



# Full wwPDB X-ray Structure Validation Report ⓘ

Sep 16, 2020 – 06:03 PM BST

PDB ID : 5HCR  
Title : Crystal structure of antimicrobial peptide Oncocin 10wt bound to the *Thermus thermophilus* 70S ribosome  
Authors : Gagnon, M.G.; Roy, R.N.; Lomakin, I.B.; Florin, T.; Mankin, A.S.; Steitz, T.A.  
Deposited on : 2016-01-04  
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.

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

MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.14.3.dev2  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.14.3.dev2

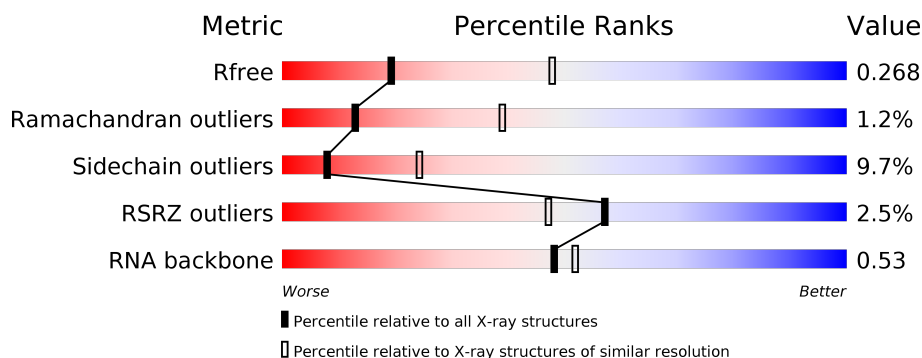
# 1 Overall quality at a glance

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.














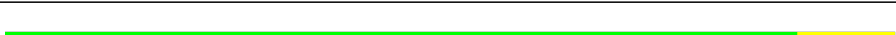


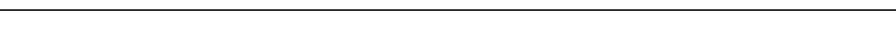
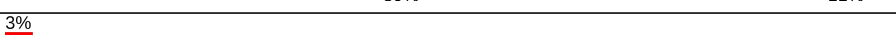

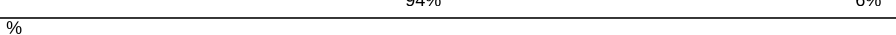
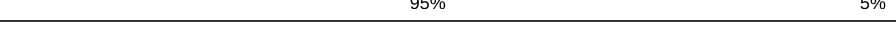






Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	130704	3140 (2.80-2.80)
Ramachandran outliers	138981	3498 (2.80-2.80)
Sidechain outliers	138945	3500 (2.80-2.80)
RSRZ outliers	127900	3078 (2.80-2.80)
RNA backbone	3102	1227 (3.10-2.50)

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

Mol	Chain	Length	Quality of chain
1	1A	2915	<div> <div>%</div> <div> <div></div> <div>80%</div> <div>14%</div> <div>6%</div> </div> </div>
1	2A	2915	<div> <div>%</div> <div> <div></div> <div>79%</div> <div>17%</div> <div></div> </div> </div>
2	1B	121	<div> <div></div> <div> <div></div> <div>91%</div> <div>8%</div> <div></div> </div> </div>
2	2B	121	<div> <div>%</div> <div> <div></div> <div>79%</div> <div>20%</div> <div></div> </div> </div>
3	1D	276	<div> <div></div> <div> <div></div> <div>90%</div> <div>9%</div> </div> </div>
3	2D	276	<div> <div></div> <div> <div></div> <div>91%</div> <div>9%</div> </div> </div>

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Mol	Chain	Length	Quality of chain
4	1E	206	
4	2E	206	
5	1F	210	
5	2F	210	
6	1G	182	
6	2G	182	
7	1H	180	
7	2H	180	
8	1I	148	
8	2I	148	
9	1N	140	
9	2N	140	
10	1O	122	
10	2O	122	
11	1P	150	
11	2P	150	
12	1Q	141	
12	2Q	141	
13	1R	118	
13	2R	118	
14	1S	112	
14	2S	112	
15	1T	146	
15	2T	146	
16	1U	118	

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Mol	Chain	Length	Quality of chain
16	2U	118	
17	1V	101	
17	2V	101	
18	1W	113	
18	2W	113	
19	1X	96	
19	2X	96	
20	1Y	110	
20	2Y	110	
21	1Z	206	
21	2Z	206	
22	10	85	
22	20	85	
23	11	98	
23	21	98	
24	12	72	
24	22	72	
25	13	60	
25	23	60	
26	14	71	
26	24	71	
27	15	60	
27	25	60	
28	16	54	
28	26	54	

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Mol	Chain	Length	Quality of chain
29	17	49	
29	27	49	
30	18	65	
30	28	65	
31	19	37	
31	29	37	
32	1a	1521	
32	2a	1521	
33	1b	256	
33	2b	256	
34	1c	239	
34	2c	239	
35	1d	209	
35	2d	209	
36	1e	162	
36	2e	162	
37	1f	101	
37	2f	101	
38	1g	156	
38	2g	156	
39	1h	138	
39	2h	138	
40	1i	128	
40	2i	128	
41	1j	105	





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Mol	Chain	Length	Quality of chain
41	2j	105	
42	1k	129	
42	2k	129	
43	1l	132	
43	2l	132	
44	1m	126	
44	2m	126	
45	1n	61	
45	2n	61	
46	1o	89	
46	2o	89	
47	1p	88	
47	2p	88	
48	1q	105	
48	2q	105	
49	1r	88	
49	2r	88	
50	1s	93	
50	2s	93	
51	1t	106	
51	2t	106	
52	1u	27	
52	2u	27	
53	1v	24	
53	2v	24	

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Mol	Chain	Length	Quality of chain
54	1x	77	
54	2x	77	
55	1z	19	
55	2z	19	

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	3307	-	-	-	X
56	MG	1A	3353	-	-	-	X
56	MG	1A	3385	-	-	-	X
56	MG	1A	3510	-	-	-	X
56	MG	1A	3545	-	-	-	X
56	MG	1A	3918	-	-	-	X
56	MG	1B	227	-	-	-	X
56	MG	1D	311	-	-	-	X
56	MG	1H	203	-	-	-	X
56	MG	1N	201	-	-	-	X
56	MG	1R	205	-	-	-	X
56	MG	1a	1902	-	-	-	X
56	MG	1m	202	-	-	-	X
56	MG	1x	101	-	-	-	X
56	MG	2A	3452	-	-	-	X
56	MG	2A	3496	-	-	-	X
56	MG	2a	1614	-	-	-	X
56	MG	2e	202	-	-	-	X

## 2 Entry composition

There are 59 unique types of molecules in this entry. The entry contains 288674 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
1	1A	2746	Total	C	N	O	P	0	0	0
			59154	26327	11077	19005	2745			
1	2A	2790	Total	C	N	O	P	0	0	0
			60091	26746	11243	19313	2789			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	1B	120	Total	C	N	O	P	0	0	0
			2572	1146	476	831	119			
2	2B	120	Total	C	N	O	P	0	0	0
			2573	1146	476	832	119			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
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
			2142	1352	426	361	3			

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	1G	181	Total	C	N	O	S	0	0	0
			1425	914	256	251	4			
6	2G	181	Total	C	N	O	S	0	0	0
			1424	911	258	251	4			

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	1I	146	Total	C	N	O	S	0	0	0
			1085	693	189	202	1			
8	2I	146	Total	C	N	O	S	0	0	0
			1061	680	186	194	1			

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	1P	149	Total	C	N	O	S	0	0	0
			1139	709	231	196	3			
11	2P	149	Total	C	N	O	S	0	0	0
			1135	706	230	196	3			

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
21	1Z	186	Total	C	N	O	S	0	0	0
			1470	937	262	269	2			
21	2Z	186	Total	C	N	O	S	0	0	0
			1454	929	256	267	2			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
22	10	75	Total	C	N	O	S	0	0	0
			598	370	127	100	1			
22	20	75	Total	C	N	O	S	0	0	0
			598	370	127	100	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
			558	352	102	99	5			

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

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

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

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

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
32	1a	1477	Total	C	N	O	P	0	0	0
			31750	14131	5883	10259	1477			
32	2a	1483	Total	C	N	O	P	0	0	0
			31877	14188	5905	10301	1483			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
33	1b	231	Total	C	N	O	S	0	0	0
			1786	1136	321	325	4			
33	2b	231	Total	C	N	O	S	0	0	0
			1697	1079	292	321	5			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
34	1c	206	Total	C	N	O	S	0	0	0
			1480	932	281	266	1			
34	2c	206	Total	C	N	O	S	0	0	0
			1412	883	269	259	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
35	1d	208	Total	C	N	O	S	0	0	0
			1618	1013	312	286	7			
35	2d	208	Total	C	N	O	S	0	0	0
			1630	1022	321	280	7			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
36	1e	148	Total	C	N	O	S	0	0	0
			1129	714	213	198	4			
36	2e	148	Total	C	N	O	S	0	0	0
			1095	695	203	193	4			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
37	1f	100	Total	C	N	O	S	0	0	0
			806	511	143	149	3			
37	2f	100	Total	C	N	O	S	0	0	0
			817	516	146	152	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
			1183	732	232	213	6			
38	2g	155	Total	C	N	O	S	0	0	0
			1167	728	220	213	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
			1074	681	202	189	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
			976	620	189	167			
40	2i	127	Total	C	N	O	0	0	0
			932	589	177	166			

- 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
			682	424	130	128			
41	2j	96	Total	C	N	O	0	0	0
			678	424	126	128			

- 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
			826	513	156	154	3			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
42	2k	114	Total	C	N	O	S	0	0	0
			829	516	155	155	3			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
43	1l	122	Total	C	N	O	S	0	0	0
			920	579	181	159	1			
43	2l	122	Total	C	N	O	S	0	0	0
			918	576	182	159	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
44	1m	118	Total	C	N	O	S	0	0	0
			923	569	191	161	2			
44	2m	116	Total	C	N	O	S	0	0	0
			903	555	187	159	2			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
45	1n	60	Total	C	N	O	S	0	0	0
			482	306	100	72	4			
45	2n	60	Total	C	N	O	S	0	0	0
			459	291	93	71	4			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
46	1o	88	Total	C	N	O	S	0	0	0
			715	447	140	126	2			
46	2o	88	Total	C	N	O	S	0	0	0
			728	456	144	126	2			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
47	1p	82	Total	C	N	O	S	0	0	0
			671	424	133	113	1			
47	2p	82	Total	C	N	O	S	0	0	0
			677	430	133	113	1			



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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
48	1q	99	Total	C	N	O	S	0	0	0
			811	519	148	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	84	Total	C	N	O	S	0	0	0
			642	409	119	112	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
			712	435	152	123	2			
51	2t	96	Total	C	N	O	S	0	0	0
			731	449	156	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
			187	116	42	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	5	Total	C	N	O	P	0	0	0
			109	49	22	33	5			
53	2v	5	Total	C	N	O	P	0	0	0
			109	49	22	33	5			

- Molecule 54 is a RNA chain called P-site tRNA.

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

- Molecule 55 is a protein called Oncocin 10wt.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
55	1z	13	Total	C	N	O	0	0	0
			108	72	20	16			
55	2z	12	Total	C	N	O	0	0	0
			101	67	19	15			

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
56	2E	4	Total	Mg	0	0
			4	4		
56	17	6	Total	Mg	0	0
			6	6		
56	2d	1	Total	Mg	0	0
			1	1		
56	1T	6	Total	Mg	0	0
			6	6		
56	1N	8	Total	Mg	0	0
			8	8		
56	1u	1	Total	Mg	0	0
			1	1		
56	18	4	Total	Mg	0	0
			4	4		
56	1o	2	Total	Mg	0	0
			2	2		
56	2W	1	Total	Mg	0	0
			1	1		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
56	1Y	1	Total 1	Mg 1	0	0
56	13	2	Total 2	Mg 2	0	0
56	1f	1	Total 1	Mg 1	0	0
56	1P	6	Total 6	Mg 6	0	0
56	2B	10	Total 10	Mg 10	0	0
56	1q	4	Total 4	Mg 4	0	0
56	2a	217	Total 217	Mg 217	0	0
56	1k	1	Total 1	Mg 1	0	0
56	1E	8	Total 8	Mg 8	0	0
56	1b	2	Total 2	Mg 2	0	0
56	2l	4	Total 4	Mg 4	0	0
56	2F	3	Total 3	Mg 3	0	0
56	16	3	Total 3	Mg 3	0	0
56	28	1	Total 1	Mg 1	0	0
56	2e	3	Total 3	Mg 3	0	0
56	1W	5	Total 5	Mg 5	0	0
56	1A	1096	Total 1096	Mg 1096	0	0
56	1t	1	Total 1	Mg 1	0	0
56	2p	1	Total 1	Mg 1	0	0
56	1n	1	Total 1	Mg 1	0	0
56	1X	1	Total 1	Mg 1	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
56	20	1	Total 1	Mg 1	0	0
56	25	1	Total 1	Mg 1	0	0
56	1D	13	Total 13	Mg 13	0	0
56	2N	1	Total 1	Mg 1	0	0
56	1e	3	Total 3	Mg 3	0	0
56	2G	1	Total 1	Mg 1	0	0
56	2f	1	Total 1	Mg 1	0	0
56	1V	1	Total 1	Mg 1	0	0
56	1a	307	Total 307	Mg 307	0	0
56	2Q	5	Total 5	Mg 5	0	0
56	15	3	Total 3	Mg 3	0	0
56	1x	10	Total 10	Mg 10	0	0
56	1R	6	Total 6	Mg 6	0	0
56	1m	2	Total 2	Mg 2	0	0
56	2U	2	Total 2	Mg 2	0	0
56	1G	3	Total 3	Mg 3	0	0
56	2O	2	Total 2	Mg 2	0	0
56	11	4	Total 4	Mg 4	0	0
56	1d	2	Total 2	Mg 2	0	0
56	2n	1	Total 1	Mg 1	0	0
56	1H	3	Total 3	Mg 3	0	0

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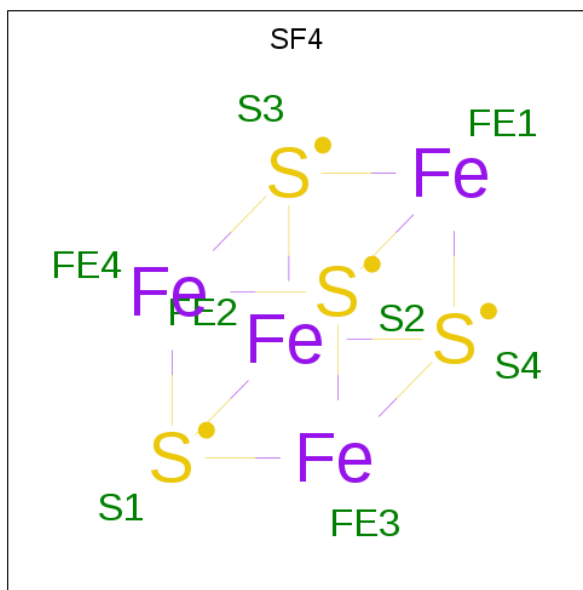
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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
56	2Y	2	Total Mg 2 2	0	0
56	2x	5	Total Mg 5 5	0	0
56	1Z	2	Total Mg 2 2	0	0
56	2D	6	Total Mg 6 6	0	0
56	2q	2	Total Mg 2 2	0	0
56	2k	1	Total Mg 1 1	0	0
56	1U	6	Total Mg 6 6	0	0
56	1O	3	Total Mg 3 3	0	0
56	1r	3	Total Mg 3 3	0	0
56	19	3	Total Mg 3 3	0	0
56	1l	1	Total Mg 1 1	0	0
56	1F	7	Total Mg 7 7	0	0
56	10	6	Total Mg 6 6	0	0
56	2t	1	Total Mg 1 1	0	0
56	1Q	7	Total Mg 7 7	0	0
56	2A	559	Total Mg 559 559	0	0
56	1h	3	Total Mg 3 3	0	0
56	2Z	1	Total Mg 1 1	0	0
56	1B	27	Total Mg 27 27	0	0
56	1c	1	Total Mg 1 1	0	0

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

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

- Molecule 58 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe<sub>4</sub>S<sub>4</sub>).



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

- Molecule 59 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
59	1A	2345	Total	O	0	0
			2345	2345		
59	1B	45	Total	O	0	0
			45	45		
59	1D	20	Total	O	0	0
			20	20		
59	1E	29	Total	O	0	0
			29	29		
59	1F	18	Total	O	0	0
			18	18		
59	1G	4	Total	O	0	0
			4	4		
59	1H	4	Total	O	0	0
			4	4		
59	1I	1	Total	O	0	0
			1	1		
59	1N	12	Total	O	0	0
			12	12		
59	1O	6	Total	O	0	0
			6	6		
59	1P	16	Total	O	0	0
			16	16		
59	1Q	12	Total	O	0	0
			12	12		
59	1R	10	Total	O	0	0
			10	10		
59	1S	1	Total	O	0	0
			1	1		
59	1T	14	Total	O	0	0
			14	14		
59	1U	11	Total	O	0	0
			11	11		
59	1V	5	Total	O	0	0
			5	5		
59	1W	9	Total	O	0	0
			9	9		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
59	1X	6	Total 6	O 6	0	0
59	1Y	1	Total 1	O 1	0	0
59	1Z	6	Total 6	O 6	0	0
59	10	7	Total 7	O 7	0	0
59	11	9	Total 9	O 9	0	0
59	12	1	Total 1	O 1	0	0
59	13	5	Total 5	O 5	0	0
59	14	1	Total 1	O 1	0	0
59	15	9	Total 9	O 9	0	0
59	16	6	Total 6	O 6	0	0
59	17	3	Total 3	O 3	0	0
59	18	15	Total 15	O 15	0	0
59	19	4	Total 4	O 4	0	0
59	1a	395	Total 395	O 395	0	0
59	1b	1	Total 1	O 1	0	0
59	1d	5	Total 5	O 5	0	0
59	1e	3	Total 3	O 3	0	0
59	1f	1	Total 1	O 1	0	0
59	1h	4	Total 4	O 4	0	0
59	1i	1	Total 1	O 1	0	0
59	1j	2	Total 2	O 2	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
59	1k	2	Total 2	O 2	0	0
59	1l	3	Total 3	O 3	0	0
59	1o	3	Total 3	O 3	0	0
59	1s	1	Total 1	O 1	0	0
59	1v	2	Total 2	O 2	0	0
59	1x	11	Total 11	O 11	0	0
59	1z	1	Total 1	O 1	0	0
59	2A	810	Total 810	O 810	0	0
59	2B	10	Total 10	O 10	0	0
59	2D	15	Total 15	O 15	0	0
59	2E	9	Total 9	O 9	0	0
59	2F	4	Total 4	O 4	0	0
59	2O	2	Total 2	O 2	0	0
59	2P	6	Total 6	O 6	0	0
59	2Q	2	Total 2	O 2	0	0
59	2R	2	Total 2	O 2	0	0
59	2T	2	Total 2	O 2	0	0
59	2U	4	Total 4	O 4	0	0
59	2V	1	Total 1	O 1	0	0
59	2W	1	Total 1	O 1	0	0
59	2X	2	Total 2	O 2	0	0

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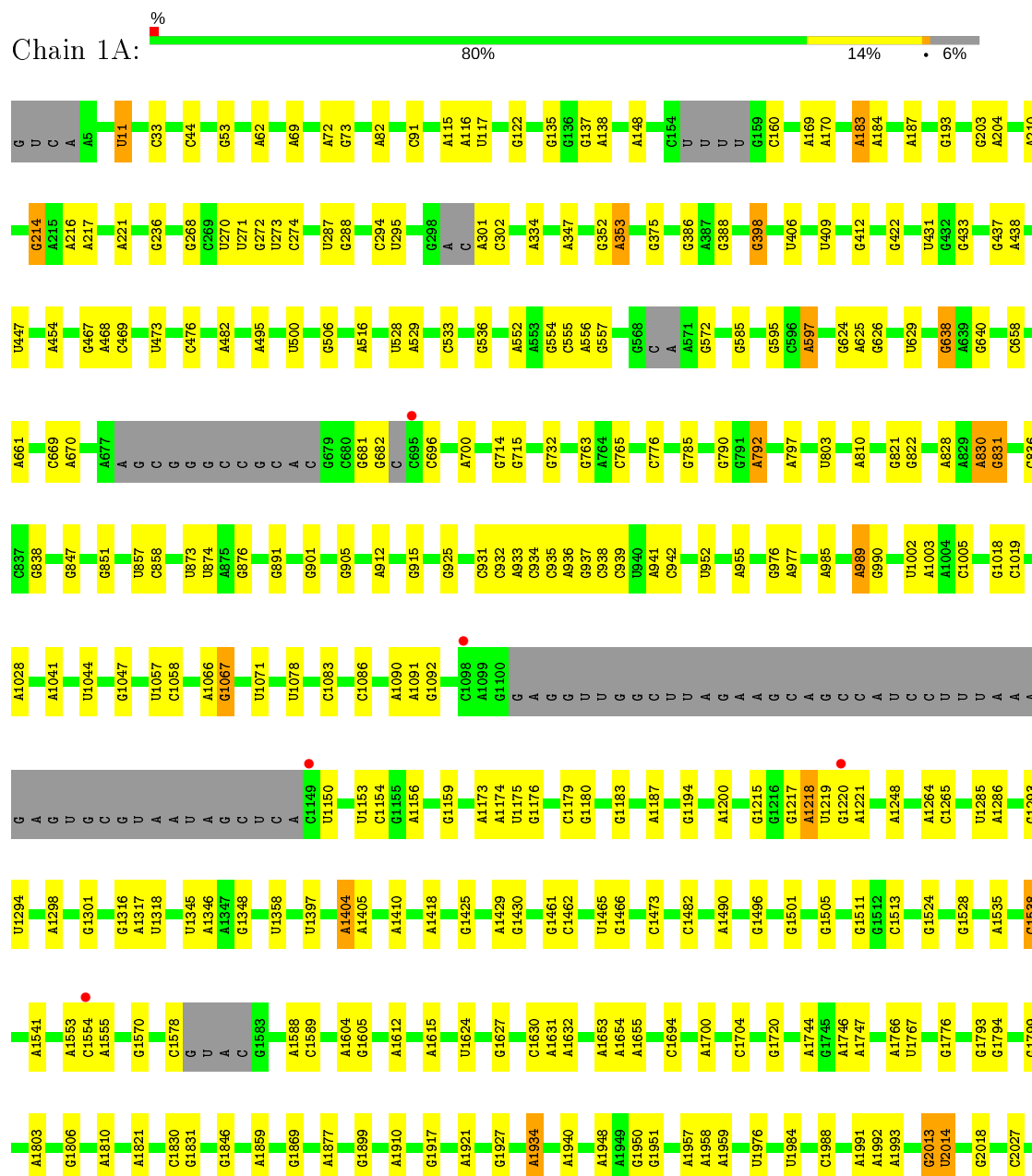
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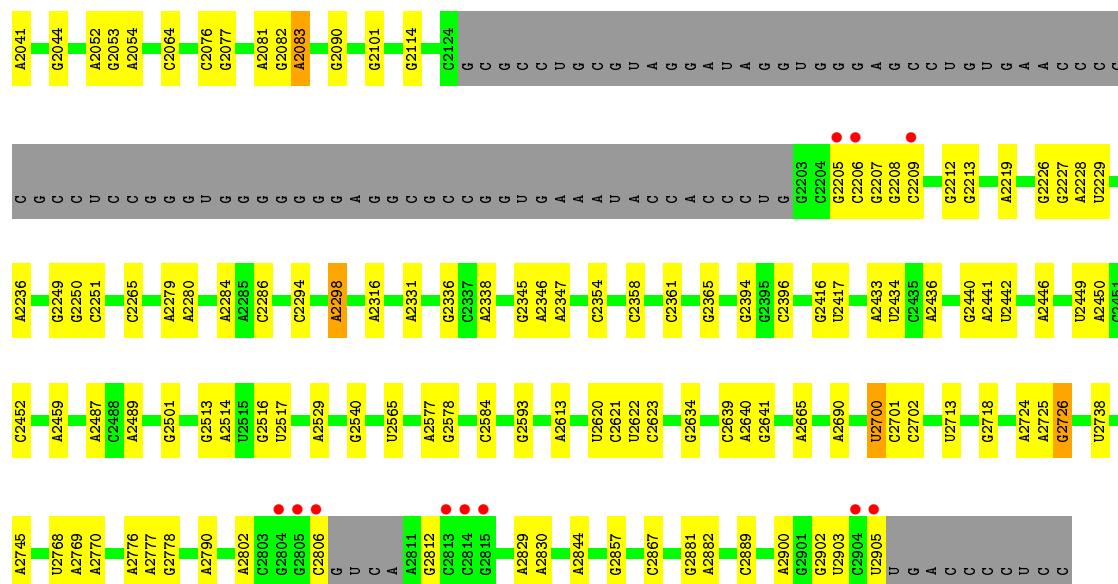
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
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59	2Z	4	Total 4	O 4	0	0
59	20	3	Total 3	O 3	0	0
59	21	1	Total 1	O 1	0	0
59	23	2	Total 2	O 2	0	0
59	28	4	Total 4	O 4	0	0
59	2a	235	Total 235	O 235	0	0
59	2d	2	Total 2	O 2	0	0
59	2e	3	Total 3	O 3	0	0
59	2i	1	Total 1	O 1	0	0
59	2m	1	Total 1	O 1	0	0
59	2n	1	Total 1	O 1	0	0
59	2p	1	Total 1	O 1	0	0
59	2t	4	Total 4	O 4	0	0
59	2x	5	Total 5	O 5	0	0
59	2z	1	Total 1	O 1	0	0

### 3 Residue-property plots

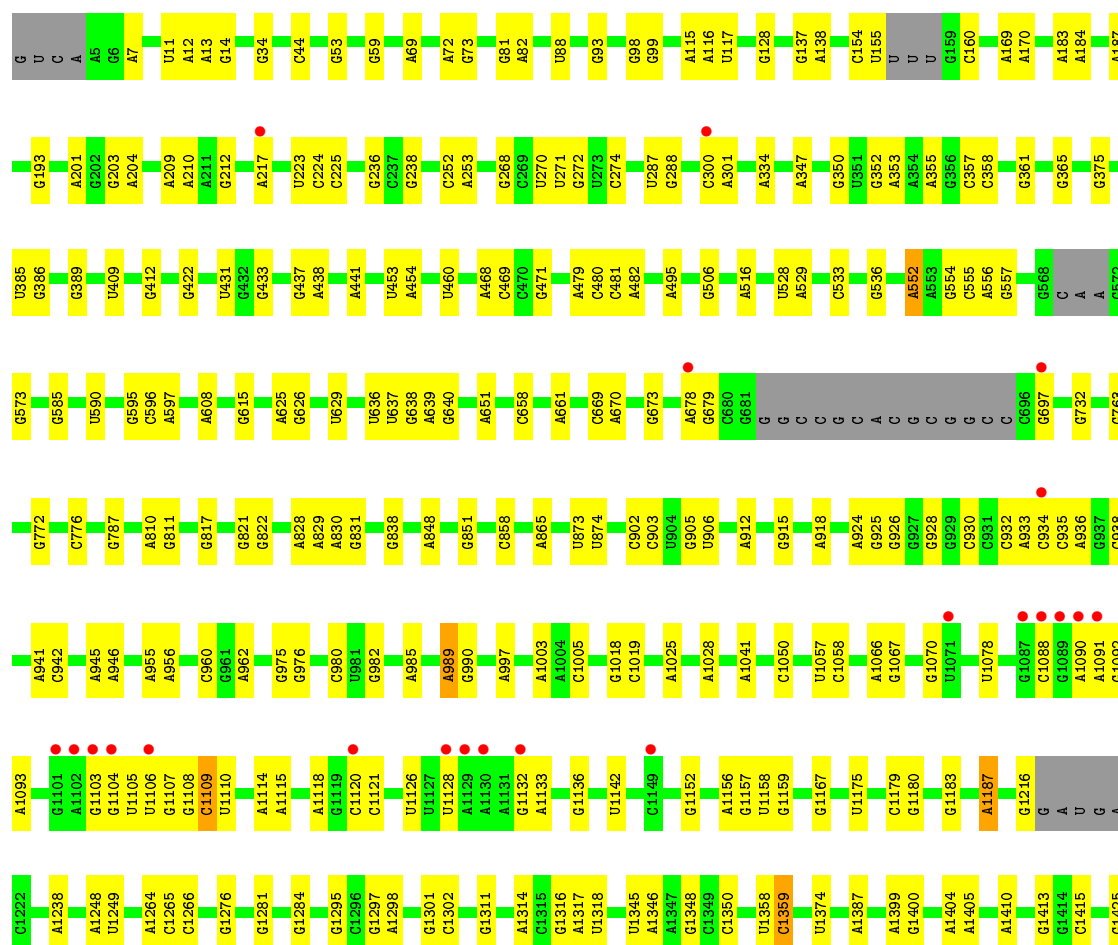
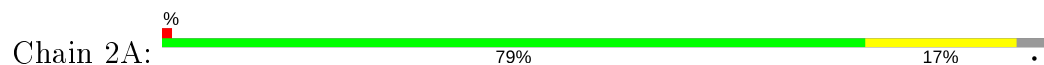
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

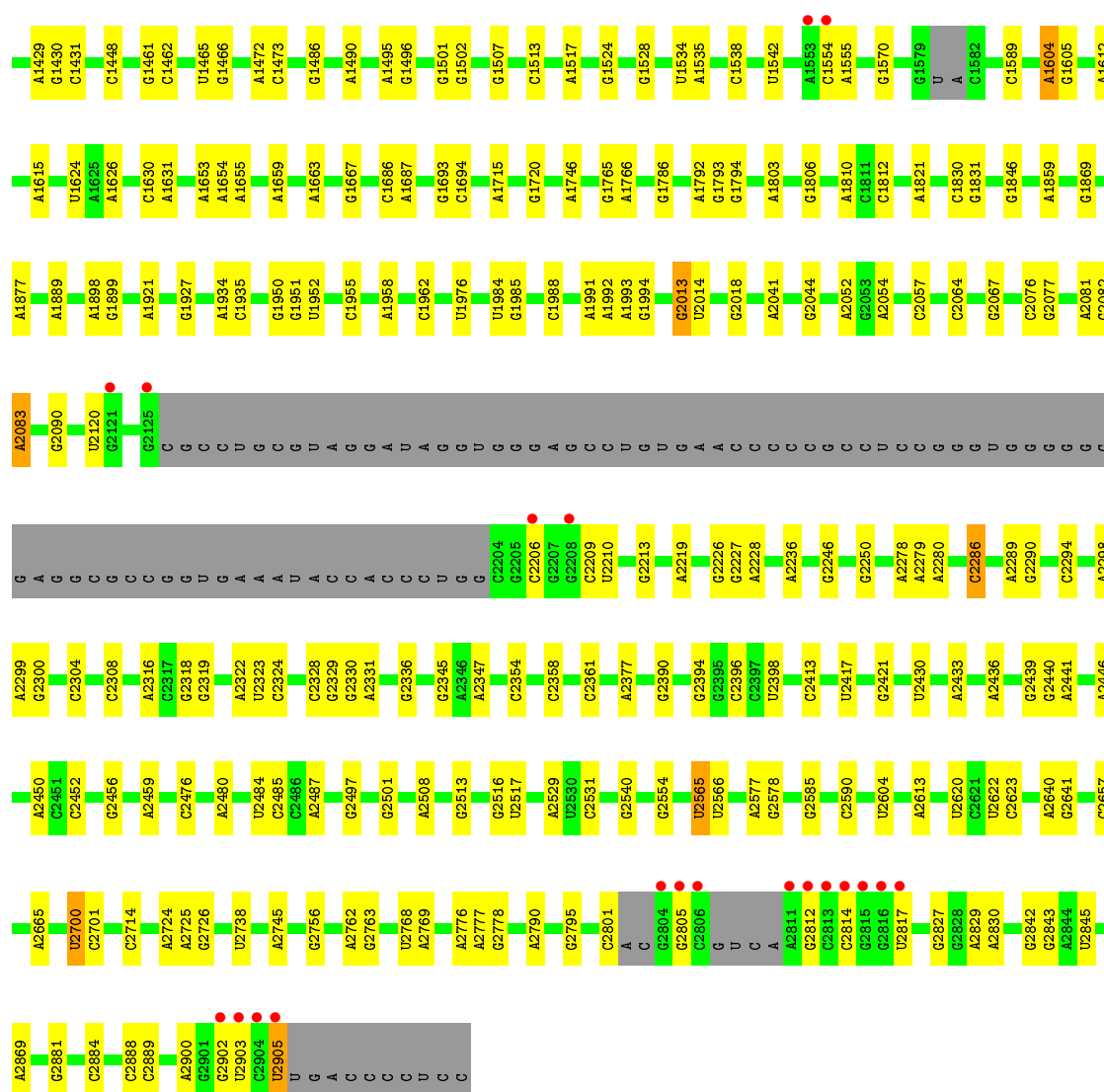
#### • Molecule 1: 23S Ribosomal RNA



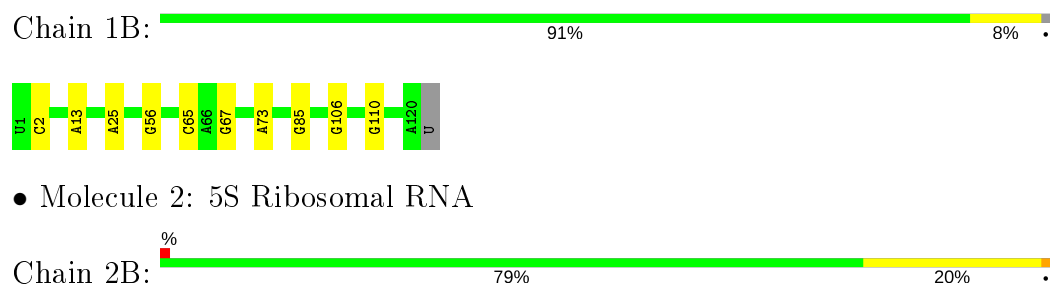


• Molecule 1: 23S Ribosomal RNA

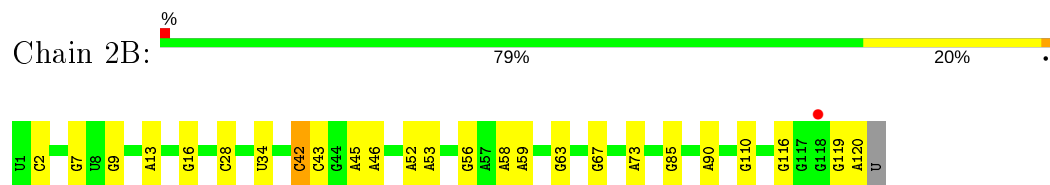




• Molecule 2: 5S Ribosomal RNA



• Molecule 2: 5S Ribosomal RNA



• Molecule 3: 50S ribosomal protein L2





- Molecule 3: 50S ribosomal protein L2



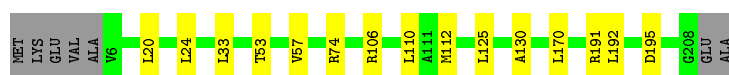
- Molecule 4: 50S ribosomal protein L3



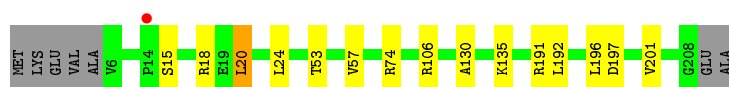
- Molecule 4: 50S ribosomal protein L3



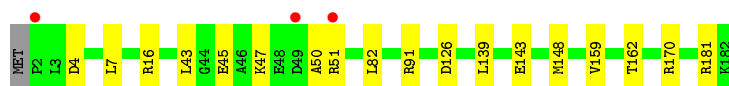
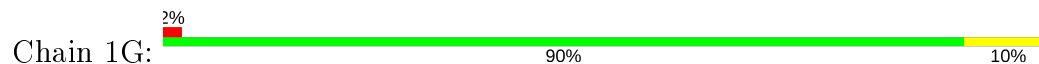
- Molecule 5: 50S ribosomal protein L4



- Molecule 5: 50S ribosomal protein L4

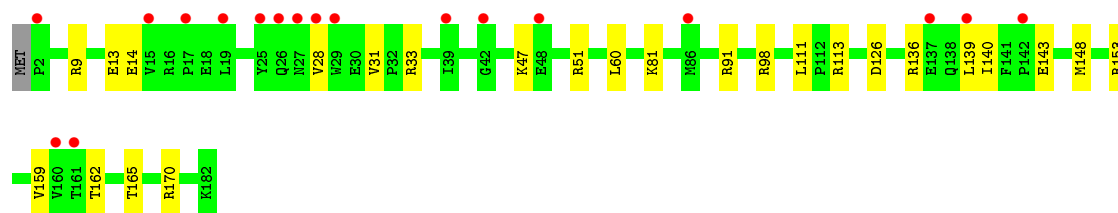


- Molecule 6: 50S ribosomal protein L5

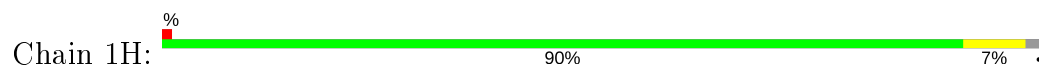


- Molecule 6: 50S ribosomal protein L5

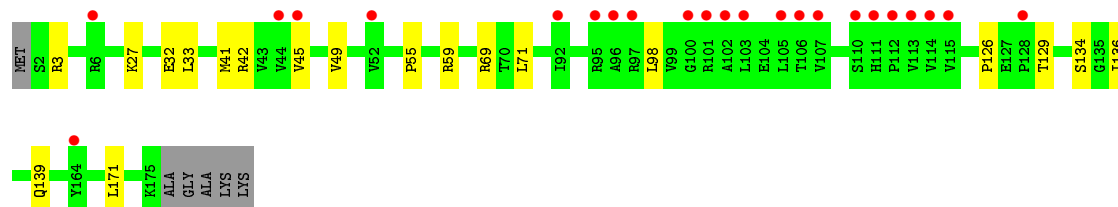
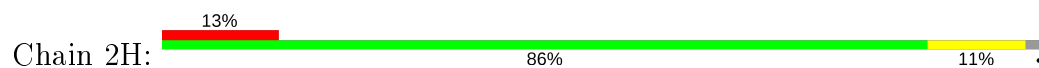




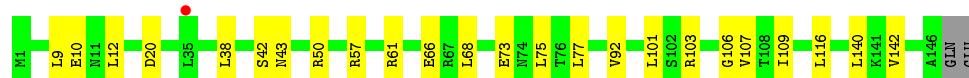
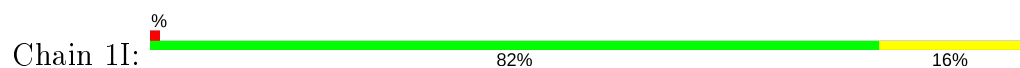
- Molecule 7: 50S ribosomal protein L6



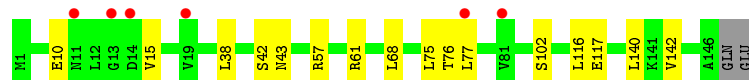
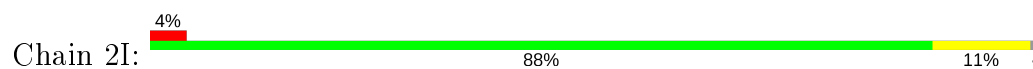
- Molecule 7: 50S ribosomal protein L6



- Molecule 8: 50S ribosomal protein L9



- Molecule 8: 50S ribosomal protein L9

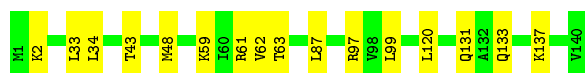


- Molecule 9: 50S ribosomal protein L13



- Molecule 9: 50S ribosomal protein L13

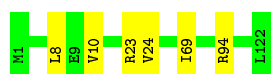




- Molecule 10: 50S ribosomal protein L14



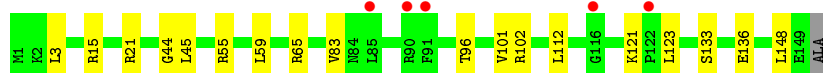
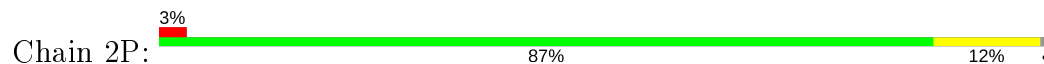
- Molecule 10: 50S ribosomal protein L14



- Molecule 11: 50S ribosomal protein L15



- Molecule 11: 50S ribosomal protein L15



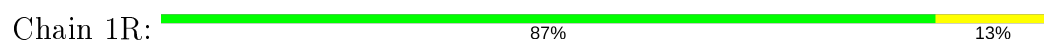
- Molecule 12: 50S ribosomal protein L16



- Molecule 12: 50S ribosomal protein L16



- Molecule 13: 50S ribosomal protein L17







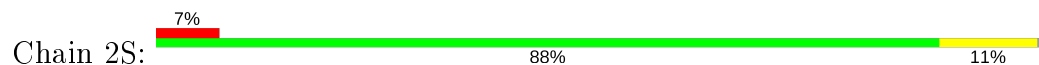
- Molecule 13: 50S ribosomal protein L17



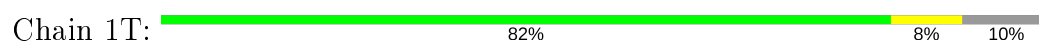
- Molecule 14: 50S ribosomal protein L18



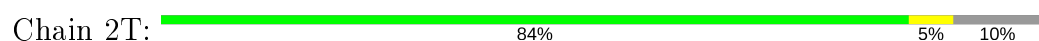
- Molecule 14: 50S ribosomal protein L18



- Molecule 15: 50S ribosomal protein L19



- Molecule 15: 50S ribosomal protein L19

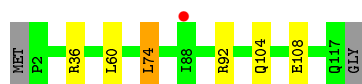


- Molecule 16: 50S ribosomal protein L20



- Molecule 16: 50S ribosomal protein L20





- Molecule 17: 50S ribosomal protein L21

Chain 1V: 88% 11% .



- Molecule 17: 50S ribosomal protein L21

Chain 2V: 91% 8% .



- Molecule 18: 50S ribosomal protein L22

Chain 1W: 94% 5% .



- Molecule 18: 50S ribosomal protein L22

Chain 2W: 94% 5% .



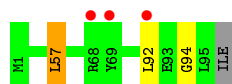
- Molecule 19: 50S ribosomal protein L23

Chain 1X: 96% ..



- Molecule 19: 50S ribosomal protein L23

Chain 2X: 96% ...

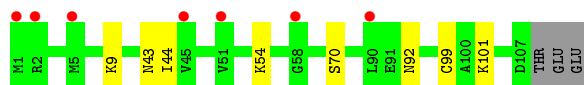
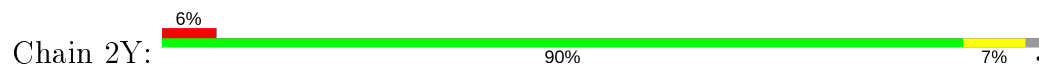


- Molecule 20: 50S ribosomal protein L24

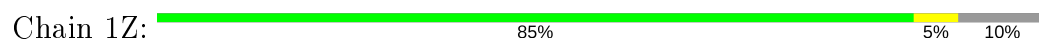
Chain 1Y: 91% 6% .



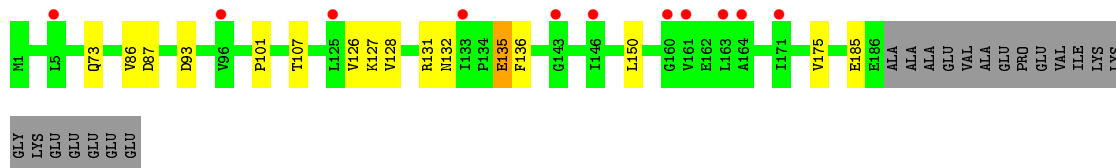
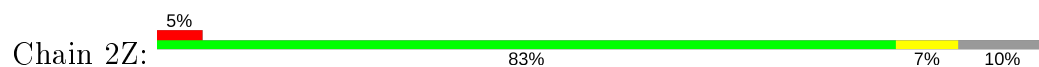
- Molecule 20: 50S ribosomal protein L24



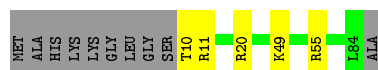
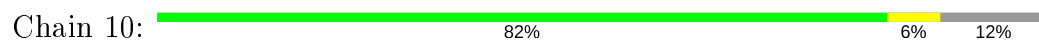
- Molecule 21: 50S ribosomal protein L25



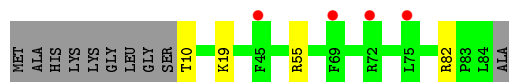
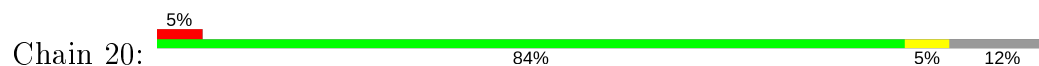
- Molecule 21: 50S ribosomal protein L25



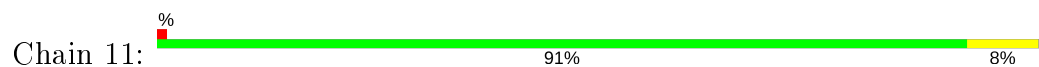
- Molecule 22: 50S ribosomal protein L27



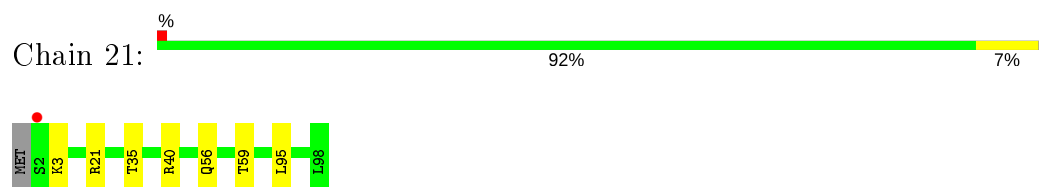
- Molecule 22: 50S ribosomal protein L27



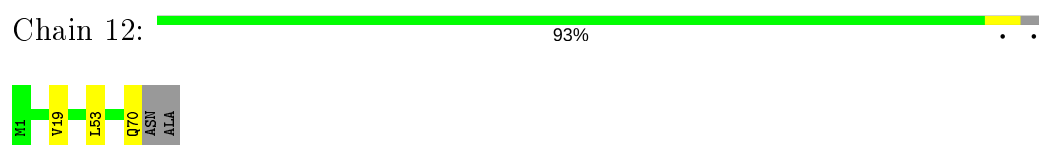
- Molecule 23: 50S ribosomal protein L28



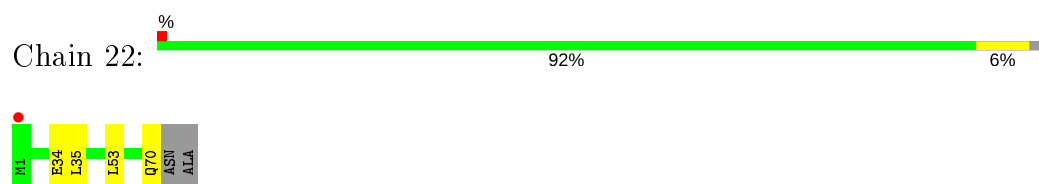
- Molecule 23: 50S ribosomal protein L28



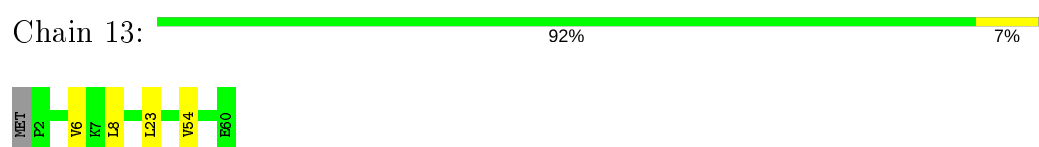
- Molecule 24: 50S ribosomal protein L29



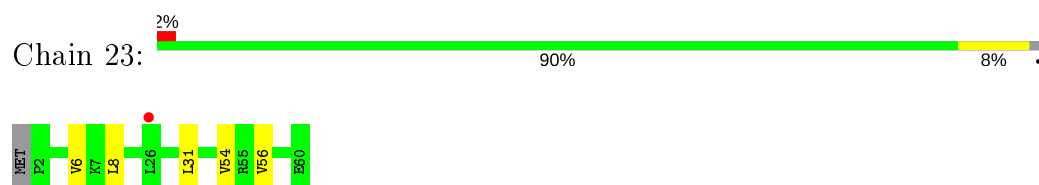
- Molecule 24: 50S ribosomal protein L29



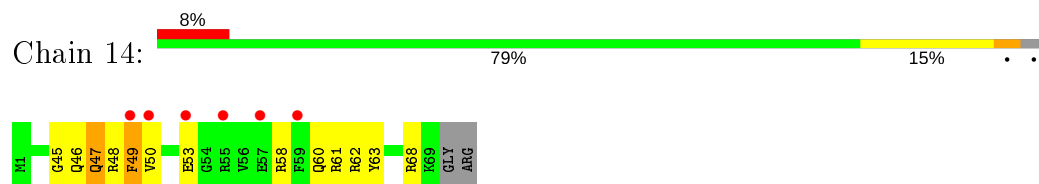
- Molecule 25: 50S ribosomal protein L30



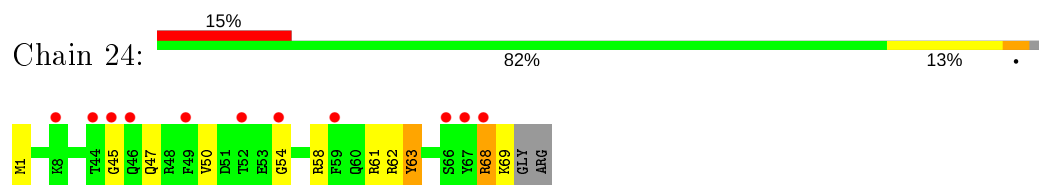
- Molecule 25: 50S ribosomal protein L30



- Molecule 26: 50S ribosomal protein L31



- Molecule 26: 50S ribosomal protein L31



- Molecule 27: 50S ribosomal protein L32

Chain 15:  92% 7% .




- Molecule 27: 50S ribosomal protein L32

Chain 25:  92% 7% .



- Molecule 28: 50S ribosomal protein L33

Chain 16:  89% 9% .




- Molecule 28: 50S ribosomal protein L33

Chain 26:  89% 9% .



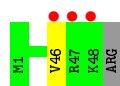
- Molecule 29: 50S ribosomal protein L34

Chain 17:  2% 90% 8% .



- Molecule 29: 50S ribosomal protein L34

Chain 27:  6% 96% . .

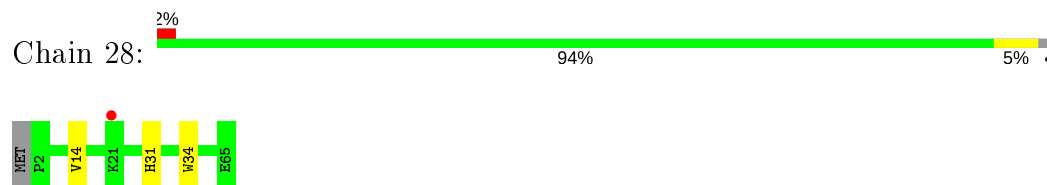


- Molecule 30: 50S ribosomal protein L35

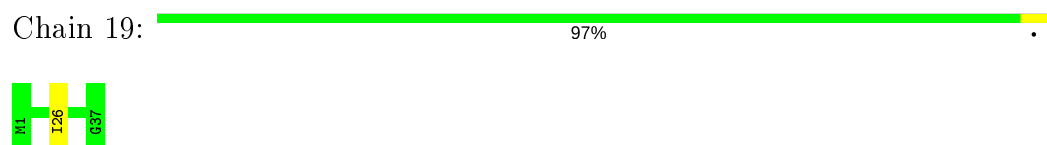
Chain 18:  91% 8% .



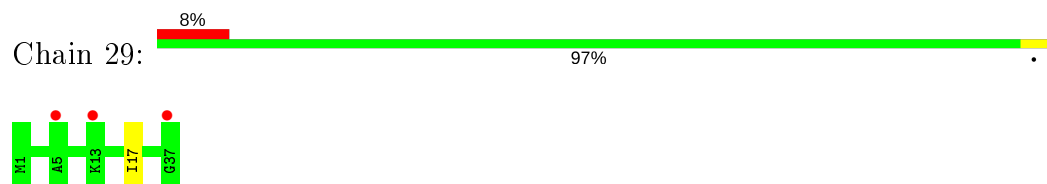
- Molecule 30: 50S ribosomal protein L35



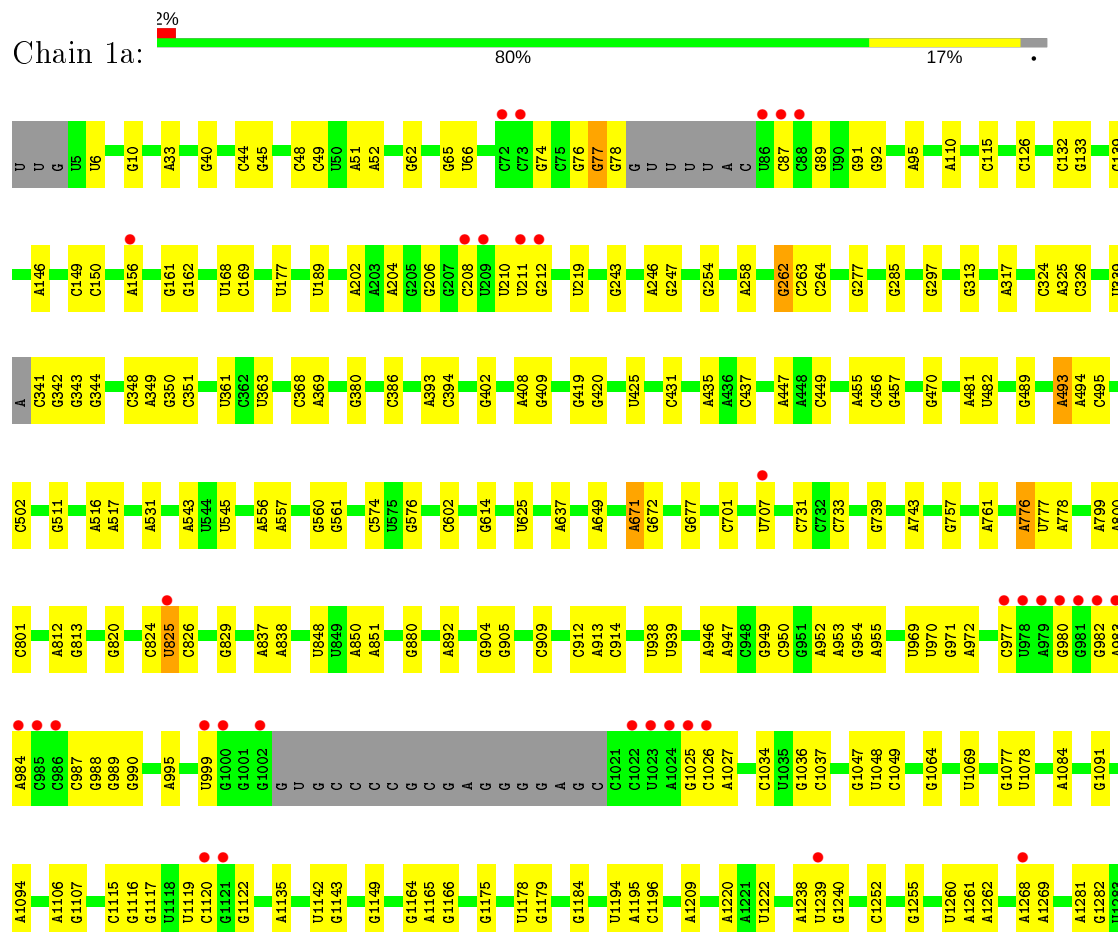
- Molecule 31: 50S ribosomal protein L36

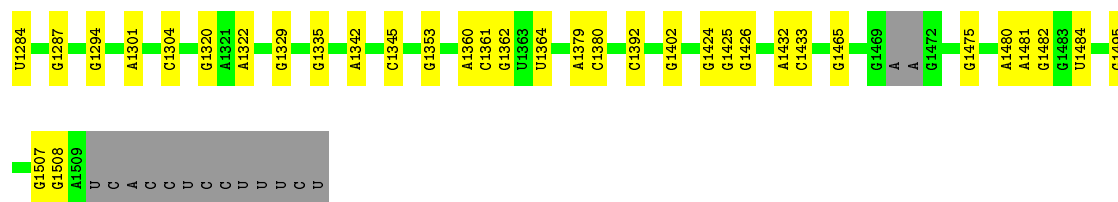


- Molecule 31: 50S ribosomal protein L36

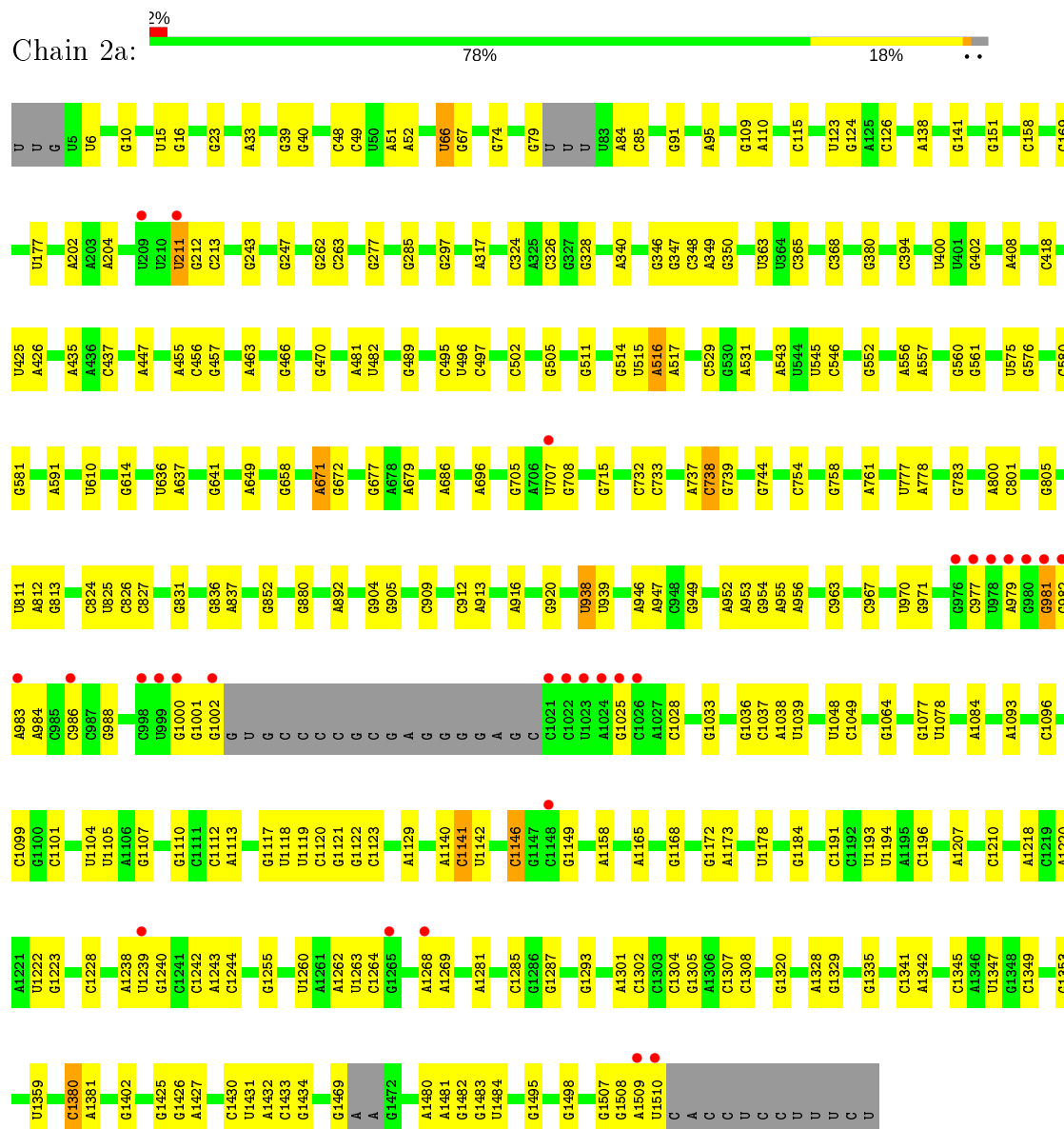


- Molecule 32: 16S Ribosomal RNA

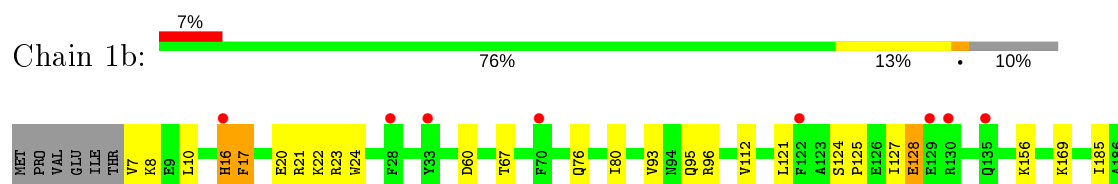


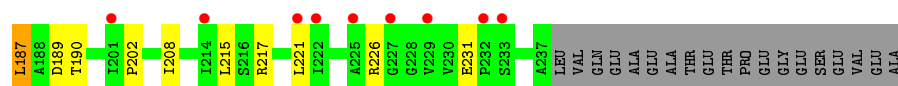


• Molecule 32: 16S Ribosomal RNA

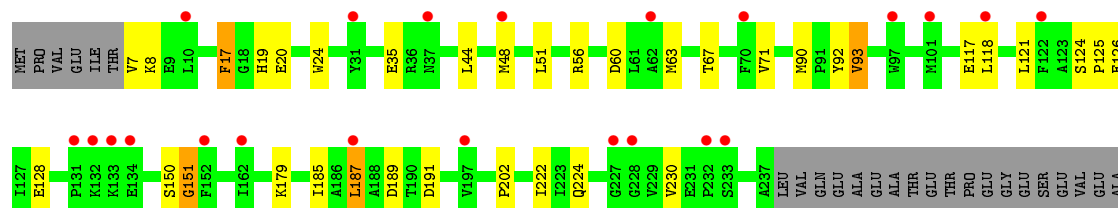
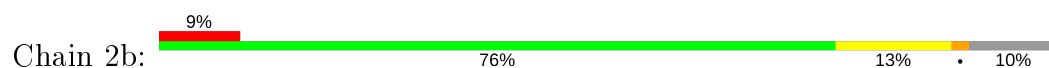


• Molecule 33: 30S ribosomal protein S2

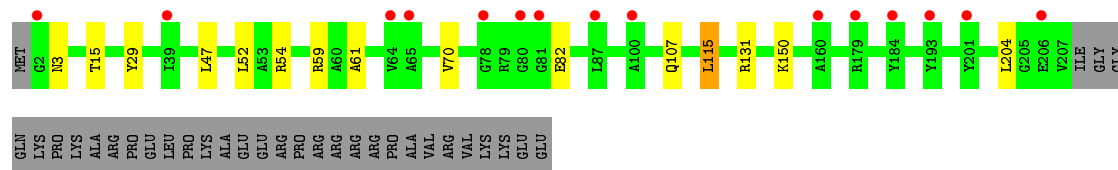
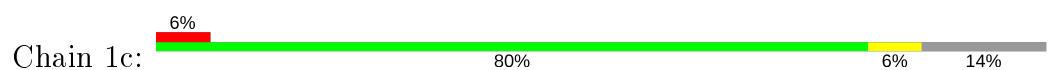




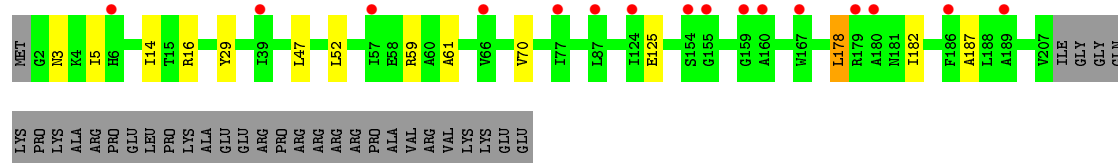
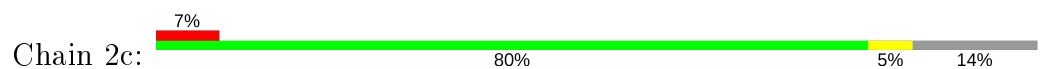
- Molecule 33: 30S ribosomal protein S2



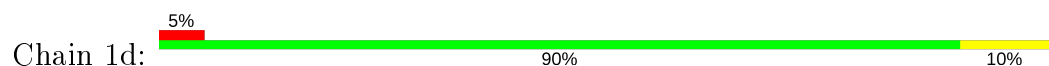
- Molecule 34: 30S ribosomal protein S3



- Molecule 34: 30S ribosomal protein S3



- Molecule 35: 30S ribosomal protein S4




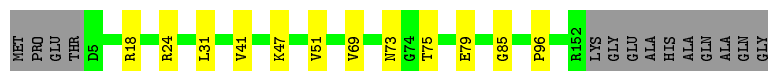
- Molecule 35: 30S ribosomal protein S4




- Molecule 36: 30S ribosomal protein S5



Chain 1e: 



- Molecule 36: 30S ribosomal protein S5

Chain 2e: 



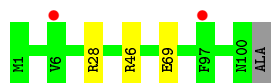
- Molecule 37: 30S ribosomal protein S6

Chain 1f: 

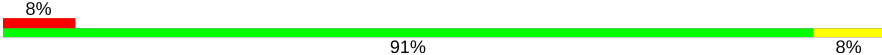


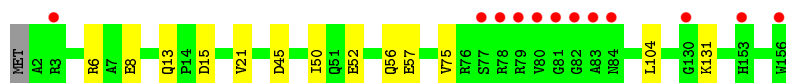
- Molecule 37: 30S ribosomal protein S6

Chain 2f: 



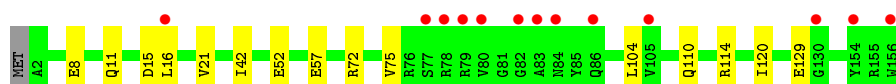
- Molecule 38: 30S ribosomal protein S7

Chain 1g: 



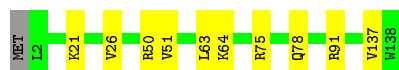
- Molecule 38: 30S ribosomal protein S7

Chain 2g: 

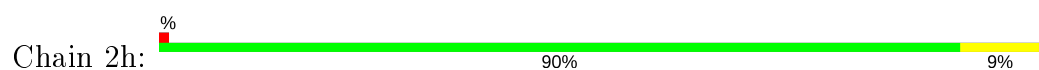


- Molecule 39: 30S ribosomal protein S8

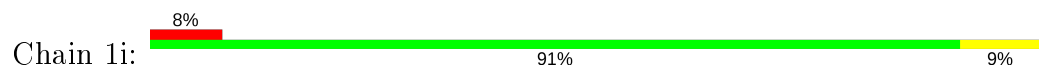
Chain 1h: 



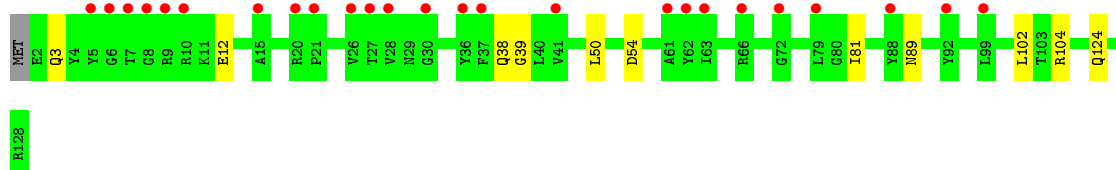
- Molecule 39: 30S ribosomal protein S8



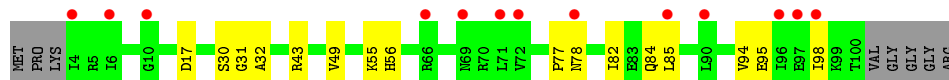
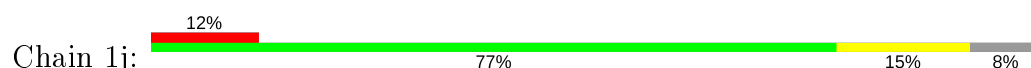
- Molecule 40: 30S ribosomal protein S9



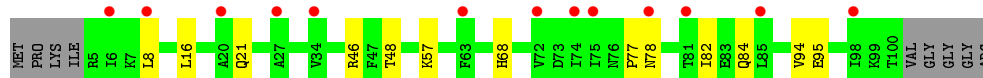
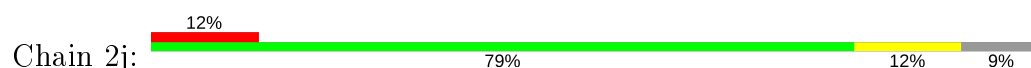
- Molecule 40: 30S ribosomal protein S9



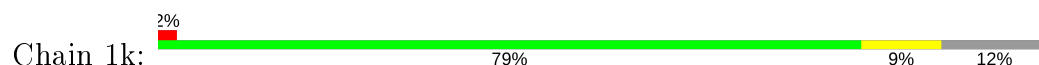
- Molecule 41: 30S ribosomal protein S10



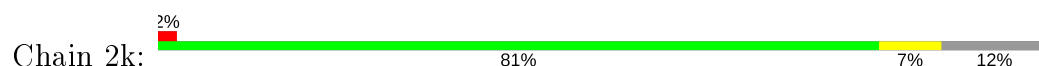
- Molecule 41: 30S ribosomal protein S10

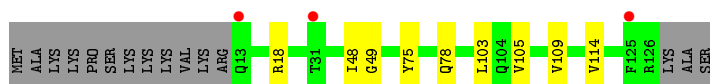


- Molecule 42: 30S ribosomal protein S11

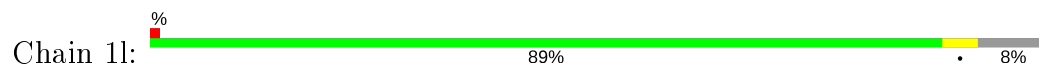


- Molecule 42: 30S ribosomal protein S11





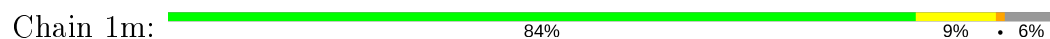
- Molecule 43: 30S ribosomal protein S12



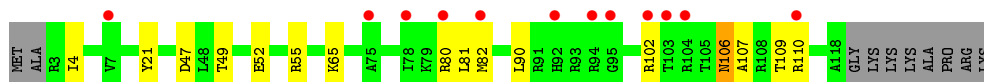
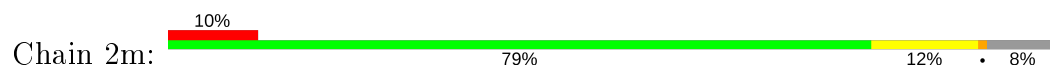
- Molecule 43: 30S ribosomal protein S12



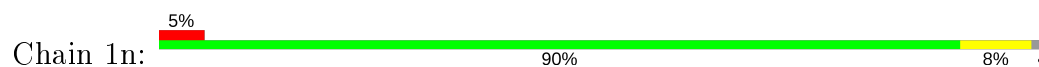
- Molecule 44: 30S ribosomal protein S13



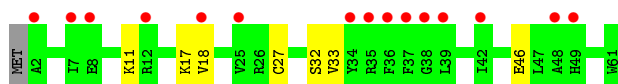
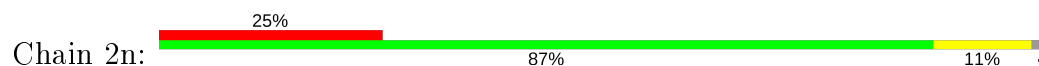
- Molecule 44: 30S ribosomal protein S13



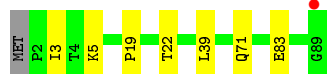
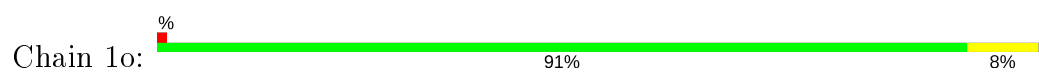
- Molecule 45: 30S ribosomal protein S14 type Z



- Molecule 45: 30S ribosomal protein S14 type Z



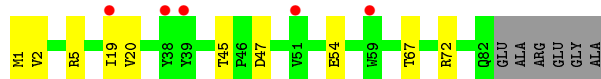
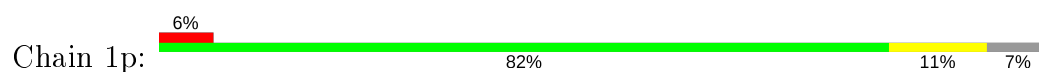
- Molecule 46: 30S ribosomal protein S15



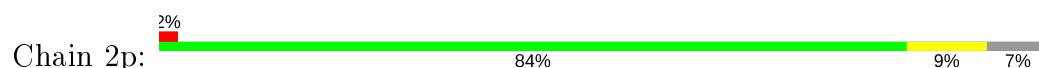
- Molecule 46: 30S ribosomal protein S15



- Molecule 47: 30S ribosomal protein S16



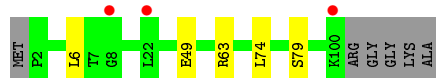
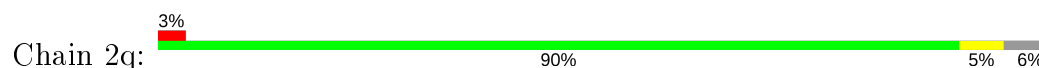
- Molecule 47: 30S ribosomal protein S16



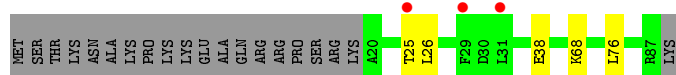
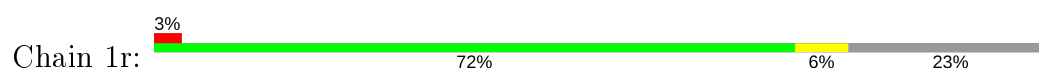
- Molecule 48: 30S ribosomal protein S17



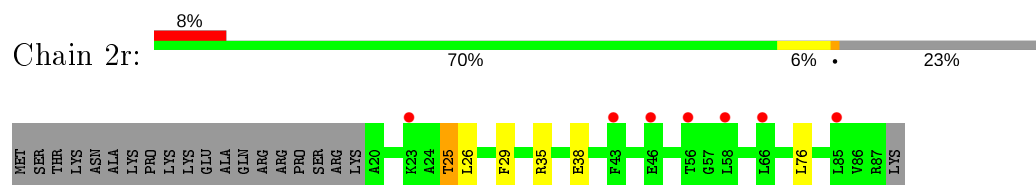
- Molecule 48: 30S ribosomal protein S17



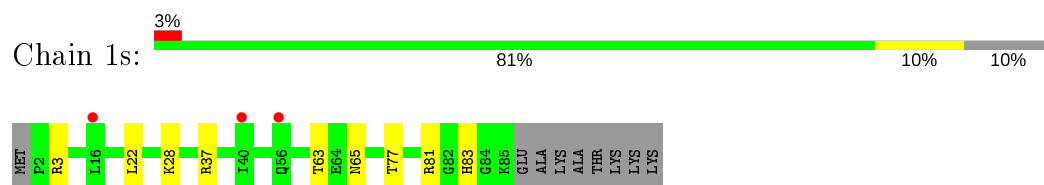
- Molecule 49: 30S ribosomal protein S18



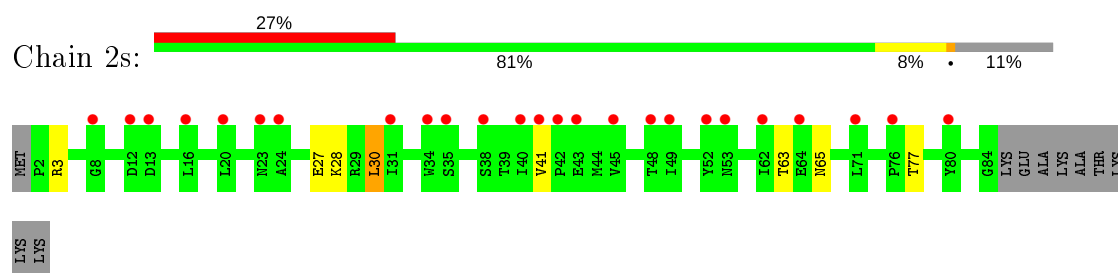
- Molecule 49: 30S ribosomal protein S18



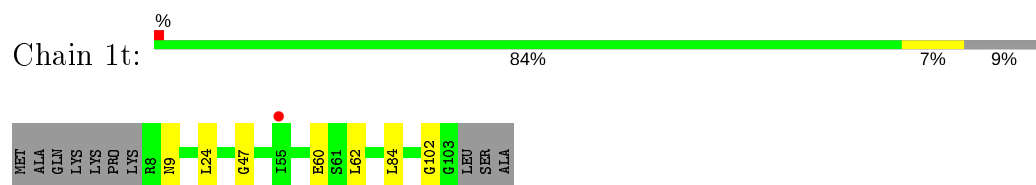
- Molecule 50: 30S ribosomal protein S19



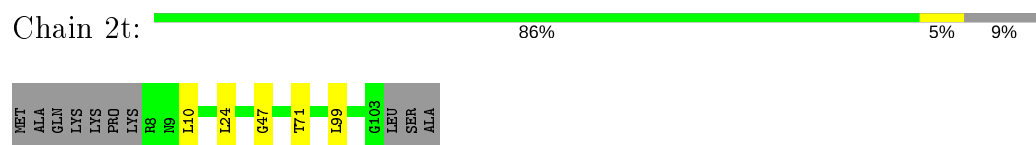
- Molecule 50: 30S ribosomal protein S19



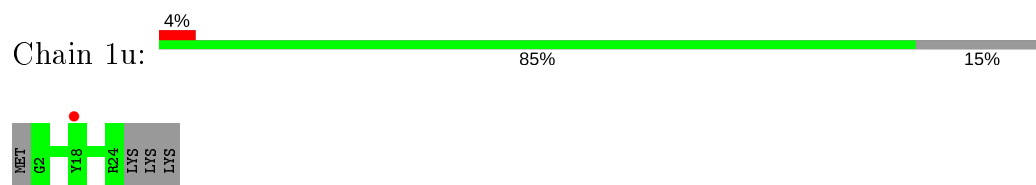
- Molecule 51: 30S ribosomal protein S20



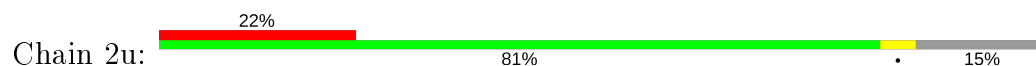
- Molecule 51: 30S ribosomal protein S20

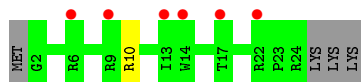


- Molecule 52: 30S ribosomal protein Thx



- Molecule 52: 30S ribosomal protein Thx

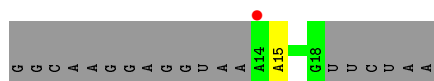




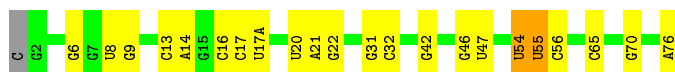
- Molecule 53: mRNA



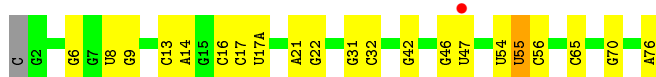
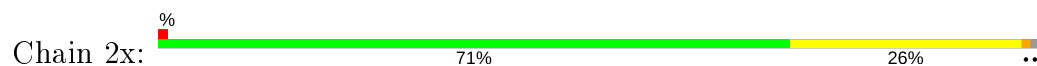
- Molecule 53: mRNA



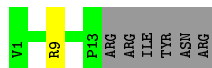
- Molecule 54: P-site tRNA



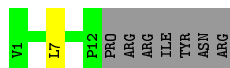
- Molecule 54: P-site tRNA



- Molecule 55: Oncocin 10wt



- Molecule 55: Oncocin 10wt



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	209.83Å 450.81Å 622.72Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.62 – 2.80 49.62 – 2.80	Depositor EDS
% Data completeness (in resolution range)	99.1 (49.62-2.80) 99.0 (49.62-2.80)	Depositor EDS
$R_{merge}$	0.22	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.20 (at 2.81Å)	Xtriage
Refinement program	PHENIX	Depositor
R, $R_{free}$	0.215 , 0.268 0.215 , 0.268	Depositor DCC
$R_{free}$ test set	71167 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	56.8	Xtriage
Anisotropy	0.225	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.28 , 59.8	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.42$ , $\langle L^2 \rangle = 0.24$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.92	EDS
Total number of atoms	288674	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	58.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.67% 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: 5MU, ZN, SF4, MG, 5MC, 4SU, PSU

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	0.58	6/66249 (0.0%)	0.96	66/103407 (0.1%)
1	2A	0.46	2/67298 (0.0%)	0.94	47/105044 (0.0%)
2	1B	0.46	0/2877	0.86	0/4488
2	2B	0.52	0/2878	0.95	1/4490 (0.0%)
3	1D	0.41	0/2186	0.56	0/2944
3	2D	0.36	0/2192	0.56	0/2951
4	1E	0.41	0/1592	0.55	0/2149
4	2E	0.36	0/1592	0.56	0/2149
5	1F	0.39	0/1619	0.56	0/2193
5	2F	0.35	0/1615	0.57	0/2188
6	1G	0.31	0/1450	0.57	1/1959 (0.1%)
6	2G	0.35	0/1449	0.58	0/1958
7	1H	0.35	0/1356	0.56	1/1834 (0.1%)
7	2H	0.34	0/1356	0.55	0/1834
8	1I	0.32	0/1100	0.57	0/1501
8	2I	0.30	0/1076	0.54	0/1471
9	1N	0.38	0/1144	0.53	0/1543
9	2N	0.34	0/1144	0.55	0/1543
10	1O	0.40	0/943	0.57	1/1269 (0.1%)
10	2O	0.36	0/943	0.60	1/1269 (0.1%)
11	1P	0.38	0/1156	0.60	0/1537
11	2P	0.36	0/1152	0.59	1/1533 (0.1%)
12	1Q	0.40	0/1143	0.56	0/1527
12	2Q	0.36	0/1143	0.56	0/1527
13	1R	0.39	0/982	0.63	1/1312 (0.1%)
13	2R	0.33	0/982	0.56	0/1312
14	1S	0.36	0/887	0.56	0/1180
14	2S	0.35	0/880	0.56	0/1172
15	1T	0.36	0/1105	0.54	0/1477
15	2T	0.34	0/1097	0.53	0/1468
16	1U	0.45	0/977	0.54	0/1301
16	2U	0.38	0/977	0.54	1/1301 (0.1%)



Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
17	1V	0.39	0/782	0.57	0/1049
17	2V	0.37	0/782	0.52	0/1049
18	1W	0.42	0/897	0.56	0/1205
18	2W	0.36	0/897	0.56	0/1205
19	1X	0.40	0/764	0.53	0/1025
19	2X	0.37	0/764	0.59	1/1025 (0.1%)
20	1Y	0.40	0/819	0.57	0/1095
20	2Y	0.35	0/819	0.57	0/1095
21	1Z	0.32	0/1502	0.52	0/2041
21	2Z	0.35	0/1486	0.53	0/2022
22	10	0.42	0/606	0.59	0/808
22	20	0.33	0/606	0.54	0/808
23	11	0.37	0/762	0.54	0/1014
23	21	0.34	0/762	0.52	0/1014
24	12	0.35	0/590	0.53	0/781
24	22	0.33	0/590	0.50	0/781
25	13	0.38	0/474	0.56	0/635
25	23	0.30	0/469	0.52	0/630
26	14	0.37	0/571	0.65	0/768
26	24	0.35	0/545	0.68	0/737
27	15	0.40	0/469	0.65	0/635
27	25	0.32	0/469	0.55	0/635
28	16	0.38	0/460	0.55	0/613
28	26	0.35	0/456	0.50	0/608
29	17	0.43	0/426	0.55	0/561
29	27	0.37	0/426	0.54	0/561
30	18	0.41	0/525	0.59	0/691
30	28	0.35	0/525	0.54	0/691
31	19	0.40	0/310	0.51	0/407
31	29	0.38	0/310	0.61	0/407
32	1a	0.40	0/35537	0.89	16/55456 (0.0%)
32	2a	0.38	0/35680	0.89	31/55681 (0.1%)
33	1b	0.32	0/1820	0.56	1/2468 (0.0%)
33	2b	2.73	8/1728 (0.5%)	0.72	4/2352 (0.2%)
34	1c	0.29	0/1504	0.52	1/2047 (0.0%)
34	2c	0.32	0/1435	0.54	1/1960 (0.1%)
35	1d	0.31	0/1648	0.52	0/2222
35	2d	0.31	0/1659	0.54	0/2230
36	1e	0.30	0/1145	0.54	0/1543
36	2e	0.30	0/1111	0.56	0/1504
37	1f	0.32	0/819	0.53	0/1111
37	2f	0.30	0/830	0.51	0/1125
38	1g	0.30	0/1198	0.47	0/1613

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
38	2g	0.30	0/1185	0.47	0/1602
39	1h	0.29	0/1108	0.51	0/1494
39	2h	0.29	0/1094	0.52	0/1478
40	1i	0.31	0/995	0.54	0/1339
40	2i	0.33	0/949	0.56	0/1284
41	1j	0.31	0/695	0.56	0/950
41	2j	0.31	0/690	0.58	0/943
42	1k	0.29	0/840	0.52	0/1138
42	2k	0.30	0/844	0.52	0/1145
43	1l	0.31	0/936	0.52	0/1263
43	2l	0.32	0/934	0.59	1/1262 (0.1%)
44	1m	0.28	0/933	0.55	0/1254
44	2m	0.32	0/913	0.55	0/1230
45	1n	0.33	0/491	0.56	0/653
45	2n	0.31	0/467	0.47	0/624
46	1o	0.31	0/726	0.51	0/970
46	2o	0.30	0/739	0.51	0/985
47	1p	0.27	0/686	0.53	0/926
47	2p	0.31	0/693	0.54	0/935
48	1q	0.32	0/824	0.53	0/1105
48	2q	0.32	0/836	0.51	0/1117
49	1r	0.31	0/560	0.55	0/746
49	2r	0.32	0/560	0.54	0/746
50	1s	0.29	0/657	0.59	0/890
50	2s	0.33	0/661	0.61	0/893
51	1t	0.29	0/714	0.60	0/948
51	2t	0.29	0/733	0.49	0/969
52	1u	0.28	0/191	0.50	0/252
52	2u	0.33	0/203	0.56	0/266
53	1v	0.58	0/122	1.23	0/188
53	2v	0.54	0/122	1.09	0/188
54	1x	0.57	2/1725 (0.1%)	1.16	17/2689 (0.6%)
54	2x	0.56	0/1725	1.17	13/2689 (0.5%)
55	1z	0.46	0/114	0.77	0/158
55	2z	0.39	0/106	0.51	0/146
All	All	0.49	18/306288 (0.0%)	0.85	207/458204 (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
5	2F	0	1

All (18) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
33	2b	92	TYR	CD1-CE1	59.29	2.28	1.39
33	2b	92	TYR	CD2-CE2	53.39	2.19	1.39
33	2b	92	TYR	CE2-CZ	41.90	1.93	1.38
33	2b	92	TYR	CE1-CZ	41.71	1.92	1.38
33	2b	92	TYR	CG-CD1	33.77	1.83	1.39
33	2b	92	TYR	CG-CD2	32.09	1.80	1.39
33	2b	151	GLY	N-CA	22.68	1.80	1.46
33	2b	150	SER	C-N	10.43	1.51	1.33
1	1A	1187	A	N9-C4	-7.08	1.33	1.37
1	1A	552	A	N9-C4	-6.81	1.33	1.37
54	1x	22	G	N7-C5	6.37	1.43	1.39
1	2A	552	A	N9-C4	-6.03	1.34	1.37
54	1x	14	A	N7-C5	-5.89	1.35	1.39
1	1A	2298	A	N9-C4	-5.80	1.34	1.37
1	1A	1066	A	N9-C4	-5.34	1.34	1.37
1	1A	1934	A	N9-C4	5.24	1.41	1.37
1	1A	353	A	N9-C4	-5.15	1.34	1.37
1	2A	1187	A	N9-C4	-5.02	1.34	1.37

All (207) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
33	2b	150	SER	C-N-CA	16.53	157.01	122.30
54	1x	46	G	C6-N1-C2	-10.98	118.51	125.10
1	1A	552	A	C2-N3-C4	-10.97	105.11	110.60
54	2x	14	A	C4-C5-C6	9.84	121.92	117.00
1	1A	847	G	O5'-P-OP2	-9.71	96.96	105.70
54	2x	46	G	C6-N1-C2	-9.65	119.31	125.10
54	1x	14	A	C4-C5-C6	9.54	121.77	117.00
54	1x	14	A	C5-N7-C8	8.92	108.36	103.90
33	2b	151	GLY	N-CA-C	8.87	135.27	113.10
1	1A	1066	A	C2-N3-C4	-8.84	106.18	110.60
32	2a	1141	C	C2-N1-C1'	8.74	128.41	118.80
1	2A	552	A	C2-N3-C4	-8.66	106.27	110.60
32	2a	1141	C	N1-C2-O2	8.61	124.07	118.90
1	2A	1109	C	C2-N1-C1'	8.53	128.18	118.80
54	2x	14	A	C5-N7-C8	8.42	108.11	103.90
1	1A	552	A	N3-C4-N9	-8.40	120.68	127.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	2a	1380	C	N1-C2-O2	8.28	123.87	118.90
1	1A	353	A	C2-N3-C4	-8.23	106.48	110.60
1	1A	552	A	N3-C4-C5	8.21	132.55	126.80
1	2A	2324	C	N1-C2-O2	8.15	123.79	118.90
1	1A	2027	C	O5'-P-OP1	-8.12	98.39	105.70
32	2a	1380	C	C2-N1-C1'	8.12	127.73	118.80
54	1x	22	G	C5-N7-C8	-8.05	100.27	104.30
54	2x	22	G	C5-N7-C8	-7.96	100.32	104.30
1	1A	536	G	O4'-C1'-N9	7.89	114.51	108.20
1	1A	1187	A	C2-N3-C4	-7.81	106.69	110.60
1	1A	11	U	C2-N1-C1'	7.68	126.92	117.70
54	1x	46	G	C5-C6-N1	7.67	115.33	111.50
1	1A	1806	G	O5'-P-OP2	-7.66	98.81	105.70
1	1A	138	A	N7-C8-N9	7.50	117.55	113.80
1	2A	2324	C	N3-C2-O2	-7.42	116.71	121.90
1	1A	214	G	O4'-C1'-N9	7.33	114.06	108.20
1	2A	300	C	C2-N1-C1'	7.29	126.82	118.80
1	1A	989	A	C5-N7-C8	-7.28	100.26	103.90
54	1x	22	G	C4-C5-C6	-7.26	114.44	118.80
1	1A	597	A	O5'-P-OP1	-7.18	99.23	105.70
1	2A	300	C	N1-C2-O2	7.17	123.20	118.90
54	2x	14	A	C5-C6-N1	-7.11	114.14	117.70
19	2X	57	LEU	CA-CB-CG	7.11	131.65	115.30
1	1A	2083	A	O4'-C1'-N9	7.08	113.87	108.20
1	1A	2298	A	C2-N3-C4	-7.07	107.07	110.60
1	2A	2324	C	C2-N1-C1'	6.99	126.49	118.80
32	1a	341	C	N1-C2-O2	6.93	123.06	118.90
54	1x	22	G	N3-C4-N9	-6.90	121.86	126.00
54	1x	22	G	N1-C6-O6	-6.86	115.78	119.90
32	2a	1380	C	N3-C2-O2	-6.83	117.12	121.90
32	1a	341	C	C6-N1-C2	-6.79	117.58	120.30
1	1A	138	A	C8-N9-C4	-6.77	103.09	105.80
1	2A	2484	U	C2-N1-C1'	6.77	125.82	117.70
1	2A	552	A	N3-C4-C5	6.73	131.51	126.80
1	2A	536	G	O4'-C1'-N9	6.73	113.58	108.20
32	1a	341	C	C2-N1-C1'	6.71	126.19	118.80
1	1A	1187	A	N3-C4-C5	6.68	131.48	126.80
32	1a	87	C	N1-C2-O2	6.67	122.90	118.90
32	2a	1380	C	C6-N1-C2	-6.62	117.65	120.30
1	2A	2484	U	N1-C2-O2	6.56	127.39	122.80
54	1x	14	A	C5-C6-N1	-6.53	114.44	117.70
1	2A	2565	U	O5'-P-OP1	-6.52	99.83	105.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	2a	1141	C	N3-C2-O2	-6.50	117.35	121.90
32	2a	982	G	N3-C4-C5	-6.42	125.39	128.60
1	2A	787	G	O5'-P-OP1	-6.41	99.94	105.70
43	2l	29	GLY	N-CA-C	-6.37	97.18	113.10
1	2A	552	A	N3-C4-N9	-6.35	122.32	127.40
54	2x	46	G	C5-C6-N1	6.34	114.67	111.50
1	1A	2083	A	C2-N3-C4	-6.33	107.44	110.60
54	2x	46	G	N3-C2-N2	-6.33	115.47	119.90
54	1x	46	G	C5-C6-O6	-6.32	124.81	128.60
1	1A	1187	A	N3-C4-N9	-6.31	122.35	127.40
1	1A	1248	A	O4'-C1'-N9	6.30	113.24	108.20
32	1a	825	U	C5-C6-N1	6.26	125.83	122.70
1	2A	1358	U	C2-N1-C1'	6.24	125.19	117.70
1	1A	138	A	C5-N7-C8	-6.23	100.78	103.90
32	2a	66	U	P-O3'-C3'	6.23	127.17	119.70
32	2a	738	C	C2-N1-C1'	6.22	125.64	118.80
1	1A	1066	A	C5-N7-C8	-6.21	100.80	103.90
1	1A	1066	A	N7-C8-N9	6.17	116.89	113.80
1	2A	1109	C	C5-C6-N1	6.16	124.08	121.00
1	1A	2014	U	O5'-P-OP1	-6.16	100.16	105.70
1	2A	1187	A	C2-N3-C4	-6.14	107.53	110.60
1	1A	353	A	N1-C2-N3	6.09	132.35	129.30
32	2a	1141	C	C6-N1-C2	-6.08	117.87	120.30
32	1a	87	C	C2-N3-C4	6.08	122.94	119.90
1	1A	830	A	P-O3'-C3'	6.03	126.94	119.70
1	2A	1109	C	N1-C2-O2	6.02	122.51	118.90
1	2A	2814	C	C6-N1-C2	-6.00	117.90	120.30
1	1A	1067	G	N3-C4-N9	-5.97	122.42	126.00
54	2x	22	G	C4-C5-C6	-5.97	115.22	118.80
1	1A	1957	A	O4'-C1'-N9	5.94	112.95	108.20
32	2a	1207	A	C5-C6-N6	5.94	128.45	123.70
1	2A	2013	G	P-O3'-C3'	5.93	126.82	119.70
1	2A	1109	C	C6-N1-C1'	-5.91	113.71	120.80
32	2a	1141	C	C6-N1-C1'	-5.91	113.71	120.80
1	1A	977	A	C5-N7-C8	-5.90	100.95	103.90
32	2a	938	U	C2-N1-C1'	5.88	124.76	117.70
1	1A	1067	G	N3-C2-N2	-5.88	115.79	119.90
1	2A	409	U	O4'-C1'-N1	5.85	112.88	108.20
1	1A	1538	C	C2-N1-C1'	5.85	125.23	118.80
54	2x	14	A	C4-N9-C1'	5.84	136.81	126.30
1	1A	1744	A	C2-N3-C4	-5.83	107.69	110.60
54	1x	22	G	C8-N9-C1'	5.82	134.56	127.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1A	2700	U	N3-C2-O2	-5.75	118.17	122.20
1	2A	2484	U	N3-C2-O2	-5.74	118.18	122.20
1	1A	1066	A	N1-C2-N3	5.72	132.16	129.30
1	1A	2013	G	P-O3'-C3'	5.69	126.53	119.70
32	1a	341	C	N3-C2-O2	-5.69	117.92	121.90
54	1x	22	G	N7-C8-N9	5.68	115.94	113.10
10	1O	8	LEU	CA-CB-CG	5.68	128.36	115.30
32	1a	361	U	C2-N1-C1'	-5.68	110.89	117.70
1	2A	1109	C	C6-N1-C2	-5.64	118.04	120.30
1	2A	989	A	N1-C6-N6	5.62	121.97	118.60
1	1A	1218	A	P-O3'-C3'	5.62	126.44	119.70
32	2a	738	C	N1-C2-O2	5.62	122.27	118.90
32	2a	1146	C	N1-C2-O2	5.59	122.25	118.90
32	2a	982	G	C4-N9-C1'	5.59	133.77	126.50
1	1A	138	A	O4'-C1'-N9	5.59	112.67	108.20
32	1a	341	C	C5-C6-N1	5.58	123.79	121.00
1	1A	409	U	C2-N1-C1'	-5.56	111.03	117.70
54	2x	14	A	C8-N9-C1'	-5.55	117.71	127.70
34	1c	115	LEU	CA-CB-CG	5.54	128.03	115.30
54	1x	22	G	C6-C5-N7	5.53	133.72	130.40
32	2a	1207	A	N1-C6-N6	-5.53	115.28	118.60
32	1a	262	G	P-O3'-C3'	5.52	126.32	119.70
33	1b	187	LEU	CA-CB-CG	5.52	127.99	115.30
1	2A	636	U	N3-C2-O2	-5.51	118.34	122.20
32	1a	77	G	C5-C6-O6	5.50	131.90	128.60
1	1A	2449	U	OP2-P-O3'	5.46	117.22	105.20
32	2a	514	G	C4-N9-C1'	5.46	133.60	126.50
33	2b	118	LEU	CA-CB-CG	5.46	127.86	115.30
32	2a	1349	C	N1-C2-O2	5.45	122.17	118.90
1	1A	790	G	O5'-P-OP2	-5.45	100.80	105.70
1	1A	1044	U	O5'-P-OP2	-5.43	100.81	105.70
32	2a	516	A	OP1-P-O3'	5.41	117.10	105.20
1	1A	398	G	O4'-C1'-N9	5.39	112.51	108.20
1	2A	2905	U	N1-C2-O2	5.39	126.58	122.80
1	1A	831	G	O5'-P-OP2	-5.37	100.87	105.70
1	1A	1404	A	C2-N3-C4	5.37	113.29	110.60
34	2c	178	LEU	CA-CB-CG	5.37	127.65	115.30
32	1a	776	A	O4'-C1'-N9	5.35	112.48	108.20
1	1A	2265	C	N1-C2-O2	-5.35	115.69	118.90
32	2a	1146	C	C2-N1-C1'	5.35	124.68	118.80
1	2A	2286	C	OP1-P-O3'	5.35	116.96	105.20
1	1A	989	A	C4-C5-N7	5.34	113.37	110.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	2a	981	G	N1-C6-O6	-5.34	116.69	119.90
1	2A	1358	U	C5-C6-N1	5.34	125.37	122.70
32	1a	77	G	N1-C6-O6	-5.33	116.70	119.90
1	2A	2905	U	C2-N1-C1'	5.33	124.09	117.70
32	2a	671	A	P-O3'-C3'	5.33	126.09	119.70
1	2A	1314	A	N1-C6-N6	5.31	121.79	118.60
1	2A	1359	C	C2-N1-C1'	5.30	124.63	118.80
1	1A	989	A	C2-N3-C4	-5.29	107.95	110.60
6	1G	82	LEU	CA-CB-CG	5.29	127.47	115.30
1	2A	1311	G	C8-N9-C4	5.29	108.52	106.40
32	2a	1380	C	C6-N1-C1'	-5.27	114.47	120.80
1	1A	989	A	N1-C6-N6	5.27	121.76	118.60
1	2A	1693	G	O4'-C1'-N9	-5.25	104.00	108.20
1	1A	891	G	O4'-C1'-N9	5.25	112.40	108.20
1	1A	2857	G	O4'-C1'-N9	5.24	112.39	108.20
1	2A	1248	A	O4'-C1'-N9	5.24	112.39	108.20
1	1A	138	A	C6-C5-N7	-5.24	128.63	132.30
1	1A	2346	A	O4'-C1'-N9	5.24	112.39	108.20
54	2x	22	G	C8-N9-C1'	5.23	133.81	127.00
2	2B	42	C	P-O3'-C3'	5.23	125.98	119.70
1	1A	183	A	P-O3'-C3'	5.23	125.98	119.70
32	1a	493	A	C8-N9-C4	-5.23	103.71	105.80
32	2a	732	C	P-O3'-C3'	5.22	125.96	119.70
1	1A	830	A	O4'-C1'-N9	5.21	112.37	108.20
32	2a	1025	G	C4-N9-C1'	-5.20	119.73	126.50
54	2x	22	G	C5-C6-N1	5.20	114.10	111.50
1	1A	638	G	O4'-C1'-N9	5.20	112.36	108.20
11	2P	44	GLY	C-N-CA	5.19	134.67	121.70
32	1a	969	U	P-O3'-C3'	5.18	125.91	119.70
1	2A	2083	A	N1-C6-N6	5.17	121.70	118.60
1	1A	1744	A	N1-C6-N6	5.17	121.70	118.60
1	1A	1294	U	O5'-P-OP1	-5.16	101.06	105.70
1	2A	300	C	N3-C2-O2	-5.15	118.29	121.90
13	1R	113	LEU	CA-CB-CG	5.14	127.13	115.30
1	2A	1604	A	P-O3'-C3'	5.14	125.87	119.70
54	1x	14	A	C8-N9-C1'	-5.13	118.46	127.70
7	1H	33	LEU	CA-CB-CG	5.12	127.09	115.30
54	2x	14	A	C4-C5-N7	-5.12	108.14	110.70
1	1A	792	A	O4'-C1'-N9	5.12	112.30	108.20
1	1A	1176	G	N1-C2-N2	-5.11	111.60	116.20
1	2A	300	C	C6-N1-C1'	-5.11	114.67	120.80
1	2A	1806	G	N3-C4-N9	5.10	129.06	126.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1A	2298	A	N3-C4-C5	5.10	130.37	126.80
54	1x	14	A	C4-C5-N7	-5.10	108.15	110.70
33	2b	187	LEU	CA-CB-CG	5.10	127.03	115.30
1	1A	830	A	OP1-P-O3'	5.08	116.38	105.20
32	2a	516	A	P-O3'-C3'	5.07	125.78	119.70
54	1x	22	G	C5-C6-N1	5.07	114.03	111.50
32	2a	211	U	C2-N1-C1'	5.06	123.77	117.70
1	1A	1358	U	C2-N1-C1'	5.05	123.76	117.70
1	1A	2726	G	O5'-P-OP2	-5.04	101.16	105.70
32	1a	671	A	P-O3'-C3'	5.04	125.75	119.70
1	2A	1359	C	C6-N1-C2	-5.04	118.28	120.30
1	2A	2905	U	N3-C2-O2	-5.04	118.67	122.20
1	2A	1659	A	O5'-P-OP1	-5.04	101.17	105.70
1	2A	1994	G	N1-C6-O6	-5.04	116.88	119.90
1	2A	2604	U	N3-C4-O4	-5.04	115.88	119.40
1	2A	2700	U	P-O3'-C3'	5.04	125.74	119.70
16	2U	74	LEU	CA-CB-CG	5.03	126.88	115.30
32	2a	109	G	P-O3'-C3'	5.03	125.73	119.70
54	1x	14	A	C4-N9-C1'	5.02	135.34	126.30
10	2O	8	LEU	CA-CB-CG	5.02	126.85	115.30
32	2a	982	G	C8-N9-C4	-5.02	104.39	106.40
1	2A	1302	C	C6-N1-C2	-5.02	118.29	120.30
1	1A	2514	A	N1-C2-N3	-5.00	126.80	129.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
5	2F	20	LEU	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%)	257 (94%)	16 (6%)	0	100	100
3	2D	273/276 (99%)	254 (93%)	17 (6%)	2 (1%)	22	53
4	1E	202/206 (98%)	194 (96%)	7 (4%)	1 (0%)	29	61
4	2E	202/206 (98%)	194 (96%)	7 (4%)	1 (0%)	29	61
5	1F	201/210 (96%)	189 (94%)	11 (6%)	1 (0%)	29	61
5	2F	201/210 (96%)	189 (94%)	10 (5%)	2 (1%)	15	44
6	1G	179/182 (98%)	158 (88%)	17 (10%)	4 (2%)	6	22
6	2G	179/182 (98%)	154 (86%)	20 (11%)	5 (3%)	5	17
7	1H	172/180 (96%)	162 (94%)	9 (5%)	1 (1%)	25	56
7	2H	172/180 (96%)	160 (93%)	10 (6%)	2 (1%)	13	39
8	1I	144/148 (97%)	121 (84%)	19 (13%)	4 (3%)	5	17
8	2I	144/148 (97%)	122 (85%)	20 (14%)	2 (1%)	11	34
9	1N	138/140 (99%)	136 (99%)	2 (1%)	0	100	100
9	2N	138/140 (99%)	135 (98%)	2 (1%)	1 (1%)	22	53
10	1O	120/122 (98%)	114 (95%)	6 (5%)	0	100	100
10	2O	120/122 (98%)	114 (95%)	6 (5%)	0	100	100
11	1P	147/150 (98%)	140 (95%)	6 (4%)	1 (1%)	22	53
11	2P	147/150 (98%)	139 (95%)	8 (5%)	0	100	100
12	1Q	139/141 (99%)	130 (94%)	8 (6%)	1 (1%)	22	53
12	2Q	139/141 (99%)	127 (91%)	12 (9%)	0	100	100
13	1R	116/118 (98%)	107 (92%)	9 (8%)	0	100	100
13	2R	116/118 (98%)	107 (92%)	9 (8%)	0	100	100
14	1S	108/112 (96%)	100 (93%)	7 (6%)	1 (1%)	17	46
14	2S	108/112 (96%)	98 (91%)	9 (8%)	1 (1%)	17	46
15	1T	129/146 (88%)	124 (96%)	4 (3%)	1 (1%)	19	49
15	2T	129/146 (88%)	126 (98%)	3 (2%)	0	100	100
16	1U	114/118 (97%)	114 (100%)	0	0	100	100
16	2U	114/118 (97%)	113 (99%)	1 (1%)	0	100	100
17	1V	99/101 (98%)	96 (97%)	2 (2%)	1 (1%)	15	44
17	2V	99/101 (98%)	95 (96%)	3 (3%)	1 (1%)	15	44

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
18	1W	110/113 (97%)	107 (97%)	3 (3%)	0	100	100
18	2W	110/113 (97%)	107 (97%)	3 (3%)	0	100	100
19	1X	93/96 (97%)	91 (98%)	1 (1%)	1 (1%)	14	41
19	2X	93/96 (97%)	90 (97%)	2 (2%)	1 (1%)	14	41
20	1Y	105/110 (96%)	94 (90%)	9 (9%)	2 (2%)	8	26
20	2Y	105/110 (96%)	97 (92%)	7 (7%)	1 (1%)	15	44
21	1Z	184/206 (89%)	167 (91%)	15 (8%)	2 (1%)	14	41
21	2Z	184/206 (89%)	163 (89%)	16 (9%)	5 (3%)	5	17
22	10	73/85 (86%)	72 (99%)	1 (1%)	0	100	100
22	20	73/85 (86%)	69 (94%)	4 (6%)	0	100	100
23	11	95/98 (97%)	94 (99%)	0	1 (1%)	14	41
23	21	95/98 (97%)	93 (98%)	1 (1%)	1 (1%)	14	41
24	12	68/72 (94%)	67 (98%)	1 (2%)	0	100	100
24	22	68/72 (94%)	65 (96%)	3 (4%)	0	100	100
25	13	57/60 (95%)	56 (98%)	1 (2%)	0	100	100
25	23	57/60 (95%)	54 (95%)	3 (5%)	0	100	100
26	14	67/71 (94%)	49 (73%)	10 (15%)	8 (12%)	0	1
26	24	67/71 (94%)	50 (75%)	10 (15%)	7 (10%)	0	1
27	15	57/60 (95%)	55 (96%)	2 (4%)	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%)	50 (98%)	1 (2%)	0	100	100
29	17	46/49 (94%)	46 (100%)	0	0	100	100
29	27	46/49 (94%)	45 (98%)	1 (2%)	0	100	100
30	18	62/65 (95%)	59 (95%)	3 (5%)	0	100	100
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%)	182 (80%)	36 (16%)	11 (5%)	2	7
33	2b	229/256 (90%)	187 (82%)	33 (14%)	9 (4%)	3	10
34	1c	204/239 (85%)	173 (85%)	28 (14%)	3 (2%)	10	33

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
34	2c	204/239 (85%)	166 (81%)	36 (18%)	2 (1%)	15	44
35	1d	206/209 (99%)	185 (90%)	20 (10%)	1 (0%)	29	61
35	2d	206/209 (99%)	188 (91%)	16 (8%)	2 (1%)	15	44
36	1e	146/162 (90%)	128 (88%)	15 (10%)	3 (2%)	7	23
36	2e	146/162 (90%)	130 (89%)	14 (10%)	2 (1%)	11	34
37	1f	98/101 (97%)	91 (93%)	7 (7%)	0	100	100
37	2f	98/101 (97%)	91 (93%)	7 (7%)	0	100	100
38	1g	153/156 (98%)	130 (85%)	23 (15%)	0	100	100
38	2g	153/156 (98%)	130 (85%)	23 (15%)	0	100	100
39	1h	135/138 (98%)	130 (96%)	5 (4%)	0	100	100
39	2h	135/138 (98%)	130 (96%)	4 (3%)	1 (1%)	22	53
40	1i	125/128 (98%)	106 (85%)	18 (14%)	1 (1%)	19	49
40	2i	125/128 (98%)	104 (83%)	19 (15%)	2 (2%)	9	31
41	1j	95/105 (90%)	82 (86%)	6 (6%)	7 (7%)	1	2
41	2j	94/105 (90%)	82 (87%)	9 (10%)	3 (3%)	4	13
42	1k	112/129 (87%)	100 (89%)	10 (9%)	2 (2%)	8	28
42	2k	112/129 (87%)	102 (91%)	8 (7%)	2 (2%)	8	28
43	1l	120/132 (91%)	115 (96%)	4 (3%)	1 (1%)	19	49
43	2l	120/132 (91%)	113 (94%)	7 (6%)	0	100	100
44	1m	116/126 (92%)	105 (90%)	8 (7%)	3 (3%)	5	18
44	2m	114/126 (90%)	100 (88%)	10 (9%)	4 (4%)	3	12
45	1n	58/61 (95%)	52 (90%)	5 (9%)	1 (2%)	9	29
45	2n	58/61 (95%)	53 (91%)	5 (9%)	0	100	100
46	1o	86/89 (97%)	80 (93%)	5 (6%)	1 (1%)	13	39
46	2o	86/89 (97%)	80 (93%)	4 (5%)	2 (2%)	6	21
47	1p	80/88 (91%)	65 (81%)	15 (19%)	0	100	100
47	2p	80/88 (91%)	65 (81%)	15 (19%)	0	100	100
48	1q	97/105 (92%)	88 (91%)	8 (8%)	1 (1%)	15	44
48	2q	97/105 (92%)	87 (90%)	10 (10%)	0	100	100
49	1r	66/88 (75%)	59 (89%)	6 (9%)	1 (2%)	10	33
49	2r	66/88 (75%)	62 (94%)	3 (4%)	1 (2%)	10	33

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
50	1s	82/93 (88%)	68 (83%)	14 (17%)	0	100	100
50	2s	81/93 (87%)	69 (85%)	11 (14%)	1 (1%)	13	39
51	1t	94/106 (89%)	80 (85%)	12 (13%)	2 (2%)	7	23
51	2t	94/106 (89%)	79 (84%)	13 (14%)	2 (2%)	7	23
52	1u	21/27 (78%)	20 (95%)	1 (5%)	0	100	100
52	2u	21/27 (78%)	20 (95%)	1 (5%)	0	100	100
55	1z	11/19 (58%)	10 (91%)	0	1 (9%)	1	1
55	2z	10/19 (53%)	10 (100%)	0	0	100	100
All	All	11431/12166 (94%)	10441 (91%)	856 (8%)	134 (1%)	13	39

All (134) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
6	1G	126	ASP
8	1I	106	GLY
21	1Z	93	ASP
23	1I	3	LYS
26	14	45	GLY
26	14	48	ARG
26	14	50	VAL
26	14	53	GLU
33	1b	16	HIS
33	1b	121	LEU
33	1b	125	PRO
34	1c	107	GLN
40	1i	54	ASP
41	1j	55	LYS
41	1j	56	HIS
42	1k	49	GLY
44	1m	4	ILE
45	1n	3	ARG
48	1q	68	ARG
6	2G	14	GLU
6	2G	47	LYS
6	2G	51	ARG
6	2G	126	ASP
7	2H	55	PRO
7	2H	126	PRO
8	2I	10	GLU

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Mol	Chain	Res	Type
17	2V	79	VAL
21	2Z	93	ASP
21	2Z	128	VAL
21	2Z	135	GLU
26	24	45	GLY
26	24	62	ARG
26	24	68	ARG
33	2b	17	PHE
33	2b	93	VAL
33	2b	124	SER
40	2i	54	ASP
42	2k	49	GLY
44	2m	106	ASN
51	2t	99	LEU
5	1F	130	ALA
7	1H	126	PRO
12	1Q	58	PHE
14	1S	60	GLY
17	1V	79	VAL
19	1X	94	GLY
33	1b	17	PHE
33	1b	95	GLN
33	1b	128	GLU
41	1j	31	GLY
43	1l	29	GLY
5	2F	130	ALA
6	2G	81	LYS
19	2X	94	GLY
20	2Y	54	LYS
26	24	54	GLY
33	2b	121	LEU
33	2b	125	PRO
36	2e	37	ARG
44	2m	4	ILE
44	2m	21	TYR
44	2m	107	ALA
6	1G	47	LYS
6	1G	51	ARG
8	1I	42	SER
8	1I	73	GLU
26	14	62	ARG
33	1b	22	LYS

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Mol	Chain	Res	Type
33	1b	23	ARG
33	1b	231	GLU
41	1j	77	PRO
44	1m	106	ASN
51	1t	47	GLY
9	2N	2	LYS
23	21	3	LYS
26	24	47	GLN
40	2i	39	GLY
41	2j	77	PRO
41	2j	78	ASN
49	2r	25	THR
4	1E	52	LEU
20	1Y	53	PRO
20	1Y	54	LYS
26	14	49	PHE
33	1b	20	GLU
44	1m	21	TYR
49	1r	25	THR
55	1z	9	ARG
4	2E	52	LEU
5	2F	18	ARG
8	2I	42	SER
26	24	63	TYR
34	2c	61	ALA
34	2c	187	ALA
35	2d	47	ARG
50	2s	30	LEU
51	2t	47	GLY
8	1I	107	VAL
21	1Z	101	PRO
26	14	46	GLN
26	14	47	GLN
33	1b	202	PRO
34	1c	3	ASN
41	1j	78	ASN
41	1j	82	ILE
3	2D	3	VAL
14	2S	84	GLN
21	2Z	101	PRO
21	2Z	127	LYS
33	2b	20	GLU

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Mol	Chain	Res	Type
33	2b	202	PRO
33	2b	230	VAL
35	2d	45	GLN
46	2o	88	ARG
6	1G	50	ALA
34	1c	61	ALA
36	1e	69	VAL
41	1j	32	ALA
36	2e	69	VAL
46	2o	19	PRO
35	1d	8	VAL
3	2D	125	ILE
26	24	50	VAL
36	1e	85	GLY
42	1k	105	VAL
42	2k	105	VAL
46	1o	19	PRO
33	2b	151	GLY
41	2j	82	ILE
11	1P	122	PRO
15	1T	37	GLY
36	1e	96	PRO
51	1t	102	GLY
39	2h	73	ASP

### 5.3.2 Protein sidechains ⓘ

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%)	189 (88%)	26 (12%)	5	15
3	2D	216/218 (99%)	194 (90%)	22 (10%)	7	22
4	1E	164/166 (99%)	144 (88%)	20 (12%)	5	15
4	2E	164/166 (99%)	149 (91%)	15 (9%)	9	27
5	1F	160/166 (96%)	146 (91%)	14 (9%)	10	29

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
5	2F	159/166 (96%)	146 (92%)	13 (8%)	11	33
6	1G	143/156 (92%)	130 (91%)	13 (9%)	9	27
6	2G	142/156 (91%)	122 (86%)	20 (14%)	3	10
7	1H	144/148 (97%)	134 (93%)	10 (7%)	15	41
7	2H	144/148 (97%)	127 (88%)	17 (12%)	5	16
8	1I	110/124 (89%)	90 (82%)	20 (18%)	1	5
8	2I	104/124 (84%)	90 (86%)	14 (14%)	4	11
9	1N	118/119 (99%)	104 (88%)	14 (12%)	5	16
9	2N	118/119 (99%)	103 (87%)	15 (13%)	4	14
10	1O	100/100 (100%)	93 (93%)	7 (7%)	15	40
10	2O	100/100 (100%)	95 (95%)	5 (5%)	24	56
11	1P	116/116 (100%)	101 (87%)	15 (13%)	4	13
11	2P	115/116 (99%)	98 (85%)	17 (15%)	3	9
12	1Q	111/111 (100%)	104 (94%)	7 (6%)	18	46
12	2Q	111/111 (100%)	104 (94%)	7 (6%)	18	46
13	1R	101/101 (100%)	87 (86%)	14 (14%)	3	11
13	2R	101/101 (100%)	90 (89%)	11 (11%)	6	19
14	1S	87/88 (99%)	80 (92%)	7 (8%)	12	34
14	2S	85/88 (97%)	74 (87%)	11 (13%)	4	13
15	1T	115/127 (91%)	105 (91%)	10 (9%)	10	30
15	2T	113/127 (89%)	105 (93%)	8 (7%)	14	39
16	1U	93/94 (99%)	84 (90%)	9 (10%)	8	24
16	2U	93/94 (99%)	87 (94%)	6 (6%)	17	44
17	1V	80/82 (98%)	68 (85%)	12 (15%)	3	9
17	2V	80/82 (98%)	71 (89%)	9 (11%)	6	18
18	1W	90/92 (98%)	84 (93%)	6 (7%)	16	43
18	2W	90/92 (98%)	84 (93%)	6 (7%)	16	43
19	1X	77/78 (99%)	75 (97%)	2 (3%)	46	79
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%)	78 (92%)	7 (8%)	11	33

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
21	1Z	159/179 (89%)	150 (94%)	9 (6%)	20	50
21	2Z	156/179 (87%)	144 (92%)	12 (8%)	13	35
22	10	60/67 (90%)	55 (92%)	5 (8%)	11	32
22	20	60/67 (90%)	56 (93%)	4 (7%)	16	43
23	11	80/83 (96%)	73 (91%)	7 (9%)	10	29
23	21	80/83 (96%)	74 (92%)	6 (8%)	13	37
24	12	65/67 (97%)	62 (95%)	3 (5%)	27	60
24	22	65/67 (97%)	61 (94%)	4 (6%)	18	47
25	13	51/52 (98%)	47 (92%)	4 (8%)	12	35
25	23	50/52 (96%)	45 (90%)	5 (10%)	7	22
26	14	60/63 (95%)	53 (88%)	7 (12%)	5	16
26	24	53/63 (84%)	47 (89%)	6 (11%)	6	18
27	15	50/52 (96%)	46 (92%)	4 (8%)	12	34
27	25	50/52 (96%)	46 (92%)	4 (8%)	12	34
28	16	51/52 (98%)	46 (90%)	5 (10%)	8	24
28	26	50/52 (96%)	45 (90%)	5 (10%)	7	22
29	17	41/42 (98%)	37 (90%)	4 (10%)	8	24
29	27	41/42 (98%)	40 (98%)	1 (2%)	49	81
30	18	54/55 (98%)	49 (91%)	5 (9%)	9	26
30	28	54/55 (98%)	51 (94%)	3 (6%)	21	51
31	19	34/34 (100%)	33 (97%)	1 (3%)	42	76
31	29	34/34 (100%)	33 (97%)	1 (3%)	42	76
33	1b	177/220 (80%)	149 (84%)	28 (16%)	2	8
33	2b	158/220 (72%)	132 (84%)	26 (16%)	2	7
34	1c	127/188 (68%)	115 (91%)	12 (9%)	8	26
34	2c	108/188 (57%)	96 (89%)	12 (11%)	6	19
35	1d	161/181 (89%)	142 (88%)	19 (12%)	5	16
35	2d	164/181 (91%)	149 (91%)	15 (9%)	9	27
36	1e	113/123 (92%)	104 (92%)	9 (8%)	12	34
36	2e	106/123 (86%)	94 (89%)	12 (11%)	6	18
37	1f	83/90 (92%)	78 (94%)	5 (6%)	19	48

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
37	2f	86/90 (96%)	83 (96%)	3 (4%)	36	70
38	1g	111/127 (87%)	98 (88%)	13 (12%)	5	16
38	2g	107/127 (84%)	92 (86%)	15 (14%)	3	11
39	1h	114/119 (96%)	104 (91%)	10 (9%)	10	29
39	2h	111/119 (93%)	99 (89%)	12 (11%)	6	19
40	1i	89/99 (90%)	79 (89%)	10 (11%)	6	18
40	2i	80/99 (81%)	71 (89%)	9 (11%)	6	18
41	1j	60/92 (65%)	51 (85%)	9 (15%)	3	9
41	2j	62/92 (67%)	52 (84%)	10 (16%)	2	7
42	1k	82/99 (83%)	72 (88%)	10 (12%)	5	15
42	2k	82/99 (83%)	75 (92%)	7 (8%)	10	31
43	1l	95/109 (87%)	91 (96%)	4 (4%)	30	63
43	2l	94/109 (86%)	91 (97%)	3 (3%)	39	73
44	1m	90/101 (89%)	80 (89%)	10 (11%)	6	19
44	2m	87/101 (86%)	74 (85%)	13 (15%)	3	9
45	1n	47/50 (94%)	43 (92%)	4 (8%)	10	31
45	2n	43/50 (86%)	36 (84%)	7 (16%)	2	7
46	1o	75/80 (94%)	69 (92%)	6 (8%)	12	34
46	2o	78/80 (98%)	74 (95%)	4 (5%)	24	55
47	1p	67/74 (90%)	57 (85%)	10 (15%)	3	9
47	2p	68/74 (92%)	60 (88%)	8 (12%)	5	16
48	1q	91/97 (94%)	85 (93%)	6 (7%)	16	44
48	2q	94/97 (97%)	89 (95%)	5 (5%)	22	54
49	1r	59/77 (77%)	55 (93%)	4 (7%)	16	42
49	2r	59/77 (77%)	53 (90%)	6 (10%)	7	22
50	1s	65/80 (81%)	56 (86%)	9 (14%)	3	11
50	2s	67/80 (84%)	59 (88%)	8 (12%)	5	16
51	1t	66/82 (80%)	61 (92%)	5 (8%)	13	36
51	2t	71/82 (87%)	68 (96%)	3 (4%)	30	63
52	1u	16/22 (73%)	16 (100%)	0	100	100
52	2u	18/22 (82%)	17 (94%)	1 (6%)	21	51

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
55	1z	13/19 (68%)	13 (100%)	0	100	100
55	2z	12/19 (63%)	11 (92%)	1 (8%)	11	32
All	All	9160/10104 (91%)	8276 (90%)	884 (10%)	8	24

All (884) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	1D	3	VAL
3	1D	13	ARG
3	1D	14	ARG
3	1D	27	THR
3	1D	54	ARG
3	1D	61	LEU
3	1D	71	ASP
3	1D	94	LEU
3	1D	99	ASP
3	1D	103	ARG
3	1D	111	LEU
3	1D	113	VAL
3	1D	115	GLN
3	1D	116	GLN
3	1D	138	VAL
3	1D	142	VAL
3	1D	171	ASP
3	1D	193	VAL
3	1D	211	ARG
3	1D	217	ARG
3	1D	221	VAL
3	1D	229	VAL
3	1D	242	ARG
3	1D	257	LEU
3	1D	260	ARG
3	1D	275	LYS
4	1E	7	VAL
4	1E	12	THR
4	1E	14	ILE
4	1E	21	VAL
4	1E	40	GLU
4	1E	49	LEU
4	1E	54	GLN
4	1E	73	GLU

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Mol	Chain	Res	Type
4	1E	75	VAL
4	1E	82	ARG
4	1E	111	ARG
4	1E	116	VAL
4	1E	119	ARG
4	1E	144	ARG
4	1E	154	LYS
4	1E	163	GLU
4	1E	167	VAL
4	1E	175	VAL
4	1E	181	LEU
4	1E	184	VAL
5	1F	20	LEU
5	1F	24	LEU
5	1F	33	LEU
5	1F	53	THR
5	1F	57	VAL
5	1F	74	ARG
5	1F	106	ARG
5	1F	110	LEU
5	1F	112	MET
5	1F	125	LEU
5	1F	170	LEU
5	1F	191	ARG
5	1F	192	LEU
5	1F	195	ASP
6	1G	4	ASP
6	1G	7	LEU
6	1G	16	ARG
6	1G	43	LEU
6	1G	45	GLU
6	1G	91	ARG
6	1G	139	LEU
6	1G	143	GLU
6	1G	148	MET
6	1G	159	VAL
6	1G	162	THR
6	1G	170	ARG
6	1G	181	ARG
7	1H	3	ARG
7	1H	45	VAL
7	1H	49	VAL

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Mol	Chain	Res	Type
7	1H	59	ARG
7	1H	60	ARG
7	1H	69	ARG
7	1H	71	LEU
7	1H	127	GLU
7	1H	129	THR
7	1H	175	LYS
8	1I	9	LEU
8	1I	10	GLU
8	1I	12	LEU
8	1I	20	ASP
8	1I	38	LEU
8	1I	43	ASN
8	1I	50	ARG
8	1I	57	ARG
8	1I	61	ARG
8	1I	66	GLU
8	1I	68	LEU
8	1I	75	LEU
8	1I	77	LEU
8	1I	92	VAL
8	1I	101	LEU
8	1I	103	ARG
8	1I	109	ILE
8	1I	116	LEU
8	1I	140	LEU
8	1I	142	VAL
9	1N	8	GLN
9	1N	28	THR
9	1N	33	LEU
9	1N	34	LEU
9	1N	48	MET
9	1N	61	ARG
9	1N	73	THR
9	1N	87	LEU
9	1N	97	ARG
9	1N	99	LEU
9	1N	120	LEU
9	1N	131	GLN
9	1N	133	GLN
9	1N	138	LEU
10	1O	10	VAL

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Mol	Chain	Res	Type
10	1O	23	ARG
10	1O	24	VAL
10	1O	69	ILE
10	1O	94	ARG
10	1O	105	GLU
10	1O	113	LYS
11	1P	3	LEU
11	1P	21	ARG
11	1P	55	ARG
11	1P	59	LEU
11	1P	70	GLN
11	1P	76	LYS
11	1P	83	VAL
11	1P	95	VAL
11	1P	98	GLU
11	1P	99	LEU
11	1P	106	LEU
11	1P	112	LEU
11	1P	125	VAL
11	1P	148	LEU
11	1P	149	GLU
12	1Q	1	MET
12	1Q	45	GLN
12	1Q	55	VAL
12	1Q	60	ARG
12	1Q	64	ILE
12	1Q	109	VAL
12	1Q	110	THR
13	1R	6	SER
13	1R	18	LEU
13	1R	28	LEU
13	1R	29	LEU
13	1R	33	ARG
13	1R	36	THR
13	1R	44	LEU
13	1R	60	LEU
13	1R	65	LEU
13	1R	67	LEU
13	1R	75	LEU
13	1R	79	LEU
13	1R	91	GLN
13	1R	111	LEU

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Mol	Chain	Res	Type
14	1S	3	ARG
14	1S	14	VAL
14	1S	20	ARG
14	1S	59	LYS
14	1S	61	ASN
14	1S	69	VAL
14	1S	85	VAL
15	1T	6	LEU
15	1T	13	ARG
15	1T	35	LYS
15	1T	49	VAL
15	1T	78	LEU
15	1T	89	VAL
15	1T	96	ARG
15	1T	107	ASP
15	1T	108	ARG
15	1T	118	ARG
16	1U	8	VAL
16	1U	36	ARG
16	1U	52	ARG
16	1U	60	LEU
16	1U	74	LEU
16	1U	77	SER
16	1U	92	ARG
16	1U	95	LEU
16	1U	104	GLN
17	1V	18	LEU
17	1V	21	ARG
17	1V	28	GLU
17	1V	35	LEU
17	1V	38	LEU
17	1V	43	GLU
17	1V	46	VAL
17	1V	61	VAL
17	1V	62	LEU
17	1V	72	VAL
17	1V	79	VAL
17	1V	95	LEU
18	1W	11	ARG
18	1W	15	ARG
18	1W	17	VAL
18	1W	19	LEU

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Mol	Chain	Res	Type
18	1W	51	LEU
18	1W	107	LEU
19	1X	35	THR
19	1X	88	LYS
20	1Y	9	LYS
20	1Y	23	ARG
20	1Y	43	ASN
20	1Y	70	SER
20	1Y	90	LEU
21	1Z	11	GLU
21	1Z	31	ARG
21	1Z	86	VAL
21	1Z	107	THR
21	1Z	150	LEU
21	1Z	155	LEU
21	1Z	162	GLU
21	1Z	170	THR
21	1Z	182	LYS
22	10	10	THR
22	10	11	ARG
22	10	20	ARG
22	10	49	LYS
22	10	55	ARG
23	11	21	ARG
23	11	35	THR
23	11	40	ARG
23	11	59	THR
23	11	78	LYS
23	11	89	GLU
23	11	95	LEU
24	12	19	VAL
24	12	53	LEU
24	12	70	GLN
25	13	6	VAL
25	13	8	LEU
25	13	23	LEU
25	13	54	VAL
26	14	47	GLN
26	14	49	PHE
26	14	58	ARG
26	14	60	GLN
26	14	61	ARG

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Mol	Chain	Res	Type
26	14	63	TYR
26	14	68	ARG
27	15	6	VAL
27	15	16	ARG
27	15	29	THR
27	15	40	LYS
28	16	4	GLU
28	16	6	ARG
28	16	14	THR
28	16	38	LYS
28	16	48	VAL
29	17	1	MET
29	17	23	ARG
29	17	24	THR
29	17	43	THR
30	18	14	VAL
30	18	31	HIS
30	18	32	LEU
30	18	34	TRP
30	18	46	ARG
31	19	26	ILE
33	1b	7	VAL
33	1b	8	LYS
33	1b	10	LEU
33	1b	16	HIS
33	1b	17	PHE
33	1b	21	ARG
33	1b	24	TRP
33	1b	60	ASP
33	1b	67	THR
33	1b	76	GLN
33	1b	80	ILE
33	1b	93	VAL
33	1b	96	ARG
33	1b	112	VAL
33	1b	124	SER
33	1b	127	ILE
33	1b	128	GLU
33	1b	156	LYS
33	1b	169	LYS
33	1b	185	ILE
33	1b	187	LEU

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Mol	Chain	Res	Type
33	1b	189	ASP
33	1b	190	THR
33	1b	208	ILE
33	1b	215	LEU
33	1b	217	ARG
33	1b	221	LEU
33	1b	226	ARG
34	1c	15	THR
34	1c	29	TYR
34	1c	47	LEU
34	1c	52	LEU
34	1c	54	ARG
34	1c	59	ARG
34	1c	70	VAL
34	1c	82	GLU
34	1c	115	LEU
34	1c	131	ARG
34	1c	150	LYS
34	1c	204	LEU
35	1d	5	ILE
35	1d	15	GLU
35	1d	28	SER
35	1d	31	CYS
35	1d	45	GLN
35	1d	49	ARG
35	1d	58	LEU
35	1d	66	ARG
35	1d	73	ARG
35	1d	101	LEU
35	1d	107	ARG
35	1d	122	ARG
35	1d	141	ARG
35	1d	160	GLN
35	1d	162	LEU
35	1d	168	ARG
35	1d	181	MET
35	1d	188	LEU
35	1d	194	LEU
36	1e	18	ARG
36	1e	24	ARG
36	1e	31	LEU
36	1e	41	VAL

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Mol	Chain	Res	Type
36	1e	47	LYS
36	1e	51	VAL
36	1e	73	ASN
36	1e	75	THR
36	1e	79	GLU
37	1f	69	GLU
37	1f	72	VAL
37	1f	74	ASP
37	1f	75	LEU
37	1f	89	MET
38	1g	6	ARG
38	1g	8	GLU
38	1g	13	GLN
38	1g	15	ASP
38	1g	21	VAL
38	1g	45	ASP
38	1g	50	ILE
38	1g	52	GLU
38	1g	56	GLN
38	1g	57	GLU
38	1g	75	VAL
38	1g	104	LEU
38	1g	131	LYS
39	1h	21	LYS
39	1h	26	VAL
39	1h	50	ARG
39	1h	51	VAL
39	1h	63	LEU
39	1h	64	LYS
39	1h	75	ARG
39	1h	78	GLN
39	1h	91	ARG
39	1h	137	VAL
40	1i	23	ASN
40	1i	27	THR
40	1i	42	ARG
40	1i	81	ILE
40	1i	86	VAL
40	1i	102	LEU
40	1i	104	ARG
40	1i	108	VAL
40	1i	113	LYS

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Mol	Chain	Res	Type
40	1i	127	LYS
41	1j	17	ASP
41	1j	30	SER
41	1j	43	ARG
41	1j	49	VAL
41	1j	84	GLN
41	1j	85	LEU
41	1j	94	VAL
41	1j	95	GLU
41	1j	98	ILE
42	1k	14	VAL
42	1k	18	ARG
42	1k	31	THR
42	1k	48	ILE
42	1k	78	GLN
42	1k	84	VAL
42	1k	87	THR
42	1k	106	LYS
42	1k	109	VAL
42	1k	114	VAL
43	1l	27	LEU
43	1l	33	ARG
43	1l	60	LEU
43	1l	67	THR
44	1m	4	ILE
44	1m	11	ARG
44	1m	19	LEU
44	1m	56	LEU
44	1m	69	GLU
44	1m	70	LEU
44	1m	102	ARG
44	1m	109	THR
44	1m	110	ARG
44	1m	117	VAL
45	1n	11	LYS
45	1n	18	VAL
45	1n	33	VAL
45	1n	46	GLU
46	1o	3	ILE
46	1o	5	LYS
46	1o	22	THR
46	1o	39	LEU

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Mol	Chain	Res	Type
46	1o	71	GLN
46	1o	83	GLU
47	1p	1	MET
47	1p	2	VAL
47	1p	5	ARG
47	1p	19	ILE
47	1p	20	VAL
47	1p	45	THR
47	1p	47	ASP
47	1p	54	GLU
47	1p	67	THR
47	1p	72	ARG
48	1q	49	GLU
48	1q	68	ARG
48	1q	74	LEU
48	1q	79	SER
48	1q	89	LEU
48	1q	98	LEU
49	1r	26	LEU
49	1r	38	GLU
49	1r	68	LYS
49	1r	76	LEU
50	1s	3	ARG
50	1s	22	LEU
50	1s	28	LYS
50	1s	37	ARG
50	1s	63	THR
50	1s	65	ASN
50	1s	77	THR
50	1s	81	ARG
50	1s	83	HIS
51	1t	9	ASN
51	1t	24	LEU
51	1t	60	GLU
51	1t	62	LEU
51	1t	84	LEU
3	2D	13	ARG
3	2D	54	ARG
3	2D	61	LEU
3	2D	94	LEU
3	2D	103	ARG
3	2D	106	ILE

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Mol	Chain	Res	Type
3	2D	113	VAL
3	2D	134	ARG
3	2D	141	VAL
3	2D	142	VAL
3	2D	154	LYS
3	2D	164	GLN
3	2D	183	ARG
3	2D	193	VAL
3	2D	217	ARG
3	2D	221	VAL
3	2D	229	VAL
3	2D	242	ARG
3	2D	257	LEU
3	2D	260	ARG
3	2D	262	ARG
3	2D	276	LYS
4	2E	12	THR
4	2E	21	VAL
4	2E	40	GLU
4	2E	49	LEU
4	2E	52	LEU
4	2E	75	VAL
4	2E	82	ARG
4	2E	111	ARG
4	2E	116	VAL
4	2E	119	ARG
4	2E	144	ARG
4	2E	154	LYS
4	2E	163	GLU
4	2E	175	VAL
4	2E	202	LYS
5	2F	15	SER
5	2F	20	LEU
5	2F	24	LEU
5	2F	53	THR
5	2F	57	VAL
5	2F	74	ARG
5	2F	106	ARG
5	2F	135	LYS
5	2F	191	ARG
5	2F	192	LEU
5	2F	196	LEU

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Mol	Chain	Res	Type
5	2F	197	ASP
5	2F	201	VAL
6	2G	9	ARG
6	2G	13	GLU
6	2G	28	VAL
6	2G	31	VAL
6	2G	33	ARG
6	2G	60	LEU
6	2G	91	ARG
6	2G	98	ARG
6	2G	111	LEU
6	2G	113	ARG
6	2G	136	ARG
6	2G	139	LEU
6	2G	140	ILE
6	2G	143	GLU
6	2G	148	MET
6	2G	153	ARG
6	2G	159	VAL
6	2G	162	THR
6	2G	165	THR
6	2G	170	ARG
7	2H	3	ARG
7	2H	27	LYS
7	2H	32	GLU
7	2H	33	LEU
7	2H	41	MET
7	2H	42	ARG
7	2H	45	VAL
7	2H	49	VAL
7	2H	59	ARG
7	2H	69	ARG
7	2H	71	LEU
7	2H	98	LEU
7	2H	129	THR
7	2H	134	SER
7	2H	136	ILE
7	2H	139	GLN
7	2H	171	LEU
8	2I	15	VAL
8	2I	38	LEU
8	2I	43	ASN

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Mol	Chain	Res	Type
8	2I	57	ARG
8	2I	61	ARG
8	2I	68	LEU
8	2I	75	LEU
8	2I	76	THR
8	2I	77	LEU
8	2I	102	SER
8	2I	116	LEU
8	2I	117	GLU
8	2I	140	LEU
8	2I	142	VAL
9	2N	33	LEU
9	2N	34	LEU
9	2N	43	THR
9	2N	48	MET
9	2N	59	LYS
9	2N	61	ARG
9	2N	62	VAL
9	2N	63	THR
9	2N	87	LEU
9	2N	97	ARG
9	2N	99	LEU
9	2N	120	LEU
9	2N	131	GLN
9	2N	133	GLN
9	2N	137	LYS
10	2O	10	VAL
10	2O	23	ARG
10	2O	24	VAL
10	2O	69	ILE
10	2O	94	ARG
11	2P	3	LEU
11	2P	15	ARG
11	2P	21	ARG
11	2P	45	LEU
11	2P	55	ARG
11	2P	59	LEU
11	2P	65	ARG
11	2P	83	VAL
11	2P	96	THR
11	2P	101	VAL
11	2P	102	ARG

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Mol	Chain	Res	Type
11	2P	112	LEU
11	2P	121	LYS
11	2P	123	LEU
11	2P	133	SER
11	2P	136	GLU
11	2P	148	LEU
12	2Q	5	ARG
12	2Q	21	THR
12	2Q	22	LYS
12	2Q	38	GLU
12	2Q	45	GLN
12	2Q	64	ILE
12	2Q	110	THR
13	2R	1	MET
13	2R	6	SER
13	2R	18	LEU
13	2R	28	LEU
13	2R	29	LEU
13	2R	44	LEU
13	2R	60	LEU
13	2R	65	LEU
13	2R	79	LEU
13	2R	100	LEU
13	2R	111	LEU
14	2S	4	LEU
14	2S	14	VAL
14	2S	20	ARG
14	2S	23	ARG
14	2S	35	ILE
14	2S	44	LYS
14	2S	67	ARG
14	2S	69	VAL
14	2S	75	GLU
14	2S	83	LYS
14	2S	85	VAL
15	2T	6	LEU
15	2T	8	LYS
15	2T	34	VAL
15	2T	49	VAL
15	2T	89	VAL
15	2T	96	ARG
15	2T	98	LYS

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Mol	Chain	Res	Type
15	2T	118	ARG
16	2U	36	ARG
16	2U	60	LEU
16	2U	74	LEU
16	2U	92	ARG
16	2U	104	GLN
16	2U	108	GLU
17	2V	18	LEU
17	2V	21	ARG
17	2V	35	LEU
17	2V	43	GLU
17	2V	46	VAL
17	2V	52	VAL
17	2V	62	LEU
17	2V	72	VAL
17	2V	79	VAL
18	2W	1	MET
18	2W	11	ARG
18	2W	15	ARG
18	2W	17	VAL
18	2W	51	LEU
18	2W	107	LEU
19	2X	57	LEU
19	2X	92	LEU
20	2Y	9	LYS
20	2Y	43	ASN
20	2Y	44	ILE
20	2Y	70	SER
20	2Y	92	ASN
20	2Y	99	CYS
20	2Y	101	LYS
21	2Z	73	GLN
21	2Z	86	VAL
21	2Z	87	ASP
21	2Z	107	THR
21	2Z	126	VAL
21	2Z	131	ARG
21	2Z	132	ASN
21	2Z	135	GLU
21	2Z	136	PHE
21	2Z	150	LEU
21	2Z	175	VAL

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Mol	Chain	Res	Type
21	2Z	185	GLU
22	20	10	THR
22	20	19	LYS
22	20	55	ARG
22	20	82	ARG
23	21	21	ARG
23	21	35	THR
23	21	40	ARG
23	21	56	GLN
23	21	59	THR
23	21	95	LEU
24	22	34	GLU
24	22	35	LEU
24	22	53	LEU
24	22	70	GLN
25	23	6	VAL
25	23	8	LEU
25	23	31	LEU
25	23	54	VAL
25	23	56	VAL
26	24	1	MET
26	24	58	ARG
26	24	61	ARG
26	24	63	TYR
26	24	68	ARG
26	24	69	LYS
27	25	6	VAL
27	25	16	ARG
27	25	29	THR
27	25	40	LYS
28	26	6	ARG
28	26	14	THR
28	26	28	ARG
28	26	38	LYS
28	26	48	VAL
29	27	46	VAL
30	28	14	VAL
30	28	31	HIS
30	28	34	TRP
31	29	17	ILE
33	2b	7	VAL
33	2b	8	LYS

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Mol	Chain	Res	Type
33	2b	17	PHE
33	2b	19	HIS
33	2b	24	TRP
33	2b	35	GLU
33	2b	44	LEU
33	2b	48	MET
33	2b	51	LEU
33	2b	56	ARG
33	2b	60	ASP
33	2b	63	MET
33	2b	67	THR
33	2b	71	VAL
33	2b	90	MET
33	2b	93	VAL
33	2b	117	GLU
33	2b	126	GLU
33	2b	128	GLU
33	2b	179	LYS
33	2b	185	ILE
33	2b	187	LEU
33	2b	189	ASP
33	2b	191	ASP
33	2b	222	ILE
33	2b	224	GLN
34	2c	3	ASN
34	2c	5	ILE
34	2c	14	ILE
34	2c	16	ARG
34	2c	29	TYR
34	2c	47	LEU
34	2c	52	LEU
34	2c	59	ARG
34	2c	70	VAL
34	2c	125	GLU
34	2c	178	LEU
34	2c	182	ILE
35	2d	3	ARG
35	2d	8	VAL
35	2d	26	CYS
35	2d	34	GLU
35	2d	38	TYR
35	2d	47	ARG

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Mol	Chain	Res	Type
35	2d	58	LEU
35	2d	61	LYS
35	2d	73	ARG
35	2d	96	LEU
35	2d	135	LEU
35	2d	157	LEU
35	2d	170	VAL
35	2d	187	ARG
35	2d	194	LEU
36	2e	24	ARG
36	2e	27	ARG
36	2e	31	LEU
36	2e	40	ARG
36	2e	41	VAL
36	2e	47	LYS
36	2e	50	GLU
36	2e	51	VAL
36	2e	68	GLU
36	2e	78	HIS
36	2e	115	VAL
36	2e	121	LYS
37	2f	28	ARG
37	2f	46	ARG
37	2f	69	GLU
38	2g	8	GLU
38	2g	11	GLN
38	2g	15	ASP
38	2g	16	LEU
38	2g	21	VAL
38	2g	42	ILE
38	2g	52	GLU
38	2g	57	GLU
38	2g	72	ARG
38	2g	75	VAL
38	2g	104	LEU
38	2g	110	GLN
38	2g	114	ARG
38	2g	120	ILE
38	2g	129	GLU
39	2h	10	LEU
39	2h	21	LYS
39	2h	26	VAL

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Mol	Chain	Res	Type
39	2h	51	VAL
39	2h	63	LEU
39	2h	78	GLN
39	2h	84	ARG
39	2h	91	ARG
39	2h	111	ILE
39	2h	120	THR
39	2h	125	ARG
39	2h	137	VAL
40	2i	3	GLN
40	2i	12	GLU
40	2i	38	GLN
40	2i	50	LEU
40	2i	81	ILE
40	2i	89	ASN
40	2i	102	LEU
40	2i	104	ARG
40	2i	124	GLN
41	2j	8	LEU
41	2j	16	LEU
41	2j	21	GLN
41	2j	46	ARG
41	2j	48	THR
41	2j	57	LYS
41	2j	68	HIS
41	2j	84	GLN
41	2j	94	VAL
41	2j	95	GLU
42	2k	18	ARG
42	2k	48	ILE
42	2k	75	TYR
42	2k	78	GLN
42	2k	103	LEU
42	2k	109	VAL
42	2k	114	VAL
43	2l	33	ARG
43	2l	115	LYS
43	2l	123	LYS
44	2m	47	ASP
44	2m	49	THR
44	2m	52	GLU
44	2m	55	ARG

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Mol	Chain	Res	Type
44	2m	65	LYS
44	2m	80	ARG
44	2m	81	LEU
44	2m	82	MET
44	2m	90	LEU
44	2m	102	ARG
44	2m	106	ASN
44	2m	109	THR
44	2m	110	ARG
45	2n	11	LYS
45	2n	17	LYS
45	2n	18	VAL
45	2n	27	CYS
45	2n	32	SER
45	2n	33	VAL
45	2n	46	GLU
46	2o	3	ILE
46	2o	5	LYS
46	2o	24	SER
46	2o	39	LEU
47	2p	1	MET
47	2p	2	VAL
47	2p	5	ARG
47	2p	11	SER
47	2p	54	GLU
47	2p	67	THR
47	2p	72	ARG
47	2p	74	LEU
48	2q	6	LEU
48	2q	49	GLU
48	2q	63	ARG
48	2q	74	LEU
48	2q	79	SER
49	2r	25	THR
49	2r	26	LEU
49	2r	29	PHE
49	2r	35	ARG
49	2r	38	GLU
49	2r	76	LEU
50	2s	3	ARG
50	2s	27	GLU
50	2s	28	LYS

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Mol	Chain	Res	Type
50	2s	30	LEU
50	2s	41	VAL
50	2s	63	THR
50	2s	65	ASN
50	2s	77	THR
51	2t	10	LEU
51	2t	24	LEU
51	2t	71	THR
52	2u	10	ARG
55	2z	7	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (138) such sidechains are listed below:

Mol	Chain	Res	Type
3	1D	126	GLN
3	1D	253	GLN
4	1E	54	GLN
5	1F	69	HIS
5	1F	203	GLN
6	1G	40	ASN
6	1G	79	ASN
8	1I	43	ASN
9	1N	8	GLN
9	1N	133	GLN
11	1P	38	GLN
11	1P	70	GLN
12	1Q	45	GLN
13	1R	71	GLN
14	1S	95	HIS
15	1T	43	GLN
15	1T	123	GLN
16	1U	104	GLN
16	1U	117	GLN
19	1X	31	HIS
20	1Y	6	HIS
20	1Y	92	ASN
21	1Z	73	GLN
21	1Z	151	HIS
24	12	38	GLN
24	12	70	GLN
26	14	47	GLN
30	18	35	GLN

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Mol	Chain	Res	Type
31	19	36	GLN
33	1b	16	HIS
33	1b	94	ASN
34	1c	6	HIS
34	1c	37	GLN
34	1c	176	HIS
35	1d	43	HIS
35	1d	45	GLN
35	1d	77	ASN
35	1d	123	HIS
35	1d	160	GLN
36	1e	38	GLN
36	1e	141	GLN
37	1f	100	ASN
38	1g	86	GLN
38	1g	97	GLN
38	1g	110	GLN
39	1h	82	HIS
40	1i	31	GLN
40	1i	38	GLN
40	1i	58	HIS
40	1i	73	GLN
40	1i	89	ASN
40	1i	124	GLN
41	1j	56	HIS
41	1j	84	GLN
42	1k	93	GLN
43	1l	78	GLN
43	1l	99	HIS
48	1q	16	GLN
48	1q	26	GLN
50	1s	14	HIS
50	1s	47	HIS
50	1s	56	GLN
50	1s	65	ASN
50	1s	69	HIS
51	1t	9	ASN
51	1t	16	HIS
51	1t	26	ASN
51	1t	45	GLN
3	2D	87	ASN
3	2D	253	GLN

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
5	2F	69	HIS
5	2F	169	ASN
5	2F	203	GLN
6	2G	108	ASN
6	2G	132	ASN
8	2I	43	ASN
8	2I	54	GLN
9	2N	8	GLN
10	2O	5	GLN
11	2P	38	GLN
12	2Q	45	GLN
13	2R	71	GLN
14	2S	68	GLN
14	2S	95	HIS
15	2T	43	GLN
15	2T	58	ASN
15	2T	123	GLN
17	2V	64	HIS
19	2X	31	HIS
20	2Y	43	ASN
20	2Y	92	ASN
21	2Z	73	GLN
21	2Z	151	HIS
23	21	56	GLN
24	22	38	GLN
25	23	33	GLN
28	26	32	ASN
30	28	35	GLN
31	29	36	GLN
33	2b	19	HIS
33	2b	45	GLN
33	2b	146	GLN
34	2c	3	ASN
34	2c	6	HIS
34	2c	123	GLN
34	2c	136	GLN
35	2d	74	GLN
35	2d	77	ASN
35	2d	123	HIS
35	2d	125	HIS
35	2d	201	GLN
38	2g	28	ASN

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Mol	Chain	Res	Type
38	2g	86	GLN
38	2g	97	GLN
38	2g	110	GLN
38	2g	122	HIS
38	2g	148	ASN
39	2h	15	ASN
40	2i	38	GLN
40	2i	73	GLN
41	2j	21	GLN
41	2j	56	HIS
41	2j	84	GLN
42	2k	22	HIS
42	2k	78	GLN
42	2k	93	GLN
42	2k	104	GLN
43	2l	75	HIS
43	2l	78	GLN
44	2m	40	ASN
44	2m	77	ASN
44	2m	106	ASN
46	2o	28	GLN
46	2o	62	GLN
50	2s	56	GLN
50	2s	69	HIS
51	2t	18	GLN
51	2t	42	GLN

### 5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	1A	2737/2915 (93%)	383 (13%)	21 (0%)
1	2A	2781/2915 (95%)	467 (16%)	21 (0%)
2	1B	119/121 (98%)	10 (8%)	0
2	2B	119/121 (98%)	24 (20%)	2 (1%)
32	1a	1472/1521 (96%)	263 (17%)	0
32	2a	1479/1521 (97%)	283 (19%)	0
53	1v	4/24 (16%)	1 (25%)	0
53	2v	4/24 (16%)	1 (25%)	0
54	1x	75/77 (97%)	17 (22%)	0
54	2x	75/77 (97%)	15 (20%)	0
All	All	8865/9316 (95%)	1464 (16%)	44 (0%)

All (1464) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	1A	11	U
1	1A	33	C
1	1A	44	C
1	1A	53	G
1	1A	62	A
1	1A	69	A
1	1A	72	A
1	1A	73	G
1	1A	82	A
1	1A	91	C
1	1A	115	A
1	1A	116	A
1	1A	117	U
1	1A	122	G
1	1A	135	G
1	1A	137	G
1	1A	148	A
1	1A	160	C
1	1A	169	A
1	1A	170	A
1	1A	184	A
1	1A	187	A
1	1A	193	G
1	1A	203	G
1	1A	204	A
1	1A	210	A
1	1A	214	G
1	1A	216	A
1	1A	217	A
1	1A	221	A
1	1A	236	G
1	1A	268	G
1	1A	271	U
1	1A	272	G
1	1A	273	U
1	1A	274	C
1	1A	287	U
1	1A	288	G
1	1A	294	C
1	1A	295	U
1	1A	302	C
1	1A	334	A

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Mol	Chain	Res	Type
1	1A	347	A
1	1A	352	G
1	1A	353	A
1	1A	375	G
1	1A	386	G
1	1A	388	G
1	1A	398	G
1	1A	406	U
1	1A	412	G
1	1A	422	G
1	1A	431	U
1	1A	433	G
1	1A	437	G
1	1A	438	A
1	1A	447	U
1	1A	454	A
1	1A	467	G
1	1A	468	A
1	1A	469	C
1	1A	473	U
1	1A	476	C
1	1A	482	A
1	1A	495	A
1	1A	500	U
1	1A	506	G
1	1A	528	U
1	1A	529	A
1	1A	533	C
1	1A	554	G
1	1A	555	C
1	1A	556	A
1	1A	557	G
1	1A	572	G
1	1A	585	G
1	1A	595	G
1	1A	597	A
1	1A	624	G
1	1A	625	A
1	1A	626	G
1	1A	629	U
1	1A	638	G
1	1A	640	G

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Mol	Chain	Res	Type
1	1A	658	C
1	1A	661	A
1	1A	669	C
1	1A	670	A
1	1A	681	G
1	1A	682	G
1	1A	696	C
1	1A	700	A
1	1A	714	G
1	1A	715	G
1	1A	732	G
1	1A	763	G
1	1A	765	C
1	1A	776	C
1	1A	785	G
1	1A	797	A
1	1A	803	U
1	1A	810	A
1	1A	821	G
1	1A	822	G
1	1A	828	A
1	1A	830	A
1	1A	831	G
1	1A	836	C
1	1A	838	G
1	1A	851	G
1	1A	857	U
1	1A	858	C
1	1A	873	U
1	1A	874	U
1	1A	876	G
1	1A	901	G
1	1A	905	G
1	1A	912	A
1	1A	915	G
1	1A	925	G
1	1A	931	C
1	1A	932	C
1	1A	933	A
1	1A	934	C
1	1A	935	C
1	1A	936	A

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Mol	Chain	Res	Type
1	1A	937	G
1	1A	938	C
1	1A	939	C
1	1A	941	A
1	1A	942	C
1	1A	952	U
1	1A	955	A
1	1A	976	G
1	1A	985	A
1	1A	989	A
1	1A	990	G
1	1A	1002	U
1	1A	1003	A
1	1A	1005	C
1	1A	1018	G
1	1A	1019	C
1	1A	1028	A
1	1A	1041	A
1	1A	1057	U
1	1A	1058	C
1	1A	1067	G
1	1A	1071	U
1	1A	1078	U
1	1A	1083	C
1	1A	1086	C
1	1A	1090	A
1	1A	1091	A
1	1A	1092	G
1	1A	1150	U
1	1A	1154	C
1	1A	1156	A
1	1A	1159	G
1	1A	1173	A
1	1A	1174	A
1	1A	1175	U
1	1A	1179	C
1	1A	1180	G
1	1A	1183	G
1	1A	1194	G
1	1A	1200	A
1	1A	1215	G
1	1A	1217	G

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Mol	Chain	Res	Type
1	1A	1218	A
1	1A	1219	U
1	1A	1220	G
1	1A	1221	A
1	1A	1264	A
1	1A	1265	C
1	1A	1285	U
1	1A	1286	A
1	1A	1293	G
1	1A	1298	A
1	1A	1301	G
1	1A	1316	G
1	1A	1317	A
1	1A	1318	U
1	1A	1345	U
1	1A	1346	A
1	1A	1348	G
1	1A	1397	U
1	1A	1404	A
1	1A	1405	A
1	1A	1410	A
1	1A	1418	A
1	1A	1429	A
1	1A	1430	G
1	1A	1461	G
1	1A	1462	C
1	1A	1465	U
1	1A	1466	G
1	1A	1473	C
1	1A	1482	C
1	1A	1490	A
1	1A	1496	G
1	1A	1501	G
1	1A	1505	G
1	1A	1511	G
1	1A	1513	C
1	1A	1524	G
1	1A	1528	G
1	1A	1535	A
1	1A	1538	C
1	1A	1541	A
1	1A	1553	A

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Mol	Chain	Res	Type
1	1A	1554	C
1	1A	1555	A
1	1A	1570	G
1	1A	1578	C
1	1A	1588	A
1	1A	1589	C
1	1A	1604	A
1	1A	1605	G
1	1A	1612	A
1	1A	1615	A
1	1A	1624	U
1	1A	1627	G
1	1A	1630	C
1	1A	1631	A
1	1A	1632	A
1	1A	1653	A
1	1A	1654	A
1	1A	1655	A
1	1A	1694	C
1	1A	1700	A
1	1A	1704	C
1	1A	1720	G
1	1A	1746	A
1	1A	1747	A
1	1A	1766	A
1	1A	1767	U
1	1A	1776	G
1	1A	1793	G
1	1A	1794	G
1	1A	1799	G
1	1A	1803	A
1	1A	1810	A
1	1A	1821	A
1	1A	1830	C
1	1A	1831	G
1	1A	1846	G
1	1A	1859	A
1	1A	1869	G
1	1A	1877	A
1	1A	1899	G
1	1A	1910	A
1	1A	1917	G

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Mol	Chain	Res	Type
1	1A	1921	A
1	1A	1927	G
1	1A	1934	A
1	1A	1940	A
1	1A	1948	A
1	1A	1950	G
1	1A	1951	G
1	1A	1958	A
1	1A	1959	A
1	1A	1976	U
1	1A	1984	U
1	1A	1988	C
1	1A	1991	A
1	1A	1992	A
1	1A	1993	A
1	1A	2013	G
1	1A	2014	U
1	1A	2018	G
1	1A	2041	A
1	1A	2044	G
1	1A	2052	A
1	1A	2053	G
1	1A	2054	A
1	1A	2064	C
1	1A	2076	C
1	1A	2077	G
1	1A	2081	A
1	1A	2082	G
1	1A	2083	A
1	1A	2090	G
1	1A	2101	G
1	1A	2114	G
1	1A	2205	G
1	1A	2206	C
1	1A	2207	G
1	1A	2209	C
1	1A	2212	G
1	1A	2213	G
1	1A	2219	A
1	1A	2226	G
1	1A	2227	G
1	1A	2228	A

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Mol	Chain	Res	Type
1	1A	2229	U
1	1A	2236	A
1	1A	2249	G
1	1A	2250	G
1	1A	2251	C
1	1A	2279	A
1	1A	2280	A
1	1A	2284	A
1	1A	2286	C
1	1A	2294	C
1	1A	2298	A
1	1A	2316	A
1	1A	2331	A
1	1A	2336	G
1	1A	2338	A
1	1A	2345	G
1	1A	2347	A
1	1A	2354	C
1	1A	2358	C
1	1A	2361	C
1	1A	2365	G
1	1A	2394	G
1	1A	2396	C
1	1A	2416	G
1	1A	2417	U
1	1A	2433	A
1	1A	2434	U
1	1A	2436	A
1	1A	2440	G
1	1A	2441	A
1	1A	2442	U
1	1A	2446	A
1	1A	2450	A
1	1A	2452	C
1	1A	2459	A
1	1A	2487	A
1	1A	2489	A
1	1A	2501	G
1	1A	2513	G
1	1A	2516	G
1	1A	2517	U
1	1A	2529	A

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Mol	Chain	Res	Type
1	1A	2540	G
1	1A	2565	U
1	1A	2577	A
1	1A	2578	G
1	1A	2584	C
1	1A	2593	G
1	1A	2613	A
1	1A	2620	U
1	1A	2621	C
1	1A	2622	U
1	1A	2623	C
1	1A	2634	G
1	1A	2639	C
1	1A	2640	A
1	1A	2641	G
1	1A	2665	A
1	1A	2690	A
1	1A	2700	U
1	1A	2701	C
1	1A	2702	C
1	1A	2713	U
1	1A	2718	G
1	1A	2724	A
1	1A	2725	A
1	1A	2726	G
1	1A	2738	U
1	1A	2745	A
1	1A	2769	A
1	1A	2770	A
1	1A	2776	A
1	1A	2777	A
1	1A	2778	G
1	1A	2790	A
1	1A	2802	A
1	1A	2806	C
1	1A	2812	G
1	1A	2829	A
1	1A	2830	A
1	1A	2844	A
1	1A	2867	C
1	1A	2881	G
1	1A	2882	A

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Mol	Chain	Res	Type
1	1A	2889	C
1	1A	2900	A
1	1A	2902	G
1	1A	2903	U
1	1A	2905	U
2	1B	2	C
2	1B	13	A
2	1B	25	A
2	1B	56	G
2	1B	65	C
2	1B	67	G
2	1B	73	A
2	1B	85	G
2	1B	106	G
2	1B	110	G
32	1a	6	U
32	1a	10	G
32	1a	33	A
32	1a	40	G
32	1a	44	C
32	1a	45	G
32	1a	48	C
32	1a	49	C
32	1a	51	A
32	1a	52	A
32	1a	62	G
32	1a	65	G
32	1a	66	U
32	1a	74	G
32	1a	76	G
32	1a	77	G
32	1a	78	G
32	1a	89	G
32	1a	91	G
32	1a	92	G
32	1a	95	A
32	1a	110	A
32	1a	115	C
32	1a	126	C
32	1a	132	C
32	1a	133	G
32	1a	139	G

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Mol	Chain	Res	Type
32	1a	146	A
32	1a	149	C
32	1a	150	C
32	1a	156	A
32	1a	161	G
32	1a	162	G
32	1a	168	U
32	1a	169	C
32	1a	177	U
32	1a	189	U
32	1a	202	A
32	1a	204	A
32	1a	206	G
32	1a	208	C
32	1a	210	U
32	1a	211	U
32	1a	212	G
32	1a	219	U
32	1a	243	G
32	1a	246	A
32	1a	247	G
32	1a	254	G
32	1a	258	A
32	1a	262	G
32	1a	263	C
32	1a	264	C
32	1a	277	G
32	1a	285	G
32	1a	297	G
32	1a	313	G
32	1a	317	A
32	1a	324	C
32	1a	325	A
32	1a	326	C
32	1a	339	U
32	1a	342	G
32	1a	343	G
32	1a	344	G
32	1a	348	C
32	1a	349	A
32	1a	350	G
32	1a	351	C

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Mol	Chain	Res	Type
32	1a	363	U
32	1a	368	C
32	1a	369	A
32	1a	380	G
32	1a	386	C
32	1a	393	A
32	1a	394	C
32	1a	402	G
32	1a	408	A
32	1a	409	G
32	1a	419	G
32	1a	420	G
32	1a	425	U
32	1a	431	C
32	1a	435	A
32	1a	437	C
32	1a	447	A
32	1a	449	C
32	1a	455	A
32	1a	456	C
32	1a	457	G
32	1a	470	G
32	1a	481	A
32	1a	482	U
32	1a	489	G
32	1a	493	A
32	1a	494	A
32	1a	495	C
32	1a	502	C
32	1a	511	G
32	1a	516	A
32	1a	517	A
32	1a	531	A
32	1a	543	A
32	1a	545	U
32	1a	556	A
32	1a	557	A
32	1a	560	G
32	1a	561	G
32	1a	574	C
32	1a	576	G
32	1a	602	C

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Mol	Chain	Res	Type
32	1a	614	G
32	1a	625	U
32	1a	637	A
32	1a	649	A
32	1a	671	A
32	1a	672	G
32	1a	677	G
32	1a	701	C
32	1a	707	U
32	1a	731	C
32	1a	733	C
32	1a	739	G
32	1a	743	A
32	1a	757	G
32	1a	761	A
32	1a	776	A
32	1a	777	U
32	1a	778	A
32	1a	799	A
32	1a	800	A
32	1a	801	C
32	1a	812	A
32	1a	813	G
32	1a	820	G
32	1a	824	C
32	1a	825	U
32	1a	826	C
32	1a	829	G
32	1a	837	A
32	1a	838	A
32	1a	848	U
32	1a	850	A
32	1a	851	A
32	1a	880	G
32	1a	892	A
32	1a	904	G
32	1a	905	G
32	1a	909	C
32	1a	912	C
32	1a	913	A
32	1a	914	C
32	1a	938	U

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Mol	Chain	Res	Type
32	1a	939	U
32	1a	946	A
32	1a	947	A
32	1a	949	G
32	1a	950	C
32	1a	952	A
32	1a	953	A
32	1a	954	G
32	1a	955	A
32	1a	970	U
32	1a	971	G
32	1a	972	A
32	1a	977	C
32	1a	980	G
32	1a	982	G
32	1a	983	A
32	1a	984	A
32	1a	987	C
32	1a	988	G
32	1a	989	G
32	1a	990	G
32	1a	995	A
32	1a	999	U
32	1a	1025	G
32	1a	1026	C
32	1a	1027	A
32	1a	1034	C
32	1a	1036	G
32	1a	1037	C
32	1a	1047	G
32	1a	1048	U
32	1a	1049	C
32	1a	1064	G
32	1a	1069	U
32	1a	1077	G
32	1a	1078	U
32	1a	1084	A
32	1a	1091	G
32	1a	1094	A
32	1a	1106	A
32	1a	1107	G
32	1a	1115	C

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
32	1a	1116	G
32	1a	1117	G
32	1a	1119	U
32	1a	1120	C
32	1a	1122	G
32	1a	1135	A
32	1a	1142	U
32	1a	1143	G
32	1a	1149	G
32	1a	1164	G
32	1a	1165	A
32	1a	1166	G
32	1a	1175	G
32	1a	1178	U
32	1a	1179	G
32	1a	1184	G
32	1a	1194	U
32	1a	1195	A
32	1a	1196	C
32	1a	1209	A
32	1a	1220	A
32	1a	1222	U
32	1a	1238	A
32	1a	1239	U
32	1a	1240	G
32	1a	1252	C
32	1a	1255	G
32	1a	1260	U
32	1a	1261	A
32	1a	1262	A
32	1a	1268	A
32	1a	1269	A
32	1a	1281	A
32	1a	1282	G
32	1a	1284	U
32	1a	1287	G
32	1a	1294	G
32	1a	1301	A
32	1a	1304	C
32	1a	1320	G
32	1a	1322	A
32	1a	1329	G

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Mol	Chain	Res	Type
32	1a	1335	G
32	1a	1342	A
32	1a	1345	C
32	1a	1353	G
32	1a	1360	A
32	1a	1361	C
32	1a	1362	G
32	1a	1364	U
32	1a	1379	A
32	1a	1380	C
32	1a	1392	C
32	1a	1402	G
32	1a	1424	G
32	1a	1425	G
32	1a	1426	G
32	1a	1432	A
32	1a	1433	C
32	1a	1465	G
32	1a	1475	G
32	1a	1480	A
32	1a	1481	A
32	1a	1482	G
32	1a	1484	U
32	1a	1495	G
32	1a	1507	G
32	1a	1508	G
53	1v	15	A
54	1x	6	G
54	1x	9	G
54	1x	13	C
54	1x	16	C
54	1x	17	C
54	1x	17(A)	U
54	1x	20	U
54	1x	21	A
54	1x	31	G
54	1x	42	G
54	1x	47	U
54	1x	54	5MU
54	1x	55	PSU
54	1x	56	C
54	1x	65	C

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Mol	Chain	Res	Type
54	1x	70	G
54	1x	76	A
1	2A	7	A
1	2A	11	U
1	2A	12	A
1	2A	13	A
1	2A	14	G
1	2A	34	G
1	2A	44	C
1	2A	53	G
1	2A	59	G
1	2A	69	A
1	2A	72	A
1	2A	73	G
1	2A	81	G
1	2A	82	A
1	2A	88	U
1	2A	93	G
1	2A	98	G
1	2A	99	G
1	2A	115	A
1	2A	116	A
1	2A	117	U
1	2A	128	G
1	2A	137	G
1	2A	138	A
1	2A	154	C
1	2A	155	U
1	2A	160	C
1	2A	169	A
1	2A	170	A
1	2A	184	A
1	2A	187	A
1	2A	193	G
1	2A	201	A
1	2A	203	G
1	2A	204	A
1	2A	209	A
1	2A	210	A
1	2A	212	G
1	2A	217	A
1	2A	223	U

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Mol	Chain	Res	Type
1	2A	224	C
1	2A	225	C
1	2A	236	G
1	2A	238	G
1	2A	252	C
1	2A	253	A
1	2A	268	G
1	2A	270	U
1	2A	271	U
1	2A	272	G
1	2A	274	C
1	2A	287	U
1	2A	288	G
1	2A	301	A
1	2A	334	A
1	2A	347	A
1	2A	350	G
1	2A	352	G
1	2A	353	A
1	2A	355	A
1	2A	357	C
1	2A	358	C
1	2A	361	G
1	2A	365	G
1	2A	375	G
1	2A	385	U
1	2A	386	G
1	2A	389	G
1	2A	412	G
1	2A	422	G
1	2A	431	U
1	2A	433	G
1	2A	437	G
1	2A	438	A
1	2A	441	A
1	2A	453	U
1	2A	454	A
1	2A	460	U
1	2A	468	A
1	2A	469	C
1	2A	471	G
1	2A	479	A

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Mol	Chain	Res	Type
1	2A	480	C
1	2A	481	C
1	2A	482	A
1	2A	495	A
1	2A	506	G
1	2A	528	U
1	2A	529	A
1	2A	533	C
1	2A	552	A
1	2A	554	G
1	2A	555	C
1	2A	556	A
1	2A	557	G
1	2A	573	G
1	2A	585	G
1	2A	590	U
1	2A	595	G
1	2A	596	C
1	2A	597	A
1	2A	608	A
1	2A	615	G
1	2A	625	A
1	2A	626	G
1	2A	629	U
1	2A	637	U
1	2A	638	G
1	2A	639	A
1	2A	640	G
1	2A	651	A
1	2A	658	C
1	2A	661	A
1	2A	669	C
1	2A	670	A
1	2A	673	G
1	2A	678	A
1	2A	679	G
1	2A	697	G
1	2A	732	G
1	2A	763	G
1	2A	772	G
1	2A	776	C
1	2A	811	G

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Mol	Chain	Res	Type
1	2A	817	G
1	2A	821	G
1	2A	822	G
1	2A	828	A
1	2A	829	A
1	2A	830	A
1	2A	831	G
1	2A	838	G
1	2A	848	A
1	2A	851	G
1	2A	858	C
1	2A	865	A
1	2A	873	U
1	2A	874	U
1	2A	903	C
1	2A	905	G
1	2A	906	U
1	2A	912	A
1	2A	915	G
1	2A	918	A
1	2A	924	A
1	2A	925	G
1	2A	926	G
1	2A	928	G
1	2A	930	C
1	2A	932	C
1	2A	933	A
1	2A	934	C
1	2A	935	C
1	2A	936	A
1	2A	938	C
1	2A	941	A
1	2A	942	C
1	2A	945	A
1	2A	946	A
1	2A	955	A
1	2A	956	A
1	2A	960	C
1	2A	962	A
1	2A	975	G
1	2A	976	G
1	2A	980	C

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Mol	Chain	Res	Type
1	2A	982	G
1	2A	985	A
1	2A	989	A
1	2A	990	G
1	2A	997	A
1	2A	1003	A
1	2A	1005	C
1	2A	1018	G
1	2A	1019	C
1	2A	1025	A
1	2A	1028	A
1	2A	1041	A
1	2A	1050	C
1	2A	1057	U
1	2A	1058	C
1	2A	1066	A
1	2A	1067	G
1	2A	1070	G
1	2A	1078	U
1	2A	1088	C
1	2A	1090	A
1	2A	1091	A
1	2A	1092	G
1	2A	1093	A
1	2A	1103	G
1	2A	1104	G
1	2A	1105	U
1	2A	1106	U
1	2A	1107	G
1	2A	1108	G
1	2A	1109	C
1	2A	1110	U
1	2A	1115	A
1	2A	1118	A
1	2A	1120	C
1	2A	1121	C
1	2A	1126	U
1	2A	1128	U
1	2A	1132	G
1	2A	1133	A
1	2A	1136	G
1	2A	1142	U

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Mol	Chain	Res	Type
1	2A	1152	G
1	2A	1156	A
1	2A	1157	G
1	2A	1158	U
1	2A	1159	G
1	2A	1167	G
1	2A	1175	U
1	2A	1179	C
1	2A	1180	G
1	2A	1183	G
1	2A	1187	A
1	2A	1216	G
1	2A	1249	U
1	2A	1264	A
1	2A	1265	C
1	2A	1266	C
1	2A	1276	G
1	2A	1281	G
1	2A	1284	G
1	2A	1295	G
1	2A	1297	G
1	2A	1298	A
1	2A	1301	G
1	2A	1316	G
1	2A	1317	A
1	2A	1318	U
1	2A	1345	U
1	2A	1346	A
1	2A	1348	G
1	2A	1350	C
1	2A	1359	C
1	2A	1374	U
1	2A	1387	A
1	2A	1399	A
1	2A	1400	G
1	2A	1404	A
1	2A	1405	A
1	2A	1410	A
1	2A	1413	G
1	2A	1415	C
1	2A	1429	A
1	2A	1430	G

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Mol	Chain	Res	Type
1	2A	1431	C
1	2A	1448	C
1	2A	1461	G
1	2A	1462	C
1	2A	1465	U
1	2A	1466	G
1	2A	1472	A
1	2A	1473	C
1	2A	1486	G
1	2A	1490	A
1	2A	1495	A
1	2A	1496	G
1	2A	1501	G
1	2A	1502	G
1	2A	1507	G
1	2A	1513	C
1	2A	1517	A
1	2A	1524	G
1	2A	1528	G
1	2A	1534	U
1	2A	1535	A
1	2A	1538	C
1	2A	1542	U
1	2A	1554	C
1	2A	1555	A
1	2A	1570	G
1	2A	1589	C
1	2A	1604	A
1	2A	1605	G
1	2A	1612	A
1	2A	1615	A
1	2A	1624	U
1	2A	1626	A
1	2A	1630	C
1	2A	1631	A
1	2A	1653	A
1	2A	1654	A
1	2A	1655	A
1	2A	1663	A
1	2A	1667	G
1	2A	1686	C
1	2A	1687	A

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Mol	Chain	Res	Type
1	2A	1694	C
1	2A	1715	A
1	2A	1720	G
1	2A	1746	A
1	2A	1765	G
1	2A	1766	A
1	2A	1786	G
1	2A	1792	A
1	2A	1793	G
1	2A	1794	G
1	2A	1803	A
1	2A	1810	A
1	2A	1812	C
1	2A	1821	A
1	2A	1830	C
1	2A	1831	G
1	2A	1846	G
1	2A	1859	A
1	2A	1869	G
1	2A	1877	A
1	2A	1889	A
1	2A	1898	A
1	2A	1899	G
1	2A	1921	A
1	2A	1927	G
1	2A	1934	A
1	2A	1935	C
1	2A	1950	G
1	2A	1951	G
1	2A	1952	U
1	2A	1955	C
1	2A	1958	A
1	2A	1962	C
1	2A	1976	U
1	2A	1984	U
1	2A	1985	G
1	2A	1988	C
1	2A	1991	A
1	2A	1992	A
1	2A	1993	A
1	2A	2014	U
1	2A	2018	G

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Mol	Chain	Res	Type
1	2A	2041	A
1	2A	2044	G
1	2A	2052	A
1	2A	2054	A
1	2A	2057	C
1	2A	2064	C
1	2A	2067	G
1	2A	2076	C
1	2A	2077	G
1	2A	2081	A
1	2A	2082	G
1	2A	2083	A
1	2A	2090	G
1	2A	2120	U
1	2A	2206	C
1	2A	2209	C
1	2A	2210	U
1	2A	2213	G
1	2A	2219	A
1	2A	2226	G
1	2A	2227	G
1	2A	2228	A
1	2A	2236	A
1	2A	2246	G
1	2A	2250	G
1	2A	2278	A
1	2A	2279	A
1	2A	2280	A
1	2A	2286	C
1	2A	2289	A
1	2A	2290	G
1	2A	2294	C
1	2A	2298	A
1	2A	2299	A
1	2A	2300	G
1	2A	2304	C
1	2A	2308	C
1	2A	2316	A
1	2A	2318	G
1	2A	2319	G
1	2A	2322	A
1	2A	2323	U

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Mol	Chain	Res	Type
1	2A	2329	G
1	2A	2330	G
1	2A	2331	A
1	2A	2336	G
1	2A	2345	G
1	2A	2347	A
1	2A	2354	C
1	2A	2358	C
1	2A	2361	C
1	2A	2377	A
1	2A	2390	G
1	2A	2394	G
1	2A	2396	C
1	2A	2398	U
1	2A	2413	C
1	2A	2417	U
1	2A	2421	G
1	2A	2430	U
1	2A	2433	A
1	2A	2436	A
1	2A	2439	G
1	2A	2440	G
1	2A	2441	A
1	2A	2446	A
1	2A	2450	A
1	2A	2452	C
1	2A	2456	G
1	2A	2459	A
1	2A	2476	C
1	2A	2480	A
1	2A	2485	C
1	2A	2487	A
1	2A	2497	G
1	2A	2501	G
1	2A	2508	A
1	2A	2513	G
1	2A	2516	G
1	2A	2517	U
1	2A	2529	A
1	2A	2531	C
1	2A	2540	G
1	2A	2554	G

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Mol	Chain	Res	Type
1	2A	2565	U
1	2A	2566	U
1	2A	2577	A
1	2A	2578	G
1	2A	2585	G
1	2A	2590	C
1	2A	2613	A
1	2A	2620	U
1	2A	2622	U
1	2A	2623	C
1	2A	2640	A
1	2A	2641	G
1	2A	2657	C
1	2A	2665	A
1	2A	2700	U
1	2A	2701	C
1	2A	2714	C
1	2A	2724	A
1	2A	2725	A
1	2A	2726	G
1	2A	2738	U
1	2A	2745	A
1	2A	2756	G
1	2A	2763	G
1	2A	2769	A
1	2A	2776	A
1	2A	2777	A
1	2A	2778	G
1	2A	2790	A
1	2A	2795	G
1	2A	2801	C
1	2A	2805	G
1	2A	2812	G
1	2A	2817	U
1	2A	2827	G
1	2A	2829	A
1	2A	2830	A
1	2A	2842	G
1	2A	2843	G
1	2A	2845	U
1	2A	2869	A
1	2A	2881	G

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Mol	Chain	Res	Type
1	2A	2884	C
1	2A	2888	C
1	2A	2889	C
1	2A	2900	A
1	2A	2902	G
1	2A	2903	U
1	2A	2905	U
2	2B	2	C
2	2B	7	G
2	2B	9	G
2	2B	13	A
2	2B	16	G
2	2B	28	C
2	2B	34	U
2	2B	43	C
2	2B	45	A
2	2B	46	A
2	2B	52	A
2	2B	53	A
2	2B	56	G
2	2B	58	A
2	2B	59	A
2	2B	63	G
2	2B	67	G
2	2B	73	A
2	2B	85	G
2	2B	90	A
2	2B	110	G
2	2B	116	G
2	2B	119	G
2	2B	120	A
32	2a	6	U
32	2a	10	G
32	2a	15	U
32	2a	16	G
32	2a	23	G
32	2a	33	A
32	2a	39	G
32	2a	40	G
32	2a	48	C
32	2a	49	C
32	2a	51	A

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Mol	Chain	Res	Type
32	2a	52	A
32	2a	66	U
32	2a	67	G
32	2a	74	G
32	2a	79	G
32	2a	84	A
32	2a	85	C
32	2a	91	G
32	2a	95	A
32	2a	110	A
32	2a	115	C
32	2a	123	U
32	2a	124	G
32	2a	126	C
32	2a	138	A
32	2a	141	G
32	2a	151	G
32	2a	158	C
32	2a	169	C
32	2a	177	U
32	2a	202	A
32	2a	204	A
32	2a	211	U
32	2a	212	G
32	2a	213	C
32	2a	243	G
32	2a	247	G
32	2a	262	G
32	2a	263	C
32	2a	277	G
32	2a	285	G
32	2a	297	G
32	2a	317	A
32	2a	324	C
32	2a	326	C
32	2a	328	G
32	2a	340	A
32	2a	346	G
32	2a	347	G
32	2a	348	C
32	2a	349	A
32	2a	350	G

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Mol	Chain	Res	Type
32	2a	363	U
32	2a	365	C
32	2a	368	C
32	2a	380	G
32	2a	394	C
32	2a	400	U
32	2a	402	G
32	2a	408	A
32	2a	418	C
32	2a	425	U
32	2a	426	A
32	2a	435	A
32	2a	437	C
32	2a	447	A
32	2a	455	A
32	2a	456	C
32	2a	457	G
32	2a	463	A
32	2a	466	G
32	2a	470	G
32	2a	481	A
32	2a	482	U
32	2a	489	G
32	2a	495	C
32	2a	496	U
32	2a	497	C
32	2a	502	C
32	2a	505	G
32	2a	511	G
32	2a	515	U
32	2a	516	A
32	2a	517	A
32	2a	529	C
32	2a	531	A
32	2a	543	A
32	2a	545	U
32	2a	546	C
32	2a	552	G
32	2a	556	A
32	2a	557	A
32	2a	560	G
32	2a	561	G

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Mol	Chain	Res	Type
32	2a	575	U
32	2a	576	G
32	2a	580	C
32	2a	581	G
32	2a	591	A
32	2a	610	U
32	2a	614	G
32	2a	636	U
32	2a	637	A
32	2a	641	G
32	2a	649	A
32	2a	658	G
32	2a	671	A
32	2a	672	G
32	2a	677	G
32	2a	679	A
32	2a	686	A
32	2a	696	A
32	2a	705	G
32	2a	707	U
32	2a	708	G
32	2a	715	G
32	2a	733	C
32	2a	737	A
32	2a	738	C
32	2a	739	G
32	2a	744	G
32	2a	754	C
32	2a	758	G
32	2a	761	A
32	2a	777	U
32	2a	778	A
32	2a	783	G
32	2a	800	A
32	2a	801	C
32	2a	805	G
32	2a	811	U
32	2a	812	A
32	2a	813	G
32	2a	824	C
32	2a	825	U
32	2a	826	C

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Mol	Chain	Res	Type
32	2a	827	C
32	2a	831	G
32	2a	836	G
32	2a	837	A
32	2a	852	G
32	2a	880	G
32	2a	892	A
32	2a	904	G
32	2a	905	G
32	2a	909	C
32	2a	912	C
32	2a	913	A
32	2a	916	A
32	2a	920	G
32	2a	938	U
32	2a	939	U
32	2a	946	A
32	2a	947	A
32	2a	949	G
32	2a	952	A
32	2a	953	A
32	2a	954	G
32	2a	955	A
32	2a	956	A
32	2a	963	C
32	2a	967	C
32	2a	970	U
32	2a	971	G
32	2a	977	C
32	2a	979	A
32	2a	981	G
32	2a	983	A
32	2a	984	A
32	2a	986	C
32	2a	988	G
32	2a	1000	G
32	2a	1001	G
32	2a	1002	G
32	2a	1028	C
32	2a	1033	G
32	2a	1036	G
32	2a	1037	C

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Mol	Chain	Res	Type
32	2a	1038	A
32	2a	1039	U
32	2a	1048	U
32	2a	1049	C
32	2a	1064	G
32	2a	1077	G
32	2a	1078	U
32	2a	1084	A
32	2a	1093	A
32	2a	1096	C
32	2a	1099	C
32	2a	1101	C
32	2a	1104	U
32	2a	1105	U
32	2a	1107	G
32	2a	1110	G
32	2a	1112	C
32	2a	1113	A
32	2a	1117	G
32	2a	1118	U
32	2a	1119	U
32	2a	1120	C
32	2a	1121	G
32	2a	1122	G
32	2a	1123	C
32	2a	1129	A
32	2a	1140	A
32	2a	1141	C
32	2a	1142	U
32	2a	1146	C
32	2a	1149	G
32	2a	1158	A
32	2a	1165	A
32	2a	1168	G
32	2a	1172	G
32	2a	1173	A
32	2a	1178	U
32	2a	1184	G
32	2a	1191	C
32	2a	1193	U
32	2a	1194	U
32	2a	1196	C

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Mol	Chain	Res	Type
32	2a	1210	C
32	2a	1218	A
32	2a	1220	A
32	2a	1222	U
32	2a	1223	G
32	2a	1228	C
32	2a	1238	A
32	2a	1239	U
32	2a	1240	G
32	2a	1242	C
32	2a	1243	A
32	2a	1244	C
32	2a	1255	G
32	2a	1260	U
32	2a	1262	A
32	2a	1263	U
32	2a	1264	C
32	2a	1268	A
32	2a	1269	A
32	2a	1281	A
32	2a	1285	C
32	2a	1287	G
32	2a	1293	G
32	2a	1301	A
32	2a	1302	C
32	2a	1304	C
32	2a	1305	G
32	2a	1307	C
32	2a	1308	C
32	2a	1320	G
32	2a	1328	A
32	2a	1329	G
32	2a	1335	G
32	2a	1341	C
32	2a	1342	A
32	2a	1345	C
32	2a	1347	U
32	2a	1353	G
32	2a	1359	U
32	2a	1380	C
32	2a	1381	A
32	2a	1402	G

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Mol	Chain	Res	Type
32	2a	1425	G
32	2a	1426	G
32	2a	1427	A
32	2a	1430	C
32	2a	1431	U
32	2a	1432	A
32	2a	1433	C
32	2a	1434	G
32	2a	1469	G
32	2a	1480	A
32	2a	1481	A
32	2a	1482	G
32	2a	1483	G
32	2a	1484	U
32	2a	1495	G
32	2a	1498	G
32	2a	1507	G
32	2a	1508	G
32	2a	1509	A
32	2a	1510	U
53	2v	15	A
54	2x	6	G
54	2x	9	G
54	2x	13	C
54	2x	16	C
54	2x	17	C
54	2x	17(A)	U
54	2x	21	A
54	2x	31	G
54	2x	42	G
54	2x	47	U
54	2x	55	PSU
54	2x	56	C
54	2x	65	C
54	2x	70	G
54	2x	76	A

All (44) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	1A	183	A
1	1A	184	A

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Mol	Chain	Res	Type
1	1A	270	U
1	1A	301	A
1	1A	516	A
1	1A	792	A
1	1A	873	U
1	1A	1018	G
1	1A	1047	G
1	1A	1153	U
1	1A	1218	A
1	1A	1220	G
1	1A	1285	U
1	1A	1425	G
1	1A	1653	A
1	1A	2013	G
1	1A	2208	G
1	1A	2417	U
1	1A	2441	A
1	1A	2700	U
1	1A	2768	U
1	2A	183	A
1	2A	184	A
1	2A	203	G
1	2A	357	C
1	2A	516	A
1	2A	810	A
1	2A	902	C
1	2A	945	A
1	2A	1114	A
1	2A	1238	A
1	2A	1425	G
1	2A	1465	U
1	2A	1604	A
1	2A	1934	A
1	2A	2013	G
1	2A	2328	C
1	2A	2417	U
1	2A	2450	A
1	2A	2700	U
1	2A	2762	A
1	2A	2768	U
2	2B	42	C
2	2B	45	A

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

8 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$
54	4SU	1x	8	54	14,21,22	1.42	2 (14%)	15,30,33	2.61	2 (13%)
54	5MU	1x	54	54	15,22,23	1.11	2 (13%)	16,32,35	2.21	2 (12%)
54	PSU	1x	55	54	17,21,22	1.64	2 (11%)	20,30,33	3.35	6 (30%)
54	PSU	2x	55	54	17,21,22	1.51	2 (11%)	20,30,33	3.16	6 (30%)
54	5MU	2x	54	54	15,22,23	1.04	1 (6%)	16,32,35	2.01	1 (6%)
54	4SU	2x	8	54	14,21,22	1.29	2 (14%)	15,30,33	2.57	2 (13%)
54	5MC	2x	32	54	15,22,23	1.26	1 (6%)	19,32,35	1.42	3 (15%)
54	5MC	1x	32	54	15,22,23	1.28	1 (6%)	19,32,35	1.44	3 (15%)

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
54	4SU	1x	8	54	-	0/5/25/26	0/2/2/2
54	5MU	1x	54	54	-	2/5/25/26	0/2/2/2
54	PSU	1x	55	54	-	2/7/25/26	0/2/2/2
54	PSU	2x	55	54	-	2/7/25/26	0/2/2/2
54	5MU	2x	54	54	-	2/5/25/26	0/2/2/2
54	4SU	2x	8	54	-	1/5/25/26	0/2/2/2
54	5MC	2x	32	54	-	0/5/25/26	0/2/2/2
54	5MC	1x	32	54	-	0/5/25/26	0/2/2/2

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
54	1x	32	5MC	C5-C4	4.56	1.48	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
54	2x	32	5MC	C5-C4	4.50	1.48	1.41
54	1x	55	PSU	C5-C1'	-4.30	1.48	1.52
54	1x	8	4SU	C4-S4	-4.10	1.60	1.67
54	2x	55	PSU	C4-C5	3.88	1.49	1.41
54	1x	55	PSU	C4-C5	3.70	1.49	1.41
54	1x	54	5MU	C4-C5	3.43	1.48	1.41
54	2x	8	4SU	C4-S4	-3.41	1.61	1.67
54	2x	55	PSU	C5-C1'	-3.38	1.49	1.52
54	2x	54	5MU	C4-C5	3.34	1.48	1.41
54	1x	8	4SU	C2-N3	-2.92	1.32	1.38
54	2x	8	4SU	C2-N3	-2.88	1.32	1.38
54	1x	54	5MU	C2-N3	-2.13	1.34	1.38

All (25) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	1x	8	4SU	C2-N3-C4	8.96	128.15	115.15
54	2x	55	PSU	N1-C2-N3	-8.92	121.34	128.43
54	1x	55	PSU	N1-C2-N3	-8.75	121.47	128.43
54	2x	8	4SU	C2-N3-C4	8.43	127.37	115.15
54	1x	54	5MU	C4-N3-C2	8.04	121.93	115.14
54	1x	55	PSU	C4-N3-C2	8.01	121.91	115.14
54	2x	54	5MU	C4-N3-C2	7.67	121.62	115.14
54	2x	55	PSU	C4-N3-C2	6.88	120.95	115.14
54	1x	55	PSU	C5-C4-N3	-6.58	116.88	125.36
54	2x	55	PSU	C5-C4-N3	-5.00	118.92	125.36
54	2x	8	4SU	C5-C4-N3	-4.87	117.32	123.83
54	1x	8	4SU	C5-C4-N3	-4.29	118.09	123.83
54	2x	55	PSU	C6-N1-C2	4.25	122.38	115.36
54	2x	32	5MC	C2-N3-C4	3.99	120.83	116.02
54	2x	55	PSU	C5-C6-N1	-3.90	119.64	124.44
54	1x	32	5MC	C2-N3-C4	3.68	120.46	116.02
54	1x	55	PSU	C6-N1-C2	3.68	121.43	115.36
54	1x	55	PSU	C5-C6-N1	-3.04	120.71	124.44
54	1x	54	5MU	C5-C6-N1	-2.79	119.19	122.19
54	1x	32	5MC	N4-C4-N3	2.77	120.94	117.03
54	1x	32	5MC	C5-C6-N1	-2.54	119.46	122.19
54	2x	32	5MC	N4-C4-N3	2.41	120.44	117.03
54	2x	55	PSU	C5-C1'-C2'	-2.22	111.36	115.32
54	1x	55	PSU	C5-C1'-C2'	-2.09	111.60	115.32
54	2x	32	5MC	C5-C6-N1	-2.08	119.95	122.19

There are no chirality outliers.

All (9) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
54	1x	55	PSU	C3'-C4'-C5'-O5'
54	1x	55	PSU	O4'-C4'-C5'-O5'
54	2x	55	PSU	C3'-C4'-C5'-O5'
54	2x	55	PSU	O4'-C4'-C5'-O5'
54	2x	8	4SU	C2'-C1'-N1-C6
54	1x	54	5MU	C3'-C4'-C5'-O5'
54	1x	54	5MU	O4'-C4'-C5'-O5'
54	2x	54	5MU	C3'-C4'-C5'-O5'
54	2x	54	5MU	O4'-C4'-C5'-O5'

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 2436 ligands modelled in this entry, 2434 are monoatomic - leaving 2 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
58	SF4	1d	501	35	0,12,12	0.00	-	-		
58	SF4	2d	501	35	0,12,12	0.00	-	-		

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

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

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

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	2746/2915 (94%)	-0.05	16 (0%) 89 86	20, 42, 84, 108	0
1	2A	2790/2915 (95%)	-0.33	42 (1%) 73 68	24, 46, 91, 108	0
2	1B	120/121 (99%)	-0.21	0 100 100	35, 63, 80, 89	0
2	2B	120/121 (99%)	-0.05	1 (0%) 86 81	41, 68, 82, 91	0
3	1D	275/276 (99%)	-0.34	0 100 100	21, 40, 56, 78	0
3	2D	275/276 (99%)	-0.45	1 (0%) 92 91	22, 42, 59, 78	0
4	1E	204/206 (99%)	-0.20	0 100 100	21, 44, 65, 84	0
4	2E	204/206 (99%)	-0.25	0 100 100	23, 47, 67, 85	0
5	1F	203/210 (96%)	-0.23	0 100 100	22, 50, 74, 88	0
5	2F	203/210 (96%)	-0.31	1 (0%) 91 88	23, 54, 77, 90	0
6	1G	181/182 (99%)	-0.19	3 (1%) 70 63	50, 67, 79, 91	0
6	2G	181/182 (99%)	0.42	18 (9%) 7 4	54, 71, 81, 92	0
7	1H	174/180 (96%)	-0.12	1 (0%) 89 86	48, 63, 75, 85	0
7	2H	174/180 (96%)	0.75	23 (13%) 3 2	52, 68, 79, 86	0
8	1I	146/148 (98%)	0.07	1 (0%) 87 84	46, 74, 84, 90	0
8	2I	146/148 (98%)	0.47	6 (4%) 37 27	48, 74, 84, 90	0
9	1N	140/140 (100%)	-0.23	0 100 100	29, 47, 65, 76	0
9	2N	140/140 (100%)	-0.04	0 100 100	33, 50, 68, 78	0
10	1O	122/122 (100%)	-0.31	0 100 100	32, 44, 61, 74	0
10	2O	122/122 (100%)	-0.40	0 100 100	34, 47, 62, 74	0
11	1P	149/150 (99%)	-0.18	0 100 100	22, 53, 74, 81	0
11	2P	149/150 (99%)	0.24	5 (3%) 45 35	24, 56, 76, 83	0
12	1Q	141/141 (100%)	-0.08	2 (1%) 75 70	32, 48, 61, 79	0
12	2Q	141/141 (100%)	-0.37	1 (0%) 87 84	35, 51, 64, 78	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
13	1R	118/118 (100%)	-0.20	0 100 100	27, 39, 50, 64	0
13	2R	118/118 (100%)	-0.36	0 100 100	30, 42, 54, 66	0
14	1S	110/112 (98%)	-0.08	0 100 100	43, 61, 71, 77	0
14	2S	110/112 (98%)	0.59	8 (7%) 15 8	48, 63, 76, 79	0
15	1T	131/146 (89%)	-0.26	0 100 100	37, 49, 72, 84	0
15	2T	131/146 (89%)	-0.39	0 100 100	40, 50, 73, 83	0
16	1U	116/118 (98%)	-0.17	0 100 100	27, 39, 56, 74	0
16	2U	116/118 (98%)	-0.33	1 (0%) 84 80	29, 43, 61, 74	0
17	1V	101/101 (100%)	-0.23	0 100 100	28, 47, 65, 75	0
17	2V	101/101 (100%)	-0.04	0 100 100	32, 53, 69, 76	0
18	1W	112/113 (99%)	-0.34	1 (0%) 84 80	27, 36, 55, 89	0
18	2W	112/113 (99%)	-0.25	0 100 100	28, 39, 57, 90	0
19	1X	95/96 (98%)	-0.18	0 100 100	26, 46, 66, 81	0
19	2X	95/96 (98%)	-0.09	3 (3%) 47 37	29, 49, 68, 81	0
20	1Y	107/110 (97%)	-0.02	1 (0%) 84 80	42, 59, 76, 86	0
20	2Y	107/110 (97%)	0.61	7 (6%) 18 11	47, 62, 79, 88	0
21	1Z	186/206 (90%)	-0.37	0 100 100	48, 66, 79, 89	0
21	2Z	186/206 (90%)	0.44	11 (5%) 22 14	53, 69, 81, 91	0
22	10	75/85 (88%)	-0.49	0 100 100	18, 36, 48, 61	0
22	20	75/85 (88%)	0.27	4 (5%) 26 17	46, 62, 73, 80	0
23	11	97/98 (98%)	-0.18	1 (1%) 82 77	28, 48, 72, 77	0
23	21	97/98 (98%)	-0.15	1 (1%) 82 77	31, 51, 72, 75	0
24	12	70/72 (97%)	-0.15	0 100 100	43, 56, 70, 74	0
24	22	70/72 (97%)	0.06	1 (1%) 75 70	46, 60, 73, 74	0
25	13	59/60 (98%)	-0.12	0 100 100	32, 44, 64, 77	0
25	23	59/60 (98%)	0.54	1 (1%) 70 63	35, 48, 66, 77	0
26	14	69/71 (97%)	0.06	6 (8%) 10 5	47, 71, 93, 97	0
26	24	69/71 (97%)	0.71	11 (15%) 1 1	56, 89, 96, 98	0
27	15	59/60 (98%)	-0.59	0 100 100	16, 28, 46, 72	0
27	25	59/60 (98%)	-0.34	0 100 100	29, 49, 66, 75	0
28	16	53/54 (98%)	-0.46	0 100 100	24, 38, 54, 63	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
28	26	53/54 (98%)	-0.29	0 100 100	41, 58, 74, 79	0
29	17	48/49 (97%)	-0.17	1 (2%) 63 54	24, 32, 64, 78	0
29	27	48/49 (97%)	-0.12	3 (6%) 20 12	27, 34, 66, 77	0
30	18	64/65 (98%)	-0.13	0 100 100	32, 39, 49, 60	0
30	28	64/65 (98%)	-0.06	1 (1%) 72 66	35, 43, 54, 62	0
31	19	37/37 (100%)	0.08	0 100 100	38, 49, 66, 70	0
31	29	37/37 (100%)	0.39	3 (8%) 12 6	44, 52, 67, 72	0
32	1a	1477/1521 (97%)	-0.10	34 (2%) 60 51	32, 70, 96, 113	0
32	2a	1483/1521 (97%)	-0.03	28 (1%) 66 59	44, 77, 98, 111	0
33	1b	231/256 (90%)	0.36	17 (7%) 14 8	66, 81, 93, 101	0
33	2b	231/256 (90%)	0.55	22 (9%) 8 4	68, 86, 96, 102	0
34	1c	206/239 (86%)	0.24	15 (7%) 15 8	65, 81, 88, 95	0
34	2c	206/239 (86%)	0.48	16 (7%) 13 7	69, 82, 89, 93	0
35	1d	208/209 (99%)	0.18	10 (4%) 30 21	51, 75, 88, 96	0
35	2d	208/209 (99%)	-0.02	1 (0%) 91 88	58, 73, 85, 90	0
36	1e	148/162 (91%)	-0.21	0 100 100	45, 67, 77, 84	0
36	2e	148/162 (91%)	-0.18	1 (0%) 87 84	56, 74, 83, 89	0
37	1f	100/101 (99%)	-0.23	0 100 100	57, 72, 80, 88	0
37	2f	100/101 (99%)	-0.24	2 (2%) 65 56	58, 73, 83, 87	0
38	1g	155/156 (99%)	0.34	12 (7%) 13 7	67, 77, 91, 95	0
38	2g	155/156 (99%)	0.68	13 (8%) 11 5	67, 78, 90, 93	0
39	1h	137/138 (99%)	-0.06	0 100 100	53, 69, 77, 85	0
39	2h	137/138 (99%)	0.12	2 (1%) 73 68	65, 76, 83, 89	0
40	1i	127/128 (99%)	0.52	10 (7%) 12 7	64, 83, 91, 95	0
40	2i	127/128 (99%)	1.22	25 (19%) 1 0	65, 84, 92, 98	0
41	1j	97/105 (92%)	0.90	13 (13%) 3 1	67, 85, 93, 97	0
41	2j	96/105 (91%)	1.07	13 (13%) 3 1	69, 86, 94, 97	0
42	1k	114/129 (88%)	-0.07	2 (1%) 68 61	43, 67, 80, 88	0
42	2k	114/129 (88%)	0.25	3 (2%) 56 46	56, 76, 86, 91	0
43	1l	122/132 (92%)	-0.17	1 (0%) 86 81	43, 61, 72, 79	0
43	2l	122/132 (92%)	-0.05	3 (2%) 57 47	52, 67, 75, 81	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
44	1m	118/126 (93%)	0.11	0 100 100	59, 77, 85, 94	0
44	2m	116/126 (92%)	0.34	12 (10%) 6 3	66, 80, 86, 93	0
45	1n	60/61 (98%)	0.30	3 (5%) 28 19	62, 73, 83, 84	0
45	2n	60/61 (98%)	1.29	15 (25%) 0 0	76, 84, 90, 92	0
46	1o	88/89 (98%)	0.04	1 (1%) 80 75	47, 64, 80, 90	0
46	2o	88/89 (98%)	0.11	1 (1%) 80 75	58, 72, 83, 86	0
47	1p	82/88 (93%)	0.58	5 (6%) 21 13	61, 76, 87, 94	0
47	2p	82/88 (93%)	0.28	2 (2%) 59 49	57, 70, 82, 90	0
48	1q	99/105 (94%)	-0.02	0 100 100	47, 67, 78, 82	0
48	2q	99/105 (94%)	0.16	3 (3%) 50 40	56, 72, 80, 87	0
49	1r	68/88 (77%)	0.40	3 (4%) 34 24	54, 68, 81, 87	0
49	2r	68/88 (77%)	0.61	7 (10%) 6 3	61, 72, 82, 92	0
50	1s	84/93 (90%)	0.59	3 (3%) 42 32	66, 78, 86, 97	0
50	2s	83/93 (89%)	1.48	25 (30%) 0 0	73, 89, 96, 103	0
51	1t	96/106 (90%)	0.26	1 (1%) 82 77	58, 73, 81, 88	0
51	2t	96/106 (90%)	0.21	0 100 100	57, 71, 81, 86	0
52	1u	23/27 (85%)	0.71	1 (4%) 35 25	68, 75, 80, 84	0
52	2u	23/27 (85%)	1.41	6 (26%) 0 0	69, 76, 83, 85	0
53	1v	5/24 (20%)	0.23	0 100 100	63, 66, 85, 92	0
53	2v	5/24 (20%)	0.96	1 (20%) 1 0	66, 69, 85, 93	0
54	1x	72/77 (93%)	-0.13	0 100 100	32, 66, 81, 96	0
54	2x	72/77 (93%)	0.04	1 (1%) 75 70	34, 69, 83, 97	0
55	1z	13/19 (68%)	0.15	0 100 100	26, 36, 52, 56	0
55	2z	12/19 (63%)	-0.05	0 100 100	28, 39, 53, 55	0
All	All	20521/21482 (95%)	-0.02	519 (2%) 57 47	16, 61, 89, 113	0

All (519) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
32	1a	980	G	8.7
32	1a	981	G	7.6
1	2A	2812	G	6.4
38	1g	81	GLY	6.3
32	1a	979	A	6.3

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Mol	Chain	Res	Type	RSRZ
20	2Y	1	MET	5.9
32	2a	981	G	5.8
41	1j	10	GLY	5.7
38	1g	79	ARG	5.5
40	2i	21	PRO	5.5
38	2g	82	GLY	5.5
20	1Y	1	MET	5.4
32	2a	979	A	5.4
32	2a	980	G	5.4
40	2i	7	THR	5.3
38	2g	83	ALA	5.2
52	2u	14	TRP	5.2
32	1a	982	G	5.1
38	2g	156	TRP	4.9
1	2A	2811	A	4.7
31	29	37	GLY	4.7
41	1j	98	ILE	4.7
45	2n	25	VAL	4.6
38	1g	80	VAL	4.6
1	1A	2815	G	4.6
1	1A	1554	C	4.6
7	2H	112	PRO	4.5
32	1a	209	U	4.4
34	2c	189	ALA	4.4
38	2g	78	ARG	4.4
32	1a	211	U	4.4
41	2j	75	ILE	4.4
26	24	49	PHE	4.4
38	1g	82	GLY	4.3
38	1g	156	TRP	4.3
29	17	48	LYS	4.3
1	2A	2815	G	4.3
33	2b	132	LYS	4.3
50	2s	12	ASP	4.3
33	2b	152	PHE	4.3
41	2j	6	ILE	4.2
33	1b	214	ILE	4.2
50	2s	31	ILE	4.2
7	2H	115	VAL	4.2
26	24	68	ARG	4.2
1	2A	1091	A	4.2
45	2n	49	HIS	4.2

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Mol	Chain	Res	Type	RSRZ
52	2u	6	ARG	4.1
7	2H	111	HIS	4.1
40	2i	8	GLY	4.0
40	2i	15	ALA	4.0
40	1i	15	ALA	4.0
33	2b	133	LYS	3.9
40	2i	61	ALA	3.9
49	1r	25	THR	3.9
26	24	45	GLY	3.9
41	2j	63	PHE	3.9
6	2G	28	VAL	3.8
32	1a	978	U	3.8
1	2A	2904	C	3.8
14	2S	58	LEU	3.8
38	2g	154	TYR	3.8
7	2H	113	VAL	3.8
34	1c	81	GLY	3.8
1	2A	2805	G	3.7
1	2A	2813	C	3.7
1	2A	1554	C	3.7
32	2a	1509	A	3.7
49	2r	66	LEU	3.7
50	2s	16	LEU	3.7
32	2a	1510	U	3.7
32	2a	978	U	3.6
32	2a	982	G	3.6
40	2i	66	ARG	3.6
41	2j	20	ALA	3.6
34	2c	159	GLY	3.6
33	2b	187	LEU	3.6
33	2b	131	PRO	3.6
45	2n	36	PHE	3.6
33	1b	227	GLY	3.6
41	1j	85	LEU	3.5
1	2A	678	A	3.5
49	2r	46	GLU	3.5
35	1d	23	GLY	3.5
38	2g	80	VAL	3.5
40	1i	19	LEU	3.4
34	1c	87	LEU	3.4
45	2n	39	LEU	3.4
26	14	55	ARG	3.4

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Mol	Chain	Res	Type	RSRZ
21	2Z	5	LEU	3.4
34	2c	180	ALA	3.4
38	2g	84	ASN	3.4
40	2i	36	TYR	3.4
19	2X	92	LEU	3.3
41	1j	90	LEU	3.3
50	2s	8	GLY	3.3
32	1a	1025	G	3.3
48	2q	8	GLY	3.3
41	1j	96	ILE	3.3
40	2i	41	VAL	3.3
35	2d	130	GLY	3.3
50	2s	38	SER	3.3
32	2a	1239	U	3.3
41	2j	72	VAL	3.3
33	2b	97	TRP	3.3
19	2X	69	TYR	3.2
33	1b	28	PHE	3.2
20	2Y	5	MET	3.2
26	24	67	TYR	3.2
32	1a	1023	U	3.2
32	2a	1000	G	3.2
41	1j	72	VAL	3.2
40	2i	62	TYR	3.2
1	1A	2206	C	3.2
7	2H	103	LEU	3.2
41	2j	85	LEU	3.2
1	2A	1106	U	3.2
34	2c	57	ILE	3.2
1	2A	217	A	3.2
1	2A	2902	G	3.2
32	1a	1024	A	3.2
1	1A	2806	C	3.2
1	2A	2806	C	3.2
40	1i	98	PRO	3.2
21	2Z	160	GLY	3.1
33	1b	135	GLN	3.1
25	23	26	LEU	3.1
50	2s	80	TYR	3.1
1	1A	2205	G	3.1
32	2a	1025	G	3.1
34	2c	179	ARG	3.1

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Mol	Chain	Res	Type	RSRZ
6	2G	137	GLU	3.1
8	2I	11	ASN	3.1
39	2h	122	ARG	3.1
40	1i	33	PHE	3.1
31	29	5	ALA	3.1
34	2c	154	SER	3.1
40	2i	9	ARG	3.1
45	2n	35	ARG	3.1
6	2G	25	TYR	3.1
32	2a	1265	G	3.1
50	2s	20	LEU	3.1
1	1A	2814	C	3.1
32	2a	1022	C	3.1
50	2s	52	TYR	3.1
1	1A	2813	C	3.1
38	1g	78	ARG	3.1
50	2s	40	ILE	3.1
50	2s	43	GLU	3.1
7	2H	114	VAL	3.0
40	2i	37	PHE	3.0
1	1A	2805	G	3.0
42	1k	13	GLN	3.0
38	2g	16	LEU	3.0
50	1s	56	GLN	3.0
32	2a	1021	C	3.0
33	2b	232	PRO	3.0
42	2k	31	THR	3.0
41	2j	98	ILE	3.0
44	2m	82	MET	3.0
38	2g	86	GLN	3.0
46	2o	87	ILE	3.0
1	2A	2121	G	3.0
1	2A	2816	G	3.0
45	2n	37	PHE	3.0
32	1a	88	C	3.0
1	2A	1130	A	3.0
32	1a	984	A	3.0
6	1G	51	ARG	3.0
49	2r	85	LEU	3.0
32	1a	208	C	3.0
7	2H	107	VAL	3.0
47	1p	51	VAL	3.0

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Mol	Chain	Res	Type	RSRZ
7	2H	6	ARG	2.9
34	2c	155	GLY	2.9
44	2m	95	GLY	2.9
42	2k	13	GLN	2.9
38	1g	153	HIS	2.9
6	2G	2	PRO	2.9
32	2a	1268	A	2.9
49	2r	43	PHE	2.9
53	2v	14	A	2.9
50	2s	76	PRO	2.9
41	1j	66	ARG	2.9
41	1j	71	LEU	2.9
32	2a	211	U	2.9
34	2c	39	ILE	2.9
1	2A	1149	C	2.9
7	2H	102	ALA	2.9
32	1a	1239	U	2.9
33	2b	227	GLY	2.9
33	1b	232	PRO	2.9
50	2s	13	ASP	2.9
50	2s	53	ASN	2.9
41	2j	81	THR	2.9
44	2m	102	ARG	2.9
32	1a	1002	G	2.9
41	2j	8	LEU	2.9
6	2G	48	GLU	2.8
8	2I	14	ASP	2.8
41	1j	4	ILE	2.8
49	2r	58	LEU	2.8
49	2r	23	LYS	2.8
1	1A	2905	U	2.8
50	2s	49	ILE	2.8
34	1c	206	GLU	2.8
19	2X	68	ARG	2.8
32	1a	977	C	2.8
1	2A	697	G	2.8
1	2A	1104	G	2.8
24	22	1	MET	2.8
35	1d	152	SER	2.8
50	2s	34	TRP	2.8
11	2P	91	PHE	2.8
49	1r	31	LEU	2.8

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Mol	Chain	Res	Type	RSRZ
7	2H	105	LEU	2.7
7	2H	110	SER	2.7
34	1c	78	GLY	2.7
50	2s	41	VAL	2.7
40	1i	36	TYR	2.7
1	2A	1129	A	2.7
20	2Y	45	VAL	2.7
33	2b	197	VAL	2.7
38	2g	105	VAL	2.7
52	2u	9	ARG	2.7
7	1H	2	SER	2.7
21	2Z	143	GLY	2.7
32	2a	1024	A	2.7
26	24	59	PHE	2.7
34	2c	77	ILE	2.7
40	2i	20	ARG	2.7
6	2G	27	ASN	2.7
38	2g	79	ARG	2.7
32	1a	999	U	2.7
21	2Z	96	VAL	2.7
1	2A	2814	C	2.7
32	1a	72	C	2.7
47	2p	59	TRP	2.6
47	1p	19	ILE	2.6
50	2s	24	ALA	2.6
1	2A	1089	G	2.6
26	14	53	GLU	2.6
32	2a	983	A	2.6
40	2i	5	TYR	2.6
50	2s	71	LEU	2.6
44	2m	75	ALA	2.6
14	2S	54	LEU	2.6
20	2Y	2	ARG	2.6
35	1d	167	GLY	2.6
8	2I	77	LEU	2.6
8	2I	19	VAL	2.6
22	20	72	ARG	2.6
1	2A	2905	U	2.6
32	2a	1023	U	2.6
33	1b	16	HIS	2.6
45	2n	42	ILE	2.6
32	1a	985	C	2.6

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
32	1a	1026	C	2.6
45	2n	38	GLY	2.6
6	1G	49	ASP	2.6
41	1j	97	GLU	2.6
43	2l	64	TYR	2.6
52	1u	18	TYR	2.6
33	2b	101	MET	2.6
33	2b	118	LEU	2.6
1	2A	2804	G	2.6
32	1a	87	C	2.6
34	2c	66	VAL	2.6
43	2l	62	SER	2.6
50	2s	35	SER	2.6
7	2H	106	THR	2.5
54	2x	47	U	2.5
38	1g	83	ALA	2.5
41	2j	27	ALA	2.5
1	2A	1128	U	2.5
6	2G	86	MET	2.5
34	2c	6	HIS	2.5
14	2S	29	PHE	2.5
33	1b	233	SER	2.5
37	2f	97	PHE	2.5
1	1A	1220	G	2.5
7	2H	128	PRO	2.5
41	1j	78	ASN	2.5
1	1A	1149	C	2.5
34	2c	186	PHE	2.5
12	2Q	59	ARG	2.5
35	1d	176	LEU	2.5
52	2u	17	THR	2.5
22	20	45	PHE	2.5
33	2b	31	TYR	2.5
34	1c	65	ALA	2.5
34	1c	100	ALA	2.5
32	2a	1002	G	2.5
7	2H	44	VAL	2.5
52	2u	22	ARG	2.5
34	2c	87	LEU	2.5
50	1s	16	LEU	2.5
6	2G	29	TRP	2.5
6	2G	142	PRO	2.5

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Mol	Chain	Res	Type	RSRZ
44	2m	7	VAL	2.5
14	2S	84	GLN	2.5
11	2P	116	GLY	2.5
33	1b	122	PHE	2.4
1	2A	1132	G	2.4
1	2A	2125	G	2.4
22	20	69	PHE	2.4
26	14	59	PHE	2.4
21	2Z	164	ALA	2.4
26	24	46	GLN	2.4
21	2Z	161	VAL	2.4
32	2a	977	C	2.4
44	2m	94	ARG	2.4
21	2Z	171	ILE	2.4
33	1b	222	ILE	2.4
49	2r	56	THR	2.4
32	2a	209	U	2.4
20	2Y	58	GLY	2.4
7	2H	95	ARG	2.4
32	2a	986	C	2.4
14	2S	34	HIS	2.4
40	2i	63	ILE	2.4
26	24	52	THR	2.4
20	2Y	51	VAL	2.4
11	2P	90	ARG	2.4
12	1Q	59	ARG	2.4
32	1a	1022	C	2.4
33	1b	225	ALA	2.4
33	1b	201	ILE	2.4
44	2m	92	HIS	2.4
3	2D	273	ARG	2.4
33	2b	122	PHE	2.4
32	2a	999	U	2.4
38	2g	130	GLY	2.4
43	2l	28	LYS	2.4
1	1A	2904	C	2.4
31	29	13	LYS	2.4
45	2n	8	GLU	2.4
47	1p	39	TYR	2.4
32	1a	1268	A	2.4
34	2c	160	ALA	2.4
45	2n	2	ALA	2.4

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Mol	Chain	Res	Type	RSRZ
1	1A	2209	C	2.4
51	1t	55	ILE	2.4
1	2A	1102	A	2.4
21	2Z	133	ILE	2.4
11	2P	122	PRO	2.3
1	1A	2804	G	2.3
45	1n	2	ALA	2.3
23	1l	2	SER	2.3
33	2b	37	ASN	2.3
35	1d	175	SER	2.3
16	2U	88	ILE	2.3
38	1g	84	ASN	2.3
50	1s	40	ILE	2.3
1	2A	300	C	2.3
39	2h	131	GLY	2.3
32	1a	86	U	2.3
1	2A	1101	G	2.3
1	2A	1553	A	2.3
40	2i	6	GLY	2.3
32	2a	1026	C	2.3
34	1c	64	VAL	2.3
40	2i	88	TYR	2.3
33	2b	48	MET	2.3
33	2b	162	ILE	2.3
40	2i	79	LEU	2.3
33	2b	228	GLY	2.3
33	1b	130	ARG	2.3
40	2i	28	VAL	2.3
26	14	57	GLU	2.3
6	2G	19	LEU	2.3
14	2S	35	ILE	2.3
41	1j	6	ILE	2.3
41	2j	74	ILE	2.3
45	1n	7	ILE	2.3
6	2G	42	GLY	2.3
44	2m	103	THR	2.3
6	2G	26	GLN	2.3
18	1W	111	HIS	2.3
7	2H	96	ALA	2.3
32	1a	1121	G	2.3
40	2i	92	TYR	2.3
40	2i	26	VAL	2.3

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Mol	Chain	Res	Type	RSRZ
5	2F	14	PRO	2.3
32	1a	707	U	2.3
33	2b	62	ALA	2.3
38	1g	3	ARG	2.3
43	1l	64	TYR	2.3
45	2n	48	ALA	2.3
34	1c	39	ILE	2.3
34	2c	124	ILE	2.3
32	2a	976	G	2.3
40	2i	72	GLY	2.3
1	2A	1071	U	2.3
33	2b	10	LEU	2.3
1	1A	1098	C	2.3
32	2a	998	C	2.3
2	2B	118	G	2.3
26	14	49	PHE	2.2
7	2H	52	VAL	2.2
32	1a	983	A	2.2
40	2i	10	ARG	2.2
1	2A	2817	U	2.2
22	20	75	LEU	2.2
46	1o	89	GLY	2.2
47	2p	19	ILE	2.2
6	2G	160	VAL	2.2
7	2H	101	ARG	2.2
32	1a	825	U	2.2
50	2s	42	PRO	2.2
34	1c	193	TYR	2.2
30	28	21	LYS	2.2
32	1a	1120	C	2.2
48	2q	100	LYS	2.2
14	2S	26	LEU	2.2
33	2b	70	PHE	2.2
40	1i	63	ILE	2.2
42	1k	25	TYR	2.2
34	1c	2	GLY	2.2
41	1j	69	ASN	2.2
41	2j	78	ASN	2.2
50	2s	23	ASN	2.2
6	2G	17	PRO	2.2
34	1c	160	ALA	2.2
44	2m	78	ILE	2.2

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Mol	Chain	Res	Type	RSRZ
35	1d	104	VAL	2.2
37	2f	6	VAL	2.2
1	2A	1120	C	2.2
1	2A	2903	U	2.2
11	2P	85	LEU	2.2
21	2Z	125	LEU	2.2
40	1i	37	PHE	2.2
47	1p	59	TRP	2.2
6	2G	139	LEU	2.2
26	24	66	SER	2.2
40	1i	28	VAL	2.2
50	2s	64	GLU	2.2
7	2H	97	ARG	2.2
29	27	47	ARG	2.2
44	2m	80	ARG	2.2
32	1a	1000	G	2.2
32	2a	707	U	2.2
6	2G	39	ILE	2.2
38	1g	77	SER	2.2
45	2n	34	TYR	2.2
21	2Z	163	LEU	2.1
32	2a	1148	C	2.1
6	1G	2	PRO	2.1
40	2i	27	THR	2.1
33	1b	229	VAL	2.1
44	2m	110	ARG	2.1
1	2A	1087	G	2.1
40	1i	41	VAL	2.1
45	2n	18	VAL	2.1
50	2s	45	VAL	2.1
26	24	8	LYS	2.1
35	1d	158	ILE	2.1
1	2A	2206	C	2.1
26	14	50	VAL	2.1
34	1c	80	GLY	2.1
40	2i	30	GLY	2.1
7	2H	164	TYR	2.1
48	2q	22	LEU	2.1
7	2H	92	ILE	2.1
33	2b	134	GLU	2.1
1	1A	695	C	2.1
35	1d	169	LYS	2.1

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Mol	Chain	Res	Type	RSRZ
41	2j	34	VAL	2.1
33	1b	221	LEU	2.1
40	2i	99	LEU	2.1
44	2m	104	ARG	2.1
49	1r	29	PHE	2.1
1	2A	1090	A	2.1
26	24	54	GLY	2.1
14	2S	31	SER	2.1
33	1b	70	PHE	2.1
33	1b	33	TYR	2.1
47	1p	38	TYR	2.1
21	2Z	146	ILE	2.1
8	2I	13	GLY	2.1
35	1d	180	GLY	2.1
40	1i	8	GLY	2.1
34	1c	179	ARG	2.1
1	2A	934	C	2.1
1	2A	1088	C	2.1
6	2G	161	THR	2.1
26	24	44	THR	2.1
52	2u	13	ILE	2.1
7	2H	45	VAL	2.1
8	2I	81	VAL	2.1
35	1d	165	MET	2.1
29	27	48	LYS	2.1
38	2g	77	SER	2.1
29	27	46	VAL	2.1
33	1b	129	GLU	2.1
32	1a	212	G	2.1
34	1c	201	TYR	2.0
45	2n	7	ILE	2.0
38	1g	130	GLY	2.0
45	1n	8	GLU	2.0
8	1I	35	LEU	2.0
42	2k	125	PHE	2.0
1	2A	1103	G	2.0
23	21	2	SER	2.0
32	1a	986	C	2.0
33	2b	233	SER	2.0
50	2s	62	ILE	2.0
6	2G	15	VAL	2.0
12	1Q	60	ARG	2.0

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Mol	Chain	Res	Type	RSRZ
36	2e	20	GLN	2.0
7	2H	100	GLY	2.0
1	2A	2208	G	2.0
32	1a	73	C	2.0
34	1c	184	TYR	2.0
34	2c	167	TRP	2.0
32	1a	156	A	2.0
45	2n	12	ARG	2.0
50	2s	48	THR	2.0
20	2Y	90	LEU	2.0

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

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
54	PSU	2x	55	20/21	0.87	0.15	54,68,77,91	0
54	5MU	2x	54	21/22	0.92	0.17	68,73,80,91	0
54	PSU	1x	55	20/21	0.93	0.15	51,64,77,80	0
54	4SU	2x	8	20/21	0.93	0.12	73,78,85,87	0
54	5MC	2x	32	21/22	0.94	0.21	61,75,84,88	0
54	5MU	1x	54	21/22	0.95	0.15	55,62,73,81	0
54	4SU	1x	8	20/21	0.95	0.13	58,63,74,74	0
54	5MC	1x	32	21/22	0.97	0.17	40,61,68,75	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	1A	3942	1/1	0.27	0.17	53,53,53,53	0
56	MG	1a	1843	1/1	0.29	0.14	69,69,69,69	0
56	MG	1A	3346	1/1	0.42	0.18	76,76,76,76	0
56	MG	1A	3899	1/1	0.49	0.11	80,80,80,80	0
56	MG	2a	1741	1/1	0.49	0.24	89,89,89,89	0
56	MG	1H	203	1/1	0.52	0.68	95,95,95,95	0
56	MG	1l	201	1/1	0.52	0.13	74,74,74,74	0
56	MG	1A	3336	1/1	0.53	0.25	62,62,62,62	0
56	MG	1a	1698	1/1	0.54	0.31	64,64,64,64	0
56	MG	2A	3496	1/1	0.59	0.42	66,66,66,66	0
56	MG	1a	1783	1/1	0.59	0.15	78,78,78,78	0
56	MG	1a	1902	1/1	0.60	0.59	92,92,92,92	0
56	MG	1A	3545	1/1	0.62	0.47	61,61,61,61	0
56	MG	1A	3307	1/1	0.62	0.50	61,61,61,61	0
56	MG	1a	1658	1/1	0.62	0.12	69,69,69,69	0
56	MG	1a	1697	1/1	0.63	0.19	67,67,67,67	0
56	MG	2A	3390	1/1	0.64	0.19	55,55,55,55	0
57	ZN	24	501	1/1	0.65	0.07	114,114,114,114	0
56	MG	1A	3505	1/1	0.66	0.27	58,58,58,58	0
56	MG	2A	3554	1/1	0.66	0.25	70,70,70,70	0
56	MG	1A	3376	1/1	0.67	0.31	55,55,55,55	0
56	MG	1x	101	1/1	0.67	0.67	89,89,89,89	0
56	MG	2a	1666	1/1	0.67	0.21	65,65,65,65	0
56	MG	1A	3069	1/1	0.68	0.14	58,58,58,58	0
56	MG	1a	1784	1/1	0.69	0.23	95,95,95,95	0
56	MG	1a	1819	1/1	0.69	0.40	59,59,59,59	0
56	MG	2A	3291	1/1	0.69	0.13	48,48,48,48	0
56	MG	1A	3287	1/1	0.69	0.36	43,43,43,43	0
56	MG	1A	3694	1/1	0.69	0.16	76,76,76,76	0
56	MG	1h	3001	1/1	0.70	0.12	70,70,70,70	0
56	MG	1N	201	1/1	0.70	0.46	73,73,73,73	0
56	MG	2a	1633	1/1	0.70	0.13	86,86,86,86	0
56	MG	2A	3492	1/1	0.71	0.18	43,43,43,43	0
56	MG	2a	1715	1/1	0.71	0.23	82,82,82,82	0
56	MG	1B	227	1/1	0.71	0.52	70,70,70,70	0
56	MG	1A	3534	1/1	0.71	0.15	64,64,64,64	0
56	MG	1A	3570	1/1	0.72	0.13	32,32,32,32	0
56	MG	1A	3496	1/1	0.72	0.16	57,57,57,57	0
56	MG	2A	3528	1/1	0.72	0.37	60,60,60,60	0
56	MG	1a	1668	1/1	0.73	0.18	81,81,81,81	0
56	MG	2a	1749	1/1	0.73	0.23	66,66,66,66	0
56	MG	1a	1901	1/1	0.73	0.25	65,65,65,65	0
56	MG	1a	1889	1/1	0.73	0.23	68,68,68,68	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	1A	3756	1/1	0.73	0.19	43,43,43,43	0
56	MG	1A	3918	1/1	0.73	0.82	47,47,47,47	0
56	MG	1B	213	1/1	0.73	0.10	68,68,68,68	0
56	MG	1A	3400	1/1	0.74	0.30	69,69,69,69	0
56	MG	2a	1614	1/1	0.74	0.43	55,55,55,55	0
56	MG	20	8001	1/1	0.74	0.21	67,67,67,67	0
56	MG	1A	3564	1/1	0.74	0.11	72,72,72,72	0
56	MG	2A	3107	1/1	0.74	0.26	54,54,54,54	0
56	MG	2A	3356	1/1	0.74	0.27	41,41,41,41	0
56	MG	1A	3280	1/1	0.74	0.11	76,76,76,76	0
56	MG	1D	311	1/1	0.75	0.45	58,58,58,58	0
56	MG	2A	3094	1/1	0.75	0.23	45,45,45,45	0
56	MG	1A	3409	1/1	0.75	0.38	51,51,51,51	0
56	MG	1A	3550	1/1	0.75	0.21	81,81,81,81	0
56	MG	1A	3353	1/1	0.75	0.63	63,63,63,63	0
56	MG	1A	4066	1/1	0.75	0.24	51,51,51,51	0
56	MG	1A	3385	1/1	0.75	0.51	56,56,56,56	0
56	MG	1a	1772	1/1	0.75	0.10	83,83,83,83	0
56	MG	2A	3438	1/1	0.76	0.14	39,39,39,39	0
56	MG	2a	1758	1/1	0.76	0.18	59,59,59,59	0
56	MG	1A	4030	1/1	0.76	0.31	77,77,77,77	0
56	MG	2A	3535	1/1	0.76	0.11	51,51,51,51	0
56	MG	1A	3871	1/1	0.76	0.27	45,45,45,45	0
56	MG	1A	3458	1/1	0.76	0.17	71,71,71,71	0
56	MG	1A	3389	1/1	0.76	0.34	50,50,50,50	0
56	MG	1A	3891	1/1	0.76	0.28	65,65,65,65	0
56	MG	2a	1687	1/1	0.76	0.10	62,62,62,62	0
56	MG	2A	3352	1/1	0.76	0.15	62,62,62,62	0
56	MG	1a	1754	1/1	0.77	0.29	60,60,60,60	0
56	MG	1x	105	1/1	0.77	0.15	65,65,65,65	0
56	MG	1A	4059	1/1	0.77	0.24	52,52,52,52	0
56	MG	1a	1606	1/1	0.77	0.09	62,62,62,62	0
56	MG	2a	1630	1/1	0.77	0.12	60,60,60,60	0
56	MG	2A	3212	1/1	0.77	0.28	64,64,64,64	0
56	MG	1a	1801	1/1	0.77	0.15	58,58,58,58	0
56	MG	2A	3437	1/1	0.77	0.20	56,56,56,56	0
56	MG	10	105	1/1	0.77	0.15	61,61,61,61	0
56	MG	13	102	1/1	0.77	0.25	72,72,72,72	0
56	MG	1A	4039	1/1	0.78	0.20	81,81,81,81	0
56	MG	2A	3452	1/1	0.78	0.46	69,69,69,69	0
56	MG	2A	3018	1/1	0.78	0.15	50,50,50,50	0
56	MG	1a	1786	1/1	0.78	0.16	71,71,71,71	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	2e	202	1/1	0.78	0.49	74,74,74,74	0
56	MG	1A	3347	1/1	0.78	0.12	47,47,47,47	0
56	MG	1A	3493	1/1	0.78	0.25	54,54,54,54	0
56	MG	2A	3365	1/1	0.78	0.17	49,49,49,49	0
56	MG	1A	3266	1/1	0.78	0.19	57,57,57,57	0
56	MG	17	106	1/1	0.78	0.16	40,40,40,40	0
56	MG	1a	1605	1/1	0.78	0.14	83,83,83,83	0
56	MG	1A	3479	1/1	0.78	0.34	75,75,75,75	0
56	MG	1A	3994	1/1	0.78	0.39	33,33,33,33	0
56	MG	1a	1635	1/1	0.78	0.26	66,66,66,66	0
56	MG	2a	1770	1/1	0.78	0.11	63,63,63,63	0
56	MG	2a	1747	1/1	0.79	0.15	45,45,45,45	0
56	MG	1A	3700	1/1	0.79	0.13	31,31,31,31	0
56	MG	1r	101	1/1	0.79	0.14	65,65,65,65	0
56	MG	1A	3921	1/1	0.79	0.10	52,52,52,52	0
56	MG	1R	205	1/1	0.79	0.53	55,55,55,55	0
56	MG	1a	1755	1/1	0.79	0.20	68,68,68,68	0
56	MG	2A	3217	1/1	0.79	0.32	46,46,46,46	0
56	MG	1A	3292	1/1	0.79	0.27	76,76,76,76	0
56	MG	1m	202	1/1	0.79	0.43	71,71,71,71	0
56	MG	1A	3912	1/1	0.79	0.17	55,55,55,55	0
56	MG	1A	3294	1/1	0.79	0.20	64,64,64,64	0
56	MG	1a	1750	1/1	0.79	0.34	73,73,73,73	0
56	MG	2a	1725	1/1	0.79	0.11	58,58,58,58	0
56	MG	1A	4050	1/1	0.79	0.37	55,55,55,55	0
56	MG	1A	3762	1/1	0.79	0.08	60,60,60,60	0
56	MG	1A	3563	1/1	0.80	0.18	62,62,62,62	0
56	MG	1a	1646	1/1	0.80	0.29	60,60,60,60	0
56	MG	2A	3059	1/1	0.80	0.28	64,64,64,64	0
56	MG	1A	3486	1/1	0.80	0.33	70,70,70,70	0
56	MG	2q	3002	1/1	0.80	0.23	59,59,59,59	0
56	MG	2a	1695	1/1	0.80	0.16	58,58,58,58	0
56	MG	1A	3274	1/1	0.80	0.15	57,57,57,57	0
56	MG	1A	3485	1/1	0.80	0.73	58,58,58,58	0
56	MG	1A	3510	1/1	0.80	0.69	62,62,62,62	0
56	MG	1a	1710	1/1	0.80	0.13	59,59,59,59	0
56	MG	1A	3148	1/1	0.80	0.41	43,43,43,43	0
56	MG	1A	4064	1/1	0.80	0.21	69,69,69,69	0
56	MG	2a	1612	1/1	0.80	0.20	67,67,67,67	0
56	MG	2a	1704	1/1	0.80	0.39	57,57,57,57	0
56	MG	1A	3521	1/1	0.80	0.32	51,51,51,51	0
56	MG	1A	3461	1/1	0.80	0.24	57,57,57,57	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	1A	3317	1/1	0.81	0.26	56,56,56,56	0
56	MG	2A	3219	1/1	0.81	0.13	61,61,61,61	0
56	MG	1A	3342	1/1	0.81	0.14	49,49,49,49	0
56	MG	1a	1894	1/1	0.81	0.37	72,72,72,72	0
56	MG	1A	3110	1/1	0.81	0.27	52,52,52,52	0
56	MG	1A	3431	1/1	0.81	0.19	64,64,64,64	0
56	MG	1A	3538	1/1	0.81	0.10	67,67,67,67	0
56	MG	1A	3689	1/1	0.81	0.16	34,34,34,34	0
56	MG	2A	3555	1/1	0.81	0.36	50,50,50,50	0
56	MG	1A	3435	1/1	0.81	0.16	71,71,71,71	0
56	MG	1a	1749	1/1	0.81	0.22	72,72,72,72	0
56	MG	2A	3081	1/1	0.81	0.31	60,60,60,60	0
56	MG	10	101	1/1	0.81	0.32	64,64,64,64	0
56	MG	1A	3343	1/1	0.81	0.16	54,54,54,54	0
56	MG	1a	1807	1/1	0.81	0.28	74,74,74,74	0
56	MG	2a	1632	1/1	0.81	0.17	76,76,76,76	0
56	MG	2a	1726	1/1	0.81	0.40	59,59,59,59	0
56	MG	2A	3421	1/1	0.81	0.28	61,61,61,61	0
56	MG	1A	3556	1/1	0.81	0.14	67,67,67,67	0
56	MG	1A	3614	1/1	0.82	0.12	58,58,58,58	0
56	MG	1B	214	1/1	0.82	0.18	69,69,69,69	0
56	MG	2a	1739	1/1	0.82	0.25	73,73,73,73	0
56	MG	2a	1623	1/1	0.82	0.51	63,63,63,63	0
56	MG	2a	1816	1/1	0.82	0.27	52,52,52,52	0
56	MG	1A	3359	1/1	0.82	0.31	43,43,43,43	0
56	MG	1A	3967	1/1	0.82	0.14	51,51,51,51	0
56	MG	2A	3029	1/1	0.82	0.30	54,54,54,54	0
56	MG	2A	3388	1/1	0.82	0.36	57,57,57,57	0
56	MG	1a	1643	1/1	0.82	0.18	47,47,47,47	0
56	MG	1A	3477	1/1	0.82	0.12	56,56,56,56	0
56	MG	1B	204	1/1	0.82	0.18	59,59,59,59	0
56	MG	1T	201	1/1	0.82	0.22	57,57,57,57	0
56	MG	1A	3501	1/1	0.82	0.33	66,66,66,66	0
56	MG	1A	3877	1/1	0.82	0.14	41,41,41,41	0
56	MG	2A	3084	1/1	0.82	0.25	39,39,39,39	0
56	MG	1A	3558	1/1	0.82	0.25	65,65,65,65	0
56	MG	2A	3472	1/1	0.82	0.22	53,53,53,53	0
56	MG	1A	3561	1/1	0.82	0.28	55,55,55,55	0
56	MG	1A	3436	1/1	0.82	0.33	66,66,66,66	0
56	MG	2a	1753	1/1	0.82	0.10	63,63,63,63	0
56	MG	1A	4013	1/1	0.82	0.39	55,55,55,55	0
56	MG	2A	3487	1/1	0.82	0.10	67,67,67,67	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	2l	203	1/1	0.82	0.09	55,55,55,55	0
56	MG	1A	3998	1/1	0.82	0.11	47,47,47,47	0
56	MG	2A	3194	1/1	0.82	0.31	48,48,48,48	0
56	MG	2a	1729	1/1	0.82	0.10	58,58,58,58	0
56	MG	1A	3062	1/1	0.82	0.25	50,50,50,50	0
56	MG	1a	1820	1/1	0.82	0.30	50,50,50,50	0
56	MG	2a	1766	1/1	0.82	0.20	83,83,83,83	0
56	MG	1a	1714	1/1	0.83	0.35	56,56,56,56	0
56	MG	2a	1667	1/1	0.83	0.37	69,69,69,69	0
56	MG	2A	3004	1/1	0.83	0.16	55,55,55,55	0
56	MG	1A	3344	1/1	0.83	0.31	73,73,73,73	0
56	MG	1A	3322	1/1	0.83	0.23	55,55,55,55	0
56	MG	1A	3935	1/1	0.83	0.23	69,69,69,69	0
56	MG	1A	3856	1/1	0.83	0.12	48,48,48,48	0
56	MG	1a	1612	1/1	0.83	0.15	58,58,58,58	0
56	MG	2A	3276	1/1	0.83	0.09	58,58,58,58	0
56	MG	1A	3495	1/1	0.83	0.15	61,61,61,61	0
56	MG	1A	4029	1/1	0.83	0.20	61,61,61,61	0
56	MG	2A	3544	1/1	0.83	0.11	48,48,48,48	0
56	MG	1A	3300	1/1	0.83	0.27	28,28,28,28	0
56	MG	2A	3339	1/1	0.83	0.09	78,78,78,78	0
56	MG	1D	307	1/1	0.83	0.20	43,43,43,43	0
56	MG	1G	3002	1/1	0.83	0.12	48,48,48,48	0
56	MG	1O	203	1/1	0.83	0.33	60,60,60,60	0
56	MG	1O	201	1/1	0.83	0.32	47,47,47,47	0
56	MG	1A	3519	1/1	0.83	0.07	62,62,62,62	0
56	MG	2A	3284	1/1	0.83	0.12	45,45,45,45	0
56	MG	1A	3301	1/1	0.83	0.17	85,85,85,85	0
56	MG	1a	1690	1/1	0.83	0.18	78,78,78,78	0
56	MG	1A	3971	1/1	0.83	0.30	82,82,82,82	0
56	MG	2A	3479	1/1	0.83	0.18	56,56,56,56	0
56	MG	1A	4003	1/1	0.83	0.19	53,53,53,53	0
56	MG	1A	3650	1/1	0.83	0.19	30,30,30,30	0
56	MG	1A	3532	1/1	0.84	0.12	54,54,54,54	0
56	MG	1a	1613	1/1	0.84	0.12	44,44,44,44	0
56	MG	1A	3722	1/1	0.84	0.14	62,62,62,62	0
56	MG	1A	3506	1/1	0.84	0.19	57,57,57,57	0
56	MG	2A	3106	1/1	0.84	0.15	58,58,58,58	0
56	MG	1A	3226	1/1	0.84	0.12	31,31,31,31	0
56	MG	1A	4038	1/1	0.84	0.26	63,63,63,63	0
56	MG	1N	203	1/1	0.84	0.24	47,47,47,47	0
56	MG	1a	1616	1/1	0.84	0.25	63,63,63,63	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	2A	3504	1/1	0.84	0.15	56,56,56,56	0
56	MG	2a	1734	1/1	0.84	0.10	69,69,69,69	0
56	MG	1a	1700	1/1	0.84	0.22	62,62,62,62	0
56	MG	1a	1869	1/1	0.84	0.20	66,66,66,66	0
56	MG	1A	3913	1/1	0.84	0.15	73,73,73,73	0
56	MG	1A	3893	1/1	0.84	0.18	53,53,53,53	0
56	MG	1a	1609	1/1	0.84	0.32	56,56,56,56	0
56	MG	1E	305	1/1	0.84	0.36	45,45,45,45	0
56	MG	1a	1817	1/1	0.84	0.14	71,71,71,71	0
56	MG	1A	3624	1/1	0.84	0.12	50,50,50,50	0
56	MG	1H	202	1/1	0.84	0.18	53,53,53,53	0
56	MG	1a	1763	1/1	0.84	0.12	57,57,57,57	0
56	MG	2e	201	1/1	0.84	0.25	71,71,71,71	0
56	MG	1A	3398	1/1	0.84	0.48	58,58,58,58	0
56	MG	1a	1604	1/1	0.84	0.18	63,63,63,63	0
56	MG	1Q	3007	1/1	0.84	0.22	60,60,60,60	0
56	MG	2A	3200	1/1	0.84	0.21	41,41,41,41	0
56	MG	1A	3328	1/1	0.84	0.11	78,78,78,78	0
56	MG	1a	1662	1/1	0.84	0.20	61,61,61,61	0
56	MG	1A	3319	1/1	0.84	0.15	50,50,50,50	0
56	MG	1a	1688	1/1	0.84	0.14	72,72,72,72	0
56	MG	1A	3576	1/1	0.84	0.13	45,45,45,45	0
56	MG	2a	1605	1/1	0.84	0.15	66,66,66,66	0
56	MG	1A	3003	1/1	0.84	0.24	41,41,41,41	0
56	MG	1A	3137	1/1	0.84	0.15	58,58,58,58	0
56	MG	2x	3005	1/1	0.84	0.08	80,80,80,80	0
56	MG	1A	3754	1/1	0.84	0.08	61,61,61,61	0
56	MG	2A	3223	1/1	0.84	0.11	82,82,82,82	0
56	MG	1A	3104	1/1	0.85	0.14	52,52,52,52	0
56	MG	1A	3490	1/1	0.85	0.36	56,56,56,56	0
56	MG	1A	3566	1/1	0.85	0.11	64,64,64,64	0
56	MG	28	8001	1/1	0.85	0.41	58,58,58,58	0
56	MG	2A	3014	1/1	0.85	0.32	59,59,59,59	0
56	MG	2A	3012	1/1	0.85	0.18	57,57,57,57	0
56	MG	2a	1752	1/1	0.85	0.21	59,59,59,59	0
56	MG	2A	3210	1/1	0.85	0.34	52,52,52,52	0
56	MG	1A	3542	1/1	0.85	0.29	53,53,53,53	0
56	MG	2A	3227	1/1	0.85	0.17	59,59,59,59	0
56	MG	1A	4014	1/1	0.85	0.31	47,47,47,47	0
56	MG	2A	3001	1/1	0.85	0.20	39,39,39,39	0
56	MG	1T	205	1/1	0.85	0.27	76,76,76,76	0
56	MG	2A	3281	1/1	0.85	0.22	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	3439	1/1	0.85	0.10	65,65,65,65	0
56	MG	1A	3380	1/1	0.85	0.28	49,49,49,49	0
56	MG	2A	3481	1/1	0.85	0.07	83,83,83,83	0
56	MG	1A	3751	1/1	0.85	0.22	20,20,20,20	0
56	MG	2A	3394	1/1	0.85	0.12	57,57,57,57	0
56	MG	1A	3732	1/1	0.85	0.12	67,67,67,67	0
56	MG	2A	3102	1/1	0.85	0.12	53,53,53,53	0
56	MG	1A	3481	1/1	0.85	0.22	56,56,56,56	0
56	MG	1A	3869	1/1	0.85	0.23	81,81,81,81	0
56	MG	2a	1763	1/1	0.85	0.14	57,57,57,57	0
56	MG	1A	3956	1/1	0.85	0.22	17,17,17,17	0
56	MG	2A	3464	1/1	0.85	0.29	59,59,59,59	0
56	MG	1h	3003	1/1	0.85	0.26	70,70,70,70	0
56	MG	1A	3703	1/1	0.85	0.23	29,29,29,29	0
56	MG	1A	3475	1/1	0.85	0.34	50,50,50,50	0
56	MG	2A	3473	1/1	0.85	0.12	42,42,42,42	0
56	MG	1a	1779	1/1	0.85	0.18	47,47,47,47	0
56	MG	1A	3219	1/1	0.85	0.34	62,62,62,62	0
56	MG	1A	3303	1/1	0.85	0.27	43,43,43,43	0
56	MG	1A	3225	1/1	0.85	0.12	49,49,49,49	0
56	MG	1A	3873	1/1	0.85	0.13	48,48,48,48	0
56	MG	1A	3430	1/1	0.85	0.25	58,58,58,58	0
56	MG	2A	3104	1/1	0.85	0.14	52,52,52,52	0
56	MG	2A	3367	1/1	0.85	0.24	41,41,41,41	0
56	MG	1a	1634	1/1	0.85	0.22	41,41,41,41	0
56	MG	1a	1742	1/1	0.85	0.12	69,69,69,69	0
56	MG	2G	3001	1/1	0.85	0.17	49,49,49,49	0
56	MG	2A	3495	1/1	0.85	0.13	44,44,44,44	0
56	MG	1A	4044	1/1	0.85	0.11	27,27,27,27	0
56	MG	1Q	3004	1/1	0.85	0.65	51,51,51,51	0
56	MG	2A	3225	1/1	0.85	0.23	50,50,50,50	0
56	MG	1a	1822	1/1	0.85	0.18	76,76,76,76	0
56	MG	1A	4065	1/1	0.86	0.15	42,42,42,42	0
56	MG	1A	3647	1/1	0.86	0.17	41,41,41,41	0
56	MG	2a	1616	1/1	0.86	0.18	61,61,61,61	0
56	MG	1A	3136	1/1	0.86	0.45	39,39,39,39	0
56	MG	2A	3079	1/1	0.86	0.08	45,45,45,45	0
56	MG	1A	3049	1/1	0.86	0.14	60,60,60,60	0
56	MG	2A	3051	1/1	0.86	0.36	62,62,62,62	0
56	MG	1A	3540	1/1	0.86	0.20	69,69,69,69	0
56	MG	2A	3088	1/1	0.86	0.14	46,46,46,46	0
56	MG	1A	3420	1/1	0.86	0.14	72,72,72,72	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	1A	3423	1/1	0.86	0.17	59,59,59,59	0
56	MG	1T	203	1/1	0.86	0.30	50,50,50,50	0
56	MG	1A	3108	1/1	0.86	0.20	51,51,51,51	0
56	MG	1a	1844	1/1	0.86	0.18	53,53,53,53	0
56	MG	1A	3910	1/1	0.86	0.22	37,37,37,37	0
56	MG	1a	1859	1/1	0.86	0.22	65,65,65,65	0
56	MG	1G	3001	1/1	0.86	0.10	45,45,45,45	0
56	MG	2a	1817	1/1	0.86	0.79	84,84,84,84	0
56	MG	1a	1707	1/1	0.86	0.15	65,65,65,65	0
56	MG	1A	3507	1/1	0.86	0.24	40,40,40,40	0
56	MG	1A	3422	1/1	0.86	0.19	63,63,63,63	0
56	MG	2a	1733	1/1	0.86	0.12	67,67,67,67	0
56	MG	1A	3242	1/1	0.86	0.22	30,30,30,30	0
56	MG	1A	3471	1/1	0.86	0.28	58,58,58,58	0
56	MG	2A	3285	1/1	0.86	0.17	48,48,48,48	0
56	MG	2a	1627	1/1	0.86	0.44	68,68,68,68	0
56	MG	1A	3577	1/1	0.86	0.18	32,32,32,32	0
56	MG	2l	202	1/1	0.86	0.13	69,69,69,69	0
56	MG	2A	3125	1/1	0.86	0.40	55,55,55,55	0
56	MG	1x	108	1/1	0.86	0.09	59,59,59,59	0
56	MG	2a	1617	1/1	0.86	0.17	67,67,67,67	0
56	MG	1A	3009	1/1	0.86	0.10	47,47,47,47	0
56	MG	1A	3180	1/1	0.86	0.17	39,39,39,39	0
56	MG	2A	3109	1/1	0.86	0.27	57,57,57,57	0
56	MG	2a	1780	1/1	0.86	0.15	64,64,64,64	0
56	MG	1a	1739	1/1	0.86	0.13	54,54,54,54	0
56	MG	2A	3546	1/1	0.86	0.26	48,48,48,48	0
56	MG	2A	3252	1/1	0.86	0.24	58,58,58,58	0
56	MG	2a	1649	1/1	0.86	0.25	51,51,51,51	0
56	MG	2A	3287	1/1	0.86	0.21	55,55,55,55	0
56	MG	1a	1675	1/1	0.86	0.26	59,59,59,59	0
56	MG	1A	3905	1/1	0.86	0.21	43,43,43,43	0
56	MG	16	103	1/1	0.86	0.13	36,36,36,36	0
56	MG	1A	3451	1/1	0.86	0.07	52,52,52,52	0
56	MG	1A	3452	1/1	0.86	0.23	69,69,69,69	0
56	MG	2a	1645	1/1	0.86	0.26	57,57,57,57	0
56	MG	2a	1721	1/1	0.86	0.12	49,49,49,49	0
56	MG	1a	1601	1/1	0.86	0.29	62,62,62,62	0
56	MG	2A	3153	1/1	0.86	0.13	45,45,45,45	0
56	MG	1A	3887	1/1	0.86	0.10	44,44,44,44	0
56	MG	1a	1617	1/1	0.86	0.19	60,60,60,60	0
56	MG	1A	3329	1/1	0.86	0.13	52,52,52,52	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	2A	3538	1/1	0.86	0.14	56,56,56,56	0
56	MG	1A	3623	1/1	0.86	0.08	61,61,61,61	0
56	MG	1A	3569	1/1	0.86	0.21	36,36,36,36	0
56	MG	1a	1756	1/1	0.86	0.19	74,74,74,74	0
56	MG	1A	3437	1/1	0.86	0.15	51,51,51,51	0
56	MG	1A	3006	1/1	0.86	0.32	48,48,48,48	0
56	MG	1A	3018	1/1	0.86	0.18	46,46,46,46	0
56	MG	2A	3192	1/1	0.86	0.11	49,49,49,49	0
56	MG	1A	3416	1/1	0.86	0.22	56,56,56,56	0
56	MG	2A	3055	1/1	0.86	0.15	57,57,57,57	0
56	MG	2A	3216	1/1	0.86	0.17	44,44,44,44	0
56	MG	1a	1870	1/1	0.86	0.25	58,58,58,58	0
56	MG	1A	3349	1/1	0.86	0.13	46,46,46,46	0
56	MG	2A	3204	1/1	0.87	0.21	46,46,46,46	0
56	MG	1A	3716	1/1	0.87	0.10	52,52,52,52	0
56	MG	2A	3468	1/1	0.87	0.20	57,57,57,57	0
56	MG	1A	3611	1/1	0.87	0.29	31,31,31,31	0
56	MG	1a	1719	1/1	0.87	0.14	53,53,53,53	0
56	MG	1A	3932	1/1	0.87	0.16	58,58,58,58	0
56	MG	1A	3489	1/1	0.87	0.12	41,41,41,41	0
56	MG	2A	3245	1/1	0.87	0.23	23,23,23,23	0
56	MG	2a	1811	1/1	0.87	0.16	66,66,66,66	0
56	MG	2A	3098	1/1	0.87	0.26	50,50,50,50	0
56	MG	2A	3203	1/1	0.87	0.19	19,19,19,19	0
56	MG	1a	1847	1/1	0.87	0.19	45,45,45,45	0
56	MG	1a	1791	1/1	0.87	0.19	71,71,71,71	0
56	MG	2q	3001	1/1	0.87	0.23	54,54,54,54	0
56	MG	2A	3060	1/1	0.87	0.14	50,50,50,50	0
56	MG	2a	1661	1/1	0.87	0.16	58,58,58,58	0
56	MG	1A	3687	1/1	0.87	0.23	53,53,53,53	0
56	MG	1A	3107	1/1	0.87	0.21	53,53,53,53	0
56	MG	2a	1662	1/1	0.87	0.09	83,83,83,83	0
56	MG	1T	204	1/1	0.87	0.20	68,68,68,68	0
56	MG	2a	1621	1/1	0.87	0.31	53,53,53,53	0
56	MG	2A	3306	1/1	0.87	0.13	32,32,32,32	0
56	MG	2a	1810	1/1	0.87	0.20	84,84,84,84	0
56	MG	2A	3258	1/1	0.87	0.23	52,52,52,52	0
56	MG	2A	3268	1/1	0.87	0.30	75,75,75,75	0
56	MG	2D	303	1/1	0.87	0.25	46,46,46,46	0
56	MG	2A	3463	1/1	0.87	0.13	57,57,57,57	0
56	MG	2a	1684	1/1	0.87	0.41	60,60,60,60	0
56	MG	1A	3549	1/1	0.87	0.26	64,64,64,64	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	1A	3105	1/1	0.87	0.13	43,43,43,43	0
56	MG	1A	4037	1/1	0.87	0.34	54,54,54,54	0
56	MG	1a	1685	1/1	0.87	0.12	37,37,37,37	0
56	MG	1A	3129	1/1	0.87	0.19	41,41,41,41	0
56	MG	1A	3177	1/1	0.87	0.11	52,52,52,52	0
56	MG	1A	3356	1/1	0.87	0.35	56,56,56,56	0
56	MG	1A	3102	1/1	0.87	0.22	51,51,51,51	0
56	MG	2D	301	1/1	0.87	0.13	50,50,50,50	0
56	MG	1A	3830	1/1	0.87	0.11	38,38,38,38	0
56	MG	1A	3028	1/1	0.87	0.28	52,52,52,52	0
56	MG	1A	3991	1/1	0.87	0.28	94,94,94,94	0
56	MG	17	105	1/1	0.87	0.21	44,44,44,44	0
56	MG	2a	1703	1/1	0.87	0.18	57,57,57,57	0
56	MG	18	102	1/1	0.87	0.38	48,48,48,48	0
56	MG	2A	3089	1/1	0.87	0.10	47,47,47,47	0
56	MG	2A	3032	1/1	0.87	0.26	59,59,59,59	0
56	MG	1A	3109	1/1	0.87	0.11	60,60,60,60	0
56	MG	1A	3142	1/1	0.87	0.08	62,62,62,62	0
56	MG	1A	3651	1/1	0.87	0.19	23,23,23,23	0
56	MG	1a	1810	1/1	0.87	0.12	69,69,69,69	0
56	MG	1A	3828	1/1	0.87	0.19	22,22,22,22	0
56	MG	2a	1639	1/1	0.87	0.09	80,80,80,80	0
56	MG	1A	3468	1/1	0.87	0.52	64,64,64,64	0
56	MG	1A	3293	1/1	0.87	0.26	50,50,50,50	0
56	MG	1B	224	1/1	0.87	0.22	58,58,58,58	0
56	MG	1A	3456	1/1	0.87	0.15	52,52,52,52	0
56	MG	1A	3745	1/1	0.87	0.19	69,69,69,69	0
56	MG	1a	1703	1/1	0.87	0.09	66,66,66,66	0
56	MG	1A	3215	1/1	0.87	0.10	50,50,50,50	0
56	MG	2a	1672	1/1	0.87	0.38	57,57,57,57	0
56	MG	2A	3191	1/1	0.88	0.31	51,51,51,51	0
56	MG	1a	1806	1/1	0.88	0.17	79,79,79,79	0
56	MG	1A	3391	1/1	0.88	0.15	44,44,44,44	0
56	MG	1A	3476	1/1	0.88	0.14	61,61,61,61	0
56	MG	1D	306	1/1	0.88	0.21	50,50,50,50	0
56	MG	2A	3547	1/1	0.88	0.38	51,51,51,51	0
56	MG	2A	3087	1/1	0.88	0.29	49,49,49,49	0
56	MG	2a	1786	1/1	0.88	0.38	71,71,71,71	0
56	MG	1A	3384	1/1	0.88	0.55	48,48,48,48	0
56	MG	2A	3370	1/1	0.88	0.11	49,49,49,49	0
56	MG	1A	3261	1/1	0.88	0.17	43,43,43,43	0
56	MG	2a	1717	1/1	0.88	0.22	57,57,57,57	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	1a	1670	1/1	0.88	0.39	60,60,60,60	0
56	MG	1A	3652	1/1	0.88	0.19	48,48,48,48	0
56	MG	1A	3865	1/1	0.88	0.24	60,60,60,60	0
56	MG	2t	3001	1/1	0.88	0.32	53,53,53,53	0
56	MG	2a	1651	1/1	0.88	0.61	56,56,56,56	0
56	MG	1a	1891	1/1	0.88	0.15	52,52,52,52	0
56	MG	1c	3001	1/1	0.88	0.13	64,64,64,64	0
56	MG	10	103	1/1	0.88	0.26	59,59,59,59	0
56	MG	1A	3492	1/1	0.88	0.23	59,59,59,59	0
56	MG	1A	3275	1/1	0.88	0.28	58,58,58,58	0
56	MG	2A	3160	1/1	0.88	0.12	52,52,52,52	0
56	MG	1A	3896	1/1	0.88	0.13	47,47,47,47	0
56	MG	1A	3954	1/1	0.88	0.18	42,42,42,42	0
56	MG	1A	3714	1/1	0.88	0.14	54,54,54,54	0
56	MG	2A	3048	1/1	0.88	0.17	43,43,43,43	0
56	MG	2A	3095	1/1	0.88	0.23	54,54,54,54	0
56	MG	2a	1796	1/1	0.88	0.15	73,73,73,73	0
56	MG	1A	3710	1/1	0.88	0.18	25,25,25,25	0
56	MG	1A	3460	1/1	0.88	0.21	61,61,61,61	0
56	MG	1A	3529	1/1	0.88	0.13	46,46,46,46	0
56	MG	2A	3409	1/1	0.88	0.12	68,68,68,68	0
56	MG	1U	206	1/1	0.88	0.45	46,46,46,46	0
56	MG	2a	1740	1/1	0.88	0.90	101,101,101,101	0
56	MG	1A	3067	1/1	0.88	0.19	48,48,48,48	0
56	MG	1A	3746	1/1	0.88	0.12	38,38,38,38	0
56	MG	2a	1814	1/1	0.88	0.13	79,79,79,79	0
56	MG	1a	1748	1/1	0.88	0.25	56,56,56,56	0
56	MG	1a	1789	1/1	0.88	0.11	62,62,62,62	0
56	MG	1a	1666	1/1	0.88	0.15	61,61,61,61	0
56	MG	1A	3378	1/1	0.88	0.24	36,36,36,36	0
56	MG	1D	304	1/1	0.88	0.23	44,44,44,44	0
56	MG	1a	1887	1/1	0.88	0.16	64,64,64,64	0
56	MG	2A	3294	1/1	0.88	0.21	41,41,41,41	0
56	MG	1A	3095	1/1	0.88	0.13	60,60,60,60	0
56	MG	1A	3796	1/1	0.88	0.23	59,59,59,59	0
56	MG	2B	3004	1/1	0.88	0.23	45,45,45,45	0
56	MG	2a	1620	1/1	0.88	0.24	66,66,66,66	0
56	MG	1a	1895	1/1	0.88	0.29	47,47,47,47	0
56	MG	1a	1812	1/1	0.88	0.29	66,66,66,66	0
56	MG	1A	3194	1/1	0.88	0.29	50,50,50,50	0
56	MG	1A	3306	1/1	0.88	0.18	47,47,47,47	0
56	MG	2A	3017	1/1	0.88	0.19	66,66,66,66	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	1A	3339	1/1	0.88	0.19	73,73,73,73	0
56	MG	1A	3415	1/1	0.88	0.32	58,58,58,58	0
56	MG	2A	3108	1/1	0.88	0.25	59,59,59,59	0
56	MG	1A	4093	1/1	0.88	0.69	39,39,39,39	0
56	MG	2A	3462	1/1	0.88	0.10	44,44,44,44	0
56	MG	1A	3392	1/1	0.88	0.14	44,44,44,44	0
56	MG	1A	3055	1/1	0.88	0.30	41,41,41,41	0
56	MG	1A	3216	1/1	0.88	0.17	41,41,41,41	0
56	MG	2A	3318	1/1	0.88	0.33	58,58,58,58	0
56	MG	1A	3123	1/1	0.88	0.20	43,43,43,43	0
56	MG	1A	4047	1/1	0.88	0.17	44,44,44,44	0
56	MG	2A	3269	1/1	0.88	0.22	52,52,52,52	0
56	MG	2a	1607	1/1	0.88	0.22	54,54,54,54	0
56	MG	1B	209	1/1	0.88	0.20	66,66,66,66	0
56	MG	1A	3483	1/1	0.88	0.27	75,75,75,75	0
56	MG	1a	1811	1/1	0.88	0.15	90,90,90,90	0
56	MG	1A	3366	1/1	0.88	0.12	48,48,48,48	0
56	MG	1A	3286	1/1	0.88	0.26	63,63,63,63	0
56	MG	2a	1785	1/1	0.88	0.14	68,68,68,68	0
56	MG	1a	1760	1/1	0.88	0.08	48,48,48,48	0
56	MG	1A	3965	1/1	0.88	0.14	39,39,39,39	0
56	MG	2a	1638	1/1	0.88	0.21	59,59,59,59	0
56	MG	1A	4077	1/1	0.88	0.10	62,62,62,62	0
56	MG	1A	3381	1/1	0.89	0.24	38,38,38,38	0
56	MG	1A	3103	1/1	0.89	0.10	53,53,53,53	0
56	MG	1a	1720	1/1	0.89	0.20	40,40,40,40	0
56	MG	17	103	1/1	0.89	0.26	49,49,49,49	0
56	MG	1A	3363	1/1	0.89	0.18	65,65,65,65	0
56	MG	2A	3274	1/1	0.89	0.14	46,46,46,46	0
56	MG	1A	3290	1/1	0.89	0.14	55,55,55,55	0
56	MG	1A	3073	1/1	0.89	0.27	49,49,49,49	0
56	MG	2A	3542	1/1	0.89	0.09	41,41,41,41	0
56	MG	1A	3551	1/1	0.89	0.16	85,85,85,85	0
56	MG	1A	4019	1/1	0.89	0.15	59,59,59,59	0
56	MG	2A	3073	1/1	0.89	0.41	43,43,43,43	0
56	MG	2A	3299	1/1	0.89	0.28	65,65,65,65	0
56	MG	1a	1792	1/1	0.89	0.27	63,63,63,63	0
56	MG	2a	1755	1/1	0.89	0.14	82,82,82,82	0
56	MG	2A	3368	1/1	0.89	0.12	43,43,43,43	0
56	MG	1A	3169	1/1	0.89	0.34	48,48,48,48	0
56	MG	1A	3715	1/1	0.89	0.26	57,57,57,57	0
56	MG	1D	308	1/1	0.89	0.32	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	3387	1/1	0.89	0.22	37,37,37,37	0
56	MG	1A	3463	1/1	0.89	0.22	54,54,54,54	0
56	MG	2A	3050	1/1	0.89	0.34	47,47,47,47	0
56	MG	2A	3074	1/1	0.89	0.17	50,50,50,50	0
56	MG	1A	3375	1/1	0.89	0.47	62,62,62,62	0
56	MG	1A	3681	1/1	0.89	0.15	43,43,43,43	0
56	MG	2A	3478	1/1	0.89	0.05	42,42,42,42	0
56	MG	2A	3447	1/1	0.89	0.10	57,57,57,57	0
56	MG	2A	3474	1/1	0.89	0.14	63,63,63,63	0
56	MG	1A	3424	1/1	0.89	0.10	45,45,45,45	0
56	MG	2Z	3001	1/1	0.89	0.05	73,73,73,73	0
56	MG	2a	1694	1/1	0.89	0.07	61,61,61,61	0
56	MG	1A	3315	1/1	0.89	0.18	50,50,50,50	0
56	MG	1a	1863	1/1	0.89	0.14	64,64,64,64	0
56	MG	2A	3186	1/1	0.89	0.28	35,35,35,35	0
56	MG	1a	1639	1/1	0.89	0.15	76,76,76,76	0
56	MG	2A	3427	1/1	0.89	0.09	43,43,43,43	0
56	MG	1A	3124	1/1	0.89	0.36	49,49,49,49	0
56	MG	1a	1623	1/1	0.89	0.30	71,71,71,71	0
56	MG	1A	3596	1/1	0.89	0.18	45,45,45,45	0
56	MG	2A	3490	1/1	0.89	0.16	48,48,48,48	0
56	MG	17	102	1/1	0.89	0.21	40,40,40,40	0
56	MG	2A	3058	1/1	0.89	0.21	46,46,46,46	0
56	MG	2A	3040	1/1	0.89	0.18	60,60,60,60	0
56	MG	1A	3178	1/1	0.89	0.19	48,48,48,48	0
56	MG	2A	3115	1/1	0.89	0.25	49,49,49,49	0
56	MG	2A	3469	1/1	0.89	0.20	60,60,60,60	0
56	MG	1A	3248	1/1	0.89	0.18	42,42,42,42	0
56	MG	2a	1795	1/1	0.89	0.15	53,53,53,53	0
56	MG	1A	3470	1/1	0.89	0.40	43,43,43,43	0
56	MG	1A	3498	1/1	0.89	0.37	44,44,44,44	0
56	MG	2a	1714	1/1	0.89	0.18	65,65,65,65	0
56	MG	2f	3001	1/1	0.89	0.14	54,54,54,54	0
56	MG	2A	3226	1/1	0.89	0.15	72,72,72,72	0
56	MG	1a	1630	1/1	0.89	0.19	59,59,59,59	0
56	MG	1A	3868	1/1	0.89	0.16	65,65,65,65	0
56	MG	2A	3371	1/1	0.89	0.26	61,61,61,61	0
56	MG	1A	3304	1/1	0.89	0.20	72,72,72,72	0
56	MG	2A	3165	1/1	0.89	0.10	35,35,35,35	0
56	MG	1A	3792	1/1	0.89	0.20	26,26,26,26	0
56	MG	2a	1806	1/1	0.89	0.33	57,57,57,57	0
56	MG	2A	3241	1/1	0.89	0.20	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	1697	1/1	0.89	0.09	60,60,60,60	0
56	MG	2A	3340	1/1	0.89	0.05	58,58,58,58	0
56	MG	2A	3413	1/1	0.89	0.12	63,63,63,63	0
56	MG	2a	1744	1/1	0.89	0.31	63,63,63,63	0
56	MG	1R	202	1/1	0.89	0.13	64,64,64,64	0
56	MG	1a	1765	1/1	0.89	0.29	69,69,69,69	0
56	MG	1a	1759	1/1	0.89	0.15	58,58,58,58	0
56	MG	1A	3690	1/1	0.89	0.22	15,15,15,15	0
56	MG	1A	3539	1/1	0.89	0.18	56,56,56,56	0
56	MG	1D	302	1/1	0.89	0.23	63,63,63,63	0
56	MG	1A	3879	1/1	0.89	0.13	48,48,48,48	0
56	MG	1A	3837	1/1	0.90	0.09	44,44,44,44	0
56	MG	1A	3345	1/1	0.90	0.13	51,51,51,51	0
56	MG	1A	4051	1/1	0.90	0.13	45,45,45,45	0
56	MG	2A	3548	1/1	0.90	0.19	53,53,53,53	0
56	MG	1N	206	1/1	0.90	0.18	37,37,37,37	0
56	MG	1a	1699	1/1	0.90	0.27	68,68,68,68	0
56	MG	1A	3455	1/1	0.90	0.11	59,59,59,59	0
56	MG	2a	1802	1/1	0.90	0.33	68,68,68,68	0
56	MG	2A	3314	1/1	0.90	0.18	49,49,49,49	0
56	MG	1A	3311	1/1	0.90	0.13	67,67,67,67	0
56	MG	1A	3544	1/1	0.90	0.60	67,67,67,67	0
56	MG	1A	4055	1/1	0.90	0.75	53,53,53,53	0
56	MG	2A	3142	1/1	0.90	0.56	53,53,53,53	0
56	MG	2A	3193	1/1	0.90	0.20	50,50,50,50	0
56	MG	2A	3077	1/1	0.90	0.27	54,54,54,54	0
56	MG	2A	3132	1/1	0.90	0.09	52,52,52,52	0
56	MG	1A	3189	1/1	0.90	0.23	37,37,37,37	0
56	MG	2A	3097	1/1	0.90	0.10	51,51,51,51	0
56	MG	1A	3699	1/1	0.90	0.18	49,49,49,49	0
56	MG	2A	3331	1/1	0.90	0.23	58,58,58,58	0
56	MG	1A	3253	1/1	0.90	0.28	54,54,54,54	0
56	MG	2A	3184	1/1	0.90	0.21	43,43,43,43	0
56	MG	2A	3188	1/1	0.90	0.14	54,54,54,54	0
56	MG	2A	3551	1/1	0.90	0.20	32,32,32,32	0
56	MG	2A	3313	1/1	0.90	0.06	57,57,57,57	0
56	MG	1A	3523	1/1	0.90	0.54	77,77,77,77	0
56	MG	1A	3023	1/1	0.90	0.14	47,47,47,47	0
56	MG	2a	1784	1/1	0.90	0.20	71,71,71,71	0
56	MG	1a	1761	1/1	0.90	0.27	77,77,77,77	0
56	MG	1a	1836	1/1	0.90	0.20	52,52,52,52	0
56	MG	1A	3890	1/1	0.90	0.21	63,63,63,63	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	1a	1751	1/1	0.90	0.22	60,60,60,60	0
56	MG	1r	103	1/1	0.90	0.12	51,51,51,51	0
56	MG	1A	3508	1/1	0.90	0.23	52,52,52,52	0
56	MG	1A	3160	1/1	0.90	0.23	53,53,53,53	0
56	MG	2A	3529	1/1	0.90	0.18	43,43,43,43	0
56	MG	1A	3777	1/1	0.90	0.15	41,41,41,41	0
56	MG	1A	3790	1/1	0.90	0.23	38,38,38,38	0
56	MG	1D	309	1/1	0.90	0.13	31,31,31,31	0
56	MG	2B	3003	1/1	0.90	0.12	60,60,60,60	0
57	ZN	2n	501	1/1	0.90	0.06	93,93,93,93	0
56	MG	1A	3072	1/1	0.90	0.29	44,44,44,44	0
56	MG	1A	3674	1/1	0.90	0.20	37,37,37,37	0
56	MG	1A	3465	1/1	0.90	0.15	49,49,49,49	0
56	MG	1A	3520	1/1	0.90	0.07	53,53,53,53	0
56	MG	1A	3039	1/1	0.90	0.18	51,51,51,51	0
56	MG	1B	220	1/1	0.90	0.11	52,52,52,52	0
56	MG	1A	3937	1/1	0.90	0.15	51,51,51,51	0
56	MG	1a	1830	1/1	0.90	0.14	59,59,59,59	0
56	MG	1B	203	1/1	0.90	0.20	53,53,53,53	0
56	MG	2a	1626	1/1	0.90	0.17	55,55,55,55	0
56	MG	1A	3447	1/1	0.90	0.23	47,47,47,47	0
56	MG	1A	3341	1/1	0.90	0.13	49,49,49,49	0
56	MG	1A	4062	1/1	0.90	0.23	62,62,62,62	0
56	MG	1a	1766	1/1	0.90	0.10	82,82,82,82	0
56	MG	2A	3036	1/1	0.90	0.26	61,61,61,61	0
56	MG	2A	3361	1/1	0.90	0.13	53,53,53,53	0
56	MG	1a	1872	1/1	0.90	0.07	50,50,50,50	0
56	MG	2A	3295	1/1	0.90	0.21	32,32,32,32	0
56	MG	1A	3662	1/1	0.90	0.22	22,22,22,22	0
56	MG	2A	3006	1/1	0.90	0.12	54,54,54,54	0
56	MG	1U	204	1/1	0.90	0.49	33,33,33,33	0
56	MG	2a	1712	1/1	0.90	0.22	67,67,67,67	0
56	MG	1A	3395	1/1	0.90	0.10	61,61,61,61	0
56	MG	1A	3441	1/1	0.90	0.23	59,59,59,59	0
56	MG	1A	4086	1/1	0.90	0.12	51,51,51,51	0
56	MG	2A	3030	1/1	0.90	0.12	45,45,45,45	0
56	MG	1A	3044	1/1	0.90	0.53	38,38,38,38	0
56	MG	1A	3779	1/1	0.90	0.19	36,36,36,36	0
56	MG	2a	1642	1/1	0.90	0.46	87,87,87,87	0
56	MG	1A	3316	1/1	0.90	0.20	48,48,48,48	0
56	MG	1a	1861	1/1	0.90	0.13	48,48,48,48	0
56	MG	1a	1664	1/1	0.90	0.12	50,50,50,50	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	2a	1764	1/1	0.90	0.31	52,52,52,52	0
56	MG	2A	3178	1/1	0.90	0.06	52,52,52,52	0
56	MG	2A	3010	1/1	0.90	0.12	46,46,46,46	0
56	MG	1A	3949	1/1	0.90	0.33	37,37,37,37	0
56	MG	1A	3234	1/1	0.90	0.13	52,52,52,52	0
56	MG	2a	1808	1/1	0.90	0.08	73,73,73,73	0
56	MG	2A	3092	1/1	0.90	0.20	52,52,52,52	0
56	MG	1A	3750	1/1	0.90	0.26	41,41,41,41	0
56	MG	1B	211	1/1	0.90	0.09	46,46,46,46	0
56	MG	2A	3093	1/1	0.90	0.36	52,52,52,52	0
56	MG	1a	1805	1/1	0.90	0.28	77,77,77,77	0
56	MG	2A	3396	1/1	0.90	0.18	64,64,64,64	0
56	MG	2a	1688	1/1	0.90	0.12	49,49,49,49	0
56	MG	1A	3941	1/1	0.90	0.24	50,50,50,50	0
56	MG	2A	3445	1/1	0.90	0.19	56,56,56,56	0
56	MG	1a	1818	1/1	0.90	0.33	69,69,69,69	0
56	MG	1A	3914	1/1	0.90	0.20	51,51,51,51	0
56	MG	1x	110	1/1	0.90	0.08	53,53,53,53	0
56	MG	2A	3237	1/1	0.90	0.14	46,46,46,46	0
56	MG	2a	1700	1/1	0.90	0.16	55,55,55,55	0
56	MG	1A	3659	1/1	0.90	0.14	25,25,25,25	0
56	MG	1B	212	1/1	0.90	0.31	50,50,50,50	0
56	MG	1A	3060	1/1	0.90	0.15	46,46,46,46	0
56	MG	2a	1745	1/1	0.90	0.31	54,54,54,54	0
56	MG	1A	4046	1/1	0.90	0.39	50,50,50,50	0
56	MG	2a	1635	1/1	0.90	0.14	88,88,88,88	0
56	MG	1A	3327	1/1	0.90	0.07	64,64,64,64	0
56	MG	2A	3266	1/1	0.90	0.20	76,76,76,76	0
56	MG	2A	3253	1/1	0.90	0.27	29,29,29,29	0
56	MG	1A	3986	1/1	0.90	0.18	38,38,38,38	0
56	MG	2A	3147	1/1	0.90	0.18	33,33,33,33	0
56	MG	1A	3522	1/1	0.90	0.10	73,73,73,73	0
56	MG	1A	3643	1/1	0.90	0.24	34,34,34,34	0
56	MG	2A	3477	1/1	0.90	0.09	52,52,52,52	0
56	MG	1a	1615	1/1	0.90	0.13	66,66,66,66	0
56	MG	2F	302	1/1	0.90	0.06	36,36,36,36	0
56	MG	1A	4073	1/1	0.90	0.44	47,47,47,47	0
56	MG	1a	1728	1/1	0.90	0.27	49,49,49,49	0
56	MG	1A	3847	1/1	0.90	0.58	40,40,40,40	0
56	MG	1A	3405	1/1	0.90	0.27	36,36,36,36	0
56	MG	2A	3366	1/1	0.90	0.12	51,51,51,51	0
56	MG	1P	205	1/1	0.90	0.47	75,75,75,75	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	1A	3283	1/1	0.90	0.15	47,47,47,47	0
56	MG	1A	3291	1/1	0.90	0.22	33,33,33,33	0
56	MG	1A	3083	1/1	0.90	0.28	48,48,48,48	0
56	MG	1F	306	1/1	0.91	0.25	49,49,49,49	0
56	MG	2B	3002	1/1	0.91	0.09	65,65,65,65	0
56	MG	1R	206	1/1	0.91	0.20	37,37,37,37	0
56	MG	1A	3141	1/1	0.91	0.29	37,37,37,37	0
56	MG	1A	4082	1/1	0.91	0.16	44,44,44,44	0
56	MG	2A	3550	1/1	0.91	0.14	51,51,51,51	0
56	MG	1A	3488	1/1	0.91	0.16	43,43,43,43	0
56	MG	2a	1792	1/1	0.91	0.16	44,44,44,44	0
56	MG	2a	1601	1/1	0.91	0.40	54,54,54,54	0
56	MG	1A	3482	1/1	0.91	0.17	55,55,55,55	0
56	MG	1A	3462	1/1	0.91	0.15	62,62,62,62	0
56	MG	1A	3621	1/1	0.91	0.13	79,79,79,79	0
56	MG	2A	3172	1/1	0.91	0.44	58,58,58,58	0
56	MG	2A	3068	1/1	0.91	0.14	50,50,50,50	0
56	MG	1A	3027	1/1	0.91	0.14	42,42,42,42	0
56	MG	1A	3433	1/1	0.91	0.14	53,53,53,53	0
56	MG	2a	1682	1/1	0.91	0.29	48,48,48,48	0
56	MG	2A	3373	1/1	0.91	0.13	41,41,41,41	0
56	MG	1A	3729	1/1	0.91	0.18	43,43,43,43	0
56	MG	2a	1748	1/1	0.91	0.14	50,50,50,50	0
56	MG	1A	3562	1/1	0.91	0.10	63,63,63,63	0
56	MG	1a	1657	1/1	0.91	0.10	25,25,25,25	0
56	MG	1A	3997	1/1	0.91	0.14	48,48,48,48	0
56	MG	1A	3500	1/1	0.91	0.23	60,60,60,60	0
56	MG	2A	3359	1/1	0.91	0.13	49,49,49,49	0
56	MG	1a	1661	1/1	0.91	0.28	58,58,58,58	0
56	MG	1U	205	1/1	0.91	0.39	30,30,30,30	0
56	MG	1a	1667	1/1	0.91	0.62	51,51,51,51	0
56	MG	1a	1876	1/1	0.91	0.18	47,47,47,47	0
56	MG	2A	3423	1/1	0.91	0.10	65,65,65,65	0
56	MG	1A	3922	1/1	0.91	0.25	52,52,52,52	0
56	MG	1a	1680	1/1	0.91	0.25	45,45,45,45	0
56	MG	2A	3399	1/1	0.91	0.07	58,58,58,58	0
56	MG	1A	3078	1/1	0.91	0.32	56,56,56,56	0
56	MG	2a	1610	1/1	0.91	0.26	60,60,60,60	0
56	MG	2A	3525	1/1	0.91	0.16	40,40,40,40	0
56	MG	1A	3235	1/1	0.91	0.08	36,36,36,36	0
56	MG	1a	1725	1/1	0.91	0.22	59,59,59,59	0
56	MG	2A	3513	1/1	0.91	0.19	66,66,66,66	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	2A	3120	1/1	0.91	0.18	33,33,33,33	0
56	MG	2A	3319	1/1	0.91	0.13	55,55,55,55	0
56	MG	1a	1797	1/1	0.91	0.17	54,54,54,54	0
56	MG	1A	3835	1/1	0.91	0.13	57,57,57,57	0
56	MG	1a	1669	1/1	0.91	0.18	45,45,45,45	0
56	MG	1A	3924	1/1	0.91	0.21	23,23,23,23	0
56	MG	1A	3025	1/1	0.91	0.27	44,44,44,44	0
56	MG	1A	3981	1/1	0.91	0.34	43,43,43,43	0
56	MG	1a	1795	1/1	0.91	0.21	56,56,56,56	0
56	MG	1A	3886	1/1	0.91	0.28	65,65,65,65	0
56	MG	1A	3696	1/1	0.91	0.13	34,34,34,34	0
56	MG	1a	1626	1/1	0.91	0.08	62,62,62,62	0
56	MG	2a	1768	1/1	0.91	0.25	70,70,70,70	0
56	MG	2A	3297	1/1	0.91	0.33	49,49,49,49	0
56	MG	2A	3151	1/1	0.91	0.34	40,40,40,40	0
56	MG	2a	1669	1/1	0.91	0.14	43,43,43,43	0
56	MG	1A	3125	1/1	0.91	0.17	56,56,56,56	0
56	MG	1A	3992	1/1	0.91	0.14	70,70,70,70	0
56	MG	1A	3857	1/1	0.91	0.18	51,51,51,51	0
56	MG	2A	3113	1/1	0.91	0.27	44,44,44,44	0
56	MG	2A	3491	1/1	0.91	0.29	53,53,53,53	0
56	MG	2A	3082	1/1	0.91	0.21	55,55,55,55	0
56	MG	2A	3121	1/1	0.91	0.20	35,35,35,35	0
56	MG	1A	3646	1/1	0.91	0.21	49,49,49,49	0
56	MG	1a	1852	1/1	0.91	0.12	51,51,51,51	0
56	MG	2A	3393	1/1	0.91	0.25	44,44,44,44	0
56	MG	1A	3676	1/1	0.91	0.11	22,22,22,22	0
56	MG	1A	3884	1/1	0.91	0.14	47,47,47,47	0
56	MG	1A	3193	1/1	0.91	0.14	50,50,50,50	0
56	MG	1A	3305	1/1	0.91	0.41	52,52,52,52	0
56	MG	2a	1774	1/1	0.91	0.07	69,69,69,69	0
56	MG	1A	3713	1/1	0.91	0.17	48,48,48,48	0
56	MG	1A	3282	1/1	0.91	0.26	36,36,36,36	0
56	MG	1a	1653	1/1	0.91	0.16	54,54,54,54	0
56	MG	1a	1702	1/1	0.91	0.20	43,43,43,43	0
56	MG	2a	1718	1/1	0.91	0.40	53,53,53,53	0
56	MG	1A	3397	1/1	0.91	0.15	46,46,46,46	0
56	MG	2A	3398	1/1	0.91	0.24	45,45,45,45	0
56	MG	2A	3185	1/1	0.91	0.15	46,46,46,46	0
56	MG	2A	3301	1/1	0.91	0.12	43,43,43,43	0
56	MG	2A	3228	1/1	0.91	0.19	52,52,52,52	0
56	MG	1A	3271	1/1	0.91	0.18	36,36,36,36	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	1A	4002	1/1	0.91	0.18	70,70,70,70	0
56	MG	1A	3829	1/1	0.91	0.19	49,49,49,49	0
56	MG	1A	3414	1/1	0.91	0.22	55,55,55,55	0
56	MG	2a	1760	1/1	0.91	0.26	59,59,59,59	0
56	MG	1a	1718	1/1	0.91	0.15	67,67,67,67	0
56	MG	1A	3320	1/1	0.91	0.10	52,52,52,52	0
56	MG	1A	3602	1/1	0.91	0.16	46,46,46,46	0
57	ZN	26	501	1/1	0.91	0.10	62,62,62,62	0
56	MG	1A	4075	1/1	0.91	0.17	36,36,36,36	0
56	MG	1A	3698	1/1	0.91	0.14	26,26,26,26	0
56	MG	1A	3980	1/1	0.91	0.09	33,33,33,33	0
56	MG	1A	3156	1/1	0.91	0.32	40,40,40,40	0
56	MG	1A	4008	1/1	0.91	0.24	68,68,68,68	0
56	MG	2a	1611	1/1	0.91	0.10	68,68,68,68	0
56	MG	2a	1668	1/1	0.91	0.32	42,42,42,42	0
56	MG	1A	3229	1/1	0.91	0.16	57,57,57,57	0
56	MG	1A	3324	1/1	0.91	0.07	62,62,62,62	0
56	MG	2A	3494	1/1	0.91	0.25	54,54,54,54	0
56	MG	2A	3242	1/1	0.91	0.28	53,53,53,53	0
56	MG	1A	4033	1/1	0.91	0.12	71,71,71,71	0
56	MG	1A	3089	1/1	0.91	0.17	50,50,50,50	0
56	MG	2A	3444	1/1	0.91	0.07	58,58,58,58	0
56	MG	1A	3326	1/1	0.91	0.09	62,62,62,62	0
56	MG	2a	1618	1/1	0.91	0.28	74,74,74,74	0
56	MG	2A	3545	1/1	0.91	0.14	69,69,69,69	0
56	MG	1A	3031	1/1	0.91	0.13	60,60,60,60	0
56	MG	1a	1737	1/1	0.91	0.07	70,70,70,70	0
56	MG	15	104	1/1	0.91	0.26	54,54,54,54	0
56	MG	1A	3844	1/1	0.91	0.14	56,56,56,56	0
56	MG	1a	1602	1/1	0.91	0.26	81,81,81,81	0
56	MG	2A	3085	1/1	0.91	0.16	31,31,31,31	0
56	MG	2a	1629	1/1	0.91	0.07	72,72,72,72	0
56	MG	2A	3056	1/1	0.91	0.11	37,37,37,37	0
56	MG	1A	3187	1/1	0.91	0.16	42,42,42,42	0
56	MG	1A	3399	1/1	0.92	0.13	39,39,39,39	0
56	MG	1A	3547	1/1	0.92	0.11	56,56,56,56	0
56	MG	1A	3809	1/1	0.92	0.12	43,43,43,43	0
56	MG	2a	1750	1/1	0.92	0.39	54,54,54,54	0
56	MG	2a	1613	1/1	0.92	0.49	63,63,63,63	0
56	MG	1A	3474	1/1	0.92	0.10	49,49,49,49	0
56	MG	2a	1628	1/1	0.92	0.55	66,66,66,66	0
56	MG	1A	3744	1/1	0.92	0.16	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	1A	3938	1/1	0.92	0.13	34,34,34,34	0
56	MG	1a	1641	1/1	0.92	0.82	64,64,64,64	0
56	MG	2A	3138	1/1	0.92	0.22	36,36,36,36	0
56	MG	2A	3005	1/1	0.92	0.18	59,59,59,59	0
56	MG	1A	3693	1/1	0.92	0.12	25,25,25,25	0
56	MG	1A	3473	1/1	0.92	0.52	47,47,47,47	0
56	MG	2A	3135	1/1	0.92	0.15	46,46,46,46	0
56	MG	1A	3312	1/1	0.92	0.12	59,59,59,59	0
56	MG	1A	3077	1/1	0.92	0.16	59,59,59,59	0
56	MG	2A	3498	1/1	0.92	0.13	63,63,63,63	0
56	MG	2A	3401	1/1	0.92	0.26	60,60,60,60	0
56	MG	1A	3677	1/1	0.92	0.17	16,16,16,16	0
56	MG	1A	3808	1/1	0.92	0.12	31,31,31,31	0
56	MG	1u	8001	1/1	0.92	0.21	69,69,69,69	0
56	MG	1a	1804	1/1	0.92	0.15	66,66,66,66	0
56	MG	1A	3332	1/1	0.92	0.12	54,54,54,54	0
56	MG	2A	3343	1/1	0.92	0.16	53,53,53,53	0
56	MG	1A	3065	1/1	0.92	0.45	53,53,53,53	0
56	MG	1l	103	1/1	0.92	0.16	50,50,50,50	0
56	MG	2A	3466	1/1	0.92	0.14	45,45,45,45	0
56	MG	2A	3183	1/1	0.92	0.20	44,44,44,44	0
56	MG	2A	3303	1/1	0.92	0.10	30,30,30,30	0
56	MG	2A	3381	1/1	0.92	0.10	52,52,52,52	0
56	MG	2A	3493	1/1	0.92	0.30	57,57,57,57	0
56	MG	1x	106	1/1	0.92	0.17	46,46,46,46	0
56	MG	1A	3626	1/1	0.92	0.21	27,27,27,27	0
56	MG	2A	3054	1/1	0.92	0.15	44,44,44,44	0
56	MG	1A	3503	1/1	0.92	0.13	56,56,56,56	0
56	MG	1A	3598	1/1	0.92	0.16	48,48,48,48	0
56	MG	1A	3706	1/1	0.92	0.34	68,68,68,68	0
56	MG	1A	3417	1/1	0.92	0.30	44,44,44,44	0
56	MG	1A	3212	1/1	0.92	0.07	50,50,50,50	0
56	MG	1a	1888	1/1	0.92	0.28	46,46,46,46	0
56	MG	1A	3923	1/1	0.92	0.18	46,46,46,46	0
56	MG	2n	502	1/1	0.92	0.48	56,56,56,56	0
56	MG	2a	1656	1/1	0.92	0.20	50,50,50,50	0
56	MG	1q	3301	1/1	0.92	0.29	49,49,49,49	0
56	MG	1A	3459	1/1	0.92	0.11	44,44,44,44	0
56	MG	1A	3265	1/1	0.92	0.20	52,52,52,52	0
56	MG	1Q	3002	1/1	0.92	0.23	36,36,36,36	0
56	MG	1A	4028	1/1	0.92	0.20	87,87,87,87	0
56	MG	2Q	3004	1/1	0.92	0.23	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	2A	3015	1/1	0.92	0.12	57,57,57,57	0
56	MG	1A	3982	1/1	0.92	0.19	40,40,40,40	0
56	MG	1A	3371	1/1	0.92	0.26	46,46,46,46	0
56	MG	1A	3578	1/1	0.92	0.37	47,47,47,47	0
56	MG	1A	3186	1/1	0.92	0.46	36,36,36,36	0
56	MG	2A	3450	1/1	0.92	0.20	52,52,52,52	0
56	MG	1B	221	1/1	0.92	0.11	57,57,57,57	0
56	MG	1a	1659	1/1	0.92	0.13	68,68,68,68	0
56	MG	2A	3175	1/1	0.92	0.35	30,30,30,30	0
56	MG	1a	1696	1/1	0.92	0.12	59,59,59,59	0
56	MG	1a	1773	1/1	0.92	0.12	65,65,65,65	0
56	MG	1A	3513	1/1	0.92	0.20	58,58,58,58	0
56	MG	1A	3438	1/1	0.92	0.21	54,54,54,54	0
56	MG	2A	3189	1/1	0.92	0.26	45,45,45,45	0
56	MG	2A	3047	1/1	0.92	0.22	48,48,48,48	0
56	MG	1a	1624	1/1	0.92	0.35	64,64,64,64	0
56	MG	1A	3373	1/1	0.92	0.14	58,58,58,58	0
56	MG	2A	3453	1/1	0.92	0.15	67,67,67,67	0
56	MG	1a	1856	1/1	0.92	0.21	68,68,68,68	0
56	MG	2a	1742	1/1	0.92	0.28	71,71,71,71	0
56	MG	1a	1644	1/1	0.92	0.18	60,60,60,60	0
56	MG	1a	1716	1/1	0.92	0.16	77,77,77,77	0
56	MG	1a	1787	1/1	0.92	0.12	61,61,61,61	0
56	MG	1A	3158	1/1	0.92	0.21	38,38,38,38	0
56	MG	1A	3393	1/1	0.92	0.08	54,54,54,54	0
56	MG	1a	1764	1/1	0.92	0.10	85,85,85,85	0
56	MG	2A	3179	1/1	0.92	0.21	47,47,47,47	0
56	MG	2A	3159	1/1	0.92	0.23	71,71,71,71	0
56	MG	1R	201	1/1	0.92	0.28	55,55,55,55	0
56	MG	2A	3176	1/1	0.92	0.30	37,37,37,37	0
56	MG	2a	1769	1/1	0.92	0.23	56,56,56,56	0
56	MG	2A	3213	1/1	0.92	0.15	53,53,53,53	0
56	MG	1A	3587	1/1	0.92	0.10	38,38,38,38	0
56	MG	2a	1813	1/1	0.92	0.33	72,72,72,72	0
56	MG	1X	3001	1/1	0.92	0.27	43,43,43,43	0
56	MG	2a	1663	1/1	0.92	0.07	51,51,51,51	0
56	MG	1A	3987	1/1	0.92	0.15	54,54,54,54	0
56	MG	1A	3126	1/1	0.92	0.26	44,44,44,44	0
56	MG	1A	3670	1/1	0.92	0.17	19,19,19,19	0
56	MG	1A	3011	1/1	0.92	0.20	49,49,49,49	0
56	MG	2A	3279	1/1	0.92	0.06	55,55,55,55	0
56	MG	1U	202	1/1	0.92	0.40	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	1B	222	1/1	0.92	0.13	62,62,62,62	0
56	MG	1A	3579	1/1	0.92	0.07	51,51,51,51	0
56	MG	1A	3849	1/1	0.92	0.07	55,55,55,55	0
56	MG	1A	3411	1/1	0.92	0.14	47,47,47,47	0
56	MG	2A	3257	1/1	0.92	0.21	35,35,35,35	0
56	MG	1A	3279	1/1	0.92	0.40	53,53,53,53	0
56	MG	2A	3220	1/1	0.92	0.16	43,43,43,43	0
56	MG	1a	1790	1/1	0.92	0.20	68,68,68,68	0
56	MG	2a	1815	1/1	0.92	0.13	56,56,56,56	0
56	MG	1A	3613	1/1	0.92	0.10	30,30,30,30	0
56	MG	1A	3122	1/1	0.92	0.15	44,44,44,44	0
56	MG	2A	3364	1/1	0.92	0.18	42,42,42,42	0
56	MG	1A	3466	1/1	0.92	0.28	57,57,57,57	0
56	MG	2A	3122	1/1	0.92	0.09	54,54,54,54	0
56	MG	2a	1678	1/1	0.92	0.09	58,58,58,58	0
56	MG	2A	3286	1/1	0.92	0.24	32,32,32,32	0
56	MG	2A	3057	1/1	0.92	0.16	54,54,54,54	0
56	MG	1a	1686	1/1	0.92	0.16	48,48,48,48	0
56	MG	1a	1692	1/1	0.92	0.05	61,61,61,61	0
56	MG	1A	3255	1/1	0.92	0.09	61,61,61,61	0
56	MG	1a	1745	1/1	0.92	0.21	50,50,50,50	0
56	MG	1A	4000	1/1	0.92	0.26	50,50,50,50	0
56	MG	2a	1737	1/1	0.92	0.10	74,74,74,74	0
56	MG	1R	204	1/1	0.92	0.23	58,58,58,58	0
56	MG	1A	3822	1/1	0.92	0.07	48,48,48,48	0
56	MG	1a	1648	1/1	0.92	0.23	60,60,60,60	0
56	MG	1A	3666	1/1	0.92	0.10	28,28,28,28	0
56	MG	1A	3022	1/1	0.92	0.14	46,46,46,46	0
56	MG	1A	3680	1/1	0.92	0.09	45,45,45,45	0
56	MG	1A	3975	1/1	0.92	0.20	50,50,50,50	0
56	MG	2a	1602	1/1	0.92	0.17	41,41,41,41	0
56	MG	2A	3389	1/1	0.92	0.11	52,52,52,52	0
56	MG	1A	3940	1/1	0.92	0.14	48,48,48,48	0
56	MG	2A	3424	1/1	0.92	0.15	44,44,44,44	0
56	MG	2A	3342	1/1	0.92	0.35	56,56,56,56	0
56	MG	2A	3243	1/1	0.92	0.14	27,27,27,27	0
56	MG	1A	4022	1/1	0.92	0.06	64,64,64,64	0
56	MG	2A	3114	1/1	0.92	0.30	45,45,45,45	0
56	MG	2A	3505	1/1	0.92	0.09	42,42,42,42	0
56	MG	2A	3062	1/1	0.92	0.16	43,43,43,43	0
56	MG	1A	3951	1/1	0.92	0.14	40,40,40,40	0
56	MG	2a	1648	1/1	0.92	0.14	68,68,68,68	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
57	ZN	2Y	202	1/1	0.92	0.05	80,80,80,80	0
56	MG	2A	3163	1/1	0.92	0.17	52,52,52,52	0
56	MG	1a	1834	1/1	0.92	0.27	48,48,48,48	0
56	MG	2A	3025	1/1	0.92	0.20	45,45,45,45	0
56	MG	1A	3390	1/1	0.92	0.14	56,56,56,56	0
56	MG	1A	3567	1/1	0.92	0.25	47,47,47,47	0
56	MG	1A	4031	1/1	0.92	0.66	64,64,64,64	0
56	MG	1A	3325	1/1	0.92	0.30	59,59,59,59	0
56	MG	1a	1776	1/1	0.92	0.08	54,54,54,54	0
56	MG	1A	3955	1/1	0.92	0.18	46,46,46,46	0
56	MG	1A	3535	1/1	0.92	0.22	57,57,57,57	0
56	MG	2A	3514	1/1	0.92	0.20	53,53,53,53	0
56	MG	2a	1716	1/1	0.92	0.14	53,53,53,53	0
56	MG	1A	3821	1/1	0.92	0.18	59,59,59,59	0
56	MG	1A	3053	1/1	0.92	0.60	41,41,41,41	0
56	MG	2A	3022	1/1	0.93	0.12	42,42,42,42	0
56	MG	1a	1880	1/1	0.93	0.12	68,68,68,68	0
56	MG	2a	1724	1/1	0.93	0.22	64,64,64,64	0
56	MG	1a	1897	1/1	0.93	0.43	53,53,53,53	0
56	MG	1A	3440	1/1	0.93	0.06	45,45,45,45	0
56	MG	1A	3413	1/1	0.93	0.28	53,53,53,53	0
56	MG	1A	3974	1/1	0.93	0.18	46,46,46,46	0
56	MG	1a	1758	1/1	0.93	0.12	50,50,50,50	0
56	MG	2a	1711	1/1	0.93	0.16	61,61,61,61	0
56	MG	2A	3380	1/1	0.93	0.10	37,37,37,37	0
56	MG	2A	3091	1/1	0.93	0.16	52,52,52,52	0
56	MG	2A	3013	1/1	0.93	0.12	52,52,52,52	0
56	MG	2A	3506	1/1	0.93	0.12	37,37,37,37	0
56	MG	2A	3372	1/1	0.93	0.08	58,58,58,58	0
56	MG	2a	1658	1/1	0.93	0.14	53,53,53,53	0
56	MG	1A	3021	1/1	0.93	0.20	43,43,43,43	0
56	MG	2A	3384	1/1	0.93	0.10	33,33,33,33	0
56	MG	2x	3002	1/1	0.93	0.06	57,57,57,57	0
56	MG	1A	3920	1/1	0.93	0.32	87,87,87,87	0
56	MG	2A	3273	1/1	0.93	0.10	70,70,70,70	0
56	MG	2A	3039	1/1	0.93	0.42	45,45,45,45	0
56	MG	1A	3402	1/1	0.93	0.20	51,51,51,51	0
56	MG	1a	1845	1/1	0.93	0.07	70,70,70,70	0
56	MG	1A	3543	1/1	0.93	0.10	41,41,41,41	0
56	MG	2A	3240	1/1	0.93	0.16	46,46,46,46	0
56	MG	2A	3117	1/1	0.93	0.15	41,41,41,41	0
56	MG	2A	3124	1/1	0.93	0.24	48,48,48,48	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	2A	3224	1/1	0.93	0.12	37,37,37,37	0
56	MG	1A	3257	1/1	0.93	0.35	55,55,55,55	0
56	MG	2A	3531	1/1	0.93	0.10	47,47,47,47	0
56	MG	1a	1637	1/1	0.93	0.14	51,51,51,51	0
56	MG	1Z	301	1/1	0.93	0.16	44,44,44,44	0
56	MG	2A	3459	1/1	0.93	0.21	46,46,46,46	0
56	MG	1A	3682	1/1	0.93	0.14	37,37,37,37	0
56	MG	1A	3368	1/1	0.93	0.12	53,53,53,53	0
56	MG	1A	3233	1/1	0.93	0.14	42,42,42,42	0
56	MG	2a	1644	1/1	0.93	0.12	47,47,47,47	0
56	MG	2A	3483	1/1	0.93	0.09	43,43,43,43	0
56	MG	1A	3351	1/1	0.93	0.29	47,47,47,47	0
56	MG	2A	3007	1/1	0.93	0.26	57,57,57,57	0
56	MG	2A	3023	1/1	0.93	0.19	49,49,49,49	0
56	MG	1A	3972	1/1	0.93	0.17	80,80,80,80	0
56	MG	1A	3730	1/1	0.93	0.42	59,59,59,59	0
56	MG	1a	1906	1/1	0.93	0.07	75,75,75,75	0
56	MG	1A	3801	1/1	0.93	0.19	15,15,15,15	0
56	MG	2A	3410	1/1	0.93	0.12	56,56,56,56	0
56	MG	2A	3533	1/1	0.93	0.35	28,28,28,28	0
56	MG	1A	3883	1/1	0.93	0.17	45,45,45,45	0
56	MG	1A	3815	1/1	0.93	0.10	52,52,52,52	0
56	MG	2A	3321	1/1	0.93	0.15	32,32,32,32	0
56	MG	2A	3497	1/1	0.93	0.23	62,62,62,62	0
56	MG	1A	3047	1/1	0.93	0.15	40,40,40,40	0
56	MG	1E	308	1/1	0.93	0.30	28,28,28,28	0
56	MG	1k	201	1/1	0.93	0.11	68,68,68,68	0
56	MG	1A	3480	1/1	0.93	0.18	47,47,47,47	0
56	MG	1A	3816	1/1	0.93	0.17	56,56,56,56	0
56	MG	2A	3502	1/1	0.93	0.09	47,47,47,47	0
56	MG	1A	3005	1/1	0.93	0.19	57,57,57,57	0
56	MG	2A	3486	1/1	0.93	0.21	70,70,70,70	0
56	MG	1A	3387	1/1	0.93	0.26	33,33,33,33	0
56	MG	2A	3412	1/1	0.93	0.11	53,53,53,53	0
56	MG	1a	1738	1/1	0.93	0.21	53,53,53,53	0
56	MG	1A	3780	1/1	0.93	0.21	23,23,23,23	0
56	MG	2A	3173	1/1	0.93	0.38	54,54,54,54	0
56	MG	2A	3484	1/1	0.93	0.15	53,53,53,53	0
56	MG	1A	3654	1/1	0.93	0.16	20,20,20,20	0
56	MG	2A	3515	1/1	0.93	0.10	53,53,53,53	0
56	MG	2A	3280	1/1	0.93	0.11	46,46,46,46	0
56	MG	2A	3209	1/1	0.93	0.22	49,49,49,49	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	2A	3482	1/1	0.93	0.38	59,59,59,59	0
56	MG	1A	3663	1/1	0.93	0.17	20,20,20,20	0
56	MG	1A	3247	1/1	0.93	0.18	62,62,62,62	0
56	MG	2A	3221	1/1	0.93	0.29	30,30,30,30	0
56	MG	1a	1631	1/1	0.93	0.41	45,45,45,45	0
56	MG	1r	102	1/1	0.93	0.12	47,47,47,47	0
56	MG	2A	3334	1/1	0.93	0.16	57,57,57,57	0
56	MG	2A	3309	1/1	0.93	0.14	39,39,39,39	0
56	MG	2A	3045	1/1	0.93	0.09	38,38,38,38	0
56	MG	1A	3655	1/1	0.93	0.28	36,36,36,36	0
56	MG	10	106	1/1	0.93	0.52	72,72,72,72	0
56	MG	2B	3001	1/1	0.93	0.21	57,57,57,57	0
56	MG	2A	3181	1/1	0.93	0.21	38,38,38,38	0
56	MG	2A	3519	1/1	0.93	0.15	44,44,44,44	0
56	MG	2A	3532	1/1	0.93	0.39	43,43,43,43	0
56	MG	1A	3806	1/1	0.93	0.07	65,65,65,65	0
56	MG	1A	3042	1/1	0.93	0.25	44,44,44,44	0
56	MG	2a	1671	1/1	0.93	0.37	53,53,53,53	0
56	MG	1A	3002	1/1	0.93	0.11	48,48,48,48	0
56	MG	1b	3002	1/1	0.93	0.38	82,82,82,82	0
56	MG	2A	3177	1/1	0.93	0.16	40,40,40,40	0
56	MG	1A	3035	1/1	0.93	0.46	59,59,59,59	0
56	MG	2A	3065	1/1	0.93	0.23	56,56,56,56	0
56	MG	1A	3407	1/1	0.93	0.17	67,67,67,67	0
56	MG	1A	3406	1/1	0.93	0.15	49,49,49,49	0
56	MG	2A	3346	1/1	0.93	0.12	44,44,44,44	0
56	MG	1A	3701	1/1	0.93	0.07	28,28,28,28	0
56	MG	1A	3197	1/1	0.93	0.18	44,44,44,44	0
56	MG	1E	307	1/1	0.93	0.14	64,64,64,64	0
56	MG	1A	3640	1/1	0.93	0.18	42,42,42,42	0
56	MG	2A	3009	1/1	0.93	0.42	45,45,45,45	0
56	MG	1A	3256	1/1	0.93	0.12	37,37,37,37	0
56	MG	1a	1808	1/1	0.93	0.18	57,57,57,57	0
56	MG	1A	4040	1/1	0.93	0.15	51,51,51,51	0
56	MG	18	103	1/1	0.93	0.27	59,59,59,59	0
56	MG	1A	3895	1/1	0.93	0.19	57,57,57,57	0
56	MG	1A	3964	1/1	0.93	0.18	20,20,20,20	0
56	MG	2A	3489	1/1	0.93	0.25	60,60,60,60	0
56	MG	1A	3014	1/1	0.93	0.32	46,46,46,46	0
56	MG	1a	1871	1/1	0.93	0.13	50,50,50,50	0
56	MG	1a	1875	1/1	0.93	0.19	61,61,61,61	0
56	MG	2A	3167	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	1659	1/1	0.93	0.27	60,60,60,60	0
56	MG	1A	3008	1/1	0.93	0.22	53,53,53,53	0
56	MG	1A	3046	1/1	0.93	0.05	51,51,51,51	0
56	MG	2a	1705	1/1	0.93	0.28	68,68,68,68	0
56	MG	2A	3162	1/1	0.93	0.32	42,42,42,42	0
56	MG	2A	3174	1/1	0.93	0.17	32,32,32,32	0
56	MG	2a	1606	1/1	0.93	0.09	78,78,78,78	0
56	MG	1a	1638	1/1	0.93	0.10	56,56,56,56	0
56	MG	2a	1791	1/1	0.93	0.36	71,71,71,71	0
56	MG	1A	3833	1/1	0.93	0.12	36,36,36,36	0
56	MG	1A	4015	1/1	0.93	0.10	29,29,29,29	0
56	MG	2B	3006	1/1	0.93	0.19	40,40,40,40	0
56	MG	2A	3264	1/1	0.93	0.11	36,36,36,36	0
56	MG	1A	3601	1/1	0.93	0.14	24,24,24,24	0
56	MG	1A	3976	1/1	0.93	0.19	46,46,46,46	0
56	MG	1A	3888	1/1	0.93	0.12	87,87,87,87	0
56	MG	2A	3278	1/1	0.93	0.12	52,52,52,52	0
56	MG	19	104	1/1	0.93	0.13	46,46,46,46	0
56	MG	1A	3767	1/1	0.93	0.15	71,71,71,71	0
56	MG	1B	206	1/1	0.93	0.21	38,38,38,38	0
56	MG	2A	3249	1/1	0.93	0.23	53,53,53,53	0
56	MG	1N	202	1/1	0.93	0.46	49,49,49,49	0
56	MG	1A	3882	1/1	0.93	0.07	49,49,49,49	0
56	MG	1a	1663	1/1	0.93	0.24	64,64,64,64	0
56	MG	2N	8001	1/1	0.93	0.18	56,56,56,56	0
56	MG	1a	1785	1/1	0.93	0.17	66,66,66,66	0
56	MG	2A	3434	1/1	0.93	0.07	49,49,49,49	0
56	MG	1B	210	1/1	0.93	0.12	50,50,50,50	0
56	MG	1a	1774	1/1	0.93	0.11	75,75,75,75	0
56	MG	1A	3165	1/1	0.93	0.12	35,35,35,35	0
56	MG	2a	1608	1/1	0.93	0.09	67,67,67,67	0
56	MG	1o	3002	1/1	0.93	0.14	57,57,57,57	0
56	MG	1Y	201	1/1	0.93	0.29	39,39,39,39	0
56	MG	2a	1735	1/1	0.93	0.15	51,51,51,51	0
56	MG	1A	3289	1/1	0.93	0.19	32,32,32,32	0
56	MG	1a	1730	1/1	0.93	0.18	49,49,49,49	0
56	MG	1m	201	1/1	0.93	0.25	73,73,73,73	0
56	MG	1a	1708	1/1	0.93	0.20	40,40,40,40	0
56	MG	1e	203	1/1	0.93	0.14	61,61,61,61	0
56	MG	1A	3217	1/1	0.93	0.14	43,43,43,43	0
56	MG	1A	4063	1/1	0.93	0.14	38,38,38,38	0
56	MG	1A	3900	1/1	0.93	0.26	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	1651	1/1	0.93	0.12	52,52,52,52	0
56	MG	1A	3565	1/1	0.93	0.18	67,67,67,67	0
56	MG	1a	1860	1/1	0.93	0.08	49,49,49,49	0
56	MG	2E	302	1/1	0.93	0.29	45,45,45,45	0
56	MG	1a	1777	1/1	0.93	0.11	64,64,64,64	0
56	MG	1A	4034	1/1	0.93	0.13	50,50,50,50	0
56	MG	1A	3950	1/1	0.93	0.41	68,68,68,68	0
56	MG	1A	3318	1/1	0.93	0.23	53,53,53,53	0
56	MG	1A	3159	1/1	0.93	0.15	69,69,69,69	0
56	MG	1A	3454	1/1	0.93	0.19	42,42,42,42	0
56	MG	1A	3464	1/1	0.93	0.28	25,25,25,25	0
56	MG	1A	3442	1/1	0.93	0.50	64,64,64,64	0
56	MG	1A	3902	1/1	0.93	0.16	70,70,70,70	0
56	MG	1A	3753	1/1	0.93	0.17	21,21,21,21	0
56	MG	11	102	1/1	0.93	0.14	58,58,58,58	0
56	MG	1A	3372	1/1	0.93	0.19	52,52,52,52	0
56	MG	2A	3311	1/1	0.93	0.26	32,32,32,32	0
56	MG	2A	3037	1/1	0.93	0.13	44,44,44,44	0
56	MG	1A	3531	1/1	0.93	0.06	68,68,68,68	0
56	MG	1A	3943	1/1	0.93	0.12	54,54,54,54	0
56	MG	1a	1693	1/1	0.93	0.19	55,55,55,55	0
56	MG	1A	3084	1/1	0.93	0.26	32,32,32,32	0
56	MG	1A	3041	1/1	0.93	0.24	50,50,50,50	0
56	MG	1A	3978	1/1	0.93	0.12	67,67,67,67	0
56	MG	1A	3574	1/1	0.93	0.23	29,29,29,29	0
56	MG	1A	3052	1/1	0.93	0.19	49,49,49,49	0
56	MG	1A	3079	1/1	0.93	0.54	46,46,46,46	0
56	MG	2A	3559	1/1	0.93	0.13	58,58,58,58	0
56	MG	2A	3111	1/1	0.93	0.13	36,36,36,36	0
56	MG	1A	3909	1/1	0.93	0.13	54,54,54,54	0
56	MG	2A	3277	1/1	0.93	0.31	42,42,42,42	0
56	MG	2A	3332	1/1	0.93	0.21	48,48,48,48	0
56	MG	1A	3702	1/1	0.93	0.23	48,48,48,48	0
56	MG	2A	3071	1/1	0.93	0.13	42,42,42,42	0
56	MG	1a	1840	1/1	0.93	0.26	57,57,57,57	0
56	MG	2A	3404	1/1	0.93	0.26	55,55,55,55	0
56	MG	1A	4018	1/1	0.93	0.19	49,49,49,49	0
56	MG	2U	201	1/1	0.93	0.17	30,30,30,30	0
56	MG	2A	3485	1/1	0.93	0.16	48,48,48,48	0
56	MG	1W	3005	1/1	0.93	0.25	32,32,32,32	0
56	MG	1A	3494	1/1	0.93	0.19	63,63,63,63	0
56	MG	18	104	1/1	0.93	0.27	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	3015	1/1	0.93	0.12	52,52,52,52	0
56	MG	1A	3350	1/1	0.93	0.28	67,67,67,67	0
56	MG	2a	1643	1/1	0.93	0.34	69,69,69,69	0
56	MG	1A	3213	1/1	0.93	0.09	63,63,63,63	0
56	MG	1A	3903	1/1	0.93	0.28	50,50,50,50	0
56	MG	1A	3258	1/1	0.93	0.23	43,43,43,43	0
56	MG	2Q	3001	1/1	0.93	0.36	39,39,39,39	0
56	MG	2A	3031	1/1	0.93	0.22	49,49,49,49	0
56	MG	1A	3533	1/1	0.93	0.16	57,57,57,57	0
56	MG	2A	3432	1/1	0.93	0.25	48,48,48,48	0
56	MG	1A	3206	1/1	0.93	0.18	37,37,37,37	0
56	MG	1A	3457	1/1	0.93	0.16	52,52,52,52	0
56	MG	1A	4011	1/1	0.94	0.12	48,48,48,48	0
56	MG	1A	3927	1/1	0.94	0.17	61,61,61,61	0
56	MG	2A	3419	1/1	0.94	0.22	45,45,45,45	0
56	MG	2a	1757	1/1	0.94	0.17	60,60,60,60	0
56	MG	2A	3406	1/1	0.94	0.09	58,58,58,58	0
56	MG	2a	1754	1/1	0.94	0.17	44,44,44,44	0
56	MG	2A	3026	1/1	0.94	0.44	54,54,54,54	0
56	MG	1T	206	1/1	0.94	0.23	69,69,69,69	0
56	MG	2A	3353	1/1	0.94	0.18	59,59,59,59	0
56	MG	1A	3408	1/1	0.94	0.04	43,43,43,43	0
56	MG	1A	3419	1/1	0.94	0.14	47,47,47,47	0
56	MG	1A	3619	1/1	0.94	0.22	24,24,24,24	0
56	MG	1a	1611	1/1	0.94	0.07	76,76,76,76	0
56	MG	1A	3931	1/1	0.94	0.10	42,42,42,42	0
56	MG	1A	3752	1/1	0.94	0.19	25,25,25,25	0
56	MG	2a	1812	1/1	0.94	0.28	42,42,42,42	0
56	MG	1A	3240	1/1	0.94	0.18	37,37,37,37	0
56	MG	1a	1672	1/1	0.94	0.10	53,53,53,53	0
56	MG	2a	1778	1/1	0.94	0.12	69,69,69,69	0
56	MG	1A	3973	1/1	0.94	0.14	29,29,29,29	0
56	MG	2A	3411	1/1	0.94	0.21	65,65,65,65	0
56	MG	1A	3858	1/1	0.94	0.24	44,44,44,44	0
56	MG	1A	4027	1/1	0.94	0.16	50,50,50,50	0
56	MG	2a	1794	1/1	0.94	0.12	68,68,68,68	0
56	MG	1A	3134	1/1	0.94	0.43	35,35,35,35	0
56	MG	1D	312	1/1	0.94	0.10	44,44,44,44	0
56	MG	1A	3019	1/1	0.94	0.29	46,46,46,46	0
56	MG	1A	3632	1/1	0.94	0.14	27,27,27,27	0
56	MG	2a	1650	1/1	0.94	0.08	70,70,70,70	0
56	MG	1A	3599	1/1	0.94	0.12	47,47,47,47	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	2D	306	1/1	0.94	0.15	55,55,55,55	0
56	MG	1a	1632	1/1	0.94	0.17	47,47,47,47	0
56	MG	2a	1674	1/1	0.94	0.14	50,50,50,50	0
56	MG	1a	1855	1/1	0.94	0.31	58,58,58,58	0
56	MG	2A	3250	1/1	0.94	0.12	70,70,70,70	0
56	MG	1A	3163	1/1	0.94	0.16	38,38,38,38	0
56	MG	2A	3379	1/1	0.94	0.23	64,64,64,64	0
56	MG	1A	3928	1/1	0.94	0.10	57,57,57,57	0
56	MG	1A	3167	1/1	0.94	0.17	35,35,35,35	0
56	MG	2a	1624	1/1	0.94	0.14	62,62,62,62	0
56	MG	1A	3075	1/1	0.94	0.60	57,57,57,57	0
56	MG	2A	3019	1/1	0.94	0.10	45,45,45,45	0
56	MG	2W	201	1/1	0.94	0.27	42,42,42,42	0
56	MG	1A	3827	1/1	0.94	0.25	44,44,44,44	0
56	MG	1A	4070	1/1	0.94	0.13	25,25,25,25	0
56	MG	1A	3733	1/1	0.94	0.15	44,44,44,44	0
56	MG	2A	3330	1/1	0.94	0.17	37,37,37,37	0
56	MG	1A	3839	1/1	0.94	0.32	28,28,28,28	0
56	MG	1A	3281	1/1	0.94	0.16	53,53,53,53	0
56	MG	2A	3214	1/1	0.94	0.11	42,42,42,42	0
56	MG	1A	3369	1/1	0.94	0.16	38,38,38,38	0
56	MG	1A	3881	1/1	0.94	0.15	43,43,43,43	0
56	MG	1A	4081	1/1	0.94	0.64	27,27,27,27	0
56	MG	1A	3057	1/1	0.94	0.21	49,49,49,49	0
56	MG	1A	3221	1/1	0.94	0.12	36,36,36,36	0
56	MG	1A	3679	1/1	0.94	0.15	41,41,41,41	0
56	MG	1A	3087	1/1	0.94	0.29	52,52,52,52	0
56	MG	1A	3657	1/1	0.94	0.17	48,48,48,48	0
56	MG	2a	1676	1/1	0.94	0.32	60,60,60,60	0
56	MG	1A	3604	1/1	0.94	0.16	30,30,30,30	0
56	MG	1a	1619	1/1	0.94	0.16	82,82,82,82	0
56	MG	2A	3086	1/1	0.94	0.12	36,36,36,36	0
56	MG	2A	3271	1/1	0.94	0.12	42,42,42,42	0
56	MG	1A	3264	1/1	0.94	0.12	51,51,51,51	0
56	MG	1F	305	1/1	0.94	0.19	48,48,48,48	0
56	MG	1A	3766	1/1	0.94	0.13	43,43,43,43	0
56	MG	1A	3066	1/1	0.94	0.09	56,56,56,56	0
56	MG	2A	3024	1/1	0.94	0.17	46,46,46,46	0
56	MG	1a	1881	1/1	0.94	0.21	40,40,40,40	0
56	MG	1A	3330	1/1	0.94	0.07	56,56,56,56	0
56	MG	1a	1798	1/1	0.94	0.13	52,52,52,52	0
56	MG	1A	3099	1/1	0.94	0.24	53,53,53,53	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	1A	3608	1/1	0.94	0.18	32,32,32,32	0
56	MG	1A	3919	1/1	0.94	0.18	48,48,48,48	0
56	MG	1A	3990	1/1	0.94	0.19	47,47,47,47	0
56	MG	1A	3272	1/1	0.94	0.16	60,60,60,60	0
56	MG	1A	3897	1/1	0.94	0.16	46,46,46,46	0
56	MG	1a	1645	1/1	0.94	0.07	59,59,59,59	0
56	MG	1A	3333	1/1	0.94	0.11	53,53,53,53	0
56	MG	1A	3518	1/1	0.94	0.12	57,57,57,57	0
56	MG	1a	1864	1/1	0.94	0.30	61,61,61,61	0
56	MG	1A	3211	1/1	0.94	0.16	43,43,43,43	0
56	MG	1l	101	1/1	0.94	0.41	75,75,75,75	0
56	MG	2A	3067	1/1	0.94	0.36	56,56,56,56	0
56	MG	1a	1694	1/1	0.94	0.12	45,45,45,45	0
56	MG	1A	4004	1/1	0.94	0.17	53,53,53,53	0
56	MG	1a	1752	1/1	0.94	0.54	60,60,60,60	0
56	MG	1A	3201	1/1	0.94	0.18	49,49,49,49	0
56	MG	1a	1734	1/1	0.94	0.34	54,54,54,54	0
56	MG	2A	3061	1/1	0.94	0.12	44,44,44,44	0
56	MG	1A	3088	1/1	0.94	0.09	47,47,47,47	0
56	MG	1A	3446	1/1	0.94	0.18	43,43,43,43	0
56	MG	1A	3610	1/1	0.94	0.26	27,27,27,27	0
56	MG	1A	4072	1/1	0.94	0.15	70,70,70,70	0
56	MG	2a	1625	1/1	0.94	0.26	42,42,42,42	0
56	MG	2A	3304	1/1	0.94	0.08	40,40,40,40	0
56	MG	1A	3448	1/1	0.94	0.10	58,58,58,58	0
56	MG	2A	3362	1/1	0.94	0.22	62,62,62,62	0
56	MG	1A	3355	1/1	0.94	0.11	54,54,54,54	0
56	MG	2A	3508	1/1	0.94	0.07	45,45,45,45	0
56	MG	2a	1660	1/1	0.94	0.07	62,62,62,62	0
56	MG	2a	1776	1/1	0.94	0.18	54,54,54,54	0
56	MG	2A	3123	1/1	0.94	0.14	53,53,53,53	0
56	MG	1A	3929	1/1	0.94	0.20	47,47,47,47	0
56	MG	1A	3499	1/1	0.94	0.11	42,42,42,42	0
56	MG	2a	1799	1/1	0.94	0.48	56,56,56,56	0
56	MG	2A	3516	1/1	0.94	0.16	30,30,30,30	0
56	MG	1a	1886	1/1	0.94	0.14	60,60,60,60	0
56	MG	2A	3442	1/1	0.94	0.12	60,60,60,60	0
56	MG	2A	3096	1/1	0.94	0.15	43,43,43,43	0
56	MG	1A	4006	1/1	0.94	0.23	51,51,51,51	0
56	MG	1A	4067	1/1	0.94	0.29	37,37,37,37	0
56	MG	2a	1619	1/1	0.94	0.21	53,53,53,53	0
56	MG	1A	3358	1/1	0.94	0.14	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	3775	1/1	0.94	0.20	14,14,14,14	0
56	MG	1A	3953	1/1	0.94	0.20	44,44,44,44	0
56	MG	1A	3944	1/1	0.94	0.49	50,50,50,50	0
56	MG	15	102	1/1	0.94	0.17	45,45,45,45	0
56	MG	1a	1724	1/1	0.94	0.09	47,47,47,47	0
56	MG	2A	3201	1/1	0.94	0.09	62,62,62,62	0
56	MG	1A	3568	1/1	0.94	0.30	53,53,53,53	0
56	MG	1a	1825	1/1	0.94	0.16	64,64,64,64	0
56	MG	1A	3983	1/1	0.94	0.20	53,53,53,53	0
56	MG	2A	3335	1/1	0.94	0.14	38,38,38,38	0
56	MG	1A	3208	1/1	0.94	0.20	51,51,51,51	0
56	MG	1A	3795	1/1	0.94	0.12	37,37,37,37	0
56	MG	2A	3116	1/1	0.94	0.17	33,33,33,33	0
56	MG	1A	4060	1/1	0.94	0.18	56,56,56,56	0
56	MG	1a	1850	1/1	0.94	0.17	47,47,47,47	0
56	MG	1A	4045	1/1	0.94	0.38	34,34,34,34	0
56	MG	1A	3297	1/1	0.94	0.15	41,41,41,41	0
56	MG	2A	3126	1/1	0.94	0.17	44,44,44,44	0
56	MG	1A	3686	1/1	0.94	0.08	36,36,36,36	0
56	MG	2a	1686	1/1	0.94	0.09	49,49,49,49	0
56	MG	2A	3337	1/1	0.94	0.31	59,59,59,59	0
56	MG	2E	303	1/1	0.94	0.40	42,42,42,42	0
56	MG	1A	3826	1/1	0.94	0.22	42,42,42,42	0
56	MG	1A	3144	1/1	0.94	0.22	34,34,34,34	0
56	MG	1a	1767	1/1	0.94	0.19	63,63,63,63	0
56	MG	2A	3070	1/1	0.94	0.15	53,53,53,53	0
56	MG	1A	3298	1/1	0.94	0.11	46,46,46,46	0
56	MG	1a	1622	1/1	0.94	0.19	59,59,59,59	0
56	MG	2A	3326	1/1	0.94	0.29	50,50,50,50	0
56	MG	2A	3317	1/1	0.94	0.11	37,37,37,37	0
56	MG	1A	4084	1/1	0.94	0.25	36,36,36,36	0
56	MG	2a	1653	1/1	0.94	0.08	60,60,60,60	0
56	MG	2a	1772	1/1	0.94	0.33	63,63,63,63	0
56	MG	1a	1713	1/1	0.94	0.11	54,54,54,54	0
56	MG	1A	3554	1/1	0.94	0.15	61,61,61,61	0
56	MG	1n	502	1/1	0.94	0.11	55,55,55,55	0
56	MG	2A	3207	1/1	0.94	0.21	41,41,41,41	0
56	MG	1A	3861	1/1	0.94	0.15	34,34,34,34	0
56	MG	1a	1907	1/1	0.94	0.24	37,37,37,37	0
56	MG	1A	4048	1/1	0.94	0.29	41,41,41,41	0
56	MG	2A	3064	1/1	0.94	0.24	33,33,33,33	0
56	MG	2a	1701	1/1	0.94	0.34	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	2A	3348	1/1	0.94	0.14	49,49,49,49	0
56	MG	2A	3501	1/1	0.94	0.08	52,52,52,52	0
56	MG	2A	3327	1/1	0.94	0.13	56,56,56,56	0
56	MG	1a	1865	1/1	0.94	0.10	55,55,55,55	0
56	MG	1a	1890	1/1	0.94	0.34	66,66,66,66	0
56	MG	1A	3237	1/1	0.94	0.11	27,27,27,27	0
56	MG	2A	3100	1/1	0.94	0.40	38,38,38,38	0
56	MG	1A	3239	1/1	0.94	0.17	25,25,25,25	0
56	MG	1A	3760	1/1	0.94	0.15	36,36,36,36	0
56	MG	1A	3874	1/1	0.94	0.10	33,33,33,33	0
56	MG	1W	3002	1/1	0.94	0.24	40,40,40,40	0
56	MG	2A	3522	1/1	0.94	0.16	50,50,50,50	0
56	MG	1A	4061	1/1	0.94	0.21	48,48,48,48	0
56	MG	2a	1723	1/1	0.94	0.41	67,67,67,67	0
56	MG	1A	3832	1/1	0.94	0.12	36,36,36,36	0
56	MG	2A	3197	1/1	0.94	0.19	47,47,47,47	0
56	MG	1A	3831	1/1	0.94	0.14	42,42,42,42	0
56	MG	2B	3009	1/1	0.94	0.35	58,58,58,58	0
56	MG	1A	3774	1/1	0.94	0.15	63,63,63,63	0
56	MG	1A	3642	1/1	0.94	0.17	39,39,39,39	0
56	MG	2A	3028	1/1	0.94	0.21	45,45,45,45	0
56	MG	1a	1654	1/1	0.94	0.14	72,72,72,72	0
56	MG	2A	3288	1/1	0.94	0.11	35,35,35,35	0
56	MG	1A	3588	1/1	0.94	0.21	14,14,14,14	0
56	MG	2A	3260	1/1	0.94	0.23	63,63,63,63	0
56	MG	1A	3112	1/1	0.94	0.14	45,45,45,45	0
56	MG	1A	3228	1/1	0.94	0.29	33,33,33,33	0
56	MG	1A	3230	1/1	0.94	0.19	28,28,28,28	0
56	MG	1A	3524	1/1	0.94	0.59	63,63,63,63	0
56	MG	2A	3443	1/1	0.94	0.09	53,53,53,53	0
56	MG	1A	4088	1/1	0.94	0.47	35,35,35,35	0
56	MG	19	103	1/1	0.94	0.11	40,40,40,40	0
56	MG	1A	4074	1/1	0.94	0.47	37,37,37,37	0
56	MG	1D	303	1/1	0.94	0.16	37,37,37,37	0
56	MG	1a	1780	1/1	0.94	0.27	62,62,62,62	0
56	MG	2A	3355	1/1	0.94	0.18	22,22,22,22	0
56	MG	1a	1904	1/1	0.94	0.12	60,60,60,60	0
56	MG	2A	3407	1/1	0.94	0.20	68,68,68,68	0
56	MG	1A	3586	1/1	0.94	0.18	55,55,55,55	0
56	MG	2Q	3005	1/1	0.94	0.30	46,46,46,46	0
56	MG	1A	3007	1/1	0.94	0.45	43,43,43,43	0
56	MG	2a	1759	1/1	0.94	0.12	68,68,68,68	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	1A	3383	1/1	0.94	0.20	43,43,43,43	0
56	MG	1A	3166	1/1	0.94	0.20	29,29,29,29	0
56	MG	1a	1701	1/1	0.94	0.13	60,60,60,60	0
56	MG	1A	3360	1/1	0.94	0.41	48,48,48,48	0
56	MG	2A	3329	1/1	0.94	0.10	36,36,36,36	0
56	MG	1A	3748	1/1	0.94	0.12	64,64,64,64	0
56	MG	1a	1717	1/1	0.94	0.09	73,73,73,73	0
56	MG	2a	1698	1/1	0.94	0.29	57,57,57,57	0
56	MG	2A	3524	1/1	0.94	0.15	46,46,46,46	0
56	MG	2A	3118	1/1	0.94	0.11	37,37,37,37	0
56	MG	1a	1796	1/1	0.94	0.15	54,54,54,54	0
56	MG	2a	1809	1/1	0.94	0.19	64,64,64,64	0
56	MG	1o	3001	1/1	0.94	0.08	64,64,64,64	0
56	MG	1A	4036	1/1	0.94	0.10	61,61,61,61	0
56	MG	1A	3995	1/1	0.94	0.22	16,16,16,16	0
56	MG	1A	3032	1/1	0.94	0.21	66,66,66,66	0
56	MG	2A	3417	1/1	0.94	0.09	42,42,42,42	0
56	MG	2A	3391	1/1	0.94	0.28	47,47,47,47	0
56	MG	1A	3894	1/1	0.94	0.13	49,49,49,49	0
56	MG	1A	3249	1/1	0.94	0.28	43,43,43,43	0
56	MG	1a	1647	1/1	0.94	0.10	45,45,45,45	0
56	MG	1A	3930	1/1	0.94	0.11	28,28,28,28	0
56	MG	2A	3149	1/1	0.94	0.14	39,39,39,39	0
56	MG	1A	3374	1/1	0.94	0.14	48,48,48,48	0
56	MG	15	103	1/1	0.94	0.17	33,33,33,33	0
56	MG	2a	1738	1/1	0.94	0.10	58,58,58,58	0
56	MG	1A	3171	1/1	0.94	0.09	45,45,45,45	0
56	MG	2A	3169	1/1	0.94	0.34	54,54,54,54	0
56	MG	1A	3034	1/1	0.94	0.18	57,57,57,57	0
56	MG	2B	3008	1/1	0.94	0.21	69,69,69,69	0
56	MG	1a	1770	1/1	0.94	0.21	60,60,60,60	0
56	MG	17	101	1/1	0.94	0.45	35,35,35,35	0
56	MG	1A	3098	1/1	0.94	0.20	44,44,44,44	0
56	MG	1A	3952	1/1	0.94	0.08	66,66,66,66	0
56	MG	2A	3134	1/1	0.94	0.12	40,40,40,40	0
56	MG	1A	3070	1/1	0.94	0.19	52,52,52,52	0
56	MG	1N	205	1/1	0.94	0.15	42,42,42,42	0
56	MG	2A	3541	1/1	0.94	0.22	31,31,31,31	0
56	MG	1A	3823	1/1	0.94	0.13	62,62,62,62	0
56	MG	2A	3354	1/1	0.94	0.12	49,49,49,49	0
56	MG	1a	1715	1/1	0.94	0.19	47,47,47,47	0
56	MG	2A	3378	1/1	0.94	0.23	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	1a	1802	1/1	0.94	0.14	56,56,56,56	0
56	MG	2A	3232	1/1	0.94	0.13	47,47,47,47	0
56	MG	2A	3526	1/1	0.94	0.32	46,46,46,46	0
56	MG	1A	3553	1/1	0.94	0.21	50,50,50,50	0
56	MG	1A	3238	1/1	0.94	0.09	63,63,63,63	0
56	MG	1A	3309	1/1	0.94	0.10	48,48,48,48	0
56	MG	2A	3157	1/1	0.94	0.12	40,40,40,40	0
56	MG	2e	203	1/1	0.94	0.18	78,78,78,78	0
56	MG	2A	3448	1/1	0.94	0.27	53,53,53,53	0
56	MG	2A	3511	1/1	0.94	0.23	45,45,45,45	0
56	MG	2A	3422	1/1	0.94	0.34	53,53,53,53	0
56	MG	1A	3048	1/1	0.94	0.32	43,43,43,43	0
56	MG	1a	1649	1/1	0.94	0.13	49,49,49,49	0
56	MG	19	101	1/1	0.94	0.22	55,55,55,55	0
56	MG	2a	1731	1/1	0.94	0.12	68,68,68,68	0
56	MG	2a	1713	1/1	0.94	0.10	60,60,60,60	0
56	MG	2A	3312	1/1	0.94	0.10	27,27,27,27	0
56	MG	1B	201	1/1	0.94	0.26	72,72,72,72	0
56	MG	1A	3582	1/1	0.94	0.28	45,45,45,45	0
56	MG	2A	3433	1/1	0.94	0.14	56,56,56,56	0
56	MG	1A	3509	1/1	0.94	0.41	43,43,43,43	0
56	MG	1B	205	1/1	0.94	0.10	57,57,57,57	0
56	MG	2A	3510	1/1	0.95	0.20	49,49,49,49	0
56	MG	1A	3410	1/1	0.95	0.22	47,47,47,47	0
56	MG	1A	3114	1/1	0.95	0.14	36,36,36,36	0
56	MG	1a	1671	1/1	0.95	0.25	54,54,54,54	0
56	MG	2A	3428	1/1	0.95	0.32	58,58,58,58	0
56	MG	1A	3631	1/1	0.95	0.10	43,43,43,43	0
56	MG	1A	3688	1/1	0.95	0.17	21,21,21,21	0
56	MG	2A	3033	1/1	0.95	0.11	57,57,57,57	0
56	MG	2O	3001	1/1	0.95	0.14	49,49,49,49	0
56	MG	2A	3239	1/1	0.95	0.13	59,59,59,59	0
56	MG	2A	3540	1/1	0.95	0.21	45,45,45,45	0
56	MG	1A	3012	1/1	0.95	0.35	46,46,46,46	0
56	MG	1A	4009	1/1	0.95	0.20	40,40,40,40	0
56	MG	2A	3534	1/1	0.95	0.31	45,45,45,45	0
56	MG	2A	3420	1/1	0.95	0.10	54,54,54,54	0
56	MG	2A	3211	1/1	0.95	0.09	58,58,58,58	0
56	MG	2E	304	1/1	0.95	0.12	58,58,58,58	0
56	MG	1a	1892	1/1	0.95	0.16	49,49,49,49	0
56	MG	1A	3121	1/1	0.95	0.15	30,30,30,30	0
56	MG	1a	1809	1/1	0.95	0.15	75,75,75,75	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	2A	3275	1/1	0.95	0.21	45,45,45,45	0
56	MG	1d	502	1/1	0.95	0.10	60,60,60,60	0
56	MG	2A	3509	1/1	0.95	0.18	44,44,44,44	0
56	MG	2A	3426	1/1	0.95	0.09	43,43,43,43	0
56	MG	1A	3321	1/1	0.95	0.18	28,28,28,28	0
56	MG	2A	3198	1/1	0.95	0.16	51,51,51,51	0
56	MG	1A	3804	1/1	0.95	0.15	58,58,58,58	0
56	MG	1A	3525	1/1	0.95	0.22	54,54,54,54	0
56	MG	1A	3783	1/1	0.95	0.16	22,22,22,22	0
56	MG	1A	3188	1/1	0.95	0.21	50,50,50,50	0
56	MG	2A	3042	1/1	0.95	0.24	50,50,50,50	0
56	MG	1A	3684	1/1	0.95	0.15	21,21,21,21	0
56	MG	1A	3252	1/1	0.95	0.18	29,29,29,29	0
56	MG	2A	3488	1/1	0.95	0.16	57,57,57,57	0
56	MG	2A	3182	1/1	0.95	0.14	47,47,47,47	0
56	MG	1A	4071	1/1	0.95	0.11	40,40,40,40	0
56	MG	2a	1743	1/1	0.95	0.23	35,35,35,35	0
56	MG	1A	3453	1/1	0.95	0.09	48,48,48,48	0
56	MG	1A	3276	1/1	0.95	0.27	37,37,37,37	0
56	MG	2a	1641	1/1	0.95	0.12	64,64,64,64	0
56	MG	1W	3001	1/1	0.95	0.20	43,43,43,43	0
56	MG	1A	3802	1/1	0.95	0.16	36,36,36,36	0
56	MG	2a	1622	1/1	0.95	0.16	53,53,53,53	0
56	MG	2A	3168	1/1	0.95	0.12	43,43,43,43	0
56	MG	1A	3379	1/1	0.95	0.20	41,41,41,41	0
56	MG	1f	3001	1/1	0.95	0.24	56,56,56,56	0
56	MG	2A	3063	1/1	0.95	0.32	47,47,47,47	0
56	MG	1A	3639	1/1	0.95	0.15	57,57,57,57	0
56	MG	1A	3644	1/1	0.95	0.11	60,60,60,60	0
56	MG	2A	3170	1/1	0.95	0.11	40,40,40,40	0
56	MG	1A	4085	1/1	0.95	0.11	46,46,46,46	0
56	MG	2a	1652	1/1	0.95	0.06	45,45,45,45	0
56	MG	1A	3170	1/1	0.95	0.24	23,23,23,23	0
56	MG	1A	3635	1/1	0.95	0.12	83,83,83,83	0
56	MG	1A	3254	1/1	0.95	0.27	29,29,29,29	0
56	MG	2a	1691	1/1	0.95	0.15	55,55,55,55	0
56	MG	1A	3898	1/1	0.95	0.06	50,50,50,50	0
56	MG	1A	3948	1/1	0.95	0.34	56,56,56,56	0
56	MG	2D	302	1/1	0.95	0.11	48,48,48,48	0
56	MG	2A	3202	1/1	0.95	0.09	47,47,47,47	0
56	MG	1A	3763	1/1	0.95	0.10	41,41,41,41	0
56	MG	1A	4052	1/1	0.95	0.41	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	3282	1/1	0.95	0.14	39,39,39,39	0
56	MG	1A	3168	1/1	0.95	0.30	38,38,38,38	0
56	MG	1a	1862	1/1	0.95	0.15	58,58,58,58	0
56	MG	2A	3480	1/1	0.95	0.14	74,74,74,74	0
56	MG	2A	3076	1/1	0.95	0.07	42,42,42,42	0
56	MG	1A	3176	1/1	0.95	0.16	38,38,38,38	0
56	MG	1A	3737	1/1	0.95	0.12	60,60,60,60	0
56	MG	1A	3528	1/1	0.95	0.22	64,64,64,64	0
56	MG	1A	3789	1/1	0.95	0.23	21,21,21,21	0
56	MG	2a	1761	1/1	0.95	0.05	45,45,45,45	0
56	MG	1A	3627	1/1	0.95	0.15	50,50,50,50	0
56	MG	1A	3157	1/1	0.95	0.14	40,40,40,40	0
56	MG	1a	1794	1/1	0.95	0.12	60,60,60,60	0
56	MG	1a	1727	1/1	0.95	0.26	66,66,66,66	0
56	MG	1A	3097	1/1	0.95	0.15	55,55,55,55	0
56	MG	2A	3435	1/1	0.95	0.25	59,59,59,59	0
56	MG	1A	3377	1/1	0.95	0.38	43,43,43,43	0
56	MG	1A	3755	1/1	0.95	0.05	51,51,51,51	0
56	MG	1A	3769	1/1	0.95	0.15	44,44,44,44	0
56	MG	1A	3854	1/1	0.95	0.13	35,35,35,35	0
56	MG	1a	1823	1/1	0.95	0.19	54,54,54,54	0
56	MG	13	101	1/1	0.95	0.16	46,46,46,46	0
56	MG	1A	3472	1/1	0.95	0.09	46,46,46,46	0
56	MG	2A	3475	1/1	0.95	0.08	53,53,53,53	0
56	MG	1A	3961	1/1	0.95	0.12	54,54,54,54	0
56	MG	1a	1839	1/1	0.95	0.14	70,70,70,70	0
56	MG	1A	3811	1/1	0.95	0.15	34,34,34,34	0
56	MG	2F	303	1/1	0.95	0.23	50,50,50,50	0
56	MG	2A	3099	1/1	0.95	0.05	57,57,57,57	0
56	MG	1A	4054	1/1	0.95	0.15	40,40,40,40	0
56	MG	1a	1769	1/1	0.95	0.22	58,58,58,58	0
56	MG	1A	3803	1/1	0.95	0.16	53,53,53,53	0
56	MG	1B	225	1/1	0.95	0.09	51,51,51,51	0
56	MG	1A	3853	1/1	0.95	0.12	44,44,44,44	0
56	MG	2A	3446	1/1	0.95	0.13	52,52,52,52	0
56	MG	1A	3182	1/1	0.95	0.18	33,33,33,33	0
56	MG	1a	1709	1/1	0.95	0.14	66,66,66,66	0
56	MG	1A	3812	1/1	0.95	0.16	59,59,59,59	0
56	MG	1B	226	1/1	0.95	0.12	47,47,47,47	0
56	MG	2A	3136	1/1	0.95	0.10	44,44,44,44	0
56	MG	2A	3041	1/1	0.95	0.17	28,28,28,28	0
56	MG	1a	1679	1/1	0.95	0.16	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	16	104	1/1	0.95	0.28	43,43,43,43	0
56	MG	2A	3512	1/1	0.95	0.36	32,32,32,32	0
56	MG	1A	3798	1/1	0.95	0.15	23,23,23,23	0
56	MG	1A	3024	1/1	0.95	0.11	48,48,48,48	0
56	MG	1A	3600	1/1	0.95	0.12	50,50,50,50	0
56	MG	2A	3298	1/1	0.95	0.18	31,31,31,31	0
56	MG	1A	3427	1/1	0.95	0.12	44,44,44,44	0
56	MG	2A	3080	1/1	0.95	0.10	41,41,41,41	0
56	MG	1A	3051	1/1	0.95	0.31	47,47,47,47	0
56	MG	1a	1732	1/1	0.95	0.45	42,42,42,42	0
56	MG	1B	208	1/1	0.95	0.14	30,30,30,30	0
56	MG	1E	306	1/1	0.95	0.12	51,51,51,51	0
56	MG	1A	3199	1/1	0.95	0.25	36,36,36,36	0
56	MG	1a	1683	1/1	0.95	0.51	51,51,51,51	0
56	MG	1a	1691	1/1	0.95	0.11	59,59,59,59	0
56	MG	1A	3080	1/1	0.95	0.23	38,38,38,38	0
56	MG	2A	3083	1/1	0.95	0.12	51,51,51,51	0
56	MG	2A	3255	1/1	0.95	0.15	42,42,42,42	0
56	MG	1a	1877	1/1	0.95	0.05	65,65,65,65	0
56	MG	2x	3004	1/1	0.95	0.06	76,76,76,76	0
56	MG	1A	3365	1/1	0.95	0.12	57,57,57,57	0
56	MG	1a	1722	1/1	0.95	0.14	65,65,65,65	0
56	MG	2a	1603	1/1	0.95	0.31	50,50,50,50	0
56	MG	2A	3066	1/1	0.95	0.27	59,59,59,59	0
56	MG	2a	1736	1/1	0.95	0.08	74,74,74,74	0
56	MG	1q	3303	1/1	0.95	0.15	60,60,60,60	0
56	MG	1A	3061	1/1	0.95	0.15	51,51,51,51	0
56	MG	2A	3208	1/1	0.95	0.19	43,43,43,43	0
56	MG	1a	1642	1/1	0.95	0.31	95,95,95,95	0
56	MG	1A	3081	1/1	0.95	0.12	57,57,57,57	0
56	MG	1A	3904	1/1	0.95	0.09	64,64,64,64	0
56	MG	2A	3451	1/1	0.95	0.18	53,53,53,53	0
56	MG	1a	1832	1/1	0.95	0.15	65,65,65,65	0
56	MG	1A	3758	1/1	0.95	0.12	28,28,28,28	0
56	MG	1Z	302	1/1	0.95	0.11	56,56,56,56	0
56	MG	2A	3457	1/1	0.95	0.07	68,68,68,68	0
56	MG	2A	3016	1/1	0.95	0.11	58,58,58,58	0
56	MG	1A	4058	1/1	0.95	0.17	56,56,56,56	0
56	MG	1a	1687	1/1	0.95	0.11	51,51,51,51	0
56	MG	1a	1782	1/1	0.95	0.20	61,61,61,61	0
56	MG	2A	3408	1/1	0.95	0.23	46,46,46,46	0
56	MG	2a	1655	1/1	0.95	0.10	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	3146	1/1	0.95	0.21	32,32,32,32	0
56	MG	1a	1879	1/1	0.95	0.14	43,43,43,43	0
56	MG	1A	3781	1/1	0.95	0.14	19,19,19,19	0
56	MG	1A	4023	1/1	0.95	0.14	39,39,39,39	0
56	MG	2A	3154	1/1	0.95	0.32	39,39,39,39	0
56	MG	1A	3016	1/1	0.95	0.30	41,41,41,41	0
56	MG	2A	3053	1/1	0.95	0.10	47,47,47,47	0
56	MG	2A	3254	1/1	0.95	0.18	55,55,55,55	0
56	MG	1A	4001	1/1	0.95	0.09	49,49,49,49	0
56	MG	1a	1652	1/1	0.95	0.12	63,63,63,63	0
56	MG	2A	3425	1/1	0.95	0.10	46,46,46,46	0
56	MG	10	102	1/1	0.95	0.05	51,51,51,51	0
56	MG	1A	3712	1/1	0.95	0.25	29,29,29,29	0
56	MG	2A	3430	1/1	0.95	0.15	59,59,59,59	0
56	MG	1a	1882	1/1	0.95	0.12	40,40,40,40	0
56	MG	2a	1708	1/1	0.95	0.15	59,59,59,59	0
56	MG	1A	3772	1/1	0.95	0.24	51,51,51,51	0
56	MG	11	104	1/1	0.95	0.19	59,59,59,59	0
56	MG	1A	3203	1/1	0.95	0.13	19,19,19,19	0
56	MG	2A	3449	1/1	0.95	0.13	52,52,52,52	0
56	MG	1a	1660	1/1	0.95	0.12	57,57,57,57	0
56	MG	2a	1647	1/1	0.95	0.12	64,64,64,64	0
56	MG	2A	3145	1/1	0.95	0.32	33,33,33,33	0
56	MG	1A	3660	1/1	0.95	0.20	30,30,30,30	0
56	MG	1A	3174	1/1	0.95	0.11	47,47,47,47	0
56	MG	1A	3664	1/1	0.95	0.12	37,37,37,37	0
56	MG	1E	304	1/1	0.95	0.15	44,44,44,44	0
56	MG	1A	3370	1/1	0.95	0.15	43,43,43,43	0
56	MG	1T	202	1/1	0.95	0.09	38,38,38,38	0
56	MG	1A	3906	1/1	0.95	0.06	67,67,67,67	0
56	MG	2a	1807	1/1	0.95	0.19	46,46,46,46	0
56	MG	1A	3450	1/1	0.95	0.16	54,54,54,54	0
56	MG	1A	3151	1/1	0.95	0.28	26,26,26,26	0
56	MG	1B	202	1/1	0.95	0.14	56,56,56,56	0
56	MG	2a	1783	1/1	0.95	0.20	59,59,59,59	0
56	MG	1A	3581	1/1	0.95	0.20	51,51,51,51	0
56	MG	1a	1721	1/1	0.95	0.34	36,36,36,36	0
56	MG	1a	1878	1/1	0.95	0.21	64,64,64,64	0
56	MG	2A	3476	1/1	0.95	0.12	72,72,72,72	0
56	MG	1A	3645	1/1	0.95	0.26	44,44,44,44	0
56	MG	1A	3946	1/1	0.95	0.21	29,29,29,29	0
56	MG	1a	1682	1/1	0.95	0.22	48,48,48,48	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	1A	3609	1/1	0.95	0.26	26,26,26,26	0
56	MG	1A	3143	1/1	0.95	0.23	41,41,41,41	0
56	MG	1A	3285	1/1	0.95	0.14	47,47,47,47	0
56	MG	2A	3416	1/1	0.95	0.09	50,50,50,50	0
56	MG	1A	3478	1/1	0.95	0.32	50,50,50,50	0
56	MG	2a	1804	1/1	0.95	0.29	60,60,60,60	0
56	MG	1a	1899	1/1	0.95	0.09	43,43,43,43	0
56	MG	1A	3214	1/1	0.95	0.11	63,63,63,63	0
56	MG	1a	1753	1/1	0.95	0.56	53,53,53,53	0
56	MG	1A	3382	1/1	0.95	0.57	59,59,59,59	0
56	MG	1a	1729	1/1	0.95	0.22	38,38,38,38	0
56	MG	2A	3400	1/1	0.95	0.22	34,34,34,34	0
56	MG	2A	3523	1/1	0.95	0.18	57,57,57,57	0
56	MG	1A	3720	1/1	0.95	0.23	67,67,67,67	0
56	MG	1A	3421	1/1	0.95	0.12	52,52,52,52	0
56	MG	2A	3075	1/1	0.95	0.20	26,26,26,26	0
56	MG	1A	3880	1/1	0.95	0.08	76,76,76,76	0
56	MG	1A	3246	1/1	0.95	0.16	23,23,23,23	0
56	MG	1A	3263	1/1	0.95	0.18	31,31,31,31	0
56	MG	1A	3794	1/1	0.95	0.06	57,57,57,57	0
56	MG	2A	3035	1/1	0.95	0.10	57,57,57,57	0
56	MG	2Y	201	1/1	0.95	0.09	58,58,58,58	0
56	MG	2a	1681	1/1	0.95	0.16	53,53,53,53	0
56	MG	2D	304	1/1	0.95	0.17	27,27,27,27	0
56	MG	1a	1816	1/1	0.95	0.07	56,56,56,56	0
56	MG	1A	3308	1/1	0.95	0.14	40,40,40,40	0
56	MG	1q	3302	1/1	0.95	0.27	53,53,53,53	0
56	MG	2a	1732	1/1	0.95	0.22	75,75,75,75	0
56	MG	2a	1751	1/1	0.95	0.37	55,55,55,55	0
56	MG	1q	3304	1/1	0.95	0.16	47,47,47,47	0
56	MG	1A	3708	1/1	0.95	0.14	46,46,46,46	0
56	MG	2A	3256	1/1	0.95	0.18	36,36,36,36	0
56	MG	2A	3402	1/1	0.95	0.15	44,44,44,44	0
56	MG	1A	3432	1/1	0.95	0.42	52,52,52,52	0
56	MG	2A	3536	1/1	0.95	0.18	37,37,37,37	0
56	MG	2a	1664	1/1	0.95	0.38	51,51,51,51	0
56	MG	1A	3771	1/1	0.95	0.21	11,11,11,11	0
56	MG	2A	3360	1/1	0.95	0.32	41,41,41,41	0
56	MG	1A	3805	1/1	0.95	0.18	21,21,21,21	0
56	MG	2A	3520	1/1	0.95	0.16	25,25,25,25	0
56	MG	1A	3704	1/1	0.95	0.13	26,26,26,26	0
56	MG	1A	3185	1/1	0.95	0.41	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	2A	3218	1/1	0.95	0.08	37,37,37,37	0
56	MG	1A	3907	1/1	0.95	0.23	15,15,15,15	0
56	MG	1A	4068	1/1	0.95	0.17	36,36,36,36	0
56	MG	1A	3685	1/1	0.95	0.19	31,31,31,31	0
56	MG	1A	3872	1/1	0.95	0.13	28,28,28,28	0
56	MG	2A	3296	1/1	0.95	0.19	40,40,40,40	0
56	MG	2A	3386	1/1	0.95	0.17	68,68,68,68	0
56	MG	1A	3314	1/1	0.95	0.15	52,52,52,52	0
56	MG	2A	3418	1/1	0.95	0.21	56,56,56,56	0
56	MG	1A	3747	1/1	0.95	0.13	64,64,64,64	0
56	MG	1a	1900	1/1	0.95	0.24	68,68,68,68	0
56	MG	1A	3572	1/1	0.95	0.14	56,56,56,56	0
56	MG	1A	4090	1/1	0.95	0.40	38,38,38,38	0
56	MG	2A	3148	1/1	0.95	0.09	54,54,54,54	0
56	MG	1A	3723	1/1	0.95	0.14	51,51,51,51	0
56	MG	2a	1788	1/1	0.95	0.29	68,68,68,68	0
56	MG	1t	3001	1/1	0.95	0.37	53,53,53,53	0
56	MG	1A	3819	1/1	0.95	0.14	80,80,80,80	0
56	MG	1A	3207	1/1	0.95	0.23	47,47,47,47	0
56	MG	2A	3530	1/1	0.96	0.14	46,46,46,46	0
56	MG	2A	3052	1/1	0.96	0.22	37,37,37,37	0
56	MG	1A	4010	1/1	0.96	0.16	37,37,37,37	0
56	MG	1A	3313	1/1	0.96	0.08	50,50,50,50	0
56	MG	1A	3838	1/1	0.96	0.10	28,28,28,28	0
56	MG	1a	1866	1/1	0.96	0.13	55,55,55,55	0
56	MG	2A	3351	1/1	0.96	0.11	52,52,52,52	0
56	MG	1a	1736	1/1	0.96	0.20	59,59,59,59	0
56	MG	1a	1829	1/1	0.96	0.28	37,37,37,37	0
56	MG	1A	3120	1/1	0.96	0.16	28,28,28,28	0
56	MG	1A	3135	1/1	0.96	0.30	36,36,36,36	0
56	MG	2A	3137	1/1	0.96	0.26	63,63,63,63	0
56	MG	2A	3144	1/1	0.96	0.07	43,43,43,43	0
56	MG	2a	1727	1/1	0.96	0.14	45,45,45,45	0
56	MG	1a	1771	1/1	0.96	0.20	52,52,52,52	0
56	MG	1A	3793	1/1	0.96	0.22	50,50,50,50	0
56	MG	1a	1762	1/1	0.96	0.13	59,59,59,59	0
56	MG	2a	1706	1/1	0.96	0.36	58,58,58,58	0
56	MG	1A	3026	1/1	0.96	0.22	49,49,49,49	0
56	MG	1A	3200	1/1	0.96	0.24	28,28,28,28	0
56	MG	2l	201	1/1	0.96	0.10	66,66,66,66	0
56	MG	1A	3277	1/1	0.96	0.12	33,33,33,33	0
56	MG	1A	3236	1/1	0.96	0.05	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	1898	1/1	0.96	0.12	47,47,47,47	0
56	MG	1A	3999	1/1	0.96	0.13	27,27,27,27	0
56	MG	2A	3338	1/1	0.96	0.09	53,53,53,53	0
56	MG	1A	3092	1/1	0.96	0.28	47,47,47,47	0
56	MG	1A	3625	1/1	0.96	0.09	43,43,43,43	0
56	MG	2A	3215	1/1	0.96	0.14	43,43,43,43	0
56	MG	1A	3810	1/1	0.96	0.06	43,43,43,43	0
56	MG	1A	3111	1/1	0.96	0.19	35,35,35,35	0
56	MG	2a	1793	1/1	0.96	0.11	58,58,58,58	0
56	MG	2A	3034	1/1	0.96	0.11	44,44,44,44	0
56	MG	1A	3338	1/1	0.96	0.17	61,61,61,61	0
56	MG	1A	3864	1/1	0.96	0.11	53,53,53,53	0
56	MG	2A	3008	1/1	0.96	0.19	58,58,58,58	0
56	MG	1a	1735	1/1	0.96	0.37	43,43,43,43	0
56	MG	1a	1695	1/1	0.96	0.10	40,40,40,40	0
56	MG	1A	3597	1/1	0.96	0.23	36,36,36,36	0
56	MG	1A	3361	1/1	0.96	0.35	53,53,53,53	0
56	MG	1a	1665	1/1	0.96	0.18	54,54,54,54	0
56	MG	1x	107	1/1	0.96	0.10	50,50,50,50	0
56	MG	1A	3090	1/1	0.96	0.07	36,36,36,36	0
56	MG	2A	3265	1/1	0.96	0.09	49,49,49,49	0
56	MG	2A	3377	1/1	0.96	0.18	39,39,39,39	0
56	MG	1A	3010	1/1	0.96	0.21	46,46,46,46	0
56	MG	2A	3461	1/1	0.96	0.23	64,64,64,64	0
56	MG	1A	3585	1/1	0.96	0.14	20,20,20,20	0
56	MG	1A	3017	1/1	0.96	0.55	53,53,53,53	0
56	MG	2Q	3002	1/1	0.96	0.14	44,44,44,44	0
56	MG	1a	1827	1/1	0.96	0.24	55,55,55,55	0
56	MG	1A	3130	1/1	0.96	0.32	35,35,35,35	0
56	MG	2A	3129	1/1	0.96	0.11	43,43,43,43	0
56	MG	2A	3539	1/1	0.96	0.09	29,29,29,29	0
56	MG	2A	3456	1/1	0.96	0.10	31,31,31,31	0
56	MG	1A	3721	1/1	0.96	0.09	51,51,51,51	0
56	MG	1A	3916	1/1	0.96	0.23	49,49,49,49	0
56	MG	1A	3302	1/1	0.96	0.28	28,28,28,28	0
56	MG	1A	3396	1/1	0.96	0.17	39,39,39,39	0
56	MG	1A	4017	1/1	0.96	0.11	42,42,42,42	0
56	MG	1A	3845	1/1	0.96	0.20	53,53,53,53	0
56	MG	1a	1625	1/1	0.96	0.14	51,51,51,51	0
56	MG	1A	3784	1/1	0.96	0.13	27,27,27,27	0
56	MG	2A	3537	1/1	0.96	0.08	45,45,45,45	0
56	MG	1A	3260	1/1	0.96	0.17	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	3444	1/1	0.96	0.15	63,63,63,63	0
56	MG	1A	3086	1/1	0.96	0.23	39,39,39,39	0
56	MG	1A	3933	1/1	0.96	0.07	42,42,42,42	0
56	MG	2A	3310	1/1	0.96	0.13	55,55,55,55	0
56	MG	1F	304	1/1	0.96	0.35	19,19,19,19	0
56	MG	1a	1833	1/1	0.96	0.12	51,51,51,51	0
56	MG	1A	3866	1/1	0.96	0.16	53,53,53,53	0
56	MG	2a	1779	1/1	0.96	0.10	39,39,39,39	0
56	MG	1A	4032	1/1	0.96	0.08	35,35,35,35	0
56	MG	1A	3132	1/1	0.96	0.15	39,39,39,39	0
56	MG	1a	1656	1/1	0.96	0.12	56,56,56,56	0
56	MG	2a	1801	1/1	0.96	0.07	63,63,63,63	0
56	MG	2a	1631	1/1	0.96	0.52	51,51,51,51	0
56	MG	1A	3192	1/1	0.96	0.30	47,47,47,47	0
56	MG	1A	3606	1/1	0.96	0.10	58,58,58,58	0
56	MG	1e	201	1/1	0.96	0.07	75,75,75,75	0
56	MG	2A	3103	1/1	0.96	0.25	50,50,50,50	0
56	MG	1A	3331	1/1	0.96	0.10	39,39,39,39	0
56	MG	1a	1681	1/1	0.96	0.08	52,52,52,52	0
56	MG	1a	1813	1/1	0.96	0.10	56,56,56,56	0
56	MG	1A	3736	1/1	0.96	0.18	34,34,34,34	0
56	MG	1A	4079	1/1	0.96	0.41	49,49,49,49	0
56	MG	2O	3002	1/1	0.96	0.10	36,36,36,36	0
56	MG	1a	1837	1/1	0.96	0.13	46,46,46,46	0
56	MG	1x	103	1/1	0.96	0.15	68,68,68,68	0
56	MG	1a	1867	1/1	0.96	0.13	56,56,56,56	0
56	MG	1A	3094	1/1	0.96	0.11	42,42,42,42	0
56	MG	1A	3731	1/1	0.96	0.26	58,58,58,58	0
56	MG	1P	206	1/1	0.96	0.34	44,44,44,44	0
56	MG	1A	3765	1/1	0.96	0.06	36,36,36,36	0
56	MG	2A	3078	1/1	0.96	0.20	51,51,51,51	0
56	MG	1A	3985	1/1	0.96	0.14	22,22,22,22	0
56	MG	1A	3013	1/1	0.96	0.06	50,50,50,50	0
56	MG	1A	3364	1/1	0.96	0.20	41,41,41,41	0
56	MG	1A	3362	1/1	0.96	0.30	41,41,41,41	0
56	MG	1a	1636	1/1	0.96	0.13	66,66,66,66	0
56	MG	1A	3778	1/1	0.96	0.16	30,30,30,30	0
56	MG	1a	1778	1/1	0.96	0.07	70,70,70,70	0
56	MG	1A	4021	1/1	0.96	0.14	18,18,18,18	0
56	MG	1A	3063	1/1	0.96	0.13	41,41,41,41	0
56	MG	1x	104	1/1	0.96	0.06	40,40,40,40	0
56	MG	1A	3323	1/1	0.96	0.11	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	3764	1/1	0.96	0.08	41,41,41,41	0
56	MG	1A	3514	1/1	0.96	0.35	46,46,46,46	0
56	MG	1A	3850	1/1	0.96	0.20	43,43,43,43	0
56	MG	1A	4024	1/1	0.96	0.25	61,61,61,61	0
56	MG	1A	3939	1/1	0.96	0.36	30,30,30,30	0
56	MG	1a	1883	1/1	0.96	0.20	47,47,47,47	0
56	MG	2A	3308	1/1	0.96	0.13	44,44,44,44	0
56	MG	1A	3770	1/1	0.96	0.24	26,26,26,26	0
56	MG	2A	3503	1/1	0.96	0.17	50,50,50,50	0
56	MG	1A	3852	1/1	0.96	0.14	41,41,41,41	0
56	MG	2A	3471	1/1	0.96	0.15	40,40,40,40	0
56	MG	2A	3549	1/1	0.96	0.24	49,49,49,49	0
56	MG	2A	3385	1/1	0.96	0.17	42,42,42,42	0
56	MG	1A	4007	1/1	0.96	0.13	68,68,68,68	0
56	MG	1A	3502	1/1	0.96	0.33	61,61,61,61	0
56	MG	2a	1765	1/1	0.96	0.25	52,52,52,52	0
56	MG	1F	302	1/1	0.96	0.07	42,42,42,42	0
56	MG	1A	3820	1/1	0.96	0.20	45,45,45,45	0
56	MG	1A	3512	1/1	0.96	0.34	34,34,34,34	0
56	MG	2A	3429	1/1	0.96	0.10	58,58,58,58	0
56	MG	2F	301	1/1	0.96	0.12	39,39,39,39	0
56	MG	2A	3556	1/1	0.96	0.39	40,40,40,40	0
56	MG	1A	3222	1/1	0.96	0.20	21,21,21,21	0
56	MG	2A	3507	1/1	0.96	0.28	63,63,63,63	0
56	MG	1A	3504	1/1	0.96	0.13	64,64,64,64	0
56	MG	1A	3911	1/1	0.96	0.11	46,46,46,46	0
56	MG	1A	3106	1/1	0.96	0.17	57,57,57,57	0
56	MG	1a	1857	1/1	0.96	0.33	47,47,47,47	0
56	MG	1A	3557	1/1	0.96	0.11	48,48,48,48	0
56	MG	2A	3003	1/1	0.96	0.12	44,44,44,44	0
56	MG	2A	3199	1/1	0.96	0.19	42,42,42,42	0
56	MG	2A	3307	1/1	0.96	0.07	63,63,63,63	0
56	MG	2a	1730	1/1	0.96	0.13	66,66,66,66	0
56	MG	1A	3834	1/1	0.96	0.14	51,51,51,51	0
56	MG	1A	3037	1/1	0.96	0.14	50,50,50,50	0
56	MG	2a	1670	1/1	0.96	0.10	60,60,60,60	0
56	MG	1Q	3003	1/1	0.96	0.33	59,59,59,59	0
56	MG	1A	3284	1/1	0.96	0.36	41,41,41,41	0
56	MG	1a	1757	1/1	0.96	0.07	50,50,50,50	0
56	MG	1A	3175	1/1	0.96	0.18	21,21,21,21	0
56	MG	2p	101	1/1	0.96	0.27	62,62,62,62	0
56	MG	2a	1762	1/1	0.96	0.08	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	1781	1/1	0.96	0.19	48,48,48,48	0
56	MG	1a	1903	1/1	0.96	0.16	72,72,72,72	0
56	MG	2a	1771	1/1	0.96	0.23	50,50,50,50	0
56	MG	2a	1689	1/1	0.96	0.07	43,43,43,43	0
56	MG	1A	3675	1/1	0.96	0.20	21,21,21,21	0
56	MG	1A	3439	1/1	0.96	0.12	64,64,64,64	0
56	MG	1A	4012	1/1	0.96	0.21	42,42,42,42	0
56	MG	1a	1854	1/1	0.96	0.10	41,41,41,41	0
56	MG	2A	3558	1/1	0.96	0.16	40,40,40,40	0
56	MG	1a	1607	1/1	0.96	0.20	62,62,62,62	0
56	MG	1A	3667	1/1	0.96	0.21	19,19,19,19	0
56	MG	1A	3367	1/1	0.96	0.24	53,53,53,53	0
56	MG	2a	1798	1/1	0.96	0.14	69,69,69,69	0
56	MG	2A	3397	1/1	0.96	0.27	27,27,27,27	0
56	MG	1A	3262	1/1	0.96	0.70	43,43,43,43	0
56	MG	2A	3139	1/1	0.96	0.16	40,40,40,40	0
56	MG	2a	1702	1/1	0.96	0.14	64,64,64,64	0
56	MG	1a	1800	1/1	0.96	0.32	67,67,67,67	0
56	MG	1A	3957	1/1	0.96	0.14	20,20,20,20	0
56	MG	2a	1805	1/1	0.96	0.09	52,52,52,52	0
56	MG	1A	3449	1/1	0.96	0.29	54,54,54,54	0
56	MG	1A	3101	1/1	0.96	0.20	46,46,46,46	0
56	MG	1A	3649	1/1	0.96	0.13	54,54,54,54	0
56	MG	1A	3962	1/1	0.96	0.10	42,42,42,42	0
56	MG	1A	3799	1/1	0.96	0.09	39,39,39,39	0
56	MG	2A	3323	1/1	0.96	0.22	56,56,56,56	0
56	MG	1D	305	1/1	0.96	0.19	46,46,46,46	0
56	MG	2A	3454	1/1	0.96	0.08	61,61,61,61	0
56	MG	2a	1637	1/1	0.96	0.22	71,71,71,71	0
56	MG	1A	3692	1/1	0.96	0.06	61,61,61,61	0
56	MG	1A	3443	1/1	0.96	0.28	50,50,50,50	0
56	MG	2A	3392	1/1	0.96	0.15	24,24,24,24	0
56	MG	1A	3140	1/1	0.96	0.58	38,38,38,38	0
56	MG	1A	3115	1/1	0.96	0.18	48,48,48,48	0
56	MG	1A	4043	1/1	0.96	0.09	24,24,24,24	0
56	MG	1A	3970	1/1	0.96	0.14	28,28,28,28	0
56	MG	1A	3040	1/1	0.96	0.23	34,34,34,34	0
56	MG	1A	3768	1/1	0.96	0.16	39,39,39,39	0
56	MG	1a	1849	1/1	0.96	0.06	59,59,59,59	0
56	MG	1A	3537	1/1	0.96	0.07	43,43,43,43	0
56	MG	1A	3150	1/1	0.96	0.14	39,39,39,39	0
56	MG	1A	3717	1/1	0.96	0.04	48,48,48,48	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	1A	3782	1/1	0.96	0.12	27,27,27,27	0
56	MG	1A	3594	1/1	0.96	0.17	36,36,36,36	0
56	MG	1a	1684	1/1	0.96	0.08	52,52,52,52	0
56	MG	1A	3840	1/1	0.96	0.16	59,59,59,59	0
56	MG	1A	3117	1/1	0.96	0.17	29,29,29,29	0
56	MG	1A	3575	1/1	0.96	0.09	62,62,62,62	0
56	MG	25	502	1/1	0.96	0.52	52,52,52,52	0
56	MG	2a	1781	1/1	0.96	0.46	68,68,68,68	0
56	MG	2l	204	1/1	0.96	0.17	43,43,43,43	0
56	MG	2B	3005	1/1	0.96	0.20	51,51,51,51	0
56	MG	2A	3325	1/1	0.96	0.20	70,70,70,70	0
56	MG	1A	3267	1/1	0.96	0.52	51,51,51,51	0
56	MG	2a	1787	1/1	0.96	0.20	67,67,67,67	0
56	MG	1d	503	1/1	0.96	0.13	56,56,56,56	0
56	MG	1a	1815	1/1	0.96	0.12	72,72,72,72	0
56	MG	1A	3245	1/1	0.96	0.23	25,25,25,25	0
56	MG	1A	3251	1/1	0.96	0.15	58,58,58,58	0
56	MG	1A	3977	1/1	0.96	0.22	54,54,54,54	0
56	MG	1A	3085	1/1	0.96	0.14	28,28,28,28	0
56	MG	1B	216	1/1	0.96	0.16	33,33,33,33	0
56	MG	1W	3004	1/1	0.96	0.23	34,34,34,34	0
56	MG	2a	1746	1/1	0.96	0.15	46,46,46,46	0
56	MG	1A	3388	1/1	0.96	0.20	60,60,60,60	0
56	MG	1A	3711	1/1	0.96	0.24	63,63,63,63	0
56	MG	1A	3138	1/1	0.96	0.24	32,32,32,32	0
56	MG	1a	1799	1/1	0.96	0.15	39,39,39,39	0
56	MG	1A	3004	1/1	0.96	0.10	49,49,49,49	0
56	MG	2a	1789	1/1	0.96	0.04	88,88,88,88	0
56	MG	1A	3155	1/1	0.96	0.28	27,27,27,27	0
56	MG	1A	3172	1/1	0.96	0.12	56,56,56,56	0
56	MG	2A	3238	1/1	0.96	0.10	45,45,45,45	0
56	MG	1A	3960	1/1	0.96	0.20	47,47,47,47	0
56	MG	1A	3403	1/1	0.96	0.07	38,38,38,38	0
56	MG	2d	502	1/1	0.96	0.30	48,48,48,48	0
56	MG	1A	3310	1/1	0.96	0.17	51,51,51,51	0
56	MG	1A	3149	1/1	0.96	0.14	35,35,35,35	0
56	MG	1A	3633	1/1	0.96	0.15	21,21,21,21	0
56	MG	1A	3241	1/1	0.96	0.31	30,30,30,30	0
56	MG	1a	1905	1/1	0.96	0.12	52,52,52,52	0
56	MG	1A	3428	1/1	0.96	0.10	36,36,36,36	0
56	MG	1A	3727	1/1	0.96	0.21	43,43,43,43	0
56	MG	2a	1634	1/1	0.96	0.13	94,94,94,94	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	1A	3618	1/1	0.96	0.08	39,39,39,39	0
56	MG	1A	3691	1/1	0.96	0.11	8,8,8,8	0
56	MG	1A	3033	1/1	0.96	0.14	39,39,39,39	0
56	MG	1A	3846	1/1	0.96	0.13	21,21,21,21	0
56	MG	2Q	3003	1/1	0.96	0.13	37,37,37,37	0
56	MG	1A	3560	1/1	0.96	0.18	37,37,37,37	0
56	MG	2a	1719	1/1	0.96	0.11	63,63,63,63	0
56	MG	1A	3855	1/1	0.96	0.10	51,51,51,51	0
56	MG	1A	3813	1/1	0.96	0.14	37,37,37,37	0
56	MG	1A	3418	1/1	0.96	0.10	53,53,53,53	0
56	MG	1P	203	1/1	0.96	0.29	52,52,52,52	0
56	MG	1A	4083	1/1	0.96	0.15	34,34,34,34	0
56	MG	1b	3001	1/1	0.96	0.23	63,63,63,63	0
56	MG	1A	3678	1/1	0.96	0.29	44,44,44,44	0
56	MG	1A	3209	1/1	0.96	0.15	45,45,45,45	0
56	MG	1A	3636	1/1	0.96	0.15	35,35,35,35	0
56	MG	2A	3027	1/1	0.96	0.18	53,53,53,53	0
56	MG	1A	3653	1/1	0.96	0.14	25,25,25,25	0
56	MG	1A	3511	1/1	0.96	0.25	47,47,47,47	0
56	MG	1A	3179	1/1	0.96	0.21	38,38,38,38	0
56	MG	1A	4087	1/1	0.96	0.10	37,37,37,37	0
56	MG	2A	3305	1/1	0.96	0.14	41,41,41,41	0
56	MG	1P	201	1/1	0.96	0.23	56,56,56,56	0
56	MG	1A	3584	1/1	0.96	0.22	33,33,33,33	0
56	MG	1E	301	1/1	0.96	0.16	14,14,14,14	0
56	MG	2A	3521	1/1	0.96	0.20	38,38,38,38	0
56	MG	1a	1821	1/1	0.96	0.11	64,64,64,64	0
56	MG	1A	3552	1/1	0.96	0.14	53,53,53,53	0
56	MG	2E	301	1/1	0.96	0.17	30,30,30,30	0
56	MG	1a	1621	1/1	0.96	0.11	68,68,68,68	0
56	MG	2a	1803	1/1	0.96	0.09	60,60,60,60	0
56	MG	1A	3484	1/1	0.96	0.09	54,54,54,54	0
56	MG	1A	3656	1/1	0.96	0.21	46,46,46,46	0
56	MG	1a	1741	1/1	0.96	0.38	58,58,58,58	0
56	MG	1A	3191	1/1	0.96	0.24	37,37,37,37	0
56	MG	1A	3555	1/1	0.96	0.28	47,47,47,47	0
56	MG	1A	3947	1/1	0.96	0.15	32,32,32,32	0
56	MG	1A	3724	1/1	0.96	0.08	50,50,50,50	0
56	MG	1A	3749	1/1	0.96	0.05	48,48,48,48	0
56	MG	1V	201	1/1	0.96	0.32	39,39,39,39	0
56	MG	1A	4091	1/1	0.96	0.07	45,45,45,45	0
56	MG	1a	1676	1/1	0.96	0.24	49,49,49,49	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	2a	1636	1/1	0.96	0.08	92,92,92,92	0
56	MG	1W	3003	1/1	0.96	0.16	43,43,43,43	0
56	MG	1A	3146	1/1	0.96	0.11	39,39,39,39	0
57	ZN	14	501	1/1	0.96	0.10	75,75,75,75	0
56	MG	2a	1710	1/1	0.96	0.15	71,71,71,71	0
56	MG	1a	1841	1/1	0.96	0.10	37,37,37,37	0
56	MG	1a	1740	1/1	0.96	0.27	46,46,46,46	0
56	MG	1A	3757	1/1	0.96	0.28	33,33,33,33	0
56	MG	2A	3127	1/1	0.96	0.59	45,45,45,45	0
56	MG	1a	1627	1/1	0.97	0.07	36,36,36,36	0
56	MG	2A	3363	1/1	0.97	0.28	52,52,52,52	0
56	MG	1a	1747	1/1	0.97	0.14	43,43,43,43	0
56	MG	1A	3630	1/1	0.97	0.21	47,47,47,47	0
56	MG	2A	3267	1/1	0.97	0.30	50,50,50,50	0
56	MG	1a	1828	1/1	0.97	0.17	45,45,45,45	0
56	MG	1A	3641	1/1	0.97	0.10	36,36,36,36	0
56	MG	2A	3405	1/1	0.97	0.16	53,53,53,53	0
56	MG	1A	4078	1/1	0.97	0.14	23,23,23,23	0
56	MG	2a	1790	1/1	0.97	0.06	72,72,72,72	0
56	MG	1A	3043	1/1	0.97	0.10	36,36,36,36	0
56	MG	2A	3261	1/1	0.97	0.28	66,66,66,66	0
56	MG	2a	1657	1/1	0.97	0.17	61,61,61,61	0
56	MG	2A	3347	1/1	0.97	0.24	60,60,60,60	0
56	MG	1a	1842	1/1	0.97	0.30	39,39,39,39	0
56	MG	1a	1640	1/1	0.97	0.17	57,57,57,57	0
56	MG	2x	3003	1/1	0.97	0.14	48,48,48,48	0
56	MG	2A	3158	1/1	0.97	0.18	39,39,39,39	0
56	MG	1A	4080	1/1	0.97	0.34	45,45,45,45	0
56	MG	2A	3517	1/1	0.97	0.09	36,36,36,36	0
56	MG	2A	3349	1/1	0.97	0.04	63,63,63,63	0
56	MG	1a	1610	1/1	0.97	0.04	48,48,48,48	0
56	MG	1a	1628	1/1	0.97	0.11	35,35,35,35	0
56	MG	1a	1873	1/1	0.97	0.17	52,52,52,52	0
56	MG	2A	3431	1/1	0.97	0.05	59,59,59,59	0
56	MG	1a	1733	1/1	0.97	0.11	41,41,41,41	0
56	MG	2A	3196	1/1	0.97	0.39	51,51,51,51	0
56	MG	2a	1720	1/1	0.97	0.29	60,60,60,60	0
56	MG	2A	3244	1/1	0.97	0.10	55,55,55,55	0
56	MG	1A	3800	1/1	0.97	0.16	25,25,25,25	0
56	MG	1a	1884	1/1	0.97	0.12	44,44,44,44	0
56	MG	1A	3875	1/1	0.97	0.13	19,19,19,19	0
56	MG	1A	3788	1/1	0.97	0.14	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	1U	203	1/1	0.97	0.20	42,42,42,42	0
56	MG	1A	3401	1/1	0.97	0.13	46,46,46,46	0
56	MG	2A	3105	1/1	0.97	0.36	29,29,29,29	0
56	MG	1B	215	1/1	0.97	0.09	36,36,36,36	0
56	MG	18	101	1/1	0.97	0.15	30,30,30,30	0
56	MG	1A	3386	1/1	0.97	0.11	34,34,34,34	0
56	MG	1A	3743	1/1	0.97	0.19	69,69,69,69	0
56	MG	1a	1868	1/1	0.97	0.14	41,41,41,41	0
56	MG	1A	3590	1/1	0.97	0.21	40,40,40,40	0
56	MG	1A	3824	1/1	0.97	0.21	19,19,19,19	0
56	MG	1a	1677	1/1	0.97	0.28	45,45,45,45	0
56	MG	1a	1674	1/1	0.97	0.12	46,46,46,46	0
56	MG	1A	3425	1/1	0.97	0.21	62,62,62,62	0
56	MG	1A	3860	1/1	0.97	0.16	59,59,59,59	0
56	MG	1A	3232	1/1	0.97	0.69	39,39,39,39	0
56	MG	2A	3011	1/1	0.97	0.48	50,50,50,50	0
56	MG	2A	3272	1/1	0.97	0.28	44,44,44,44	0
56	MG	1A	3259	1/1	0.97	0.09	52,52,52,52	0
56	MG	2A	3543	1/1	0.97	0.06	47,47,47,47	0
56	MG	1A	3412	1/1	0.97	0.13	77,77,77,77	0
56	MG	2a	1773	1/1	0.97	0.14	53,53,53,53	0
56	MG	1a	1726	1/1	0.97	0.15	53,53,53,53	0
56	MG	2A	3246	1/1	0.97	0.21	56,56,56,56	0
56	MG	1A	3595	1/1	0.97	0.12	27,27,27,27	0
56	MG	1A	3707	1/1	0.97	0.17	50,50,50,50	0
56	MG	1A	4005	1/1	0.97	0.12	65,65,65,65	0
56	MG	1A	3719	1/1	0.97	0.12	34,34,34,34	0
56	MG	1A	3785	1/1	0.97	0.12	21,21,21,21	0
56	MG	1A	3959	1/1	0.97	0.23	27,27,27,27	0
56	MG	1A	3050	1/1	0.97	0.31	62,62,62,62	0
56	MG	1A	3429	1/1	0.97	0.12	45,45,45,45	0
56	MG	1A	3671	1/1	0.97	0.14	16,16,16,16	0
56	MG	2A	3251	1/1	0.97	0.21	40,40,40,40	0
56	MG	1a	1678	1/1	0.97	0.12	54,54,54,54	0
56	MG	2A	3557	1/1	0.97	0.18	52,52,52,52	0
56	MG	2a	1692	1/1	0.97	0.08	67,67,67,67	0
56	MG	2A	3187	1/1	0.97	0.21	40,40,40,40	0
56	MG	2B	3007	1/1	0.97	0.15	48,48,48,48	0
56	MG	1A	3527	1/1	0.97	0.18	68,68,68,68	0
56	MG	1A	3797	1/1	0.97	0.17	15,15,15,15	0
56	MG	1A	3592	1/1	0.97	0.12	35,35,35,35	0
56	MG	2A	3110	1/1	0.97	0.35	44,44,44,44	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
57	ZN	16	102	1/1	0.97	0.18	57,57,57,57	0
56	MG	1A	3536	1/1	0.97	0.12	45,45,45,45	0
56	MG	1A	3988	1/1	0.97	0.39	37,37,37,37	0
56	MG	1a	1788	1/1	0.97	0.12	71,71,71,71	0
56	MG	1A	3901	1/1	0.97	0.07	40,40,40,40	0
56	MG	1A	4026	1/1	0.97	0.22	45,45,45,45	0
56	MG	2A	3090	1/1	0.97	0.29	33,33,33,33	0
56	MG	1A	3546	1/1	0.97	0.19	62,62,62,62	0
56	MG	1A	4057	1/1	0.97	0.32	40,40,40,40	0
56	MG	1A	4016	1/1	0.97	0.17	26,26,26,26	0
56	MG	1A	3926	1/1	0.97	0.06	52,52,52,52	0
56	MG	1A	3059	1/1	0.97	0.25	43,43,43,43	0
56	MG	1A	3352	1/1	0.97	0.15	37,37,37,37	0
56	MG	2A	3460	1/1	0.97	0.24	44,44,44,44	0
56	MG	2A	3553	1/1	0.97	0.42	42,42,42,42	0
56	MG	1F	301	1/1	0.97	0.23	36,36,36,36	0
56	MG	1A	3154	1/1	0.97	0.23	34,34,34,34	0
56	MG	1a	1826	1/1	0.97	0.24	47,47,47,47	0
56	MG	1A	4042	1/1	0.97	0.30	32,32,32,32	0
56	MG	2A	3302	1/1	0.97	0.19	48,48,48,48	0
56	MG	2A	3518	1/1	0.97	0.22	58,58,58,58	0
56	MG	2A	3164	1/1	0.97	0.15	37,37,37,37	0
56	MG	1A	4092	1/1	0.97	0.48	33,33,33,33	0
56	MG	2a	1722	1/1	0.97	0.24	47,47,47,47	0
56	MG	2A	3382	1/1	0.97	0.26	47,47,47,47	0
56	MG	1a	1705	1/1	0.97	0.15	38,38,38,38	0
56	MG	2a	1777	1/1	0.97	0.09	66,66,66,66	0
56	MG	1A	3580	1/1	0.97	0.14	22,22,22,22	0
56	MG	2A	3552	1/1	0.97	0.17	47,47,47,47	0
56	MG	1A	3622	1/1	0.97	0.08	61,61,61,61	0
56	MG	1a	1620	1/1	0.97	0.12	72,72,72,72	0
56	MG	1A	3181	1/1	0.97	0.08	41,41,41,41	0
56	MG	2A	3527	1/1	0.97	0.16	37,37,37,37	0
56	MG	1A	3787	1/1	0.97	0.18	33,33,33,33	0
56	MG	1A	3738	1/1	0.97	0.13	46,46,46,46	0
56	MG	2a	1728	1/1	0.97	0.09	75,75,75,75	0
56	MG	2A	3441	1/1	0.97	0.07	43,43,43,43	0
56	MG	1A	3334	1/1	0.97	0.30	37,37,37,37	0
56	MG	2a	1673	1/1	0.97	0.45	52,52,52,52	0
56	MG	2a	1665	1/1	0.97	0.28	41,41,41,41	0
56	MG	1A	3541	1/1	0.97	0.11	44,44,44,44	0
56	MG	2A	3150	1/1	0.97	0.24	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	3231	1/1	0.97	0.13	42,42,42,42	0
56	MG	1A	3851	1/1	0.97	0.28	52,52,52,52	0
56	MG	1a	1744	1/1	0.97	0.10	53,53,53,53	0
56	MG	1e	202	1/1	0.97	0.25	81,81,81,81	0
56	MG	1A	3742	1/1	0.97	0.31	37,37,37,37	0
56	MG	1A	3093	1/1	0.97	0.32	54,54,54,54	0
56	MG	1a	1723	1/1	0.97	0.33	48,48,48,48	0
56	MG	2A	3021	1/1	0.97	0.29	42,42,42,42	0
56	MG	1A	3517	1/1	0.97	0.06	55,55,55,55	0
56	MG	2A	3234	1/1	0.97	0.27	55,55,55,55	0
56	MG	2A	3002	1/1	0.97	0.17	47,47,47,47	0
56	MG	2a	1693	1/1	0.97	0.19	67,67,67,67	0
56	MG	10	104	1/1	0.97	0.06	46,46,46,46	0
56	MG	1A	3164	1/1	0.97	0.41	20,20,20,20	0
56	MG	1A	3074	1/1	0.97	0.24	34,34,34,34	0
56	MG	1A	3064	1/1	0.97	0.07	57,57,57,57	0
56	MG	1B	207	1/1	0.97	0.11	43,43,43,43	0
56	MG	1a	1846	1/1	0.97	0.15	55,55,55,55	0
56	MG	2A	3455	1/1	0.97	0.09	45,45,45,45	0
56	MG	2A	3458	1/1	0.97	0.09	64,64,64,64	0
56	MG	1A	3162	1/1	0.97	0.46	35,35,35,35	0
56	MG	1A	3791	1/1	0.97	0.18	19,19,19,19	0
56	MG	2a	1699	1/1	0.97	0.15	71,71,71,71	0
56	MG	1A	3848	1/1	0.97	0.12	69,69,69,69	0
56	MG	1A	3709	1/1	0.97	0.13	15,15,15,15	0
56	MG	1A	3673	1/1	0.97	0.27	32,32,32,32	0
56	MG	2x	3001	1/1	0.97	0.09	57,57,57,57	0
56	MG	2A	3333	1/1	0.97	0.16	45,45,45,45	0
56	MG	1A	3487	1/1	0.97	0.12	41,41,41,41	0
56	MG	1a	1689	1/1	0.97	0.05	61,61,61,61	0
56	MG	2A	3156	1/1	0.97	0.26	28,28,28,28	0
56	MG	1h	3002	1/1	0.97	0.09	63,63,63,63	0
56	MG	1A	3113	1/1	0.97	0.14	27,27,27,27	0
56	MG	1A	3295	1/1	0.97	0.27	50,50,50,50	0
56	MG	2A	3131	1/1	0.97	0.11	46,46,46,46	0
56	MG	2A	3038	1/1	0.97	0.20	46,46,46,46	0
56	MG	2A	3322	1/1	0.97	0.30	41,41,41,41	0
56	MG	1A	3139	1/1	0.97	0.23	21,21,21,21	0
56	MG	1a	1848	1/1	0.97	0.14	45,45,45,45	0
56	MG	1A	4035	1/1	0.97	0.20	57,57,57,57	0
56	MG	1A	3127	1/1	0.97	0.25	39,39,39,39	0
56	MG	1a	1885	1/1	0.97	0.21	49,49,49,49	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	2A	3112	1/1	0.97	0.13	40,40,40,40	0
56	MG	1A	3357	1/1	0.97	0.06	54,54,54,54	0
56	MG	1N	204	1/1	0.97	0.20	36,36,36,36	0
56	MG	2A	3229	1/1	0.97	0.31	64,64,64,64	0
56	MG	2a	1709	1/1	0.97	0.10	64,64,64,64	0
56	MG	2A	3222	1/1	0.97	0.18	34,34,34,34	0
56	MG	2A	3283	1/1	0.97	0.07	57,57,57,57	0
56	MG	1A	4049	1/1	0.97	0.36	18,18,18,18	0
56	MG	2A	3470	1/1	0.97	0.20	67,67,67,67	0
56	MG	1A	3993	1/1	0.97	0.20	30,30,30,30	0
56	MG	1A	3573	1/1	0.97	0.11	38,38,38,38	0
56	MG	1H	201	1/1	0.97	0.30	49,49,49,49	0
56	MG	2A	3190	1/1	0.97	0.28	44,44,44,44	0
56	MG	2A	3467	1/1	0.97	0.18	39,39,39,39	0
56	MG	1A	3629	1/1	0.97	0.17	40,40,40,40	0
56	MG	17	104	1/1	0.97	0.10	31,31,31,31	0
56	MG	1A	3668	1/1	0.97	0.20	31,31,31,31	0
56	MG	1A	3273	1/1	0.97	0.10	16,16,16,16	0
56	MG	2a	1679	1/1	0.97	0.23	52,52,52,52	0
56	MG	2A	3375	1/1	0.97	0.09	57,57,57,57	0
56	MG	2A	3499	1/1	0.97	0.17	56,56,56,56	0
56	MG	1A	3195	1/1	0.97	0.24	38,38,38,38	0
56	MG	1Q	3001	1/1	0.97	0.25	31,31,31,31	0
56	MG	1A	3867	1/1	0.97	0.26	48,48,48,48	0
56	MG	2A	3262	1/1	0.97	0.13	35,35,35,35	0
57	ZN	29	501	1/1	0.97	0.07	58,58,58,58	0
56	MG	2A	3195	1/1	0.97	0.32	38,38,38,38	0
56	MG	1A	4056	1/1	0.97	0.20	30,30,30,30	0
56	MG	1A	3725	1/1	0.97	0.14	56,56,56,56	0
56	MG	2A	3166	1/1	0.97	0.14	40,40,40,40	0
56	MG	2A	3043	1/1	0.97	0.20	46,46,46,46	0
56	MG	1A	4076	1/1	0.97	0.16	36,36,36,36	0
56	MG	1A	3288	1/1	0.97	0.07	82,82,82,82	0
56	MG	2a	1767	1/1	0.97	0.07	57,57,57,57	0
56	MG	1A	3082	1/1	0.97	0.38	65,65,65,65	0
56	MG	1a	1673	1/1	0.97	0.05	51,51,51,51	0
56	MG	2A	3133	1/1	0.97	0.11	33,33,33,33	0
56	MG	1a	1743	1/1	0.97	0.07	73,73,73,73	0
56	MG	1A	3695	1/1	0.97	0.22	29,29,29,29	0
56	MG	2a	1690	1/1	0.97	0.35	55,55,55,55	0
56	MG	1A	3862	1/1	0.97	0.07	45,45,45,45	0
56	MG	1A	3068	1/1	0.97	0.04	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	3270	1/1	0.97	0.26	27,27,27,27	0
56	MG	1A	3776	1/1	0.97	0.23	42,42,42,42	0
56	MG	2A	3500	1/1	0.97	0.36	53,53,53,53	0
56	MG	1A	3516	1/1	0.97	0.08	54,54,54,54	0
56	MG	1A	3934	1/1	0.97	0.06	52,52,52,52	0
56	MG	2a	1797	1/1	0.97	0.14	57,57,57,57	0
56	MG	2A	3141	1/1	0.97	0.23	37,37,37,37	0
56	MG	1A	3220	1/1	0.97	0.15	30,30,30,30	0
56	MG	1P	202	1/1	0.97	0.14	41,41,41,41	0
56	MG	2A	3171	1/1	0.97	0.21	40,40,40,40	0
56	MG	1A	3892	1/1	0.97	0.12	44,44,44,44	0
56	MG	1A	3889	1/1	0.97	0.14	46,46,46,46	0
56	MG	1A	3761	1/1	0.97	0.12	47,47,47,47	0
56	MG	2A	3369	1/1	0.97	0.34	45,45,45,45	0
56	MG	1a	1824	1/1	0.97	0.33	52,52,52,52	0
56	MG	1A	3996	1/1	0.97	0.47	32,32,32,32	0
56	MG	1A	3268	1/1	0.97	0.16	51,51,51,51	0
56	MG	1A	3184	1/1	0.97	0.30	35,35,35,35	0
56	MG	1A	3583	1/1	0.97	0.20	47,47,47,47	0
56	MG	2A	3259	1/1	0.97	0.07	36,36,36,36	0
56	MG	2A	3247	1/1	0.97	0.16	47,47,47,47	0
56	MG	1A	3335	1/1	0.97	0.10	46,46,46,46	0
57	ZN	1Y	202	1/1	0.97	0.11	65,65,65,65	0
56	MG	2k	3001	1/1	0.97	0.07	60,60,60,60	0
56	MG	2A	3069	1/1	0.97	0.36	52,52,52,52	0
56	MG	2A	3395	1/1	0.97	0.23	51,51,51,51	0
56	MG	1a	1893	1/1	0.97	0.37	71,71,71,71	0
56	MG	1A	3071	1/1	0.97	0.10	41,41,41,41	0
56	MG	1a	1711	1/1	0.97	0.20	60,60,60,60	0
56	MG	1A	3469	1/1	0.97	0.17	16,16,16,16	0
56	MG	1A	3036	1/1	0.97	0.17	41,41,41,41	0
56	MG	1A	3394	1/1	0.97	0.07	60,60,60,60	0
56	MG	1A	3526	1/1	0.97	0.40	41,41,41,41	0
56	MG	1A	3548	1/1	0.97	0.13	44,44,44,44	0
56	MG	1A	3128	1/1	0.97	0.27	27,27,27,27	0
56	MG	1A	4089	1/1	0.97	0.21	34,34,34,34	0
56	MG	1A	3559	1/1	0.97	0.21	47,47,47,47	0
56	MG	2A	3072	1/1	0.97	0.36	40,40,40,40	0
56	MG	2a	1707	1/1	0.97	0.09	58,58,58,58	0
56	MG	1A	4069	1/1	0.97	0.15	38,38,38,38	0
56	MG	2A	3341	1/1	0.97	0.06	54,54,54,54	0
56	MG	2A	3152	1/1	0.97	0.14	30,30,30,30	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	1A	3029	1/1	0.97	0.28	40,40,40,40	0
56	MG	1A	3515	1/1	0.97	0.10	57,57,57,57	0
56	MG	2A	3119	1/1	0.97	0.15	25,25,25,25	0
56	MG	1G	3003	1/1	0.97	0.04	45,45,45,45	0
56	MG	1A	3665	1/1	0.97	0.11	40,40,40,40	0
56	MG	2A	3230	1/1	0.97	0.16	45,45,45,45	0
56	MG	1A	3020	1/1	0.97	0.26	47,47,47,47	0
56	MG	2Y	203	1/1	0.97	0.10	41,41,41,41	0
56	MG	2A	3336	1/1	0.97	0.14	38,38,38,38	0
56	MG	1A	3936	1/1	0.97	0.10	37,37,37,37	0
56	MG	2A	3155	1/1	0.97	0.14	33,33,33,33	0
56	MG	1R	203	1/1	0.97	0.20	24,24,24,24	0
56	MG	2A	3316	1/1	0.97	0.20	33,33,33,33	0
56	MG	1A	3337	1/1	0.97	0.08	39,39,39,39	0
56	MG	2a	1640	1/1	0.97	0.08	81,81,81,81	0
56	MG	1a	1603	1/1	0.97	0.17	56,56,56,56	0
56	MG	2a	1604	1/1	0.97	0.41	47,47,47,47	0
56	MG	1a	1793	1/1	0.97	0.19	29,29,29,29	0
56	MG	1A	3925	1/1	0.97	0.16	50,50,50,50	0
56	MG	1A	3870	1/1	0.97	0.09	47,47,47,47	0
56	MG	1A	3270	1/1	0.97	0.25	41,41,41,41	0
56	MG	1D	313	1/1	0.97	0.18	39,39,39,39	0
56	MG	2A	3049	1/1	0.97	0.15	35,35,35,35	0
56	MG	1a	1851	1/1	0.97	0.20	64,64,64,64	0
56	MG	2a	1685	1/1	0.97	0.20	53,53,53,53	0
56	MG	2A	3358	1/1	0.97	0.23	47,47,47,47	0
56	MG	1A	3340	1/1	0.97	0.08	43,43,43,43	0
56	MG	1a	1608	1/1	0.97	0.12	73,73,73,73	0
56	MG	1A	3945	1/1	0.97	0.27	36,36,36,36	0
56	MG	1F	307	1/1	0.97	0.19	41,41,41,41	0
56	MG	2A	3143	1/1	0.97	0.32	49,49,49,49	0
56	MG	1a	1633	1/1	0.97	0.26	51,51,51,51	0
56	MG	1a	1896	1/1	0.97	0.16	72,72,72,72	0
56	MG	1A	3224	1/1	0.97	0.11	37,37,37,37	0
56	MG	1A	3278	1/1	0.97	0.10	28,28,28,28	0
56	MG	1A	3196	1/1	0.97	0.11	54,54,54,54	0
56	MG	1A	3205	1/1	0.97	0.21	40,40,40,40	0
56	MG	1A	3908	1/1	0.97	0.16	49,49,49,49	0
56	MG	1A	3638	1/1	0.97	0.16	56,56,56,56	0
56	MG	1A	3697	1/1	0.97	0.10	23,23,23,23	0
56	MG	1A	3190	1/1	0.97	0.07	55,55,55,55	0
56	MG	2a	1775	1/1	0.97	0.33	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	3243	1/1	0.97	0.25	51,51,51,51	0
56	MG	16	101	1/1	0.97	0.16	42,42,42,42	0
57	ZN	1n	501	1/1	0.97	0.12	84,84,84,84	0
56	MG	1A	3571	1/1	0.97	0.18	42,42,42,42	0
56	MG	1A	3591	1/1	0.97	0.18	52,52,52,52	0
56	MG	1A	3878	1/1	0.98	0.08	20,20,20,20	0
56	MG	2A	3205	1/1	0.98	0.13	46,46,46,46	0
56	MG	1A	3759	1/1	0.98	0.19	41,41,41,41	0
56	MG	1a	1803	1/1	0.98	0.05	57,57,57,57	0
56	MG	1A	3530	1/1	0.98	0.07	41,41,41,41	0
56	MG	1A	3210	1/1	0.98	0.14	45,45,45,45	0
56	MG	1A	3434	1/1	0.98	0.18	47,47,47,47	0
56	MG	1A	3817	1/1	0.98	0.17	49,49,49,49	0
56	MG	1A	3876	1/1	0.98	0.10	26,26,26,26	0
56	MG	2A	3315	1/1	0.98	0.25	50,50,50,50	0
56	MG	1a	1853	1/1	0.98	0.08	31,31,31,31	0
56	MG	1A	3672	1/1	0.98	0.11	17,17,17,17	0
56	MG	1E	303	1/1	0.98	0.20	14,14,14,14	0
56	MG	2A	3206	1/1	0.98	0.35	55,55,55,55	0
56	MG	1x	102	1/1	0.98	0.14	42,42,42,42	0
56	MG	2a	1675	1/1	0.98	0.13	59,59,59,59	0
56	MG	1Q	3005	1/1	0.98	0.16	38,38,38,38	0
56	MG	1A	3984	1/1	0.98	0.14	51,51,51,51	0
56	MG	1A	3404	1/1	0.98	0.14	38,38,38,38	0
56	MG	1A	3131	1/1	0.98	0.27	50,50,50,50	0
56	MG	1A	3056	1/1	0.98	0.30	57,57,57,57	0
56	MG	1A	3299	1/1	0.98	0.29	16,16,16,16	0
56	MG	2A	3044	1/1	0.98	0.12	32,32,32,32	0
56	MG	1A	3958	1/1	0.98	0.16	18,18,18,18	0
56	MG	2A	3263	1/1	0.98	0.29	41,41,41,41	0
56	MG	2A	3403	1/1	0.98	0.33	53,53,53,53	0
56	MG	1a	1650	1/1	0.98	0.14	42,42,42,42	0
56	MG	1A	3969	1/1	0.98	0.13	40,40,40,40	0
56	MG	2a	1696	1/1	0.98	0.16	43,43,43,43	0
56	MG	2A	3345	1/1	0.98	0.24	51,51,51,51	0
56	MG	1A	3467	1/1	0.98	0.11	50,50,50,50	0
56	MG	1A	3968	1/1	0.98	0.16	21,21,21,21	0
56	MG	1A	3739	1/1	0.98	0.17	16,16,16,16	0
56	MG	1A	3116	1/1	0.98	0.12	21,21,21,21	0
56	MG	2B	3010	1/1	0.98	0.21	55,55,55,55	0
56	MG	2a	1654	1/1	0.98	0.07	49,49,49,49	0
56	MG	1A	3741	1/1	0.98	0.18	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	3445	1/1	0.98	0.18	55,55,55,55	0
56	MG	1A	3669	1/1	0.98	0.14	17,17,17,17	0
56	MG	1A	3683	1/1	0.98	0.21	48,48,48,48	0
56	MG	2a	1800	1/1	0.98	0.42	73,73,73,73	0
56	MG	1A	3354	1/1	0.98	0.06	56,56,56,56	0
56	MG	1A	3885	1/1	0.98	0.09	51,51,51,51	0
56	MG	2A	3128	1/1	0.98	0.12	46,46,46,46	0
56	MG	1A	3605	1/1	0.98	0.09	42,42,42,42	0
56	MG	1A	3607	1/1	0.98	0.09	27,27,27,27	0
56	MG	1a	1768	1/1	0.98	0.09	56,56,56,56	0
56	MG	2D	305	1/1	0.98	0.34	27,27,27,27	0
56	MG	1A	3989	1/1	0.98	0.15	38,38,38,38	0
56	MG	1a	1618	1/1	0.98	0.16	58,58,58,58	0
56	MG	2A	3344	1/1	0.98	0.12	43,43,43,43	0
56	MG	1F	303	1/1	0.98	0.09	35,35,35,35	0
56	MG	1Q	3006	1/1	0.98	0.29	37,37,37,37	0
56	MG	2A	3320	1/1	0.98	0.29	46,46,46,46	0
56	MG	1A	3173	1/1	0.98	0.27	44,44,44,44	0
56	MG	2A	3290	1/1	0.98	0.21	40,40,40,40	0
56	MG	1A	3917	1/1	0.98	0.13	58,58,58,58	0
56	MG	1A	3773	1/1	0.98	0.06	49,49,49,49	0
56	MG	1A	3223	1/1	0.98	0.15	24,24,24,24	0
56	MG	1A	3966	1/1	0.98	0.14	56,56,56,56	0
56	MG	1A	3818	1/1	0.98	0.19	19,19,19,19	0
56	MG	1A	3841	1/1	0.98	0.18	17,17,17,17	0
56	MG	2A	3324	1/1	0.98	0.20	24,24,24,24	0
56	MG	1E	302	1/1	0.98	0.18	55,55,55,55	0
56	MG	1A	3734	1/1	0.98	0.04	45,45,45,45	0
56	MG	1a	1874	1/1	0.98	0.16	48,48,48,48	0
56	MG	2A	3414	1/1	0.98	0.31	67,67,67,67	0
56	MG	2A	3248	1/1	0.98	0.25	45,45,45,45	0
56	MG	2A	3235	1/1	0.98	0.38	54,54,54,54	0
56	MG	2A	3465	1/1	0.98	0.34	52,52,52,52	0
56	MG	1A	3825	1/1	0.98	0.20	13,13,13,13	0
56	MG	1A	3045	1/1	0.98	0.34	42,42,42,42	0
56	MG	1A	3161	1/1	0.98	0.18	27,27,27,27	0
56	MG	1A	3842	1/1	0.98	0.09	47,47,47,47	0
56	MG	1A	3038	1/1	0.98	0.15	51,51,51,51	0
56	MG	1A	4094	1/1	0.98	0.22	27,27,27,27	0
56	MG	1A	3979	1/1	0.98	0.22	32,32,32,32	0
56	MG	2A	3440	1/1	0.98	0.34	56,56,56,56	0
56	MG	1A	4096	1/1	0.98	0.29	69,69,69,69	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	1a	1814	1/1	0.98	0.11	61,61,61,61	0
56	MG	1A	3250	1/1	0.98	0.14	52,52,52,52	0
56	MG	1A	3628	1/1	0.98	0.08	26,26,26,26	0
56	MG	1A	3497	1/1	0.98	0.14	36,36,36,36	0
56	MG	2A	3415	1/1	0.98	0.20	47,47,47,47	0
56	MG	1a	1629	1/1	0.98	0.15	33,33,33,33	0
56	MG	1A	3615	1/1	0.98	0.17	16,16,16,16	0
56	MG	1A	3658	1/1	0.98	0.12	36,36,36,36	0
56	MG	1A	3030	1/1	0.98	0.08	38,38,38,38	0
56	MG	1A	3054	1/1	0.98	0.31	50,50,50,50	0
56	MG	1a	1655	1/1	0.98	0.18	50,50,50,50	0
56	MG	1a	1831	1/1	0.98	0.18	32,32,32,32	0
56	MG	1A	3915	1/1	0.98	0.09	13,13,13,13	0
56	MG	2A	3233	1/1	0.98	0.17	58,58,58,58	0
56	MG	1a	1775	1/1	0.98	0.17	55,55,55,55	0
56	MG	1A	3616	1/1	0.98	0.17	32,32,32,32	0
56	MG	2A	3357	1/1	0.98	0.10	55,55,55,55	0
56	MG	1A	3076	1/1	0.98	0.17	40,40,40,40	0
56	MG	1A	3218	1/1	0.98	0.42	28,28,28,28	0
56	MG	1A	3096	1/1	0.98	0.07	46,46,46,46	0
56	MG	1A	3963	1/1	0.98	0.04	33,33,33,33	0
56	MG	2a	1609	1/1	0.98	0.41	60,60,60,60	0
56	MG	1D	301	1/1	0.98	0.13	31,31,31,31	0
56	MG	1A	3118	1/1	0.98	0.08	33,33,33,33	0
56	MG	1A	3735	1/1	0.98	0.13	32,32,32,32	0
56	MG	1a	1731	1/1	0.98	0.44	42,42,42,42	0
56	MG	1N	207	1/1	0.98	0.05	19,19,19,19	0
56	MG	1A	3091	1/1	0.98	0.18	46,46,46,46	0
56	MG	1B	219	1/1	0.98	0.12	25,25,25,25	0
56	MG	1A	3718	1/1	0.98	0.10	8,8,8,8	0
56	MG	1A	3661	1/1	0.98	0.17	16,16,16,16	0
56	MG	1A	3726	1/1	0.98	0.12	23,23,23,23	0
56	MG	1B	223	1/1	0.98	0.18	48,48,48,48	0
56	MG	1B	218	1/1	0.98	0.12	43,43,43,43	0
56	MG	1N	208	1/1	0.98	0.08	47,47,47,47	0
56	MG	1A	3269	1/1	0.98	0.18	17,17,17,17	0
56	MG	1a	1614	1/1	0.98	0.06	74,74,74,74	0
56	MG	1A	3617	1/1	0.98	0.17	38,38,38,38	0
56	MG	1A	3491	1/1	0.98	0.11	45,45,45,45	0
56	MG	1a	1746	1/1	0.98	0.11	54,54,54,54	0
56	MG	1A	3153	1/1	0.98	0.21	36,36,36,36	0
56	MG	1A	3296	1/1	0.98	0.20	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	3289	1/1	0.98	0.23	49,49,49,49	0
56	MG	2a	1680	1/1	0.98	0.10	49,49,49,49	0
56	MG	1P	204	1/1	0.98	0.30	34,34,34,34	0
56	MG	1A	3198	1/1	0.98	0.11	46,46,46,46	0
56	MG	2A	3161	1/1	0.98	0.18	37,37,37,37	0
56	MG	1A	3145	1/1	0.98	0.19	29,29,29,29	0
56	MG	2A	3350	1/1	0.98	0.09	55,55,55,55	0
56	MG	1A	4025	1/1	0.98	0.18	30,30,30,30	0
56	MG	1A	3863	1/1	0.98	0.25	45,45,45,45	0
56	MG	1A	3058	1/1	0.98	0.37	63,63,63,63	0
56	MG	2A	3020	1/1	0.98	0.37	44,44,44,44	0
56	MG	1U	201	1/1	0.98	0.11	33,33,33,33	0
56	MG	1a	1858	1/1	0.98	0.21	35,35,35,35	0
56	MG	1a	1835	1/1	0.98	0.14	54,54,54,54	0
56	MG	1A	3859	1/1	0.98	0.26	41,41,41,41	0
56	MG	1A	3133	1/1	0.98	0.14	28,28,28,28	0
56	MG	1A	3183	1/1	0.98	0.29	43,43,43,43	0
56	MG	2A	3130	1/1	0.98	0.13	43,43,43,43	0
56	MG	1O	202	1/1	0.98	0.10	52,52,52,52	0
56	MG	1A	4053	1/1	0.98	0.12	29,29,29,29	0
56	MG	2A	3300	1/1	0.98	0.15	50,50,50,50	0
56	MG	2U	202	1/1	0.98	0.42	48,48,48,48	0
56	MG	1A	3348	1/1	0.98	0.21	20,20,20,20	0
56	MG	1A	3814	1/1	0.98	0.17	35,35,35,35	0
56	MG	1A	3836	1/1	0.98	0.41	57,57,57,57	0
56	MG	1D	310	1/1	0.98	0.32	31,31,31,31	0
56	MG	1A	3001	1/1	0.98	0.27	30,30,30,30	0
56	MG	1A	3227	1/1	0.98	0.14	27,27,27,27	0
56	MG	2a	1677	1/1	0.98	0.09	55,55,55,55	0
56	MG	1A	3119	1/1	0.98	0.13	31,31,31,31	0
56	MG	2A	3236	1/1	0.98	0.14	55,55,55,55	0
56	MG	1A	3634	1/1	0.98	0.05	32,32,32,32	0
56	MG	1A	3620	1/1	0.99	0.15	7,7,7,7	0
56	MG	1A	3204	1/1	0.99	0.19	36,36,36,36	0
56	MG	1A	3244	1/1	0.99	0.07	14,14,14,14	0
56	MG	2a	1683	1/1	0.99	0.12	43,43,43,43	0
56	MG	2A	3374	1/1	0.99	0.12	41,41,41,41	0
56	MG	1a	1712	1/1	0.99	0.19	53,53,53,53	0
56	MG	1A	4095	1/1	0.99	0.14	32,32,32,32	0
56	MG	1A	3589	1/1	0.99	0.14	31,31,31,31	0
56	MG	1A	3843	1/1	0.99	0.10	29,29,29,29	0
56	MG	1A	3612	1/1	0.99	0.15	37,37,37,37	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
57	ZN	19	102	1/1	0.99	0.13	46,46,46,46	0
56	MG	1A	3637	1/1	0.99	0.31	31,31,31,31	0
56	MG	1A	3705	1/1	0.99	0.09	16,16,16,16	0
56	MG	2A	3436	1/1	0.99	0.17	32,32,32,32	0
56	MG	2A	3292	1/1	0.99	0.22	43,43,43,43	0
56	MG	1A	3426	1/1	0.99	0.18	56,56,56,56	0
56	MG	2a	1756	1/1	0.99	0.18	47,47,47,47	0
56	MG	1x	109	1/1	0.99	0.05	78,78,78,78	0
56	MG	2A	3180	1/1	0.99	0.32	34,34,34,34	0
56	MG	1A	3152	1/1	0.99	0.20	29,29,29,29	0
56	MG	1A	4041	1/1	0.99	0.22	12,12,12,12	0
56	MG	1A	3740	1/1	0.99	0.20	23,23,23,23	0
56	MG	1A	3807	1/1	0.99	0.15	47,47,47,47	0
56	MG	1A	3100	1/1	0.99	0.19	34,34,34,34	0
56	MG	2A	3376	1/1	0.99	0.19	48,48,48,48	0
57	ZN	15	101	1/1	0.99	0.13	48,48,48,48	0
56	MG	2a	1615	1/1	0.99	0.10	56,56,56,56	0
56	MG	1A	3593	1/1	0.99	0.14	38,38,38,38	0
56	MG	2A	3101	1/1	0.99	0.16	52,52,52,52	0
56	MG	2A	3328	1/1	0.99	0.05	47,47,47,47	0
56	MG	1A	3147	1/1	0.99	0.13	33,33,33,33	0
56	MG	1A	4020	1/1	0.99	0.07	30,30,30,30	0
56	MG	2a	1646	1/1	0.99	0.14	70,70,70,70	0
56	MG	1A	3648	1/1	0.99	0.09	24,24,24,24	0
56	MG	1B	217	1/1	0.99	0.15	55,55,55,55	0
56	MG	2A	3231	1/1	0.99	0.15	42,42,42,42	0
56	MG	1A	3202	1/1	0.99	0.34	33,33,33,33	0
56	MG	1A	3603	1/1	0.99	0.14	45,45,45,45	0
57	ZN	25	501	1/1	0.99	0.11	47,47,47,47	0
56	MG	2A	3140	1/1	0.99	0.39	35,35,35,35	0
56	MG	1A	3728	1/1	0.99	0.12	17,17,17,17	0
56	MG	1a	1706	1/1	0.99	0.11	53,53,53,53	0
56	MG	1a	1704	1/1	0.99	0.14	40,40,40,40	0
56	MG	2A	3046	1/1	0.99	0.17	38,38,38,38	0
56	MG	1A	3786	1/1	0.99	0.13	31,31,31,31	0
56	MG	2A	3383	1/1	0.99	0.17	49,49,49,49	0
58	SF4	2d	501	8/8	0.99	0.12	56,71,81,82	0
56	MG	2a	1782	1/1	0.99	0.27	46,46,46,46	0
58	SF4	1d	501	8/8	0.99	0.13	56,73,76,77	0
56	MG	2A	3293	1/1	0.99	0.17	36,36,36,36	0
56	MG	1a	1838	1/1	1.00	0.09	34,34,34,34	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.