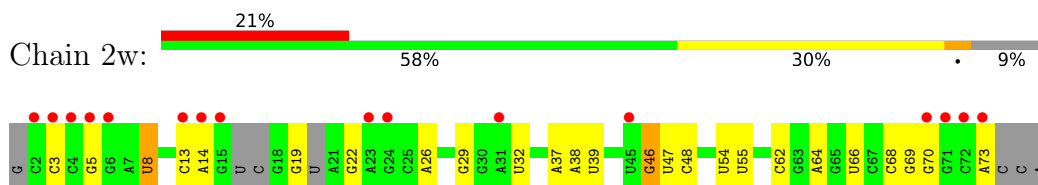
• Molecule 54: A-site and E-site tRNAs



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

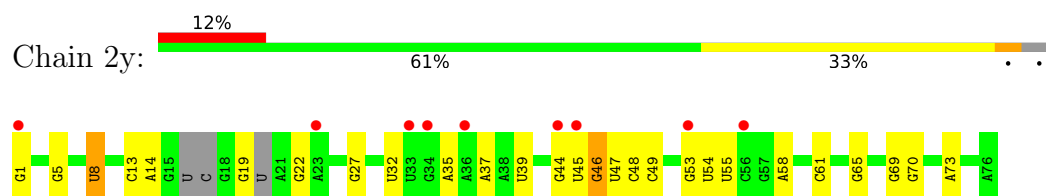


• Molecule 54: A-site and E-site tRNAs

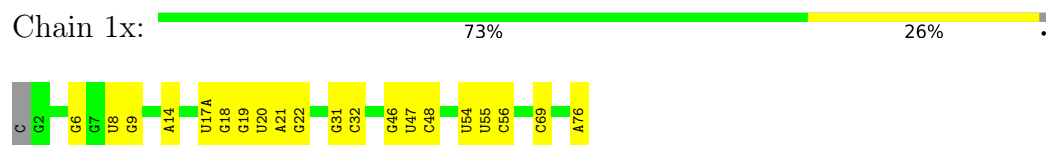


• Molecule 54: A-site and E-site tRNAs

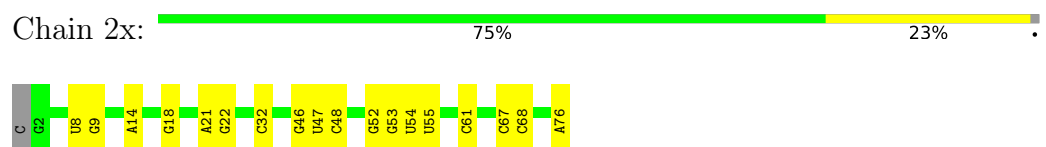




- Molecule 55: P-site tRNA



- Molecule 55: P-site tRNA



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	209.94Å 451.23Å 622.44Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	155.61 – 2.80 311.22 – 2.80	Depositor EDS
% Data completeness (in resolution range)	96.6 (155.61-2.80) 96.6 (311.22-2.80)	Depositor EDS
$R_{merge}$	0.15	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.32 (at 2.82Å)	Xtrriage
Refinement program	PHENIX 1.8.2	Depositor
R, $R_{free}$	0.229 , 0.278 0.228 , 0.278	Depositor DCC
$R_{free}$ test set	69403 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	53.5	Xtrriage
Anisotropy	0.220	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.29 , 60.4	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.39$ , $\langle L^2 \rangle = 0.21$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.89	EDS
Total number of atoms	300935	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	51.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.66% 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: 2MU, SF4, UR3, 4SU, M2G, MA6, 5MU, 2MG, ZN, K, MIA, MG, 7MG, 5MC, 2MA, PSU, 4OC, OMG, 0TD, M2D

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	0.31	0/69009	0.80	23/107712 (0.0%)
1	2A	0.25	0/67293	0.78	13/105034 (0.0%)
2	1B	0.31	1/2882 (0.0%)	0.74	0/4494
2	2B	0.30	1/2879 (0.0%)	0.78	1/4487 (0.0%)
3	1D	0.28	0/2186	0.50	0/2944
3	2D	0.27	0/2186	0.48	0/2944
4	1E	0.27	0/1592	0.49	0/2149
4	2E	0.25	0/1592	0.47	0/2149
5	1F	0.28	0/1619	0.46	0/2193
5	2F	0.26	0/1615	0.44	0/2188
6	1G	0.26	0/1448	0.45	0/1957
6	2G	0.25	0/1453	0.46	0/1963
7	1H	0.26	0/1356	0.45	0/1834
7	2H	0.25	0/1356	0.43	0/1834
8	1I	0.24	0/1112	0.46	0/1514
8	2I	0.24	0/1079	0.45	0/1475
9	1N	0.28	0/1144	0.47	0/1543
9	2N	0.25	0/1144	0.43	0/1543
10	1O	0.29	0/943	0.48	0/1269
10	2O	0.27	0/943	0.47	0/1269
11	1P	0.30	0/1152	0.47	0/1533
11	2P	0.26	0/1152	0.48	0/1533
12	1Q	0.28	0/1143	0.45	0/1527
12	2Q	0.26	0/1143	0.42	0/1527
13	1R	0.25	0/982	0.47	0/1312
13	2R	0.24	0/982	0.44	0/1312
14	1S	0.26	0/883	0.45	0/1176
14	2S	0.25	0/880	0.44	0/1172
15	1T	0.26	0/1105	0.45	0/1477
15	2T	0.25	0/1097	0.43	0/1468
16	1U	0.28	0/977	0.43	0/1301

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
16	2U	0.25	0/977	0.38	0/1301
17	1V	0.32	0/782	0.50	0/1049
17	2V	0.27	0/782	0.48	0/1049
18	1W	0.28	0/897	0.47	0/1205
18	2W	0.25	0/897	0.43	0/1205
19	1X	0.29	0/764	0.50	0/1025
19	2X	0.25	0/764	0.45	0/1025
20	1Y	0.28	0/819	0.49	0/1095
20	2Y	0.27	0/819	0.47	0/1095
21	1Z	0.27	0/1267	0.46	0/1717
21	2Z	0.26	0/1299	0.48	0/1763
22	10	0.28	0/662	0.48	0/881
22	20	0.27	0/662	0.48	0/881
23	11	0.32	0/762	0.49	0/1014
23	21	0.26	0/762	0.48	0/1014
24	12	0.26	0/590	0.40	0/781
24	22	0.24	0/590	0.37	0/781
25	13	0.26	0/474	0.48	0/635
25	23	0.24	0/469	0.42	0/630
26	14	0.33	0/565	0.54	0/761
26	24	0.27	0/545	0.50	0/737
27	15	0.27	0/469	0.50	0/635
27	25	0.27	0/469	0.45	0/635
28	16	0.27	0/460	0.48	0/613
28	26	0.26	0/456	0.47	0/608
29	17	0.27	0/426	0.45	0/561
29	27	0.25	0/426	0.47	0/561
30	18	0.27	0/525	0.50	0/691
30	28	0.25	0/525	0.44	0/691
31	19	0.27	0/310	0.48	0/407
31	29	0.24	0/310	0.49	0/407
32	1a	0.25	0/35795	0.79	22/55864 (0.0%)
32	2a	0.26	3/35886 (0.0%)	0.83	29/56005 (0.1%)
33	1b	0.25	0/1881	0.45	0/2542
33	2b	0.26	0/1860	0.46	0/2518
34	1c	0.25	0/1572	0.43	0/2126
34	2c	0.25	0/1566	0.45	0/2119
35	1d	0.25	0/1685	0.42	0/2262
35	2d	0.25	0/1704	0.44	0/2284
36	1e	0.26	0/1145	0.47	0/1543
36	2e	0.27	0/1149	0.48	0/1548
37	1f	0.25	0/823	0.44	0/1115
37	2f	0.25	0/829	0.43	0/1123

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
38	1g	0.24	0/1250	0.41	0/1679
38	2g	0.26	0/1254	0.44	0/1683
39	1h	0.25	0/1108	0.45	0/1494
39	2h	0.25	0/1108	0.43	0/1494
40	1i	0.26	0/1002	0.46	0/1346
40	2i	0.26	0/997	0.45	0/1343
41	1j	0.24	0/722	0.45	0/982
41	2j	0.25	0/727	0.48	0/988
42	1k	0.25	0/844	0.44	0/1145
42	2k	0.25	0/848	0.43	0/1149
43	1l	0.26	0/937	0.49	0/1260
43	2l	0.26	0/937	0.46	0/1260
44	1m	0.26	0/969	0.47	0/1302
44	2m	0.25	0/961	0.47	0/1291
45	1n	0.26	0/501	0.43	0/664
45	2n	0.26	0/501	0.42	0/664
46	1o	0.24	0/739	0.40	0/985
46	2o	0.24	0/739	0.40	0/985
47	1p	0.24	0/697	0.44	0/939
47	2p	0.24	0/693	0.45	0/935
48	1q	0.24	0/836	0.44	0/1117
48	2q	0.25	0/836	0.45	0/1117
49	1r	0.25	0/560	0.42	0/746
49	2r	0.24	0/560	0.40	0/746
50	1s	0.25	0/667	0.51	0/900
50	2s	0.24	0/661	0.48	0/893
51	1t	0.24	0/730	0.40	0/965
51	2t	0.23	0/729	0.39	0/965
52	1u	0.23	0/203	0.42	0/266
52	2u	0.26	0/203	0.46	0/266
53	1v	0.25	0/310	0.80	0/480
53	2v	0.34	0/310	0.83	0/480
54	1w	0.41	1/1559 (0.1%)	0.99	1/2424 (0.0%)
54	1y	0.39	1/1606 (0.1%)	0.93	2/2497 (0.1%)
54	2w	0.32	0/1487	0.99	0/2311
54	2y	0.40	1/1583 (0.1%)	0.91	0/2459
55	1x	0.38	0/1725	1.01	12/2689 (0.4%)
55	2x	0.32	0/1725	0.94	2/2689 (0.1%)
All	All	0.27	8/316570 (0.0%)	0.73	105/473933 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a

sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
26	24	0	2

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	2B	1	U	OP3-P	-10.45	1.48	1.61
54	1y	1	G	OP3-P	-10.37	1.48	1.61
54	2y	1	G	OP3-P	-10.37	1.48	1.61
54	1w	1	G	OP3-P	-10.33	1.48	1.61
2	1B	1	U	OP3-P	-10.29	1.48	1.61
32	2a	1272	G	N1-C2	-8.23	1.31	1.37
32	2a	1272	G	C6-N1	-7.72	1.34	1.39
32	2a	1263	C	N3-C4	-5.02	1.30	1.33

All (105) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	2a	1263	C	N1-C2-O2	19.01	130.31	118.90
32	2a	1272	G	N3-C2-N2	18.64	132.95	119.90
32	2a	1272	G	C5-C6-O6	17.98	139.39	128.60
32	2a	1272	G	N1-C2-N2	-15.35	102.39	116.20
32	2a	1263	C	C2-N3-C4	12.95	126.37	119.90
32	2a	1272	G	C6-N1-C2	11.26	131.85	125.10
32	2a	1272	G	N1-C6-O6	-10.83	113.40	119.90
1	1A	1132	A	N1-C6-N6	-10.80	112.12	118.60
32	2a	1263	C	N3-C2-O2	-10.26	114.72	121.90
1	1A	1121	C	N1-C2-O2	9.67	124.70	118.90
32	2a	1263	C	C5-C6-N1	9.20	125.60	121.00
32	2a	1272	G	C5-C6-N1	-8.64	107.18	111.50
1	1A	1121	C	C2-N3-C4	8.53	124.16	119.90
1	1A	834	U	O5'-P-OP1	-8.38	98.16	105.70
55	1x	46	G	C6-N1-C2	-8.09	120.25	125.10
2	2B	80	U	O4'-C1'-N1	7.98	114.59	108.20
1	2A	2473	U	C2-N1-C1'	7.86	127.14	117.70
1	1A	1109	G	C5-C6-O6	7.71	133.23	128.60
32	2a	754	C	C2-N1-C1'	7.68	127.25	118.80
1	1A	2189	U	C2-N1-C1'	7.61	126.83	117.70
32	2a	754	C	N1-C2-O2	7.27	123.26	118.90
55	1x	22	G	C8-N9-C1'	7.18	136.33	127.00
1	1A	1132	A	C5-C6-N6	7.07	129.35	123.70
1	1A	2189	U	N1-C2-O2	7.05	127.73	122.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1A	1109	G	C6-N1-C2	7.01	129.31	125.10
32	2a	1263	C	C5-C4-N4	6.98	125.09	120.20
32	1a	1002	G	C4-N9-C1'	6.85	135.40	126.50
55	1x	22	G	N3-C4-N9	-6.85	121.89	126.00
32	2a	1028	C	C2-N3-C4	6.85	123.32	119.90
32	1a	1030(B)	C	C2-N1-C1'	6.82	126.30	118.80
55	2x	14	A	C4-C5-C6	6.80	120.40	117.00
1	1A	894	U	C2-N1-C1'	6.76	125.81	117.70
32	1a	1027	C	N3-C4-C5	-6.72	119.21	121.90
32	2a	1263	C	C6-N1-C2	-6.70	117.62	120.30
1	1A	2189	U	N3-C2-O2	-6.69	117.52	122.20
1	2A	2139	C	C2-N1-C1'	6.61	126.07	118.80
54	1y	33	U	C2-N1-C1'	6.59	125.61	117.70
32	1a	266	G	P-O3'-C3'	6.55	127.56	119.70
32	2a	1263	C	C4-C5-C6	-6.53	114.14	117.40
32	1a	1002	G	N3-C4-N9	6.50	129.90	126.00
55	1x	22	G	C4-C5-C6	-6.40	114.96	118.80
55	1x	22	G	C4-N9-C1'	-6.39	118.19	126.50
1	2A	2136	C	N1-C2-O2	6.38	122.73	118.90
32	2a	1263	C	C2-N1-C1'	6.36	125.80	118.80
1	2A	2149	G	N3-C4-N9	6.32	129.79	126.00
32	2a	1272	G	C4-N9-C1'	6.31	134.70	126.50
32	1a	1002	G	C8-N9-C1'	-6.29	118.83	127.00
32	1a	1027	C	C5-C4-N4	6.28	124.59	120.20
32	2a	1272	G	C8-N9-C1'	-6.25	118.87	127.00
32	1a	1027	C	C6-N1-C1'	6.17	128.20	120.80
32	1a	1065	U	P-O3'-C3'	6.14	127.07	119.70
1	2A	1313	U	C2-N1-C1'	6.12	125.05	117.70
32	1a	1034	G	C6-N1-C2	6.12	128.77	125.10
32	2a	1263	C	N3-C4-N4	-6.12	113.72	118.00
32	2a	1263	C	N1-C2-N3	-6.10	114.93	119.20
55	1x	22	G	N1-C6-O6	-5.95	116.33	119.90
32	2a	1272	G	C2-N3-C4	-5.94	108.93	111.90
55	1x	22	G	C6-C5-N7	5.91	133.95	130.40
1	1A	1020	C	N1-C2-O2	-5.89	115.37	118.90
1	1A	2641	A	P-O3'-C3'	5.87	126.74	119.70
55	1x	14	A	C4-C5-C6	5.84	119.92	117.00
32	2a	1025	U	N1-C2-O2	5.76	126.83	122.80
32	2a	754	C	N3-C2-O2	-5.73	117.89	121.90
1	2A	1530	C	P-O3'-C3'	5.68	126.51	119.70
32	1a	1030	C	N1-C2-O2	5.64	122.28	118.90
55	1x	46	G	N3-C2-N2	-5.63	115.96	119.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1A	1219	A	OP1-P-O3'	5.61	117.55	105.20
1	2A	2139	C	C6-N1-C1'	-5.59	114.09	120.80
55	1x	14	A	C5-N7-C8	5.57	106.68	103.90
1	1A	1121	C	N3-C2-O2	-5.54	118.02	121.90
1	1A	795	G	O4'-C1'-N9	5.53	112.62	108.20
32	1a	1034	G	C5-C6-O6	5.46	131.88	128.60
32	1a	1030(B)	C	N1-C2-O2	5.41	122.14	118.90
1	1A	12	U	C2-N1-C1'	5.40	124.18	117.70
1	1A	1109	G	N3-C2-N2	5.40	123.68	119.90
1	1A	1128	U	N3-C4-C5	5.40	117.84	114.60
1	2A	2473	U	N1-C2-O2	5.39	126.58	122.80
32	2a	754	C	C6-N1-C1'	-5.39	114.34	120.80
32	1a	1158	C	C2-N1-C1'	5.37	124.71	118.80
32	1a	1002	G	N3-C4-C5	-5.33	125.93	128.60
1	2A	1992	G	P-O3'-C3'	5.33	126.10	119.70
32	2a	65	U	P-O3'-C3'	5.30	126.06	119.70
1	2A	228	A	P-O3'-C3'	5.30	126.06	119.70
32	1a	1034	G	N3-C2-N2	5.30	123.61	119.90
32	1a	1030(B)	C	C6-N1-C2	-5.25	118.20	120.30
32	1a	266	G	OP2-P-O3'	5.25	116.74	105.20
1	1A	1359	U	C2-N1-C1'	5.21	123.96	117.70
55	2x	46	G	C6-N1-C2	-5.19	121.99	125.10
32	1a	841	U	C5-C6-N1	5.17	125.29	122.70
1	1A	537	G	O4'-C1'-N9	5.17	112.33	108.20
32	2a	266	G	P-O3'-C3'	5.16	125.89	119.70
32	1a	1067	A	P-O3'-C3'	5.14	125.87	119.70
55	1x	46	G	N9-C4-C5	5.12	107.45	105.40
1	2A	2473	U	N3-C2-O2	-5.12	118.62	122.20
32	2a	1028	C	C5-C6-N1	5.12	123.56	121.00
1	2A	845	G	C4-N9-C1'	5.11	133.15	126.50
32	1a	748	C	P-O3'-C3'	5.10	125.82	119.70
54	1w	47	U	C2-N1-C1'	5.09	123.81	117.70
32	2a	1262	C	N1-C2-O2	5.07	121.94	118.90
1	2A	2473	U	C6-N1-C1'	-5.06	114.12	121.20
32	1a	1065	U	OP2-P-O3'	5.05	116.32	105.20
1	1A	1132	A	N9-C4-C5	5.04	107.82	105.80
55	1x	22	G	C5-N7-C8	-5.04	101.78	104.30
54	1y	33	U	N1-C2-O2	5.03	126.32	122.80
1	1A	1219	A	P-O3'-C3'	5.01	125.71	119.70

There are no chirality outliers.

All (2) planarity outliers are listed below:



Mol	Chain	Res	Type	Group
26	24	56	VAL	Peptide
26	24	63	TYR	Peptide

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

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

## 5.3 Torsion angles [i](#)

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

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	1D	273/276 (99%)	258 (94%)	15 (6%)	0	100	100
3	2D	273/276 (99%)	260 (95%)	13 (5%)	0	100	100
4	1E	202/206 (98%)	192 (95%)	9 (4%)	1 (0%)	29	61
4	2E	202/206 (98%)	192 (95%)	8 (4%)	2 (1%)	15	44
5	1F	201/210 (96%)	195 (97%)	5 (2%)	1 (0%)	29	61
5	2F	201/210 (96%)	192 (96%)	9 (4%)	0	100	100
6	1G	179/182 (98%)	163 (91%)	12 (7%)	4 (2%)	6	22
6	2G	179/182 (98%)	164 (92%)	12 (7%)	3 (2%)	9	29
7	1H	172/180 (96%)	160 (93%)	10 (6%)	2 (1%)	13	39
7	2H	172/180 (96%)	154 (90%)	17 (10%)	1 (1%)	25	56
8	1I	144/148 (97%)	129 (90%)	14 (10%)	1 (1%)	22	53
8	2I	144/148 (97%)	124 (86%)	17 (12%)	3 (2%)	7	23
9	1N	138/140 (99%)	134 (97%)	4 (3%)	0	100	100
9	2N	138/140 (99%)	133 (96%)	5 (4%)	0	100	100
10	1O	120/122 (98%)	111 (92%)	8 (7%)	1 (1%)	19	49
10	2O	120/122 (98%)	109 (91%)	11 (9%)	0	100	100
11	1P	147/150 (98%)	139 (95%)	8 (5%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
11	2P	147/150 (98%)	136 (92%)	11 (8%)	0	100	100
12	1Q	139/141 (99%)	128 (92%)	11 (8%)	0	100	100
12	2Q	139/141 (99%)	129 (93%)	9 (6%)	1 (1%)	22	53
13	1R	116/118 (98%)	112 (97%)	4 (3%)	0	100	100
13	2R	116/118 (98%)	109 (94%)	7 (6%)	0	100	100
14	1S	108/112 (96%)	104 (96%)	4 (4%)	0	100	100
14	2S	108/112 (96%)	103 (95%)	4 (4%)	1 (1%)	17	46
15	1T	129/146 (88%)	122 (95%)	7 (5%)	0	100	100
15	2T	129/146 (88%)	119 (92%)	10 (8%)	0	100	100
16	1U	114/118 (97%)	113 (99%)	1 (1%)	0	100	100
16	2U	114/118 (97%)	113 (99%)	1 (1%)	0	100	100
17	1V	99/101 (98%)	92 (93%)	6 (6%)	1 (1%)	15	44
17	2V	99/101 (98%)	91 (92%)	7 (7%)	1 (1%)	15	44
18	1W	110/113 (97%)	110 (100%)	0	0	100	100
18	2W	110/113 (97%)	107 (97%)	3 (3%)	0	100	100
19	1X	93/96 (97%)	89 (96%)	3 (3%)	1 (1%)	14	41
19	2X	93/96 (97%)	91 (98%)	2 (2%)	0	100	100
20	1Y	105/110 (96%)	97 (92%)	6 (6%)	2 (2%)	8	26
20	2Y	105/110 (96%)	97 (92%)	6 (6%)	2 (2%)	8	26
21	1Z	148/206 (72%)	134 (90%)	14 (10%)	0	100	100
21	2Z	156/206 (76%)	132 (85%)	23 (15%)	1 (1%)	25	56
22	10	81/85 (95%)	79 (98%)	2 (2%)	0	100	100
22	20	81/85 (95%)	78 (96%)	3 (4%)	0	100	100
23	11	95/98 (97%)	94 (99%)	1 (1%)	0	100	100
23	21	95/98 (97%)	92 (97%)	3 (3%)	0	100	100
24	12	68/72 (94%)	68 (100%)	0	0	100	100
24	22	68/72 (94%)	64 (94%)	4 (6%)	0	100	100
25	13	57/60 (95%)	56 (98%)	1 (2%)	0	100	100
25	23	57/60 (95%)	56 (98%)	1 (2%)	0	100	100
26	14	67/71 (94%)	52 (78%)	12 (18%)	3 (4%)	2	8
26	24	67/71 (94%)	57 (85%)	9 (13%)	1 (2%)	10	33

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
27	15	57/60 (95%)	56 (98%)	1 (2%)	0	100	100
27	25	57/60 (95%)	55 (96%)	2 (4%)	0	100	100
28	16	51/54 (94%)	50 (98%)	1 (2%)	0	100	100
28	26	51/54 (94%)	49 (96%)	2 (4%)	0	100	100
29	17	46/49 (94%)	45 (98%)	1 (2%)	0	100	100
29	27	46/49 (94%)	45 (98%)	1 (2%)	0	100	100
30	18	62/65 (95%)	61 (98%)	0	1 (2%)	9	31
30	28	62/65 (95%)	60 (97%)	2 (3%)	0	100	100
31	19	35/37 (95%)	35 (100%)	0	0	100	100
31	29	35/37 (95%)	35 (100%)	0	0	100	100
33	1b	229/256 (90%)	193 (84%)	29 (13%)	7 (3%)	4	14
33	2b	229/256 (90%)	202 (88%)	20 (9%)	7 (3%)	4	14
34	1c	204/239 (85%)	185 (91%)	18 (9%)	1 (0%)	29	61
34	2c	204/239 (85%)	184 (90%)	17 (8%)	3 (2%)	10	33
35	1d	206/209 (99%)	196 (95%)	10 (5%)	0	100	100
35	2d	206/209 (99%)	189 (92%)	17 (8%)	0	100	100
36	1e	146/162 (90%)	131 (90%)	12 (8%)	3 (2%)	7	23
36	2e	146/162 (90%)	135 (92%)	11 (8%)	0	100	100
37	1f	98/101 (97%)	93 (95%)	4 (4%)	1 (1%)	15	44
37	2f	98/101 (97%)	97 (99%)	1 (1%)	0	100	100
38	1g	153/156 (98%)	141 (92%)	10 (6%)	2 (1%)	12	36
38	2g	153/156 (98%)	140 (92%)	11 (7%)	2 (1%)	12	36
39	1h	135/138 (98%)	130 (96%)	5 (4%)	0	100	100
39	2h	135/138 (98%)	130 (96%)	5 (4%)	0	100	100
40	1i	125/128 (98%)	110 (88%)	15 (12%)	0	100	100
40	2i	125/128 (98%)	109 (87%)	16 (13%)	0	100	100
41	1j	95/105 (90%)	81 (85%)	10 (10%)	4 (4%)	3	9
41	2j	94/105 (90%)	79 (84%)	10 (11%)	5 (5%)	2	6
42	1k	112/129 (87%)	104 (93%)	7 (6%)	1 (1%)	17	46
42	2k	112/129 (87%)	99 (88%)	10 (9%)	3 (3%)	5	17
43	1l	119/132 (90%)	112 (94%)	7 (6%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
43	2l	119/132 (90%)	108 (91%)	11 (9%)	0	100	100
44	1m	121/126 (96%)	104 (86%)	15 (12%)	2 (2%)	9	29
44	2m	120/126 (95%)	108 (90%)	12 (10%)	0	100	100
45	1n	58/61 (95%)	54 (93%)	4 (7%)	0	100	100
45	2n	58/61 (95%)	53 (91%)	5 (9%)	0	100	100
46	1o	86/89 (97%)	81 (94%)	4 (5%)	1 (1%)	13	39
46	2o	86/89 (97%)	77 (90%)	9 (10%)	0	100	100
47	1p	80/88 (91%)	72 (90%)	7 (9%)	1 (1%)	12	36
47	2p	80/88 (91%)	69 (86%)	10 (12%)	1 (1%)	12	36
48	1q	97/105 (92%)	89 (92%)	8 (8%)	0	100	100
48	2q	97/105 (92%)	87 (90%)	6 (6%)	4 (4%)	3	9
49	1r	66/88 (75%)	60 (91%)	6 (9%)	0	100	100
49	2r	66/88 (75%)	61 (92%)	5 (8%)	0	100	100
50	1s	81/93 (87%)	68 (84%)	11 (14%)	2 (2%)	5	19
50	2s	81/93 (87%)	71 (88%)	9 (11%)	1 (1%)	13	39
51	1t	94/106 (89%)	89 (95%)	3 (3%)	2 (2%)	7	23
51	2t	94/106 (89%)	83 (88%)	8 (8%)	3 (3%)	4	13
52	1u	21/27 (78%)	19 (90%)	2 (10%)	0	100	100
52	2u	21/27 (78%)	18 (86%)	3 (14%)	0	100	100
All	All	11370/12128 (94%)	10535 (93%)	745 (7%)	90 (1%)	19	49

All (90) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
5	1F	130	ALA
6	1G	47	LYS
6	1G	49	ASP
7	1H	126	PRO
8	1I	10	GLU
17	1V	79	VAL
20	1Y	55	TYR
33	1b	17	PHE
33	1b	22	LYS
51	1t	100	ILE
6	2G	49	ASP

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
7	2H	126	PRO
8	2I	10	GLU
14	2S	96	GLY
33	2b	125	PRO
41	2j	75	ILE
47	2p	53	VAL
33	1b	20	GLU
41	1j	29	ARG
41	1j	75	ILE
44	1m	67	GLU
50	1s	29	ARG
50	1s	81	ARG
51	1t	47	GLY
26	24	65	ASP
33	2b	9	GLU
33	2b	10	LEU
33	2b	17	PHE
33	2b	22	LYS
42	2k	49	GLY
51	2t	47	GLY
51	2t	100	ILE
7	1H	47	GLU
10	1O	25	LEU
19	1X	93	GLU
33	1b	21	ARG
36	1e	27	ARG
37	1f	38	GLU
38	1g	114	ARG
46	1o	17	ARG
17	2V	79	VAL
21	2Z	2	GLU
38	2g	4	ARG
41	2j	78	ASN
42	2k	89	ALA
48	2q	68	ARG
48	2q	81	ARG
50	2s	29	ARG
51	2t	10	LEU
4	1E	52	LEU
6	1G	43	LEU
20	1Y	54	LYS
26	14	44	THR

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Mol	Chain	Res	Type
26	14	57	GLU
38	1g	80	VAL
41	1j	77	PRO
41	1j	78	ASN
4	2E	28	ALA
4	2E	52	LEU
6	2G	47	LYS
8	2I	85	GLU
33	2b	20	GLU
34	2c	3	ASN
26	14	55	ARG
30	18	37	SER
44	1m	21	TYR
38	2g	80	VAL
41	2j	79	ARG
48	2q	74	LEU
33	1b	8	LYS
33	1b	194	PRO
12	2Q	17	LEU
20	2Y	43	ASN
34	2c	47	LEU
34	2c	66	VAL
41	2j	91	PRO
34	1c	66	VAL
42	1k	49	GLY
47	1p	63	GLY
6	2G	52	ILE
41	2j	39	PRO
36	1e	69	VAL
36	1e	85	GLY
8	2I	145	VAL
20	2Y	51	VAL
6	1G	52	ILE
33	2b	165	VAL
42	2k	105	VAL
48	2q	77	VAL
33	1b	125	PRO

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

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

resolution.

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	1D	215/218 (99%)	205 (95%)	10 (5%)	26	59
3	2D	215/218 (99%)	206 (96%)	9 (4%)	30	63
4	1E	164/166 (99%)	153 (93%)	11 (7%)	16	43
4	2E	164/166 (99%)	154 (94%)	10 (6%)	18	48
5	1F	160/166 (96%)	149 (93%)	11 (7%)	15	41
5	2F	159/166 (96%)	151 (95%)	8 (5%)	24	56
6	1G	143/156 (92%)	137 (96%)	6 (4%)	30	63
6	2G	143/156 (92%)	135 (94%)	8 (6%)	21	51
7	1H	144/148 (97%)	139 (96%)	5 (4%)	36	70
7	2H	144/148 (97%)	139 (96%)	5 (4%)	36	70
8	1I	113/124 (91%)	103 (91%)	10 (9%)	10	29
8	2I	105/124 (85%)	101 (96%)	4 (4%)	33	67
9	1N	118/119 (99%)	112 (95%)	6 (5%)	24	55
9	2N	118/119 (99%)	107 (91%)	11 (9%)	9	26
10	1O	100/100 (100%)	96 (96%)	4 (4%)	31	65
10	2O	100/100 (100%)	99 (99%)	1 (1%)	76	93
11	1P	115/116 (99%)	109 (95%)	6 (5%)	23	55
11	2P	115/116 (99%)	112 (97%)	3 (3%)	46	79
12	1Q	111/111 (100%)	107 (96%)	4 (4%)	35	69
12	2Q	111/111 (100%)	107 (96%)	4 (4%)	35	69
13	1R	101/101 (100%)	91 (90%)	10 (10%)	8	23
13	2R	101/101 (100%)	95 (94%)	6 (6%)	19	49
14	1S	86/88 (98%)	83 (96%)	3 (4%)	36	70
14	2S	85/88 (97%)	84 (99%)	1 (1%)	71	92
15	1T	115/127 (91%)	109 (95%)	6 (5%)	23	55
15	2T	113/127 (89%)	110 (97%)	3 (3%)	44	78
16	1U	93/94 (99%)	90 (97%)	3 (3%)	39	73
16	2U	93/94 (99%)	91 (98%)	2 (2%)	52	83
17	1V	80/82 (98%)	74 (92%)	6 (8%)	13	37

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
17	2V	80/82 (98%)	73 (91%)	7 (9%)	10	29
18	1W	90/92 (98%)	84 (93%)	6 (7%)	16	43
18	2W	90/92 (98%)	90 (100%)	0	100	100
19	1X	77/78 (99%)	77 (100%)	0	100	100
19	2X	77/78 (99%)	75 (97%)	2 (3%)	46	79
20	1Y	85/91 (93%)	80 (94%)	5 (6%)	19	49
20	2Y	85/91 (93%)	80 (94%)	5 (6%)	19	49
21	1Z	135/179 (75%)	124 (92%)	11 (8%)	11	33
21	2Z	137/179 (76%)	131 (96%)	6 (4%)	28	61
22	10	65/67 (97%)	63 (97%)	2 (3%)	40	74
22	20	65/67 (97%)	63 (97%)	2 (3%)	40	74
23	11	80/83 (96%)	76 (95%)	4 (5%)	24	56
23	21	80/83 (96%)	77 (96%)	3 (4%)	33	67
24	12	65/67 (97%)	63 (97%)	2 (3%)	40	74
24	22	65/67 (97%)	63 (97%)	2 (3%)	40	74
25	13	51/52 (98%)	48 (94%)	3 (6%)	19	49
25	23	50/52 (96%)	47 (94%)	3 (6%)	19	48
26	14	59/63 (94%)	53 (90%)	6 (10%)	7	22
26	24	53/63 (84%)	47 (89%)	6 (11%)	6	18
27	15	50/52 (96%)	47 (94%)	3 (6%)	19	48
27	25	50/52 (96%)	46 (92%)	4 (8%)	12	34
28	16	51/52 (98%)	49 (96%)	2 (4%)	32	66
28	26	50/52 (96%)	49 (98%)	1 (2%)	55	84
29	17	41/42 (98%)	38 (93%)	3 (7%)	14	38
29	27	41/42 (98%)	39 (95%)	2 (5%)	25	57
30	18	54/55 (98%)	51 (94%)	3 (6%)	21	51
30	28	54/55 (98%)	50 (93%)	4 (7%)	13	37
31	19	34/34 (100%)	33 (97%)	1 (3%)	42	76
31	29	34/34 (100%)	33 (97%)	1 (3%)	42	76
33	1b	192/220 (87%)	189 (98%)	3 (2%)	62	88
33	2b	187/220 (85%)	178 (95%)	9 (5%)	25	58

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
34	1c	142/188 (76%)	139 (98%)	3 (2%)	53	84
34	2c	140/188 (74%)	138 (99%)	2 (1%)	67	90
35	1d	169/181 (93%)	162 (96%)	7 (4%)	30	64
35	2d	173/181 (96%)	168 (97%)	5 (3%)	42	76
36	1e	113/123 (92%)	107 (95%)	6 (5%)	22	54
36	2e	114/123 (93%)	110 (96%)	4 (4%)	36	70
37	1f	84/90 (93%)	84 (100%)	0	100	100
37	2f	85/90 (94%)	82 (96%)	3 (4%)	36	70
38	1g	119/127 (94%)	115 (97%)	4 (3%)	37	71
38	2g	120/127 (94%)	117 (98%)	3 (2%)	47	80
39	1h	114/119 (96%)	110 (96%)	4 (4%)	36	70
39	2h	114/119 (96%)	107 (94%)	7 (6%)	18	48
40	1i	90/99 (91%)	86 (96%)	4 (4%)	28	61
40	2i	89/99 (90%)	84 (94%)	5 (6%)	21	51
41	1j	66/92 (72%)	64 (97%)	2 (3%)	41	75
41	2j	69/92 (75%)	67 (97%)	2 (3%)	42	76
42	1k	82/99 (83%)	81 (99%)	1 (1%)	71	92
42	2k	83/99 (84%)	80 (96%)	3 (4%)	35	69
43	1l	96/108 (89%)	92 (96%)	4 (4%)	30	63
43	2l	96/108 (89%)	93 (97%)	3 (3%)	40	74
44	1m	93/101 (92%)	91 (98%)	2 (2%)	52	83
44	2m	92/101 (91%)	91 (99%)	1 (1%)	73	92
45	1n	49/50 (98%)	43 (88%)	6 (12%)	5	15
45	2n	49/50 (98%)	44 (90%)	5 (10%)	7	22
46	1o	78/80 (98%)	78 (100%)	0	100	100
46	2o	78/80 (98%)	77 (99%)	1 (1%)	69	91
47	1p	69/74 (93%)	66 (96%)	3 (4%)	29	62
47	2p	68/74 (92%)	62 (91%)	6 (9%)	10	29
48	1q	94/97 (97%)	93 (99%)	1 (1%)	73	92
48	2q	94/97 (97%)	93 (99%)	1 (1%)	73	92
49	1r	59/77 (77%)	58 (98%)	1 (2%)	60	87

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
49	2r	59/77 (77%)	56 (95%)	3 (5%)	24	55
50	1s	69/80 (86%)	66 (96%)	3 (4%)	29	62
50	2s	67/80 (84%)	65 (97%)	2 (3%)	41	75
51	1t	70/82 (85%)	69 (99%)	1 (1%)	67	90
51	2t	70/82 (85%)	69 (99%)	1 (1%)	67	90
52	1u	18/22 (82%)	17 (94%)	1 (6%)	21	51
52	2u	18/22 (82%)	18 (100%)	0	100	100
All	All	9303/10064 (92%)	8906 (96%)	397 (4%)	29	62

All (397) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	1D	22	SER
3	1D	61	LEU
3	1D	99	ASP
3	1D	142	VAL
3	1D	155	LEU
3	1D	211	ARG
3	1D	217	ARG
3	1D	221	VAL
3	1D	229	VAL
3	1D	242	ARG
4	1E	12	THR
4	1E	21	VAL
4	1E	24	THR
4	1E	42	ASP
4	1E	75	VAL
4	1E	116	VAL
4	1E	136	ARG
4	1E	152	LYS
4	1E	175	VAL
4	1E	181	LEU
4	1E	195	LEU
5	1F	28	ILE
5	1F	33	LEU
5	1F	53	THR
5	1F	57	VAL
5	1F	74	ARG
5	1F	106	ARG
5	1F	110	LEU

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
5	1F	170	LEU
5	1F	183	VAL
5	1F	192	LEU
5	1F	195	ASP
6	1G	3	LEU
6	1G	31	VAL
6	1G	43	LEU
6	1G	133	LEU
6	1G	159	VAL
6	1G	175	LEU
7	1H	15	VAL
7	1H	71	LEU
7	1H	81	GLU
7	1H	84	SER
7	1H	129	THR
8	1I	9	LEU
8	1I	38	LEU
8	1I	43	ASN
8	1I	74	ASN
8	1I	75	LEU
8	1I	77	LEU
8	1I	92	VAL
8	1I	101	LEU
8	1I	109	ILE
8	1I	123	LEU
9	1N	28	THR
9	1N	32	THR
9	1N	33	LEU
9	1N	34	LEU
9	1N	67	LEU
9	1N	99	LEU
10	1O	10	VAL
10	1O	42	SER
10	1O	70	LYS
10	1O	120	GLU
11	1P	55	ARG
11	1P	59	LEU
11	1P	95	VAL
11	1P	125	VAL
11	1P	133	SER
11	1P	147	LEU
12	1Q	35	VAL

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
12	1Q	109	VAL
12	1Q	110	THR
12	1Q	133	ARG
13	1R	24	GLN
13	1R	29	LEU
13	1R	36	THR
13	1R	44	LEU
13	1R	54	LEU
13	1R	65	LEU
13	1R	67	LEU
13	1R	100	LEU
13	1R	111	LEU
13	1R	114	VAL
14	1S	36	TYR
14	1S	69	VAL
14	1S	85	VAL
15	1T	28	VAL
15	1T	51	ARG
15	1T	67	SER
15	1T	70	VAL
15	1T	96	ARG
15	1T	103	ARG
16	1U	17	ILE
16	1U	77	SER
16	1U	95	LEU
17	1V	46	VAL
17	1V	51	VAL
17	1V	62	LEU
17	1V	72	VAL
17	1V	73	SER
17	1V	79	VAL
18	1W	11	ARG
18	1W	15	ARG
18	1W	17	VAL
18	1W	23	LEU
18	1W	92	ARG
18	1W	107	LEU
20	1Y	63	LYS
20	1Y	72	VAL
20	1Y	76	CYS
20	1Y	99	CYS
20	1Y	107	ASP

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
21	1Z	33	LEU
21	1Z	49	ARG
21	1Z	70	LEU
21	1Z	129	SER
21	1Z	138	GLU
21	1Z	150	LEU
21	1Z	153	SER
21	1Z	154	ASP
21	1Z	155	LEU
21	1Z	170	THR
21	1Z	171	ILE
22	10	14	ARG
22	10	39	ARG
23	11	3	LYS
23	11	11	ARG
23	11	33	LYS
23	11	95	LEU
24	12	40	SER
24	12	52	ASP
25	13	23	LEU
25	13	34	GLU
25	13	54	VAL
26	14	44	THR
26	14	49	PHE
26	14	50	VAL
26	14	52	THR
26	14	56	VAL
26	14	60	GLN
27	15	6	VAL
27	15	16	ARG
27	15	29	THR
28	16	9	LEU
28	16	48	VAL
29	17	1	MET
29	17	39	ARG
29	17	43	THR
30	18	30	ARG
30	18	31	HIS
30	18	32	LEU
31	19	4	ARG
33	1b	94	ASN
33	1b	187	LEU

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
33	1b	200	ILE
34	1c	3	ASN
34	1c	64	VAL
34	1c	195	VAL
35	1d	10	ARG
35	1d	19	LEU
35	1d	31	CYS
35	1d	83	SER
35	1d	91	SER
35	1d	135	LEU
35	1d	177	ASP
36	1e	16	THR
36	1e	31	LEU
36	1e	41	VAL
36	1e	56	GLN
36	1e	81	GLU
36	1e	152	ARG
38	1g	12	LEU
38	1g	79	ARG
38	1g	92	SER
38	1g	115	ARG
39	1h	52	ASP
39	1h	63	LEU
39	1h	69	ARG
39	1h	104	ARG
40	1i	75	ASP
40	1i	83	ARG
40	1i	92	TYR
40	1i	128	ARG
41	1j	16	LEU
41	1j	55	LYS
42	1k	33	THR
43	1l	54	LYS
43	1l	58	VAL
43	1l	59	ARG
43	1l	83	VAL
44	1m	15	VAL
44	1m	91	ARG
45	1n	6	LEU
45	1n	18	VAL
45	1n	23	ARG
45	1n	29	ARG

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
45	1n	33	VAL
45	1n	56	VAL
47	1p	11	SER
47	1p	21	VAL
47	1p	67	THR
48	1q	68	ARG
49	1r	31	LEU
50	1s	12	ASP
50	1s	41	VAL
50	1s	77	THR
51	1t	90	GLN
52	1u	15	ARG
3	2D	3	VAL
3	2D	38	LYS
3	2D	68	LYS
3	2D	99	ASP
3	2D	138	VAL
3	2D	142	VAL
3	2D	169	GLU
3	2D	242	ARG
3	2D	259	THR
4	2E	9	VAL
4	2E	12	THR
4	2E	21	VAL
4	2E	58	ARG
4	2E	75	VAL
4	2E	101	ARG
4	2E	116	VAL
4	2E	170	LEU
4	2E	175	VAL
4	2E	181	LEU
5	2F	51	THR
5	2F	53	THR
5	2F	60	SER
5	2F	72	ARG
5	2F	88	VAL
5	2F	132	VAL
5	2F	158	THR
5	2F	183	VAL
6	2G	3	LEU
6	2G	9	ARG
6	2G	43	LEU

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
6	2G	51	ARG
6	2G	133	LEU
6	2G	140	ILE
6	2G	161	THR
6	2G	165	THR
7	2H	52	VAL
7	2H	70	THR
7	2H	71	LEU
7	2H	129	THR
7	2H	134	SER
8	2I	74	ASN
8	2I	76	THR
8	2I	92	VAL
8	2I	144	VAL
9	2N	14	VAL
9	2N	28	THR
9	2N	33	LEU
9	2N	35	ARG
9	2N	48	MET
9	2N	58	ASP
9	2N	62	VAL
9	2N	63	THR
9	2N	73	THR
9	2N	99	LEU
9	2N	140	VAL
10	2O	64	ARG
11	2P	95	VAL
11	2P	105	LEU
11	2P	112	LEU
12	2Q	35	VAL
12	2Q	38	GLU
12	2Q	75	THR
12	2Q	110	THR
13	2R	24	GLN
13	2R	29	LEU
13	2R	44	LEU
13	2R	65	LEU
13	2R	100	LEU
13	2R	111	LEU
14	2S	84	GLN
15	2T	41	ARG
15	2T	89	VAL

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
15	2T	96	ARG
16	2U	8	VAL
16	2U	78	THR
17	2V	39	LEU
17	2V	51	VAL
17	2V	56	SER
17	2V	62	LEU
17	2V	72	VAL
17	2V	79	VAL
17	2V	100	ARG
19	2X	35	THR
19	2X	70	LEU
20	2Y	23	ARG
20	2Y	37	VAL
20	2Y	55	TYR
20	2Y	99	CYS
20	2Y	107	ASP
21	2Z	52	SER
21	2Z	72	ARG
21	2Z	129	SER
21	2Z	144	LEU
21	2Z	154	ASP
21	2Z	170	THR
22	20	10	THR
22	20	74	ARG
23	21	21	ARG
23	21	35	THR
23	21	95	LEU
24	22	19	VAL
24	22	52	ASP
25	23	30	ARG
25	23	31	LEU
25	23	34	GLU
26	24	26	SER
26	24	34	GLU
26	24	44	THR
26	24	49	PHE
26	24	50	VAL
26	24	63	TYR
27	25	6	VAL
27	25	29	THR
27	25	33	CYS

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
27	25	58	LEU
28	26	5	VAL
29	27	1	MET
29	27	39	ARG
30	28	14	VAL
30	28	30	ARG
30	28	32	LEU
30	28	41	ILE
31	29	7	VAL
33	2b	19	HIS
33	2b	93	VAL
33	2b	94	ASN
33	2b	112	VAL
33	2b	127	ILE
33	2b	140	HIS
33	2b	185	ILE
33	2b	189	ASP
33	2b	192	SER
34	2c	15	THR
34	2c	166	GLU
35	2d	31	CYS
35	2d	115	ARG
35	2d	135	LEU
35	2d	181	MET
35	2d	208	SER
36	2e	41	VAL
36	2e	68	GLU
36	2e	75	THR
36	2e	152	ARG
37	2f	72	VAL
37	2f	75	LEU
37	2f	83	ASP
38	2g	79	ARG
38	2g	98	SER
38	2g	111	ARG
39	2h	3	THR
39	2h	54	ASP
39	2h	56	LYS
39	2h	84	ARG
39	2h	104	ARG
39	2h	112	LEU
39	2h	114	THR

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Mol	Chain	Res	Type
40	2i	3	GLN
40	2i	64	THR
40	2i	65	VAL
40	2i	102	LEU
40	2i	127	LYS
41	2j	16	LEU
41	2j	69	ASN
42	2k	14	VAL
42	2k	24	SER
42	2k	109	VAL
43	2l	27	LEU
43	2l	97	ARG
43	2l	116	SER
44	2m	91	ARG
45	2n	6	LEU
45	2n	18	VAL
45	2n	19	ARG
45	2n	25	VAL
45	2n	33	VAL
46	2o	51	HIS
47	2p	2	VAL
47	2p	20	VAL
47	2p	21	VAL
47	2p	44	THR
47	2p	62	VAL
47	2p	69	THR
48	2q	68	ARG
49	2r	31	LEU
49	2r	47	THR
49	2r	76	LEU
50	2s	5	LEU
50	2s	41	VAL
51	2t	84	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (76) such sidechains are listed below:

Mol	Chain	Res	Type
4	1E	60	ASN
5	1F	8	GLN
5	1F	69	HIS
6	1G	26	GLN
6	1G	58	GLN

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
8	1I	105	HIS
10	1O	3	GLN
12	1Q	12	GLN
12	1Q	57	HIS
13	1R	71	GLN
14	1S	61	ASN
15	1T	58	ASN
19	1X	31	HIS
19	1X	82	GLN
23	11	47	GLN
23	11	56	GLN
24	12	9	GLN
27	15	4	HIS
33	1b	40	HIS
34	1c	6	HIS
34	1c	162	GLN
34	1c	176	HIS
36	1e	78	HIS
37	1f	100	ASN
38	1g	28	ASN
38	1g	148	ASN
40	1i	3	GLN
40	1i	31	GLN
40	1i	87	GLN
40	1i	124	GLN
43	1l	99	HIS
47	1p	13	HIS
50	1s	23	ASN
50	1s	47	HIS
50	1s	69	HIS
50	1s	83	HIS
3	2D	87	ASN
3	2D	143	HIS
4	2E	48	GLN
5	2F	69	HIS
8	2I	139	GLN
10	2O	5	GLN
12	2Q	12	GLN
12	2Q	123	HIS
13	2R	13	HIS
18	2W	60	ASN
18	2W	62	HIS

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Mol	Chain	Res	Type
19	2X	31	HIS
20	2Y	6	HIS
21	2Z	32	HIS
21	2Z	55	HIS
24	22	65	ASN
29	27	6	GLN
31	29	20	HIS
33	2b	78	GLN
33	2b	94	ASN
34	2c	102	ASN
34	2c	162	GLN
35	2d	77	ASN
35	2d	119	GLN
35	2d	123	HIS
35	2d	125	HIS
36	2e	78	HIS
38	2g	28	ASN
38	2g	109	ASN
38	2g	148	ASN
40	2i	31	GLN
40	2i	87	GLN
40	2i	89	ASN
40	2i	124	GLN
41	2j	56	HIS
42	2k	104	GLN
44	2m	77	ASN
47	2p	16	HIS
49	2r	63	GLN
50	2s	23	ASN

### 5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	1A	2861/2915 (98%)	450 (15%)	29 (1%)
1	2A	2788/2915 (95%)	473 (16%)	20 (0%)
2	1B	120/121 (99%)	9 (7%)	1 (0%)
2	2B	118/121 (97%)	28 (23%)	0
32	1a	1494/1521 (98%)	242 (16%)	0
32	2a	1498/1521 (98%)	288 (19%)	0
53	1v	12/24 (50%)	2 (16%)	0
53	2v	12/24 (50%)	3 (25%)	0

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Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
54	1w	69/76 (90%)	22 (31%)	0
54	1y	71/76 (93%)	22 (30%)	0
54	2w	65/76 (85%)	20 (30%)	0
54	2y	69/76 (90%)	21 (30%)	0
55	1x	75/77 (97%)	13 (17%)	0
55	2x	75/77 (97%)	12 (16%)	0
All	All	9327/9620 (96%)	1605 (17%)	50 (0%)

All (1605) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	1A	12	U
1	1A	13	A
1	1A	14	A
1	1A	15	G
1	1A	34	C
1	1A	36	G
1	1A	45	C
1	1A	50	G
1	1A	54	G
1	1A	57	G
1	1A	70	A
1	1A	71	U
1	1A	73	A
1	1A	74	G
1	1A	77	A
1	1A	83	A
1	1A	90	A
1	1A	94	G
1	1A	116	A
1	1A	117	A
1	1A	118	U
1	1A	121	G
1	1A	123	G
1	1A	138	G
1	1A	145	G
1	1A	177	G
1	1A	185	A
1	1A	188	A
1	1A	194	G
1	1A	203	G
1	1A	204	G

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	1A	205	A
1	1A	211	A
1	1A	217	A
1	1A	218	A
1	1A	222	A
1	1A	237	G
1	1A	258	U
1	1A	262	C
1	1A	272	U
1	1A	273	G
1	1A	275	C
1	1A	278	G
1	1A	279	G
1	1A	289	G
1	1A	299	G
1	1A	303	C
1	1A	309	C
1	1A	335	A
1	1A	353	G
1	1A	354	A
1	1A	360	C
1	1A	376	G
1	1A	387	G
1	1A	388	A
1	1A	389	G
1	1A	407	U
1	1A	413	G
1	1A	423	G
1	1A	432	U
1	1A	438	G
1	1A	448	U
1	1A	455	A
1	1A	469	A
1	1A	470	C
1	1A	474	U
1	1A	480	A
1	1A	482	C
1	1A	507	G
1	1A	519	G
1	1A	526	A
1	1A	529	U
1	1A	530	A

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	1A	534	C
1	1A	538	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	579	G
1	1A	586	G
1	1A	591	U
1	1A	596	G
1	1A	598	A
1	1A	607	C
1	1A	616	G
1	1A	626	A
1	1A	627	G
1	1A	630	U
1	1A	639	G
1	1A	641	G
1	1A	642	G
1	1A	652	A
1	1A	662	A
1	1A	670	C
1	1A	671	A
1	1A	693	G
1	1A	697	C
1	1A	716	G
1	1A	732	A
1	1A	733	G
1	1A	777	C
1	1A	811	A
1	1A	822	G
1	1A	823	G
1	1A	829	A
1	1A	830	A
1	1A	831	A
1	1A	832	G
1	1A	837	C
1	1A	839	G
1	1A	852	G
1	1A	859	C

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	1A	866	A
1	1A	874	U
1	1A	875	U
1	1A	913	A
1	1A	924	U
1	1A	926	G
1	1A	927	G
1	1A	931	C
1	1A	932	C
1	1A	933	C
1	1A	934	A
1	1A	935	C
1	1A	936	C
1	1A	937	A
1	1A	940	C
1	1A	941	U
1	1A	942	A
1	1A	943	C
1	1A	944	C
1	1A	953	U
1	1A	956	A
1	1A	977	G
1	1A	983	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	1008	U
1	1A	1019	G
1	1A	1020	C
1	1A	1029	A
1	1A	1042	A
1	1A	1058	U
1	1A	1059	C
1	1A	1068	G
1	1A	1072	U
1	1A	1073	A
1	1A	1079	U
1	1A	1084	C
1	1A	1090	G

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	1A	1091	A
1	1A	1092	A
1	1A	1093	G
1	1A	1094	A
1	1A	1100	A
1	1A	1101	G
1	1A	1104	G
1	1A	1109	G
1	1A	1112	U
1	1A	1113	A
1	1A	1114	G
1	1A	1116	A
1	1A	1117	G
1	1A	1119	A
1	1A	1120	G
1	1A	1121	C
1	1A	1122	C
1	1A	1124	U
1	1A	1127	U
1	1A	1131	A
1	1A	1134	A
1	1A	1135	G
1	1A	1136	U
1	1A	1140	U
1	1A	1142	A
1	1A	1147	U
1	1A	1154	U
1	1A	1157	A
1	1A	1158	G
1	1A	1161	G
1	1A	1162	C
1	1A	1174	A
1	1A	1176	U
1	1A	1180	C
1	1A	1181	G
1	1A	1195	G
1	1A	1214	G
1	1A	1217	G
1	1A	1218	G
1	1A	1219	A
1	1A	1220	U
1	1A	1221	G

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	1A	1222	A
1	1A	1223	C
1	1A	1256	U
1	1A	1263	C
1	1A	1282	G
1	1A	1294	G
1	1A	1296	G
1	1A	1299	A
1	1A	1302	G
1	1A	1317	G
1	1A	1318	A
1	1A	1322	A
1	1A	1327	G
1	1A	1346	U
1	1A	1347	A
1	1A	1349	G
1	1A	1366	C
1	1A	1391	C
1	1A	1398	U
1	1A	1405	A
1	1A	1406	A
1	1A	1411	A
1	1A	1430	A
1	1A	1431	G
1	1A	1432	C
1	1A	1441	A
1	1A	1442	U
1	1A	1462	G
1	1A	1463	C
1	1A	1466	U
1	1A	1467	G
1	1A	1474	C
1	1A	1491	A
1	1A	1497	G
1	1A	1502	G
1	1A	1514	C
1	1A	1529	G
1	1A	1539	C
1	1A	1543	U
1	1A	1554	A
1	1A	1555	C
1	1A	1556	A

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	1A	1586	G
1	1A	1587	U
1	1A	1605	A
1	1A	1613	A
1	1A	1616	A
1	1A	1625	U
1	1A	1627	A
1	1A	1628	G
1	1A	1631	C
1	1A	1632	A
1	1A	1654	A
1	1A	1655	A
1	1A	1656	A
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	1750	G
1	1A	1767	A
1	1A	1768	U
1	1A	1776	G
1	1A	1787	G
1	1A	1793	A
1	1A	1794	G
1	1A	1795	G
1	1A	1804	A
1	1A	1811	A
1	1A	1813	C
1	1A	1817	A
1	1A	1822	A
1	1A	1831	C
1	1A	1832	G
1	1A	1847	G
1	1A	1860	A
1	1A	1870	G
1	1A	1878	A
1	1A	1889	G
1	1A	1899	A
1	1A	1911	A
1	1A	1922	A

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	1A	1928	G
1	1A	1936	C
1	1A	1951	G
1	1A	1952	G
1	1A	1959	A
1	1A	1960	A
1	1A	1977	U
1	1A	1982	A
1	1A	1985	U
1	1A	1989	C
1	1A	1992	A
1	1A	1993	A
1	1A	1994	A
1	1A	2014	G
1	1A	2015	U
1	1A	2019	G
1	1A	2042	A
1	1A	2045	G
1	1A	2053	A
1	1A	2055	A
1	1A	2065	C
1	1A	2074	G
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	2114	U
1	1A	2115	G
1	1A	2124	U
1	1A	2132	G
1	1A	2133	C
1	1A	2134	G
1	1A	2135	U
1	1A	2136	A
1	1A	2138	G
1	1A	2142	G
1	1A	2143	G
1	1A	2144	U
1	1A	2148	A
1	1A	2149	G

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	1A	2151	C
1	1A	2152	U
1	1A	2153	G
1	1A	2154	U
1	1A	2155	G
1	1A	2156	A
1	1A	2157	A
1	1A	2158	C
1	1A	2162	C
1	1A	2163	G
1	1A	2164	C
1	1A	2165	C
1	1A	2166	U
1	1A	2168	C
1	1A	2170	G
1	1A	2172	U
1	1A	2173	G
1	1A	2178	G
1	1A	2179	G
1	1A	2180	A
1	1A	2181	G
1	1A	2182	G
1	1A	2184	G
1	1A	2188	G
1	1A	2189	U
1	1A	2193	A
1	1A	2194	U
1	1A	2195	A
1	1A	2204	G
1	1A	2206	G
1	1A	2211	U
1	1A	2214	G
1	1A	2220	A
1	1A	2227	G
1	1A	2228	G
1	1A	2229	A
1	1A	2237	A
1	1A	2250	G
1	1A	2251	G
1	1A	2280	A
1	1A	2281	A
1	1A	2285	A

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	1A	2291	G
1	1A	2292	G
1	1A	2295	C
1	1A	2299	A
1	1A	2301	G
1	1A	2306	C
1	1A	2317	A
1	1A	2319	G
1	1A	2320	G
1	1A	2321	A
1	1A	2332	A
1	1A	2337	G
1	1A	2346	G
1	1A	2348	A
1	1A	2359	C
1	1A	2362	C
1	1A	2373	A
1	1A	2395	G
1	1A	2397	C
1	1A	2408	G
1	1A	2412	G
1	1A	2418	U
1	1A	2436	C
1	1A	2437	A
1	1A	2440	G
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	2460	A
1	1A	2488	A
1	1A	2490	A
1	1A	2514	G
1	1A	2517	G
1	1A	2518	U
1	1A	2530	A
1	1A	2537	G
1	1A	2541	G
1	1A	2547	G
1	1A	2561	G

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	1A	2566	U
1	1A	2578	A
1	1A	2579	G
1	1A	2585	C
1	1A	2614	A
1	1A	2621	U
1	1A	2623	U
1	1A	2624	C
1	1A	2640	C
1	1A	2641	A
1	1A	2642	G
1	1A	2666	A
1	1A	2701	U
1	1A	2702	C
1	1A	2714	U
1	1A	2715	C
1	1A	2725	A
1	1A	2726	A
1	1A	2727	G
1	1A	2739	U
1	1A	2746	A
1	1A	2757	G
1	1A	2770	A
1	1A	2771	A
1	1A	2777	A
1	1A	2778	A
1	1A	2779	G
1	1A	2791	A
1	1A	2793	G
1	1A	2802	C
1	1A	2803	A
1	1A	2804	C
1	1A	2806	G
1	1A	2813	G
1	1A	2830	A
1	1A	2831	A
1	1A	2845	A
1	1A	2882	G
1	1A	2890	C
1	1A	2901	A
1	1A	2903	G
2	1B	2	C

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
2	1B	30	C
2	1B	35	U
2	1B	52	A
2	1B	56	G
2	1B	67	G
2	1B	73	A
2	1B	106	G
2	1B	110	G
32	1a	7	G
32	1a	9	G
32	1a	32	A
32	1a	39	G
32	1a	47	C
32	1a	48	C
32	1a	50	A
32	1a	51	A
32	1a	61	G
32	1a	70	G
32	1a	73	G
32	1a	79	G
32	1a	96	U
32	1a	98	G
32	1a	101	A
32	1a	116	A
32	1a	120	A
32	1a	121	C
32	1a	131	C
32	1a	163	C
32	1a	174	C
32	1a	182	U
32	1a	189(B)	C
32	1a	189(F)	U
32	1a	189(G)	G
32	1a	189(J)	G
32	1a	195	A
32	1a	197	A
32	1a	202	U
32	1a	203	U
32	1a	204	U
32	1a	216	G
32	1a	217	C
32	1a	220	G

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
32	1a	247	G
32	1a	251	G
32	1a	258	G
32	1a	266	G
32	1a	267	C
32	1a	289	G
32	1a	301	G
32	1a	321	A
32	1a	328	C
32	1a	332	G
32	1a	341	C
32	1a	342	C
32	1a	344	A
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	382	A
32	1a	384	G
32	1a	397	A
32	1a	398	C
32	1a	406	G
32	1a	412	A
32	1a	421	U
32	1a	424	G
32	1a	429	U
32	1a	430	A
32	1a	439	A
32	1a	442	C
32	1a	452	A
32	1a	453	A
32	1a	461	A
32	1a	470	C
32	1a	471	G
32	1a	485	G
32	1a	496	A
32	1a	498	U
32	1a	505	G

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
32	1a	509	A
32	1a	510	A
32	1a	511	C
32	1a	518	C
32	1a	521	G
32	1a	527	7MG
32	1a	531	U
32	1a	532	A
32	1a	547	A
32	1a	559	A
32	1a	560	U
32	1a	561	U
32	1a	562	C
32	1a	568	G
32	1a	572	A
32	1a	573	A
32	1a	574	A
32	1a	576	G
32	1a	577	G
32	1a	596	C
32	1a	630	G
32	1a	653	A
32	1a	665	A
32	1a	666	G
32	1a	687	A
32	1a	688	G
32	1a	703	G
32	1a	717	C
32	1a	723	U
32	1a	731	G
32	1a	734	G
32	1a	747	C
32	1a	749	C
32	1a	755	G
32	1a	759	A
32	1a	760	G
32	1a	777	A
32	1a	792	A
32	1a	793	U
32	1a	794	A
32	1a	815	A
32	1a	816	A

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
32	1a	817	C
32	1a	821	G
32	1a	828	A
32	1a	840	C
32	1a	841	U
32	1a	851	G
32	1a	859	A
32	1a	870	U
32	1a	872	A
32	1a	902	G
32	1a	914	A
32	1a	926	G
32	1a	927	G
32	1a	931	C
32	1a	934	C
32	1a	935	A
32	1a	942	G
32	1a	960	U
32	1a	961	U
32	1a	967	5MC
32	1a	968	A
32	1a	969	A
32	1a	971	G
32	1a	974	A
32	1a	975	A
32	1a	976	G
32	1a	977	A
32	1a	982	U
32	1a	992	U
32	1a	993	G
32	1a	994	A
32	1a	997	U
32	1a	1000	U
32	1a	1001	A
32	1a	1003	G
32	1a	1005	A
32	1a	1006	C
32	1a	1009	G
32	1a	1011	G
32	1a	1020	U
32	1a	1022	G
32	1a	1024	G

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
32	1a	1025	U
32	1a	1026	G
32	1a	1027	C
32	1a	1028	C
32	1a	1030(A)	G
32	1a	1030(C)	G
32	1a	1030(D)	A
32	1a	1031	G
32	1a	1033	G
32	1a	1039	C
32	1a	1043	C
32	1a	1054	C
32	1a	1066	C
32	1a	1068	G
32	1a	1081	G
32	1a	1094	G
32	1a	1095	U
32	1a	1096	C
32	1a	1101	A
32	1a	1125	U
32	1a	1137	C
32	1a	1138	G
32	1a	1139	G
32	1a	1146	A
32	1a	1152	A
32	1a	1154	G
32	1a	1159	U
32	1a	1160	G
32	1a	1184	G
32	1a	1187	G
32	1a	1196	U
32	1a	1197	G
32	1a	1202	G
32	1a	1212	U
32	1a	1213	A
32	1a	1227	A
32	1a	1238	A
32	1a	1250	A
32	1a	1256	A
32	1a	1257	U
32	1a	1260	C
32	1a	1275	A

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
32	1a	1278	U
32	1a	1279	A
32	1a	1280	A
32	1a	1286	A
32	1a	1287	A
32	1a	1299	A
32	1a	1300	G
32	1a	1302	U
32	1a	1305	G
32	1a	1320	C
32	1a	1338	G
32	1a	1346	A
32	1a	1347	G
32	1a	1353	G
32	1a	1358	U
32	1a	1363	C
32	1a	1363(A)	A
32	1a	1364	U
32	1a	1370	G
32	1a	1378	C
32	1a	1390	U
32	1a	1394	A
32	1a	1397	C
32	1a	1419	G
32	1a	1442	G
32	1a	1442(A)	G
32	1a	1442(B)	A
32	1a	1446	U
32	1a	1447	A
32	1a	1452	C
32	1a	1487	G
32	1a	1492	A
32	1a	1494	G
32	1a	1503	A
32	1a	1504	G
32	1a	1506	U
32	1a	1517	G
32	1a	1529	G
32	1a	1530	G
32	1a	1532	U
53	1v	13	A
53	1v	24	A

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
54	1w	2	C
54	1w	3	C
54	1w	7	A
54	1w	9	A
54	1w	14	A
54	1w	19	G
54	1w	20	U
54	1w	21	A
54	1w	23	A
54	1w	24	G
54	1w	45	U
54	1w	46	7MG
54	1w	47	U
54	1w	48	C
54	1w	50	U
54	1w	62	C
54	1w	63	G
54	1w	68	C
54	1w	69	G
54	1w	70	G
54	1w	73	A
54	1w	74	C
55	1x	6	G
55	1x	9	G
55	1x	17(A)	U
55	1x	18	G
55	1x	19	G
55	1x	20	U
55	1x	21	A
55	1x	31	G
55	1x	47	U
55	1x	48	C
55	1x	56	C
55	1x	69	C
55	1x	76	A
54	1y	6	G
54	1y	8	4SU
54	1y	13	C
54	1y	14	A
54	1y	19	G
54	1y	20	U
54	1y	21	A

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
54	1y	35	A
54	1y	44	G
54	1y	45	U
54	1y	46	7MG
54	1y	48	C
54	1y	49	C
54	1y	53	G
54	1y	57	G
54	1y	59	U
54	1y	61	C
54	1y	65	G
54	1y	66	U
54	1y	69	G
54	1y	70	G
54	1y	73	A
1	2A	15	G
1	2A	35	G
1	2A	36	G
1	2A	45	C
1	2A	71	A
1	2A	74	A
1	2A	75	G
1	2A	83	G
1	2A	84	A
1	2A	90	U
1	2A	95	G
1	2A	100	G
1	2A	102	G
1	2A	118	A
1	2A	119	A
1	2A	120	U
1	2A	125	G
1	2A	126	A
1	2A	136	G
1	2A	154(A)	C
1	2A	157	U
1	2A	172	C
1	2A	173	G
1	2A	181	A
1	2A	196	A
1	2A	199	A
1	2A	205	G

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	2A	214	G
1	2A	216	A
1	2A	222	A
1	2A	228	A
1	2A	229	A
1	2A	233	A
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	272(B)	G
1	2A	274	G
1	2A	277	C
1	2A	278	A
1	2A	279	C
1	2A	294	A
1	2A	308	G
1	2A	311	A
1	2A	323	G
1	2A	324	A
1	2A	327	G
1	2A	329	G
1	2A	330	A
1	2A	342	G
1	2A	352	G
1	2A	362	U
1	2A	363	G
1	2A	363(B)	G
1	2A	363(D)	G
1	2A	363(E)	U
1	2A	363(F)	A
1	2A	386	G
1	2A	396	G
1	2A	403	U
1	2A	405	U
1	2A	411	G
1	2A	412	A
1	2A	421	U
1	2A	422	A
1	2A	444	C

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	2A	447	A
1	2A	454	A
1	2A	457	A
1	2A	479	A
1	2A	481	G
1	2A	494	G
1	2A	505	A
1	2A	509	C
1	2A	529	A
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	567	A
1	2A	568	U
1	2A	573	G
1	2A	575	A
1	2A	588	U
1	2A	599	G
1	2A	603	A
1	2A	604	G
1	2A	606	U
1	2A	607	U
1	2A	614(B)	G
1	2A	615	G
1	2A	616	G
1	2A	627	A
1	2A	634	C
1	2A	637	A
1	2A	645	C
1	2A	652(B)	A
1	2A	652(U)	G
1	2A	669	G
1	2A	686	G
1	2A	709	U
1	2A	717	G
1	2A	730	C
1	2A	753	C
1	2A	771	G
1	2A	775	G

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	2A	776	G
1	2A	779	U
1	2A	782	A
1	2A	784	A
1	2A	785	G
1	2A	792	G
1	2A	805	G
1	2A	811	U
1	2A	812	C
1	2A	819	A
1	2A	827	U
1	2A	828	U
1	2A	847	U
1	2A	854	G
1	2A	857	C
1	2A	859	G
1	2A	866	A
1	2A	869	G
1	2A	873	G
1	2A	874	G
1	2A	875	G
1	2A	877	U
1	2A	878	A
1	2A	879	G
1	2A	880	G
1	2A	883	G
1	2A	884	C
1	2A	886	C
1	2A	887	A
1	2A	888	C
1	2A	890	A
1	2A	893	C
1	2A	894	C
1	2A	896	A
1	2A	900	A
1	2A	901	A
1	2A	910	A
1	2A	914	C
1	2A	915	C
1	2A	917	A
1	2A	932	G
1	2A	941	A

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	2A	945	A
1	2A	946	G
1	2A	953	A
1	2A	957	A
1	2A	958	U
1	2A	959	A
1	2A	961	C
1	2A	974	G
1	2A	975	C
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	1017	G
1	2A	1022	G
1	2A	1025	G
1	2A	1026	U
1	2A	1033	U
1	2A	1036	G
1	2A	1038	C
1	2A	1039	G
1	2A	1041	C
1	2A	1043	C
1	2A	1116	C
1	2A	1122	G
1	2A	1130	U
1	2A	1135	C
1	2A	1136	G
1	2A	1139	G
1	2A	1142(A)	A
1	2A	1144	G
1	2A	1166	C
1	2A	1171	G
1	2A	1180	C
1	2A	1206	G
1	2A	1211	U
1	2A	1220	A
1	2A	1237	A
1	2A	1244	G

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	2A	1250	G
1	2A	1253	A
1	2A	1256	G
1	2A	1271	G
1	2A	1272	A
1	2A	1273	U
1	2A	1284	A
1	2A	1300	U
1	2A	1301	A
1	2A	1308	A
1	2A	1314	C
1	2A	1320	C
1	2A	1345	C
1	2A	1352	U
1	2A	1359	A
1	2A	1360	A
1	2A	1365	A
1	2A	1368	G
1	2A	1370	C
1	2A	1380	G
1	2A	1384	A
1	2A	1385	G
1	2A	1386	C
1	2A	1398	C
1	2A	1411	C
1	2A	1416	G
1	2A	1417	C
1	2A	1420	U
1	2A	1421	G
1	2A	1427	A
1	2A	1428	C
1	2A	1437	C
1	2A	1445	A
1	2A	1449	A
1	2A	1450	G
1	2A	1455	G
1	2A	1460	A
1	2A	1463	C
1	2A	1467	C
1	2A	1471	A
1	2A	1482	G
1	2A	1490	A

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	2A	1493	C
1	2A	1497	U
1	2A	1508	A
1	2A	1509	C
1	2A	1509(A)	A
1	2A	1531	C
1	2A	1532	C
1	2A	1542	A
1	2A	1545	A
1	2A	1558	A
1	2A	1566	A
1	2A	1569	A
1	2A	1578	U
1	2A	1579	A
1	2A	1580	A
1	2A	1583	A
1	2A	1584	C
1	2A	1586	A
1	2A	1608	A
1	2A	1609	A
1	2A	1610	A
1	2A	1640	C
1	2A	1648	C
1	2A	1654	A
1	2A	1674	G
1	2A	1675	C
1	2A	1696	G
1	2A	1700	A
1	2A	1701	A
1	2A	1703	G
1	2A	1721	G
1	2A	1722	A
1	2A	1739	U
1	2A	1740	G
1	2A	1746	G
1	2A	1747	G
1	2A	1750	G
1	2A	1756	G
1	2A	1758	G
1	2A	1762	A
1	2A	1763	G
1	2A	1764	G

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	2A	1773	A
1	2A	1780	A
1	2A	1782	C
1	2A	1786	A
1	2A	1791	A
1	2A	1800	C
1	2A	1801	G
1	2A	1811	G
1	2A	1812	A
1	2A	1816	G
1	2A	1829	A
1	2A	1835	G
1	2A	1847	A
1	2A	1848	A
1	2A	1857	G
1	2A	1877	A
1	2A	1878	G
1	2A	1889	A
1	2A	1896	G
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	1938	A
1	2A	1955	U
1	2A	1963	U
1	2A	1964	G
1	2A	1967	C
1	2A	1970	A
1	2A	1971	A
1	2A	1972	A
1	2A	1993	U
1	2A	1997	G
1	2A	2023	G
1	2A	2027	G
1	2A	2031	A
1	2A	2033	A
1	2A	2043	C
1	2A	2055	C

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	2A	2056	G
1	2A	2060	A
1	2A	2061	G
1	2A	2062	A
1	2A	2069	G
1	2A	2093	G
1	2A	2105	C
1	2A	2108	C
1	2A	2111	C
1	2A	2112	G
1	2A	2116	G
1	2A	2117	A
1	2A	2119	A
1	2A	2120	G
1	2A	2122	U
1	2A	2124	G
1	2A	2126	A
1	2A	2127	G
1	2A	2129	C
1	2A	2131	G
1	2A	2132	U
1	2A	2133	G
1	2A	2134	A
1	2A	2135	A
1	2A	2136	C
1	2A	2137	C
1	2A	2138	C
1	2A	2140	C
1	2A	2142	C
1	2A	2146	C
1	2A	2147	G
1	2A	2150	U
1	2A	2153	G
1	2A	2154	G
1	2A	2155	G
1	2A	2156	G
1	2A	2157	G
1	2A	2158	A
1	2A	2161	C
1	2A	2165	G
1	2A	2166	G
1	2A	2167	U

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	2A	2168	G
1	2A	2172	U
1	2A	2174	C
1	2A	2178	C
1	2A	2185	C
1	2A	2189	U
1	2A	2192	G
1	2A	2198	A
1	2A	2206	G
1	2A	2207	G
1	2A	2208	A
1	2A	2218	U
1	2A	2225	A
1	2A	2239	G
1	2A	2275	C
1	2A	2278	A
1	2A	2279	G
1	2A	2282	G
1	2A	2283	C
1	2A	2287	A
1	2A	2288	A
1	2A	2305	A
1	2A	2308	G
1	2A	2319	G
1	2A	2320	A
1	2A	2322	A
1	2A	2325	G
1	2A	2327	A
1	2A	2334	G
1	2A	2336	A
1	2A	2341	G
1	2A	2346	A
1	2A	2347	C
1	2A	2350	C
1	2A	2376	A
1	2A	2383	G
1	2A	2385	C
1	2A	2396	G
1	2A	2403	C
1	2A	2406	U
1	2A	2419	U
1	2A	2425	A

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	2A	2429	G
1	2A	2430	A
1	2A	2434	A
1	2A	2435	A
1	2A	2439	A
1	2A	2441	C
1	2A	2445	G
1	2A	2448	A
1	2A	2465	C
1	2A	2468	G
1	2A	2469	A
1	2A	2476	A
1	2A	2487	G
1	2A	2490	G
1	2A	2491	U
1	2A	2497	A
1	2A	2502	G
1	2A	2505	G
1	2A	2506	U
1	2A	2518	A
1	2A	2520	C
1	2A	2554	U
1	2A	2555	U
1	2A	2566	A
1	2A	2567	G
1	2A	2576	G
1	2A	2579	C
1	2A	2582	G
1	2A	2602	A
1	2A	2609	U
1	2A	2610	C
1	2A	2611	U
1	2A	2612	C
1	2A	2629	A
1	2A	2630	G
1	2A	2634	G
1	2A	2654	A
1	2A	2669	G
1	2A	2686	G
1	2A	2689	U
1	2A	2690	C
1	2A	2702	U

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	2A	2703	C
1	2A	2712(A)	A
1	2A	2713	A
1	2A	2714	G
1	2A	2726	U
1	2A	2733	A
1	2A	2751	G
1	2A	2758	A
1	2A	2764	A
1	2A	2765	A
1	2A	2778	A
1	2A	2793	G
1	2A	2802	G
1	2A	2803	C
1	2A	2804	C
1	2A	2807	G
1	2A	2818	G
1	2A	2820	A
1	2A	2821	A
1	2A	2833	G
1	2A	2839	G
1	2A	2872	G
1	2A	2873	A
1	2A	2879	C
1	2A	2894	G
1	2A	2897	U
2	2B	2	C
2	2B	4	C
2	2B	5	C
2	2B	8	U
2	2B	13	A
2	2B	19	G
2	2B	23	G
2	2B	30	C
2	2B	34	U
2	2B	38	C
2	2B	42	C
2	2B	53	A
2	2B	56	G
2	2B	57	A
2	2B	63	G
2	2B	67	G

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
2	2B	73	A
2	2B	74	U
2	2B	75	G
2	2B	85	G
2	2B	106	G
2	2B	108	U
2	2B	109	C
2	2B	110	G
2	2B	114	C
2	2B	116	G
2	2B	119	G
2	2B	120	A
32	2a	6	G
32	2a	9	G
32	2a	13	U
32	2a	15	G
32	2a	32	A
32	2a	39	G
32	2a	47	C
32	2a	48	C
32	2a	50	A
32	2a	51	A
32	2a	66	G
32	2a	73	G
32	2a	79	G
32	2a	80	G
32	2a	89	C
32	2a	98	G
32	2a	101	A
32	2a	116	A
32	2a	121	C
32	2a	129(A)	G
32	2a	131	C
32	2a	142	G
32	2a	152	A
32	2a	156	G
32	2a	163	C
32	2a	174	C
32	2a	182	U
32	2a	189(E)	U
32	2a	189(F)	U
32	2a	195	A

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
32	2a	196	A
32	2a	197	A
32	2a	201	C
32	2a	202	U
32	2a	203	U
32	2a	204	U
32	2a	216	G
32	2a	247	G
32	2a	251	G
32	2a	258	G
32	2a	266	G
32	2a	267	C
32	2a	281	G
32	2a	289	G
32	2a	318	G
32	2a	321	A
32	2a	328	C
32	2a	332	G
32	2a	350	G
32	2a	351	G
32	2a	352	C
32	2a	353	A
32	2a	354	G
32	2a	365	U
32	2a	367	U
32	2a	372	C
32	2a	373	A
32	2a	381	C
32	2a	384	G
32	2a	397	A
32	2a	398	C
32	2a	406	G
32	2a	412	A
32	2a	413	G
32	2a	421	U
32	2a	423	G
32	2a	424	G
32	2a	429	U
32	2a	441	A
32	2a	442	C
32	2a	443	C
32	2a	452	A

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
32	2a	461	A
32	2a	470	C
32	2a	477	A
32	2a	484	G
32	2a	485	G
32	2a	496	A
32	2a	498	U
32	2a	505	G
32	2a	510	A
32	2a	511	C
32	2a	518	C
32	2a	524	G
32	2a	531	U
32	2a	532	A
32	2a	533	A
32	2a	547	A
32	2a	559	A
32	2a	560	U
32	2a	564	C
32	2a	568	G
32	2a	572	A
32	2a	573	A
32	2a	575	G
32	2a	576	G
32	2a	577	G
32	2a	588	G
32	2a	596	C
32	2a	630	G
32	2a	653	A
32	2a	656	C
32	2a	665	A
32	2a	672	U
32	2a	688	G
32	2a	695	A
32	2a	702	A
32	2a	703	G
32	2a	721	G
32	2a	723	U
32	2a	724	G
32	2a	731	G
32	2a	749	C
32	2a	755	G

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
32	2a	777	A
32	2a	793	U
32	2a	794	A
32	2a	816	A
32	2a	817	C
32	2a	821	G
32	2a	828	A
32	2a	833	U
32	2a	838	G
32	2a	840	C
32	2a	841	U
32	2a	853	G
32	2a	859	A
32	2a	873	A
32	2a	881	G
32	2a	885	G
32	2a	902	G
32	2a	914	A
32	2a	926	G
32	2a	927	G
32	2a	930	C
32	2a	931	C
32	2a	932	C
32	2a	934	C
32	2a	935	A
32	2a	960	U
32	2a	961	U
32	2a	968	A
32	2a	969	A
32	2a	971	G
32	2a	974	A
32	2a	975	A
32	2a	976	G
32	2a	977	A
32	2a	982	U
32	2a	984	C
32	2a	989	C
32	2a	992	U
32	2a	993	G
32	2a	997	U
32	2a	999	C
32	2a	1001	A

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
32	2a	1001(A)	G
32	2a	1002	G
32	2a	1003	G
32	2a	1005	A
32	2a	1006	C
32	2a	1009	G
32	2a	1016	A
32	2a	1020	U
32	2a	1021	G
32	2a	1022	G
32	2a	1023	G
32	2a	1025	U
32	2a	1026	G
32	2a	1027	C
32	2a	1029	C
32	2a	1030(A)	G
32	2a	1031	G
32	2a	1032	G
32	2a	1033	G
32	2a	1034	G
32	2a	1036	G
32	2a	1037	C
32	2a	1038	C
32	2a	1039	C
32	2a	1040	U
32	2a	1045	C
32	2a	1055	A
32	2a	1065	U
32	2a	1066	C
32	2a	1068	G
32	2a	1077	G
32	2a	1079	G
32	2a	1081	G
32	2a	1094	G
32	2a	1095	U
32	2a	1101	A
32	2a	1108	G
32	2a	1113	C
32	2a	1115	C
32	2a	1117	G
32	2a	1121	U
32	2a	1122	U

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
32	2a	1125	U
32	2a	1129	C
32	2a	1130	A
32	2a	1136	U
32	2a	1137	C
32	2a	1138	G
32	2a	1139	G
32	2a	1146	A
32	2a	1147	C
32	2a	1152	A
32	2a	1154	G
32	2a	1157	A
32	2a	1158	C
32	2a	1159	U
32	2a	1160	G
32	2a	1161	C
32	2a	1163	C
32	2a	1172	C
32	2a	1182	G
32	2a	1183	A
32	2a	1184	G
32	2a	1191	A
32	2a	1192	C
32	2a	1196	U
32	2a	1197	G
32	2a	1202	G
32	2a	1204	A
32	2a	1209	C
32	2a	1211	U
32	2a	1212	U
32	2a	1213	A
32	2a	1214	C
32	2a	1227	A
32	2a	1236	A
32	2a	1238	A
32	2a	1240	U
32	2a	1241	G
32	2a	1256	A
32	2a	1257	U
32	2a	1260	C
32	2a	1262	C
32	2a	1264	C

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
32	2a	1267	C
32	2a	1270	C
32	2a	1272	G
32	2a	1273	G
32	2a	1277	C
32	2a	1278	U
32	2a	1279	A
32	2a	1280	A
32	2a	1286	A
32	2a	1287	A
32	2a	1290	G
32	2a	1294	G
32	2a	1302	U
32	2a	1303	C
32	2a	1305	G
32	2a	1313	U
32	2a	1319	A
32	2a	1320	C
32	2a	1323	G
32	2a	1340	A
32	2a	1346	A
32	2a	1347	G
32	2a	1358	U
32	2a	1363	C
32	2a	1364	U
32	2a	1368	G
32	2a	1370	G
32	2a	1378	C
32	2a	1419	G
32	2a	1442	G
32	2a	1442(A)	G
32	2a	1446	U
32	2a	1447	A
32	2a	1452	C
32	2a	1456	G
32	2a	1457	G
32	2a	1492	A
32	2a	1494	G
32	2a	1504	G
32	2a	1506	U
32	2a	1507	A
32	2a	1508	G

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
32	2a	1517	G
32	2a	1520	G
32	2a	1529	G
32	2a	1530	G
32	2a	1531	A
32	2a	1532	U
53	2v	13	A
53	2v	15	A
53	2v	19	U
54	2w	3	C
54	2w	5	G
54	2w	8	4SU
54	2w	13	C
54	2w	14	A
54	2w	19	G
54	2w	22	G
54	2w	26	A
54	2w	29	G
54	2w	38	A
54	2w	46	7MG
54	2w	47	U
54	2w	48	C
54	2w	62	C
54	2w	64	A
54	2w	66	U
54	2w	68	C
54	2w	69	G
54	2w	70	G
54	2w	73	A
55	2x	9	G
55	2x	18	G
55	2x	21	A
55	2x	22	G
55	2x	47	U
55	2x	48	C
55	2x	52	G
55	2x	53	G
55	2x	61	C
55	2x	67	C
55	2x	68	C
55	2x	76	A
54	2y	5	G

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Mol	Chain	Res	Type
54	2y	8	4SU
54	2y	13	C
54	2y	14	A
54	2y	19	G
54	2y	22	G
54	2y	27	G
54	2y	35	A
54	2y	44	G
54	2y	45	U
54	2y	46	7MG
54	2y	47	U
54	2y	48	C
54	2y	49	C
54	2y	53	G
54	2y	58	A
54	2y	61	C
54	2y	65	G
54	2y	69	G
54	2y	70	G
54	2y	73	A

All (50) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	1A	115	G
1	1A	271	U
1	1A	302	A
1	1A	509	A
1	1A	572	A
1	1A	913	A
1	1A	941	U
1	1A	1065	U
1	1A	1067	A
1	1A	1093	G
1	1A	1201	A
1	1A	1219	A
1	1A	1220	U
1	1A	1221	G
1	1A	1255	A
1	1A	1321	A
1	1A	1466	U
1	1A	1554	A

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Mol	Chain	Res	Type
1	1A	1654	A
1	1A	1700	G
1	1A	1710	C
1	1A	2014	G
1	1A	2156	A
1	1A	2203	G
1	1A	2205	C
1	1A	2418	U
1	1A	2641	A
1	1A	2701	U
1	1A	2769	U
2	1B	1	U
1	2A	195	A
1	2A	228	A
1	2A	266	G
1	2A	271(K)	U
1	2A	271(M)	G
1	2A	277	C
1	2A	528	A
1	2A	752	A
1	2A	827	U
1	2A	856	C
1	2A	900	A
1	2A	1210	A
1	2A	1379	A
1	2A	1420	U
1	2A	1442	G
1	2A	1530	C
1	2A	1653	G
1	2A	1913	A
1	2A	1992	G
1	2A	2689	U

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

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

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

RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
32	UR3	2a	1498	32	19,22,23	1.03	1 (5%)	26,32,35	1.50	1 (3%)
54	PSU	2w	32	54	18,21,22	1.32	2 (11%)	22,30,33	1.85	3 (13%)
32	M2G	2a	966	32	20,27,28	1.42	3 (15%)	22,40,43	1.01	2 (9%)
32	5MC	2a	1407	32	18,22,23	0.95	2 (11%)	26,32,35	1.15	3 (11%)
32	7MG	2a	527	56,32	22,26,27	1.34	4 (18%)	29,39,42	2.51	7 (24%)
1	2MU	2A	2552	1,56	19,22,24	1.28	2 (10%)	26,31,36	1.69	5 (19%)
1	PSU	1A	1933	1	18,21,22	1.35	2 (11%)	22,30,33	1.86	3 (13%)
43	0TD	1l	92	43	7,9,10	4.71	1 (14%)	6,11,13	4.76	2 (33%)
54	MIA	1y	37	54	18,24,32	1.10	2 (11%)	18,35,47	1.26	2 (11%)
32	2MG	1a	1207	32	18,26,27	0.95	1 (5%)	16,38,41	1.06	1 (6%)
55	5MC	2x	32	55	18,22,23	1.01	2 (11%)	26,32,35	1.21	3 (11%)
54	4SU	2w	8	54	18,21,22	1.70	4 (22%)	26,30,33	2.32	5 (19%)
55	5MC	1x	32	55	18,22,23	0.98	2 (11%)	26,32,35	1.15	2 (7%)
54	5MU	1y	54	54	19,22,23	1.44	6 (31%)	28,32,35	2.04	6 (21%)
32	MA6	1a	1518	32	18,26,27	0.97	1 (5%)	19,38,41	1.64	6 (31%)
55	5MU	1x	54	56,55	19,22,23	1.39	5 (26%)	28,32,35	1.94	7 (25%)
55	4SU	1x	8	55	18,21,22	2.00	5 (27%)	26,30,33	1.63	5 (19%)
32	MA6	2a	1518	32	18,26,27	1.00	1 (5%)	19,38,41	1.64	4 (21%)
54	PSU	2y	32	54	18,21,22	1.35	2 (11%)	22,30,33	1.82	3 (13%)
1	PSU	1A	2617	1,56	18,21,22	1.35	2 (11%)	22,30,33	1.81	3 (13%)
55	PSU	2x	55	56,55	18,21,22	1.34	2 (11%)	22,30,33	1.88	3 (13%)
55	4SU	2x	8	55	18,21,22	1.93	6 (33%)	26,30,33	1.70	6 (23%)
1	5MC	1A	1964	1,56	18,22,23	0.93	2 (11%)	26,32,35	1.12	2 (7%)
32	5MC	1a	1404	32	18,22,23	0.97	2 (11%)	26,32,35	1.13	2 (7%)
32	5MC	2a	1400	32	18,22,23	0.95	2 (11%)	26,32,35	1.16	2 (7%)
54	5MU	2y	54	54	19,22,23	1.46	5 (26%)	28,32,35	1.73	7 (25%)
32	4OC	1a	1402	32	20,23,24	0.74	0	26,32,35	0.91	1 (3%)
54	PSU	1y	32	54	18,21,22	1.35	2 (11%)	22,30,33	1.83	3 (13%)
32	UR3	1a	1498	32	19,22,23	0.98	1 (5%)	26,32,35	1.39	1 (3%)
54	7MG	1w	46	54	22,26,27	1.43	4 (18%)	29,39,42	2.48	7 (24%)
32	5MC	1a	967	32	18,22,23	0.97	2 (11%)	26,32,35	1.19	3 (11%)
54	PSU	1w	39	54	18,21,22	1.31	2 (11%)	22,30,33	1.92	3 (13%)
54	PSU	1y	55	54	18,21,22	1.37	2 (11%)	22,30,33	1.91	3 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
32	5MC	1a	1400	32	18,22,23	0.97	2 (11%)	26,32,35	1.16	3 (11%)
32	PSU	1a	516	56,32	18,21,22	1.35	2 (11%)	22,30,33	1.90	4 (18%)
54	PSU	2y	39	54	18,21,22	1.26	2 (11%)	22,30,33	2.03	4 (18%)
32	5MC	2a	967	32	18,22,23	0.97	2 (11%)	26,32,35	1.12	2 (7%)
1	PSU	2A	1911	1	18,21,22	1.32	2 (11%)	22,30,33	1.84	3 (13%)
1	5MC	2A	1942	1	18,22,23	0.96	2 (11%)	26,32,35	1.14	2 (7%)
1	5MU	2A	1915	1	19,22,23	1.47	6 (31%)	28,32,35	2.07	6 (21%)
1	5MU	2A	1939	1,56	19,22,23	1.41	6 (31%)	28,32,35	2.13	6 (21%)
32	5MC	2a	1404	32	18,22,23	0.97	2 (11%)	26,32,35	1.20	3 (11%)
1	2MA	1A	2515	1,56	17,25,26	0.95	1 (5%)	17,37,40	0.99	2 (11%)
32	M2G	1a	966	32	20,27,28	1.45	3 (15%)	22,40,43	0.95	2 (9%)
32	MA6	1a	1519	32	18,26,27	1.05	1 (5%)	19,38,41	1.61	4 (21%)
54	4SU	1y	8	54	18,21,22	1.68	4 (22%)	26,30,33	2.15	4 (15%)
1	5MU	1A	1961	1,56	19,22,23	1.42	6 (31%)	28,32,35	2.19	6 (21%)
54	PSU	2w	39	54	18,21,22	1.34	2 (11%)	22,30,33	1.75	3 (13%)
32	5MC	1a	1407	32	18,22,23	0.91	2 (11%)	26,32,35	1.14	2 (7%)
54	PSU	2w	55	54	18,21,22	1.36	2 (11%)	22,30,33	1.88	3 (13%)
54	7MG	1y	46	54	22,26,27	1.35	3 (13%)	29,39,42	2.60	6 (20%)
1	4OC	1A	1942	1	19,22,24	0.81	0	26,31,35	0.95	1 (3%)
1	2MA	2A	2503	1,56	17,25,26	0.98	1 (5%)	17,37,40	0.97	2 (11%)
32	2MG	2a	1207	32	18,26,27	0.88	1 (5%)	16,38,41	1.18	2 (12%)
54	PSU	1w	55	54	18,21,22	1.36	2 (11%)	22,30,33	1.90	3 (13%)
55	5MU	2x	54	55	19,22,23	1.41	5 (26%)	28,32,35	2.16	6 (21%)
1	OMG	1A	2263	1,56,55	18,26,27	0.95	1 (5%)	19,38,41	1.12	2 (10%)
54	PSU	1w	32	54	18,21,22	1.35	2 (11%)	22,30,33	1.78	3 (13%)
1	OMG	2A	2251	1,56,55	18,26,27	0.95	1 (5%)	19,38,41	1.04	2 (10%)
1	PSU	2A	1917	1	18,21,22	1.33	2 (11%)	22,30,33	1.87	3 (13%)
54	MIA	2w	37	54	20,27,32	1.78	3 (15%)	22,39,47	1.83	7 (31%)
1	5MC	1A	1984	1	18,22,23	0.97	2 (11%)	26,32,35	1.11	2 (7%)
1	PSU	2A	2605	1	18,21,22	1.34	2 (11%)	22,30,33	1.87	4 (18%)
1	2MU	1A	2564	1,56	19,22,24	1.29	3 (15%)	26,31,36	1.75	6 (23%)
54	MIA	1w	37	54	24,31,32	2.23	3 (12%)	26,44,47	2.56	10 (38%)
54	MIA	2y	37	54	18,24,32	1.09	2 (11%)	18,35,47	1.32	2 (11%)
32	PSU	2a	516	32	18,21,22	1.33	2 (11%)	22,30,33	1.84	4 (18%)
54	5MU	1w	54	54	19,22,23	1.40	5 (26%)	28,32,35	1.99	6 (21%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
1	5MU	1A	1937	1	19,22,23	1.43	5 (26%)	28,32,35	2.02	6 (21%)
1	4OC	2A	1920	1	19,22,24	0.81	0	26,31,35	0.86	0
32	4OC	2a	1402	32	20,23,24	0.80	0	26,32,35	1.05	2 (7%)
32	MA6	2a	1519	32	18,26,27	1.01	1 (5%)	19,38,41	1.57	4 (21%)
1	5MC	2A	1962	1,56	18,22,23	0.97	2 (11%)	26,32,35	1.10	2 (7%)
54	4SU	2y	8	54,56	18,21,22	1.76	5 (27%)	26,30,33	2.10	4 (15%)
54	PSU	1y	39	54	18,21,22	1.32	2 (11%)	22,30,33	1.95	3 (13%)
54	4SU	1w	8	54	18,21,22	1.78	5 (27%)	26,30,33	1.95	5 (19%)
54	7MG	2w	46	54	22,26,27	1.35	4 (18%)	29,39,42	2.52	7 (24%)
54	5MU	2w	54	54	19,22,23	1.36	5 (26%)	28,32,35	1.97	7 (25%)
55	PSU	1x	55	55	18,21,22	1.35	2 (11%)	22,30,33	1.89	3 (13%)
43	0TD	2l	92	43	7,9,10	4.85	1 (14%)	6,11,13	5.20	3 (50%)
54	7MG	2y	46	54	22,26,27	1.35	3 (13%)	29,39,42	2.67	8 (27%)
54	PSU	2y	55	54	18,21,22	1.33	2 (11%)	22,30,33	1.91	3 (13%)
1	PSU	1A	1939	1	18,21,22	1.34	2 (11%)	22,30,33	1.89	3 (13%)
32	7MG	1a	527	56,32	22,26,27	1.34	4 (18%)	29,39,42	2.48	7 (24%)

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	UR3	2a	1498	32	-	0/7/25/26	0/2/2/2
54	PSU	2w	32	54	-	0/7/25/26	0/2/2/2
32	M2G	2a	966	32	-	0/7/29/30	0/3/3/3
32	5MC	2a	1407	32	-	0/7/25/26	0/2/2/2
32	7MG	2a	527	56,32	-	2/7/37/38	0/3/3/3
1	2MU	2A	2552	1,56	-	0/9/27/28	0/2/2/2
1	PSU	1A	1933	1	-	0/7/25/26	0/2/2/2
43	0TD	1l	92	43	-	3/7/12/14	-
54	MIA	1y	37	54	-	2/3/25/34	0/3/3/3
32	2MG	1a	1207	32	-	1/5/27/28	0/3/3/3
55	5MC	2x	32	55	-	0/7/25/26	0/2/2/2
54	4SU	2w	8	54	-	1/7/25/26	0/2/2/2
55	5MC	1x	32	55	-	0/7/25/26	0/2/2/2
54	5MU	1y	54	54	-	0/7/25/26	0/2/2/2
32	MA6	1a	1518	32	-	2/7/29/30	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
55	5MU	1x	54	56,55	-	0/7/25/26	0/2/2/2
55	4SU	1x	8	55	-	0/7/25/26	0/2/2/2
32	MA6	2a	1518	32	-	3/7/29/30	0/3/3/3
54	PSU	2y	32	54	-	0/7/25/26	0/2/2/2
1	PSU	1A	2617	1,56	-	0/7/25/26	0/2/2/2
55	PSU	2x	55	56,55	-	0/7/25/26	0/2/2/2
55	4SU	2x	8	55	-	1/7/25/26	0/2/2/2
1	5MC	1A	1964	1,56	-	0/7/25/26	0/2/2/2
32	5MC	1a	1404	32	-	0/7/25/26	0/2/2/2
32	5MC	2a	1400	32	-	0/7/25/26	0/2/2/2
54	5MU	2y	54	54	-	0/7/25/26	0/2/2/2
32	4OC	1a	1402	32	-	2/9/29/30	0/2/2/2
54	PSU	1y	32	54	-	0/7/25/26	0/2/2/2
32	UR3	1a	1498	32	-	0/7/25/26	0/2/2/2
54	7MG	1w	46	54	-	3/7/37/38	0/3/3/3
32	5MC	1a	967	32	-	2/7/25/26	0/2/2/2
54	PSU	1w	39	54	-	0/7/25/26	0/2/2/2
54	PSU	1y	55	54	-	2/7/25/26	0/2/2/2
32	5MC	1a	1400	32	-	0/7/25/26	0/2/2/2
32	PSU	1a	516	56,32	-	0/7/25/26	0/2/2/2
54	PSU	2y	39	54	-	0/7/25/26	0/2/2/2
32	5MC	2a	967	32	-	1/7/25/26	0/2/2/2
1	PSU	2A	1911	1	-	0/7/25/26	0/2/2/2
1	5MC	2A	1942	1	-	0/7/25/26	0/2/2/2
1	5MU	2A	1915	1	-	0/7/25/26	0/2/2/2
1	5MU	2A	1939	1,56	-	0/7/25/26	0/2/2/2
32	5MC	2a	1404	32	-	0/7/25/26	0/2/2/2
1	2MA	1A	2515	1,56	-	2/3/25/26	0/3/3/3
32	M2G	1a	966	32	-	0/7/29/30	0/3/3/3
32	MA6	1a	1519	32	-	3/7/29/30	0/3/3/3
54	4SU	1y	8	54	-	3/7/25/26	0/2/2/2
1	5MU	1A	1961	1,56	-	0/7/25/26	0/2/2/2
54	PSU	2w	39	54	-	0/7/25/26	0/2/2/2
32	5MC	1a	1407	32	-	0/7/25/26	0/2/2/2
54	PSU	2w	55	54	-	0/7/25/26	0/2/2/2
54	7MG	1y	46	54	-	2/7/37/38	0/3/3/3
1	4OC	1A	1942	1	-	1/9/27/30	0/2/2/2
1	2MA	2A	2503	1,56	-	2/3/25/26	0/3/3/3
32	2MG	2a	1207	32	-	2/5/27/28	0/3/3/3
54	PSU	1w	55	54	-	0/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
55	5MU	2x	54	55	-	0/7/25/26	0/2/2/2
1	OMG	1A	2263	1,56,55	-	0/5/27/28	0/3/3/3
54	PSU	1w	32	54	-	0/7/25/26	0/2/2/2
1	OMG	2A	2251	1,56,55	-	1/5/27/28	0/3/3/3
1	PSU	2A	1917	1	-	0/7/25/26	0/2/2/2
54	MIA	2w	37	54	-	2/7/29/34	0/3/3/3
1	5MC	1A	1984	1	-	0/7/25/26	0/2/2/2
1	PSU	2A	2605	1	-	0/7/25/26	0/2/2/2
1	2MU	1A	2564	1,56	-	0/9/27/28	0/2/2/2
54	MIA	1w	37	54	-	1/11/33/34	0/3/3/3
54	MIA	2y	37	54	-	2/3/25/34	0/3/3/3
32	PSU	2a	516	32	-	0/7/25/26	0/2/2/2
54	5MU	1w	54	54	-	0/7/25/26	0/2/2/2
1	5MU	1A	1937	1	-	0/7/25/26	0/2/2/2
1	4OC	2A	1920	1	-	2/9/27/30	0/2/2/2
32	4OC	2a	1402	32	-	2/9/29/30	0/2/2/2
32	MA6	2a	1519	32	-	5/7/29/30	0/3/3/3
1	5MC	2A	1962	1,56	-	1/7/25/26	0/2/2/2
54	4SU	2y	8	54,56	-	2/7/25/26	0/2/2/2
54	PSU	1y	39	54	-	0/7/25/26	0/2/2/2
54	4SU	1w	8	54	-	0/7/25/26	0/2/2/2
54	7MG	2w	46	54	-	4/7/37/38	0/3/3/3
54	5MU	2w	54	54	-	0/7/25/26	0/2/2/2
55	PSU	1x	55	55	-	0/7/25/26	0/2/2/2
43	0TD	2l	92	43	-	2/7/12/14	-
54	7MG	2y	46	54	-	3/7/37/38	0/3/3/3
54	PSU	2y	55	54	-	2/7/25/26	0/2/2/2
1	PSU	1A	1939	1	-	0/7/25/26	0/2/2/2
32	7MG	1a	527	56,32	-	2/7/37/38	0/3/3/3

All (212) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
43	2l	92	0TD	CB-SB	-12.55	1.69	1.82
43	1l	92	0TD	CB-SB	-12.15	1.69	1.82
54	1w	37	MIA	C13-C14	7.14	1.52	1.32
54	1w	37	MIA	C2-S10	-6.84	1.69	1.75
54	2w	37	MIA	C2-S10	-6.53	1.70	1.75
54	2y	8	4SU	C4-S4	-4.57	1.59	1.68
32	1a	966	M2G	C2-N3	4.55	1.36	1.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	2a	966	M2G	C2-N3	4.54	1.36	1.30
54	1w	8	4SU	C4-S4	-4.47	1.59	1.68
54	2w	8	4SU	C4-S4	-4.43	1.60	1.68
55	1x	8	4SU	C4-S4	-4.42	1.60	1.68
55	2x	8	4SU	C4-S4	-4.42	1.60	1.68
54	1y	8	4SU	C4-S4	-4.30	1.60	1.68
55	1x	8	4SU	C4-N3	-4.29	1.33	1.37
55	2x	8	4SU	C4-N3	-3.98	1.33	1.37
54	2w	55	PSU	C6-C5	3.63	1.39	1.35
54	1w	55	PSU	C6-C5	3.62	1.39	1.35
54	1y	32	PSU	C6-C5	3.54	1.39	1.35
54	2y	32	PSU	C6-C5	3.47	1.39	1.35
54	2y	55	PSU	C6-C5	3.45	1.39	1.35
54	1y	55	PSU	C6-C5	3.43	1.39	1.35
55	1x	55	PSU	C6-C5	3.39	1.39	1.35
54	2w	39	PSU	C6-C5	3.38	1.39	1.35
54	1w	46	7MG	C4-N9	-3.36	1.33	1.37
54	1y	39	PSU	C6-C5	3.34	1.39	1.35
55	2x	55	PSU	C6-C5	3.34	1.39	1.35
1	1A	1939	PSU	C6-C5	3.33	1.39	1.35
32	2a	516	PSU	C6-C5	3.29	1.39	1.35
54	1w	8	4SU	C4-N3	-3.28	1.34	1.37
54	2w	32	PSU	C6-C5	3.27	1.39	1.35
54	2y	46	7MG	C5-C4	3.26	1.48	1.38
1	1A	1933	PSU	C6-C5	3.25	1.39	1.35
1	2A	1911	PSU	C6-C5	3.24	1.39	1.35
1	2A	1917	PSU	C6-C5	3.23	1.39	1.35
55	1x	8	4SU	C2-N3	-3.22	1.32	1.38
54	1w	39	PSU	C6-C5	3.22	1.39	1.35
54	1y	46	7MG	C5-C4	3.22	1.48	1.38
54	1w	32	PSU	C6-C5	3.21	1.39	1.35
32	1a	516	PSU	C6-C5	3.20	1.39	1.35
55	1x	8	4SU	C5-C4	-3.15	1.38	1.42
54	2y	8	4SU	C4-N3	-3.13	1.34	1.37
1	2A	2605	PSU	C6-C5	3.11	1.38	1.35
54	1y	8	4SU	C4-N3	-3.11	1.34	1.37
54	2y	39	PSU	C6-C5	3.10	1.38	1.35
54	1w	46	7MG	C5-C4	3.09	1.48	1.38
32	1a	527	7MG	C5-C4	3.08	1.48	1.38
1	2A	1915	5MU	C6-C5	3.08	1.39	1.34
55	2x	8	4SU	C5-C4	-3.06	1.38	1.42
32	2a	527	7MG	C4-N9	-3.00	1.34	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
54	2w	46	7MG	C4-N9	-2.99	1.34	1.37
54	2w	46	7MG	C5-C4	2.99	1.47	1.38
1	1A	2617	PSU	C6-C5	2.98	1.38	1.35
32	2a	527	7MG	C5-C4	2.94	1.47	1.38
32	2a	1404	5MC	C6-C5	2.91	1.39	1.34
55	2x	32	5MC	C6-C5	2.90	1.39	1.34
55	1x	32	5MC	C6-C5	2.89	1.39	1.34
54	1y	54	5MU	C6-C5	2.89	1.39	1.34
1	1A	2564	2MU	C4-N3	-2.87	1.33	1.38
1	1A	1961	5MU	C4-N3	-2.87	1.33	1.38
32	1a	966	M2G	C2-N2	2.85	1.40	1.35
1	1A	1937	5MU	C6-C5	2.85	1.39	1.34
55	2x	54	5MU	C6-C5	2.82	1.39	1.34
32	1a	1404	5MC	C6-C5	2.82	1.39	1.34
1	1A	1961	5MU	C6-C5	2.81	1.39	1.34
32	1a	1400	5MC	C6-C5	2.80	1.39	1.34
54	2w	8	4SU	C4-N3	-2.79	1.34	1.37
54	1w	54	5MU	C6-C5	2.79	1.39	1.34
32	2a	967	5MC	C6-C5	2.79	1.39	1.34
1	2A	2605	PSU	C4-N3	-2.77	1.33	1.38
1	1A	1984	5MC	C6-C5	2.76	1.39	1.34
54	2y	54	5MU	C6-C5	2.76	1.39	1.34
32	1a	527	7MG	C4-N9	-2.75	1.34	1.37
1	2A	1962	5MC	C6-C5	2.75	1.39	1.34
1	2A	1942	5MC	C6-C5	2.74	1.39	1.34
1	1A	2617	PSU	C4-N3	-2.73	1.33	1.38
54	2w	54	5MU	C6-C5	2.73	1.39	1.34
1	2A	1939	5MU	C6-C5	2.73	1.39	1.34
32	1a	967	5MC	C6-C5	2.71	1.39	1.34
54	2y	8	4SU	C5-C4	-2.70	1.39	1.42
1	2A	1939	5MU	C4-N3	-2.70	1.33	1.38
32	2a	1400	5MC	C6-C5	2.69	1.39	1.34
32	2a	1518	MA6	C5-C4	2.69	1.48	1.40
1	2A	1915	5MU	C4-N3	-2.68	1.33	1.38
54	2y	54	5MU	C4-N3	-2.67	1.33	1.38
54	1y	54	5MU	C4-N3	-2.66	1.33	1.38
54	2y	54	5MU	C2-N1	2.66	1.42	1.38
54	1w	8	4SU	C5-C4	-2.65	1.39	1.42
1	1A	1964	5MC	C6-C5	2.64	1.38	1.34
32	2a	1519	MA6	C5-C4	2.64	1.47	1.40
54	2w	8	4SU	C5-C4	-2.63	1.39	1.42
1	2A	2552	2MU	C4-N3	-2.62	1.33	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
54	2y	37	MIA	C5-C4	2.62	1.47	1.40
32	2a	966	M2G	C2-N2	2.61	1.40	1.35
32	1a	516	PSU	C4-N3	-2.61	1.34	1.38
55	1x	54	5MU	C6-C5	2.61	1.38	1.34
1	1A	1937	5MU	C4-N3	-2.61	1.34	1.38
1	2A	1915	5MU	C4-C5	2.60	1.49	1.44
32	1a	1519	MA6	C5-C4	2.60	1.47	1.40
54	1y	37	MIA	C5-C4	2.60	1.47	1.40
54	1w	54	5MU	C4-N3	-2.60	1.34	1.38
1	1A	1933	PSU	C4-N3	-2.59	1.34	1.38
54	1w	37	MIA	C5-C4	2.59	1.47	1.40
32	2a	1407	5MC	C6-C5	2.59	1.38	1.34
1	1A	1939	PSU	C4-N3	-2.58	1.34	1.38
55	1x	54	5MU	C4-N3	-2.58	1.34	1.38
54	1w	46	7MG	C6-N1	-2.57	1.34	1.38
32	1a	966	M2G	C6-N1	-2.56	1.34	1.37
54	1w	32	PSU	C4-N3	-2.56	1.34	1.38
32	1a	1207	2MG	C6-N1	-2.55	1.34	1.37
54	1y	37	MIA	C2-N3	2.55	1.36	1.32
54	2y	55	PSU	C4-N3	-2.55	1.34	1.38
54	2w	39	PSU	C4-N3	-2.55	1.34	1.38
54	1y	55	PSU	C4-N3	-2.54	1.34	1.38
1	2A	1917	PSU	C4-N3	-2.54	1.34	1.38
54	2y	37	MIA	C2-N3	2.53	1.36	1.32
55	2x	54	5MU	C4-N3	-2.52	1.34	1.38
54	2w	8	4SU	C2-N1	2.52	1.42	1.38
54	2w	37	MIA	C5-C4	2.51	1.47	1.40
54	1y	39	PSU	C4-N3	-2.51	1.34	1.38
32	1a	1407	5MC	C6-C5	2.50	1.38	1.34
1	2A	1911	PSU	C4-N3	-2.50	1.34	1.38
54	1y	54	5MU	C4-C5	2.49	1.48	1.44
55	2x	55	PSU	C4-N3	-2.49	1.34	1.38
54	2w	55	PSU	C4-N3	-2.48	1.34	1.38
1	2A	2251	OMG	C6-N1	-2.47	1.34	1.37
55	2x	8	4SU	C2-N3	-2.47	1.33	1.38
54	2w	32	PSU	C4-N3	-2.46	1.34	1.38
1	1A	1937	5MU	C2-N1	2.45	1.42	1.38
32	1a	1518	MA6	C5-C4	2.43	1.47	1.40
54	1y	32	PSU	C4-N3	-2.43	1.34	1.38
54	1w	39	PSU	C4-N3	-2.43	1.34	1.38
32	2a	516	PSU	C4-N3	-2.42	1.34	1.38
55	2x	54	5MU	C4-C5	2.42	1.48	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
54	2w	54	5MU	C4-N3	-2.42	1.34	1.38
54	1y	46	7MG	C6-N1	-2.41	1.34	1.38
55	1x	55	PSU	C4-N3	-2.41	1.34	1.38
54	2y	32	PSU	C4-N3	-2.40	1.34	1.38
32	2a	966	M2G	C6-N1	-2.40	1.34	1.37
54	2y	46	7MG	C6-N1	-2.40	1.34	1.38
54	1w	54	5MU	C4-C5	2.39	1.48	1.44
54	2w	54	5MU	C4-C5	2.38	1.48	1.44
1	1A	1937	5MU	C4-C5	2.37	1.48	1.44
1	2A	2552	2MU	C5-C4	2.37	1.48	1.43
54	2w	46	7MG	C8-N9	2.36	1.47	1.46
1	1A	1961	5MU	C2-N3	-2.34	1.33	1.38
55	2x	8	4SU	C2-N1	2.34	1.42	1.38
54	1w	55	PSU	C4-N3	-2.34	1.34	1.38
1	2A	1915	5MU	C2-N1	2.33	1.42	1.38
1	1A	2564	2MU	C2-N3	-2.32	1.33	1.38
54	1y	8	4SU	C5-C4	-2.32	1.39	1.42
1	1A	1984	5MC	C6-N1	-2.32	1.34	1.38
54	1y	46	7MG	C8-N9	2.32	1.47	1.46
1	2A	1939	5MU	C6-N1	-2.32	1.34	1.38
1	2A	1939	5MU	C4-C5	2.31	1.48	1.44
32	2a	527	7MG	C6-N1	-2.30	1.34	1.38
32	2a	1400	5MC	C6-N1	-2.29	1.34	1.38
1	1A	2564	2MU	C5-C4	2.29	1.48	1.43
1	1A	2263	OMG	C6-N1	-2.29	1.34	1.37
55	2x	54	5MU	C2-N1	2.28	1.42	1.38
54	2y	54	5MU	C4-C5	2.28	1.48	1.44
54	2y	46	7MG	C8-N9	2.27	1.47	1.46
55	1x	54	5MU	C4-C5	2.26	1.48	1.44
55	1x	54	5MU	C2-N1	2.25	1.42	1.38
32	1a	527	7MG	C6-N1	-2.25	1.34	1.38
32	1a	967	5MC	C6-N1	-2.24	1.34	1.38
32	2a	1207	2MG	C6-N1	-2.23	1.34	1.37
32	1a	1407	5MC	C6-N1	-2.23	1.34	1.38
1	2A	1962	5MC	C6-N1	-2.22	1.34	1.38
32	2a	1407	5MC	C6-N1	-2.22	1.34	1.38
54	2y	39	PSU	C4-N3	-2.22	1.34	1.38
1	1A	1961	5MU	C6-N1	-2.21	1.34	1.38
54	1w	8	4SU	C2-N1	2.21	1.42	1.38
54	2y	8	4SU	C2-N1	2.21	1.42	1.38
1	1A	1964	5MC	C6-N1	-2.21	1.34	1.38
54	1y	54	5MU	C2-N1	2.21	1.42	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
55	1x	32	5MC	C6-N1	-2.20	1.34	1.38
54	1y	8	4SU	C2-N1	2.20	1.42	1.38
1	2A	1942	5MC	C6-N1	-2.19	1.34	1.38
1	1A	1961	5MU	C4-C5	2.18	1.48	1.44
55	2x	54	5MU	C6-N1	-2.17	1.34	1.38
32	1a	1404	5MC	C6-N1	-2.17	1.34	1.38
32	2a	1404	5MC	C6-N1	-2.16	1.34	1.38
54	1y	54	5MU	C6-N1	-2.16	1.34	1.38
54	2w	37	MIA	C6-N1	2.16	1.35	1.32
32	1a	1400	5MC	C6-N1	-2.15	1.34	1.38
1	2A	2503	2MA	C2-N3	2.14	1.35	1.31
32	2a	1498	UR3	C2-N1	2.13	1.41	1.38
55	1x	54	5MU	C6-N1	-2.13	1.34	1.38
54	1w	8	4SU	C2-N3	-2.13	1.34	1.38
1	2A	1915	5MU	C6-N1	-2.12	1.34	1.38
1	2A	1939	5MU	C2-N1	2.12	1.41	1.38
54	1w	54	5MU	C2-N1	2.11	1.41	1.38
1	1A	2515	2MA	C2-N3	2.10	1.35	1.31
54	2w	54	5MU	C6-N1	-2.10	1.34	1.38
54	1w	46	7MG	C8-N9	2.08	1.47	1.46
54	1w	54	5MU	C6-N1	-2.08	1.34	1.38
1	2A	1939	5MU	C2-N3	-2.07	1.34	1.38
32	2a	967	5MC	C6-N1	-2.07	1.34	1.38
1	1A	1937	5MU	C6-N1	-2.07	1.34	1.38
32	1a	1498	UR3	C6-C5	2.06	1.39	1.35
55	2x	8	4SU	O2-C2	2.06	1.26	1.23
54	1y	54	5MU	C2-N3	-2.05	1.34	1.38
1	2A	1915	5MU	C2-N3	-2.05	1.34	1.38
32	2a	527	7MG	C8-N9	2.05	1.47	1.46
55	1x	8	4SU	C2-N1	2.05	1.41	1.38
1	1A	1961	5MU	C2-N1	2.05	1.41	1.38
54	2w	46	7MG	C6-N1	-2.04	1.35	1.38
55	2x	32	5MC	C6-N1	-2.03	1.34	1.38
32	1a	527	7MG	C8-N9	2.03	1.47	1.46
54	2y	54	5MU	C2-N3	-2.03	1.34	1.38
54	2y	8	4SU	C2-N3	-2.01	1.34	1.38
54	2w	54	5MU	C2-N1	2.00	1.41	1.38

All (313) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
43	2l	92	0TD	CSB-SB-CB	-11.92	80.88	102.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
43	1l	92	0TD	CSB-SB-CB	-10.99	82.56	102.44
54	2y	46	7MG	N9-C4-N3	9.91	140.30	125.47
54	1y	46	7MG	N9-C4-N3	9.56	139.78	125.47
54	1w	46	7MG	N9-C4-N3	8.91	138.79	125.47
32	1a	527	7MG	N9-C4-N3	8.72	138.51	125.47
32	2a	527	7MG	N9-C4-N3	8.68	138.45	125.47
54	2w	46	7MG	N9-C4-N3	8.65	138.41	125.47
54	1w	37	MIA	C12-C13-C14	-8.10	111.38	127.14
54	2w	8	4SU	C4-N3-C2	-7.02	120.52	127.34
54	1y	8	4SU	C4-N3-C2	-6.72	120.81	127.34
32	2a	1498	UR3	C4-N3-C2	-6.34	118.59	124.56
54	2y	39	PSU	N1-C2-N3	6.22	122.17	115.13
54	2y	8	4SU	C4-N3-C2	-6.17	121.34	127.34
54	1y	55	PSU	N1-C2-N3	6.11	122.05	115.13
54	1y	39	PSU	N1-C2-N3	6.05	121.99	115.13
54	2y	55	PSU	N1-C2-N3	6.04	121.98	115.13
55	1x	55	PSU	N1-C2-N3	6.03	121.96	115.13
32	1a	516	PSU	N1-C2-N3	6.03	121.96	115.13
55	2x	55	PSU	N1-C2-N3	5.97	121.89	115.13
54	1w	39	PSU	N1-C2-N3	5.95	121.87	115.13
54	2y	46	7MG	C5-C4-N3	-5.90	116.88	128.13
1	2A	1917	PSU	N1-C2-N3	5.90	121.81	115.13
54	2y	8	4SU	C5-C4-N3	5.89	120.15	114.69
54	1w	55	PSU	N1-C2-N3	5.87	121.78	115.13
54	2w	8	4SU	C5-C4-N3	5.86	120.12	114.69
1	1A	1939	PSU	N1-C2-N3	5.85	121.76	115.13
54	2w	55	PSU	N1-C2-N3	5.84	121.75	115.13
54	1y	46	7MG	C5-C4-N3	-5.84	117.00	128.13
54	2w	32	PSU	N1-C2-N3	5.83	121.73	115.13
32	2a	516	PSU	N1-C2-N3	5.82	121.72	115.13
54	1y	32	PSU	N1-C2-N3	5.80	121.70	115.13
54	2y	32	PSU	N1-C2-N3	5.80	121.70	115.13
1	1A	1933	PSU	N1-C2-N3	5.78	121.68	115.13
1	2A	1911	PSU	N1-C2-N3	5.75	121.65	115.13
54	1w	32	PSU	N1-C2-N3	5.73	121.62	115.13
1	2A	2605	PSU	N1-C2-N3	5.72	121.61	115.13
54	1w	8	4SU	C5-C4-N3	5.66	119.94	114.69
32	1a	1498	UR3	C4-N3-C2	-5.63	119.26	124.56
1	1A	2617	PSU	N1-C2-N3	5.60	121.47	115.13
54	1w	8	4SU	C4-N3-C2	-5.57	121.93	127.34
1	1A	1961	5MU	C4-N3-C2	-5.57	120.15	127.35
54	1y	8	4SU	C5-C4-N3	5.52	119.81	114.69

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
55	2x	54	5MU	C4-N3-C2	-5.49	120.25	127.35
54	2w	39	PSU	N1-C2-N3	5.42	121.27	115.13
32	1a	527	7MG	C5-C4-N3	-5.41	117.83	128.13
32	2a	527	7MG	N9-C8-N7	-5.38	95.68	103.38
1	2A	1939	5MU	C4-N3-C2	-5.36	120.42	127.35
54	2w	46	7MG	C5-C4-N3	-5.30	118.03	128.13
1	2A	1915	5MU	C4-N3-C2	-5.29	120.50	127.35
1	2A	1915	5MU	N3-C2-N1	5.24	121.85	114.89
54	2w	46	7MG	N9-C8-N7	-5.23	95.89	103.38
32	2a	527	7MG	C5-C4-N3	-5.23	118.16	128.13
54	1w	46	7MG	N9-C8-N7	-5.23	95.90	103.38
1	1A	1961	5MU	N3-C2-N1	5.18	121.77	114.89
55	2x	54	5MU	N3-C2-N1	5.17	121.76	114.89
54	1y	54	5MU	C4-N3-C2	-5.09	120.77	127.35
1	1A	2564	2MU	N3-C2-N1	5.08	121.63	114.89
1	1A	1937	5MU	C4-N3-C2	-5.05	120.82	127.35
1	1A	1961	5MU	C5-C4-N3	5.01	119.58	115.31
54	1y	54	5MU	N3-C2-N1	4.98	121.50	114.89
32	1a	527	7MG	N9-C8-N7	-4.97	96.26	103.38
54	1w	54	5MU	C4-N3-C2	-4.94	120.95	127.35
1	1A	1937	5MU	N3-C2-N1	4.91	121.41	114.89
1	2A	2552	2MU	N3-C2-N1	4.90	121.40	114.89
1	2A	1939	5MU	N3-C2-N1	4.87	121.35	114.89
54	1w	54	5MU	N3-C2-N1	4.85	121.33	114.89
54	2w	54	5MU	C4-N3-C2	-4.82	121.11	127.35
1	2A	1939	5MU	C5-C4-N3	4.80	119.41	115.31
54	1w	46	7MG	C5-C4-N3	-4.74	119.10	128.13
55	2x	8	4SU	C5-C4-N3	4.69	119.04	114.69
55	1x	54	5MU	C4-N3-C2	-4.68	121.29	127.35
54	1y	46	7MG	N9-C8-N7	-4.68	96.68	103.38
54	2y	46	7MG	N9-C8-N7	-4.65	96.72	103.38
54	2w	54	5MU	N3-C2-N1	4.64	121.05	114.89
55	1x	54	5MU	N3-C2-N1	4.63	121.03	114.89
55	2x	54	5MU	C5-C4-N3	4.61	119.24	115.31
54	2y	46	7MG	C2-N3-C4	4.53	120.37	112.30
1	1A	1937	5MU	C5-C4-N3	4.51	119.16	115.31
55	1x	8	4SU	C5-C4-N3	4.50	118.86	114.69
54	1y	46	7MG	C2-N3-C4	4.49	120.30	112.30
54	2y	39	PSU	C4-N3-C2	-4.44	119.94	126.34
1	1A	1961	5MU	C5-C6-N1	-4.41	118.80	123.34
54	2w	46	7MG	C2-N3-C4	4.40	120.14	112.30
54	2w	37	MIA	C2-N3-C4	4.39	121.37	115.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	2A	1915	5MU	C5-C4-N3	4.39	119.05	115.31
54	1y	54	5MU	C5-C4-N3	4.34	119.02	115.31
32	2a	527	7MG	C2-N3-C4	4.30	119.97	112.30
54	1w	54	5MU	C5-C4-N3	4.29	118.97	115.31
32	1a	527	7MG	C2-N3-C4	4.28	119.93	112.30
1	1A	2564	2MU	C4-N3-C2	-4.28	120.94	126.58
54	2w	54	5MU	C5-C4-N3	4.27	118.96	115.31
1	2A	2552	2MU	C4-N3-C2	-4.25	120.97	126.58
54	1y	8	4SU	N3-C2-N1	4.24	120.52	114.89
54	1w	37	MIA	C2-N3-C4	4.23	121.15	115.32
54	1w	37	MIA	C15-C14-C13	-4.20	110.51	122.65
1	1A	1961	5MU	O4-C4-C5	-4.15	120.09	124.90
54	2w	8	4SU	N3-C2-N1	4.15	120.40	114.89
54	1y	39	PSU	C4-N3-C2	-4.12	120.40	126.34
55	2x	8	4SU	C1'-N1-C2	4.10	124.99	117.57
55	2x	54	5MU	O4-C4-C5	-4.09	120.16	124.90
1	2A	1915	5MU	C5-C6-N1	-4.09	119.14	123.34
1	2A	2605	PSU	C4-N3-C2	-4.08	120.46	126.34
55	1x	54	5MU	C5-C4-N3	4.06	118.77	115.31
1	2A	1939	5MU	C5-C6-N1	-4.04	119.18	123.34
1	2A	1939	5MU	O4-C4-C5	-4.02	120.24	124.90
54	2w	54	5MU	O4-C4-C5	-4.02	120.25	124.90
54	1w	39	PSU	C4-N3-C2	-4.01	120.57	126.34
1	1A	1939	PSU	C4-N3-C2	-4.00	120.58	126.34
54	2w	8	4SU	C5-C4-S4	-4.00	119.32	124.47
54	2y	39	PSU	O2-C2-N1	-3.97	118.42	122.79
54	2y	54	5MU	C5-C4-N3	3.95	118.68	115.31
54	2y	55	PSU	C4-N3-C2	-3.94	120.67	126.34
54	1w	37	MIA	C16-C14-C13	-3.91	111.35	122.65
32	1a	516	PSU	C4-N3-C2	-3.89	120.73	126.34
54	2w	32	PSU	C4-N3-C2	-3.86	120.77	126.34
1	2A	1917	PSU	C4-N3-C2	-3.83	120.82	126.34
32	2a	1400	5MC	C5-C6-N1	-3.83	119.40	123.34
54	1y	54	5MU	C5-C6-N1	-3.81	119.42	123.34
54	1w	55	PSU	O2-C2-N1	-3.81	118.60	122.79
54	1y	55	PSU	O2-C2-N1	-3.80	118.60	122.79
1	1A	1933	PSU	C4-N3-C2	-3.80	120.87	126.34
55	2x	55	PSU	C4-N3-C2	-3.79	120.87	126.34
55	2x	54	5MU	C5-C6-N1	-3.79	119.44	123.34
54	1w	46	7MG	C2-N3-C4	3.79	119.05	112.30
54	2y	8	4SU	C5-C4-S4	-3.78	119.59	124.47
1	2A	1911	PSU	C4-N3-C2	-3.78	120.89	126.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	2a	516	PSU	C4-N3-C2	-3.77	120.91	126.34
54	1w	54	5MU	O4-C4-C5	-3.77	120.54	124.90
1	1A	1937	5MU	O4-C4-C5	-3.75	120.56	124.90
54	1y	55	PSU	C4-N3-C2	-3.74	120.95	126.34
55	1x	55	PSU	C4-N3-C2	-3.74	120.95	126.34
54	1w	39	PSU	O2-C2-N1	-3.72	118.70	122.79
54	2w	55	PSU	C4-N3-C2	-3.71	120.99	126.34
32	2a	1518	MA6	C4-C5-N7	-3.71	105.54	109.40
1	1A	2617	PSU	C4-N3-C2	-3.69	121.02	126.34
32	2a	1518	MA6	C9-N6-C6	-3.68	108.36	119.51
32	1a	1404	5MC	C5-C6-N1	-3.67	119.56	123.34
54	2y	32	PSU	C4-N3-C2	-3.66	121.06	126.34
55	1x	32	5MC	C5-C6-N1	-3.66	119.57	123.34
54	1w	55	PSU	C4-N3-C2	-3.66	121.07	126.34
55	1x	55	PSU	O2-C2-N1	-3.65	118.77	122.79
55	1x	54	5MU	O4-C4-C5	-3.65	120.67	124.90
54	2y	54	5MU	C4-N3-C2	-3.65	122.63	127.35
54	1y	39	PSU	O2-C2-N1	-3.64	118.78	122.79
32	1a	1400	5MC	C5-C6-N1	-3.62	119.61	123.34
54	1y	32	PSU	C4-N3-C2	-3.62	121.12	126.34
54	2y	8	4SU	N3-C2-N1	3.61	119.68	114.89
54	2y	54	5MU	N3-C2-N1	3.56	119.61	114.89
1	1A	1984	5MC	C5-C6-N1	-3.55	119.69	123.34
54	1w	32	PSU	C4-N3-C2	-3.54	121.24	126.34
54	2w	39	PSU	C4-N3-C2	-3.52	121.26	126.34
1	2A	1911	PSU	O2-C2-N1	-3.51	118.92	122.79
32	2a	1404	5MC	C5-C6-N1	-3.51	119.73	123.34
54	1y	54	5MU	O4-C4-C5	-3.50	120.84	124.90
54	2w	55	PSU	O2-C2-N1	-3.50	118.93	122.79
55	2x	55	PSU	O2-C2-N1	-3.50	118.93	122.79
1	1A	1933	PSU	O2-C2-N1	-3.50	118.94	122.79
32	2a	967	5MC	C5-C6-N1	-3.50	119.74	123.34
1	2A	1962	5MC	C5-C6-N1	-3.50	119.74	123.34
54	2y	37	MIA	N3-C2-N1	-3.47	123.25	128.68
54	1y	8	4SU	C5-C4-S4	-3.45	120.02	124.47
54	1w	37	MIA	C5-C6-N1	-3.45	117.95	120.81
1	1A	1937	5MU	C5-C6-N1	-3.43	119.81	123.34
1	2A	1917	PSU	O2-C2-N1	-3.43	119.01	122.79
43	2l	92	0TD	OD2-CG-CB	3.43	120.56	113.15
54	1w	54	5MU	C5-C6-N1	-3.43	119.81	123.34
54	1y	37	MIA	N3-C2-N1	-3.42	123.33	128.68
54	2y	54	5MU	O4-C4-C5	-3.42	120.94	124.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	1y	32	PSU	O2-C2-N1	-3.42	119.03	122.79
32	2a	1519	MA6	C9-N6-C6	-3.41	109.19	119.51
54	2w	37	MIA	C5-C6-N1	-3.41	117.98	120.81
1	1A	2617	PSU	O2-C2-N1	-3.38	119.06	122.79
32	1a	1518	MA6	N3-C2-N1	-3.37	123.41	128.68
1	2A	1915	5MU	O4-C4-C5	-3.37	121.00	124.90
1	1A	1939	PSU	O2-C2-N1	-3.37	119.08	122.79
54	2y	55	PSU	O2-C2-N1	-3.36	119.09	122.79
55	1x	8	4SU	C1'-N1-C2	3.36	123.65	117.57
54	2w	32	PSU	O2-C2-N1	-3.35	119.10	122.79
32	1a	1518	MA6	C4-C5-N7	-3.34	105.92	109.40
1	2A	1942	5MC	C5-C6-N1	-3.32	119.92	123.34
32	1a	1518	MA6	C9-N6-C6	-3.30	109.52	119.51
32	2a	1519	MA6	C4-C5-N7	-3.30	105.96	109.40
54	2y	32	PSU	O2-C2-N1	-3.30	119.16	122.79
1	1A	1964	5MC	C5-C6-N1	-3.30	119.95	123.34
32	1a	1407	5MC	C5-C6-N1	-3.29	119.95	123.34
54	2w	37	MIA	C12-N6-C6	-3.29	120.03	122.87
54	2w	8	4SU	C1'-N1-C2	3.28	123.51	117.57
54	1w	46	7MG	C5-C4-N9	-3.28	102.09	106.35
54	1w	8	4SU	C5-C4-S4	-3.27	120.25	124.47
54	1w	8	4SU	N3-C2-N1	3.26	119.22	114.89
32	1a	1519	MA6	C4-C5-N7	-3.26	106.01	109.40
32	2a	1518	MA6	N3-C2-N1	-3.24	123.61	128.68
32	2a	1519	MA6	N3-C2-N1	-3.24	123.62	128.68
32	2a	516	PSU	O2-C2-N1	-3.21	119.26	122.79
32	1a	516	PSU	O2-C2-N1	-3.19	119.27	122.79
54	1w	37	MIA	C12-N6-C6	-3.16	117.86	122.55
55	2x	32	5MC	C5-C6-N1	-3.15	120.10	123.34
32	1a	1519	MA6	C9-N6-C6	-3.15	109.98	119.51
54	1w	32	PSU	O2-C2-N1	-3.14	119.33	122.79
55	1x	54	5MU	C5-C6-N1	-3.14	120.11	123.34
54	2w	54	5MU	C5-C6-N1	-3.11	120.14	123.34
32	1a	1519	MA6	N3-C2-N1	-3.11	123.82	128.68
1	1A	2564	2MU	O2-C2-N1	-3.09	118.68	122.79
32	2a	1407	5MC	C5-C6-N1	-3.09	120.16	123.34
32	1a	967	5MC	C5-C6-N1	-3.04	120.21	123.34
1	2A	2605	PSU	O2-C2-N1	-2.96	119.53	122.79
55	1x	8	4SU	C6-C5-C4	-2.92	117.43	119.95
54	2y	37	MIA	C4-C5-N7	-2.90	106.38	109.40
32	1a	1519	MA6	N1-C6-N6	2.88	120.09	117.06
43	1l	92	0TD	OD2-CG-CB	2.85	119.32	113.15

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	2a	527	7MG	C5-C6-N1	2.85	116.01	110.99
54	1y	37	MIA	C4-C5-N7	-2.83	106.45	109.40
54	2y	54	5MU	C5-C6-N1	-2.83	120.42	123.34
1	2A	2552	2MU	C5-C4-N3	2.82	119.06	114.84
54	2w	39	PSU	O2-C2-N1	-2.82	119.69	122.79
55	1x	32	5MC	C5-C4-N3	-2.81	118.64	121.67
1	1A	2564	2MU	C5-C4-N3	2.77	118.98	114.84
54	2w	46	7MG	C5-C6-N1	2.77	115.86	110.99
54	1w	37	MIA	C2-N1-C6	2.76	122.13	117.19
54	2y	46	7MG	C5-C4-N9	-2.72	102.81	106.35
32	2a	1404	5MC	C5-C4-N3	-2.70	118.76	121.67
55	2x	54	5MU	O2-C2-N1	-2.69	119.21	122.79
55	1x	8	4SU	O2-C2-N1	2.68	126.34	122.79
55	2x	32	5MC	O2-C2-N3	-2.67	117.98	122.33
32	1a	527	7MG	C5-C6-N1	2.67	115.70	110.99
54	2w	37	MIA	C2-N1-C6	2.66	121.95	117.19
32	2a	1407	5MC	C5-C4-N3	-2.66	118.81	121.67
32	1a	1407	5MC	C5-C4-N3	-2.65	118.81	121.67
1	2A	2552	2MU	O2-C2-N1	-2.64	119.28	122.79
1	1A	1964	5MC	C5-C4-N3	-2.60	118.87	121.67
1	2A	1942	5MC	C5-C4-N3	-2.59	118.88	121.67
32	1a	967	5MC	C5-C4-N3	-2.57	118.90	121.67
1	1A	1984	5MC	C5-C4-N3	-2.57	118.90	121.67
54	2y	46	7MG	C5-C6-N1	2.57	115.51	110.99
55	2x	32	5MC	C5-C4-N3	-2.57	118.91	121.67
54	1w	54	5MU	O2-C2-N1	-2.56	119.38	122.79
54	1w	37	MIA	C11-S10-C2	-2.56	100.36	102.27
54	2w	37	MIA	C4-C5-N7	-2.56	106.73	109.40
32	1a	1404	5MC	C5-C4-N3	-2.53	118.95	121.67
54	2w	54	5MU	O2-C2-N1	-2.53	119.43	122.79
55	2x	8	4SU	C5-C4-S4	-2.52	121.22	124.47
54	1y	54	5MU	O2-C2-N1	-2.52	119.44	122.79
54	1w	37	MIA	C4-C5-N7	-2.51	106.78	109.40
32	2a	967	5MC	C5-C4-N3	-2.51	118.97	121.67
54	1y	46	7MG	C5-C6-N1	2.51	115.41	110.99
1	1A	2263	OMG	C8-N7-C5	2.49	107.73	102.99
32	2a	1518	MA6	C10-N6-C9	-2.48	108.12	116.12
32	1a	1400	5MC	C5-C4-N3	-2.48	119.00	121.67
1	2A	1915	5MU	O2-C2-N1	-2.48	119.49	122.79
1	2A	2552	2MU	O4-C4-C5	-2.47	120.81	125.16
43	2l	92	0TD	OD1-CG-CB	-2.47	117.27	122.44
32	1a	1207	2MG	C8-N7-C5	2.45	107.67	102.99

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
55	2x	8	4SU	C4-N3-C2	-2.45	124.97	127.34
32	2a	1404	5MC	O2-C2-N3	-2.44	118.36	122.33
54	2w	37	MIA	N3-C2-N1	-2.44	122.49	126.98
54	2w	37	MIA	N6-C6-N1	2.44	121.55	118.50
32	1a	1402	4OC	C6-C5-C4	2.44	119.94	116.96
1	1A	2564	2MU	C2'-C1'-N1	-2.44	109.49	114.22
1	2A	1939	5MU	O2-C2-N1	-2.42	119.57	122.79
32	2a	1207	2MG	C8-N7-C5	2.42	107.60	102.99
1	2A	1962	5MC	C5-C4-N3	-2.42	119.07	121.67
55	1x	8	4SU	O2-C2-N3	-2.41	117.00	121.50
54	1y	46	7MG	C5-C4-N9	-2.41	103.22	106.35
32	1a	966	M2G	C8-N7-C5	2.39	107.53	102.99
1	1A	2515	2MA	C5-C6-N1	2.38	118.13	114.02
55	2x	8	4SU	C6-C5-C4	-2.38	117.89	119.95
54	2y	54	5MU	C1'-N1-C2	2.38	121.88	117.57
1	2A	2503	2MA	C8-N7-C5	2.37	107.51	102.99
1	1A	1961	5MU	O2-C2-N1	-2.37	119.64	122.79
1	2A	2503	2MA	C5-C6-N1	2.35	118.07	114.02
1	2A	2251	OMG	C8-N7-C5	2.34	107.45	102.99
1	1A	1937	5MU	O2-C2-N1	-2.32	119.70	122.79
32	1a	966	M2G	C5-C6-N1	2.32	118.05	113.95
32	2a	1402	4OC	C6-C5-C4	2.31	119.79	116.96
32	2a	966	M2G	C8-N7-C5	2.30	107.38	102.99
1	1A	2515	2MA	C8-N7-C5	2.30	107.37	102.99
1	1A	2263	OMG	C5-C6-N1	2.29	118.00	113.95
54	1w	37	MIA	N3-C2-N1	-2.29	122.77	126.98
32	2a	527	7MG	C5-C4-N9	-2.29	103.38	106.35
55	1x	54	5MU	O2-C2-N1	-2.29	119.75	122.79
32	2a	1400	5MC	C5-C4-N3	-2.28	119.21	121.67
55	2x	8	4SU	C1'-N1-C6	-2.28	115.88	120.84
32	1a	1400	5MC	O2-C2-N3	-2.27	118.64	122.33
54	2y	54	5MU	C1'-N1-C6	-2.27	117.35	121.12
54	2w	46	7MG	O6-C6-C5	-2.26	122.00	127.54
32	2a	966	M2G	C5-C6-N1	2.24	117.91	113.95
1	2A	2251	OMG	C5-C6-N1	2.23	117.89	113.95
1	1A	1942	4OC	O2-C2-N3	-2.22	118.72	122.33
32	2a	1207	2MG	C5-C6-N1	2.22	117.87	113.95
55	1x	54	5MU	C5M-C5-C4	2.21	121.19	118.77
1	1A	2564	2MU	O4-C4-C5	-2.20	121.30	125.16
32	1a	1518	MA6	C10-N6-C9	-2.20	109.04	116.12
32	1a	967	5MC	C1'-N1-C6	-2.20	117.47	121.12
32	1a	1518	MA6	N1-C6-N6	2.18	119.35	117.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	1a	516	PSU	O4'-C1'-C2'	2.17	108.21	105.14
32	2a	1407	5MC	O2-C2-N3	-2.17	118.81	122.33
32	2a	1402	4OC	O2-C2-N3	-2.15	118.83	122.33
54	2w	46	7MG	C5-C4-N9	-2.15	103.56	106.35
32	2a	527	7MG	O6-C6-C5	-2.14	122.29	127.54
32	2a	1519	MA6	N1-C6-N6	2.12	119.28	117.06
32	1a	527	7MG	CM7-N7-C5	2.11	131.84	126.40
54	1w	46	7MG	C5-C6-N1	2.09	114.67	110.99
1	2A	2605	PSU	C5-C6-N1	-2.09	118.98	122.11
54	2y	46	7MG	O6-C6-C5	-2.08	122.43	127.54
32	1a	527	7MG	C5-C4-N9	-2.07	103.66	106.35
54	1w	46	7MG	CM7-N7-C5	2.06	131.72	126.40
54	2y	39	PSU	C5-C6-N1	-2.05	119.03	122.11
32	1a	1518	MA6	C10-N6-C6	-2.04	113.33	119.51
54	2y	46	7MG	CM7-N7-C5	2.03	131.64	126.40
54	2w	54	5MU	C5M-C5-C4	2.02	120.99	118.77
32	2a	516	PSU	O4'-C1'-C2'	2.02	107.99	105.14
54	1w	8	4SU	C1'-N1-C2	2.01	121.21	117.57

There are no chirality outliers.

All (71) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
32	1a	527	7MG	C3'-C4'-C5'-O5'
32	1a	967	5MC	O4'-C4'-C5'-O5'
32	1a	967	5MC	C3'-C4'-C5'-O5'
32	1a	1207	2MG	N3-C2-N2-CM2
32	1a	1518	MA6	C5-C6-N6-C10
43	1l	92	0TD	O-C-CA-CB
32	2a	1402	4OC	O4'-C4'-C5'-O5'
32	2a	1518	MA6	C5-C6-N6-C9
32	2a	1519	MA6	O4'-C4'-C5'-O5'
32	2a	1519	MA6	C3'-C4'-C5'-O5'
32	2a	1519	MA6	C5-C6-N6-C10
43	2l	92	0TD	O-C-CA-CB
54	1y	8	4SU	O4'-C4'-C5'-O5'
54	1w	37	MIA	C12-C13-C14-C16
54	2w	37	MIA	N1-C6-N6-C12
32	1a	1519	MA6	O4'-C4'-C5'-O5'
32	1a	1519	MA6	C3'-C4'-C5'-O5'
32	2a	1402	4OC	C3'-C4'-C5'-O5'
54	1y	8	4SU	C3'-C4'-C5'-O5'

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Mol	Chain	Res	Type	Atoms
54	2y	8	4SU	O4'-C4'-C5'-O5'
54	1w	46	7MG	C4'-C5'-O5'-P
54	2y	8	4SU	C3'-C4'-C5'-O5'
32	2a	1518	MA6	N1-C6-N6-C9
54	1y	37	MIA	C3'-C4'-C5'-O5'
54	2y	37	MIA	C3'-C4'-C5'-O5'
32	1a	527	7MG	O4'-C4'-C5'-O5'
32	2a	1207	2MG	O4'-C4'-C5'-O5'
32	1a	1518	MA6	C5-C6-N6-C9
32	1a	1519	MA6	C5-C6-N6-C10
32	2a	1519	MA6	C5-C6-N6-C9
54	2w	46	7MG	C2'-C1'-N9-C8
54	2y	37	MIA	O4'-C4'-C5'-O5'
54	1w	46	7MG	C3'-C4'-C5'-O5'
32	1a	1402	4OC	O4'-C4'-C5'-O5'
54	1y	37	MIA	O4'-C4'-C5'-O5'
54	1w	46	7MG	O4'-C4'-C5'-O5'
1	2A	1920	4OC	C1'-C2'-O2'-CM2
43	2l	92	0TD	CG-CB-SB-CSB
32	2a	1519	MA6	C4'-C5'-O5'-P
54	2y	46	7MG	C4'-C5'-O5'-P
54	2w	46	7MG	O4'-C4'-C5'-O5'
54	2y	46	7MG	C2'-C1'-N9-C8
32	2a	1518	MA6	C5-C6-N6-C10
54	1y	46	7MG	C4'-C5'-O5'-P
32	2a	527	7MG	C4'-C5'-O5'-P
32	2a	527	7MG	C3'-C4'-C5'-O5'
54	1y	55	PSU	O4'-C1'-C5-C4
54	2y	55	PSU	O4'-C1'-C5-C4
1	2A	2503	2MA	O4'-C4'-C5'-O5'
54	2w	46	7MG	O4'-C1'-N9-C8
1	2A	2251	OMG	C4'-C5'-O5'-P
1	2A	2503	2MA	C4'-C5'-O5'-P
32	2a	967	5MC	O4'-C4'-C5'-O5'
32	2a	1207	2MG	C3'-C4'-C5'-O5'
54	2w	37	MIA	C5-C6-N6-C12
43	1l	92	0TD	SB-CB-CG-OD2
54	2w	46	7MG	C3'-C4'-C5'-O5'
1	2A	1920	4OC	C3'-C2'-O2'-CM2
1	1A	1942	4OC	C2'-C1'-N1-C2
43	1l	92	0TD	CG-CB-SB-CSB
54	1y	55	PSU	O4'-C1'-C5-C6

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Mol	Chain	Res	Type	Atoms
54	2y	55	PSU	O4'-C1'-C5-C6
54	2w	8	4SU	C2'-C1'-N1-C2
54	2y	46	7MG	O4'-C1'-N9-C8
1	1A	2515	2MA	O4'-C4'-C5'-O5'
32	1a	1402	4OC	C3'-C4'-C5'-O5'
54	1y	46	7MG	C2'-C1'-N9-C8
55	2x	8	4SU	C2'-C1'-N1-C2
1	1A	2515	2MA	C4'-C5'-O5'-P
1	2A	1962	5MC	C2'-C1'-N1-C6
54	1y	8	4SU	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 2821 ligands modelled in this entry, 2817 are monoatomic - leaving 4 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
58	M2D	2A	3864	-	33,37,37	3.99	13 (39%)	38,50,50	1.75	7 (18%)
58	M2D	1A	4118	-	33,37,37	3.82	14 (42%)	38,50,50	1.78	5 (13%)
60	SF4	1d	501	35	0,12,12	-	-	-	-	-
60	SF4	2d	302	35	0,12,12	-	-	-	-	-

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
58	M2D	2A	3864	-	-	6/42/48/48	0/1/2/2
58	M2D	1A	4118	-	-	5/42/48/48	0/1/2/2
60	SF4	1d	501	35	-	-	0/6/5/5
60	SF4	2d	302	35	-	-	0/6/5/5

All (27) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
58	2A	3864	M2D	CAP-CAQ	-16.22	1.39	1.49
58	1A	4118	M2D	CAP-CAQ	-15.16	1.39	1.49
58	2A	3864	M2D	CAM-CAL	-8.05	1.40	1.50
58	1A	4118	M2D	CAM-CAL	-7.27	1.41	1.50
58	2A	3864	M2D	CAT-CAY	-7.25	1.33	1.50
58	1A	4118	M2D	CAT-CAY	-7.14	1.33	1.50
58	1A	4118	M2D	CBD-CAK	-5.43	1.39	1.50
58	2A	3864	M2D	CBD-CAK	-5.27	1.40	1.50
58	1A	4118	M2D	CAC-CAD	-4.34	1.40	1.51
58	2A	3864	M2D	CAE-CAF	-4.23	1.39	1.48
58	2A	3864	M2D	CAC-CAD	-4.17	1.40	1.51
58	1A	4118	M2D	CAE-CAF	-4.12	1.39	1.48
58	1A	4118	M2D	CAF-NAG	3.75	1.42	1.34
58	2A	3864	M2D	CAF-NAG	3.61	1.42	1.34
58	1A	4118	M2D	CAJ-CAI	3.56	1.41	1.32
58	1A	4118	M2D	CA-C	-3.53	1.39	1.51
58	2A	3864	M2D	CAJ-CAI	3.50	1.41	1.32
58	2A	3864	M2D	CA-C	-3.46	1.39	1.51
58	2A	3864	M2D	CAE-CAD	3.13	1.39	1.32
58	1A	4118	M2D	CAE-CAD	3.12	1.39	1.32
58	2A	3864	M2D	CAY-N	2.70	1.40	1.34
58	2A	3864	M2D	CAH-CAI	-2.54	1.40	1.50
58	1A	4118	M2D	CAH-CAI	-2.49	1.40	1.50
58	2A	3864	M2D	CAJ-CAK	-2.43	1.40	1.45
58	1A	4118	M2D	CAJ-CAK	-2.38	1.40	1.45
58	1A	4118	M2D	CAY-N	2.36	1.39	1.34
58	1A	4118	M2D	CAL-CAK	2.12	1.41	1.34

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
58	1A	4118	M2D	CAI-CAJ-CAK	7.81	137.69	125.89
58	2A	3864	M2D	CAI-CAJ-CAK	6.59	135.85	125.89
58	2A	3864	M2D	CBD-CAK-CAJ	3.48	123.56	118.08
58	1A	4118	M2D	CBD-CAK-CAJ	3.24	123.19	118.08

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
58	1A	4118	M2D	CAH-NAG-CAF	2.80	126.56	122.03
58	2A	3864	M2D	CAH-NAG-CAF	2.63	126.28	122.03
58	2A	3864	M2D	CAB-OAA-C	-2.54	113.42	117.78
58	2A	3864	M2D	CAN-CAM-CAL	2.47	116.91	111.94
58	2A	3864	M2D	CAC-CAB-CAZ	-2.44	109.97	115.98
58	1A	4118	M2D	CAE-CAF-NAG	2.32	119.35	114.97
58	1A	4118	M2D	CAN-CAO-CAP	-2.28	108.66	113.19
58	2A	3864	M2D	CAC-CAD-CAE	-2.08	120.75	126.44

There are no chirality outliers.

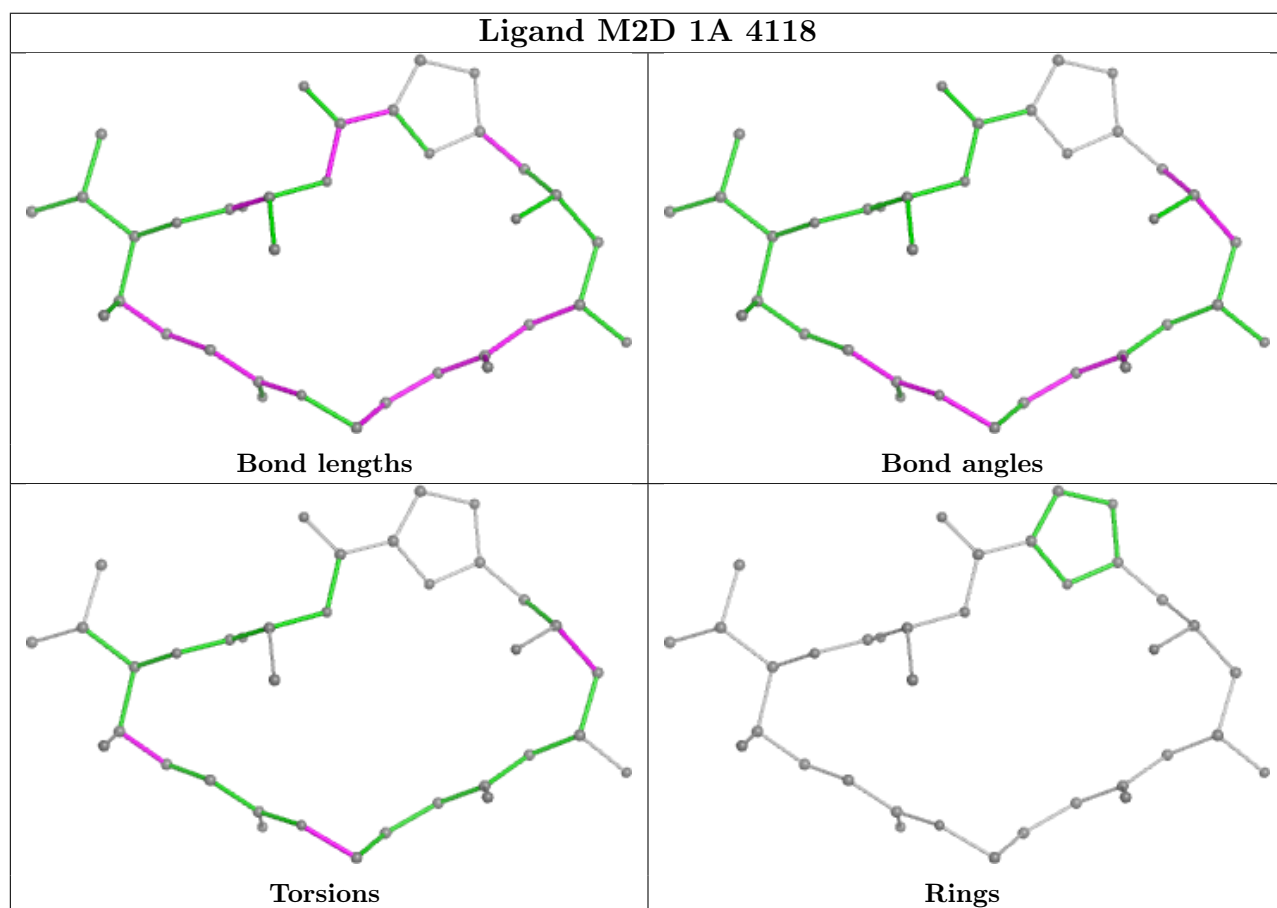
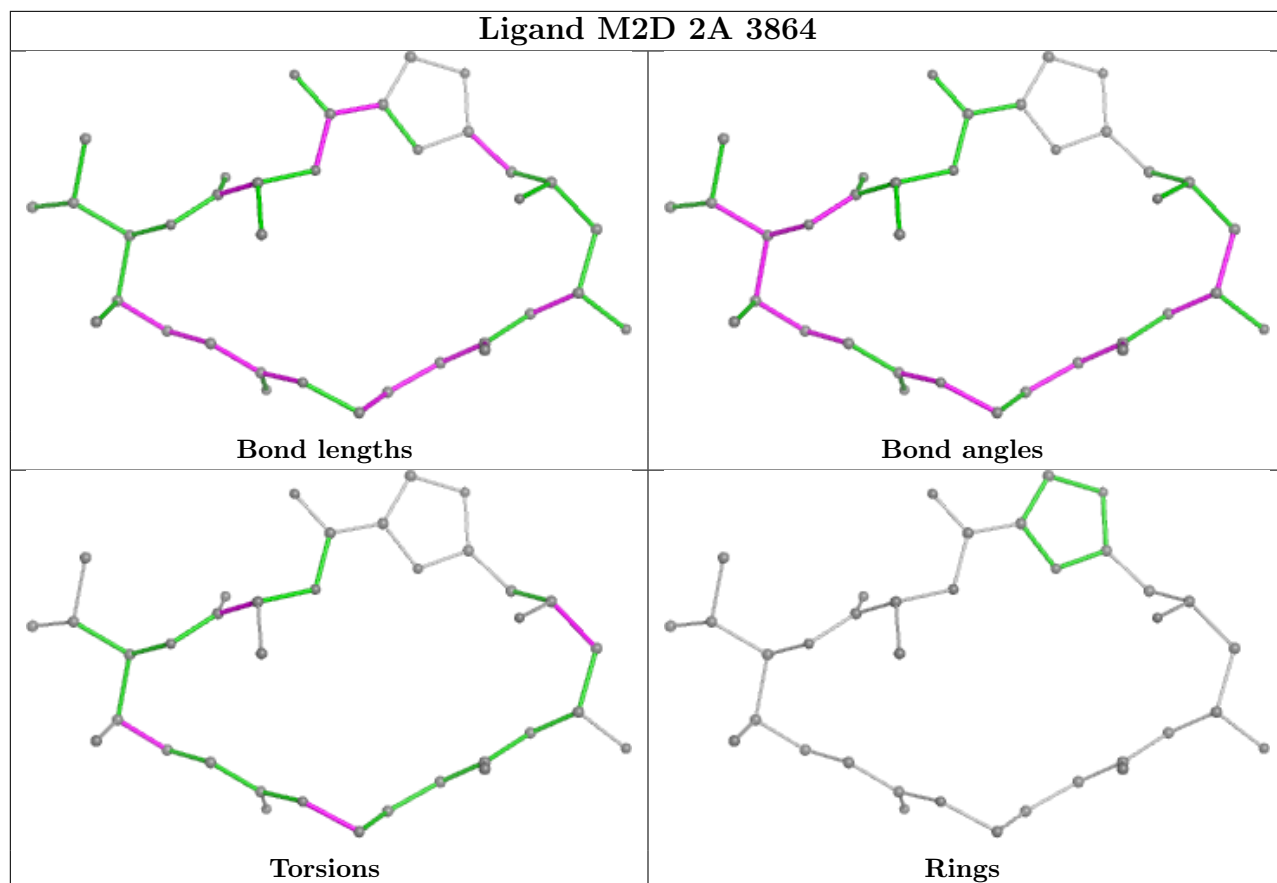
All (11) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
58	1A	4118	M2D	CAM-CAN-CAO-CAP
58	1A	4118	M2D	CAM-CAN-CAO-OBF
58	2A	3864	M2D	CAM-CAN-CAO-OBF
58	2A	3864	M2D	CAI-CAH-NAG-CAF
58	2A	3864	M2D	CBB-CAC-CAD-CAE
58	1A	4118	M2D	CAI-CAH-NAG-CAF
58	1A	4118	M2D	CBB-CAC-CAD-CAE
58	1A	4118	M2D	CAB-CAC-CAD-CAE
58	2A	3864	M2D	CAB-CAC-CAD-CAE
58	2A	3864	M2D	O-C-CA-CB
58	2A	3864	M2D	OAA-C-CA-CB

There are no ring outliers.

No monomer is involved in short contacts.

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



## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data 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	2860/2915 (98%)	0.58	12 (0%) 92 91	10, 26, 82, 97	0
1	2A	2789/2915 (95%)	0.49	39 (1%) 75 70	25, 51, 82, 96	0
2	1B	120/121 (99%)	0.32	0 100 100	19, 38, 50, 74	0
2	2B	120/121 (99%)	0.21	0 100 100	55, 70, 76, 82	0
3	1D	275/276 (99%)	0.46	2 (0%) 87 84	12, 29, 43, 62	0
3	2D	275/276 (99%)	0.69	10 (3%) 42 32	25, 43, 56, 69	0
4	1E	204/206 (99%)	0.33	0 100 100	11, 29, 48, 68	0
4	2E	204/206 (99%)	0.35	2 (0%) 82 77	29, 51, 62, 71	0
5	1F	203/210 (96%)	0.21	0 100 100	12, 32, 62, 75	0
5	2F	203/210 (96%)	0.38	5 (2%) 57 47	28, 58, 70, 80	0
6	1G	181/182 (99%)	0.11	0 100 100	28, 46, 61, 72	0
6	2G	181/182 (99%)	0.80	24 (13%) 3 2	59, 69, 78, 88	0
7	1H	174/180 (96%)	0.10	0 100 100	24, 42, 54, 60	0
7	2H	174/180 (96%)	0.70	11 (6%) 20 12	55, 72, 81, 84	0
8	1I	146/148 (98%)	0.10	0 100 100	35, 63, 72, 78	0
8	2I	146/148 (98%)	0.06	1 (0%) 87 84	44, 62, 72, 76	0
9	1N	140/140 (100%)	0.21	0 100 100	15, 27, 47, 57	0
9	2N	140/140 (100%)	0.51	6 (4%) 35 25	40, 57, 67, 74	0
10	1O	122/122 (100%)	0.34	0 100 100	20, 30, 45, 55	0
10	2O	122/122 (100%)	0.60	3 (2%) 57 47	38, 53, 63, 68	0
11	1P	149/150 (99%)	0.26	0 100 100	12, 36, 59, 70	0
11	2P	149/150 (99%)	0.73	10 (6%) 17 10	31, 59, 71, 79	0
12	1Q	141/141 (100%)	0.34	0 100 100	19, 32, 44, 66	0
12	2Q	141/141 (100%)	0.72	10 (7%) 16 9	44, 60, 73, 77	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
13	1R	118/118 (100%)	0.37	0 100 100	14, 24, 36, 43	0
13	2R	118/118 (100%)	0.38	1 (0%) 86 81	33, 44, 55, 64	0
14	1S	110/112 (98%)	0.12	0 100 100	27, 38, 50, 59	0
14	2S	110/112 (98%)	0.58	6 (5%) 25 16	55, 65, 71, 75	0
15	1T	131/146 (89%)	0.17	0 100 100	23, 33, 55, 64	0
15	2T	131/146 (89%)	0.45	2 (1%) 73 68	41, 55, 68, 81	0
16	1U	116/118 (98%)	0.40	1 (0%) 84 80	12, 19, 37, 59	0
16	2U	116/118 (98%)	0.59	3 (2%) 56 46	38, 53, 68, 76	0
17	1V	101/101 (100%)	0.16	0 100 100	12, 27, 43, 51	0
17	2V	101/101 (100%)	0.37	4 (3%) 38 28	39, 60, 69, 78	0
18	1W	112/113 (99%)	0.28	0 100 100	15, 21, 44, 69	0
18	2W	112/113 (99%)	0.43	0 100 100	30, 41, 55, 81	0
19	1X	95/96 (98%)	0.31	0 100 100	17, 29, 46, 63	0
19	2X	95/96 (98%)	0.51	1 (1%) 80 75	37, 53, 62, 68	0
20	1Y	107/110 (97%)	0.18	0 100 100	26, 40, 55, 72	0
20	2Y	107/110 (97%)	0.79	9 (8%) 11 5	51, 61, 69, 75	0
21	1Z	154/206 (74%)	0.14	0 100 100	30, 50, 75, 82	0
21	2Z	160/206 (77%)	0.81	16 (10%) 7 4	61, 73, 81, 84	0
22	10	83/85 (97%)	1.07	7 (8%) 11 5	19, 28, 59, 80	0
22	20	83/85 (97%)	0.98	8 (9%) 8 4	46, 57, 69, 78	0
23	11	97/98 (98%)	0.50	1 (1%) 82 77	15, 35, 58, 63	0
23	21	97/98 (98%)	0.58	2 (2%) 63 54	32, 49, 67, 71	0
24	12	70/72 (97%)	0.28	1 (1%) 75 70	25, 39, 50, 69	0
24	22	70/72 (97%)	0.23	1 (1%) 75 70	49, 60, 69, 73	0
25	13	59/60 (98%)	0.18	0 100 100	15, 26, 46, 64	0
25	23	59/60 (98%)	0.94	10 (16%) 1 1	46, 56, 70, 78	0
26	14	69/71 (97%)	-0.01	0 100 100	40, 59, 76, 82	0
26	24	69/71 (97%)	0.59	6 (8%) 10 5	64, 75, 83, 84	0
27	15	59/60 (98%)	0.32	1 (1%) 70 63	11, 22, 41, 58	0
27	25	59/60 (98%)	0.29	0 100 100	31, 44, 54, 65	0
28	16	53/54 (98%)	0.19	0 100 100	22, 32, 46, 48	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
28	26	53/54 (98%)	0.76	5 (9%) 8 4	43, 53, 61, 66	0
29	17	48/49 (97%)	0.59	3 (6%) 20 12	13, 19, 51, 54	0
29	27	48/49 (97%)	1.09	6 (12%) 3 2	26, 33, 54, 65	0
30	18	64/65 (98%)	0.45	2 (3%) 49 39	17, 24, 32, 43	0
30	28	64/65 (98%)	0.90	6 (9%) 8 4	39, 47, 55, 57	0
31	19	37/37 (100%)	0.35	0 100 100	18, 30, 46, 50	0
31	29	37/37 (100%)	1.36	10 (27%) 0 0	51, 63, 68, 70	0
32	1a	1488/1521 (97%)	0.43	13 (0%) 84 80	28, 57, 81, 96	0
32	2a	1491/1521 (98%)	0.56	51 (3%) 45 35	48, 69, 85, 95	0
33	1b	231/256 (90%)	0.46	12 (5%) 27 18	55, 68, 79, 83	0
33	2b	231/256 (90%)	1.02	40 (17%) 1 1	65, 77, 83, 86	0
34	1c	206/239 (86%)	0.35	7 (3%) 45 35	50, 63, 74, 80	0
34	2c	206/239 (86%)	1.05	39 (18%) 1 1	65, 75, 82, 88	0
35	1d	208/209 (99%)	0.70	20 (9%) 8 4	47, 62, 71, 82	0
35	2d	208/209 (99%)	0.86	20 (9%) 8 4	52, 63, 72, 73	0
36	1e	148/162 (91%)	0.46	3 (2%) 65 56	44, 56, 62, 69	0
36	2e	148/162 (91%)	1.00	28 (18%) 1 1	58, 69, 77, 80	0
37	1f	100/101 (99%)	0.24	0 100 100	46, 59, 68, 71	0
37	2f	100/101 (99%)	0.12	2 (2%) 65 56	52, 63, 70, 72	0
38	1g	155/156 (99%)	0.40	11 (7%) 16 9	48, 59, 70, 81	0
38	2g	155/156 (99%)	0.84	25 (16%) 1 1	60, 69, 78, 90	0
39	1h	137/138 (99%)	0.48	3 (2%) 62 52	47, 58, 66, 72	0
39	2h	137/138 (99%)	1.01	18 (13%) 3 2	59, 69, 75, 78	0
40	1i	127/128 (99%)	0.76	11 (8%) 10 5	42, 66, 74, 76	0
40	2i	127/128 (99%)	1.70	51 (40%) 0 0	65, 75, 82, 85	0
41	1j	97/105 (92%)	0.77	13 (13%) 3 1	50, 68, 77, 80	0
41	2j	96/105 (91%)	1.84	35 (36%) 0 0	67, 76, 84, 94	0
42	1k	114/129 (88%)	0.49	0 100 100	36, 54, 65, 69	0
42	2k	114/129 (88%)	0.80	10 (8%) 10 5	44, 65, 72, 75	0
43	1l	121/132 (91%)	0.44	3 (2%) 57 47	38, 46, 58, 65	0
43	2l	121/132 (91%)	0.80	15 (12%) 4 2	49, 61, 69, 74	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
44	1m	123/126 (97%)	0.24	4 (3%) 46 36	44, 57, 67, 72	0
44	2m	122/126 (96%)	1.28	28 (22%) 0 0	60, 72, 77, 82	0
45	1n	60/61 (98%)	0.94	5 (8%) 11 6	52, 58, 65, 71	0
45	2n	60/61 (98%)	2.75	36 (60%) 0 0	69, 75, 81, 84	0
46	1o	88/89 (98%)	0.50	5 (5%) 23 15	41, 55, 65, 69	0
46	2o	88/89 (98%)	0.80	10 (11%) 5 3	50, 64, 71, 77	0
47	1p	82/88 (93%)	0.98	10 (12%) 4 2	49, 60, 68, 73	0
47	2p	82/88 (93%)	0.70	6 (7%) 15 8	48, 60, 68, 70	0
48	1q	99/105 (94%)	0.78	6 (6%) 21 13	44, 56, 66, 70	0
48	2q	99/105 (94%)	1.13	22 (22%) 0 0	56, 64, 71, 74	0
49	1r	68/88 (77%)	0.34	1 (1%) 73 68	45, 56, 68, 74	0
49	2r	68/88 (77%)	0.40	1 (1%) 73 68	55, 63, 70, 77	0
50	1s	83/93 (89%)	0.22	1 (1%) 79 73	48, 60, 68, 73	0
50	2s	83/93 (89%)	1.51	24 (28%) 0 0	67, 76, 81, 84	0
51	1t	96/106 (90%)	0.63	5 (5%) 27 18	47, 59, 70, 75	0
51	2t	96/106 (90%)	0.66	10 (10%) 6 3	50, 61, 71, 75	0
52	1u	23/27 (85%)	1.75	9 (39%) 0 0	50, 55, 61, 62	0
52	2u	23/27 (85%)	2.24	13 (56%) 0 0	64, 69, 74, 76	0
53	1v	13/24 (54%)	1.15	3 (23%) 0 0	39, 52, 75, 87	0
53	2v	13/24 (54%)	2.28	7 (53%) 0 0	60, 75, 88, 90	0
54	1w	65/76 (85%)	0.75	6 (9%) 9 5	48, 76, 89, 95	0
54	1y	67/76 (88%)	0.55	2 (2%) 50 40	25, 79, 88, 91	0
54	2w	62/76 (81%)	1.46	16 (25%) 0 0	71, 83, 91, 97	0
54	2y	66/76 (86%)	1.16	9 (13%) 3 1	45, 86, 91, 92	0
55	1x	72/77 (93%)	0.39	0 100 100	35, 52, 70, 80	0
55	2x	72/77 (93%)	0.47	0 100 100	55, 70, 80, 83	0
All	All	20870/21748 (95%)	0.56	916 (4%) 34 24	10, 55, 80, 97	0

All (916) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
22	10	6	GLY	10.0
22	10	2	ALA	9.4

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
22	10	4	LYS	8.8
45	2n	34	TYR	8.5
22	10	5	LYS	8.4
41	2j	59	SER	7.7
22	10	3	HIS	7.7
44	2m	124	PRO	7.5
38	2g	81	GLY	7.3
38	1g	80	VAL	7.1
38	2g	82	GLY	7.0
22	10	7	LEU	6.8
22	20	7	LEU	6.7
41	2j	50	ILE	6.6
22	20	2	ALA	6.5
41	2j	47	PHE	6.4
45	2n	38	GLY	6.3
45	2n	25	VAL	6.3
44	2m	123	ALA	6.2
45	2n	39	LEU	6.1
38	2g	16	LEU	6.1
22	20	6	GLY	6.0
22	20	4	LYS	5.9
41	2j	48	THR	5.9
44	2m	122	LYS	5.9
44	2m	4	ILE	5.9
34	2c	198	VAL	5.8
1	1A	1555	C	5.8
50	2s	82	GLY	5.7
45	2n	37	PHE	5.7
40	2i	109	VAL	5.7
44	2m	102	ARG	5.7
33	2b	165	VAL	5.6
52	2u	14	TRP	5.4
1	2A	883	G	5.3
45	2n	56	VAL	5.3
54	2w	73	A	5.2
33	2b	101	MET	5.2
45	2n	2	ALA	5.2
45	2n	10	ALA	5.2
34	2c	39	ILE	5.2
40	2i	114	TYR	5.1
22	20	3	HIS	5.0
45	2n	57	ARG	5.0

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
54	2y	36	A	5.0
48	1q	98	LEU	5.0
52	2u	16	GLY	4.9
44	2m	5	ALA	4.9
29	27	48	LYS	4.9
41	2j	55	LYS	4.9
45	2n	42	ILE	4.8
44	2m	60	VAL	4.8
53	2v	24	A	4.8
41	2j	54	PHE	4.8
45	2n	7	ILE	4.7
54	1w	71	G	4.7
33	2b	92	TYR	4.7
45	1n	2	ALA	4.7
38	2g	80	VAL	4.7
40	2i	14	VAL	4.6
36	2e	12	LEU	4.6
44	2m	6	GLY	4.6
38	2g	4	ARG	4.6
41	2j	51	ARG	4.6
40	2i	115	GLY	4.6
41	2j	98	ILE	4.6
29	27	47	ARG	4.5
41	2j	63	PHE	4.5
41	2j	85	LEU	4.5
41	2j	62	HIS	4.5
45	2n	36	PHE	4.5
41	2j	56	HIS	4.5
41	1j	72	VAL	4.4
6	2G	157	ILE	4.4
29	27	46	VAL	4.4
52	1u	17	THR	4.4
44	1m	123	ALA	4.4
35	2d	161	ASN	4.4
36	2e	31	LEU	4.4
48	2q	9	VAL	4.4
32	2a	1030(B)	C	4.4
1	2A	2802	G	4.4
54	2w	6	G	4.3
6	2G	28	VAL	4.2
35	2d	198	VAL	4.2
41	2j	72	VAL	4.2

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
34	2c	182	ILE	4.2
23	11	2	SER	4.2
33	2b	187	LEU	4.1
34	2c	188	LEU	4.1
53	2v	14	A	4.1
31	29	37	GLY	4.1
50	2s	12	ASP	4.1
52	2u	6	ARG	4.1
45	2n	51	GLY	4.1
7	2H	105	LEU	4.0
40	2i	90	PRO	4.0
23	21	2	SER	4.0
35	1d	180	GLY	3.9
41	2j	60	ARG	3.9
50	2s	80	TYR	3.9
44	1m	124	PRO	3.9
46	2o	60	VAL	3.9
36	2e	109	ILE	3.9
40	2i	17	VAL	3.9
48	1q	36	ILE	3.9
20	2Y	48	ALA	3.9
6	2G	140	ILE	3.9
45	2n	44	LEU	3.9
38	2g	85	TYR	3.8
45	1n	61	TRP	3.8
32	2a	1257	U	3.8
1	1A	942	A	3.8
36	2e	10	MET	3.8
36	2e	105	VAL	3.8
53	1v	12	A	3.8
43	2l	29	GLY	3.8
50	2s	14	HIS	3.8
6	2G	146	TYR	3.8
34	2c	33	LEU	3.8
41	2j	71	LEU	3.8
6	2G	2	PRO	3.8
12	2Q	104	PHE	3.8
32	1a	1001(A)	G	3.8
45	2n	11	LYS	3.7
50	2s	13	ASP	3.7
50	2s	30	LEU	3.7
54	2y	34	G	3.7

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
22	10	8	GLY	3.7
41	2j	10	GLY	3.7
34	2c	189	ALA	3.7
40	2i	65	VAL	3.7
33	2b	152	PHE	3.7
31	29	25	VAL	3.7
33	2b	81	VAL	3.7
32	1a	1002	G	3.6
32	2a	1033	G	3.6
36	2e	84	PHE	3.6
48	2q	92	ARG	3.6
52	2u	24	ARG	3.6
45	2n	60	SER	3.6
34	2c	158	GLY	3.6
40	2i	117	HIS	3.6
48	2q	42	TYR	3.6
40	2i	7	THR	3.6
45	2n	41	ARG	3.6
33	2b	188	ALA	3.6
41	2j	52	GLY	3.6
43	2l	13	LYS	3.5
40	2i	81	ILE	3.5
54	2w	71	G	3.5
32	2a	1116	C	3.5
44	2m	78	ILE	3.5
38	2g	86	GLN	3.5
45	1n	8	GLU	3.5
34	2c	124	ILE	3.5
47	1p	27	LYS	3.5
34	2c	13	GLY	3.5
1	2A	888	C	3.5
34	2c	154	SER	3.5
40	2i	28	VAL	3.5
45	2n	12	ARG	3.5
54	1w	74	C	3.5
41	1j	46	ARG	3.4
47	1p	1	MET	3.4
33	1b	136	VAL	3.4
34	2c	10	PHE	3.4
1	2A	1026	U	3.4
35	1d	122	ARG	3.4
50	2s	79	THR	3.4

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
36	2e	11	ILE	3.4
45	2n	29	ARG	3.4
14	2S	32	LEU	3.4
19	2X	92	LEU	3.4
33	2b	118	LEU	3.4
34	2c	190	ARG	3.4
50	2s	81	ARG	3.4
54	2w	3	C	3.4
6	2G	41	GLN	3.4
38	1g	82	GLY	3.4
3	2D	38	LYS	3.4
54	2w	13	C	3.4
53	2v	12	A	3.4
47	1p	67	THR	3.4
53	2v	13	A	3.4
40	1i	113	LYS	3.4
51	2t	63	ILE	3.4
41	2j	49	VAL	3.4
6	2G	138	GLN	3.4
21	2Z	122	ARG	3.4
35	1d	135	LEU	3.4
38	2g	7	ALA	3.4
40	2i	116	LYS	3.3
6	2G	62	LEU	3.3
44	2m	92	HIS	3.3
52	2u	17	THR	3.3
12	2Q	86	GLY	3.3
40	2i	106	ALA	3.3
38	2g	84	ASN	3.3
1	2A	2154	G	3.3
41	1j	36	GLY	3.3
45	2n	61	TRP	3.3
32	2a	1286	A	3.3
12	2Q	22	LYS	3.3
34	2c	6	HIS	3.3
50	2s	53	ASN	3.3
32	2a	1034	G	3.3
51	2t	24	LEU	3.3
38	2g	3	ARG	3.2
39	2h	133	LEU	3.2
47	1p	4	ILE	3.2
38	1g	83	ALA	3.2

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
6	2G	34	LEU	3.2
40	2i	124	GLN	3.2
41	2j	65	LEU	3.2
34	1c	187	ALA	3.2
34	2c	160	ALA	3.2
53	2v	21	C	3.2
45	2n	45	ARG	3.2
38	2g	154	TYR	3.2
25	23	51	ALA	3.2
48	2q	88	TYR	3.2
1	2A	2133	G	3.2
40	1i	106	ALA	3.2
31	29	16	VAL	3.2
36	2e	90	VAL	3.2
38	2g	83	ALA	3.2
45	2n	31	ARG	3.2
47	1p	25	ARG	3.2
15	2T	90	GLN	3.2
51	1t	74	LYS	3.2
39	2h	2	LEU	3.2
54	1w	1	G	3.1
33	2b	26	PRO	3.1
1	2A	2146	C	3.1
36	1e	89	ILE	3.1
26	24	56	VAL	3.1
40	2i	102	LEU	3.1
32	1a	1003	G	3.1
40	2i	110	GLU	3.1
35	2d	160	GLN	3.1
35	2d	166	LYS	3.1
33	2b	71	VAL	3.1
50	2s	62	ILE	3.1
1	2A	2155	G	3.1
6	2G	169	ALA	3.1
36	2e	115	VAL	3.1
41	1j	10	GLY	3.1
50	2s	24	ALA	3.1
50	2s	41	VAL	3.1
53	2v	23	A	3.1
1	2A	1509	C	3.1
47	2p	74	LEU	3.1
40	2i	112	LYS	3.1

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
48	2q	90	ILE	3.1
40	2i	9	ARG	3.1
40	2i	79	LEU	3.1
3	1D	276	LYS	3.1
3	2D	276	LYS	3.1
34	2c	145	GLY	3.1
1	1A	932	C	3.1
40	2i	49	PRO	3.1
34	1c	12	LEU	3.0
6	2G	29	TRP	3.0
11	2P	79	ARG	3.0
39	2h	84	ARG	3.0
44	2m	88	ARG	3.0
48	1q	27	PHE	3.0
1	2A	2145	C	3.0
54	2w	72	C	3.0
43	2l	55	VAL	3.0
48	2q	84	LEU	3.0
22	20	5	LYS	3.0
22	20	8	GLY	3.0
32	1a	1531	A	3.0
43	2l	30	ALA	3.0
31	29	33	LYS	3.0
34	1c	39	ILE	3.0
34	2c	157	ILE	3.0
40	1i	15	ALA	3.0
1	2A	2111	C	3.0
35	2d	168	ARG	3.0
41	1j	98	ILE	3.0
43	2l	64	TYR	3.0
44	2m	90	LEU	3.0
46	1o	57	LEU	3.0
50	2s	77	THR	3.0
52	2u	11	GLY	3.0
40	2i	121	ARG	3.0
38	1g	32	ARG	3.0
43	2l	15	ARG	3.0
33	1b	133	LYS	3.0
29	17	46	VAL	3.0
47	2p	2	VAL	3.0
21	2Z	5	LEU	2.9
43	2l	32	PHE	2.9

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
45	2n	6	LEU	2.9
45	2n	53	LEU	2.9
52	1u	14	TRP	2.9
38	1g	79	ARG	2.9
40	2i	123	PRO	2.9
54	2w	15	G	2.9
35	1d	11	LEU	2.9
45	2n	55	GLY	2.9
41	1j	97	GLU	2.9
33	2b	185	ILE	2.9
32	2a	821	G	2.9
54	1w	73	A	2.9
54	2w	14	A	2.9
32	1a	1257	U	2.9
33	2b	37	ASN	2.9
9	2N	85	ILE	2.9
33	1b	215	LEU	2.9
4	2E	134	ILE	2.9
34	2c	134	ILE	2.9
21	2Z	149	SER	2.9
35	1d	165	MET	2.9
51	1t	69	GLY	2.9
6	2G	136	ARG	2.9
32	2a	1503	A	2.9
25	23	60	GLU	2.9
33	2b	122	PHE	2.9
41	2j	44	VAL	2.9
46	1o	66	LEU	2.9
7	2H	113	VAL	2.9
35	1d	118	ARG	2.9
28	26	4	GLU	2.8
39	2h	83	ILE	2.8
1	2A	2119	A	2.8
20	2Y	1	MET	2.8
51	1t	59	ALA	2.8
3	2D	5	LYS	2.8
32	2a	1532	U	2.8
44	2m	121	LYS	2.8
52	2u	23	PRO	2.8
21	2Z	139	VAL	2.8
29	17	48	LYS	2.8
33	1b	188	ALA	2.8

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
32	2a	1287	A	2.8
1	2A	2115	G	2.8
34	2c	5	ILE	2.8
47	2p	19	ILE	2.8
50	2s	71	LEU	2.8
48	2q	44	ALA	2.8
41	2j	61	GLU	2.8
36	2e	125	SER	2.8
51	1t	80	ARG	2.8
33	2b	201	ILE	2.8
32	2a	1224	G	2.8
34	2c	186	PHE	2.8
41	2j	89	ASP	2.8
46	2o	64	ARG	2.8
36	2e	9	LYS	2.8
40	2i	27	THR	2.8
45	2n	49	HIS	2.8
21	2Z	154	ASP	2.8
39	2h	112	LEU	2.8
46	2o	56	LEU	2.8
38	2g	79	ARG	2.8
40	2i	76	ALA	2.8
29	27	1	MET	2.8
35	2d	183	GLY	2.8
28	26	9	LEU	2.8
34	2c	201	TYR	2.8
54	2w	4	C	2.8
32	2a	1061	G	2.8
6	2G	39	ILE	2.8
15	2T	37	GLY	2.8
45	2n	24	CYS	2.8
44	2m	120	LYS	2.8
32	1a	204	U	2.8
38	2g	24	THR	2.8
32	2a	1354	C	2.8
30	28	34	TRP	2.7
34	2c	171	GLY	2.7
20	2Y	60	PHE	2.7
33	1b	163	PHE	2.7
17	2V	5	VAL	2.7
35	2d	108	LEU	2.7
14	2S	33	LYS	2.7

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
25	23	29	ARG	2.7
25	23	47	VAL	2.7
36	2e	120	THR	2.7
52	1u	18	TYR	2.7
46	2o	68	ARG	2.7
46	2o	72	ARG	2.7
38	1g	84	ASN	2.7
48	1q	23	VAL	2.7
40	1i	117	HIS	2.7
41	2j	46	ARG	2.7
1	2A	882	G	2.7
32	2a	1030(A)	G	2.7
33	1b	214	ILE	2.7
41	2j	6	ILE	2.7
41	2j	57	LYS	2.7
44	2m	101	GLN	2.7
38	1g	154	TYR	2.7
1	2A	2112	G	2.7
1	2A	2149	G	2.7
21	2Z	137	ILE	2.7
54	2w	2	C	2.7
44	2m	70	LEU	2.7
28	26	2	ALA	2.7
38	1g	85	TYR	2.7
40	2i	36	TYR	2.7
33	2b	94	ASN	2.7
35	2d	146	ILE	2.7
44	1m	122	LYS	2.7
1	2A	2116	G	2.7
21	2Z	24	LEU	2.7
21	2Z	155	LEU	2.7
39	2h	10	LEU	2.7
32	2a	965	A	2.7
40	2i	119	ALA	2.7
31	29	26	ILE	2.7
39	2h	92	ARG	2.7
52	2u	22	ARG	2.7
32	2a	1223	C	2.7
41	2j	34	VAL	2.7
48	2q	11	VAL	2.7
1	1A	1221	G	2.7
32	1a	1001	A	2.7

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
54	2y	23	A	2.7
54	2y	33	U	2.7
6	2G	139	LEU	2.7
35	1d	157	LEU	2.7
44	2m	19	LEU	2.7
33	2b	70	PHE	2.6
39	2h	111	ILE	2.6
40	2i	125	TYR	2.6
44	2m	84	ILE	2.6
50	2s	40	ILE	2.6
54	2y	45	U	2.6
6	2G	149	VAL	2.6
17	2V	72	VAL	2.6
33	2b	184	VAL	2.6
34	2c	41	GLY	2.6
32	2a	89	C	2.6
35	2d	164	ALA	2.6
32	2a	1202	G	2.6
34	2c	17	ASP	2.6
11	2P	77	ARG	2.6
38	2g	5	ARG	2.6
26	24	49	PHE	2.6
32	2a	1219	U	2.6
4	2E	10	GLY	2.6
6	2G	159	VAL	2.6
46	2o	89	GLY	2.6
32	2a	1092	A	2.6
32	2a	1531	A	2.6
39	1h	86	ILE	2.6
52	2u	10	ARG	2.6
11	2P	45	LEU	2.6
31	29	24	TYR	2.6
35	1d	167	GLY	2.6
25	23	12	PRO	2.6
34	2c	200	ALA	2.6
32	2a	1183	A	2.6
41	2j	100	THR	2.6
41	2j	74	ILE	2.6
52	2u	15	ARG	2.6
1	2A	2138	C	2.6
38	2g	40	ALA	2.6
35	2d	115	ARG	2.6

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
44	2m	104	ARG	2.6
7	2H	72	ILE	2.6
34	2c	14	ILE	2.6
27	15	60	VAL	2.6
41	1j	44	VAL	2.6
42	2k	25	TYR	2.6
44	2m	87	TYR	2.6
11	2P	18	ARG	2.6
40	2i	111	ARG	2.6
42	2k	35	PRO	2.6
44	1m	121	LYS	2.6
51	2t	26	ASN	2.6
38	2g	27	ILE	2.6
39	2h	120	THR	2.6
41	2j	96	ILE	2.6
32	2a	1220	G	2.6
5	2F	57	VAL	2.6
43	2l	18	VAL	2.6
52	2u	9	ARG	2.6
45	1n	7	ILE	2.5
33	2b	203	GLY	2.5
34	2c	91	LEU	2.5
46	1o	89	GLY	2.5
48	2q	22	LEU	2.5
1	2A	2896	C	2.5
6	2G	15	VAL	2.5
32	2a	1357	A	2.5
32	2a	1397	C	2.5
41	2j	53	PRO	2.5
9	2N	83	LYS	2.5
20	2Y	75	ILE	2.5
36	2e	24	ARG	2.5
46	2o	88	ARG	2.5
25	23	54	VAL	2.5
6	2G	163	ALA	2.5
3	2D	241	PRO	2.5
7	2H	35	VAL	2.5
35	1d	110	PHE	2.5
21	2Z	156	LYS	2.5
43	1l	16	GLU	2.5
1	2A	910	A	2.5
40	2i	83	ARG	2.5

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
54	1y	20	U	2.5
12	2Q	136	ALA	2.5
40	2i	120	ARG	2.5
6	2G	134	GLY	2.5
32	2a	1060	C	2.5
39	2h	87	SER	2.5
52	1u	2	GLY	2.5
1	2A	896	A	2.5
20	2Y	106	LEU	2.5
21	2Z	150	LEU	2.5
28	26	5	VAL	2.5
38	2g	75	VAL	2.5
40	2i	105	ASP	2.5
1	2A	884	C	2.5
25	23	26	LEU	2.5
52	2u	13	ILE	2.5
54	2w	31	A	2.5
34	2c	159	GLY	2.5
43	2l	7	ILE	2.5
48	2q	36	ILE	2.5
39	2h	101	PRO	2.5
48	2q	98	LEU	2.5
31	29	19	ARG	2.5
35	1d	133	VAL	2.5
40	2i	53	VAL	2.5
35	2d	110	PHE	2.5
26	24	40	HIS	2.5
40	1i	8	GLY	2.5
42	2k	69	ALA	2.5
14	2S	58	LEU	2.5
32	2a	1036	G	2.5
40	1i	114	TYR	2.5
32	2a	90	U	2.4
26	24	51	ASP	2.4
34	2c	80	GLY	2.4
36	2e	114	GLY	2.4
44	2m	105	THR	2.4
49	2r	66	LEU	2.4
3	2D	275	LYS	2.4
32	2a	1030	C	2.4
34	1c	13	GLY	2.4
40	2i	80	GLY	2.4

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
50	2s	69	HIS	2.4
7	2H	55	PRO	2.4
9	2N	1	MET	2.4
11	2P	75	ILE	2.4
31	29	13	LYS	2.4
33	2b	222	ILE	2.4
35	2d	148	VAL	2.4
34	2c	185	GLY	2.4
36	2e	13	ILE	2.4
39	2h	6	ILE	2.4
50	2s	47	HIS	2.4
40	2i	64	THR	2.4
42	2k	87	THR	2.4
52	1u	15	ARG	2.4
21	2Z	50	GLN	2.4
33	2b	186	ALA	2.4
6	2G	152	LEU	2.4
45	2n	47	LEU	2.4
11	2P	51	PHE	2.4
29	27	23	ARG	2.4
37	2f	6	VAL	2.4
40	2i	62	TYR	2.4
43	2l	43	VAL	2.4
54	2w	23	A	2.4
54	1w	20	U	2.4
38	2g	147	ALA	2.4
38	2g	152	ALA	2.4
44	2m	66	LEU	2.4
32	1a	1033	G	2.4
32	2a	1064	G	2.4
9	2N	103	VAL	2.4
17	2V	85	LYS	2.4
33	2b	105	PHE	2.4
35	1d	115	ARG	2.4
40	1i	112	LYS	2.4
41	1j	57	LYS	2.4
45	2n	8	GLU	2.4
39	2h	9	MET	2.4
46	2o	57	LEU	2.4
6	2G	48	GLU	2.4
39	2h	128	GLY	2.4
10	2O	81	ASP	2.4

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
32	2a	928	G	2.4
3	2D	153	ALA	2.4
53	1v	24	A	2.4
54	1y	35	A	2.4
3	2D	217	ARG	2.4
17	2V	71	LEU	2.4
33	1b	227	GLY	2.3
40	2i	88	TYR	2.3
11	2P	58	THR	2.3
42	2k	73	MET	2.3
42	2k	112	THR	2.3
46	2o	59	MET	2.3
40	2i	20	ARG	2.3
54	2w	70	G	2.3
1	1A	1142	A	2.3
12	2Q	37	LEU	2.3
24	22	60	LEU	2.3
46	2o	61	GLY	2.3
34	2c	174	PRO	2.3
45	2n	58	LYS	2.3
41	1j	66	ARG	2.3
32	1a	1034	G	2.3
34	2c	8	ILE	2.3
36	2e	29	GLY	2.3
42	2k	86	GLY	2.3
1	2A	2139	C	2.3
28	26	52	VAL	2.3
36	2e	33	VAL	2.3
6	2G	115	ARG	2.3
39	2h	37	ARG	2.3
47	1p	68	ASP	2.3
3	1D	2	ALA	2.3
41	2j	42	THR	2.3
32	2a	1398	A	2.3
40	1i	121	ARG	2.3
43	2l	39	VAL	2.3
54	1w	72	C	2.3
33	1b	232	PRO	2.3
12	2Q	103	MET	2.3
49	1r	31	LEU	2.3
11	2P	76	LYS	2.3
48	2q	37	LYS	2.3

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
50	2s	38	SER	2.3
44	2m	80	ARG	2.3
45	2n	18	VAL	2.3
32	2a	969	A	2.3
32	2a	973	G	2.3
1	1A	271	U	2.3
41	2j	58	ASP	2.3
12	2Q	121	ALA	2.3
16	2U	96	ALA	2.3
48	2q	95	TYR	2.3
51	1t	66	ALA	2.3
35	2d	204	ILE	2.3
38	2g	32	ARG	2.3
40	2i	67	GLY	2.3
1	2A	2113	U	2.3
1	2A	2137	C	2.3
21	2Z	148	ASP	2.3
32	2a	84	U	2.3
54	2w	45	U	2.3
32	2a	1035	A	2.3
5	2F	41	LEU	2.3
10	2O	19	ILE	2.3
33	2b	69	LEU	2.3
33	2b	211	ILE	2.3
40	1i	19	LEU	2.3
40	2i	19	LEU	2.3
51	2t	25	ARG	2.3
41	2j	87	THR	2.3
47	1p	22	THR	2.3
36	2e	21	ALA	2.3
43	1l	64	TYR	2.3
43	2l	52	LEU	2.3
47	1p	7	ALA	2.3
47	1p	39	TYR	2.3
1	2A	2147	G	2.3
54	2y	1	G	2.3
9	2N	69	GLN	2.3
33	2b	164	VAL	2.3
40	2i	126	SER	2.3
23	2l	76	ARG	2.3
40	2i	66	ARG	2.3
41	1j	62	HIS	2.3

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
35	1d	101	LEU	2.3
40	2i	122	ALA	2.3
46	1o	69	TYR	2.3
34	2c	4	LYS	2.3
53	1v	13	A	2.3
32	2a	1353	G	2.3
43	2l	8	ASN	2.2
34	2c	197	GLY	2.2
35	2d	165	MET	2.2
35	2d	176	LEU	2.2
38	2g	156	TRP	2.2
39	1h	35	ILE	2.2
40	2i	30	GLY	2.2
48	2q	43	LEU	2.2
48	2q	53	LEU	2.2
22	20	45	PHE	2.2
51	2t	55	ILE	2.2
24	12	70	GLN	2.2
39	2h	136	GLU	2.2
32	2a	1385	G	2.2
1	2A	2897	U	2.2
32	2a	1393	U	2.2
33	2b	163	PHE	2.2
21	2Z	38	TYR	2.2
25	23	6	VAL	2.2
29	17	47	ARG	2.2
33	2b	136	VAL	2.2
45	2n	15	LYS	2.2
32	2a	1392	G	2.2
34	2c	155	GLY	2.2
54	2w	5	G	2.2
36	2e	81	GLU	2.2
50	2s	48	THR	2.2
40	1i	81	ILE	2.2
51	2t	73	HIS	2.2
36	2e	107	ARG	2.2
41	1j	9	ARG	2.2
12	2Q	109	VAL	2.2
43	1l	90	VAL	2.2
45	1n	56	VAL	2.2
35	1d	102	ASP	2.2
33	2b	210	SER	2.2

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
40	2i	82	ALA	2.2
48	2q	7	THR	2.2
52	1u	24	ARG	2.2
1	2A	2153	G	2.2
54	2y	53	G	2.2
44	2m	7	VAL	2.2
48	2q	86	GLU	2.2
7	2H	2	SER	2.2
14	2S	21	THR	2.2
30	28	2	PRO	2.2
31	29	1	MET	2.2
1	2A	2159	G	2.2
32	2a	1117	G	2.2
31	29	2	LYS	2.2
32	2a	879	C	2.2
37	2f	92	LYS	2.2
40	2i	10	ARG	2.2
1	1A	2906	U	2.2
42	2k	29	ILE	2.2
7	2H	41	MET	2.2
33	1b	101	MET	2.2
43	2l	9	GLN	2.2
44	2m	10	PRO	2.2
1	1A	1141	A	2.2
34	1c	198	VAL	2.2
1	2A	614(B)	G	2.2
6	2G	133	LEU	2.2
32	2a	1283	G	2.2
30	28	10	ALA	2.2
36	1e	21	ALA	2.2
36	2e	28	PHE	2.2
41	1j	11	PHE	2.2
30	18	2	PRO	2.2
33	2b	90	MET	2.2
33	2b	216	SER	2.2
40	1i	49	PRO	2.2
36	2e	98	THR	2.2
45	2n	13	THR	2.2
34	2c	164	ARG	2.2
35	1d	139	ARG	2.2
52	1u	3	LYS	2.2
32	2a	1093	A	2.2

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
40	2i	108	VAL	2.2
50	2s	9	VAL	2.2
16	2U	98	LEU	2.1
33	2b	17	PHE	2.1
34	2c	178	LEU	2.1
36	2e	142	LEU	2.1
38	2g	22	LEU	2.1
47	2p	6	LEU	2.1
33	1b	201	ILE	2.1
33	2b	214	ILE	2.1
1	2A	881	G	2.1
1	2A	1816	G	2.1
1	2A	2127	G	2.1
7	2H	38	SER	2.1
20	2Y	50	ARG	2.1
35	2d	156	GLU	2.1
35	2d	159	ARG	2.1
45	2n	26	ARG	2.1
48	2q	91	ARG	2.1
30	18	14	VAL	2.1
39	2h	135	CYS	2.1
40	2i	5	TYR	2.1
50	2s	68	GLY	2.1
38	2g	39	ALA	2.1
1	1A	931	C	2.1
40	2i	107	ARG	2.1
3	2D	180	GLY	2.1
36	2e	133	TYR	2.1
50	2s	52	TYR	2.1
13	2R	69	ASP	2.1
40	2i	33	PHE	2.1
45	2n	16	PHE	2.1
3	2D	126	GLN	2.1
12	2Q	13	GLN	2.1
33	2b	41	ILE	2.1
34	1c	14	ILE	2.1
36	2e	20	GLN	2.1
38	1g	4	ARG	2.1
1	1A	2807	C	2.1
1	2A	2160	G	2.1
32	1a	1032	G	2.1
34	2c	45	LYS	2.1

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
44	2m	103	THR	2.1
50	2s	70	LYS	2.1
54	2y	44	G	2.1
8	2I	38	LEU	2.1
10	2O	7	TYR	2.1
34	1c	87	LEU	2.1
35	1d	120	LEU	2.1
1	2A	6	A	2.1
1	2A	901	A	2.1
45	2n	27	CYS	2.1
5	2F	163	VAL	2.1
20	2Y	45	VAL	2.1
30	28	9	GLY	2.1
48	2q	21	VAL	2.1
21	2Z	48	PHE	2.1
33	2b	31	TYR	2.1
34	2c	12	LEU	2.1
41	1j	45	ARG	2.1
32	2a	1401	G	2.1
33	2b	220	ASP	2.1
54	2w	24	G	2.1
40	2i	63	ILE	2.1
47	1p	24	ALA	2.1
48	2q	65	ILE	2.1
20	2Y	4	LYS	2.1
42	2k	117	ASN	2.1
35	2d	73	ARG	2.1
46	1o	65	ARG	2.1
3	2D	17	THR	2.1
50	2s	15	LEU	2.1
26	24	32	TYR	2.1
52	1u	21	TYR	2.1
53	2v	22	U	2.1
1	2A	2100	G	2.1
32	1a	1030(A)	G	2.1
32	1a	1030(C)	G	2.1
32	2a	584	G	2.1
26	24	54	GLY	2.1
29	27	27	GLY	2.1
52	2u	2	GLY	2.1
11	2P	1	MET	2.1
35	2d	56	VAL	2.1

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
52	1u	22	ARG	2.1
1	1A	935	C	2.1
32	2a	1114	C	2.1
48	2q	31	LEU	2.1
30	28	29	LYS	2.1
5	2F	80	ALA	2.1
30	28	16	ILE	2.1
44	2m	107	ALA	2.1
47	2p	24	ALA	2.1
48	1q	90	ILE	2.1
33	2b	48	MET	2.1
35	1d	168	ARG	2.1
38	2g	78	ARG	2.1
51	2t	23	ARG	2.1
36	1e	55	VAL	2.1
1	2A	2174	C	2.1
32	1a	1030	C	2.1
32	2a	977	A	2.1
32	2a	1115	C	2.1
33	2b	123	ALA	2.1
36	2e	76	ILE	2.1
35	1d	66	ARG	2.1
48	1q	25	ARG	2.1
7	2H	32	GLU	2.1
35	2d	133	VAL	2.1
36	2e	19	MET	2.1
43	2l	5	PRO	2.1
33	2b	215	LEU	2.0
51	2t	20	LEU	2.0
54	2y	56	C	2.0
33	1b	41	ILE	2.0
38	1g	42	ILE	2.0
39	2h	94	TYR	2.0
6	2G	160	VAL	2.0
25	23	16	PRO	2.0
35	1d	62	GLN	2.0
38	1g	153	HIS	2.0
1	1A	943	C	2.0
5	2F	64	ILE	2.0
35	1d	137	SER	2.0
7	2H	96	ALA	2.0
33	2b	67	THR	2.0

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Mol	Chain	Res	Type	RSRZ
34	2c	206	GLU	2.0
35	1d	207	TYR	2.0
40	2i	45	ALA	2.0
48	2q	23	VAL	2.0
44	2m	97	PRO	2.0
9	2N	116	LEU	2.0
21	2Z	121	HIS	2.0
14	2S	57	LYS	2.0
25	23	17	LYS	2.0
39	1h	83	ILE	2.0
41	2j	12	ASP	2.0
11	2P	74	GLU	2.0
20	2Y	10	GLY	2.0
1	2A	2144	U	2.0
33	1b	207	ALA	2.0
33	2b	66	GLY	2.0
36	2e	86	ALA	2.0
21	2Z	99	TYR	2.0
32	2a	1185	G	2.0
32	2a	1521	G	2.0
47	2p	22	THR	2.0
7	2H	103	LEU	2.0
16	1U	117	GLN	2.0
33	2b	96	ARG	2.0
14	2S	34	HIS	2.0
16	2U	17	ILE	2.0
41	2j	73	ASP	2.0
12	2Q	2	LEU	2.0
42	2k	13	GLN	2.0
50	1s	71	LEU	2.0
51	2t	21	LYS	2.0
51	2t	29	LYS	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
54	7MG	2y	46	24/25	0.69	0.26	84,90,96,114	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
54	PSU	2y	55	20/21	0.69	0.37	79,93,100,105	0
54	PSU	1y	55	20/21	0.72	0.25	78,86,93,105	0
54	5MU	2y	54	21/22	0.74	0.31	76,85,92,102	0
54	MIA	2y	37	22/30	0.78	0.39	64,78,97,111	0
54	7MG	1w	46	24/25	0.78	0.20	67,77,94,110	0
54	PSU	2y	32	20/21	0.80	0.27	65,77,84,86	0
54	7MG	1y	46	24/25	0.81	0.23	73,85,99,104	0
54	7MG	2w	46	24/25	0.81	0.26	71,87,94,109	0
54	4SU	2w	8	20/21	0.82	0.22	78,86,91,102	0
43	0TD	2l	92	10/11	0.83	0.25	52,60,64,75	0
54	PSU	2w	55	20/21	0.85	0.20	64,79,86,88	0
54	5MU	1y	54	21/22	0.85	0.26	78,82,88,97	0
54	PSU	2y	39	20/21	0.86	0.32	72,77,89,97	0
54	PSU	1y	32	20/21	0.86	0.24	64,71,75,82	0
54	MIA	1y	37	22/30	0.87	0.17	62,72,77,85	0
32	2MG	2a	1207	24/25	0.87	0.19	68,74,82,88	0
54	4SU	2y	8	20/21	0.87	0.19	79,88,94,100	0
55	4SU	2x	8	20/21	0.87	0.16	64,75,77,77	0
54	4SU	1y	8	20/21	0.88	0.19	77,82,89,92	0
54	PSU	1w	55	20/21	0.88	0.20	54,67,73,75	0
54	PSU	2w	32	20/21	0.89	0.31	70,78,89,93	0
54	5MU	2w	54	21/22	0.89	0.16	66,71,77,82	0
1	PSU	2A	1911	20/21	0.90	0.18	54,62,67,68	0
54	PSU	1y	39	20/21	0.90	0.16	61,69,75,82	0
43	0TD	1l	92	10/11	0.90	0.30	38,44,52,72	0
54	MIA	2w	37	25/30	0.91	0.28	63,70,76,85	0
1	5MU	2A	1915	21/22	0.91	0.17	63,70,76,88	0
1	PSU	2A	1917	20/21	0.91	0.22	52,61,72,74	0
32	PSU	2a	516	20/21	0.91	0.22	61,68,74,74	0
32	M2G	2a	966	25/26	0.92	0.29	48,59,69,78	0
32	4OC	2a	1402	22/23	0.92	0.26	52,62,65,65	0
32	5MC	2a	967	21/22	0.92	0.25	56,62,70,74	0
54	PSU	1w	32	20/21	0.92	0.25	54,60,77,78	0
55	5MC	2x	32	21/22	0.92	0.23	57,66,73,74	0
55	5MU	2x	54	21/22	0.92	0.19	65,73,79,82	0
55	PSU	2x	55	20/21	0.92	0.18	66,75,77,78	0
32	5MC	2a	1400	21/22	0.93	0.31	63,66,71,75	0
54	PSU	2w	39	20/21	0.93	0.28	63,71,75,79	0
1	5MU	1A	1937	21/22	0.93	0.20	38,48,53,61	0
32	5MC	2a	1404	21/22	0.93	0.27	50,56,61,66	0
1	4OC	2A	1920	21/23	0.93	0.20	53,60,63,65	0
54	4SU	1w	8	20/21	0.93	0.16	65,70,76,79	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
55	4SU	1x	8	20/21	0.94	0.21	46,54,68,74	0
54	5MU	1w	54	21/22	0.94	0.18	46,56,65,71	0
32	7MG	2a	527	24/25	0.94	0.23	51,57,66,74	0
32	UR3	2a	1498	21/22	0.94	0.28	44,57,63,66	0
32	7MG	1a	527	24/25	0.94	0.20	39,45,48,52	0
1	5MC	2A	1962	21/22	0.95	0.22	39,48,55,58	0
32	5MC	2a	1407	21/22	0.95	0.22	45,53,58,61	0
32	5MC	1a	967	21/22	0.95	0.23	38,49,53,55	0
32	PSU	1a	516	20/21	0.95	0.19	39,50,55,56	0
1	PSU	1A	1939	20/21	0.95	0.24	38,45,50,52	0
1	5MC	2A	1942	21/22	0.96	0.20	44,52,59,61	0
32	5MC	1a	1404	21/22	0.96	0.26	30,36,40,44	0
32	MA6	2a	1518	24/25	0.96	0.28	46,64,67,69	0
32	MA6	2a	1519	24/25	0.96	0.32	46,57,63,65	0
1	OMG	2A	2251	24/25	0.96	0.25	34,40,45,47	0
54	MIA	1w	37	29/30	0.96	0.23	35,48,55,63	0
1	PSU	2A	2605	20/21	0.96	0.21	26,37,41,42	0
55	5MC	1x	32	21/22	0.96	0.23	43,50,54,58	0
1	4OC	1A	1942	21/23	0.96	0.24	27,36,42,43	0
55	5MU	1x	54	21/22	0.96	0.17	50,57,63,68	0
32	2MG	1a	1207	24/25	0.96	0.17	50,59,63,65	0
55	PSU	1x	55	20/21	0.96	0.17	41,51,60,65	0
54	PSU	1w	39	20/21	0.96	0.23	44,55,60,63	0
32	M2G	1a	966	25/26	0.97	0.25	33,45,55,56	0
1	5MC	1A	1964	21/22	0.97	0.21	24,30,36,39	0
1	5MC	1A	1984	21/22	0.97	0.21	20,27,30,40	0
32	4OC	1a	1402	22/23	0.97	0.22	37,41,51,56	0
1	5MU	2A	1939	21/22	0.97	0.20	30,38,42,42	0
1	PSU	1A	1933	20/21	0.97	0.21	33,40,47,48	0
32	MA6	1a	1518	24/25	0.97	0.25	25,33,39,39	0
1	5MU	1A	1961	21/22	0.97	0.24	15,21,26,34	0
1	2MA	2A	2503	23/24	0.97	0.23	26,29,33,34	0
1	2MU	2A	2552	21/23	0.97	0.21	32,38,45,57	0
32	UR3	1a	1498	21/22	0.98	0.23	28,35,39,40	0
1	PSU	1A	2617	20/21	0.98	0.21	15,18,23,23	0
32	MA6	1a	1519	24/25	0.98	0.23	29,35,39,41	0
1	OMG	1A	2263	24/25	0.98	0.23	13,19,21,24	0
32	5MC	1a	1400	21/22	0.98	0.20	33,44,49,57	0
1	2MA	1A	2515	23/24	0.98	0.23	7,11,15,21	0
1	2MU	1A	2564	21/23	0.98	0.24	14,20,26,28	0
32	5MC	1a	1407	21/22	0.98	0.21	29,34,39,42	0

### 6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

### 6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	2A	3675	1/1	0.28	0.44	63,63,63,63	0
56	MG	2a	3113	1/1	0.38	0.79	72,72,72,72	0
56	MG	2a	3116	1/1	0.39	0.17	73,73,73,73	0
56	MG	2a	3166	1/1	0.39	0.13	66,66,66,66	0
56	MG	2A	3674	1/1	0.40	0.09	62,62,62,62	0
56	MG	2a	3161	1/1	0.44	0.18	70,70,70,70	0
56	MG	1A	3966	1/1	0.47	0.14	41,41,41,41	0
56	MG	2A	3723	1/1	0.49	0.39	65,65,65,65	0
56	MG	2A	3766	1/1	0.49	0.36	85,85,85,85	0
56	MG	1v	3001	1/1	0.49	0.63	67,67,67,67	0
56	MG	2A	3542	1/1	0.50	0.18	52,52,52,52	0
56	MG	1A	3861	1/1	0.51	0.15	15,15,15,15	0
56	MG	1A	3891	1/1	0.51	0.56	74,74,74,74	0
56	MG	1x	115	1/1	0.51	0.31	62,62,62,62	0
56	MG	2A	3651	1/1	0.52	0.26	56,56,56,56	0
56	MG	1A	3998	1/1	0.53	0.13	51,51,51,51	0
56	MG	2x	3002	1/1	0.53	0.14	69,69,69,69	0
56	MG	1a	3171	1/1	0.54	0.11	55,55,55,55	0
56	MG	1A	3949	1/1	0.54	0.13	58,58,58,58	0
56	MG	2A	3850	1/1	0.56	0.38	67,67,67,67	0
56	MG	1a	3174	1/1	0.56	0.14	76,76,76,76	0
56	MG	2a	3123	1/1	0.58	0.19	75,75,75,75	0
56	MG	2A	3343	1/1	0.58	0.25	65,65,65,65	0
56	MG	1A	3034	1/1	0.59	0.19	56,56,56,56	0
56	MG	2A	3021	1/1	0.59	0.19	64,64,64,64	0
56	MG	2A	3022	1/1	0.60	0.27	51,51,51,51	0
56	MG	2a	3129	1/1	0.60	0.14	64,64,64,64	0
56	MG	2U	202	1/1	0.60	0.50	63,63,63,63	0
56	MG	1A	3752	1/1	0.60	0.15	58,58,58,58	0
56	MG	2A	3460	1/1	0.60	0.19	35,35,35,35	0
56	MG	1A	3981	1/1	0.61	0.09	49,49,49,49	0
56	MG	2A	3072	1/1	0.61	0.32	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	3785	1/1	0.61	0.09	63,63,63,63	0
56	MG	2A	3227	1/1	0.61	0.22	69,69,69,69	0
56	MG	2A	3432	1/1	0.62	0.51	65,65,65,65	0
56	MG	1a	3202	1/1	0.62	0.17	53,53,53,53	0
56	MG	1A	3923	1/1	0.62	0.15	56,56,56,56	0
56	MG	2x	3003	1/1	0.62	0.14	66,66,66,66	0
56	MG	2A	3762	1/1	0.63	0.11	51,51,51,51	0
56	MG	2A	3579	1/1	0.64	0.24	65,65,65,65	0
56	MG	2A	3818	1/1	0.65	0.13	38,38,38,38	0
56	MG	2a	3096	1/1	0.65	0.39	62,62,62,62	0
56	MG	1a	3194	1/1	0.65	0.23	55,55,55,55	0
56	MG	2a	3152	1/1	0.65	0.27	67,67,67,67	0
56	MG	1a	3218	1/1	0.66	0.13	55,55,55,55	0
56	MG	2A	3260	1/1	0.66	0.14	48,48,48,48	0
56	MG	1w	103	1/1	0.66	0.12	55,55,55,55	0
56	MG	1a	3038	1/1	0.67	0.31	50,50,50,50	0
56	MG	2A	3187	1/1	0.67	0.68	43,43,43,43	0
56	MG	2A	3192	1/1	0.67	0.14	67,67,67,67	0
56	MG	1a	3211	1/1	0.67	0.16	65,65,65,65	0
56	MG	2A	3056	1/1	0.67	0.33	56,56,56,56	0
56	MG	2A	3643	1/1	0.67	0.10	57,57,57,57	0
56	MG	2A	3767	1/1	0.67	0.11	39,39,39,39	0
56	MG	2A	3339	1/1	0.68	0.46	68,68,68,68	0
56	MG	1a	3108	1/1	0.68	0.33	60,60,60,60	0
56	MG	2A	3743	1/1	0.68	0.16	47,47,47,47	0
56	MG	2A	3749	1/1	0.68	0.14	66,66,66,66	0
56	MG	2A	3404	1/1	0.68	0.22	65,65,65,65	0
56	MG	1A	4049	1/1	0.68	0.14	36,36,36,36	0
56	MG	1A	3475	1/1	0.68	0.53	67,67,67,67	0
56	MG	2y	104	1/1	0.68	0.22	85,85,85,85	0
56	MG	1A	4036	1/1	0.69	0.14	37,37,37,37	0
56	MG	1a	3210	1/1	0.69	0.08	57,57,57,57	0
56	MG	1A	3558	1/1	0.69	0.39	42,42,42,42	0
56	MG	1O	3001	1/1	0.69	0.46	60,60,60,60	0
56	MG	1A	3926	1/1	0.69	0.14	31,31,31,31	0
56	MG	2A	3741	1/1	0.69	0.59	76,76,76,76	0
56	MG	1A	3452	1/1	0.69	0.21	40,40,40,40	0
56	MG	2A	3390	1/1	0.69	0.18	57,57,57,57	0
56	MG	1a	3129	1/1	0.69	0.10	46,46,46,46	0
56	MG	1a	3153	1/1	0.69	0.16	43,43,43,43	0
56	MG	1A	3766	1/1	0.69	0.25	44,44,44,44	0
56	MG	1A	3498	1/1	0.69	0.15	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	3502	1/1	0.69	0.19	62,62,62,62	0
56	MG	1A	4019	1/1	0.70	0.14	29,29,29,29	0
56	MG	1A	3571	1/1	0.70	0.17	28,28,28,28	0
56	MG	1A	3777	1/1	0.70	0.20	37,37,37,37	0
56	MG	1A	3717	1/1	0.70	0.17	23,23,23,23	0
56	MG	1a	3029	1/1	0.70	0.19	63,63,63,63	0
56	MG	1A	3328	1/1	0.70	0.32	44,44,44,44	0
56	MG	2A	3268	1/1	0.70	0.19	59,59,59,59	0
56	MG	2A	3269	1/1	0.70	0.17	54,54,54,54	0
56	MG	1a	3055	1/1	0.70	0.11	68,68,68,68	0
56	MG	1A	3895	1/1	0.70	0.09	61,61,61,61	0
56	MG	2A	3748	1/1	0.70	0.16	48,48,48,48	0
56	MG	1A	3991	1/1	0.70	0.32	41,41,41,41	0
56	MG	1A	3916	1/1	0.70	0.18	26,26,26,26	0
56	MG	2A	3414	1/1	0.70	0.25	55,55,55,55	0
56	MG	1A	4018	1/1	0.70	0.24	52,52,52,52	0
56	MG	1A	3924	1/1	0.71	0.19	40,40,40,40	0
56	MG	1A	3983	1/1	0.71	0.18	14,14,14,14	0
56	MG	1w	102	1/1	0.71	0.36	54,54,54,54	0
56	MG	1A	3492	1/1	0.71	0.47	71,71,71,71	0
56	MG	1A	3932	1/1	0.71	0.10	25,25,25,25	0
56	MG	2A	3794	1/1	0.71	0.09	67,67,67,67	0
56	MG	2A	3727	1/1	0.71	0.08	45,45,45,45	0
56	MG	1A	3840	1/1	0.71	0.13	29,29,29,29	0
56	MG	1A	3894	1/1	0.71	0.10	36,36,36,36	0
56	MG	1A	3980	1/1	0.71	0.09	61,61,61,61	0
56	MG	2A	3493	1/1	0.72	0.19	46,46,46,46	0
56	MG	2a	3110	1/1	0.72	0.22	60,60,60,60	0
56	MG	1A	3896	1/1	0.72	0.16	60,60,60,60	0
56	MG	1a	3138	1/1	0.72	0.10	30,30,30,30	0
56	MG	1A	3834	1/1	0.72	0.14	57,57,57,57	0
56	MG	2A	3082	1/1	0.72	0.19	52,52,52,52	0
56	MG	2A	3091	1/1	0.72	0.17	50,50,50,50	0
56	MG	2E	301	1/1	0.72	0.12	53,53,53,53	0
56	MG	2Q	204	1/1	0.72	0.27	49,49,49,49	0
56	MG	1a	3160	1/1	0.72	0.19	62,62,62,62	0
56	MG	2V	201	1/1	0.72	0.44	58,58,58,58	0
56	MG	2a	3063	1/1	0.72	0.14	46,46,46,46	0
56	MG	2A	3048	1/1	0.73	0.15	43,43,43,43	0
56	MG	1A	3591	1/1	0.73	0.23	38,38,38,38	0
56	MG	2B	3019	1/1	0.73	0.33	75,75,75,75	0
56	MG	2D	304	1/1	0.73	0.20	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	3290	1/1	0.73	0.12	77,77,77,77	0
56	MG	2A	3655	1/1	0.73	0.09	55,55,55,55	0
56	MG	1A	4023	1/1	0.73	0.18	31,31,31,31	0
56	MG	1a	3047	1/1	0.73	0.16	52,52,52,52	0
56	MG	28	101	1/1	0.73	0.19	60,60,60,60	0
56	MG	1A	4033	1/1	0.73	0.26	55,55,55,55	0
56	MG	2A	3397	1/1	0.73	0.23	59,59,59,59	0
56	MG	2A	3099	1/1	0.73	0.17	43,43,43,43	0
56	MG	2A	3411	1/1	0.73	0.21	71,71,71,71	0
56	MG	2a	3115	1/1	0.73	0.14	56,56,56,56	0
56	MG	1a	3180	1/1	0.73	0.14	55,55,55,55	0
56	MG	2A	3191	1/1	0.73	0.13	43,43,43,43	0
56	MG	1A	3671	1/1	0.73	0.16	40,40,40,40	0
56	MG	2a	3141	1/1	0.73	0.09	71,71,71,71	0
56	MG	1A	3929	1/1	0.73	0.17	28,28,28,28	0
56	MG	1A	3405	1/1	0.73	0.20	30,30,30,30	0
56	MG	2A	3773	1/1	0.73	0.09	57,57,57,57	0
56	MG	2a	3173	1/1	0.73	0.18	62,62,62,62	0
56	MG	2A	3553	1/1	0.73	0.12	39,39,39,39	0
56	MG	2A	3562	1/1	0.73	0.12	32,32,32,32	0
56	MG	2A	3806	1/1	0.73	0.28	55,55,55,55	0
56	MG	2a	3144	1/1	0.74	0.15	76,76,76,76	0
56	MG	2a	3151	1/1	0.74	0.12	53,53,53,53	0
56	MG	1A	3962	1/1	0.74	0.18	15,15,15,15	0
56	MG	2A	3522	1/1	0.74	0.16	30,30,30,30	0
56	MG	1a	3152	1/1	0.74	0.08	55,55,55,55	0
56	MG	1A	3965	1/1	0.74	0.08	65,65,65,65	0
56	MG	2a	3195	1/1	0.74	0.36	69,69,69,69	0
56	MG	2j	8001	1/1	0.74	0.16	77,77,77,77	0
56	MG	1w	104	1/1	0.74	0.14	54,54,54,54	0
56	MG	1A	3495	1/1	0.74	0.17	61,61,61,61	0
56	MG	2A	3483	1/1	0.74	0.13	35,35,35,35	0
56	MG	1A	3372	1/1	0.75	0.51	25,25,25,25	0
56	MG	2a	3142	1/1	0.75	0.13	56,56,56,56	0
56	MG	25	105	1/1	0.75	0.21	55,55,55,55	0
56	MG	2A	3418	1/1	0.75	0.22	65,65,65,65	0
56	MG	2a	3017	1/1	0.75	0.13	65,65,65,65	0
56	MG	2A	3338	1/1	0.75	0.14	66,66,66,66	0
56	MG	2a	3165	1/1	0.75	0.19	52,52,52,52	0
56	MG	10	101	1/1	0.75	0.34	43,43,43,43	0
56	MG	2B	3018	1/1	0.75	0.20	74,74,74,74	0
56	MG	1a	3062	1/1	0.75	0.11	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	1A	3806	1/1	0.75	0.21	41,41,41,41	0
56	MG	1A	3635	1/1	0.75	0.15	18,18,18,18	0
56	MG	2A	3136	1/1	0.75	0.20	54,54,54,54	0
56	MG	2A	3158	1/1	0.75	0.24	47,47,47,47	0
56	MG	2a	3021	1/1	0.76	0.17	64,64,64,64	0
56	MG	2a	3054	1/1	0.76	0.11	65,65,65,65	0
56	MG	2A	3006	1/1	0.76	0.14	51,51,51,51	0
56	MG	1a	3012	1/1	0.76	0.22	50,50,50,50	0
56	MG	1A	3387	1/1	0.76	0.13	42,42,42,42	0
56	MG	2A	3769	1/1	0.76	0.10	46,46,46,46	0
56	MG	1A	3583	1/1	0.76	0.11	31,31,31,31	0
56	MG	1A	3900	1/1	0.76	0.16	42,42,42,42	0
56	MG	2a	3120	1/1	0.76	0.15	75,75,75,75	0
56	MG	1A	3906	1/1	0.76	0.08	43,43,43,43	0
56	MG	1A	3845	1/1	0.76	0.39	41,41,41,41	0
56	MG	2a	3131	1/1	0.76	0.07	87,87,87,87	0
56	MG	2a	3137	1/1	0.76	0.10	48,48,48,48	0
56	MG	2A	3384	1/1	0.76	0.13	42,42,42,42	0
56	MG	1a	3097	1/1	0.76	0.37	59,59,59,59	0
56	MG	2A	3873	1/1	0.76	0.73	41,41,41,41	0
56	MG	2B	3014	1/1	0.76	0.22	58,58,58,58	0
56	MG	2A	3669	1/1	0.76	0.17	64,64,64,64	0
56	MG	1A	3858	1/1	0.76	0.16	21,21,21,21	0
56	MG	2A	3125	1/1	0.76	0.18	51,51,51,51	0
56	MG	1A	3057	1/1	0.76	0.21	36,36,36,36	0
56	MG	1A	4053	1/1	0.76	0.15	45,45,45,45	0
56	MG	2A	3734	1/1	0.76	0.20	65,65,65,65	0
56	MG	1A	4105	1/1	0.76	0.23	44,44,44,44	0
56	MG	1A	3509	1/1	0.76	0.32	47,47,47,47	0
56	MG	1w	108	1/1	0.76	0.80	80,80,80,80	0
56	MG	1A	3227	1/1	0.76	0.39	28,28,28,28	0
59	ZN	24	501	1/1	0.76	0.10	86,86,86,86	0
56	MG	2A	3261	1/1	0.77	0.36	57,57,57,57	0
56	MG	1A	3994	1/1	0.77	0.37	48,48,48,48	0
56	MG	2A	3869	1/1	0.77	0.10	55,55,55,55	0
56	MG	2A	3718	1/1	0.77	0.26	56,56,56,56	0
56	MG	2A	3719	1/1	0.77	0.12	64,64,64,64	0
56	MG	1A	3244	1/1	0.77	0.33	65,65,65,65	0
56	MG	1A	3430	1/1	0.77	0.26	32,32,32,32	0
56	MG	1A	3812	1/1	0.77	0.09	38,38,38,38	0
56	MG	2A	3140	1/1	0.77	0.28	44,44,44,44	0
56	MG	2A	3342	1/1	0.77	0.19	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	2A	3545	1/1	0.77	0.09	56,56,56,56	0
56	MG	1A	3770	1/1	0.77	0.10	43,43,43,43	0
56	MG	20	3001	1/1	0.77	0.17	57,57,57,57	0
56	MG	2a	3156	1/1	0.77	0.14	56,56,56,56	0
56	MG	1A	4108	1/1	0.77	0.35	28,28,28,28	0
56	MG	1B	3031	1/1	0.77	0.23	59,59,59,59	0
56	MG	2A	3597	1/1	0.77	0.25	50,50,50,50	0
56	MG	2A	3080	1/1	0.77	0.14	59,59,59,59	0
56	MG	2a	3050	1/1	0.77	0.23	57,57,57,57	0
56	MG	1w	109	1/1	0.77	0.17	51,51,51,51	0
56	MG	2A	3255	1/1	0.77	0.15	63,63,63,63	0
56	MG	2a	3068	1/1	0.77	0.23	70,70,70,70	0
56	MG	2A	3663	1/1	0.77	0.36	55,55,55,55	0
56	MG	2A	3087	1/1	0.77	0.13	61,61,61,61	0
56	MG	1B	3027	1/1	0.78	0.09	59,59,59,59	0
56	MG	2A	3403	1/1	0.78	0.23	52,52,52,52	0
56	MG	1A	3928	1/1	0.78	0.11	42,42,42,42	0
56	MG	2A	3239	1/1	0.78	0.25	46,46,46,46	0
56	MG	1A	4042	1/1	0.78	0.46	64,64,64,64	0
56	MG	1A	3979	1/1	0.78	0.07	63,63,63,63	0
56	MG	1a	3201	1/1	0.78	0.11	51,51,51,51	0
56	MG	2A	3266	1/1	0.78	0.26	53,53,53,53	0
56	MG	2A	3124	1/1	0.78	0.23	52,52,52,52	0
56	MG	1a	3001	1/1	0.78	0.20	65,65,65,65	0
56	MG	2a	3140	1/1	0.78	0.08	52,52,52,52	0
56	MG	2E	304	1/1	0.78	0.18	58,58,58,58	0
56	MG	2A	3516	1/1	0.78	0.15	74,74,74,74	0
56	MG	1A	3964	1/1	0.78	0.10	73,73,73,73	0
56	MG	2A	3746	1/1	0.78	0.12	58,58,58,58	0
56	MG	1a	3023	1/1	0.78	0.24	47,47,47,47	0
56	MG	2A	3154	1/1	0.78	0.16	56,56,56,56	0
56	MG	1a	3028	1/1	0.78	0.21	53,53,53,53	0
56	MG	2A	3176	1/1	0.78	0.21	62,62,62,62	0
56	MG	2A	3348	1/1	0.78	0.23	50,50,50,50	0
56	MG	2a	3031	1/1	0.78	0.14	62,62,62,62	0
56	MG	2a	3032	1/1	0.78	0.15	59,59,59,59	0
56	MG	2a	3211	1/1	0.78	0.13	62,62,62,62	0
56	MG	2a	3036	1/1	0.78	0.09	50,50,50,50	0
56	MG	2A	3588	1/1	0.78	0.20	70,70,70,70	0
56	MG	2A	3378	1/1	0.78	0.26	57,57,57,57	0
56	MG	1A	4030	1/1	0.78	0.12	32,32,32,32	0
56	MG	1A	3187	1/1	0.78	0.22	51,51,51,51	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
56	MG	1A	3545	1/1	0.79	0.19	60,60,60,60	0
56	MG	1a	3056	1/1	0.79	0.19	56,56,56,56	0
56	MG	2a	3091	1/1	0.79	0.13	60,60,60,60	0
56	MG	2A	3042	1/1	0.79	0.27	52,52,52,52	0
56	MG	1A	3423	1/1	0.79	0.18	53,53,53,53	0
56	MG	2A	3681	1/1	0.79	0.19	52,52,52,52	0
56	MG	2A	3685	1/1	0.79	0.27	47,47,47,47	0
56	MG	2A	3295	1/1	0.79	0.24	62,62,62,62	0
56	MG	2A	3297	1/1	0.79	0.19	52,52,52,52	0
56	MG	1E	307	1/1	0.79	0.16	55,55,55,55	0
56	MG	2a	3128	1/1	0.79	0.17	57,57,57,57	0
56	MG	1A	4004	1/1	0.79	0.15	62,62,62,62	0
56	MG	1A	4016	1/1	0.79	0.09	32,32,32,32	0
56	MG	2a	3132	1/1	0.79	0.23	67,67,67,67	0
56	MG	2E	307	1/1	0.79	0.15	49,49,49,49	0
56	MG	2F	301	1/1	0.79	0.42	58,58,58,58	0
56	MG	2A	3736	1/1	0.79	0.38	72,72,72,72	0
56	MG	1a	3181	1/1	0.79	0.18	68,68,68,68	0
56	MG	1A	3467	1/1	0.79	0.31	31,31,31,31	0
56	MG	2A	3212	1/1	0.79	0.20	54,54,54,54	0
56	MG	25	102	1/1	0.79	0.18	60,60,60,60	0
56	MG	2A	3563	1/1	0.79	0.12	46,46,46,46	0
56	MG	2A	3225	1/1	0.79	0.21	69,69,69,69	0
56	MG	2a	3008	1/1	0.79	0.21	54,54,54,54	0
56	MG	2A	3089	1/1	0.79	0.20	56,56,56,56	0
56	MG	1a	3195	1/1	0.79	0.12	51,51,51,51	0
56	MG	2a	3024	1/1	0.79	0.56	58,58,58,58	0
56	MG	2A	3607	1/1	0.79	0.23	56,56,56,56	0
56	MG	2A	3624	1/1	0.79	0.14	50,50,50,50	0
56	MG	2v	102	1/1	0.79	0.24	62,62,62,62	0
56	MG	2x	3001	1/1	0.79	0.20	60,60,60,60	0
56	MG	2A	3098	1/1	0.79	0.17	32,32,32,32	0
56	MG	2a	3044	1/1	0.79	0.15	68,68,68,68	0
56	MG	1a	3140	1/1	0.79	0.10	37,37,37,37	0
56	MG	1a	3143	1/1	0.79	0.12	52,52,52,52	0
56	MG	2A	3575	1/1	0.80	0.17	38,38,38,38	0
56	MG	2A	3576	1/1	0.80	0.18	35,35,35,35	0
56	MG	2A	3031	1/1	0.80	0.19	55,55,55,55	0
56	MG	2a	3127	1/1	0.80	0.05	66,66,66,66	0
56	MG	1a	3016	1/1	0.80	0.25	51,51,51,51	0
56	MG	2Z	8001	1/1	0.80	0.23	47,47,47,47	0
56	MG	1A	3301	1/1	0.80	0.29	54,54,54,54	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	1A	3958	1/1	0.80	0.18	8,8,8,8	0
56	MG	1A	4014	1/1	0.80	0.23	35,35,35,35	0
56	MG	1A	3324	1/1	0.80	0.17	42,42,42,42	0
56	MG	2a	3003	1/1	0.80	0.17	53,53,53,53	0
56	MG	1A	3673	1/1	0.80	0.15	24,24,24,24	0
56	MG	2A	3294	1/1	0.80	0.32	61,61,61,61	0
56	MG	2a	3019	1/1	0.80	0.22	50,50,50,50	0
56	MG	1a	3199	1/1	0.80	0.11	61,61,61,61	0
56	MG	1a	3149	1/1	0.80	0.16	67,67,67,67	0
56	MG	1A	3248	1/1	0.80	0.17	35,35,35,35	0
56	MG	2A	3503	1/1	0.80	0.11	25,25,25,25	0
56	MG	2A	3203	1/1	0.80	0.18	53,53,53,53	0
56	MG	1A	4080	1/1	0.80	0.15	39,39,39,39	0
56	MG	2A	3686	1/1	0.80	0.45	52,52,52,52	0
56	MG	2A	3695	1/1	0.80	0.15	55,55,55,55	0
56	MG	2A	3712	1/1	0.80	0.08	59,59,59,59	0
56	MG	1A	3933	1/1	0.80	0.11	46,46,46,46	0
56	MG	2A	3347	1/1	0.80	0.22	58,58,58,58	0
56	MG	2A	3115	1/1	0.80	0.24	64,64,64,64	0
56	MG	2A	3726	1/1	0.80	0.08	61,61,61,61	0
56	MG	2A	3120	1/1	0.80	0.20	56,56,56,56	0
56	MG	2A	3247	1/1	0.80	0.20	64,64,64,64	0
56	MG	1A	3472	1/1	0.81	0.33	52,52,52,52	0
56	MG	1A	3731	1/1	0.81	0.14	20,20,20,20	0
56	MG	2A	3740	1/1	0.81	0.16	55,55,55,55	0
56	MG	1A	3400	1/1	0.81	0.24	50,50,50,50	0
56	MG	1A	3868	1/1	0.81	0.14	43,43,43,43	0
56	MG	2A	3494	1/1	0.81	0.14	46,46,46,46	0
56	MG	1A	4001	1/1	0.81	0.10	59,59,59,59	0
56	MG	1A	3883	1/1	0.81	0.17	13,13,13,13	0
56	MG	2A	3252	1/1	0.81	0.18	35,35,35,35	0
56	MG	1A	3884	1/1	0.81	0.17	35,35,35,35	0
56	MG	2a	3084	1/1	0.81	0.11	60,60,60,60	0
56	MG	2A	3051	1/1	0.81	0.11	40,40,40,40	0
56	MG	1A	3885	1/1	0.81	0.18	18,18,18,18	0
56	MG	2A	3770	1/1	0.81	0.14	40,40,40,40	0
56	MG	2A	3265	1/1	0.81	0.79	39,39,39,39	0
56	MG	1a	3175	1/1	0.81	0.08	70,70,70,70	0
56	MG	2A	3791	1/1	0.81	0.11	45,45,45,45	0
56	MG	1A	3950	1/1	0.81	0.21	46,46,46,46	0
56	MG	1A	3756	1/1	0.81	0.14	37,37,37,37	0
56	MG	1A	4021	1/1	0.81	0.08	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	1A	3155	1/1	0.81	0.49	56,56,56,56	0
56	MG	1A	3084	1/1	0.81	0.27	50,50,50,50	0
56	MG	1a	3046	1/1	0.81	0.18	55,55,55,55	0
56	MG	2B	3009	1/1	0.81	0.19	60,60,60,60	0
56	MG	2A	3622	1/1	0.81	0.25	56,56,56,56	0
56	MG	2A	3306	1/1	0.81	0.27	45,45,45,45	0
56	MG	2A	3328	1/1	0.81	0.17	45,45,45,45	0
56	MG	1A	3332	1/1	0.81	0.27	46,46,46,46	0
56	MG	1A	3634	1/1	0.81	0.23	12,12,12,12	0
56	MG	1A	3970	1/1	0.81	0.16	25,25,25,25	0
56	MG	2A	3667	1/1	0.81	0.15	33,33,33,33	0
56	MG	2a	3153	1/1	0.81	0.17	68,68,68,68	0
56	MG	2a	3155	1/1	0.81	0.09	75,75,75,75	0
56	MG	1A	3978	1/1	0.81	0.18	57,57,57,57	0
56	MG	1a	3224	1/1	0.81	0.16	49,49,49,49	0
56	MG	1a	3085	1/1	0.81	0.14	53,53,53,53	0
56	MG	1A	3297	1/1	0.81	0.19	42,42,42,42	0
56	MG	1a	3104	1/1	0.81	0.25	49,49,49,49	0
56	MG	2a	3185	1/1	0.81	0.15	47,47,47,47	0
56	MG	2A	3386	1/1	0.81	0.28	51,51,51,51	0
56	MG	1A	4058	1/1	0.81	0.09	71,71,71,71	0
56	MG	2a	3212	1/1	0.81	0.13	54,54,54,54	0
56	MG	1A	3132	1/1	0.81	0.41	32,32,32,32	0
56	MG	1A	3511	1/1	0.81	0.20	15,15,15,15	0
56	MG	2w	3003	1/1	0.81	0.18	51,51,51,51	0
56	MG	1w	110	1/1	0.81	0.17	79,79,79,79	0
56	MG	1x	110	1/1	0.81	0.17	63,63,63,63	0
56	MG	2a	3013	1/1	0.81	0.26	44,44,44,44	0
56	MG	2x	3004	1/1	0.81	0.14	59,59,59,59	0
56	MG	2A	3200	1/1	0.81	0.15	51,51,51,51	0
56	MG	2A	3201	1/1	0.81	0.08	52,52,52,52	0
56	MG	1A	3940	1/1	0.82	0.38	36,36,36,36	0
56	MG	2A	3248	1/1	0.82	0.21	51,51,51,51	0
56	MG	1A	3912	1/1	0.82	0.07	43,43,43,43	0
56	MG	1a	3081	1/1	0.82	0.15	47,47,47,47	0
56	MG	2A	3257	1/1	0.82	0.19	43,43,43,43	0
56	MG	1A	3239	1/1	0.82	0.11	49,49,49,49	0
56	MG	2A	3480	1/1	0.82	0.14	33,33,33,33	0
56	MG	1y	104	1/1	0.82	0.23	63,63,63,63	0
56	MG	1A	4031	1/1	0.82	0.15	37,37,37,37	0
56	MG	1a	3196	1/1	0.82	0.12	51,51,51,51	0
56	MG	2A	3142	1/1	0.82	0.14	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	3508	1/1	0.82	0.13	30,30,30,30	0
56	MG	19	101	1/1	0.82	0.48	33,33,33,33	0
56	MG	2A	3156	1/1	0.82	0.17	52,52,52,52	0
56	MG	1A	3988	1/1	0.82	0.13	28,28,28,28	0
56	MG	2A	3168	1/1	0.82	0.15	71,71,71,71	0
56	MG	1A	3446	1/1	0.82	0.17	54,54,54,54	0
56	MG	2A	3186	1/1	0.82	0.24	43,43,43,43	0
56	MG	2a	3149	1/1	0.82	0.11	62,62,62,62	0
56	MG	1a	3013	1/1	0.82	0.17	48,48,48,48	0
56	MG	1A	3608	1/1	0.82	0.13	15,15,15,15	0
56	MG	2a	3004	1/1	0.82	0.26	58,58,58,58	0
56	MG	1A	3481	1/1	0.82	0.17	66,66,66,66	0
56	MG	2A	3577	1/1	0.82	0.36	49,49,49,49	0
56	MG	1A	3447	1/1	0.82	0.27	32,32,32,32	0
56	MG	1a	3235	1/1	0.82	0.37	68,68,68,68	0
56	MG	1A	3281	1/1	0.82	0.17	40,40,40,40	0
56	MG	1A	3104	1/1	0.82	0.15	29,29,29,29	0
56	MG	2A	3353	1/1	0.82	0.24	44,44,44,44	0
56	MG	2A	3213	1/1	0.82	0.26	61,61,61,61	0
56	MG	2a	3033	1/1	0.82	0.13	61,61,61,61	0
56	MG	2A	3216	1/1	0.82	0.18	53,53,53,53	0
56	MG	2a	3229	1/1	0.82	0.26	72,72,72,72	0
56	MG	2a	3041	1/1	0.82	0.21	43,43,43,43	0
56	MG	2r	102	1/1	0.82	0.11	75,75,75,75	0
56	MG	1A	3975	1/1	0.82	0.23	21,21,21,21	0
56	MG	1A	3712	1/1	0.82	0.17	10,10,10,10	0
56	MG	1A	3939	1/1	0.82	0.24	32,32,32,32	0
56	MG	2A	3847	1/1	0.82	0.12	54,54,54,54	0
56	MG	2A	3245	1/1	0.82	0.22	58,58,58,58	0
56	MG	2a	3070	1/1	0.82	0.21	46,46,46,46	0
56	MG	2a	3075	1/1	0.82	0.13	54,54,54,54	0
56	MG	2A	3858	1/1	0.82	0.42	57,57,57,57	0
56	MG	1A	3204	1/1	0.83	0.16	41,41,41,41	0
56	MG	1A	3258	1/1	0.83	0.22	47,47,47,47	0
56	MG	1A	3161	1/1	0.83	0.22	49,49,49,49	0
56	MG	2A	3735	1/1	0.83	0.23	46,46,46,46	0
56	MG	2A	3198	1/1	0.83	0.21	58,58,58,58	0
56	MG	1A	3443	1/1	0.83	0.17	46,46,46,46	0
56	MG	1A	4133	1/1	0.83	0.17	29,29,29,29	0
56	MG	1a	3121	1/1	0.83	0.21	59,59,59,59	0
56	MG	2a	3055	1/1	0.83	0.11	70,70,70,70	0
56	MG	1A	3345	1/1	0.83	0.31	34,34,34,34	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	2A	3444	1/1	0.83	0.17	35,35,35,35	0
56	MG	1a	3137	1/1	0.83	0.14	46,46,46,46	0
56	MG	2A	3753	1/1	0.83	0.11	36,36,36,36	0
56	MG	2A	3215	1/1	0.83	0.14	49,49,49,49	0
56	MG	1A	4006	1/1	0.83	0.11	53,53,53,53	0
56	MG	2A	3217	1/1	0.83	0.16	40,40,40,40	0
56	MG	2a	3108	1/1	0.83	0.14	48,48,48,48	0
56	MG	1E	306	1/1	0.83	0.34	32,32,32,32	0
56	MG	1A	4007	1/1	0.83	0.17	45,45,45,45	0
56	MG	1a	3146	1/1	0.83	0.17	44,44,44,44	0
56	MG	1F	308	1/1	0.83	0.40	44,44,44,44	0
56	MG	1A	4009	1/1	0.83	0.33	56,56,56,56	0
56	MG	1A	3960	1/1	0.83	0.15	25,25,25,25	0
56	MG	12	3001	1/1	0.83	0.35	45,45,45,45	0
56	MG	1a	3167	1/1	0.83	0.14	51,51,51,51	0
56	MG	2A	3075	1/1	0.83	0.32	62,62,62,62	0
56	MG	1A	3176	1/1	0.83	0.10	52,52,52,52	0
56	MG	1a	3173	1/1	0.83	0.15	55,55,55,55	0
56	MG	1A	3658	1/1	0.83	0.18	15,15,15,15	0
56	MG	1A	3830	1/1	0.83	0.14	40,40,40,40	0
56	MG	1A	3915	1/1	0.83	0.20	8,8,8,8	0
56	MG	2B	3012	1/1	0.83	0.19	63,63,63,63	0
56	MG	1A	3507	1/1	0.83	0.22	36,36,36,36	0
56	MG	1a	3190	1/1	0.83	0.08	44,44,44,44	0
56	MG	2A	3292	1/1	0.83	0.20	51,51,51,51	0
56	MG	2A	3608	1/1	0.83	0.50	63,63,63,63	0
56	MG	1A	3380	1/1	0.83	0.16	37,37,37,37	0
56	MG	1a	3026	1/1	0.83	0.21	48,48,48,48	0
56	MG	1A	3462	1/1	0.83	0.24	38,38,38,38	0
56	MG	2A	3302	1/1	0.83	0.13	50,50,50,50	0
56	MG	1A	3715	1/1	0.83	0.12	48,48,48,48	0
56	MG	2A	3661	1/1	0.83	0.15	53,53,53,53	0
56	MG	2a	3169	1/1	0.83	0.09	59,59,59,59	0
56	MG	2A	3321	1/1	0.83	0.14	50,50,50,50	0
56	MG	2a	3178	1/1	0.83	0.26	70,70,70,70	0
56	MG	2A	3132	1/1	0.83	0.23	57,57,57,57	0
56	MG	1A	4034	1/1	0.83	0.20	53,53,53,53	0
56	MG	2a	3202	1/1	0.83	0.16	57,57,57,57	0
56	MG	2A	3139	1/1	0.83	0.12	69,69,69,69	0
56	MG	2A	3341	1/1	0.83	0.59	43,43,43,43	0
56	MG	1a	3041	1/1	0.83	0.15	59,59,59,59	0
56	MG	2a	3002	1/1	0.83	0.14	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	3143	1/1	0.83	0.51	30,30,30,30	0
56	MG	1A	3323	1/1	0.83	0.22	41,41,41,41	0
56	MG	2v	103	1/1	0.83	0.20	60,60,60,60	0
56	MG	1A	4047	1/1	0.83	0.07	32,32,32,32	0
56	MG	1A	3734	1/1	0.83	0.20	14,14,14,14	0
56	MG	1A	3738	1/1	0.83	0.15	23,23,23,23	0
56	MG	1a	3063	1/1	0.83	0.34	41,41,41,41	0
56	MG	1a	3077	1/1	0.83	0.15	58,58,58,58	0
56	MG	2A	3725	1/1	0.83	0.29	67,67,67,67	0
56	MG	2a	3025	1/1	0.83	0.25	58,58,58,58	0
56	MG	1A	3859	1/1	0.84	0.18	27,27,27,27	0
56	MG	2a	3098	1/1	0.84	0.14	58,58,58,58	0
56	MG	1A	3655	1/1	0.84	0.12	17,17,17,17	0
56	MG	1A	3004	1/1	0.84	0.18	23,23,23,23	0
56	MG	2A	3440	1/1	0.84	0.21	40,40,40,40	0
56	MG	1a	3010	1/1	0.84	0.15	53,53,53,53	0
56	MG	2A	3446	1/1	0.84	0.09	30,30,30,30	0
56	MG	2a	3118	1/1	0.84	0.13	68,68,68,68	0
56	MG	2D	307	1/1	0.84	1.04	43,43,43,43	0
56	MG	1A	3665	1/1	0.84	0.14	14,14,14,14	0
56	MG	2a	3124	1/1	0.84	0.11	56,56,56,56	0
56	MG	2A	3478	1/1	0.84	0.23	40,40,40,40	0
56	MG	1A	4041	1/1	0.84	0.31	45,45,45,45	0
56	MG	1A	3448	1/1	0.84	0.19	28,28,28,28	0
56	MG	1A	3217	1/1	0.84	0.25	33,33,33,33	0
56	MG	2A	3280	1/1	0.84	0.48	43,43,43,43	0
56	MG	1A	3801	1/1	0.84	0.19	56,56,56,56	0
56	MG	1a	3163	1/1	0.84	0.11	47,47,47,47	0
56	MG	1A	3458	1/1	0.84	0.19	49,49,49,49	0
56	MG	1A	3714	1/1	0.84	0.15	59,59,59,59	0
56	MG	2A	3739	1/1	0.84	0.32	69,69,69,69	0
56	MG	2a	3146	1/1	0.84	0.19	76,76,76,76	0
56	MG	1A	4078	1/1	0.84	0.17	37,37,37,37	0
56	MG	1A	3825	1/1	0.84	0.12	28,28,28,28	0
56	MG	1A	3957	1/1	0.84	0.07	37,37,37,37	0
56	MG	2A	3320	1/1	0.84	0.24	62,62,62,62	0
56	MG	1A	3353	1/1	0.84	0.39	23,23,23,23	0
56	MG	1A	3599	1/1	0.84	0.16	16,16,16,16	0
56	MG	1a	3183	1/1	0.84	0.14	64,64,64,64	0
56	MG	2A	3757	1/1	0.84	0.13	50,50,50,50	0
56	MG	1a	3187	1/1	0.84	0.37	77,77,77,77	0
56	MG	2a	3023	1/1	0.84	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	1B	3004	1/1	0.84	0.24	43,43,43,43	0
56	MG	2A	3584	1/1	0.84	0.26	52,52,52,52	0
56	MG	1B	3007	1/1	0.84	0.18	56,56,56,56	0
56	MG	1A	3908	1/1	0.84	0.10	18,18,18,18	0
56	MG	2a	3199	1/1	0.84	0.12	57,57,57,57	0
56	MG	2a	3201	1/1	0.84	0.23	70,70,70,70	0
56	MG	1A	3251	1/1	0.84	0.12	49,49,49,49	0
56	MG	2a	3204	1/1	0.84	0.17	66,66,66,66	0
56	MG	2a	3035	1/1	0.84	0.16	53,53,53,53	0
56	MG	2A	3083	1/1	0.84	0.13	51,51,51,51	0
56	MG	1A	3077	1/1	0.84	0.38	21,21,21,21	0
56	MG	1A	3852	1/1	0.84	0.18	17,17,17,17	0
56	MG	2A	3797	1/1	0.84	0.35	57,57,57,57	0
56	MG	1F	302	1/1	0.84	0.20	31,31,31,31	0
56	MG	2A	3810	1/1	0.84	0.18	44,44,44,44	0
56	MG	2A	3235	1/1	0.84	0.21	47,47,47,47	0
56	MG	1A	3918	1/1	0.84	0.13	51,51,51,51	0
56	MG	1A	3922	1/1	0.84	0.07	63,63,63,63	0
56	MG	2A	3109	1/1	0.84	0.14	52,52,52,52	0
56	MG	1A	3123	1/1	0.84	0.13	62,62,62,62	0
56	MG	2a	3089	1/1	0.84	0.16	56,56,56,56	0
56	MG	10	104	1/1	0.84	0.13	30,30,30,30	0
56	MG	1A	3091	1/1	0.85	0.13	35,35,35,35	0
56	MG	2A	3472	1/1	0.85	0.15	50,50,50,50	0
56	MG	2a	3043	1/1	0.85	0.10	51,51,51,51	0
56	MG	2A	3477	1/1	0.85	0.15	44,44,44,44	0
56	MG	1A	3311	1/1	0.85	0.30	40,40,40,40	0
56	MG	2A	3745	1/1	0.85	0.12	56,56,56,56	0
56	MG	1A	3575	1/1	0.85	0.17	21,21,21,21	0
56	MG	2A	3482	1/1	0.85	0.16	54,54,54,54	0
56	MG	2A	3108	1/1	0.85	0.15	43,43,43,43	0
56	MG	1A	3018	1/1	0.85	0.19	28,28,28,28	0
56	MG	1a	3107	1/1	0.85	0.15	55,55,55,55	0
56	MG	2A	3495	1/1	0.85	0.13	22,22,22,22	0
56	MG	2A	3499	1/1	0.85	0.12	33,33,33,33	0
56	MG	2A	3501	1/1	0.85	0.13	24,24,24,24	0
56	MG	2A	3117	1/1	0.85	0.16	36,36,36,36	0
56	MG	1A	3813	1/1	0.85	0.16	51,51,51,51	0
56	MG	2A	3509	1/1	0.85	0.17	51,51,51,51	0
56	MG	18	101	1/1	0.85	0.33	59,59,59,59	0
56	MG	2A	3786	1/1	0.85	0.08	57,57,57,57	0
56	MG	2A	3276	1/1	0.85	0.24	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	3713	1/1	0.85	0.13	66,66,66,66	0
56	MG	2A	3126	1/1	0.85	0.15	39,39,39,39	0
56	MG	1f	3002	1/1	0.85	0.25	60,60,60,60	0
56	MG	2a	3121	1/1	0.85	0.10	62,62,62,62	0
56	MG	1n	502	1/1	0.85	0.20	57,57,57,57	0
56	MG	1A	3943	1/1	0.85	0.08	52,52,52,52	0
56	MG	1a	3003	1/1	0.85	0.22	49,49,49,49	0
56	MG	1a	3007	1/1	0.85	0.18	56,56,56,56	0
56	MG	1A	3393	1/1	0.85	0.46	44,44,44,44	0
56	MG	2A	3312	1/1	0.85	0.20	51,51,51,51	0
56	MG	1a	3145	1/1	0.85	0.19	78,78,78,78	0
56	MG	1A	3144	1/1	0.85	0.47	39,39,39,39	0
56	MG	2A	3323	1/1	0.85	0.25	54,54,54,54	0
56	MG	1A	3205	1/1	0.85	0.17	47,47,47,47	0
56	MG	2B	3015	1/1	0.85	0.18	54,54,54,54	0
56	MG	1x	108	1/1	0.85	0.19	47,47,47,47	0
56	MG	1A	3611	1/1	0.85	0.13	63,63,63,63	0
56	MG	1A	4104	1/1	0.85	0.10	47,47,47,47	0
56	MG	2A	3627	1/1	0.85	0.29	60,60,60,60	0
56	MG	1A	3847	1/1	0.85	0.31	26,26,26,26	0
56	MG	1A	4011	1/1	0.85	0.13	35,35,35,35	0
56	MG	2A	3346	1/1	0.85	0.17	70,70,70,70	0
56	MG	2A	3011	1/1	0.85	0.34	42,42,42,42	0
56	MG	1A	3213	1/1	0.85	0.69	27,27,27,27	0
56	MG	2R	202	1/1	0.85	0.23	51,51,51,51	0
56	MG	2T	3001	1/1	0.85	0.42	57,57,57,57	0
56	MG	2A	3352	1/1	0.85	0.11	57,57,57,57	0
56	MG	1A	3917	1/1	0.85	0.19	52,52,52,52	0
56	MG	1A	3107	1/1	0.85	0.23	25,25,25,25	0
56	MG	2A	3382	1/1	0.85	0.12	62,62,62,62	0
56	MG	2a	3188	1/1	0.85	0.10	72,72,72,72	0
56	MG	2a	3189	1/1	0.85	0.48	73,73,73,73	0
56	MG	1B	3008	1/1	0.85	0.16	53,53,53,53	0
56	MG	2A	3682	1/1	0.85	0.17	37,37,37,37	0
56	MG	1B	3023	1/1	0.85	0.15	65,65,65,65	0
56	MG	1a	3049	1/1	0.85	0.10	35,35,35,35	0
56	MG	1A	3637	1/1	0.85	0.17	14,14,14,14	0
56	MG	2a	3210	1/1	0.85	0.16	56,56,56,56	0
56	MG	2A	3710	1/1	0.85	0.23	71,71,71,71	0
56	MG	1A	3647	1/1	0.85	0.17	27,27,27,27	0
56	MG	2A	3714	1/1	0.85	0.11	44,44,44,44	0
56	MG	2a	3014	1/1	0.85	0.13	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	3518	1/1	0.85	0.15	48,48,48,48	0
56	MG	1a	3188	1/1	0.85	0.25	55,55,55,55	0
56	MG	1A	3925	1/1	0.85	0.09	39,39,39,39	0
56	MG	2w	3002	1/1	0.85	0.12	46,46,46,46	0
56	MG	1a	3068	1/1	0.85	0.17	54,54,54,54	0
56	MG	2w	3007	1/1	0.85	0.13	60,60,60,60	0
56	MG	2A	3243	1/1	0.85	0.15	62,62,62,62	0
56	MG	2A	3084	1/1	0.85	0.31	71,71,71,71	0
56	MG	2A	3730	1/1	0.85	0.09	63,63,63,63	0
56	MG	1a	3075	1/1	0.85	0.18	58,58,58,58	0
56	MG	1A	3089	1/1	0.85	0.24	51,51,51,51	0
56	MG	2A	3459	1/1	0.85	0.25	64,64,64,64	0
56	MG	1A	3277	1/1	0.86	0.38	49,49,49,49	0
56	MG	1a	3192	1/1	0.86	0.09	53,53,53,53	0
56	MG	1A	4045	1/1	0.86	0.09	30,30,30,30	0
56	MG	2A	3369	1/1	0.86	0.20	58,58,58,58	0
56	MG	2A	3377	1/1	0.86	0.14	56,56,56,56	0
56	MG	2a	3101	1/1	0.86	0.09	66,66,66,66	0
56	MG	1A	3784	1/1	0.86	0.11	42,42,42,42	0
56	MG	2A	3224	1/1	0.86	0.23	58,58,58,58	0
56	MG	2A	3650	1/1	0.86	0.18	53,53,53,53	0
56	MG	2A	3874	1/1	0.86	0.19	37,37,37,37	0
56	MG	15	104	1/1	0.86	0.23	40,40,40,40	0
56	MG	1A	3892	1/1	0.86	0.13	30,30,30,30	0
56	MG	2A	3659	1/1	0.86	0.17	64,64,64,64	0
56	MG	2A	3085	1/1	0.86	0.19	49,49,49,49	0
56	MG	2A	3396	1/1	0.86	0.13	58,58,58,58	0
56	MG	1A	3525	1/1	0.86	0.27	51,51,51,51	0
56	MG	2A	3242	1/1	0.86	0.20	47,47,47,47	0
56	MG	1A	3317	1/1	0.86	0.19	36,36,36,36	0
56	MG	2A	3409	1/1	0.86	0.29	65,65,65,65	0
56	MG	1A	4076	1/1	0.86	0.16	34,34,34,34	0
56	MG	1A	3947	1/1	0.86	0.15	23,23,23,23	0
56	MG	2a	3134	1/1	0.86	0.12	60,60,60,60	0
56	MG	1a	3134	1/1	0.86	0.17	38,38,38,38	0
56	MG	2A	3427	1/1	0.86	0.35	58,58,58,58	0
56	MG	1A	3346	1/1	0.86	0.13	45,45,45,45	0
56	MG	1A	3403	1/1	0.86	0.16	29,29,29,29	0
56	MG	1A	3676	1/1	0.86	0.13	32,32,32,32	0
56	MG	1l	202	1/1	0.86	0.08	61,61,61,61	0
56	MG	1A	3572	1/1	0.86	0.13	34,34,34,34	0
56	MG	1A	4117	1/1	0.86	0.22	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	3156	1/1	0.86	0.35	28,28,28,28	0
56	MG	25	103	1/1	0.86	0.62	47,47,47,47	0
56	MG	2A	3724	1/1	0.86	0.13	55,55,55,55	0
56	MG	2A	3473	1/1	0.86	0.38	71,71,71,71	0
56	MG	2a	3157	1/1	0.86	0.16	73,73,73,73	0
56	MG	1A	3356	1/1	0.86	0.70	47,47,47,47	0
56	MG	2A	3131	1/1	0.86	0.12	51,51,51,51	0
56	MG	1A	3490	1/1	0.86	0.29	31,31,31,31	0
56	MG	1a	3033	1/1	0.86	0.14	56,56,56,56	0
56	MG	2a	3009	1/1	0.86	0.11	58,58,58,58	0
56	MG	1A	3426	1/1	0.86	0.17	48,48,48,48	0
56	MG	1B	3009	1/1	0.86	0.22	34,34,34,34	0
56	MG	2a	3015	1/1	0.86	0.20	46,46,46,46	0
56	MG	1a	3164	1/1	0.86	0.14	41,41,41,41	0
56	MG	2A	3146	1/1	0.86	0.16	51,51,51,51	0
56	MG	1A	3360	1/1	0.86	0.17	27,27,27,27	0
56	MG	1a	3168	1/1	0.86	0.20	44,44,44,44	0
56	MG	1A	3215	1/1	0.86	0.17	29,29,29,29	0
56	MG	1A	3376	1/1	0.86	0.26	39,39,39,39	0
56	MG	2A	3319	1/1	0.86	0.42	51,51,51,51	0
56	MG	2A	3510	1/1	0.86	0.19	37,37,37,37	0
56	MG	2A	3171	1/1	0.86	0.30	48,48,48,48	0
56	MG	1a	3051	1/1	0.86	0.34	65,65,65,65	0
56	MG	2d	301	1/1	0.86	0.28	58,58,58,58	0
56	MG	1D	313	1/1	0.86	0.44	35,35,35,35	0
56	MG	1a	3177	1/1	0.86	0.18	46,46,46,46	0
56	MG	2A	3332	1/1	0.86	0.13	43,43,43,43	0
56	MG	2A	3026	1/1	0.86	0.17	47,47,47,47	0
56	MG	2a	3047	1/1	0.86	0.13	56,56,56,56	0
56	MG	2a	3048	1/1	0.86	0.09	61,61,61,61	0
56	MG	1A	3074	1/1	0.86	0.18	37,37,37,37	0
56	MG	1A	3382	1/1	0.86	0.14	41,41,41,41	0
56	MG	1A	3871	1/1	0.86	0.19	18,18,18,18	0
56	MG	2A	3049	1/1	0.86	0.15	30,30,30,30	0
56	MG	2A	3345	1/1	0.86	0.17	54,54,54,54	0
56	MG	1A	3385	1/1	0.86	0.24	35,35,35,35	0
56	MG	2y	105	1/1	0.86	0.05	65,65,65,65	0
56	MG	1A	3654	1/1	0.86	0.22	51,51,51,51	0
56	MG	2A	3415	1/1	0.87	0.23	56,56,56,56	0
56	MG	1A	3485	1/1	0.87	0.53	33,33,33,33	0
56	MG	1A	3971	1/1	0.87	0.10	43,43,43,43	0
56	MG	2A	3429	1/1	0.87	0.22	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	3039	1/1	0.87	0.27	61,61,61,61	0
56	MG	2A	3732	1/1	0.87	0.14	43,43,43,43	0
56	MG	1a	3186	1/1	0.87	0.11	57,57,57,57	0
56	MG	1A	3212	1/1	0.87	0.33	36,36,36,36	0
56	MG	1A	3086	1/1	0.87	0.20	40,40,40,40	0
56	MG	2A	3246	1/1	0.87	0.13	55,55,55,55	0
56	MG	2A	3452	1/1	0.87	0.15	42,42,42,42	0
56	MG	1A	3096	1/1	0.87	0.14	54,54,54,54	0
56	MG	1E	309	1/1	0.87	0.11	45,45,45,45	0
56	MG	2A	3249	1/1	0.87	0.17	48,48,48,48	0
56	MG	1E	310	1/1	0.87	0.20	28,28,28,28	0
56	MG	1A	4037	1/1	0.87	0.08	45,45,45,45	0
56	MG	2A	3090	1/1	0.87	0.17	38,38,38,38	0
56	MG	2a	3078	1/1	0.87	0.28	60,60,60,60	0
56	MG	2a	3080	1/1	0.87	0.17	56,56,56,56	0
56	MG	1A	4039	1/1	0.87	0.10	54,54,54,54	0
56	MG	2A	3095	1/1	0.87	0.16	39,39,39,39	0
56	MG	2A	3264	1/1	0.87	0.61	47,47,47,47	0
56	MG	1a	3080	1/1	0.87	0.14	40,40,40,40	0
56	MG	1G	3003	1/1	0.87	0.13	47,47,47,47	0
56	MG	1A	3377	1/1	0.87	0.13	25,25,25,25	0
56	MG	1Q	3003	1/1	0.87	0.18	40,40,40,40	0
56	MG	2A	3110	1/1	0.87	0.15	49,49,49,49	0
56	MG	1V	201	1/1	0.87	0.19	25,25,25,25	0
56	MG	2A	3116	1/1	0.87	0.14	41,41,41,41	0
56	MG	2A	3787	1/1	0.87	0.07	48,48,48,48	0
56	MG	2A	3789	1/1	0.87	0.31	62,62,62,62	0
56	MG	1a	3216	1/1	0.87	0.06	62,62,62,62	0
56	MG	1A	3197	1/1	0.87	0.17	44,44,44,44	0
56	MG	2A	3123	1/1	0.87	0.36	50,50,50,50	0
56	MG	2A	3521	1/1	0.87	0.09	50,50,50,50	0
56	MG	2a	3126	1/1	0.87	0.19	70,70,70,70	0
56	MG	1a	3220	1/1	0.87	0.08	42,42,42,42	0
56	MG	2A	3538	1/1	0.87	0.17	47,47,47,47	0
56	MG	2A	3838	1/1	0.87	0.16	61,61,61,61	0
56	MG	2A	3839	1/1	0.87	0.17	55,55,55,55	0
56	MG	2A	3298	1/1	0.87	0.13	47,47,47,47	0
56	MG	1A	3325	1/1	0.87	0.30	44,44,44,44	0
56	MG	1a	3109	1/1	0.87	0.16	70,70,70,70	0
56	MG	2A	3308	1/1	0.87	0.19	50,50,50,50	0
56	MG	2A	3871	1/1	0.87	0.57	36,36,36,36	0
56	MG	2A	3127	1/1	0.87	0.32	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	1a	3111	1/1	0.87	0.16	54,54,54,54	0
56	MG	2B	3007	1/1	0.87	0.10	53,53,53,53	0
56	MG	10	105	1/1	0.87	0.41	30,30,30,30	0
56	MG	1A	3160	1/1	0.87	0.10	66,66,66,66	0
56	MG	1A	3235	1/1	0.87	0.28	46,46,46,46	0
56	MG	1A	3455	1/1	0.87	0.17	23,23,23,23	0
56	MG	1A	3287	1/1	0.87	0.17	25,25,25,25	0
56	MG	1A	4061	1/1	0.87	0.19	27,27,27,27	0
56	MG	1A	3154	1/1	0.87	0.20	34,34,34,34	0
56	MG	2D	305	1/1	0.87	0.14	27,27,27,27	0
56	MG	1A	3240	1/1	0.87	0.13	31,31,31,31	0
56	MG	1A	3560	1/1	0.87	0.19	21,21,21,21	0
56	MG	2A	3163	1/1	0.87	0.15	53,53,53,53	0
56	MG	1A	3564	1/1	0.87	0.13	51,51,51,51	0
56	MG	1A	3308	1/1	0.87	0.29	29,29,29,29	0
56	MG	1A	3903	1/1	0.87	0.09	34,34,34,34	0
56	MG	1a	3017	1/1	0.87	0.13	37,37,37,37	0
56	MG	2A	3349	1/1	0.87	0.27	45,45,45,45	0
56	MG	1A	3822	1/1	0.87	0.10	47,47,47,47	0
56	MG	1A	4122	1/1	0.87	0.11	35,35,35,35	0
56	MG	1a	3166	1/1	0.87	0.10	55,55,55,55	0
56	MG	2A	3371	1/1	0.87	0.22	49,49,49,49	0
56	MG	1A	3680	1/1	0.87	0.10	46,46,46,46	0
56	MG	2a	3207	1/1	0.87	0.16	57,57,57,57	0
56	MG	2a	3208	1/1	0.87	0.13	69,69,69,69	0
56	MG	1A	3692	1/1	0.87	0.14	56,56,56,56	0
56	MG	1A	3709	1/1	0.87	0.19	12,12,12,12	0
56	MG	1a	3036	1/1	0.87	0.29	40,40,40,40	0
56	MG	2a	3224	1/1	0.87	0.14	51,51,51,51	0
56	MG	2A	3044	1/1	0.87	0.15	36,36,36,36	0
56	MG	2A	3389	1/1	0.87	0.14	49,49,49,49	0
56	MG	2A	3047	1/1	0.87	0.23	46,46,46,46	0
56	MG	2p	3001	1/1	0.87	0.13	45,45,45,45	0
56	MG	2A	3690	1/1	0.87	0.13	68,68,68,68	0
56	MG	1A	3412	1/1	0.87	0.25	41,41,41,41	0
56	MG	2a	3011	1/1	0.87	0.19	62,62,62,62	0
56	MG	2A	3703	1/1	0.87	0.20	41,41,41,41	0
56	MG	2A	3707	1/1	0.87	0.24	65,65,65,65	0
56	MG	1A	3421	1/1	0.87	0.17	46,46,46,46	0
56	MG	1B	3022	1/1	0.87	0.16	48,48,48,48	0
56	MG	1A	4026	1/1	0.87	0.46	42,42,42,42	0
56	MG	2A	3715	1/1	0.87	0.13	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	2A	3406	1/1	0.87	0.27	59,59,59,59	0
56	MG	2A	3062	1/1	0.87	0.42	56,56,56,56	0
56	MG	2A	3068	1/1	0.87	0.14	54,54,54,54	0
56	MG	2A	3229	1/1	0.87	0.12	44,44,44,44	0
56	MG	1A	3829	1/1	0.88	0.16	52,52,52,52	0
56	MG	1a	3091	1/1	0.88	0.28	38,38,38,38	0
56	MG	1t	3001	1/1	0.88	0.15	53,53,53,53	0
56	MG	2A	3672	1/1	0.88	0.10	67,67,67,67	0
56	MG	2a	3010	1/1	0.88	0.13	56,56,56,56	0
56	MG	1A	3548	1/1	0.88	0.32	45,45,45,45	0
56	MG	1a	3103	1/1	0.88	0.15	57,57,57,57	0
56	MG	1A	3553	1/1	0.88	0.17	32,32,32,32	0
56	MG	2A	3175	1/1	0.88	0.14	45,45,45,45	0
56	MG	2A	3358	1/1	0.88	0.16	35,35,35,35	0
56	MG	1a	3106	1/1	0.88	0.23	55,55,55,55	0
56	MG	2A	3178	1/1	0.88	0.35	41,41,41,41	0
56	MG	2A	3693	1/1	0.88	0.07	54,54,54,54	0
56	MG	1A	3838	1/1	0.88	0.11	35,35,35,35	0
56	MG	2A	3699	1/1	0.88	0.10	60,60,60,60	0
56	MG	1A	3473	1/1	0.88	0.18	23,23,23,23	0
56	MG	1A	3842	1/1	0.88	0.23	28,28,28,28	0
56	MG	1x	102	1/1	0.88	0.20	50,50,50,50	0
56	MG	2A	3195	1/1	0.88	0.22	41,41,41,41	0
56	MG	1x	103	1/1	0.88	0.17	38,38,38,38	0
56	MG	1A	3306	1/1	0.88	0.14	43,43,43,43	0
56	MG	2A	3716	1/1	0.88	0.23	63,63,63,63	0
56	MG	1A	3477	1/1	0.88	0.40	30,30,30,30	0
56	MG	1A	3850	1/1	0.88	0.10	33,33,33,33	0
56	MG	2A	3207	1/1	0.88	0.16	48,48,48,48	0
56	MG	1a	3130	1/1	0.88	0.11	53,53,53,53	0
56	MG	2A	3002	1/1	0.88	0.10	49,49,49,49	0
56	MG	1a	3131	1/1	0.88	0.15	46,46,46,46	0
56	MG	1A	4027	1/1	0.88	0.19	59,59,59,59	0
56	MG	2a	3062	1/1	0.88	0.12	48,48,48,48	0
56	MG	1A	3479	1/1	0.88	0.19	38,38,38,38	0
56	MG	2A	3221	1/1	0.88	0.38	46,46,46,46	0
56	MG	2A	3222	1/1	0.88	0.11	53,53,53,53	0
56	MG	1A	3047	1/1	0.88	0.22	47,47,47,47	0
56	MG	1A	4032	1/1	0.88	0.16	19,19,19,19	0
56	MG	2A	3737	1/1	0.88	0.20	47,47,47,47	0
56	MG	1Y	503	1/1	0.88	0.24	58,58,58,58	0
56	MG	1A	3439	1/1	0.88	0.15	35,35,35,35	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	2A	3443	1/1	0.88	0.11	50,50,50,50	0
56	MG	2a	3092	1/1	0.88	0.28	59,59,59,59	0
56	MG	1A	3265	1/1	0.88	0.18	25,25,25,25	0
56	MG	1a	3147	1/1	0.88	0.11	32,32,32,32	0
56	MG	1A	3726	1/1	0.88	0.21	12,12,12,12	0
56	MG	2a	3103	1/1	0.88	0.16	68,68,68,68	0
56	MG	1A	3350	1/1	0.88	0.34	34,34,34,34	0
56	MG	13	101	1/1	0.88	0.19	31,31,31,31	0
56	MG	2A	3750	1/1	0.88	0.13	48,48,48,48	0
56	MG	2a	3114	1/1	0.88	0.19	47,47,47,47	0
56	MG	2A	3752	1/1	0.88	0.14	47,47,47,47	0
56	MG	1A	4038	1/1	0.88	0.13	39,39,39,39	0
56	MG	2A	3060	1/1	0.88	0.21	47,47,47,47	0
56	MG	2A	3759	1/1	0.88	0.10	74,74,74,74	0
56	MG	1A	3874	1/1	0.88	0.12	35,35,35,35	0
56	MG	1A	4040	1/1	0.88	0.18	52,52,52,52	0
56	MG	1A	3878	1/1	0.88	0.19	30,30,30,30	0
56	MG	2A	3481	1/1	0.88	0.23	47,47,47,47	0
56	MG	1A	3881	1/1	0.88	0.15	18,18,18,18	0
56	MG	1A	4044	1/1	0.88	0.08	17,17,17,17	0
56	MG	2A	3780	1/1	0.88	0.15	37,37,37,37	0
56	MG	1a	3170	1/1	0.88	0.11	49,49,49,49	0
56	MG	1A	3733	1/1	0.88	0.14	15,15,15,15	0
56	MG	2A	3262	1/1	0.88	0.18	59,59,59,59	0
56	MG	2a	3136	1/1	0.88	0.08	60,60,60,60	0
56	MG	2A	3263	1/1	0.88	0.11	68,68,68,68	0
56	MG	1A	3139	1/1	0.88	0.16	28,28,28,28	0
56	MG	1A	3397	1/1	0.88	0.23	27,27,27,27	0
56	MG	1A	4050	1/1	0.88	0.19	34,34,34,34	0
56	MG	1a	3176	1/1	0.88	0.12	63,63,63,63	0
56	MG	1A	3967	1/1	0.88	0.17	56,56,56,56	0
56	MG	2A	3273	1/1	0.88	0.19	51,51,51,51	0
56	MG	1a	3179	1/1	0.88	0.14	64,64,64,64	0
56	MG	2A	3279	1/1	0.88	0.13	51,51,51,51	0
56	MG	2A	3846	1/1	0.88	0.09	41,41,41,41	0
56	MG	2A	3530	1/1	0.88	0.13	45,45,45,45	0
56	MG	2A	3536	1/1	0.88	0.12	32,32,32,32	0
56	MG	2A	3854	1/1	0.88	0.22	50,50,50,50	0
56	MG	2a	3159	1/1	0.88	0.09	58,58,58,58	0
56	MG	1A	3450	1/1	0.88	0.15	22,22,22,22	0
56	MG	2A	3863	1/1	0.88	0.38	70,70,70,70	0
56	MG	1A	3631	1/1	0.88	0.13	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	1A	3762	1/1	0.88	0.13	13,13,13,13	0
56	MG	2A	3547	1/1	0.88	0.22	48,48,48,48	0
56	MG	2a	3176	1/1	0.88	0.10	55,55,55,55	0
56	MG	1A	3318	1/1	0.88	0.16	25,25,25,25	0
56	MG	2a	3181	1/1	0.88	0.16	52,52,52,52	0
56	MG	2A	3876	1/1	0.88	0.20	43,43,43,43	0
56	MG	1A	3768	1/1	0.88	0.15	47,47,47,47	0
56	MG	2B	3008	1/1	0.88	0.19	49,49,49,49	0
56	MG	2a	3194	1/1	0.88	0.13	71,71,71,71	0
56	MG	1A	4088	1/1	0.88	0.13	49,49,49,49	0
56	MG	1A	4096	1/1	0.88	0.17	39,39,39,39	0
56	MG	1A	3898	1/1	0.88	0.19	23,23,23,23	0
56	MG	1A	3088	1/1	0.88	0.23	43,43,43,43	0
56	MG	1A	3231	1/1	0.88	0.13	25,25,25,25	0
56	MG	2A	3582	1/1	0.88	0.09	57,57,57,57	0
56	MG	2A	3310	1/1	0.88	0.21	59,59,59,59	0
56	MG	1A	3200	1/1	0.88	0.21	47,47,47,47	0
56	MG	2A	3595	1/1	0.88	0.22	73,73,73,73	0
56	MG	1A	3253	1/1	0.88	0.22	43,43,43,43	0
56	MG	2a	3219	1/1	0.88	0.19	53,53,53,53	0
56	MG	2a	3221	1/1	0.88	0.11	57,57,57,57	0
56	MG	1A	3536	1/1	0.88	0.16	33,33,33,33	0
56	MG	1A	3811	1/1	0.88	0.15	41,41,41,41	0
56	MG	1A	3540	1/1	0.88	0.17	29,29,29,29	0
56	MG	2F	303	1/1	0.88	0.21	38,38,38,38	0
56	MG	2Q	202	1/1	0.88	0.19	31,31,31,31	0
56	MG	1A	4002	1/1	0.88	0.08	53,53,53,53	0
56	MG	2A	3625	1/1	0.88	0.12	53,53,53,53	0
56	MG	1A	3379	1/1	0.88	0.16	39,39,39,39	0
56	MG	2A	3638	1/1	0.88	0.06	48,48,48,48	0
56	MG	1a	3070	1/1	0.88	0.23	44,44,44,44	0
56	MG	2w	3005	1/1	0.88	0.17	66,66,66,66	0
56	MG	2W	201	1/1	0.88	0.14	42,42,42,42	0
56	MG	2A	3649	1/1	0.88	0.15	54,54,54,54	0
56	MG	1B	3018	1/1	0.88	0.15	51,51,51,51	0
56	MG	2A	3340	1/1	0.88	0.16	48,48,48,48	0
56	MG	1B	3021	1/1	0.88	0.17	50,50,50,50	0
56	MG	1A	3546	1/1	0.88	0.16	57,57,57,57	0
56	MG	1A	3547	1/1	0.88	0.12	39,39,39,39	0
56	MG	2A	3662	1/1	0.88	0.10	34,34,34,34	0
56	MG	1A	3735	1/1	0.89	0.13	25,25,25,25	0
56	MG	2A	3468	1/1	0.89	0.15	53,53,53,53	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	2A	3112	1/1	0.89	0.25	34,34,34,34	0
56	MG	1A	3736	1/1	0.89	0.18	16,16,16,16	0
56	MG	1U	203	1/1	0.89	0.22	22,22,22,22	0
56	MG	1A	3628	1/1	0.89	0.17	17,17,17,17	0
56	MG	2a	3042	1/1	0.89	0.10	63,63,63,63	0
56	MG	1A	3451	1/1	0.89	0.15	35,35,35,35	0
56	MG	1A	3044	1/1	0.89	0.24	14,14,14,14	0
56	MG	1d	502	1/1	0.89	0.18	41,41,41,41	0
56	MG	2A	3274	1/1	0.89	0.11	47,47,47,47	0
56	MG	1A	3296	1/1	0.89	0.15	34,34,34,34	0
56	MG	2a	3053	1/1	0.89	0.20	57,57,57,57	0
56	MG	2A	3278	1/1	0.89	0.14	35,35,35,35	0
56	MG	1a	3117	1/1	0.89	0.17	31,31,31,31	0
56	MG	1A	3887	1/1	0.89	0.15	50,50,50,50	0
56	MG	2A	3285	1/1	0.89	0.30	68,68,68,68	0
56	MG	2A	3751	1/1	0.89	0.15	68,68,68,68	0
56	MG	2a	3069	1/1	0.89	0.09	55,55,55,55	0
56	MG	2A	3286	1/1	0.89	0.19	46,46,46,46	0
56	MG	1A	3764	1/1	0.89	0.18	16,16,16,16	0
56	MG	1A	3340	1/1	0.89	0.67	44,44,44,44	0
56	MG	1A	3538	1/1	0.89	0.17	45,45,45,45	0
56	MG	2A	3512	1/1	0.89	0.10	29,29,29,29	0
56	MG	16	102	1/1	0.89	0.36	46,46,46,46	0
56	MG	1A	3652	1/1	0.89	0.18	41,41,41,41	0
56	MG	1w	105	1/1	0.89	0.10	48,48,48,48	0
56	MG	1A	3776	1/1	0.89	0.14	46,46,46,46	0
56	MG	1A	3344	1/1	0.89	0.13	29,29,29,29	0
56	MG	1A	3252	1/1	0.89	0.16	53,53,53,53	0
56	MG	2A	3783	1/1	0.89	0.10	40,40,40,40	0
56	MG	2A	3541	1/1	0.89	0.20	50,50,50,50	0
56	MG	2A	3157	1/1	0.89	0.14	58,58,58,58	0
56	MG	2A	3543	1/1	0.89	0.10	51,51,51,51	0
56	MG	1A	3793	1/1	0.89	0.12	25,25,25,25	0
56	MG	2A	3318	1/1	0.89	0.17	52,52,52,52	0
56	MG	2A	3548	1/1	0.89	0.16	25,25,25,25	0
56	MG	2A	3550	1/1	0.89	0.09	43,43,43,43	0
56	MG	2A	3159	1/1	0.89	0.12	28,28,28,28	0
56	MG	1A	3080	1/1	0.89	0.63	28,28,28,28	0
56	MG	1A	4086	1/1	0.89	0.28	31,31,31,31	0
56	MG	2A	3821	1/1	0.89	0.11	47,47,47,47	0
56	MG	2a	3125	1/1	0.89	0.22	78,78,78,78	0
56	MG	1A	3660	1/1	0.89	0.17	8,8,8,8	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	2A	3326	1/1	0.89	0.18	50,50,50,50	0
56	MG	1A	3910	1/1	0.89	0.17	45,45,45,45	0
56	MG	2A	3331	1/1	0.89	0.24	51,51,51,51	0
56	MG	1A	3997	1/1	0.89	0.19	52,52,52,52	0
56	MG	2A	3853	1/1	0.89	0.16	37,37,37,37	0
56	MG	1a	3159	1/1	0.89	0.08	52,52,52,52	0
56	MG	2A	3003	1/1	0.89	0.19	44,44,44,44	0
56	MG	1A	3663	1/1	0.89	0.13	32,32,32,32	0
56	MG	2A	3596	1/1	0.89	0.10	63,63,63,63	0
56	MG	2A	3188	1/1	0.89	1.51	41,41,41,41	0
56	MG	1a	3161	1/1	0.89	0.15	45,45,45,45	0
56	MG	1A	3913	1/1	0.89	0.13	34,34,34,34	0
56	MG	2A	3612	1/1	0.89	0.44	60,60,60,60	0
56	MG	2B	3001	1/1	0.89	0.12	54,54,54,54	0
56	MG	2B	3002	1/1	0.89	0.42	50,50,50,50	0
56	MG	2A	3193	1/1	0.89	0.66	40,40,40,40	0
56	MG	2A	3623	1/1	0.89	0.22	57,57,57,57	0
56	MG	1A	3243	1/1	0.89	0.13	38,38,38,38	0
56	MG	1A	3260	1/1	0.89	0.17	44,44,44,44	0
56	MG	1a	3031	1/1	0.89	0.15	48,48,48,48	0
56	MG	2A	3038	1/1	0.89	0.15	46,46,46,46	0
56	MG	1A	4125	1/1	0.89	0.19	27,27,27,27	0
56	MG	2A	3648	1/1	0.89	0.12	33,33,33,33	0
56	MG	2A	3204	1/1	0.89	0.18	68,68,68,68	0
56	MG	1A	3821	1/1	0.89	0.12	49,49,49,49	0
56	MG	1A	3550	1/1	0.89	0.22	26,26,26,26	0
56	MG	1a	3172	1/1	0.89	0.10	65,65,65,65	0
56	MG	2A	3374	1/1	0.89	0.24	39,39,39,39	0
56	MG	2A	3660	1/1	0.89	0.17	31,31,31,31	0
56	MG	1A	3674	1/1	0.89	0.23	38,38,38,38	0
56	MG	2a	3187	1/1	0.89	0.11	54,54,54,54	0
56	MG	1A	3354	1/1	0.89	0.30	36,36,36,36	0
56	MG	2O	8001	1/1	0.89	0.16	54,54,54,54	0
56	MG	1A	3262	1/1	0.89	0.45	36,36,36,36	0
56	MG	2Q	203	1/1	0.89	0.29	47,47,47,47	0
56	MG	1A	3681	1/1	0.89	0.27	49,49,49,49	0
56	MG	2a	3200	1/1	0.89	0.09	64,64,64,64	0
56	MG	1A	3424	1/1	0.89	0.29	31,31,31,31	0
56	MG	1A	3264	1/1	0.89	0.23	48,48,48,48	0
56	MG	1A	3489	1/1	0.89	0.29	47,47,47,47	0
56	MG	2A	3394	1/1	0.89	0.13	48,48,48,48	0
56	MG	2A	3677	1/1	0.89	0.58	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	2A	3395	1/1	0.89	0.21	45,45,45,45	0
56	MG	1a	3060	1/1	0.89	0.18	59,59,59,59	0
56	MG	1A	3159	1/1	0.89	0.27	26,26,26,26	0
56	MG	2A	3234	1/1	0.89	0.68	53,53,53,53	0
56	MG	1A	3374	1/1	0.89	0.20	27,27,27,27	0
56	MG	1B	3033	1/1	0.89	0.20	53,53,53,53	0
56	MG	1A	3319	1/1	0.89	0.26	38,38,38,38	0
56	MG	1a	3189	1/1	0.89	0.25	56,56,56,56	0
56	MG	2A	3244	1/1	0.89	0.23	65,65,65,65	0
56	MG	2a	3006	1/1	0.89	0.13	53,53,53,53	0
56	MG	1a	3074	1/1	0.89	0.11	49,49,49,49	0
56	MG	1A	3322	1/1	0.89	0.16	31,31,31,31	0
56	MG	2A	3421	1/1	0.89	0.21	54,54,54,54	0
56	MG	1A	3271	1/1	0.89	0.49	25,25,25,25	0
56	MG	1a	3078	1/1	0.89	0.12	47,47,47,47	0
56	MG	2A	3430	1/1	0.89	0.35	61,61,61,61	0
56	MG	1A	3602	1/1	0.89	0.14	24,24,24,24	0
56	MG	2A	3250	1/1	0.89	0.18	46,46,46,46	0
56	MG	1A	3732	1/1	0.89	0.17	16,16,16,16	0
56	MG	1A	3181	1/1	0.89	0.42	24,24,24,24	0
56	MG	2A	3105	1/1	0.89	0.19	51,51,51,51	0
56	MG	2y	101	1/1	0.89	0.12	59,59,59,59	0
56	MG	2y	103	1/1	0.89	0.08	51,51,51,51	0
56	MG	1A	3955	1/1	0.89	0.25	48,48,48,48	0
56	MG	1A	3249	1/1	0.89	0.15	49,49,49,49	0
56	MG	2A	3729	1/1	0.89	0.29	66,66,66,66	0
56	MG	2A	3376	1/1	0.90	0.22	47,47,47,47	0
56	MG	1A	3494	1/1	0.90	0.22	41,41,41,41	0
56	MG	1A	3314	1/1	0.90	0.12	44,44,44,44	0
56	MG	1A	3496	1/1	0.90	1.05	40,40,40,40	0
56	MG	2A	3679	1/1	0.90	0.23	54,54,54,54	0
56	MG	2A	3680	1/1	0.90	0.12	52,52,52,52	0
56	MG	1A	3800	1/1	0.90	0.13	35,35,35,35	0
56	MG	1F	303	1/1	0.90	0.26	14,14,14,14	0
56	MG	2a	3012	1/1	0.90	0.18	59,59,59,59	0
56	MG	2A	3683	1/1	0.90	0.13	51,51,51,51	0
56	MG	2A	3388	1/1	0.90	0.12	45,45,45,45	0
56	MG	1A	4025	1/1	0.90	0.16	18,18,18,18	0
56	MG	2a	3016	1/1	0.90	0.34	47,47,47,47	0
56	MG	1a	3114	1/1	0.90	0.14	26,26,26,26	0
56	MG	1A	3642	1/1	0.90	0.15	15,15,15,15	0
56	MG	1a	3119	1/1	0.90	0.12	28,28,28,28	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	1a	3120	1/1	0.90	0.15	46,46,46,46	0
56	MG	2A	3702	1/1	0.90	0.14	37,37,37,37	0
56	MG	1A	3803	1/1	0.90	0.13	24,24,24,24	0
56	MG	2a	3029	1/1	0.90	0.12	43,43,43,43	0
56	MG	1A	3359	1/1	0.90	0.14	33,33,33,33	0
56	MG	1T	3003	1/1	0.90	0.14	34,34,34,34	0
56	MG	1A	3431	1/1	0.90	0.24	40,40,40,40	0
56	MG	2a	3034	1/1	0.90	0.25	51,51,51,51	0
56	MG	2A	3407	1/1	0.90	0.22	45,45,45,45	0
56	MG	1U	204	1/1	0.90	0.28	22,22,22,22	0
56	MG	1U	205	1/1	0.90	0.13	35,35,35,35	0
56	MG	2A	3013	1/1	0.90	0.30	52,52,52,52	0
56	MG	2A	3016	1/1	0.90	0.18	58,58,58,58	0
56	MG	2A	3722	1/1	0.90	0.26	57,57,57,57	0
56	MG	2A	3018	1/1	0.90	0.61	36,36,36,36	0
56	MG	2a	3046	1/1	0.90	0.26	52,52,52,52	0
56	MG	1A	3435	1/1	0.90	0.45	51,51,51,51	0
56	MG	2A	3424	1/1	0.90	0.14	35,35,35,35	0
56	MG	2a	3049	1/1	0.90	0.21	79,79,79,79	0
56	MG	1W	201	1/1	0.90	0.32	28,28,28,28	0
56	MG	2A	3025	1/1	0.90	0.13	28,28,28,28	0
56	MG	2A	3728	1/1	0.90	0.15	55,55,55,55	0
56	MG	1A	3013	1/1	0.90	0.30	9,9,9,9	0
56	MG	2a	3056	1/1	0.90	0.10	46,46,46,46	0
56	MG	2A	3028	1/1	0.90	0.18	30,30,30,30	0
56	MG	1A	3017	1/1	0.90	0.13	17,17,17,17	0
56	MG	1A	4035	1/1	0.90	0.16	13,13,13,13	0
56	MG	1A	3225	1/1	0.90	0.41	42,42,42,42	0
56	MG	2A	3043	1/1	0.90	0.12	53,53,53,53	0
56	MG	1A	3524	1/1	0.90	0.26	30,30,30,30	0
56	MG	1a	3150	1/1	0.90	0.16	56,56,56,56	0
56	MG	1a	3151	1/1	0.90	0.14	45,45,45,45	0
56	MG	2A	3464	1/1	0.90	0.11	29,29,29,29	0
56	MG	2A	3465	1/1	0.90	0.18	54,54,54,54	0
56	MG	1A	3116	1/1	0.90	0.19	28,28,28,28	0
56	MG	1A	3531	1/1	0.90	0.22	35,35,35,35	0
56	MG	2a	3095	1/1	0.90	0.25	59,59,59,59	0
56	MG	1a	3157	1/1	0.90	0.12	46,46,46,46	0
56	MG	1A	3173	1/1	0.90	0.18	30,30,30,30	0
56	MG	1A	3537	1/1	0.90	0.18	38,38,38,38	0
56	MG	2A	3067	1/1	0.90	0.20	35,35,35,35	0
56	MG	2a	3105	1/1	0.90	0.20	55,55,55,55	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	1A	3948	1/1	0.90	0.11	42,42,42,42	0
56	MG	1A	3083	1/1	0.90	0.22	41,41,41,41	0
56	MG	1A	3125	1/1	0.90	0.13	17,17,17,17	0
56	MG	1a	3004	1/1	0.90	0.13	43,43,43,43	0
56	MG	1A	3326	1/1	0.90	0.30	32,32,32,32	0
56	MG	1A	3956	1/1	0.90	0.17	58,58,58,58	0
56	MG	2a	3117	1/1	0.90	0.13	51,51,51,51	0
56	MG	2A	3496	1/1	0.90	0.14	42,42,42,42	0
56	MG	2A	3768	1/1	0.90	0.12	24,24,24,24	0
56	MG	1a	3169	1/1	0.90	0.13	57,57,57,57	0
56	MG	1A	3327	1/1	0.90	0.19	40,40,40,40	0
56	MG	1A	3693	1/1	0.90	0.11	45,45,45,45	0
56	MG	2A	3505	1/1	0.90	0.10	34,34,34,34	0
56	MG	1A	3701	1/1	0.90	0.13	42,42,42,42	0
56	MG	1A	3853	1/1	0.90	0.17	7,7,7,7	0
56	MG	1A	3456	1/1	0.90	0.18	41,41,41,41	0
56	MG	1A	3052	1/1	0.90	0.18	29,29,29,29	0
56	MG	1A	3459	1/1	0.90	0.17	41,41,41,41	0
56	MG	1A	4085	1/1	0.90	0.10	25,25,25,25	0
56	MG	1A	3552	1/1	0.90	0.40	44,44,44,44	0
56	MG	1A	3391	1/1	0.90	0.62	47,47,47,47	0
56	MG	2A	3804	1/1	0.90	0.25	40,40,40,40	0
56	MG	2a	3139	1/1	0.90	0.09	41,41,41,41	0
56	MG	2A	3288	1/1	0.90	0.14	48,48,48,48	0
56	MG	1A	3554	1/1	0.90	0.16	36,36,36,36	0
56	MG	1A	3877	1/1	0.90	0.30	31,31,31,31	0
56	MG	2A	3819	1/1	0.90	0.09	48,48,48,48	0
56	MG	2a	3145	1/1	0.90	0.07	64,64,64,64	0
56	MG	2A	3293	1/1	0.90	0.08	67,67,67,67	0
56	MG	1A	3556	1/1	0.90	0.18	9,9,9,9	0
56	MG	1A	3464	1/1	0.90	0.37	29,29,29,29	0
56	MG	2A	3840	1/1	0.90	0.17	68,68,68,68	0
56	MG	1A	4111	1/1	0.90	0.14	20,20,20,20	0
56	MG	1A	3466	1/1	0.90	0.30	19,19,19,19	0
56	MG	2A	3299	1/1	0.90	0.14	46,46,46,46	0
56	MG	1A	3054	1/1	0.90	0.27	37,37,37,37	0
56	MG	2A	3558	1/1	0.90	0.09	29,29,29,29	0
56	MG	2a	3160	1/1	0.90	0.13	66,66,66,66	0
56	MG	2A	3856	1/1	0.90	0.46	35,35,35,35	0
56	MG	1A	3396	1/1	0.90	0.18	29,29,29,29	0
56	MG	2A	3861	1/1	0.90	0.07	51,51,51,51	0
56	MG	1A	3038	1/1	0.90	0.23	26,26,26,26	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	2A	3573	1/1	0.90	0.07	44,44,44,44	0
56	MG	2A	3309	1/1	0.90	0.35	55,55,55,55	0
56	MG	1a	3058	1/1	0.90	0.10	53,53,53,53	0
56	MG	1A	3399	1/1	0.90	0.11	42,42,42,42	0
56	MG	2A	3315	1/1	0.90	0.23	40,40,40,40	0
56	MG	2A	3581	1/1	0.90	0.09	42,42,42,42	0
56	MG	1A	3737	1/1	0.90	0.15	17,17,17,17	0
56	MG	1A	3065	1/1	0.90	0.26	20,20,20,20	0
56	MG	2A	3585	1/1	0.90	0.19	45,45,45,45	0
56	MG	1A	3298	1/1	0.90	0.15	45,45,45,45	0
56	MG	2a	3198	1/1	0.90	0.30	59,59,59,59	0
56	MG	1B	3010	1/1	0.90	0.39	32,32,32,32	0
56	MG	1a	3073	1/1	0.90	0.14	34,34,34,34	0
56	MG	1A	3069	1/1	0.90	0.10	16,16,16,16	0
56	MG	2B	3016	1/1	0.90	0.15	63,63,63,63	0
56	MG	2A	3141	1/1	0.90	0.22	53,53,53,53	0
56	MG	1A	3483	1/1	0.90	0.32	23,23,23,23	0
56	MG	2A	3610	1/1	0.90	0.09	42,42,42,42	0
56	MG	1a	3219	1/1	0.90	0.09	53,53,53,53	0
56	MG	2A	3618	1/1	0.90	0.13	35,35,35,35	0
56	MG	2A	3337	1/1	0.90	0.25	44,44,44,44	0
56	MG	2A	3149	1/1	0.90	0.17	56,56,56,56	0
56	MG	2a	3220	1/1	0.90	0.14	57,57,57,57	0
56	MG	2E	306	1/1	0.90	0.14	45,45,45,45	0
56	MG	1A	3604	1/1	0.90	0.11	29,29,29,29	0
56	MG	1a	3222	1/1	0.90	0.14	60,60,60,60	0
56	MG	1A	3347	1/1	0.90	0.29	34,34,34,34	0
56	MG	2G	3001	1/1	0.90	0.15	62,62,62,62	0
56	MG	2l	202	1/1	0.90	0.16	62,62,62,62	0
56	MG	1A	3767	1/1	0.90	0.26	25,25,25,25	0
56	MG	1b	3001	1/1	0.90	0.17	69,69,69,69	0
56	MG	2t	3001	1/1	0.90	0.12	48,48,48,48	0
56	MG	2A	3647	1/1	0.90	0.21	39,39,39,39	0
56	MG	2A	3161	1/1	0.90	0.16	36,36,36,36	0
56	MG	1A	3206	1/1	0.90	0.20	34,34,34,34	0
56	MG	2A	3164	1/1	0.90	0.16	18,18,18,18	0
56	MG	1e	201	1/1	0.90	0.09	63,63,63,63	0
56	MG	2w	3006	1/1	0.90	0.10	78,78,78,78	0
56	MG	2U	205	1/1	0.90	0.37	46,46,46,46	0
56	MG	1a	3083	1/1	0.90	0.19	53,53,53,53	0
56	MG	2A	3174	1/1	0.90	0.18	43,43,43,43	0
56	MG	1A	3093	1/1	0.90	0.29	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	1D	312	1/1	0.90	0.28	20,20,20,20	0
56	MG	1A	3773	1/1	0.90	0.10	26,26,26,26	0
56	MG	1a	3099	1/1	0.90	0.24	51,51,51,51	0
56	MG	1A	3043	1/1	0.90	0.22	28,28,28,28	0
56	MG	2A	3375	1/1	0.90	0.17	47,47,47,47	0
56	MG	2a	3001	1/1	0.90	0.39	56,56,56,56	0
56	MG	1A	4084	1/1	0.91	0.18	24,24,24,24	0
56	MG	1A	3404	1/1	0.91	0.28	21,21,21,21	0
56	MG	1A	3484	1/1	0.91	0.36	33,33,33,33	0
56	MG	2A	3587	1/1	0.91	0.24	68,68,68,68	0
56	MG	2A	3103	1/1	0.91	0.21	59,59,59,59	0
56	MG	1A	3203	1/1	0.91	0.48	25,25,25,25	0
56	MG	2A	3303	1/1	0.91	0.15	35,35,35,35	0
56	MG	2T	3003	1/1	0.91	0.13	59,59,59,59	0
56	MG	2A	3304	1/1	0.91	0.13	44,44,44,44	0
56	MG	1A	3601	1/1	0.91	0.15	55,55,55,55	0
56	MG	1A	3409	1/1	0.91	0.20	52,52,52,52	0
56	MG	1A	3882	1/1	0.91	0.14	25,25,25,25	0
56	MG	2A	3611	1/1	0.91	0.09	61,61,61,61	0
56	MG	1A	3748	1/1	0.91	0.13	29,29,29,29	0
56	MG	1A	3010	1/1	0.91	0.20	22,22,22,22	0
56	MG	1a	3034	1/1	0.91	0.17	49,49,49,49	0
56	MG	25	104	1/1	0.91	0.11	45,45,45,45	0
56	MG	1A	4113	1/1	0.91	0.12	44,44,44,44	0
56	MG	2A	3119	1/1	0.91	0.32	30,30,30,30	0
56	MG	1A	4116	1/1	0.91	0.13	38,38,38,38	0
56	MG	1a	3040	1/1	0.91	0.32	39,39,39,39	0
56	MG	1A	3133	1/1	0.91	0.21	17,17,17,17	0
56	MG	2A	3640	1/1	0.91	0.12	34,34,34,34	0
56	MG	2a	3005	1/1	0.91	0.21	42,42,42,42	0
56	MG	1a	3042	1/1	0.91	0.15	55,55,55,55	0
56	MG	2a	3007	1/1	0.91	0.12	38,38,38,38	0
56	MG	1a	3044	1/1	0.91	0.19	50,50,50,50	0
56	MG	2A	3329	1/1	0.91	0.20	29,29,29,29	0
56	MG	2A	3330	1/1	0.91	0.23	47,47,47,47	0
56	MG	1a	3045	1/1	0.91	0.14	38,38,38,38	0
56	MG	1A	3303	1/1	0.91	0.47	25,25,25,25	0
56	MG	1A	3616	1/1	0.91	0.15	23,23,23,23	0
56	MG	2A	3135	1/1	0.91	0.79	53,53,53,53	0
56	MG	1A	4128	1/1	0.91	0.13	22,22,22,22	0
56	MG	1A	4131	1/1	0.91	0.41	16,16,16,16	0
56	MG	1a	3200	1/1	0.91	0.08	42,42,42,42	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	2a	3018	1/1	0.91	0.10	50,50,50,50	0
56	MG	1a	3052	1/1	0.91	0.22	45,45,45,45	0
56	MG	2A	3664	1/1	0.91	0.17	50,50,50,50	0
56	MG	2a	3022	1/1	0.91	0.17	53,53,53,53	0
56	MG	2A	3665	1/1	0.91	0.13	47,47,47,47	0
56	MG	1A	3765	1/1	0.91	0.19	18,18,18,18	0
56	MG	2A	3344	1/1	0.91	0.13	48,48,48,48	0
56	MG	2A	3670	1/1	0.91	0.10	50,50,50,50	0
56	MG	2A	3145	1/1	0.91	0.12	33,33,33,33	0
56	MG	1a	3203	1/1	0.91	0.06	56,56,56,56	0
56	MG	1A	3247	1/1	0.91	0.35	31,31,31,31	0
56	MG	2A	3676	1/1	0.91	0.11	48,48,48,48	0
56	MG	1B	3005	1/1	0.91	0.19	50,50,50,50	0
56	MG	2A	3678	1/1	0.91	0.12	60,60,60,60	0
56	MG	2a	3037	1/1	0.91	0.12	53,53,53,53	0
56	MG	1A	3110	1/1	0.91	0.29	22,22,22,22	0
56	MG	2A	3350	1/1	0.91	0.27	60,60,60,60	0
56	MG	1A	3429	1/1	0.91	0.20	39,39,39,39	0
56	MG	1A	3357	1/1	0.91	0.15	12,12,12,12	0
56	MG	1A	3207	1/1	0.91	0.30	25,25,25,25	0
56	MG	2A	3160	1/1	0.91	0.15	33,33,33,33	0
56	MG	1B	3011	1/1	0.91	0.38	29,29,29,29	0
56	MG	2A	3162	1/1	0.91	0.10	42,42,42,42	0
56	MG	2A	3691	1/1	0.91	0.16	51,51,51,51	0
56	MG	1a	3071	1/1	0.91	0.14	41,41,41,41	0
56	MG	1a	3225	1/1	0.91	0.23	62,62,62,62	0
56	MG	1A	3209	1/1	0.91	0.41	45,45,45,45	0
56	MG	2A	3170	1/1	0.91	0.22	66,66,66,66	0
56	MG	1A	3510	1/1	0.91	0.26	29,29,29,29	0
56	MG	1A	3362	1/1	0.91	0.89	41,41,41,41	0
56	MG	1A	3791	1/1	0.91	0.42	32,32,32,32	0
56	MG	2a	3064	1/1	0.91	0.14	51,51,51,51	0
56	MG	2a	3067	1/1	0.91	0.12	45,45,45,45	0
56	MG	2A	3711	1/1	0.91	0.32	61,61,61,61	0
56	MG	2A	3387	1/1	0.91	0.14	39,39,39,39	0
56	MG	1A	3514	1/1	0.91	0.17	33,33,33,33	0
56	MG	2a	3073	1/1	0.91	0.23	73,73,73,73	0
56	MG	2a	3074	1/1	0.91	0.21	43,43,43,43	0
56	MG	1B	3028	1/1	0.91	0.24	38,38,38,38	0
56	MG	1m	3001	1/1	0.91	0.24	48,48,48,48	0
56	MG	1A	4015	1/1	0.91	0.15	40,40,40,40	0
56	MG	2a	3081	1/1	0.91	0.07	70,70,70,70	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	1A	3441	1/1	0.91	0.22	40,40,40,40	0
56	MG	2A	3189	1/1	0.91	0.20	38,38,38,38	0
56	MG	1A	3370	1/1	0.91	0.15	29,29,29,29	0
56	MG	2A	3400	1/1	0.91	0.14	51,51,51,51	0
56	MG	2a	3094	1/1	0.91	0.09	64,64,64,64	0
56	MG	2A	3402	1/1	0.91	0.16	39,39,39,39	0
56	MG	1a	3087	1/1	0.91	0.17	63,63,63,63	0
56	MG	1a	3089	1/1	0.91	0.27	37,37,37,37	0
56	MG	1A	3142	1/1	0.91	0.20	16,16,16,16	0
56	MG	2A	3197	1/1	0.91	0.11	46,46,46,46	0
56	MG	1a	3093	1/1	0.91	0.23	35,35,35,35	0
56	MG	1A	4020	1/1	0.91	0.46	44,44,44,44	0
56	MG	2A	3733	1/1	0.91	0.13	70,70,70,70	0
56	MG	2a	3111	1/1	0.91	0.12	46,46,46,46	0
56	MG	1a	3098	1/1	0.91	0.09	60,60,60,60	0
56	MG	1A	3060	1/1	0.91	0.17	32,32,32,32	0
56	MG	1a	3101	1/1	0.91	0.20	48,48,48,48	0
56	MG	2A	3420	1/1	0.91	0.12	40,40,40,40	0
56	MG	2A	3205	1/1	0.91	0.13	44,44,44,44	0
56	MG	1A	3810	1/1	0.91	0.17	27,27,27,27	0
56	MG	2A	3425	1/1	0.91	0.45	56,56,56,56	0
56	MG	1A	3375	1/1	0.91	0.15	25,25,25,25	0
56	MG	2a	3122	1/1	0.91	0.04	73,73,73,73	0
56	MG	1A	3255	1/1	0.91	0.33	38,38,38,38	0
56	MG	1x	112	1/1	0.91	0.17	67,67,67,67	0
56	MG	2A	3431	1/1	0.91	0.13	47,47,47,47	0
56	MG	1A	3320	1/1	0.91	0.22	28,28,28,28	0
56	MG	2A	3433	1/1	0.91	0.18	51,51,51,51	0
56	MG	2A	3435	1/1	0.91	0.12	62,62,62,62	0
56	MG	2A	3439	1/1	0.91	0.21	51,51,51,51	0
56	MG	1A	3819	1/1	0.91	0.14	10,10,10,10	0
56	MG	2A	3220	1/1	0.91	0.10	60,60,60,60	0
56	MG	1y	105	1/1	0.91	0.24	81,81,81,81	0
56	MG	1A	3121	1/1	0.91	0.27	32,32,32,32	0
56	MG	1I	3001	1/1	0.91	0.19	50,50,50,50	0
56	MG	2A	3453	1/1	0.91	0.14	52,52,52,52	0
56	MG	1N	3002	1/1	0.91	0.11	25,25,25,25	0
56	MG	2A	3226	1/1	0.91	0.27	47,47,47,47	0
56	MG	1A	3184	1/1	0.91	0.32	37,37,37,37	0
56	MG	1O	3004	1/1	0.91	0.19	41,41,41,41	0
56	MG	2A	3778	1/1	0.91	0.19	57,57,57,57	0
56	MG	2A	3232	1/1	0.91	0.10	42,42,42,42	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	2A	3782	1/1	0.91	0.07	44,44,44,44	0
56	MG	1P	202	1/1	0.91	0.49	16,16,16,16	0
56	MG	1A	3823	1/1	0.91	0.16	17,17,17,17	0
56	MG	2A	3236	1/1	0.91	0.13	50,50,50,50	0
56	MG	1R	203	1/1	0.91	0.28	30,30,30,30	0
56	MG	2A	3788	1/1	0.91	0.14	57,57,57,57	0
56	MG	2A	3240	1/1	0.91	0.14	43,43,43,43	0
56	MG	1A	3381	1/1	0.91	0.12	25,25,25,25	0
56	MG	2A	3792	1/1	0.91	0.11	37,37,37,37	0
56	MG	2A	3023	1/1	0.91	0.16	34,34,34,34	0
56	MG	2A	3795	1/1	0.91	0.11	34,34,34,34	0
56	MG	1A	3221	1/1	0.91	0.19	34,34,34,34	0
56	MG	2A	3798	1/1	0.91	0.12	51,51,51,51	0
56	MG	2a	3170	1/1	0.91	0.16	55,55,55,55	0
56	MG	2a	3171	1/1	0.91	0.14	53,53,53,53	0
56	MG	2A	3491	1/1	0.91	0.09	35,35,35,35	0
56	MG	1A	3934	1/1	0.91	0.10	14,14,14,14	0
56	MG	1A	3684	1/1	0.91	0.10	24,24,24,24	0
56	MG	2a	3179	1/1	0.91	0.10	53,53,53,53	0
56	MG	2A	3815	1/1	0.91	0.21	59,59,59,59	0
56	MG	2A	3030	1/1	0.91	0.28	56,56,56,56	0
56	MG	1A	3831	1/1	0.91	0.08	40,40,40,40	0
56	MG	2A	3497	1/1	0.91	0.23	46,46,46,46	0
56	MG	2A	3034	1/1	0.91	0.15	43,43,43,43	0
56	MG	1A	3224	1/1	0.91	0.14	41,41,41,41	0
56	MG	2A	3251	1/1	0.91	0.09	52,52,52,52	0
56	MG	2A	3041	1/1	0.91	0.18	46,46,46,46	0
56	MG	2A	3254	1/1	0.91	0.27	53,53,53,53	0
56	MG	1A	3944	1/1	0.91	0.05	53,53,53,53	0
56	MG	1A	3837	1/1	0.91	0.23	22,22,22,22	0
56	MG	2A	3511	1/1	0.91	0.15	38,38,38,38	0
56	MG	2a	3203	1/1	0.91	0.16	64,64,64,64	0
56	MG	2A	3258	1/1	0.91	0.10	40,40,40,40	0
56	MG	1A	3009	1/1	0.91	0.13	16,16,16,16	0
56	MG	1A	4043	1/1	0.91	0.10	30,30,30,30	0
56	MG	1a	3148	1/1	0.91	0.15	31,31,31,31	0
56	MG	2A	3867	1/1	0.91	0.13	36,36,36,36	0
56	MG	2A	3523	1/1	0.91	0.14	58,58,58,58	0
56	MG	10	106	1/1	0.91	0.12	48,48,48,48	0
56	MG	2A	3531	1/1	0.91	0.22	51,51,51,51	0
56	MG	11	102	1/1	0.91	0.21	47,47,47,47	0
56	MG	1A	3551	1/1	0.91	0.19	26,26,26,26	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	1A	3388	1/1	0.91	0.16	39,39,39,39	0
56	MG	1A	3268	1/1	0.91	0.26	15,15,15,15	0
56	MG	2d	303	1/1	0.91	0.10	65,65,65,65	0
56	MG	2A	3063	1/1	0.91	0.11	33,33,33,33	0
56	MG	2A	3272	1/1	0.91	0.24	43,43,43,43	0
56	MG	1a	3154	1/1	0.91	0.17	38,38,38,38	0
56	MG	1A	3195	1/1	0.91	0.11	8,8,8,8	0
56	MG	2A	3549	1/1	0.91	0.20	34,34,34,34	0
56	MG	16	103	1/1	0.91	0.14	33,33,33,33	0
56	MG	1A	3124	1/1	0.91	0.28	17,17,17,17	0
56	MG	2A	3554	1/1	0.91	0.42	51,51,51,51	0
56	MG	1A	3233	1/1	0.91	0.58	24,24,24,24	0
56	MG	2B	3021	1/1	0.91	0.09	69,69,69,69	0
56	MG	2D	301	1/1	0.91	0.22	36,36,36,36	0
56	MG	2D	302	1/1	0.91	0.11	38,38,38,38	0
56	MG	2A	3560	1/1	0.91	0.11	40,40,40,40	0
56	MG	1a	3162	1/1	0.91	0.13	42,42,42,42	0
56	MG	1A	3342	1/1	0.91	0.47	31,31,31,31	0
56	MG	1A	3476	1/1	0.91	0.20	44,44,44,44	0
56	MG	1A	3015	1/1	0.91	0.29	20,20,20,20	0
56	MG	1A	3401	1/1	0.91	0.14	29,29,29,29	0
56	MG	1a	3009	1/1	0.91	0.16	44,44,44,44	0
56	MG	1A	3201	1/1	0.91	0.16	26,26,26,26	0
56	MG	1A	4082	1/1	0.91	0.17	29,29,29,29	0
56	MG	1A	3588	1/1	0.92	0.20	24,24,24,24	0
56	MG	2A	3351	1/1	0.92	0.24	59,59,59,59	0
56	MG	1A	3453	1/1	0.92	0.22	44,44,44,44	0
56	MG	1A	4092	1/1	0.92	0.19	10,10,10,10	0
56	MG	2A	3356	1/1	0.92	0.19	51,51,51,51	0
56	MG	2A	3150	1/1	0.92	0.14	53,53,53,53	0
56	MG	1A	3597	1/1	0.92	0.12	25,25,25,25	0
56	MG	1A	4101	1/1	0.92	0.07	23,23,23,23	0
56	MG	1a	3035	1/1	0.92	0.10	43,43,43,43	0
56	MG	1A	3282	1/1	0.92	0.13	48,48,48,48	0
56	MG	1A	3725	1/1	0.92	0.16	29,29,29,29	0
56	MG	1A	3600	1/1	0.92	0.18	14,14,14,14	0
56	MG	1A	3729	1/1	0.92	0.19	10,10,10,10	0
56	MG	1a	3208	1/1	0.92	0.18	62,62,62,62	0
56	MG	1A	4112	1/1	0.92	0.51	31,31,31,31	0
56	MG	1A	3284	1/1	0.92	0.22	27,27,27,27	0
56	MG	2A	3165	1/1	0.92	0.11	53,53,53,53	0
56	MG	1a	3215	1/1	0.92	0.11	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	3402	1/1	0.92	0.28	27,27,27,27	0
56	MG	1A	3968	1/1	0.92	0.16	53,53,53,53	0
56	MG	2A	3173	1/1	0.92	0.16	39,39,39,39	0
56	MG	1A	3177	1/1	0.92	0.17	26,26,26,26	0
56	MG	1A	3607	1/1	0.92	0.19	40,40,40,40	0
56	MG	1A	4127	1/1	0.92	0.27	23,23,23,23	0
56	MG	2A	3399	1/1	0.92	0.28	53,53,53,53	0
56	MG	2a	3028	1/1	0.92	0.18	58,58,58,58	0
56	MG	2A	3696	1/1	0.92	0.16	42,42,42,42	0
56	MG	2a	3030	1/1	0.92	0.18	51,51,51,51	0
56	MG	1A	3363	1/1	0.92	0.46	29,29,29,29	0
56	MG	2A	3701	1/1	0.92	0.16	32,32,32,32	0
56	MG	2A	3401	1/1	0.92	0.13	52,52,52,52	0
56	MG	1A	3862	1/1	0.92	0.22	15,15,15,15	0
56	MG	1A	3865	1/1	0.92	0.23	14,14,14,14	0
56	MG	1A	4137	1/1	0.92	0.17	20,20,20,20	0
56	MG	1A	3365	1/1	0.92	0.15	17,17,17,17	0
56	MG	1A	3615	1/1	0.92	0.10	22,22,22,22	0
56	MG	2a	3040	1/1	0.92	0.12	47,47,47,47	0
56	MG	2A	3713	1/1	0.92	0.09	55,55,55,55	0
56	MG	1A	3873	1/1	0.92	0.12	40,40,40,40	0
56	MG	1A	3984	1/1	0.92	0.11	21,21,21,21	0
56	MG	2A	3413	1/1	0.92	0.17	50,50,50,50	0
56	MG	1A	3985	1/1	0.92	0.22	20,20,20,20	0
56	MG	1A	3290	1/1	0.92	0.21	37,37,37,37	0
56	MG	1A	3989	1/1	0.92	0.14	21,21,21,21	0
56	MG	2A	3199	1/1	0.92	0.34	44,44,44,44	0
56	MG	1B	3013	1/1	0.92	0.11	31,31,31,31	0
56	MG	2A	3423	1/1	0.92	0.46	48,48,48,48	0
56	MG	1A	3740	1/1	0.92	0.11	44,44,44,44	0
56	MG	1A	3743	1/1	0.92	0.07	17,17,17,17	0
56	MG	1A	3744	1/1	0.92	0.11	55,55,55,55	0
56	MG	2a	3058	1/1	0.92	0.10	50,50,50,50	0
56	MG	2a	3059	1/1	0.92	0.11	52,52,52,52	0
56	MG	2a	3060	1/1	0.92	0.22	49,49,49,49	0
56	MG	1A	3746	1/1	0.92	0.12	15,15,15,15	0
56	MG	1w	107	1/1	0.92	0.11	48,48,48,48	0
56	MG	2A	3210	1/1	0.92	0.30	42,42,42,42	0
56	MG	1B	3024	1/1	0.92	0.20	49,49,49,49	0
56	MG	1B	3025	1/1	0.92	0.20	21,21,21,21	0
56	MG	1A	3528	1/1	0.92	0.19	45,45,45,45	0
56	MG	2A	3436	1/1	0.92	0.10	40,40,40,40	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	2a	3071	1/1	0.92	0.30	55,55,55,55	0
56	MG	1w	111	1/1	0.92	0.09	37,37,37,37	0
56	MG	1A	3750	1/1	0.92	0.37	41,41,41,41	0
56	MG	1a	3088	1/1	0.92	0.20	52,52,52,52	0
56	MG	1x	106	1/1	0.92	0.12	52,52,52,52	0
56	MG	1B	3030	1/1	0.92	0.08	44,44,44,44	0
56	MG	2A	3744	1/1	0.92	0.21	76,76,76,76	0
56	MG	1A	3630	1/1	0.92	0.21	12,12,12,12	0
56	MG	2a	3086	1/1	0.92	0.12	57,57,57,57	0
56	MG	2a	3088	1/1	0.92	0.15	67,67,67,67	0
56	MG	1A	4005	1/1	0.92	0.12	34,34,34,34	0
56	MG	2a	3090	1/1	0.92	0.11	64,64,64,64	0
56	MG	2A	3454	1/1	0.92	0.14	52,52,52,52	0
56	MG	1a	3096	1/1	0.92	0.24	45,45,45,45	0
56	MG	1D	307	1/1	0.92	0.16	41,41,41,41	0
56	MG	1A	3292	1/1	0.92	0.13	22,22,22,22	0
56	MG	2A	3001	1/1	0.92	0.32	41,41,41,41	0
56	MG	2A	3467	1/1	0.92	0.13	32,32,32,32	0
56	MG	1A	3890	1/1	0.92	0.12	51,51,51,51	0
56	MG	2a	3102	1/1	0.92	0.17	60,60,60,60	0
56	MG	1E	301	1/1	0.92	0.44	18,18,18,18	0
56	MG	2A	3761	1/1	0.92	0.13	42,42,42,42	0
56	MG	1A	3469	1/1	0.92	0.15	36,36,36,36	0
56	MG	2A	3765	1/1	0.92	0.12	39,39,39,39	0
56	MG	2A	3008	1/1	0.92	0.10	39,39,39,39	0
56	MG	1A	4010	1/1	0.92	0.37	54,54,54,54	0
56	MG	2A	3241	1/1	0.92	0.42	66,66,66,66	0
56	MG	1A	3420	1/1	0.92	0.16	62,62,62,62	0
56	MG	1A	3228	1/1	0.92	0.27	18,18,18,18	0
56	MG	1A	3638	1/1	0.92	0.11	27,27,27,27	0
56	MG	1A	3085	1/1	0.92	0.25	37,37,37,37	0
56	MG	1F	305	1/1	0.92	0.17	36,36,36,36	0
56	MG	1a	3112	1/1	0.92	0.15	48,48,48,48	0
56	MG	1a	3113	1/1	0.92	0.12	37,37,37,37	0
56	MG	1A	4017	1/1	0.92	0.44	57,57,57,57	0
56	MG	1a	3115	1/1	0.92	0.22	38,38,38,38	0
56	MG	2A	3029	1/1	0.92	0.18	52,52,52,52	0
56	MG	1G	3002	1/1	0.92	0.13	38,38,38,38	0
56	MG	1a	3118	1/1	0.92	0.27	37,37,37,37	0
56	MG	2A	3790	1/1	0.92	0.09	32,32,32,32	0
56	MG	1A	3542	1/1	0.92	0.16	29,29,29,29	0
56	MG	2A	3037	1/1	0.92	0.15	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	1A	3899	1/1	0.92	0.11	28,28,28,28	0
56	MG	1A	3769	1/1	0.92	0.12	37,37,37,37	0
56	MG	1a	3122	1/1	0.92	0.25	46,46,46,46	0
56	MG	1a	3125	1/1	0.92	0.21	37,37,37,37	0
56	MG	2A	3800	1/1	0.92	0.12	26,26,26,26	0
56	MG	1a	3128	1/1	0.92	0.13	36,36,36,36	0
56	MG	1N	3006	1/1	0.92	0.55	46,46,46,46	0
56	MG	1A	3651	1/1	0.92	0.23	12,12,12,12	0
56	MG	1A	3094	1/1	0.92	0.11	43,43,43,43	0
56	MG	1A	3774	1/1	0.92	0.09	25,25,25,25	0
56	MG	2A	3053	1/1	0.92	0.45	30,30,30,30	0
56	MG	2A	3532	1/1	0.92	0.18	42,42,42,42	0
56	MG	2A	3825	1/1	0.92	0.09	58,58,58,58	0
56	MG	2A	3826	1/1	0.92	0.23	62,62,62,62	0
56	MG	2A	3533	1/1	0.92	0.18	54,54,54,54	0
56	MG	1a	3135	1/1	0.92	0.08	46,46,46,46	0
56	MG	2A	3057	1/1	0.92	0.36	42,42,42,42	0
56	MG	1A	3336	1/1	0.92	0.11	27,27,27,27	0
56	MG	2A	3061	1/1	0.92	0.15	38,38,38,38	0
56	MG	2A	3848	1/1	0.92	0.24	33,33,33,33	0
56	MG	1Q	3004	1/1	0.92	0.18	36,36,36,36	0
56	MG	1A	3338	1/1	0.92	0.16	37,37,37,37	0
56	MG	1R	204	1/1	0.92	0.24	34,34,34,34	0
56	MG	1A	3055	1/1	0.92	0.11	63,63,63,63	0
56	MG	2A	3069	1/1	0.92	0.21	43,43,43,43	0
56	MG	1A	3787	1/1	0.92	0.16	40,40,40,40	0
56	MG	1A	3482	1/1	0.92	0.21	18,18,18,18	0
56	MG	2a	3175	1/1	0.92	0.09	51,51,51,51	0
56	MG	1A	3189	1/1	0.92	0.28	29,29,29,29	0
56	MG	1A	3068	1/1	0.92	0.38	50,50,50,50	0
56	MG	2A	3870	1/1	0.92	0.45	40,40,40,40	0
56	MG	1V	202	1/1	0.92	0.14	52,52,52,52	0
56	MG	2a	3184	1/1	0.92	0.09	46,46,46,46	0
56	MG	1A	3920	1/1	0.92	0.13	41,41,41,41	0
56	MG	1A	3921	1/1	0.92	0.10	45,45,45,45	0
56	MG	2A	3569	1/1	0.92	0.13	31,31,31,31	0
56	MG	2A	3570	1/1	0.92	0.17	33,33,33,33	0
56	MG	2a	3191	1/1	0.92	0.10	61,61,61,61	0
56	MG	2A	3572	1/1	0.92	0.14	25,25,25,25	0
56	MG	1A	3307	1/1	0.92	0.21	32,32,32,32	0
56	MG	2A	3574	1/1	0.92	0.10	49,49,49,49	0
56	MG	1A	3040	1/1	0.92	0.18	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	1a	3155	1/1	0.92	0.12	50,50,50,50	0
56	MG	1A	3165	1/1	0.92	0.38	29,29,29,29	0
56	MG	2A	3092	1/1	0.92	0.34	41,41,41,41	0
56	MG	1A	3807	1/1	0.92	0.09	42,42,42,42	0
56	MG	1A	3246	1/1	0.92	0.16	28,28,28,28	0
56	MG	1A	3392	1/1	0.92	0.27	33,33,33,33	0
56	MG	1A	3153	1/1	0.92	0.81	23,23,23,23	0
56	MG	2A	3104	1/1	0.92	0.10	30,30,30,30	0
56	MG	15	102	1/1	0.92	0.53	28,28,28,28	0
56	MG	1A	3931	1/1	0.92	0.10	36,36,36,36	0
56	MG	2a	3214	1/1	0.92	0.10	51,51,51,51	0
56	MG	1a	3165	1/1	0.92	0.12	45,45,45,45	0
56	MG	1A	3682	1/1	0.92	0.13	12,12,12,12	0
56	MG	1A	3568	1/1	0.92	0.16	51,51,51,51	0
56	MG	17	102	1/1	0.92	0.32	36,36,36,36	0
56	MG	2E	305	1/1	0.92	0.14	39,39,39,39	0
56	MG	17	103	1/1	0.92	0.10	36,36,36,36	0
56	MG	2A	3327	1/1	0.92	0.21	40,40,40,40	0
56	MG	1A	3690	1/1	0.92	0.11	40,40,40,40	0
56	MG	2A	3613	1/1	0.92	0.09	38,38,38,38	0
56	MG	2A	3614	1/1	0.92	0.13	68,68,68,68	0
56	MG	2q	202	1/1	0.92	0.09	64,64,64,64	0
56	MG	2q	203	1/1	0.92	0.13	55,55,55,55	0
56	MG	2r	101	1/1	0.92	0.23	75,75,75,75	0
56	MG	1A	3175	1/1	0.92	0.15	35,35,35,35	0
56	MG	1A	3280	1/1	0.92	0.17	25,25,25,25	0
56	MG	1A	4054	1/1	0.92	0.16	37,37,37,37	0
56	MG	1A	3006	1/1	0.92	0.20	44,44,44,44	0
56	MG	2R	201	1/1	0.92	0.15	39,39,39,39	0
56	MG	1a	3006	1/1	0.92	0.30	49,49,49,49	0
56	MG	1A	3826	1/1	0.92	0.11	41,41,41,41	0
56	MG	1A	4072	1/1	0.92	0.14	44,44,44,44	0
56	MG	2A	3128	1/1	0.92	0.11	50,50,50,50	0
56	MG	1A	4075	1/1	0.92	0.20	39,39,39,39	0
56	MG	1A	3945	1/1	0.92	0.12	39,39,39,39	0
56	MG	1A	3702	1/1	0.92	0.15	31,31,31,31	0
56	MG	1A	3706	1/1	0.92	0.12	48,48,48,48	0
56	MG	1A	3579	1/1	0.92	0.17	27,27,27,27	0
56	MG	1A	3832	1/1	0.92	0.14	34,34,34,34	0
56	MG	1a	3025	1/1	0.92	0.12	42,42,42,42	0
56	MG	1A	3505	1/1	0.92	0.27	25,25,25,25	0
56	MG	2A	3143	1/1	0.92	0.49	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	4099	1/1	0.93	0.10	43,43,43,43	0
56	MG	1A	3183	1/1	0.93	0.36	24,24,24,24	0
56	MG	1A	4103	1/1	0.93	0.19	16,16,16,16	0
56	MG	1A	3398	1/1	0.93	0.51	48,48,48,48	0
56	MG	2A	3228	1/1	0.93	0.13	41,41,41,41	0
56	MG	2A	3697	1/1	0.93	0.24	51,51,51,51	0
56	MG	2A	3426	1/1	0.93	0.26	39,39,39,39	0
56	MG	18	103	1/1	0.93	0.20	29,29,29,29	0
56	MG	1A	3643	1/1	0.93	0.15	15,15,15,15	0
56	MG	2A	3233	1/1	0.93	0.11	41,41,41,41	0
56	MG	2A	3706	1/1	0.93	0.11	58,58,58,58	0
56	MG	1A	3302	1/1	0.93	0.27	23,23,23,23	0
56	MG	2A	3708	1/1	0.93	0.06	48,48,48,48	0
56	MG	2A	3709	1/1	0.93	0.12	43,43,43,43	0
56	MG	1A	3148	1/1	0.93	0.30	23,23,23,23	0
56	MG	1A	3541	1/1	0.93	0.27	29,29,29,29	0
56	MG	1A	3986	1/1	0.93	0.14	13,13,13,13	0
56	MG	2A	3046	1/1	0.93	0.12	56,56,56,56	0
56	MG	1A	4115	1/1	0.93	0.22	32,32,32,32	0
56	MG	1A	3036	1/1	0.93	0.51	25,25,25,25	0
56	MG	1A	3122	1/1	0.93	0.13	24,24,24,24	0
56	MG	1A	3990	1/1	0.93	0.17	19,19,19,19	0
56	MG	1A	3656	1/1	0.93	0.18	12,12,12,12	0
56	MG	2A	3054	1/1	0.93	0.19	39,39,39,39	0
56	MG	1a	3014	1/1	0.93	0.14	36,36,36,36	0
56	MG	1A	3470	1/1	0.93	0.19	33,33,33,33	0
56	MG	2A	3455	1/1	0.93	0.15	61,61,61,61	0
56	MG	2A	3457	1/1	0.93	0.15	51,51,51,51	0
56	MG	1A	3996	1/1	0.93	0.10	50,50,50,50	0
56	MG	1a	3020	1/1	0.93	0.10	33,33,33,33	0
56	MG	1A	3056	1/1	0.93	0.18	33,33,33,33	0
56	MG	1A	3309	1/1	0.93	0.32	37,37,37,37	0
56	MG	2A	3065	1/1	0.93	0.18	37,37,37,37	0
56	MG	1A	3045	1/1	0.93	0.24	22,22,22,22	0
56	MG	1A	3780	1/1	0.93	0.13	41,41,41,41	0
56	MG	1A	3667	1/1	0.93	0.14	35,35,35,35	0
56	MG	2A	3259	1/1	0.93	0.37	46,46,46,46	0
56	MG	2A	3070	1/1	0.93	0.11	34,34,34,34	0
56	MG	1B	3006	1/1	0.93	0.18	29,29,29,29	0
56	MG	2a	3051	1/1	0.93	0.12	52,52,52,52	0
56	MG	1A	3902	1/1	0.93	0.08	34,34,34,34	0
56	MG	2A	3078	1/1	0.93	0.15	31,31,31,31	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	2A	3742	1/1	0.93	0.41	69,69,69,69	0
56	MG	1A	3408	1/1	0.93	0.18	39,39,39,39	0
56	MG	2A	3484	1/1	0.93	0.13	32,32,32,32	0
56	MG	1A	3313	1/1	0.93	0.15	23,23,23,23	0
56	MG	1A	3263	1/1	0.93	0.41	31,31,31,31	0
56	MG	2A	3747	1/1	0.93	0.08	59,59,59,59	0
56	MG	1A	3794	1/1	0.93	0.19	37,37,37,37	0
56	MG	1A	3911	1/1	0.93	0.14	34,34,34,34	0
56	MG	1A	3675	1/1	0.93	0.20	32,32,32,32	0
56	MG	1a	3178	1/1	0.93	0.10	41,41,41,41	0
56	MG	1A	3316	1/1	0.93	0.19	49,49,49,49	0
56	MG	1A	3059	1/1	0.93	0.20	42,42,42,42	0
56	MG	2A	3756	1/1	0.93	0.14	45,45,45,45	0
56	MG	2A	3277	1/1	0.93	0.10	46,46,46,46	0
56	MG	1A	3129	1/1	0.93	0.44	20,20,20,20	0
56	MG	1A	3367	1/1	0.93	0.36	14,14,14,14	0
56	MG	1a	3185	1/1	0.93	0.10	60,60,60,60	0
56	MG	1A	3234	1/1	0.93	0.13	25,25,25,25	0
56	MG	1a	3048	1/1	0.93	0.17	52,52,52,52	0
56	MG	1A	3487	1/1	0.93	0.33	25,25,25,25	0
56	MG	2A	3513	1/1	0.93	0.16	36,36,36,36	0
56	MG	2a	3087	1/1	0.93	0.17	53,53,53,53	0
56	MG	1A	3569	1/1	0.93	0.18	23,23,23,23	0
56	MG	1B	3029	1/1	0.93	0.14	59,59,59,59	0
56	MG	1a	3053	1/1	0.93	0.16	46,46,46,46	0
56	MG	1a	3193	1/1	0.93	0.17	37,37,37,37	0
56	MG	2A	3526	1/1	0.93	0.07	57,57,57,57	0
56	MG	1A	3021	1/1	0.93	0.37	20,20,20,20	0
56	MG	1A	3272	1/1	0.93	0.18	30,30,30,30	0
56	MG	1A	3573	1/1	0.93	0.19	22,22,22,22	0
56	MG	1D	301	1/1	0.93	0.38	29,29,29,29	0
56	MG	2A	3118	1/1	0.93	0.28	35,35,35,35	0
56	MG	1a	3061	1/1	0.93	0.09	50,50,50,50	0
56	MG	1A	3704	1/1	0.93	0.09	37,37,37,37	0
56	MG	2A	3122	1/1	0.93	0.26	41,41,41,41	0
56	MG	1A	3237	1/1	0.93	0.15	28,28,28,28	0
56	MG	1A	3707	1/1	0.93	0.14	40,40,40,40	0
56	MG	1a	3206	1/1	0.93	0.10	54,54,54,54	0
56	MG	2A	3311	1/1	0.93	0.12	38,38,38,38	0
56	MG	2A	3796	1/1	0.93	0.13	25,25,25,25	0
56	MG	1A	3432	1/1	0.93	0.15	25,25,25,25	0
56	MG	1A	3930	1/1	0.93	0.14	40,40,40,40	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	2A	3552	1/1	0.93	0.10	40,40,40,40	0
56	MG	2A	3316	1/1	0.93	0.17	52,52,52,52	0
56	MG	2a	3119	1/1	0.93	0.09	59,59,59,59	0
56	MG	2A	3317	1/1	0.93	0.13	55,55,55,55	0
56	MG	1A	3278	1/1	0.93	0.22	37,37,37,37	0
56	MG	2A	3813	1/1	0.93	0.14	51,51,51,51	0
56	MG	1a	3214	1/1	0.93	0.20	70,70,70,70	0
56	MG	1A	3587	1/1	0.93	0.12	39,39,39,39	0
56	MG	1A	3437	1/1	0.93	0.24	27,27,27,27	0
56	MG	1E	311	1/1	0.93	0.22	41,41,41,41	0
56	MG	1A	3164	1/1	0.93	0.17	31,31,31,31	0
56	MG	1A	3593	1/1	0.93	0.14	41,41,41,41	0
56	MG	2A	3829	1/1	0.93	0.20	40,40,40,40	0
56	MG	2A	3830	1/1	0.93	0.23	51,51,51,51	0
56	MG	2A	3831	1/1	0.93	0.09	56,56,56,56	0
56	MG	2A	3835	1/1	0.93	0.11	53,53,53,53	0
56	MG	1A	3719	1/1	0.93	0.09	37,37,37,37	0
56	MG	1A	3061	1/1	0.93	0.20	22,22,22,22	0
56	MG	1a	3084	1/1	0.93	0.08	42,42,42,42	0
56	MG	2A	3841	1/1	0.93	0.10	62,62,62,62	0
56	MG	2A	3844	1/1	0.93	0.21	34,34,34,34	0
56	MG	1a	3228	1/1	0.93	0.18	58,58,58,58	0
56	MG	1a	3230	1/1	0.93	0.09	49,49,49,49	0
56	MG	1a	3234	1/1	0.93	0.12	38,38,38,38	0
56	MG	1A	3503	1/1	0.93	0.22	30,30,30,30	0
56	MG	1A	3106	1/1	0.93	0.25	28,28,28,28	0
56	MG	2A	3583	1/1	0.93	0.11	27,27,27,27	0
56	MG	2A	3155	1/1	0.93	0.16	37,37,37,37	0
56	MG	2A	3857	1/1	0.93	0.09	51,51,51,51	0
56	MG	1G	3004	1/1	0.93	0.11	39,39,39,39	0
56	MG	2A	3586	1/1	0.93	0.25	41,41,41,41	0
56	MG	1A	3946	1/1	0.93	0.15	30,30,30,30	0
56	MG	2A	3866	1/1	0.93	0.13	31,31,31,31	0
56	MG	1N	3001	1/1	0.93	0.42	34,34,34,34	0
56	MG	2A	3868	1/1	0.93	0.27	35,35,35,35	0
56	MG	2A	3592	1/1	0.93	0.12	48,48,48,48	0
56	MG	1A	3062	1/1	0.93	0.21	36,36,36,36	0
56	MG	2a	3168	1/1	0.93	0.09	61,61,61,61	0
56	MG	1a	3094	1/1	0.93	0.24	39,39,39,39	0
56	MG	1N	3003	1/1	0.93	0.21	32,32,32,32	0
56	MG	1n	503	1/1	0.93	0.13	43,43,43,43	0
56	MG	2a	3172	1/1	0.93	0.12	67,67,67,67	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
56	MG	1A	3245	1/1	0.93	0.20	19,19,19,19	0
56	MG	2A	3609	1/1	0.93	0.39	35,35,35,35	0
56	MG	1A	3849	1/1	0.93	0.09	28,28,28,28	0
56	MG	1A	4048	1/1	0.93	0.13	17,17,17,17	0
56	MG	1A	3002	1/1	0.93	0.22	40,40,40,40	0
56	MG	2A	3169	1/1	0.93	0.18	61,61,61,61	0
56	MG	2B	3011	1/1	0.93	0.27	48,48,48,48	0
56	MG	1a	3102	1/1	0.93	0.25	59,59,59,59	0
56	MG	2B	3013	1/1	0.93	0.17	57,57,57,57	0
56	MG	1A	3951	1/1	0.93	0.32	56,56,56,56	0
56	MG	2A	3619	1/1	0.93	0.16	50,50,50,50	0
56	MG	2A	3620	1/1	0.93	0.18	50,50,50,50	0
56	MG	1A	4051	1/1	0.93	0.10	44,44,44,44	0
56	MG	2A	3368	1/1	0.93	0.21	49,49,49,49	0
56	MG	1a	3105	1/1	0.93	0.26	35,35,35,35	0
56	MG	1A	3953	1/1	0.93	0.21	36,36,36,36	0
56	MG	1A	3337	1/1	0.93	0.28	38,38,38,38	0
56	MG	2A	3632	1/1	0.93	0.15	42,42,42,42	0
56	MG	1A	3035	1/1	0.93	0.11	27,27,27,27	0
56	MG	2A	3179	1/1	0.93	0.35	56,56,56,56	0
56	MG	2A	3182	1/1	0.93	0.14	51,51,51,51	0
56	MG	2a	3206	1/1	0.93	0.12	58,58,58,58	0
56	MG	2E	302	1/1	0.93	0.16	28,28,28,28	0
56	MG	2E	303	1/1	0.93	0.12	55,55,55,55	0
56	MG	2A	3646	1/1	0.93	0.15	23,23,23,23	0
56	MG	1A	3856	1/1	0.93	0.12	40,40,40,40	0
56	MG	2A	3380	1/1	0.93	0.18	36,36,36,36	0
56	MG	1A	4068	1/1	0.93	0.10	42,42,42,42	0
56	MG	2a	3217	1/1	0.93	0.13	62,62,62,62	0
56	MG	1A	4069	1/1	0.93	0.17	26,26,26,26	0
56	MG	2A	3385	1/1	0.93	0.11	36,36,36,36	0
56	MG	1U	207	1/1	0.93	0.43	22,22,22,22	0
56	MG	1A	3515	1/1	0.93	0.19	49,49,49,49	0
56	MG	1A	3390	1/1	0.93	0.18	32,32,32,32	0
56	MG	1A	3520	1/1	0.93	0.12	55,55,55,55	0
56	MG	1y	103	1/1	0.93	0.17	80,80,80,80	0
56	MG	2f	3001	1/1	0.93	0.09	42,42,42,42	0
56	MG	1Y	502	1/1	0.93	0.18	37,37,37,37	0
56	MG	1A	3618	1/1	0.93	0.17	34,34,34,34	0
56	MG	1Z	304	1/1	0.93	0.24	40,40,40,40	0
56	MG	1A	3864	1/1	0.93	0.13	23,23,23,23	0
56	MG	10	102	1/1	0.93	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	3180	1/1	0.93	0.13	38,38,38,38	0
56	MG	2A	3671	1/1	0.93	0.09	47,47,47,47	0
56	MG	1a	3126	1/1	0.93	0.18	45,45,45,45	0
56	MG	2W	202	1/1	0.93	0.14	38,38,38,38	0
56	MG	2X	3002	1/1	0.93	0.17	40,40,40,40	0
56	MG	2A	3010	1/1	0.93	0.28	31,31,31,31	0
56	MG	1A	3341	1/1	0.93	0.29	29,29,29,29	0
56	MG	2w	3004	1/1	0.93	0.15	60,60,60,60	0
56	MG	20	3002	1/1	0.93	0.10	40,40,40,40	0
56	MG	1A	3526	1/1	0.93	0.25	18,18,18,18	0
56	MG	2A	3405	1/1	0.93	0.09	34,34,34,34	0
56	MG	1A	3214	1/1	0.93	0.10	46,46,46,46	0
56	MG	1l	103	1/1	0.93	0.18	27,27,27,27	0
56	MG	1A	3147	1/1	0.93	0.18	36,36,36,36	0
56	MG	1A	3535	1/1	0.93	0.21	38,38,38,38	0
56	MG	1A	4093	1/1	0.93	0.28	25,25,25,25	0
56	MG	1A	3755	1/1	0.93	0.09	34,34,34,34	0
56	MG	1A	4097	1/1	0.93	0.22	40,40,40,40	0
56	MG	1a	3142	1/1	0.93	0.27	63,63,63,63	0
56	MG	2A	3689	1/1	0.93	0.26	56,56,56,56	0
59	ZN	29	501	1/1	0.93	0.10	77,77,77,77	0
59	ZN	2n	501	1/1	0.93	0.08	93,93,93,93	0
56	MG	2A	3568	1/1	0.94	0.10	42,42,42,42	0
56	MG	1A	3442	1/1	0.94	0.51	40,40,40,40	0
56	MG	1A	3241	1/1	0.94	0.09	46,46,46,46	0
56	MG	1A	3632	1/1	0.94	0.13	27,27,27,27	0
56	MG	2A	3281	1/1	0.94	0.45	60,60,60,60	0
56	MG	2A	3284	1/1	0.94	0.14	41,41,41,41	0
56	MG	1X	101	1/1	0.94	0.13	25,25,25,25	0
56	MG	1A	3919	1/1	0.94	0.13	35,35,35,35	0
56	MG	1A	3517	1/1	0.94	0.17	37,37,37,37	0
56	MG	2A	3578	1/1	0.94	0.15	31,31,31,31	0
56	MG	1Z	303	1/1	0.94	0.14	56,56,56,56	0
56	MG	1A	3146	1/1	0.94	0.40	38,38,38,38	0
56	MG	1A	3208	1/1	0.94	0.33	24,24,24,24	0
56	MG	1A	3775	1/1	0.94	0.41	19,19,19,19	0
56	MG	1A	3081	1/1	0.94	0.38	23,23,23,23	0
56	MG	2A	3296	1/1	0.94	0.19	63,63,63,63	0
56	MG	1A	4055	1/1	0.94	0.17	56,56,56,56	0
56	MG	1A	3641	1/1	0.94	0.17	9,9,9,9	0
56	MG	10	107	1/1	0.94	0.15	53,53,53,53	0
56	MG	2A	3591	1/1	0.94	0.20	54,54,54,54	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	1A	3449	1/1	0.94	0.61	49,49,49,49	0
56	MG	2A	3593	1/1	0.94	0.09	58,58,58,58	0
56	MG	1A	3082	1/1	0.94	0.22	34,34,34,34	0
56	MG	11	104	1/1	0.94	0.24	53,53,53,53	0
56	MG	2A	3305	1/1	0.94	0.12	53,53,53,53	0
56	MG	2A	3603	1/1	0.94	0.08	44,44,44,44	0
56	MG	2A	3605	1/1	0.94	0.14	46,46,46,46	0
56	MG	2A	3086	1/1	0.94	0.16	39,39,39,39	0
56	MG	2A	3307	1/1	0.94	0.15	41,41,41,41	0
56	MG	2T	3002	1/1	0.94	0.14	38,38,38,38	0
56	MG	1A	3384	1/1	0.94	0.13	33,33,33,33	0
56	MG	2A	3088	1/1	0.94	0.12	35,35,35,35	0
56	MG	2U	204	1/1	0.94	0.68	57,57,57,57	0
56	MG	12	3002	1/1	0.94	0.44	41,41,41,41	0
56	MG	1A	4070	1/1	0.94	0.20	49,49,49,49	0
56	MG	1A	3329	1/1	0.94	0.60	22,22,22,22	0
56	MG	15	103	1/1	0.94	0.19	17,17,17,17	0
56	MG	2A	3615	1/1	0.94	0.14	54,54,54,54	0
56	MG	2A	3617	1/1	0.94	0.13	48,48,48,48	0
56	MG	1A	3291	1/1	0.94	0.16	36,36,36,36	0
56	MG	1A	3150	1/1	0.94	0.29	39,39,39,39	0
56	MG	1A	3795	1/1	0.94	0.12	32,32,32,32	0
56	MG	2A	3101	1/1	0.94	0.39	34,34,34,34	0
56	MG	1A	3293	1/1	0.94	0.20	41,41,41,41	0
56	MG	1A	3938	1/1	0.94	0.10	32,32,32,32	0
56	MG	2A	3322	1/1	0.94	0.14	32,32,32,32	0
56	MG	1A	4083	1/1	0.94	0.14	41,41,41,41	0
56	MG	2A	3631	1/1	0.94	0.12	44,44,44,44	0
56	MG	1A	3457	1/1	0.94	0.26	56,56,56,56	0
56	MG	1A	3802	1/1	0.94	0.34	20,20,20,20	0
56	MG	1A	3942	1/1	0.94	0.09	31,31,31,31	0
56	MG	1A	3657	1/1	0.94	0.18	17,17,17,17	0
56	MG	2A	3113	1/1	0.94	0.15	47,47,47,47	0
56	MG	2A	3114	1/1	0.94	0.22	52,52,52,52	0
56	MG	1A	3539	1/1	0.94	0.15	27,27,27,27	0
56	MG	2A	3334	1/1	0.94	0.17	63,63,63,63	0
56	MG	1a	3005	1/1	0.94	0.08	52,52,52,52	0
56	MG	1A	3659	1/1	0.94	0.15	6,6,6,6	0
56	MG	2A	3654	1/1	0.94	0.09	46,46,46,46	0
56	MG	1A	3809	1/1	0.94	0.19	32,32,32,32	0
56	MG	2A	3658	1/1	0.94	0.13	31,31,31,31	0
56	MG	1A	3046	1/1	0.94	0.25	40,40,40,40	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	1A	3662	1/1	0.94	0.19	26,26,26,26	0
56	MG	2A	3121	1/1	0.94	0.14	49,49,49,49	0
56	MG	1A	3339	1/1	0.94	0.22	44,44,44,44	0
56	MG	1A	3460	1/1	0.94	0.17	20,20,20,20	0
56	MG	1A	3543	1/1	0.94	0.30	47,47,47,47	0
56	MG	1A	3669	1/1	0.94	0.11	15,15,15,15	0
56	MG	1A	3544	1/1	0.94	0.19	32,32,32,32	0
56	MG	2A	3668	1/1	0.94	0.11	57,57,57,57	0
56	MG	2a	3026	1/1	0.94	0.34	43,43,43,43	0
56	MG	1a	3018	1/1	0.94	0.13	44,44,44,44	0
56	MG	1A	3461	1/1	0.94	0.36	40,40,40,40	0
56	MG	2A	3129	1/1	0.94	0.14	31,31,31,31	0
56	MG	1a	3022	1/1	0.94	0.11	52,52,52,52	0
56	MG	2A	3673	1/1	0.94	0.23	38,38,38,38	0
56	MG	1A	3097	1/1	0.94	0.27	15,15,15,15	0
56	MG	1A	3463	1/1	0.94	0.17	49,49,49,49	0
56	MG	2A	3355	1/1	0.94	0.18	29,29,29,29	0
56	MG	1A	3827	1/1	0.94	0.36	22,22,22,22	0
56	MG	2A	3138	1/1	0.94	0.13	40,40,40,40	0
56	MG	1a	3027	1/1	0.94	0.25	42,42,42,42	0
56	MG	1a	3197	1/1	0.94	0.17	46,46,46,46	0
56	MG	1A	3961	1/1	0.94	0.14	19,19,19,19	0
56	MG	2A	3372	1/1	0.94	0.17	51,51,51,51	0
56	MG	1A	3126	1/1	0.94	0.39	35,35,35,35	0
56	MG	1a	3030	1/1	0.94	0.15	46,46,46,46	0
56	MG	1A	3299	1/1	0.94	0.14	27,27,27,27	0
56	MG	2A	3688	1/1	0.94	0.12	50,50,50,50	0
56	MG	1a	3032	1/1	0.94	0.19	20,20,20,20	0
56	MG	2A	3147	1/1	0.94	0.17	37,37,37,37	0
56	MG	2A	3379	1/1	0.94	0.11	36,36,36,36	0
56	MG	1A	3186	1/1	0.94	0.64	31,31,31,31	0
56	MG	1a	3207	1/1	0.94	0.10	33,33,33,33	0
56	MG	2A	3153	1/1	0.94	0.46	47,47,47,47	0
56	MG	1A	3468	1/1	0.94	0.19	26,26,26,26	0
56	MG	1A	3100	1/1	0.94	0.18	15,15,15,15	0
56	MG	2a	3057	1/1	0.94	0.27	53,53,53,53	0
56	MG	2A	3700	1/1	0.94	0.21	36,36,36,36	0
56	MG	1A	3835	1/1	0.94	0.16	26,26,26,26	0
56	MG	1a	3212	1/1	0.94	0.15	54,54,54,54	0
56	MG	1a	3037	1/1	0.94	0.13	44,44,44,44	0
56	MG	1A	3686	1/1	0.94	0.26	34,34,34,34	0
56	MG	1A	3005	1/1	0.94	0.15	32,32,32,32	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	1B	3001	1/1	0.94	0.28	27,27,27,27	0
56	MG	1B	3003	1/1	0.94	0.29	49,49,49,49	0
56	MG	1A	3691	1/1	0.94	0.16	34,34,34,34	0
56	MG	1A	3555	1/1	0.94	0.27	11,11,11,11	0
56	MG	1a	3223	1/1	0.94	0.12	48,48,48,48	0
56	MG	1A	3843	1/1	0.94	0.34	23,23,23,23	0
56	MG	1A	3304	1/1	0.94	0.29	49,49,49,49	0
56	MG	1A	3348	1/1	0.94	0.26	46,46,46,46	0
56	MG	1A	3349	1/1	0.94	0.17	47,47,47,47	0
56	MG	1A	3256	1/1	0.94	0.23	20,20,20,20	0
56	MG	1A	3226	1/1	0.94	0.22	42,42,42,42	0
56	MG	2A	3720	1/1	0.94	0.21	54,54,54,54	0
56	MG	2A	3721	1/1	0.94	0.08	49,49,49,49	0
56	MG	1B	3012	1/1	0.94	0.07	39,39,39,39	0
56	MG	2A	3408	1/1	0.94	0.11	48,48,48,48	0
56	MG	1A	3194	1/1	0.94	0.17	35,35,35,35	0
56	MG	2A	3410	1/1	0.94	0.18	22,22,22,22	0
56	MG	2A	3177	1/1	0.94	0.17	42,42,42,42	0
56	MG	1A	3854	1/1	0.94	0.15	18,18,18,18	0
56	MG	1A	3855	1/1	0.94	0.21	32,32,32,32	0
56	MG	2A	3181	1/1	0.94	0.20	49,49,49,49	0
56	MG	2A	3416	1/1	0.94	0.14	52,52,52,52	0
56	MG	2a	3097	1/1	0.94	0.23	54,54,54,54	0
56	MG	1A	3708	1/1	0.94	0.17	27,27,27,27	0
56	MG	2A	3184	1/1	0.94	0.38	36,36,36,36	0
56	MG	2A	3185	1/1	0.94	0.47	46,46,46,46	0
56	MG	2A	3422	1/1	0.94	0.24	31,31,31,31	0
56	MG	1A	3261	1/1	0.94	0.28	23,23,23,23	0
56	MG	1A	3992	1/1	0.94	0.15	28,28,28,28	0
56	MG	1A	3410	1/1	0.94	0.32	20,20,20,20	0
56	MG	1p	101	1/1	0.94	0.13	46,46,46,46	0
56	MG	2a	3112	1/1	0.94	0.28	61,61,61,61	0
56	MG	1s	3001	1/1	0.94	0.25	42,42,42,42	0
56	MG	1a	3066	1/1	0.94	0.08	49,49,49,49	0
56	MG	1B	3026	1/1	0.94	0.16	27,27,27,27	0
56	MG	1A	3860	1/1	0.94	0.13	14,14,14,14	0
56	MG	1A	3310	1/1	0.94	0.16	43,43,43,43	0
56	MG	1A	3574	1/1	0.94	0.20	27,27,27,27	0
56	MG	1A	4000	1/1	0.94	0.17	34,34,34,34	0
56	MG	1A	3418	1/1	0.94	0.16	36,36,36,36	0
56	MG	2A	3437	1/1	0.94	0.12	43,43,43,43	0
56	MG	2A	3438	1/1	0.94	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	1A	3576	1/1	0.94	0.19	39,39,39,39	0
56	MG	2A	3202	1/1	0.94	0.25	51,51,51,51	0
56	MG	1B	3036	1/1	0.94	0.13	27,27,27,27	0
56	MG	2A	3755	1/1	0.94	0.12	53,53,53,53	0
56	MG	1A	3718	1/1	0.94	0.20	42,42,42,42	0
56	MG	1D	304	1/1	0.94	0.63	48,48,48,48	0
56	MG	2A	3758	1/1	0.94	0.07	42,42,42,42	0
56	MG	1A	3050	1/1	0.94	0.15	39,39,39,39	0
56	MG	2A	3760	1/1	0.94	0.14	34,34,34,34	0
56	MG	2A	3208	1/1	0.94	0.16	29,29,29,29	0
56	MG	2a	3135	1/1	0.94	0.10	55,55,55,55	0
56	MG	1A	3720	1/1	0.94	0.18	19,19,19,19	0
56	MG	1x	104	1/1	0.94	0.08	51,51,51,51	0
56	MG	1A	3229	1/1	0.94	0.25	32,32,32,32	0
56	MG	2A	3214	1/1	0.94	0.11	38,38,38,38	0
56	MG	1A	3876	1/1	0.94	0.11	30,30,30,30	0
56	MG	2A	3461	1/1	0.94	0.21	30,30,30,30	0
56	MG	2a	3143	1/1	0.94	0.09	51,51,51,51	0
56	MG	2A	3463	1/1	0.94	0.10	40,40,40,40	0
56	MG	2A	3771	1/1	0.94	0.15	30,30,30,30	0
56	MG	2A	3772	1/1	0.94	0.10	30,30,30,30	0
56	MG	2a	3147	1/1	0.94	0.14	45,45,45,45	0
56	MG	1A	3230	1/1	0.94	0.27	19,19,19,19	0
56	MG	2A	3776	1/1	0.94	0.14	48,48,48,48	0
56	MG	1A	3315	1/1	0.94	0.13	31,31,31,31	0
56	MG	2A	3779	1/1	0.94	0.24	27,27,27,27	0
56	MG	2a	3154	1/1	0.94	0.07	66,66,66,66	0
56	MG	2A	3466	1/1	0.94	0.18	48,48,48,48	0
56	MG	2A	3218	1/1	0.94	0.15	49,49,49,49	0
56	MG	2A	3219	1/1	0.94	0.14	42,42,42,42	0
56	MG	1E	308	1/1	0.94	0.18	14,14,14,14	0
56	MG	1y	102	1/1	0.94	0.19	40,40,40,40	0
56	MG	2A	3474	1/1	0.94	0.14	40,40,40,40	0
56	MG	1A	3879	1/1	0.94	0.26	20,20,20,20	0
56	MG	2A	3223	1/1	0.94	0.24	55,55,55,55	0
56	MG	1A	3022	1/1	0.94	0.23	38,38,38,38	0
56	MG	1A	3592	1/1	0.94	0.17	46,46,46,46	0
56	MG	1A	3493	1/1	0.94	0.13	63,63,63,63	0
56	MG	1A	3427	1/1	0.94	0.15	35,35,35,35	0
56	MG	1A	3428	1/1	0.94	0.18	26,26,26,26	0
56	MG	2A	3485	1/1	0.94	0.10	33,33,33,33	0
56	MG	2A	3004	1/1	0.94	0.14	40,40,40,40	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	2A	3231	1/1	0.94	0.30	52,52,52,52	0
56	MG	2A	3799	1/1	0.94	0.10	59,59,59,59	0
56	MG	1F	306	1/1	0.94	0.17	34,34,34,34	0
56	MG	2a	3180	1/1	0.94	0.11	65,65,65,65	0
56	MG	2A	3803	1/1	0.94	0.07	52,52,52,52	0
56	MG	2A	3007	1/1	0.94	0.10	29,29,29,29	0
56	MG	2A	3805	1/1	0.94	0.10	42,42,42,42	0
56	MG	1A	3162	1/1	0.94	0.76	32,32,32,32	0
56	MG	2A	3807	1/1	0.94	0.14	42,42,42,42	0
56	MG	2A	3808	1/1	0.94	0.24	46,46,46,46	0
56	MG	2a	3190	1/1	0.94	0.11	61,61,61,61	0
56	MG	1G	3001	1/1	0.94	0.23	28,28,28,28	0
56	MG	1A	3888	1/1	0.94	0.12	23,23,23,23	0
56	MG	2A	3238	1/1	0.94	0.15	30,30,30,30	0
56	MG	2a	3197	1/1	0.94	0.18	54,54,54,54	0
56	MG	2A	3012	1/1	0.94	0.12	24,24,24,24	0
56	MG	1A	4022	1/1	0.94	0.13	29,29,29,29	0
56	MG	1A	3497	1/1	0.94	0.18	34,34,34,34	0
56	MG	2A	3822	1/1	0.94	0.14	48,48,48,48	0
56	MG	2A	3017	1/1	0.94	0.50	37,37,37,37	0
56	MG	1A	3368	1/1	0.94	0.22	42,42,42,42	0
56	MG	2A	3827	1/1	0.94	0.18	64,64,64,64	0
56	MG	1A	3369	1/1	0.94	0.24	44,44,44,44	0
56	MG	1A	3028	1/1	0.94	0.65	22,22,22,22	0
56	MG	1A	3078	1/1	0.94	0.14	20,20,20,20	0
56	MG	2A	3832	1/1	0.94	0.28	41,41,41,41	0
56	MG	2A	3834	1/1	0.94	0.22	47,47,47,47	0
56	MG	2A	3024	1/1	0.94	0.15	45,45,45,45	0
56	MG	2A	3837	1/1	0.94	0.14	62,62,62,62	0
56	MG	1N	3005	1/1	0.94	0.23	18,18,18,18	0
56	MG	2a	3218	1/1	0.94	0.06	60,60,60,60	0
56	MG	1A	3610	1/1	0.94	0.14	51,51,51,51	0
56	MG	1A	3747	1/1	0.94	0.13	18,18,18,18	0
56	MG	1A	3166	1/1	0.94	0.37	22,22,22,22	0
56	MG	2A	3842	1/1	0.94	0.14	41,41,41,41	0
56	MG	2a	3225	1/1	0.94	0.12	72,72,72,72	0
56	MG	2a	3227	1/1	0.94	0.11	49,49,49,49	0
56	MG	2a	3228	1/1	0.94	0.14	53,53,53,53	0
56	MG	1a	3116	1/1	0.94	0.15	35,35,35,35	0
56	MG	1O	3005	1/1	0.94	0.13	62,62,62,62	0
56	MG	1P	201	1/1	0.94	0.20	20,20,20,20	0
56	MG	2A	3256	1/1	0.94	0.15	35,35,35,35	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	2A	3534	1/1	0.94	0.12	52,52,52,52	0
56	MG	2j	8002	1/1	0.94	0.09	77,77,77,77	0
56	MG	2A	3535	1/1	0.94	0.19	48,48,48,48	0
56	MG	1A	3612	1/1	0.94	0.24	16,16,16,16	0
56	MG	1Q	3002	1/1	0.94	0.15	21,21,21,21	0
56	MG	2A	3539	1/1	0.94	0.23	46,46,46,46	0
56	MG	1A	3751	1/1	0.94	0.20	14,14,14,14	0
56	MG	2A	3859	1/1	0.94	0.57	38,38,38,38	0
56	MG	1A	3170	1/1	0.94	0.16	13,13,13,13	0
56	MG	1a	3123	1/1	0.94	0.27	40,40,40,40	0
56	MG	2A	3865	1/1	0.94	0.66	39,39,39,39	0
56	MG	1R	202	1/1	0.94	0.36	25,25,25,25	0
56	MG	1A	3440	1/1	0.94	0.35	54,54,54,54	0
56	MG	1A	3617	1/1	0.94	0.19	36,36,36,36	0
56	MG	1T	3001	1/1	0.94	0.23	50,50,50,50	0
56	MG	1T	3002	1/1	0.94	0.12	33,33,33,33	0
56	MG	1A	3757	1/1	0.94	0.20	8,8,8,8	0
56	MG	2A	3052	1/1	0.94	0.25	37,37,37,37	0
56	MG	1A	3030	1/1	0.94	0.17	27,27,27,27	0
56	MG	2A	3875	1/1	0.94	0.34	32,32,32,32	0
56	MG	2A	3556	1/1	0.94	0.13	52,52,52,52	0
56	MG	1A	3622	1/1	0.94	0.12	37,37,37,37	0
56	MG	2A	3055	1/1	0.94	0.11	24,24,24,24	0
56	MG	1A	3624	1/1	0.94	0.19	39,39,39,39	0
56	MG	1A	3513	1/1	0.94	0.10	34,34,34,34	0
58	M2D	2A	3864	36/36	0.94	0.38	32,41,50,52	0
59	ZN	14	501	1/1	0.94	0.18	71,71,71,71	0
56	MG	2A	3565	1/1	0.94	0.15	51,51,51,51	0
56	MG	2A	3566	1/1	0.94	0.15	35,35,35,35	0
56	MG	2A	3567	1/1	0.94	0.13	45,45,45,45	0
56	MG	1Q	3005	1/1	0.95	0.10	25,25,25,25	0
56	MG	2X	3001	1/1	0.95	0.22	52,52,52,52	0
56	MG	1y	101	1/1	0.95	0.23	22,22,22,22	0
56	MG	1A	3007	1/1	0.95	0.12	27,27,27,27	0
56	MG	1A	3653	1/1	0.95	0.15	9,9,9,9	0
56	MG	1A	4081	1/1	0.95	0.10	40,40,40,40	0
56	MG	2A	3194	1/1	0.95	0.25	30,30,30,30	0
56	MG	1A	3559	1/1	0.95	0.68	30,30,30,30	0
56	MG	1A	3963	1/1	0.95	0.17	16,16,16,16	0
56	MG	1A	3749	1/1	0.95	0.10	38,38,38,38	0
56	MG	1A	3445	1/1	0.95	0.20	33,33,33,33	0
56	MG	1A	3070	1/1	0.95	0.09	23,23,23,23	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	0.95	0.16	38,38,38,38	0
56	MG	1A	3275	1/1	0.95	0.11	30,30,30,30	0
56	MG	2A	3412	1/1	0.95	0.22	37,37,37,37	0
56	MG	1U	206	1/1	0.95	0.40	24,24,24,24	0
56	MG	1A	4089	1/1	0.95	0.16	34,34,34,34	0
56	MG	1A	4091	1/1	0.95	0.15	28,28,28,28	0
56	MG	1A	3866	1/1	0.95	0.14	35,35,35,35	0
56	MG	1A	3969	1/1	0.95	0.11	33,33,33,33	0
56	MG	2A	3687	1/1	0.95	0.49	37,37,37,37	0
56	MG	2A	3209	1/1	0.95	0.41	55,55,55,55	0
56	MG	1W	203	1/1	0.95	0.18	35,35,35,35	0
56	MG	2A	3211	1/1	0.95	0.11	58,58,58,58	0
56	MG	1W	207	1/1	0.95	0.16	9,9,9,9	0
56	MG	2A	3692	1/1	0.95	0.10	43,43,43,43	0
56	MG	1A	4095	1/1	0.95	0.24	19,19,19,19	0
56	MG	1X	103	1/1	0.95	0.20	22,22,22,22	0
56	MG	2A	3019	1/1	0.95	0.64	45,45,45,45	0
56	MG	1X	104	1/1	0.95	0.51	30,30,30,30	0
56	MG	2A	3698	1/1	0.95	0.14	51,51,51,51	0
56	MG	1X	105	1/1	0.95	0.16	36,36,36,36	0
56	MG	1A	3754	1/1	0.95	0.07	21,21,21,21	0
56	MG	1A	3395	1/1	0.95	0.29	35,35,35,35	0
56	MG	1Z	301	1/1	0.95	0.33	35,35,35,35	0
56	MG	1A	3149	1/1	0.95	0.21	18,18,18,18	0
56	MG	2A	3705	1/1	0.95	0.17	51,51,51,51	0
56	MG	2A	3434	1/1	0.95	0.11	38,38,38,38	0
56	MG	1A	3037	1/1	0.95	0.38	28,28,28,28	0
56	MG	1a	3132	1/1	0.95	0.13	51,51,51,51	0
56	MG	1A	3661	1/1	0.95	0.14	48,48,48,48	0
56	MG	1A	3211	1/1	0.95	0.17	33,33,33,33	0
56	MG	2A	3032	1/1	0.95	0.09	56,56,56,56	0
56	MG	2A	3033	1/1	0.95	0.20	44,44,44,44	0
56	MG	2A	3441	1/1	0.95	0.12	47,47,47,47	0
56	MG	1A	3151	1/1	0.95	0.25	14,14,14,14	0
56	MG	1A	4106	1/1	0.95	0.16	17,17,17,17	0
56	MG	2A	3445	1/1	0.95	0.14	50,50,50,50	0
56	MG	2A	3230	1/1	0.95	0.16	40,40,40,40	0
56	MG	2A	3448	1/1	0.95	0.14	23,23,23,23	0
56	MG	2A	3449	1/1	0.95	0.14	53,53,53,53	0
56	MG	1A	3982	1/1	0.95	0.09	31,31,31,31	0
56	MG	2A	3039	1/1	0.95	0.18	54,54,54,54	0
56	MG	2A	3040	1/1	0.95	0.21	38,38,38,38	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	1A	4109	1/1	0.95	0.98	32,32,32,32	0
56	MG	10	108	1/1	0.95	0.07	45,45,45,45	0
56	MG	1a	3144	1/1	0.95	0.15	43,43,43,43	0
56	MG	1A	4110	1/1	0.95	0.34	31,31,31,31	0
56	MG	1A	3098	1/1	0.95	0.47	25,25,25,25	0
56	MG	1A	3666	1/1	0.95	0.11	33,33,33,33	0
56	MG	1A	3454	1/1	0.95	0.15	29,29,29,29	0
56	MG	1A	4114	1/1	0.95	0.15	25,25,25,25	0
56	MG	1A	3668	1/1	0.95	0.16	21,21,21,21	0
56	MG	1A	3283	1/1	0.95	0.11	46,46,46,46	0
56	MG	1A	3771	1/1	0.95	0.10	13,13,13,13	0
56	MG	1A	3580	1/1	0.95	0.20	33,33,33,33	0
56	MG	1A	3182	1/1	0.95	0.36	25,25,25,25	0
56	MG	1A	4126	1/1	0.95	0.26	34,34,34,34	0
56	MG	1A	3584	1/1	0.95	0.12	7,7,7,7	0
56	MG	1A	3993	1/1	0.95	0.12	30,30,30,30	0
56	MG	2A	3479	1/1	0.95	0.12	37,37,37,37	0
56	MG	1A	3285	1/1	0.95	0.28	32,32,32,32	0
56	MG	1A	3076	1/1	0.95	0.19	26,26,26,26	0
56	MG	1A	4134	1/1	0.95	0.43	31,31,31,31	0
56	MG	2a	3072	1/1	0.95	0.13	44,44,44,44	0
56	MG	1A	3893	1/1	0.95	0.14	21,21,21,21	0
56	MG	2A	3066	1/1	0.95	0.12	43,43,43,43	0
56	MG	1A	4144	1/1	0.95	0.39	27,27,27,27	0
56	MG	2a	3077	1/1	0.95	0.14	44,44,44,44	0
56	MG	2A	3486	1/1	0.95	0.09	46,46,46,46	0
56	MG	2a	3079	1/1	0.95	0.15	53,53,53,53	0
56	MG	1A	4145	1/1	0.95	0.51	28,28,28,28	0
56	MG	2A	3492	1/1	0.95	0.10	27,27,27,27	0
56	MG	2a	3082	1/1	0.95	0.15	50,50,50,50	0
56	MG	1A	3679	1/1	0.95	0.25	43,43,43,43	0
56	MG	1A	3781	1/1	0.95	0.19	42,42,42,42	0
56	MG	2A	3071	1/1	0.95	0.22	53,53,53,53	0
56	MG	1A	3783	1/1	0.95	0.19	24,24,24,24	0
56	MG	2A	3073	1/1	0.95	0.15	25,25,25,25	0
56	MG	1A	3366	1/1	0.95	0.48	24,24,24,24	0
56	MG	2A	3076	1/1	0.95	0.17	53,53,53,53	0
56	MG	2A	3077	1/1	0.95	0.10	44,44,44,44	0
56	MG	2a	3093	1/1	0.95	0.10	60,60,60,60	0
56	MG	2A	3504	1/1	0.95	0.07	41,41,41,41	0
56	MG	2A	3267	1/1	0.95	0.17	49,49,49,49	0
56	MG	2A	3507	1/1	0.95	0.11	52,52,52,52	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	1A	3216	1/1	0.95	0.25	42,42,42,42	0
56	MG	1A	3019	1/1	0.95	0.17	8,8,8,8	0
56	MG	2A	3271	1/1	0.95	0.09	50,50,50,50	0
56	MG	1A	3901	1/1	0.95	0.14	37,37,37,37	0
56	MG	1A	3596	1/1	0.95	0.07	20,20,20,20	0
56	MG	2a	3104	1/1	0.95	0.24	34,34,34,34	0
56	MG	1a	3015	1/1	0.95	0.10	60,60,60,60	0
56	MG	2a	3106	1/1	0.95	0.09	43,43,43,43	0
56	MG	2A	3515	1/1	0.95	0.14	42,42,42,42	0
56	MG	2a	3109	1/1	0.95	0.15	43,43,43,43	0
56	MG	2A	3275	1/1	0.95	0.18	47,47,47,47	0
56	MG	2A	3775	1/1	0.95	0.09	51,51,51,51	0
56	MG	2A	3517	1/1	0.95	0.10	32,32,32,32	0
56	MG	2A	3520	1/1	0.95	0.10	62,62,62,62	0
56	MG	1A	3521	1/1	0.95	0.30	17,17,17,17	0
56	MG	1A	3905	1/1	0.95	0.19	43,43,43,43	0
56	MG	1A	3218	1/1	0.95	0.50	33,33,33,33	0
56	MG	1A	3131	1/1	0.95	0.20	29,29,29,29	0
56	MG	1A	3909	1/1	0.95	0.09	23,23,23,23	0
56	MG	1B	3020	1/1	0.95	0.18	28,28,28,28	0
56	MG	2A	3283	1/1	0.95	0.09	38,38,38,38	0
56	MG	1A	3414	1/1	0.95	0.37	27,27,27,27	0
56	MG	1A	3416	1/1	0.95	0.58	27,27,27,27	0
56	MG	1A	3694	1/1	0.95	0.17	49,49,49,49	0
56	MG	2A	3287	1/1	0.95	0.63	45,45,45,45	0
56	MG	2A	3097	1/1	0.95	0.19	38,38,38,38	0
56	MG	1A	3804	1/1	0.95	0.15	30,30,30,30	0
56	MG	2A	3291	1/1	0.95	0.13	67,67,67,67	0
56	MG	1A	3805	1/1	0.95	0.12	40,40,40,40	0
56	MG	1A	3700	1/1	0.95	0.13	49,49,49,49	0
56	MG	2a	3130	1/1	0.95	0.13	67,67,67,67	0
56	MG	1A	3529	1/1	0.95	0.17	32,32,32,32	0
56	MG	1A	3606	1/1	0.95	0.14	37,37,37,37	0
56	MG	2a	3133	1/1	0.95	0.07	69,69,69,69	0
56	MG	1A	3157	1/1	0.95	0.33	17,17,17,17	0
56	MG	2A	3802	1/1	0.95	0.07	60,60,60,60	0
56	MG	2A	3106	1/1	0.95	0.26	37,37,37,37	0
56	MG	1A	3534	1/1	0.95	0.22	40,40,40,40	0
56	MG	2A	3551	1/1	0.95	0.13	29,29,29,29	0
56	MG	1A	3373	1/1	0.95	0.13	30,30,30,30	0
56	MG	1B	3032	1/1	0.95	0.10	35,35,35,35	0
56	MG	2A	3111	1/1	0.95	0.23	29,29,29,29	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	1A	4028	1/1	0.95	0.14	24,24,24,24	0
56	MG	2A	3557	1/1	0.95	0.29	41,41,41,41	0
56	MG	1B	3034	1/1	0.95	0.13	59,59,59,59	0
56	MG	2A	3559	1/1	0.95	0.14	23,23,23,23	0
56	MG	1a	3198	1/1	0.95	0.11	48,48,48,48	0
56	MG	2A	3561	1/1	0.95	0.18	46,46,46,46	0
56	MG	1a	3039	1/1	0.95	0.10	59,59,59,59	0
56	MG	2A	3824	1/1	0.95	0.18	43,43,43,43	0
56	MG	1A	3254	1/1	0.95	0.12	32,32,32,32	0
56	MG	2A	3564	1/1	0.95	0.19	34,34,34,34	0
56	MG	1A	3188	1/1	0.95	0.15	24,24,24,24	0
56	MG	1D	302	1/1	0.95	0.65	29,29,29,29	0
56	MG	1A	3614	1/1	0.95	0.14	22,22,22,22	0
56	MG	1a	3204	1/1	0.95	0.11	27,27,27,27	0
56	MG	1D	306	1/1	0.95	0.16	14,14,14,14	0
56	MG	1A	3471	1/1	0.95	0.18	41,41,41,41	0
56	MG	2a	3162	1/1	0.95	0.09	57,57,57,57	0
56	MG	2a	3164	1/1	0.95	0.13	49,49,49,49	0
56	MG	1D	309	1/1	0.95	0.23	23,23,23,23	0
56	MG	2A	3836	1/1	0.95	0.08	44,44,44,44	0
56	MG	1D	311	1/1	0.95	0.29	29,29,29,29	0
56	MG	1A	3008	1/1	0.95	0.13	9,9,9,9	0
56	MG	1a	3050	1/1	0.95	0.11	51,51,51,51	0
56	MG	1A	3079	1/1	0.95	0.24	25,25,25,25	0
56	MG	1D	314	1/1	0.95	0.58	34,34,34,34	0
56	MG	1A	3378	1/1	0.95	0.11	25,25,25,25	0
56	MG	2A	3325	1/1	0.95	0.08	33,33,33,33	0
56	MG	2A	3580	1/1	0.95	0.20	45,45,45,45	0
56	MG	2A	3130	1/1	0.95	0.12	49,49,49,49	0
56	MG	1E	304	1/1	0.95	0.19	44,44,44,44	0
56	MG	2A	3849	1/1	0.95	0.14	24,24,24,24	0
56	MG	1A	3259	1/1	0.95	0.24	37,37,37,37	0
56	MG	2a	3182	1/1	0.95	0.19	56,56,56,56	0
56	MG	2A	3851	1/1	0.95	0.27	43,43,43,43	0
56	MG	2A	3852	1/1	0.95	0.10	43,43,43,43	0
56	MG	2A	3134	1/1	0.95	0.15	42,42,42,42	0
56	MG	1a	3057	1/1	0.95	0.32	47,47,47,47	0
56	MG	1A	3136	1/1	0.95	0.11	48,48,48,48	0
56	MG	1A	3626	1/1	0.95	0.18	19,19,19,19	0
56	MG	1A	3090	1/1	0.95	0.25	22,22,22,22	0
56	MG	2a	3193	1/1	0.95	0.10	54,54,54,54	0
56	MG	1A	3629	1/1	0.95	0.14	13,13,13,13	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	1a	3226	1/1	0.95	0.12	55,55,55,55	0
56	MG	1A	3727	1/1	0.95	0.20	32,32,32,32	0
56	MG	2A	3594	1/1	0.95	0.12	38,38,38,38	0
56	MG	1a	3064	1/1	0.95	0.13	57,57,57,57	0
56	MG	1a	3065	1/1	0.95	0.15	54,54,54,54	0
56	MG	1E	312	1/1	0.95	0.07	20,20,20,20	0
56	MG	2A	3598	1/1	0.95	0.14	27,27,27,27	0
56	MG	2A	3600	1/1	0.95	0.16	53,53,53,53	0
56	MG	1a	3067	1/1	0.95	0.16	44,44,44,44	0
56	MG	1A	3480	1/1	0.95	0.21	34,34,34,34	0
56	MG	1A	3836	1/1	0.95	0.16	39,39,39,39	0
56	MG	2A	3152	1/1	0.95	0.19	37,37,37,37	0
56	MG	1A	3941	1/1	0.95	0.12	40,40,40,40	0
56	MG	1l	201	1/1	0.95	0.18	29,29,29,29	0
56	MG	1A	3730	1/1	0.95	0.16	21,21,21,21	0
56	MG	2a	3213	1/1	0.95	0.07	56,56,56,56	0
56	MG	2B	3003	1/1	0.95	0.21	44,44,44,44	0
56	MG	2a	3216	1/1	0.95	0.16	51,51,51,51	0
56	MG	1A	3163	1/1	0.95	0.23	32,32,32,32	0
56	MG	1A	3383	1/1	0.95	0.18	28,28,28,28	0
56	MG	1A	3434	1/1	0.95	0.15	24,24,24,24	0
56	MG	1A	3549	1/1	0.95	0.15	45,45,45,45	0
56	MG	1A	3343	1/1	0.95	0.18	32,32,32,32	0
56	MG	2a	3223	1/1	0.95	0.09	54,54,54,54	0
56	MG	1A	3111	1/1	0.95	0.27	15,15,15,15	0
56	MG	1A	3848	1/1	0.95	0.10	48,48,48,48	0
56	MG	2a	3226	1/1	0.95	0.17	55,55,55,55	0
56	MG	2A	3362	1/1	0.95	0.26	26,26,26,26	0
56	MG	2A	3367	1/1	0.95	0.51	35,35,35,35	0
56	MG	2B	3017	1/1	0.95	0.13	58,58,58,58	0
56	MG	1A	4056	1/1	0.95	0.19	45,45,45,45	0
56	MG	1A	3438	1/1	0.95	0.21	30,30,30,30	0
56	MG	1a	3086	1/1	0.95	0.22	46,46,46,46	0
56	MG	2A	3166	1/1	0.95	0.24	36,36,36,36	0
56	MG	2A	3628	1/1	0.95	0.14	34,34,34,34	0
56	MG	1A	3386	1/1	0.95	0.10	34,34,34,34	0
56	MG	1A	4065	1/1	0.95	0.07	41,41,41,41	0
56	MG	2A	3635	1/1	0.95	0.21	50,50,50,50	0
56	MG	2A	3636	1/1	0.95	0.31	62,62,62,62	0
56	MG	1A	4067	1/1	0.95	0.11	40,40,40,40	0
56	MG	1a	3090	1/1	0.95	0.23	27,27,27,27	0
56	MG	1O	3002	1/1	0.95	0.57	40,40,40,40	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	2v	101	1/1	0.95	0.20	48,48,48,48	0
56	MG	2A	3644	1/1	0.95	0.23	55,55,55,55	0
56	MG	1O	3003	1/1	0.95	0.11	42,42,42,42	0
56	MG	1A	3739	1/1	0.95	0.18	21,21,21,21	0
56	MG	2A	3381	1/1	0.95	0.12	43,43,43,43	0
56	MG	1A	3954	1/1	0.95	0.20	50,50,50,50	0
56	MG	1A	3113	1/1	0.95	0.50	40,40,40,40	0
56	MG	1x	105	1/1	0.95	0.13	66,66,66,66	0
56	MG	2Q	201	1/1	0.95	0.13	43,43,43,43	0
56	MG	2A	3652	1/1	0.95	0.15	50,50,50,50	0
56	MG	1A	3741	1/1	0.95	0.13	11,11,11,11	0
56	MG	2A	3180	1/1	0.95	0.23	45,45,45,45	0
56	MG	2A	3656	1/1	0.95	0.19	44,44,44,44	0
56	MG	1x	107	1/1	0.95	0.06	53,53,53,53	0
56	MG	2y	102	1/1	0.95	0.15	59,59,59,59	0
56	MG	1A	4074	1/1	0.95	0.13	36,36,36,36	0
56	MG	2A	3183	1/1	0.95	0.13	54,54,54,54	0
56	MG	2A	3391	1/1	0.95	0.29	36,36,36,36	0
56	MG	2y	106	1/1	0.95	0.11	64,64,64,64	0
56	MG	1x	109	1/1	0.95	0.10	68,68,68,68	0
56	MG	1A	3011	1/1	0.95	0.15	26,26,26,26	0
56	MG	1x	111	1/1	0.95	0.12	52,52,52,52	0
56	MG	1A	3058	1/1	0.95	0.19	36,36,36,36	0
56	MG	2A	3666	1/1	0.95	0.21	58,58,58,58	0
56	MG	1F	307	1/1	0.96	0.27	34,34,34,34	0
56	MG	2A	3502	1/1	0.96	0.17	35,35,35,35	0
56	MG	1A	3049	1/1	0.96	0.13	24,24,24,24	0
56	MG	1a	3217	1/1	0.96	0.10	35,35,35,35	0
56	MG	1A	4060	1/1	0.96	0.14	25,25,25,25	0
56	MG	1A	3108	1/1	0.96	0.10	23,23,23,23	0
56	MG	2A	3731	1/1	0.96	0.07	64,64,64,64	0
56	MG	1A	4063	1/1	0.96	0.16	17,17,17,17	0
56	MG	1a	3221	1/1	0.96	0.09	61,61,61,61	0
56	MG	1A	3419	1/1	0.96	0.27	23,23,23,23	0
56	MG	1A	3633	1/1	0.96	0.15	24,24,24,24	0
56	MG	1A	3190	1/1	0.96	0.19	31,31,31,31	0
56	MG	1A	3364	1/1	0.96	0.41	23,23,23,23	0
56	MG	2A	3514	1/1	0.96	0.16	42,42,42,42	0
56	MG	1A	3109	1/1	0.96	0.33	28,28,28,28	0
56	MG	1A	3041	1/1	0.96	0.12	16,16,16,16	0
56	MG	1A	3266	1/1	0.96	0.26	32,32,32,32	0
56	MG	2A	3519	1/1	0.96	0.18	39,39,39,39	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	1a	3232	1/1	0.96	0.14	54,54,54,54	0
56	MG	1A	3138	1/1	0.96	0.34	16,16,16,16	0
56	MG	1A	3199	1/1	0.96	0.20	37,37,37,37	0
56	MG	1A	4077	1/1	0.96	0.18	53,53,53,53	0
56	MG	1b	3002	1/1	0.96	0.19	54,54,54,54	0
56	MG	2A	3133	1/1	0.96	0.30	44,44,44,44	0
56	MG	2a	3045	1/1	0.96	0.13	55,55,55,55	0
56	MG	1a	3076	1/1	0.96	0.53	46,46,46,46	0
56	MG	2A	3314	1/1	0.96	0.08	40,40,40,40	0
56	MG	1A	3844	1/1	0.96	0.37	21,21,21,21	0
56	MG	1A	3952	1/1	0.96	0.10	52,52,52,52	0
56	MG	2A	3754	1/1	0.96	0.10	42,42,42,42	0
56	MG	2A	3137	1/1	0.96	0.18	35,35,35,35	0
56	MG	2a	3052	1/1	0.96	0.22	55,55,55,55	0
56	MG	1A	3042	1/1	0.96	0.15	15,15,15,15	0
56	MG	2A	3537	1/1	0.96	0.15	54,54,54,54	0
56	MG	1A	3486	1/1	0.96	0.44	26,26,26,26	0
56	MG	1l	203	1/1	0.96	0.22	55,55,55,55	0
56	MG	1P	203	1/1	0.96	0.31	34,34,34,34	0
56	MG	1A	3273	1/1	0.96	0.31	46,46,46,46	0
56	MG	1A	3274	1/1	0.96	0.21	28,28,28,28	0
56	MG	2A	3763	1/1	0.96	0.11	29,29,29,29	0
56	MG	2A	3764	1/1	0.96	0.14	23,23,23,23	0
56	MG	1A	3745	1/1	0.96	0.10	28,28,28,28	0
56	MG	1A	3851	1/1	0.96	0.14	28,28,28,28	0
56	MG	1A	3141	1/1	0.96	0.29	21,21,21,21	0
56	MG	1A	3202	1/1	0.96	0.10	22,22,22,22	0
56	MG	1A	3112	1/1	0.96	0.47	29,29,29,29	0
56	MG	1S	3003	1/1	0.96	0.18	69,69,69,69	0
56	MG	1a	3092	1/1	0.96	0.16	62,62,62,62	0
56	MG	1A	3565	1/1	0.96	0.12	25,25,25,25	0
56	MG	1w	106	1/1	0.96	0.12	50,50,50,50	0
56	MG	2A	3555	1/1	0.96	0.13	55,55,55,55	0
56	MG	1A	3566	1/1	0.96	0.23	25,25,25,25	0
56	MG	2A	3777	1/1	0.96	0.11	55,55,55,55	0
56	MG	1a	3095	1/1	0.96	0.22	42,42,42,42	0
56	MG	1A	4094	1/1	0.96	0.32	22,22,22,22	0
56	MG	1U	201	1/1	0.96	0.41	22,22,22,22	0
56	MG	1A	3279	1/1	0.96	0.22	12,12,12,12	0
56	MG	1x	101	1/1	0.96	0.22	43,43,43,43	0
56	MG	1A	3238	1/1	0.96	0.28	25,25,25,25	0
56	MG	2a	3085	1/1	0.96	0.12	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	1a	3100	1/1	0.96	0.20	41,41,41,41	0
56	MG	1A	3092	1/1	0.96	0.18	11,11,11,11	0
56	MG	1A	3169	1/1	0.96	0.14	18,18,18,18	0
56	MG	1A	4100	1/1	0.96	0.53	18,18,18,18	0
56	MG	1A	3114	1/1	0.96	0.23	18,18,18,18	0
56	MG	1A	4102	1/1	0.96	0.12	11,11,11,11	0
56	MG	1A	3863	1/1	0.96	0.15	46,46,46,46	0
56	MG	1A	3330	1/1	0.96	0.39	20,20,20,20	0
56	MG	1W	205	1/1	0.96	0.22	24,24,24,24	0
56	MG	1W	206	1/1	0.96	0.21	17,17,17,17	0
56	MG	2A	3354	1/1	0.96	0.11	43,43,43,43	0
56	MG	1x	114	1/1	0.96	0.11	54,54,54,54	0
56	MG	1a	3110	1/1	0.96	0.11	50,50,50,50	0
56	MG	2a	3099	1/1	0.96	0.16	51,51,51,51	0
56	MG	1A	3973	1/1	0.96	0.19	23,23,23,23	0
56	MG	2A	3359	1/1	0.96	0.26	43,43,43,43	0
56	MG	1A	3758	1/1	0.96	0.19	59,59,59,59	0
56	MG	2A	3363	1/1	0.96	0.10	52,52,52,52	0
56	MG	2A	3364	1/1	0.96	0.26	34,34,34,34	0
56	MG	2A	3366	1/1	0.96	0.17	31,31,31,31	0
56	MG	2a	3107	1/1	0.96	0.19	38,38,38,38	0
56	MG	1A	3760	1/1	0.96	0.15	40,40,40,40	0
56	MG	1A	3867	1/1	0.96	0.13	18,18,18,18	0
56	MG	1A	3761	1/1	0.96	0.11	47,47,47,47	0
56	MG	2A	3812	1/1	0.96	0.14	52,52,52,52	0
56	MG	2A	3370	1/1	0.96	0.21	43,43,43,43	0
56	MG	1A	3870	1/1	0.96	0.13	25,25,25,25	0
56	MG	2A	3817	1/1	0.96	0.10	47,47,47,47	0
56	MG	1A	3331	1/1	0.96	0.45	14,14,14,14	0
56	MG	2A	3373	1/1	0.96	0.35	47,47,47,47	0
56	MG	1A	3872	1/1	0.96	0.29	12,12,12,12	0
56	MG	1A	3504	1/1	0.96	0.17	39,39,39,39	0
56	MG	1A	3444	1/1	0.96	0.21	37,37,37,37	0
56	MG	1A	3875	1/1	0.96	0.12	22,22,22,22	0
56	MG	1A	3987	1/1	0.96	0.09	21,21,21,21	0
56	MG	1A	4121	1/1	0.96	0.47	23,23,23,23	0
56	MG	2A	3828	1/1	0.96	0.10	40,40,40,40	0
56	MG	2A	3190	1/1	0.96	0.24	30,30,30,30	0
56	MG	2A	3599	1/1	0.96	0.28	52,52,52,52	0
56	MG	1a	3124	1/1	0.96	0.12	40,40,40,40	0
56	MG	2A	3601	1/1	0.96	0.17	45,45,45,45	0
56	MG	2A	3833	1/1	0.96	0.19	42,42,42,42	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	1A	3242	1/1	0.96	0.46	33,33,33,33	0
56	MG	2A	3383	1/1	0.96	0.16	43,43,43,43	0
56	MG	1A	4124	1/1	0.96	0.34	17,17,17,17	0
56	MG	1A	3582	1/1	0.96	0.14	13,13,13,13	0
56	MG	1A	3333	1/1	0.96	0.22	37,37,37,37	0
56	MG	1I	101	1/1	0.96	0.13	39,39,39,39	0
56	MG	1A	3334	1/1	0.96	0.10	46,46,46,46	0
56	MG	1A	3880	1/1	0.96	0.28	16,16,16,16	0
56	MG	1a	3133	1/1	0.96	0.10	48,48,48,48	0
56	MG	2A	3843	1/1	0.96	0.21	32,32,32,32	0
56	MG	1A	3586	1/1	0.96	0.25	16,16,16,16	0
56	MG	2A	3392	1/1	0.96	0.23	35,35,35,35	0
56	MG	2A	3393	1/1	0.96	0.25	30,30,30,30	0
56	MG	1A	4132	1/1	0.96	0.27	29,29,29,29	0
56	MG	1a	3136	1/1	0.96	0.09	52,52,52,52	0
56	MG	1A	3172	1/1	0.96	0.39	22,22,22,22	0
56	MG	2A	3621	1/1	0.96	0.11	62,62,62,62	0
56	MG	1A	3995	1/1	0.96	0.08	52,52,52,52	0
56	MG	2a	3148	1/1	0.96	0.08	65,65,65,65	0
56	MG	2A	3027	1/1	0.96	0.12	30,30,30,30	0
56	MG	1A	3772	1/1	0.96	0.30	14,14,14,14	0
56	MG	2A	3855	1/1	0.96	0.12	48,48,48,48	0
56	MG	1a	3141	1/1	0.96	0.09	53,53,53,53	0
56	MG	2A	3626	1/1	0.96	0.15	31,31,31,31	0
56	MG	1A	3024	1/1	0.96	0.26	26,26,26,26	0
56	MG	1A	3590	1/1	0.96	0.12	21,21,21,21	0
56	MG	2A	3629	1/1	0.96	0.11	56,56,56,56	0
56	MG	2A	3862	1/1	0.96	0.07	35,35,35,35	0
56	MG	1A	3389	1/1	0.96	0.19	36,36,36,36	0
56	MG	1A	3120	1/1	0.96	0.31	16,16,16,16	0
56	MG	2A	3633	1/1	0.96	0.09	59,59,59,59	0
56	MG	2A	3634	1/1	0.96	0.10	54,54,54,54	0
56	MG	1A	3889	1/1	0.96	0.07	57,57,57,57	0
56	MG	2A	3035	1/1	0.96	0.16	19,19,19,19	0
56	MG	2a	3167	1/1	0.96	0.18	37,37,37,37	0
56	MG	2A	3036	1/1	0.96	0.09	66,66,66,66	0
56	MG	1A	4003	1/1	0.96	0.14	33,33,33,33	0
56	MG	1A	3516	1/1	0.96	0.22	37,37,37,37	0
56	MG	1A	3779	1/1	0.96	0.10	25,25,25,25	0
56	MG	2A	3645	1/1	0.96	0.22	42,42,42,42	0
56	MG	1A	3685	1/1	0.96	0.12	37,37,37,37	0
56	MG	2A	3877	1/1	0.96	0.28	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	19	103	1/1	0.96	0.20	26,26,26,26	0
56	MG	1A	3594	1/1	0.96	0.14	18,18,18,18	0
56	MG	1a	3002	1/1	0.96	0.16	50,50,50,50	0
56	MG	2B	3004	1/1	0.96	0.21	53,53,53,53	0
56	MG	2B	3005	1/1	0.96	0.14	55,55,55,55	0
56	MG	2B	3006	1/1	0.96	0.17	60,60,60,60	0
56	MG	1A	3782	1/1	0.96	0.21	35,35,35,35	0
56	MG	2A	3045	1/1	0.96	0.16	52,52,52,52	0
56	MG	1A	3688	1/1	0.96	0.17	20,20,20,20	0
56	MG	1A	3066	1/1	0.96	0.30	21,21,21,21	0
56	MG	1a	3158	1/1	0.96	0.09	43,43,43,43	0
56	MG	1A	3025	1/1	0.96	0.35	12,12,12,12	0
56	MG	1B	3015	1/1	0.96	0.08	29,29,29,29	0
56	MG	1a	3008	1/1	0.96	0.11	37,37,37,37	0
56	MG	1A	3788	1/1	0.96	0.10	15,15,15,15	0
56	MG	1A	3789	1/1	0.96	0.14	26,26,26,26	0
56	MG	2A	3428	1/1	0.96	0.11	41,41,41,41	0
56	MG	1A	3519	1/1	0.96	0.10	43,43,43,43	0
56	MG	1A	3792	1/1	0.96	0.13	22,22,22,22	0
56	MG	1A	3178	1/1	0.96	0.25	42,42,42,42	0
56	MG	2A	3058	1/1	0.96	0.46	47,47,47,47	0
56	MG	2D	303	1/1	0.96	0.21	40,40,40,40	0
56	MG	1A	3904	1/1	0.96	0.18	6,6,6,6	0
56	MG	1A	3295	1/1	0.96	0.17	42,42,42,42	0
56	MG	1A	3522	1/1	0.96	0.24	26,26,26,26	0
56	MG	1A	3907	1/1	0.96	0.16	11,11,11,11	0
56	MG	2A	3064	1/1	0.96	0.20	59,59,59,59	0
56	MG	1a	3019	1/1	0.96	0.35	49,49,49,49	0
56	MG	1A	3796	1/1	0.96	0.17	41,41,41,41	0
56	MG	1a	3021	1/1	0.96	0.21	43,43,43,43	0
56	MG	1A	3798	1/1	0.96	0.17	39,39,39,39	0
56	MG	1A	3799	1/1	0.96	0.17	32,32,32,32	0
56	MG	1a	3024	1/1	0.96	0.24	37,37,37,37	0
56	MG	1A	3523	1/1	0.96	0.42	31,31,31,31	0
56	MG	2F	304	1/1	0.96	0.31	46,46,46,46	0
56	MG	1A	4029	1/1	0.96	0.17	35,35,35,35	0
56	MG	2A	3447	1/1	0.96	0.20	44,44,44,44	0
56	MG	1A	3020	1/1	0.96	0.17	18,18,18,18	0
56	MG	2a	3222	1/1	0.96	0.15	51,51,51,51	0
56	MG	2A	3253	1/1	0.96	0.26	58,58,58,58	0
56	MG	1A	3016	1/1	0.96	0.20	33,33,33,33	0
56	MG	1A	3152	1/1	0.96	0.37	20,20,20,20	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
56	MG	1a	3182	1/1	0.96	0.13	56,56,56,56	0
56	MG	1A	3609	1/1	0.96	0.18	6,6,6,6	0
56	MG	1A	3003	1/1	0.96	0.14	13,13,13,13	0
56	MG	2A	3081	1/1	0.96	0.18	38,38,38,38	0
56	MG	2a	3230	1/1	0.96	0.11	61,61,61,61	0
56	MG	1A	3300	1/1	0.96	0.21	40,40,40,40	0
56	MG	2U	201	1/1	0.96	0.20	39,39,39,39	0
56	MG	1D	305	1/1	0.96	0.43	24,24,24,24	0
56	MG	1A	3710	1/1	0.96	0.24	22,22,22,22	0
56	MG	1A	3075	1/1	0.96	0.33	14,14,14,14	0
56	MG	2l	201	1/1	0.96	0.24	53,53,53,53	0
56	MG	2U	206	1/1	0.96	0.13	32,32,32,32	0
56	MG	2A	3694	1/1	0.96	0.14	44,44,44,44	0
56	MG	2q	201	1/1	0.96	0.19	46,46,46,46	0
56	MG	1A	3219	1/1	0.96	0.25	24,24,24,24	0
56	MG	1A	3220	1/1	0.96	0.33	17,17,17,17	0
56	MG	1A	3351	1/1	0.96	0.28	27,27,27,27	0
56	MG	1A	3257	1/1	0.96	0.15	18,18,18,18	0
56	MG	2A	3469	1/1	0.96	0.13	50,50,50,50	0
56	MG	1A	3815	1/1	0.96	0.09	48,48,48,48	0
56	MG	1A	3816	1/1	0.96	0.13	36,36,36,36	0
56	MG	2A	3270	1/1	0.96	0.14	41,41,41,41	0
56	MG	2A	3475	1/1	0.96	0.15	28,28,28,28	0
56	MG	1E	303	1/1	0.96	0.25	23,23,23,23	0
56	MG	1a	3043	1/1	0.96	0.12	49,49,49,49	0
56	MG	1A	3927	1/1	0.96	0.12	33,33,33,33	0
56	MG	1A	3818	1/1	0.96	0.31	28,28,28,28	0
56	MG	1A	3407	1/1	0.96	0.21	29,29,29,29	0
56	MG	1A	3305	1/1	0.96	0.31	23,23,23,23	0
56	MG	1A	3355	1/1	0.96	0.16	43,43,43,43	0
56	MG	1A	3722	1/1	0.96	0.09	28,28,28,28	0
56	MG	1A	3724	1/1	0.96	0.22	34,34,34,34	0
56	MG	2x	3005	1/1	0.96	0.14	59,59,59,59	0
56	MG	1A	4052	1/1	0.96	0.12	49,49,49,49	0
56	MG	2A	3487	1/1	0.96	0.13	27,27,27,27	0
56	MG	2A	3107	1/1	0.96	0.21	30,30,30,30	0
56	MG	2A	3717	1/1	0.96	0.09	39,39,39,39	0
56	MG	2A	3282	1/1	0.96	0.10	41,41,41,41	0
56	MG	1F	301	1/1	0.96	0.54	26,26,26,26	0
58	M2D	1A	4118	36/36	0.96	0.31	13,19,23,24	0
56	MG	1a	3209	1/1	0.96	0.06	44,44,44,44	0
56	MG	1A	3128	1/1	0.96	0.11	38,38,38,38	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	1A	3935	1/1	0.96	0.26	41,41,41,41	0
56	MG	1A	3222	1/1	0.96	0.30	28,28,28,28	0
56	MG	1A	3048	1/1	0.96	0.25	26,26,26,26	0
56	MG	1a	3184	1/1	0.97	0.15	63,63,63,63	0
56	MG	1a	3069	1/1	0.97	0.17	53,53,53,53	0
56	MG	1W	204	1/1	0.97	0.12	21,21,21,21	0
56	MG	1A	3232	1/1	0.97	0.29	15,15,15,15	0
56	MG	2A	3470	1/1	0.97	0.13	32,32,32,32	0
56	MG	2a	3076	1/1	0.97	0.17	64,64,64,64	0
56	MG	2A	3471	1/1	0.97	0.08	34,34,34,34	0
56	MG	2A	3313	1/1	0.97	0.13	46,46,46,46	0
56	MG	2A	3172	1/1	0.97	0.73	44,44,44,44	0
56	MG	1A	3411	1/1	0.97	0.49	22,22,22,22	0
56	MG	2A	3653	1/1	0.97	0.13	51,51,51,51	0
56	MG	1A	3191	1/1	0.97	0.19	14,14,14,14	0
56	MG	1A	3613	1/1	0.97	0.14	18,18,18,18	0
56	MG	1X	102	1/1	0.97	0.27	20,20,20,20	0
56	MG	2A	3657	1/1	0.97	0.06	45,45,45,45	0
56	MG	1A	3413	1/1	0.97	0.33	32,32,32,32	0
56	MG	1A	3696	1/1	0.97	0.11	31,31,31,31	0
56	MG	1a	3079	1/1	0.97	0.18	30,30,30,30	0
56	MG	1A	3697	1/1	0.97	0.16	8,8,8,8	0
56	MG	1A	3698	1/1	0.97	0.14	8,8,8,8	0
56	MG	1a	3082	1/1	0.97	0.14	45,45,45,45	0
56	MG	1A	3699	1/1	0.97	0.14	55,55,55,55	0
56	MG	1A	3499	1/1	0.97	0.24	21,21,21,21	0
56	MG	1A	3312	1/1	0.97	0.26	41,41,41,41	0
56	MG	2A	3488	1/1	0.97	0.17	30,30,30,30	0
56	MG	2A	3490	1/1	0.97	0.08	65,65,65,65	0
56	MG	1A	4046	1/1	0.97	0.09	38,38,38,38	0
56	MG	1B	3017	1/1	0.97	0.13	19,19,19,19	0
56	MG	2A	3050	1/1	0.97	0.15	38,38,38,38	0
56	MG	1A	3869	1/1	0.97	0.24	39,39,39,39	0
56	MG	2A	3333	1/1	0.97	0.12	33,33,33,33	0
56	MG	1a	3205	1/1	0.97	0.13	55,55,55,55	0
56	MG	2A	3335	1/1	0.97	0.10	48,48,48,48	0
56	MG	2A	3498	1/1	0.97	0.16	39,39,39,39	0
56	MG	2A	3336	1/1	0.97	0.13	45,45,45,45	0
56	MG	2A	3500	1/1	0.97	0.13	60,60,60,60	0
56	MG	10	103	1/1	0.97	0.22	24,24,24,24	0
56	MG	1A	3415	1/1	0.97	0.42	23,23,23,23	0
56	MG	1A	3193	1/1	0.97	0.12	24,24,24,24	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	1A	3705	1/1	0.97	0.20	39,39,39,39	0
56	MG	1A	3786	1/1	0.97	0.12	42,42,42,42	0
56	MG	2A	3684	1/1	0.97	0.27	46,46,46,46	0
56	MG	2A	3506	1/1	0.97	0.15	50,50,50,50	0
56	MG	2A	3196	1/1	0.97	0.50	38,38,38,38	0
56	MG	1A	3417	1/1	0.97	0.22	19,19,19,19	0
56	MG	2A	3059	1/1	0.97	0.12	29,29,29,29	0
56	MG	1A	3087	1/1	0.97	0.18	8,8,8,8	0
56	MG	1a	3213	1/1	0.97	0.13	44,44,44,44	0
56	MG	1A	3286	1/1	0.97	0.30	38,38,38,38	0
56	MG	2A	3878	1/1	0.97	0.16	36,36,36,36	0
56	MG	1A	3790	1/1	0.97	0.14	19,19,19,19	0
56	MG	1A	3236	1/1	0.97	0.45	23,23,23,23	0
56	MG	1A	4057	1/1	0.97	0.10	50,50,50,50	0
56	MG	1A	3562	1/1	0.97	0.62	26,26,26,26	0
56	MG	1A	4059	1/1	0.97	0.14	34,34,34,34	0
56	MG	2A	3518	1/1	0.97	0.09	49,49,49,49	0
56	MG	1A	3563	1/1	0.97	0.33	19,19,19,19	0
56	MG	1A	3288	1/1	0.97	0.14	17,17,17,17	0
56	MG	1A	4062	1/1	0.97	0.18	23,23,23,23	0
56	MG	2B	3010	1/1	0.97	0.17	64,64,64,64	0
56	MG	1A	3512	1/1	0.97	0.21	30,30,30,30	0
56	MG	1A	4064	1/1	0.97	0.11	48,48,48,48	0
56	MG	2A	3524	1/1	0.97	0.13	44,44,44,44	0
56	MG	2A	3704	1/1	0.97	0.09	58,58,58,58	0
56	MG	2A	3525	1/1	0.97	0.12	38,38,38,38	0
56	MG	2a	3138	1/1	0.97	0.17	48,48,48,48	0
56	MG	17	101	1/1	0.97	0.11	15,15,15,15	0
56	MG	2A	3528	1/1	0.97	0.14	28,28,28,28	0
56	MG	2A	3529	1/1	0.97	0.14	31,31,31,31	0
56	MG	2A	3074	1/1	0.97	0.14	47,47,47,47	0
56	MG	2B	3020	1/1	0.97	0.18	66,66,66,66	0
56	MG	1A	3422	1/1	0.97	0.10	24,24,24,24	0
56	MG	1a	3227	1/1	0.97	0.13	46,46,46,46	0
56	MG	1A	3567	1/1	0.97	0.12	41,41,41,41	0
56	MG	1A	3289	1/1	0.97	0.20	33,33,33,33	0
56	MG	1a	3231	1/1	0.97	0.19	41,41,41,41	0
56	MG	1A	3095	1/1	0.97	0.10	29,29,29,29	0
56	MG	1A	3977	1/1	0.97	0.10	17,17,17,17	0
56	MG	1A	4071	1/1	0.97	0.12	34,34,34,34	0
56	MG	1D	310	1/1	0.97	0.20	34,34,34,34	0
56	MG	2A	3540	1/1	0.97	0.25	32,32,32,32	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	1A	3570	1/1	0.97	0.15	16,16,16,16	0
56	MG	1A	3639	1/1	0.97	0.07	19,19,19,19	0
56	MG	1A	3640	1/1	0.97	0.14	12,12,12,12	0
56	MG	2a	3158	1/1	0.97	0.40	66,66,66,66	0
56	MG	1A	3425	1/1	0.97	0.22	21,21,21,21	0
56	MG	2A	3546	1/1	0.97	0.17	57,57,57,57	0
56	MG	2F	302	1/1	0.97	0.14	39,39,39,39	0
56	MG	1A	3029	1/1	0.97	0.35	28,28,28,28	0
56	MG	1A	3352	1/1	0.97	0.17	34,34,34,34	0
56	MG	1A	3728	1/1	0.97	0.14	27,27,27,27	0
56	MG	1A	3644	1/1	0.97	0.13	12,12,12,12	0
56	MG	2A	3093	1/1	0.97	0.10	55,55,55,55	0
56	MG	2A	3094	1/1	0.97	0.18	43,43,43,43	0
56	MG	1A	3646	1/1	0.97	0.20	15,15,15,15	0
56	MG	1a	3011	1/1	0.97	0.16	19,19,19,19	0
56	MG	1A	3198	1/1	0.97	0.26	26,26,26,26	0
56	MG	1A	3053	1/1	0.97	0.13	38,38,38,38	0
56	MG	2A	3100	1/1	0.97	0.17	43,43,43,43	0
56	MG	2a	3174	1/1	0.97	0.14	47,47,47,47	0
56	MG	1a	3127	1/1	0.97	0.15	33,33,33,33	0
56	MG	2A	3102	1/1	0.97	0.41	33,33,33,33	0
56	MG	2A	3738	1/1	0.97	0.10	46,46,46,46	0
56	MG	1A	3294	1/1	0.97	0.17	30,30,30,30	0
56	MG	1w	101	1/1	0.97	0.18	67,67,67,67	0
56	MG	1A	3578	1/1	0.97	0.15	47,47,47,47	0
56	MG	1A	3023	1/1	0.97	0.23	18,18,18,18	0
56	MG	2a	3183	1/1	0.97	0.10	59,59,59,59	0
56	MG	1A	3817	1/1	0.97	0.12	28,28,28,28	0
56	MG	1A	3474	1/1	0.97	0.17	21,21,21,21	0
56	MG	2a	3186	1/1	0.97	0.12	37,37,37,37	0
56	MG	1A	3581	1/1	0.97	0.19	30,30,30,30	0
56	MG	1A	3063	1/1	0.97	0.27	14,14,14,14	0
56	MG	1A	3358	1/1	0.97	0.40	21,21,21,21	0
56	MG	1A	3101	1/1	0.97	0.31	24,24,24,24	0
56	MG	1A	3824	1/1	0.97	0.19	10,10,10,10	0
56	MG	2a	3192	1/1	0.97	0.13	64,64,64,64	0
56	MG	1A	3999	1/1	0.97	0.11	35,35,35,35	0
56	MG	1a	3139	1/1	0.97	0.18	31,31,31,31	0
56	MG	1A	3585	1/1	0.97	0.21	15,15,15,15	0
56	MG	2a	3196	1/1	0.97	0.20	53,53,53,53	0
56	MG	1A	3742	1/1	0.97	0.16	15,15,15,15	0
56	MG	1A	3478	1/1	0.97	0.19	38,38,38,38	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	26	502	1/1	0.97	0.40	62,62,62,62	0
56	MG	1G	3005	1/1	0.97	0.10	50,50,50,50	0
56	MG	1A	3267	1/1	0.97	0.29	16,16,16,16	0
56	MG	1A	3127	1/1	0.97	0.15	19,19,19,19	0
56	MG	1A	3664	1/1	0.97	0.14	13,13,13,13	0
56	MG	1A	3532	1/1	0.97	0.21	29,29,29,29	0
56	MG	2a	3205	1/1	0.97	0.07	66,66,66,66	0
56	MG	1A	3833	1/1	0.97	0.07	46,46,46,46	0
56	MG	1A	4008	1/1	0.97	0.08	22,22,22,22	0
56	MG	1A	3533	1/1	0.97	0.34	39,39,39,39	0
56	MG	2a	3209	1/1	0.97	0.12	55,55,55,55	0
56	MG	1x	113	1/1	0.97	0.16	46,46,46,46	0
56	MG	1A	3223	1/1	0.97	0.15	47,47,47,47	0
56	MG	2A	3417	1/1	0.97	0.14	22,22,22,22	0
56	MG	1A	3073	1/1	0.97	0.14	19,19,19,19	0
56	MG	2A	3589	1/1	0.97	0.12	38,38,38,38	0
56	MG	2a	3215	1/1	0.97	0.12	68,68,68,68	0
56	MG	1A	3115	1/1	0.97	0.29	19,19,19,19	0
56	MG	1A	3130	1/1	0.97	0.43	30,30,30,30	0
56	MG	1A	3839	1/1	0.97	0.42	30,30,30,30	0
56	MG	1a	3156	1/1	0.97	0.16	30,30,30,30	0
56	MG	1A	3753	1/1	0.97	0.16	31,31,31,31	0
56	MG	1A	3841	1/1	0.97	0.29	12,12,12,12	0
56	MG	2A	3774	1/1	0.97	0.07	27,27,27,27	0
56	MG	2a	3020	1/1	0.97	0.08	32,32,32,32	0
56	MG	1Q	3001	1/1	0.97	0.12	26,26,26,26	0
56	MG	1A	3001	1/1	0.97	0.14	22,22,22,22	0
56	MG	1A	4120	1/1	0.97	0.25	23,23,23,23	0
56	MG	1A	3598	1/1	0.97	0.10	7,7,7,7	0
56	MG	1A	3335	1/1	0.97	0.21	28,28,28,28	0
56	MG	2A	3602	1/1	0.97	0.12	37,37,37,37	0
56	MG	2A	3781	1/1	0.97	0.10	33,33,33,33	0
56	MG	1A	3250	1/1	0.97	0.11	56,56,56,56	0
56	MG	1A	3677	1/1	0.97	0.45	44,44,44,44	0
56	MG	2e	3001	1/1	0.97	0.13	58,58,58,58	0
56	MG	2A	3009	1/1	0.97	0.15	36,36,36,36	0
56	MG	2g	8001	1/1	0.97	0.06	70,70,70,70	0
56	MG	2A	3144	1/1	0.97	0.13	42,42,42,42	0
56	MG	1A	4024	1/1	0.97	0.22	14,14,14,14	0
56	MG	1A	3488	1/1	0.97	0.23	42,42,42,42	0
56	MG	1A	3117	1/1	0.97	0.15	24,24,24,24	0
56	MG	2A	3148	1/1	0.97	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	1A	3603	1/1	0.97	0.13	15,15,15,15	0
56	MG	2A	3289	1/1	0.97	0.11	58,58,58,58	0
56	MG	2A	3793	1/1	0.97	0.11	19,19,19,19	0
56	MG	2A	3014	1/1	0.97	0.13	28,28,28,28	0
56	MG	2A	3442	1/1	0.97	0.09	41,41,41,41	0
56	MG	2A	3151	1/1	0.97	0.29	46,46,46,46	0
56	MG	2A	3015	1/1	0.97	0.28	35,35,35,35	0
56	MG	1A	3371	1/1	0.97	0.47	32,32,32,32	0
56	MG	1A	3491	1/1	0.97	0.09	40,40,40,40	0
56	MG	1U	202	1/1	0.97	0.14	19,19,19,19	0
56	MG	2A	3801	1/1	0.97	0.29	47,47,47,47	0
56	MG	1A	3118	1/1	0.97	0.45	29,29,29,29	0
56	MG	1a	3059	1/1	0.97	0.44	40,40,40,40	0
56	MG	2A	3450	1/1	0.97	0.18	46,46,46,46	0
56	MG	1A	3210	1/1	0.97	0.43	37,37,37,37	0
56	MG	1A	4139	1/1	0.97	0.24	23,23,23,23	0
56	MG	2A	3300	1/1	0.97	0.15	37,37,37,37	0
56	MG	2A	3301	1/1	0.97	0.35	39,39,39,39	0
56	MG	2A	3456	1/1	0.97	0.22	31,31,31,31	0
56	MG	1A	4140	1/1	0.97	0.30	21,21,21,21	0
56	MG	2x	3006	1/1	0.97	0.15	58,58,58,58	0
56	MG	2A	3458	1/1	0.97	0.31	40,40,40,40	0
56	MG	1A	4141	1/1	0.97	0.23	27,27,27,27	0
56	MG	1A	4143	1/1	0.97	0.46	26,26,26,26	0
56	MG	1A	3135	1/1	0.97	0.23	42,42,42,42	0
56	MG	1A	3689	1/1	0.97	0.17	12,12,12,12	0
56	MG	2A	3639	1/1	0.97	0.15	62,62,62,62	0
57	K	1A	3527	1/1	0.97	0.25	57,57,57,57	0
57	K	2A	3398	1/1	0.97	0.55	70,70,70,70	0
56	MG	2a	3065	1/1	0.97	0.11	36,36,36,36	0
56	MG	2a	3066	1/1	0.97	0.24	49,49,49,49	0
56	MG	1W	202	1/1	0.97	0.32	31,31,31,31	0
56	MG	2A	3823	1/1	0.97	0.14	48,48,48,48	0
59	ZN	26	501	1/1	0.97	0.17	55,55,55,55	0
56	MG	2A	3641	1/1	0.97	0.08	56,56,56,56	0
56	MG	1A	3857	1/1	0.97	0.14	22,22,22,22	0
56	MG	2A	3816	1/1	0.98	0.13	55,55,55,55	0
56	MG	2A	3451	1/1	0.98	0.11	29,29,29,29	0
56	MG	2A	3020	1/1	0.98	0.12	26,26,26,26	0
56	MG	1A	3361	1/1	0.98	0.18	25,25,25,25	0
56	MG	2A	3820	1/1	0.98	0.13	41,41,41,41	0
56	MG	1A	3561	1/1	0.98	0.29	16,16,16,16	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	0.98	0.17	38,38,38,38	0
56	MG	1A	4119	1/1	0.98	0.48	27,27,27,27	0
56	MG	1F	304	1/1	0.98	0.41	28,28,28,28	0
56	MG	2A	3237	1/1	0.98	0.20	31,31,31,31	0
56	MG	1A	3072	1/1	0.98	0.44	23,23,23,23	0
56	MG	1A	3605	1/1	0.98	0.11	32,32,32,32	0
56	MG	1A	3716	1/1	0.98	0.10	25,25,25,25	0
56	MG	2a	3150	1/1	0.98	0.11	68,68,68,68	0
56	MG	1A	4123	1/1	0.98	0.36	18,18,18,18	0
56	MG	2A	3462	1/1	0.98	0.10	20,20,20,20	0
56	MG	1A	3972	1/1	0.98	0.16	35,35,35,35	0
56	MG	1A	3051	1/1	0.98	0.20	25,25,25,25	0
56	MG	1A	3103	1/1	0.98	0.35	18,18,18,18	0
56	MG	1A	3976	1/1	0.98	0.13	17,17,17,17	0
56	MG	1A	3145	1/1	0.98	0.12	18,18,18,18	0
56	MG	1A	4129	1/1	0.98	0.17	16,16,16,16	0
56	MG	1A	4130	1/1	0.98	0.36	20,20,20,20	0
56	MG	1A	3394	1/1	0.98	0.17	39,39,39,39	0
56	MG	2A	3357	1/1	0.98	0.20	37,37,37,37	0
56	MG	1A	3721	1/1	0.98	0.14	16,16,16,16	0
56	MG	2a	3163	1/1	0.98	0.08	65,65,65,65	0
56	MG	2A	3590	1/1	0.98	0.14	41,41,41,41	0
56	MG	1N	3004	1/1	0.98	0.22	27,27,27,27	0
56	MG	2a	3027	1/1	0.98	0.26	45,45,45,45	0
56	MG	2A	3360	1/1	0.98	0.26	30,30,30,30	0
56	MG	2A	3361	1/1	0.98	0.25	36,36,36,36	0
56	MG	2A	3845	1/1	0.98	0.14	44,44,44,44	0
56	MG	2A	3476	1/1	0.98	0.10	52,52,52,52	0
56	MG	1A	3027	1/1	0.98	0.50	16,16,16,16	0
56	MG	1A	3723	1/1	0.98	0.16	46,46,46,46	0
56	MG	1A	4135	1/1	0.98	0.14	20,20,20,20	0
56	MG	2A	3365	1/1	0.98	0.13	23,23,23,23	0
56	MG	1A	4136	1/1	0.98	0.78	28,28,28,28	0
56	MG	1A	3105	1/1	0.98	0.19	25,25,25,25	0
56	MG	2a	3177	1/1	0.98	0.06	58,58,58,58	0
56	MG	2a	3038	1/1	0.98	0.18	37,37,37,37	0
56	MG	1A	4138	1/1	0.98	0.35	29,29,29,29	0
56	MG	1A	3785	1/1	0.98	0.47	21,21,21,21	0
56	MG	1A	3914	1/1	0.98	0.09	26,26,26,26	0
56	MG	2A	3604	1/1	0.98	0.27	35,35,35,35	0
56	MG	1A	3530	1/1	0.98	0.29	42,42,42,42	0
56	MG	2A	3606	1/1	0.98	0.16	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	1A	4142	1/1	0.98	0.15	16,16,16,16	0
56	MG	1A	3031	1/1	0.98	0.19	21,21,21,21	0
56	MG	2A	3489	1/1	0.98	0.19	38,38,38,38	0
56	MG	1A	3119	1/1	0.98	0.52	24,24,24,24	0
56	MG	1a	3229	1/1	0.98	0.11	42,42,42,42	0
56	MG	1A	3167	1/1	0.98	0.29	20,20,20,20	0
56	MG	1A	3168	1/1	0.98	0.18	20,20,20,20	0
56	MG	1A	3192	1/1	0.98	0.21	20,20,20,20	0
56	MG	1a	3233	1/1	0.98	0.20	32,32,32,32	0
56	MG	2A	3616	1/1	0.98	0.17	31,31,31,31	0
56	MG	1R	201	1/1	0.98	0.23	23,23,23,23	0
56	MG	2A	3872	1/1	0.98	0.65	37,37,37,37	0
56	MG	1A	3067	1/1	0.98	0.17	8,8,8,8	0
56	MG	1A	3619	1/1	0.98	0.18	18,18,18,18	0
56	MG	1A	3620	1/1	0.98	0.16	26,26,26,26	0
56	MG	1A	3621	1/1	0.98	0.16	34,34,34,34	0
56	MG	2a	3061	1/1	0.98	0.18	40,40,40,40	0
56	MG	1A	4066	1/1	0.98	0.18	32,32,32,32	0
56	MG	1A	3465	1/1	0.98	0.45	22,22,22,22	0
56	MG	1A	3797	1/1	0.98	0.21	25,25,25,25	0
56	MG	1A	3678	1/1	0.98	0.23	43,43,43,43	0
56	MG	1A	3577	1/1	0.98	0.17	16,16,16,16	0
56	MG	1A	3433	1/1	0.98	0.20	12,12,12,12	0
56	MG	1B	3014	1/1	0.98	0.20	31,31,31,31	0
56	MG	1A	3500	1/1	0.98	0.38	27,27,27,27	0
56	MG	1B	3016	1/1	0.98	0.23	22,22,22,22	0
56	MG	1A	4073	1/1	0.98	0.12	39,39,39,39	0
56	MG	1A	3501	1/1	0.98	0.28	22,22,22,22	0
56	MG	1B	3019	1/1	0.98	0.13	34,34,34,34	0
56	MG	1A	3683	1/1	0.98	0.09	39,39,39,39	0
56	MG	1A	3134	1/1	0.98	0.14	8,8,8,8	0
56	MG	2A	3637	1/1	0.98	0.10	53,53,53,53	0
56	MG	1A	3171	1/1	0.98	0.14	21,21,21,21	0
56	MG	1A	3436	1/1	0.98	0.20	24,24,24,24	0
56	MG	1a	3054	1/1	0.98	0.11	57,57,57,57	0
56	MG	1A	3936	1/1	0.98	0.07	40,40,40,40	0
56	MG	2A	3642	1/1	0.98	0.16	37,37,37,37	0
56	MG	2A	3079	1/1	0.98	0.14	50,50,50,50	0
56	MG	2a	3083	1/1	0.98	0.14	42,42,42,42	0
56	MG	1A	3937	1/1	0.98	0.25	33,33,33,33	0
56	MG	1A	3687	1/1	0.98	0.14	30,30,30,30	0
56	MG	1A	3808	1/1	0.98	0.12	29,29,29,29	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	1A	3321	1/1	0.98	0.21	16,16,16,16	0
56	MG	1A	3506	1/1	0.98	0.25	18,18,18,18	0
56	MG	1A	4013	1/1	0.98	0.10	26,26,26,26	0
56	MG	1A	4087	1/1	0.98	0.09	14,14,14,14	0
56	MG	2D	306	1/1	0.98	0.42	34,34,34,34	0
56	MG	1A	3406	1/1	0.98	0.34	24,24,24,24	0
56	MG	1A	3636	1/1	0.98	0.16	6,6,6,6	0
56	MG	1Y	504	1/1	0.98	0.72	45,45,45,45	0
56	MG	1A	3196	1/1	0.98	0.22	21,21,21,21	0
56	MG	1Z	302	1/1	0.98	0.20	26,26,26,26	0
56	MG	1B	3035	1/1	0.98	0.15	21,21,21,21	0
56	MG	1A	3269	1/1	0.98	0.31	20,20,20,20	0
56	MG	1A	3589	1/1	0.98	0.15	19,19,19,19	0
56	MG	2a	3100	1/1	0.98	0.17	51,51,51,51	0
56	MG	1A	3270	1/1	0.98	0.49	18,18,18,18	0
56	MG	2A	3096	1/1	0.98	0.17	33,33,33,33	0
56	MG	1a	3072	1/1	0.98	0.07	36,36,36,36	0
56	MG	2A	3784	1/1	0.98	0.10	17,17,17,17	0
56	MG	1D	303	1/1	0.98	0.20	23,23,23,23	0
56	MG	1A	3014	1/1	0.98	0.27	15,15,15,15	0
56	MG	1A	3039	1/1	0.98	0.09	23,23,23,23	0
56	MG	1A	3820	1/1	0.98	0.18	27,27,27,27	0
56	MG	1A	3174	1/1	0.98	0.08	48,48,48,48	0
56	MG	2w	3001	1/1	0.98	0.19	34,34,34,34	0
56	MG	2A	3544	1/1	0.98	0.12	40,40,40,40	0
56	MG	1D	308	1/1	0.98	0.47	26,26,26,26	0
56	MG	1A	3026	1/1	0.98	0.34	14,14,14,14	0
56	MG	1A	3886	1/1	0.98	0.23	34,34,34,34	0
56	MG	1A	3645	1/1	0.98	0.13	14,14,14,14	0
56	MG	1A	3071	1/1	0.98	0.28	26,26,26,26	0
56	MG	1A	3703	1/1	0.98	0.34	24,24,24,24	0
56	MG	1A	3140	1/1	0.98	0.13	32,32,32,32	0
56	MG	2U	203	1/1	0.98	0.44	47,47,47,47	0
56	MG	1A	3648	1/1	0.98	0.20	38,38,38,38	0
56	MG	1E	302	1/1	0.98	0.18	16,16,16,16	0
56	MG	1A	4107	1/1	0.98	0.43	17,17,17,17	0
56	MG	1A	3959	1/1	0.98	0.15	26,26,26,26	0
56	MG	1E	305	1/1	0.98	0.15	26,26,26,26	0
56	MG	1A	3828	1/1	0.98	0.35	21,21,21,21	0
56	MG	1A	3649	1/1	0.98	0.12	13,13,13,13	0
56	MG	1a	3191	1/1	0.98	0.26	64,64,64,64	0
56	MG	1A	3099	1/1	0.98	0.25	24,24,24,24	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	1A	3557	1/1	0.98	0.34	19,19,19,19	0
56	MG	1A	3179	1/1	0.98	0.24	24,24,24,24	0
56	MG	23	3001	1/1	0.98	0.17	46,46,46,46	0
56	MG	18	102	1/1	0.98	0.29	19,19,19,19	0
59	ZN	1Y	501	1/1	0.98	0.19	49,49,49,49	0
56	MG	2A	3811	1/1	0.98	0.06	54,54,54,54	0
59	ZN	15	101	1/1	0.98	0.21	37,37,37,37	0
59	ZN	16	101	1/1	0.98	0.23	33,33,33,33	0
59	ZN	1n	501	1/1	0.98	0.14	55,55,55,55	0
59	ZN	2Y	501	1/1	0.98	0.16	75,75,75,75	0
56	MG	1A	3158	1/1	0.98	0.13	12,12,12,12	0
59	ZN	25	101	1/1	0.98	0.17	44,44,44,44	0
56	MG	18	104	1/1	0.98	0.21	19,19,19,19	0
56	MG	1A	3711	1/1	0.98	0.09	28,28,28,28	0
56	MG	27	101	1/1	0.98	0.18	32,32,32,32	0
60	SF4	1d	501	8/8	0.98	0.15	51,59,62,71	0
60	SF4	2d	302	8/8	0.98	0.13	53,66,72,75	0
56	MG	1A	3763	1/1	0.99	0.21	7,7,7,7	0
56	MG	2A	3206	1/1	0.99	0.11	57,57,57,57	0
56	MG	1A	3846	1/1	0.99	0.24	18,18,18,18	0
56	MG	1A	3185	1/1	0.99	0.48	22,22,22,22	0
56	MG	1A	3695	1/1	0.99	0.12	24,24,24,24	0
56	MG	1A	3623	1/1	0.99	0.19	17,17,17,17	0
56	MG	2A	3527	1/1	0.99	0.24	41,41,41,41	0
56	MG	2A	3419	1/1	0.99	0.19	28,28,28,28	0
56	MG	1A	3650	1/1	0.99	0.30	43,43,43,43	0
56	MG	1A	4012	1/1	0.99	0.14	17,17,17,17	0
56	MG	1A	3137	1/1	0.99	0.46	24,24,24,24	0
56	MG	1B	3002	1/1	0.99	0.26	27,27,27,27	0
56	MG	1A	4090	1/1	0.99	0.10	32,32,32,32	0
56	MG	1A	3625	1/1	0.99	0.10	23,23,23,23	0
56	MG	1f	3001	1/1	0.99	0.17	34,34,34,34	0
56	MG	1A	3897	1/1	0.99	0.11	40,40,40,40	0
56	MG	1A	3102	1/1	0.99	0.28	23,23,23,23	0
56	MG	1A	3627	1/1	0.99	0.20	15,15,15,15	0
56	MG	1A	3595	1/1	0.99	0.12	32,32,32,32	0
56	MG	2A	3324	1/1	0.99	0.07	58,58,58,58	0
56	MG	1A	3670	1/1	0.99	0.14	8,8,8,8	0
56	MG	1A	3814	1/1	0.99	0.09	38,38,38,38	0
56	MG	1A	4098	1/1	0.99	0.14	14,14,14,14	0
56	MG	1A	3032	1/1	0.99	0.16	8,8,8,8	0
56	MG	2A	3809	1/1	0.99	0.09	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	1S	3001	1/1	0.99	0.29	30,30,30,30	0
56	MG	1S	3002	1/1	0.99	0.16	37,37,37,37	0
56	MG	1A	3672	1/1	0.99	0.18	9,9,9,9	0
56	MG	1A	3974	1/1	0.99	0.13	8,8,8,8	0
56	MG	2A	3814	1/1	0.99	0.14	45,45,45,45	0
56	MG	1A	3033	1/1	0.99	0.53	23,23,23,23	0
56	MG	1A	3064	1/1	0.99	0.20	6,6,6,6	0
59	ZN	19	102	1/1	0.99	0.19	31,31,31,31	0
56	MG	1A	3778	1/1	0.99	0.12	22,22,22,22	0
56	MG	1A	3759	1/1	0.99	0.19	35,35,35,35	0
56	MG	2A	3167	1/1	0.99	0.12	44,44,44,44	0
56	MG	2A	3860	1/1	0.99	0.18	38,38,38,38	0
56	MG	1A	3012	1/1	0.99	0.12	14,14,14,14	0
56	MG	1A	4079	1/1	0.99	0.17	29,29,29,29	0
56	MG	2A	3630	1/1	0.99	0.13	49,49,49,49	0
56	MG	1A	3508	1/1	0.99	0.17	13,13,13,13	0
56	MG	1A	3276	1/1	0.99	0.22	33,33,33,33	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.