



# Full wwPDB X-ray Structure Validation Report ⓘ

Dec 15, 2020 – 11:12 PM EST

PDB ID : 6XHX  
Title : Crystal structure of the A2058-unmethylated *Thermus thermophilus* 70S ribosome in complex with erythromycin and protein Y (YfiA) at 2.55Å resolution  
Authors : Svetlov, M.S.; Syroegin, E.A.; Aleksandrova, E.V.; Atkinson, G.C.; Gregory, S.T.; Mankin, A.S.; Polikanov, Y.S.  
Deposited on : 2020-06-19  
Resolution : 2.55 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 : 2.15.1  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.15.1

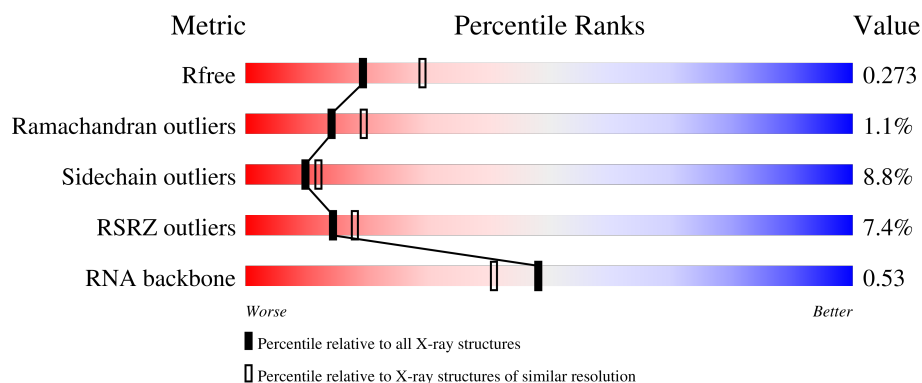
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.55 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	1284 (2.56-2.52)
Ramachandran outliers	138981	1315 (2.56-2.52)
Sidechain outliers	138945	1315 (2.56-2.52)
RSRZ outliers	127900	1272 (2.56-2.52)
RNA backbone	3102	1026 (2.88-2.20)

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

Mol	Chain	Length	Quality of chain
1	1A	2915	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red, orange, yellow, green);"></div> <div style="display: flex; justify-content: space-between; margin-top: 5px;"> <span>81%</span> <span>16%</span> <span>..</span> </div> </div>
1	2A	2915	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red, orange, yellow, green);"></div> <div style="display: flex; justify-content: space-between; margin-top: 5px;"> <span>80%</span> <span>18%</span> <span>..</span> </div> </div>
2	1B	121	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, green, yellow, orange, red);"></div> <div style="display: flex; justify-content: space-between; margin-top: 5px;"> <span>91%</span> <span>8%</span> <span>.</span> </div> </div>
2	2B	121	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, green, yellow, orange, red);"></div> <div style="display: flex; justify-content: space-between; margin-top: 5px;"> <span>86%</span> <span>13%</span> <span>.</span> </div> </div>
3	1D	276	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red, orange, yellow, green);"></div> <div style="display: flex; justify-content: space-between; margin-top: 5px;"> <span>93%</span> <span>6%</span> </div> </div>

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Mol	Chain	Length	Quality of chain
3	2D	276	<div> <div>16%</div> <div>93%</div> <div>7%</div> </div>
4	1E	206	<div> <div>%</div> <div>92%</div> <div>7%</div> </div>
4	2E	206	<div> <div>4%</div> <div>94%</div> <div>5%</div> </div>
5	1F	210	<div> <div></div> <div>89%</div> <div>8%</div> </div>
5	2F	210	<div> <div>5%</div> <div>90%</div> <div>7%</div> </div>
6	1G	182	<div> <div>3%</div> <div>92%</div> <div>7%</div> </div>
6	2G	182	<div> <div>32%</div> <div>85%</div> <div>15%</div> </div>
7	1H	180	<div> <div>%</div> <div>92%</div> <div>5%</div> </div>
7	2H	180	<div> <div>32%</div> <div>82%</div> <div>14%</div> </div>
8	1I	148	<div> <div>4%</div> <div>85%</div> <div>14%</div> </div>
8	2I	148	<div> <div>16%</div> <div>91%</div> <div>8%</div> </div>
9	1N	140	<div> <div></div> <div>94%</div> <div>6%</div> </div>
9	2N	140	<div> <div>6%</div> <div>93%</div> <div>7%</div> </div>
10	1O	122	<div> <div></div> <div>95%</div> <div>5%</div> </div>
10	2O	122	<div> <div>4%</div> <div>93%</div> <div>7%</div> </div>
11	1P	150	<div> <div>%</div> <div>95%</div> <div></div> </div>
11	2P	150	<div> <div>10%</div> <div>95%</div> <div>5%</div> </div>
12	1Q	141	<div> <div>%</div> <div>94%</div> <div>6%</div> </div>
12	2Q	141	<div> <div>9%</div> <div>96%</div> <div></div> </div>
13	1R	118	<div> <div>%</div> <div>92%</div> <div>8%</div> </div>
13	2R	118	<div> <div>8%</div> <div>92%</div> <div>8%</div> </div>
14	1S	112	<div> <div></div> <div>89%</div> <div>8%</div> </div>
14	2S	112	<div> <div>14%</div> <div>89%</div> <div>9%</div> </div>
15	1T	146	<div> <div>%</div> <div>85%</div> <div>5%</div> </div>
15	2T	146	<div> <div>5%</div> <div>84%</div> <div>5%</div> </div>

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Mol	Chain	Length	Quality of chain
16	1U	118	
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	

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Mol	Chain	Length	Quality of chain
28	26	54	
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	

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Mol	Chain	Length	Quality of chain
41	1j	105	
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	1y	113	

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Mol	Chain	Length	Quality of chain
53	2y	113	

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
54	MG	1A	3989	-	-	-	X
54	MG	2A	3024	-	-	-	X

## 2 Entry composition

There are 60 unique types of molecules in this entry. The entry contains 296819 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	2872	Total	C	N	O	P	0	0	0
			61869	27540	11574	19884	2871			
1	2A	2867	Total	C	N	O	P	0	0	0
			61758	27491	11552	19850	2865			

- 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	1145	476	832	119			
2	2B	120	Total	C	N	O	P	0	0	0
			2573	1146	476	832	119			

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
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
			1426	916	253	253	4			
6	2G	181	Total	C	N	O	S	0	0	0
			1424	912	259	249	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	173	Total	C	N	O	S	0	0	0
			1324	842	247	234	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	1I	147	Total	C	N	O	S	0	0	0
			1094	699	191	203	1			
8	2I	146	Total	C	N	O	S	0	0	0
			1076	687	186	202	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
			1121	722	208	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
			1135	706	230	196	3			
11	2P	149	Total	C	N	O	S	0	0	0
			1135	706	230	196	3			

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

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
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
			775	498	141	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
			810	520	153	131	6			
20	2Y	107	Total	C	N	O	S	0	0	0
			810	519	153	132	6			

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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



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

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

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

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

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

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

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

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

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

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

- Molecule 53 is a protein called Ribosome-associated inhibitor A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
53	1y	97	Total	C	N	O	S	0	0	0
			764	478	144	139	3			
53	2y	96	Total	C	N	O	S	0	0	0
			749	468	141	137	3			

- Molecule 54 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
54	2E	7	Total	Mg	0	0
			7	7		
54	17	5	Total	Mg	0	0
			5	5		
54	1T	3	Total	Mg	0	0
			3	3		
54	1N	4	Total	Mg	0	0
			4	4		
54	20	2	Total	Mg	0	0
			2	2		
54	18	2	Total	Mg	0	0
			2	2		
54	1o	1	Total	Mg	0	0
			1	1		
54	2W	3	Total	Mg	0	0
			3	3		
54	1Y	2	Total	Mg	0	0
			2	2		
54	2I	1	Total	Mg	0	0
			1	1		
54	13	4	Total	Mg	0	0
			4	4		
54	1f	2	Total	Mg	0	0
			2	2		
54	1P	6	Total	Mg	0	0
			6	6		
54	2B	18	Total	Mg	0	0
			18	18		
54	2a	183	Total	Mg	0	0
			183	183		
54	1E	10	Total	Mg	0	0
			10	10		
54	1b	1	Total	Mg	0	0
			1	1		
54	2l	1	Total	Mg	0	0
			1	1		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
54	2F	4	Total 4	Mg 4	0	0
54	28	2	Total 2	Mg 2	0	0
54	2e	2	Total 2	Mg 2	0	0
54	1W	4	Total 4	Mg 4	0	0
54	1A	1020	Total 1020	Mg 1020	0	0
54	1t	2	Total 2	Mg 2	0	0
54	1n	3	Total 3	Mg 3	0	0
54	2P	2	Total 2	Mg 2	0	0
54	1y	3	Total 3	Mg 3	0	0
54	25	2	Total 2	Mg 2	0	0
54	2T	3	Total 3	Mg 3	0	0
54	1D	16	Total 16	Mg 16	0	0
54	2N	1	Total 1	Mg 1	0	0
54	1e	3	Total 3	Mg 3	0	0
54	2G	3	Total 3	Mg 3	0	0
54	2f	1	Total 1	Mg 1	0	0
54	1V	7	Total 7	Mg 7	0	0
54	2X	1	Total 1	Mg 1	0	0
54	1a	274	Total 274	Mg 274	0	0
54	2Q	2	Total 2	Mg 2	0	0
54	15	6	Total 6	Mg 6	0	0

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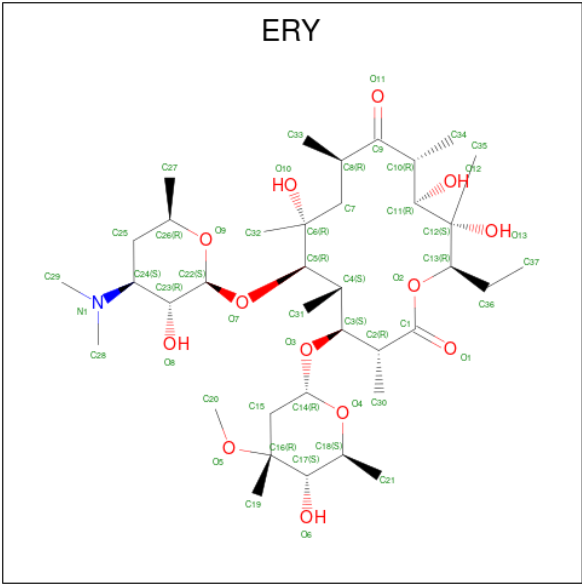
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
54	2j	1	Total 1	Mg 1	0	0
54	1R	5	Total 5	Mg 5	0	0
54	2t	1	Total 1	Mg 1	0	0
54	1m	1	Total 1	Mg 1	0	0
54	1G	4	Total 4	Mg 4	0	0
54	2O	2	Total 2	Mg 2	0	0
54	1l	4	Total 4	Mg 4	0	0
54	1d	5	Total 5	Mg 5	0	0
54	2n	1	Total 1	Mg 1	0	0
54	1H	2	Total 2	Mg 2	0	0
54	2l	1	Total 1	Mg 1	0	0
54	1i	1	Total 1	Mg 1	0	0
54	23	1	Total 1	Mg 1	0	0
54	2R	2	Total 2	Mg 2	0	0
54	1Z	1	Total 1	Mg 1	0	0
54	2D	10	Total 10	Mg 10	0	0
54	1U	8	Total 8	Mg 8	0	0
54	1O	1	Total 1	Mg 1	0	0
54	27	1	Total 1	Mg 1	0	0
54	19	1	Total 1	Mg 1	0	0
54	1l	2	Total 2	Mg 2	0	0

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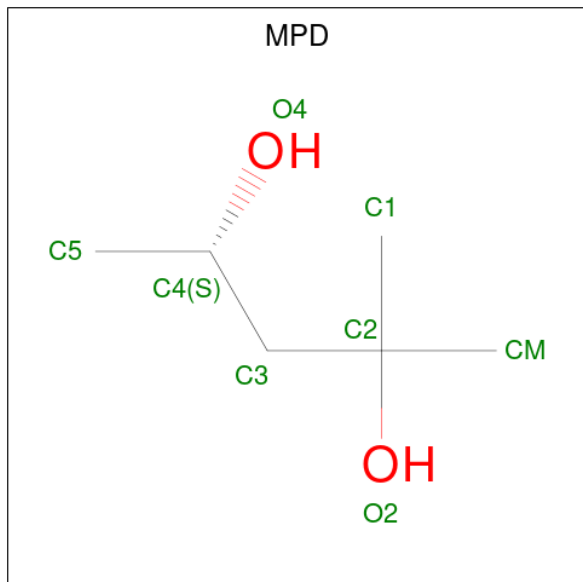
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
54	2V	3	Total	Mg	0	0
			3	3		
54	1F	18	Total	Mg	0	0
			18	18		
54	10	7	Total	Mg	0	0
			7	7		
54	1g	3	Total	Mg	0	0
			3	3		
54	2o	1	Total	Mg	0	0
			1	1		
54	1Q	4	Total	Mg	0	0
			4	4		
54	2A	733	Total	Mg	0	0
			733	733		
54	1h	2	Total	Mg	0	0
			2	2		
54	1B	32	Total	Mg	0	0
			32	32		

- Molecule 55 is ERYTHROMYCIN A (three-letter code: ERY) (formula: C<sub>37</sub>H<sub>67</sub>NO<sub>13</sub>).



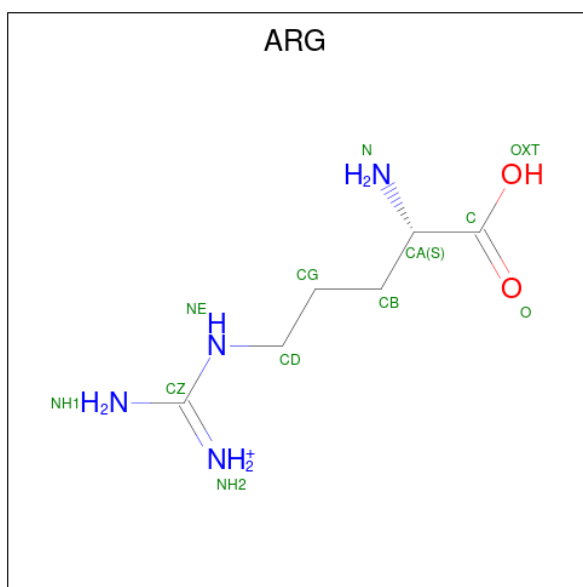
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
55	1A	1	Total	C	N	O	0	0
			51	37	1	13		
55	2A	1	Total	C	N	O	0	0
			51	37	1	13		

- Molecule 56 is (4S)-2-METHYL-2,4-PENTANEDIOL (three-letter code: MPD) (formula:  $C_6H_{14}O_2$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
56	1A	1	Total	C	O	0	0
			8	6	2		
56	1T	1	Total	C	O	0	0
			8	6	2		
56	18	1	Total	C	O	0	0
			8	6	2		
56	1a	1	Total	C	O	0	0
			8	6	2		
56	2A	1	Total	C	O	0	0
			8	6	2		
56	2A	1	Total	C	O	0	0
			8	6	2		
56	2B	1	Total	C	O	0	0
			8	6	2		

- Molecule 57 is ARGinine (three-letter code: ARG) (formula:  $C_6H_{15}N_4O_2$ ).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
57	1B	1	Total	C	N	O	0	0
			12	6	4	2		
57	1F	1	Total	C	N	O	0	0
			12	6	4	2		

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

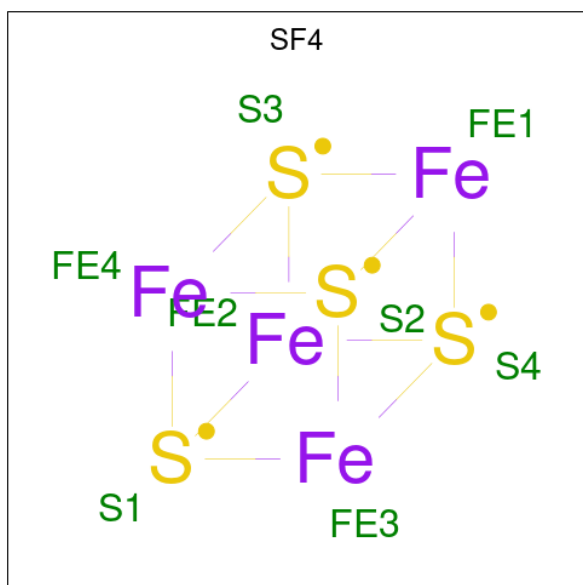
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
58	1Y	1	Total	Zn	0	0
			1	1		
58	14	1	Total	Zn	0	0
			1	1		
58	1n	1	Total	Zn	0	0
			1	1		
58	15	1	Total	Zn	0	0
			1	1		
58	29	1	Total	Zn	0	0
			1	1		
58	19	1	Total	Zn	0	0
			1	1		
58	26	1	Total	Zn	0	0
			1	1		
58	25	1	Total	Zn	0	0
			1	1		
58	24	1	Total	Zn	0	0
			1	1		
58	2n	1	Total	Zn	0	0
			1	1		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
58	2Y	1	Total	Zn	0	0
			1	1		
58	16	1	Total	Zn	0	0
			1	1		

- Molecule 59 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe<sub>4</sub>S<sub>4</sub>).



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

- Molecule 60 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
60	1A	3765	Total	O	0	0
			3765	3765		
60	1B	106	Total	O	0	0
			106	106		
60	1D	90	Total	O	0	0
			90	90		
60	1E	74	Total	O	0	0
			74	74		
60	1F	67	Total	O	0	0
			67	67		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
60	1G	18	Total	O	0	0
			18	18		
60	1H	14	Total	O	0	0
			14	14		
60	1I	8	Total	O	0	0
			8	8		
60	1N	51	Total	O	0	0
			51	51		
60	1O	26	Total	O	0	0
			26	26		
60	1P	57	Total	O	0	0
			57	57		
60	1Q	41	Total	O	0	0
			41	41		
60	1R	32	Total	O	0	0
			32	32		
60	1S	14	Total	O	0	0
			14	14		
60	1T	33	Total	O	0	0
			33	33		
60	1U	42	Total	O	0	0
			42	42		
60	1V	39	Total	O	0	0
			39	39		
60	1W	27	Total	O	0	0
			27	27		
60	1X	24	Total	O	0	0
			24	24		
60	1Y	18	Total	O	0	0
			18	18		
60	1Z	13	Total	O	0	0
			13	13		
60	10	20	Total	O	0	0
			20	20		
60	11	25	Total	O	0	0
			25	25		
60	12	12	Total	O	0	0
			12	12		
60	13	26	Total	O	0	0
			26	26		
60	14	2	Total	O	0	0
			2	2		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
60	15	28	Total 28	O 28	0	0
60	16	19	Total 19	O 19	0	0
60	17	14	Total 14	O 14	0	0
60	18	28	Total 28	O 28	0	0
60	19	5	Total 5	O 5	0	0
60	1a	465	Total 465	O 465	0	0
60	1d	9	Total 9	O 9	0	0
60	1e	1	Total 1	O 1	0	0
60	1f	2	Total 2	O 2	0	0
60	1h	1	Total 1	O 1	0	0
60	1i	1	Total 1	O 1	0	0
60	1j	1	Total 1	O 1	0	0
60	1k	1	Total 1	O 1	0	0
60	1l	5	Total 5	O 5	0	0
60	1m	3	Total 3	O 3	0	0
60	1o	3	Total 3	O 3	0	0
60	1p	1	Total 1	O 1	0	0
60	1u	1	Total 1	O 1	0	0
60	1y	3	Total 3	O 3	0	0
60	2A	1860	Total 1860	O 1860	0	0
60	2B	53	Total 53	O 53	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
60	2D	40	Total 40	O 40	0	0
60	2E	19	Total 19	O 19	0	0
60	2F	22	Total 22	O 22	0	0
60	2G	7	Total 7	O 7	0	0
60	2H	4	Total 4	O 4	0	0
60	2I	4	Total 4	O 4	0	0
60	2N	3	Total 3	O 3	0	0
60	2O	19	Total 19	O 19	0	0
60	2P	19	Total 19	O 19	0	0
60	2Q	18	Total 18	O 18	0	0
60	2R	17	Total 17	O 17	0	0
60	2S	3	Total 3	O 3	0	0
60	2T	8	Total 8	O 8	0	0
60	2U	16	Total 16	O 16	0	0
60	2V	3	Total 3	O 3	0	0
60	2W	13	Total 13	O 13	0	0
60	2X	6	Total 6	O 6	0	0
60	2Y	5	Total 5	O 5	0	0
60	2Z	7	Total 7	O 7	0	0
60	20	10	Total 10	O 10	0	0
60	21	20	Total 20	O 20	0	0

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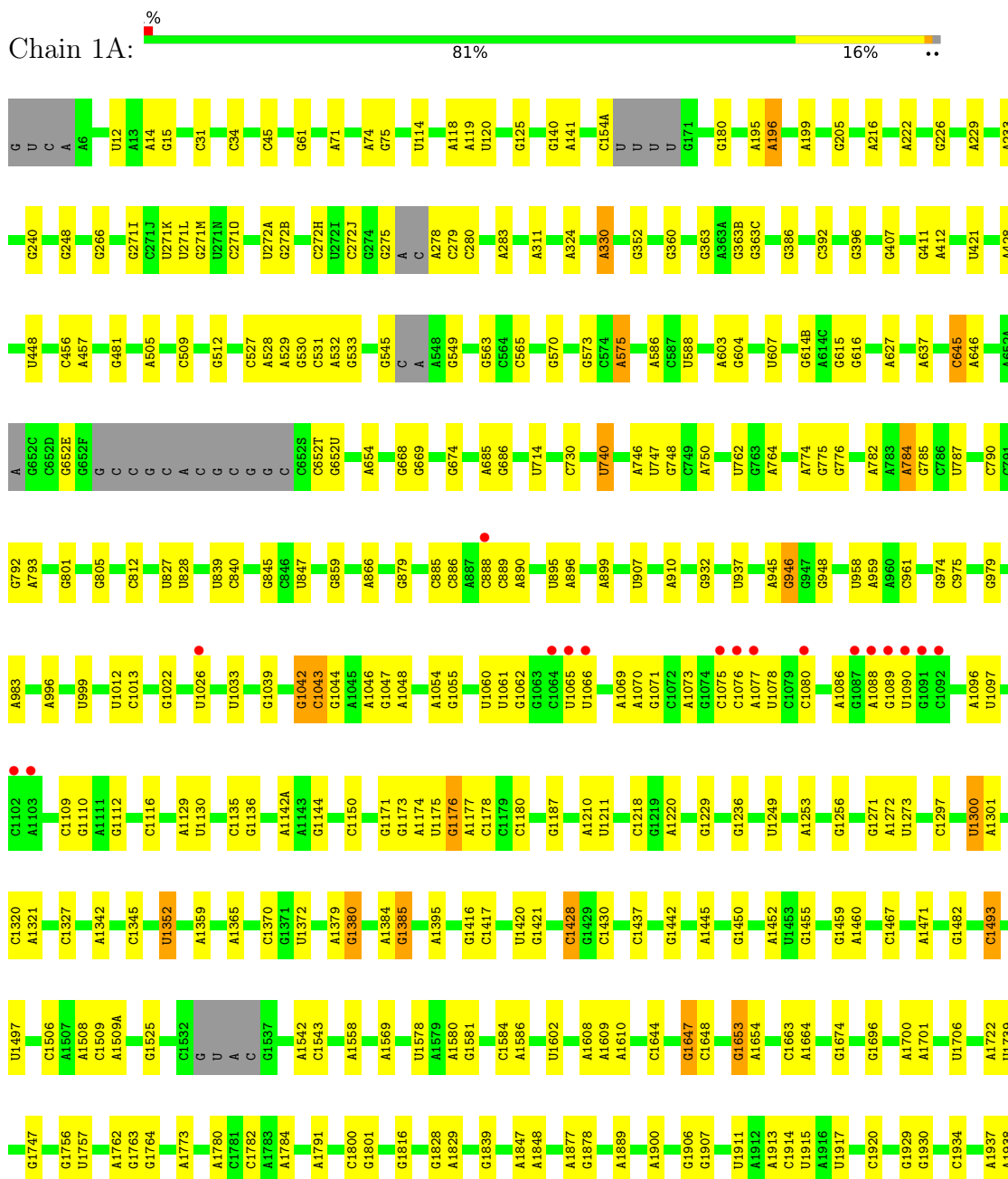
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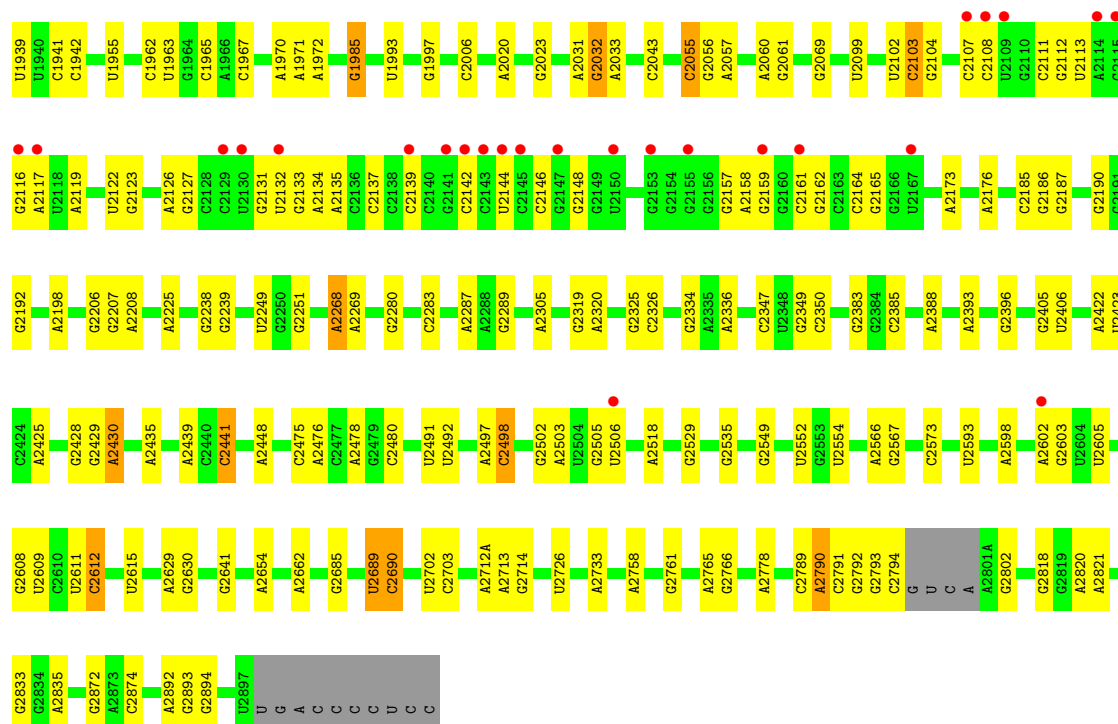
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
60	22	2	Total	O	0	0
			2	2		
60	23	3	Total	O	0	0
			3	3		
60	25	6	Total	O	0	0
			6	6		
60	26	5	Total	O	0	0
			5	5		
60	27	9	Total	O	0	0
			9	9		
60	28	9	Total	O	0	0
			9	9		
60	29	1	Total	O	0	0
			1	1		
60	2a	303	Total	O	0	0
			303	303		
60	2d	2	Total	O	0	0
			2	2		
60	2e	1	Total	O	0	0
			1	1		
60	2f	2	Total	O	0	0
			2	2		
60	2j	2	Total	O	0	0
			2	2		
60	2l	2	Total	O	0	0
			2	2		
60	2m	3	Total	O	0	0
			3	3		
60	2n	1	Total	O	0	0
			1	1		
60	2o	2	Total	O	0	0
			2	2		
60	2p	2	Total	O	0	0
			2	2		
60	2q	1	Total	O	0	0
			1	1		
60	2r	4	Total	O	0	0
			4	4		
60	2y	3	Total	O	0	0
			3	3		

### 3 Residue-property plots

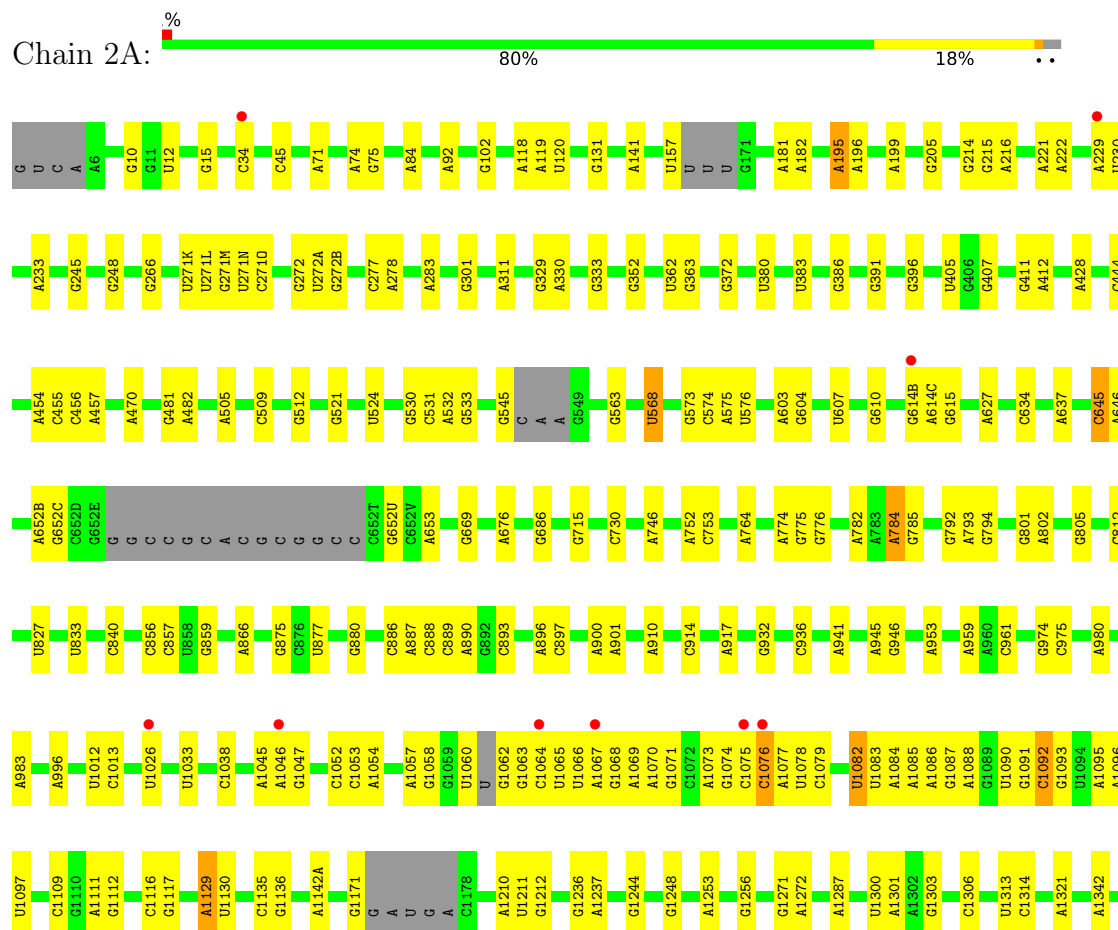
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

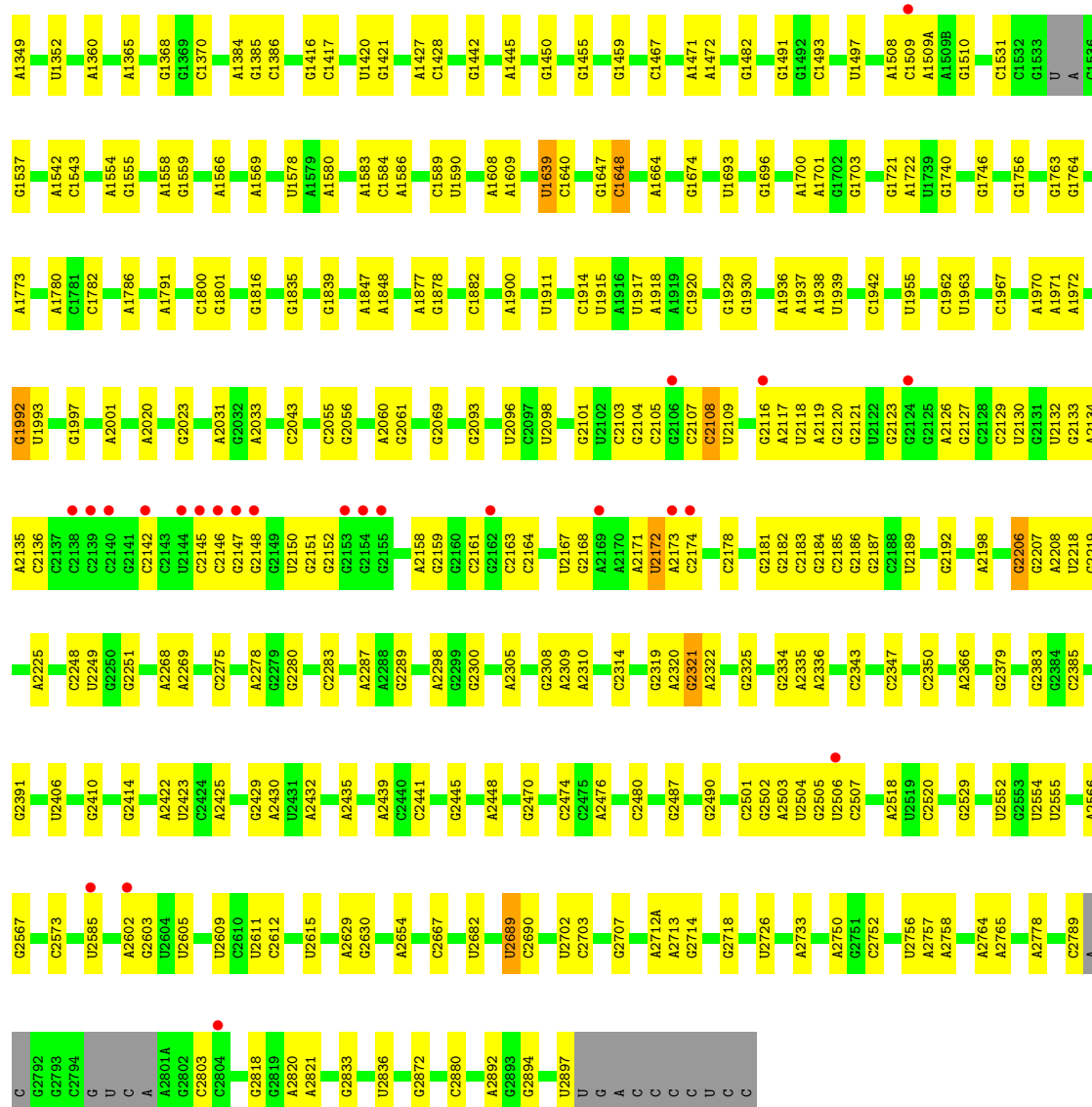
#### • Molecule 1: 23S Ribosomal RNA





- Molecule 1: 23S Ribosomal RNA





- Molecule 2: 5S Ribosomal RNA

Chain 1B: 91% 8% .



- Molecule 2: 5S Ribosomal RNA

Chain 2B: 86% 13% .

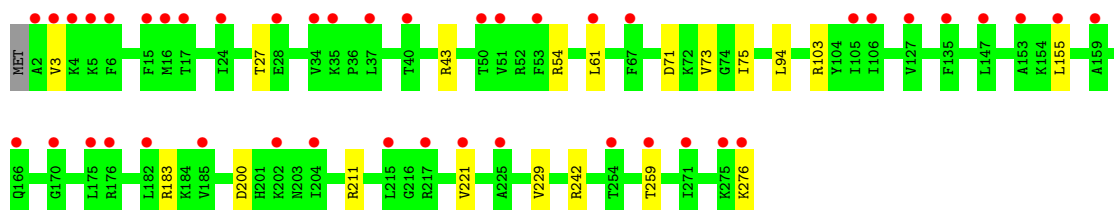


- Molecule 3: 50S ribosomal protein L2

Chain 1D: 3% 93% 6% .



- Molecule 3: 50S ribosomal protein L2



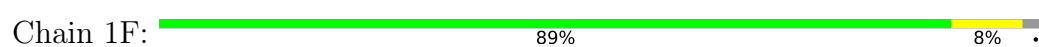
- Molecule 4: 50S ribosomal protein L3



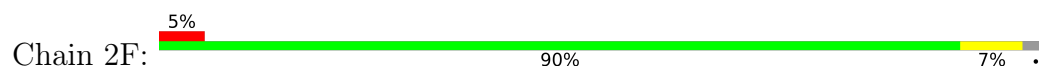
- Molecule 4: 50S ribosomal protein L3



- Molecule 5: 50S ribosomal protein L4



- Molecule 5: 50S ribosomal protein L4



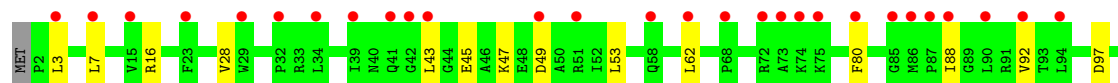
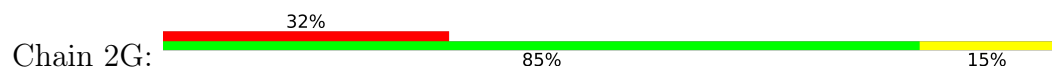
- Molecule 6: 50S ribosomal protein L5



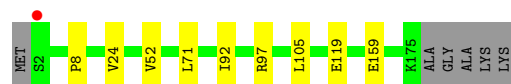




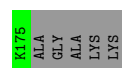
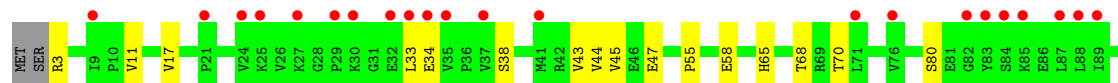
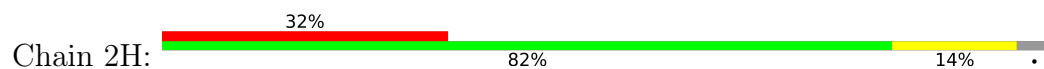
- Molecule 6: 50S ribosomal protein L5



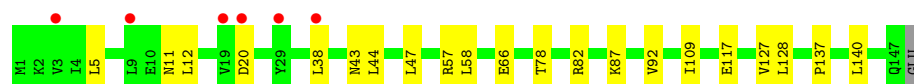
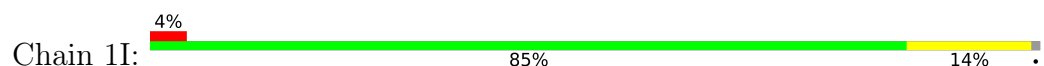
- Molecule 7: 50S ribosomal protein L6



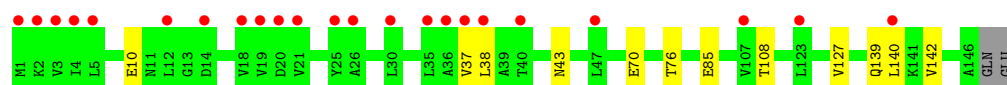
- Molecule 7: 50S ribosomal protein L6



- Molecule 8: 50S ribosomal protein L9



- Molecule 8: 50S ribosomal protein L9



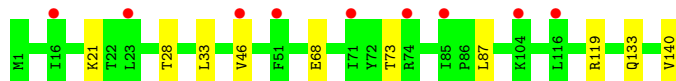
- Molecule 9: 50S ribosomal protein L13

Chain 1N:  94% 6%



- Molecule 9: 50S ribosomal protein L13

Chain 2N:  6% 93% 7%



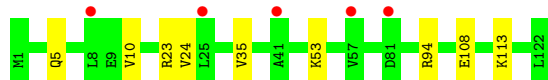
- Molecule 10: 50S ribosomal protein L14

Chain 1O:  95% 5%



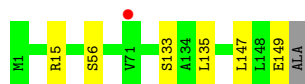
- Molecule 10: 50S ribosomal protein L14

Chain 2O:  4% 93% 7%



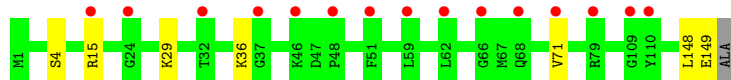
- Molecule 11: 50S ribosomal protein L15

Chain 1P:  % 95% 5%



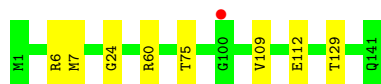
- Molecule 11: 50S ribosomal protein L15

Chain 2P:  10% 95% 5%



- Molecule 12: 50S ribosomal protein L16

Chain 1Q:  % 94% 6%



- Molecule 12: 50S ribosomal protein L16



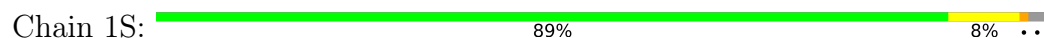
- Molecule 13: 50S ribosomal protein L17



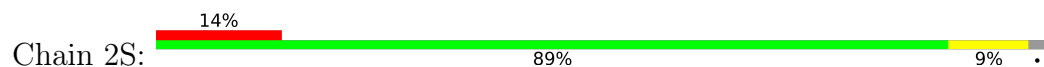
- Molecule 13: 50S ribosomal protein L17



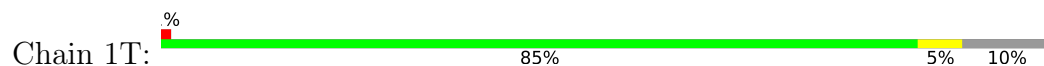
- Molecule 14: 50S ribosomal protein L18



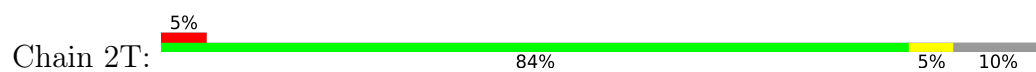
- Molecule 14: 50S ribosomal protein L18



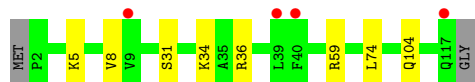
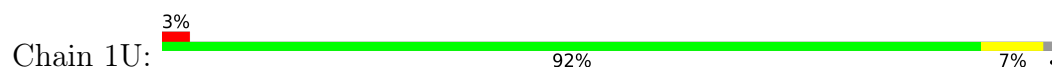
- Molecule 15: 50S ribosomal protein L19



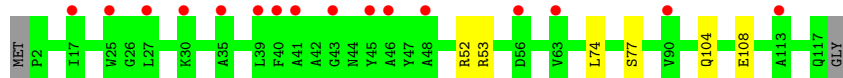
- Molecule 15: 50S ribosomal protein L19



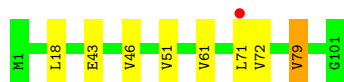
- Molecule 16: 50S ribosomal protein L20



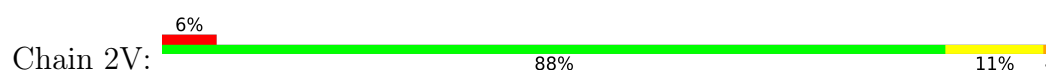
- Molecule 16: 50S ribosomal protein L20



- Molecule 17: 50S ribosomal protein L21



- Molecule 17: 50S ribosomal protein L21



- Molecule 18: 50S ribosomal protein L22

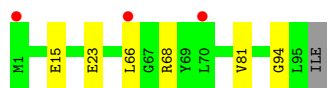


- Molecule 18: 50S ribosomal protein L22



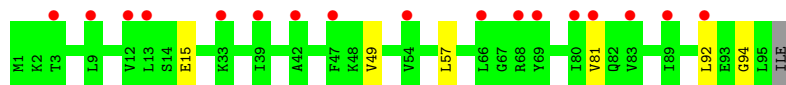
## • Molecule 19: 50S ribosomal protein L23

Chain 1X:  3% 93% 6%




## • Molecule 19: 50S ribosomal protein L23

Chain 2X:  18% 93% 6%




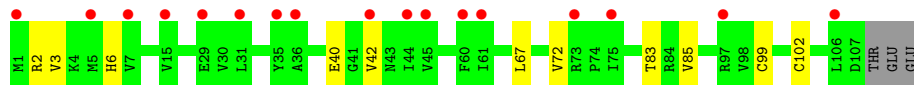
## • Molecule 20: 50S ribosomal protein L24

Chain 1Y:  90% 7%



## • Molecule 20: 50S ribosomal protein L24

Chain 2Y:  15% 87% 10%




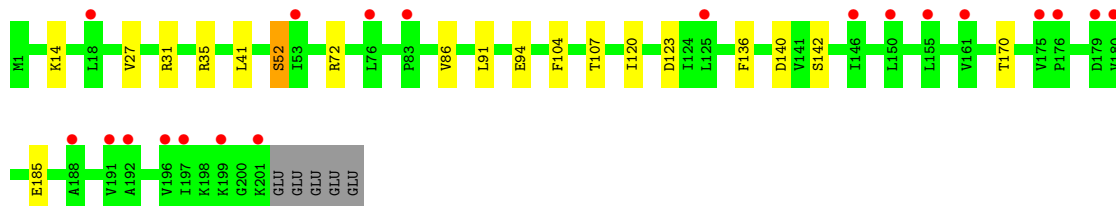
## • Molecule 21: 50S ribosomal protein L25

Chain 1Z:  92% 7%




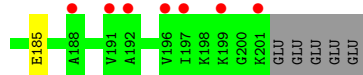
## • Molecule 21: 50S ribosomal protein L25

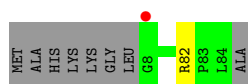
Chain 2Z:  10% 88% 9%



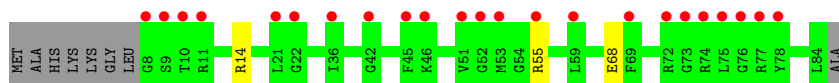
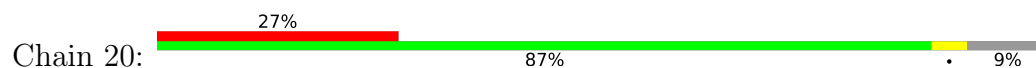
## • Molecule 22: 50S ribosomal protein L27

Chain 10:  89% 9%

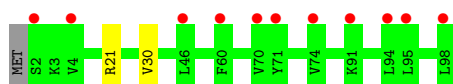




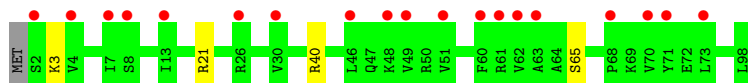
- Molecule 22: 50S ribosomal protein L27



- Molecule 23: 50S ribosomal protein L28



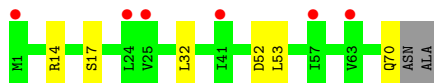
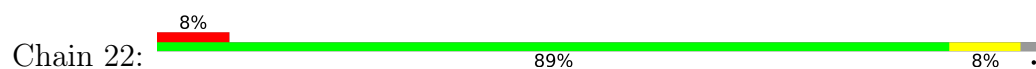
- Molecule 23: 50S ribosomal protein L28



- Molecule 24: 50S ribosomal protein L29



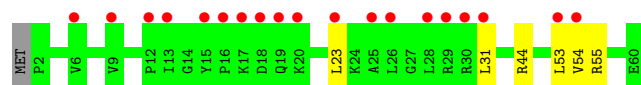
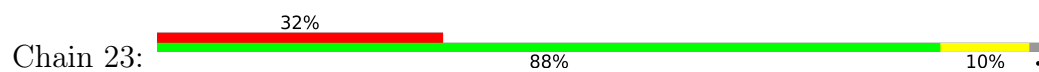
- Molecule 24: 50S ribosomal protein L29



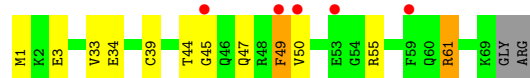
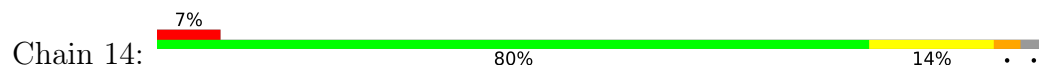
- Molecule 25: 50S ribosomal protein L30



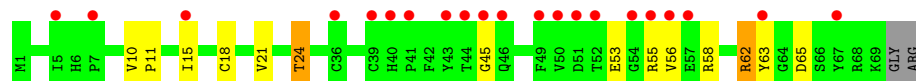
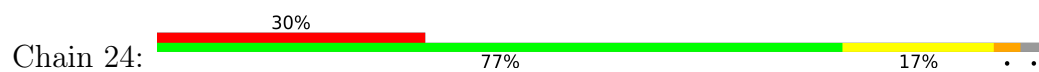
- Molecule 25: 50S ribosomal protein L30



- Molecule 26: 50S ribosomal protein L31



- Molecule 26: 50S ribosomal protein L31



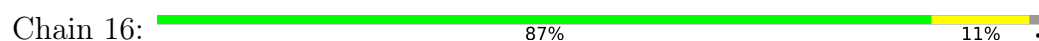
- Molecule 27: 50S ribosomal protein L32



- Molecule 27: 50S ribosomal protein L32



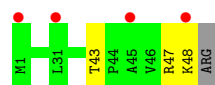
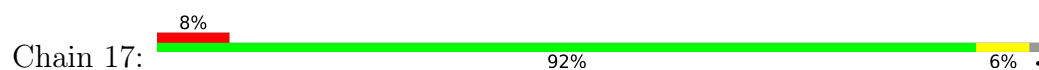
- Molecule 28: 50S ribosomal protein L33



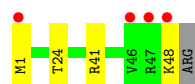
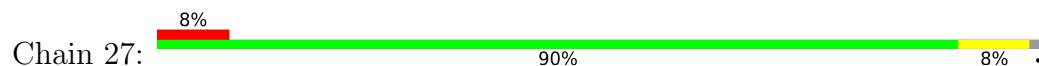
- Molecule 28: 50S ribosomal protein L33



- Molecule 29: 50S ribosomal protein L34



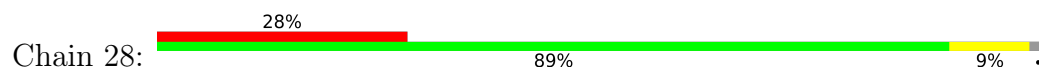
- Molecule 29: 50S ribosomal protein L34



- Molecule 30: 50S ribosomal protein L35



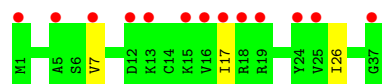
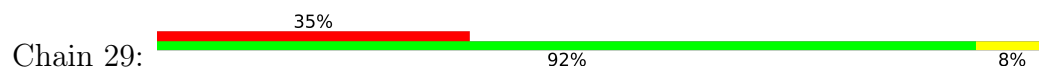
- Molecule 30: 50S ribosomal protein L35



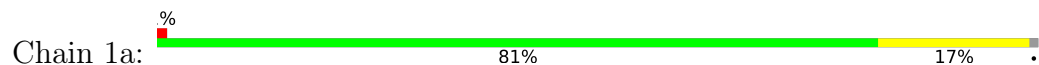
- Molecule 31: 50S ribosomal protein L36



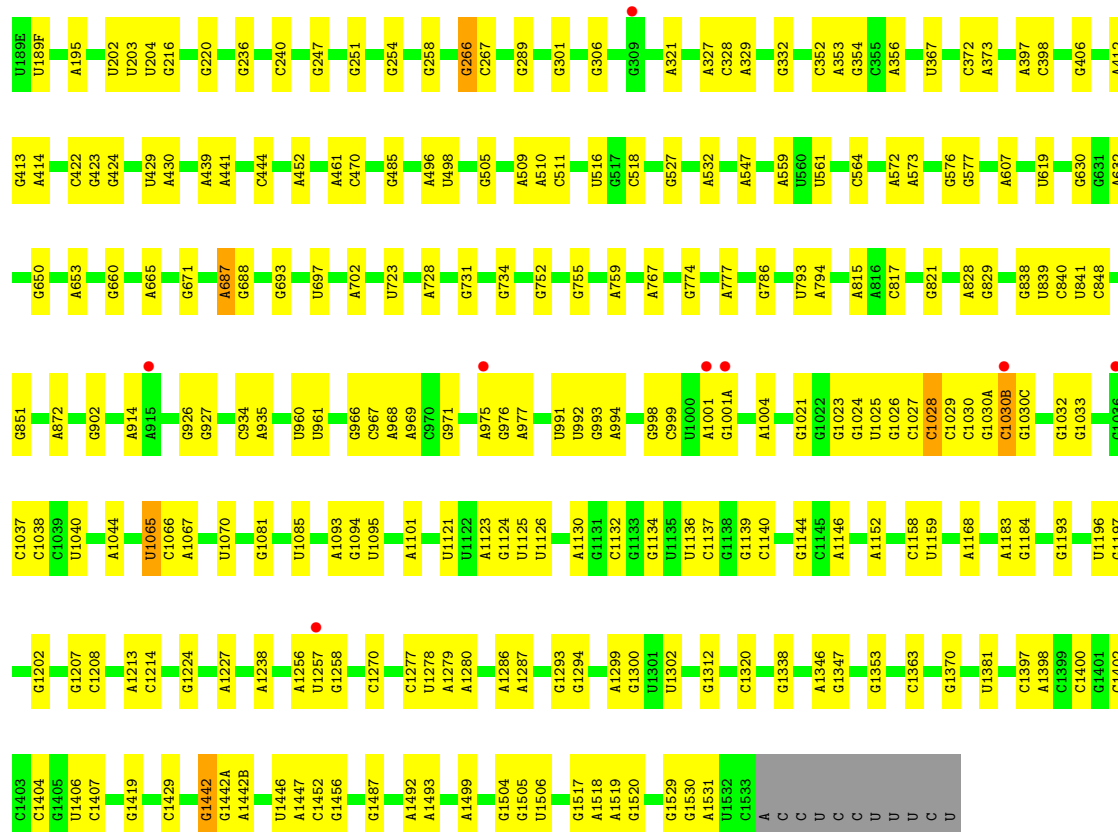
- Molecule 31: 50S ribosomal protein L36



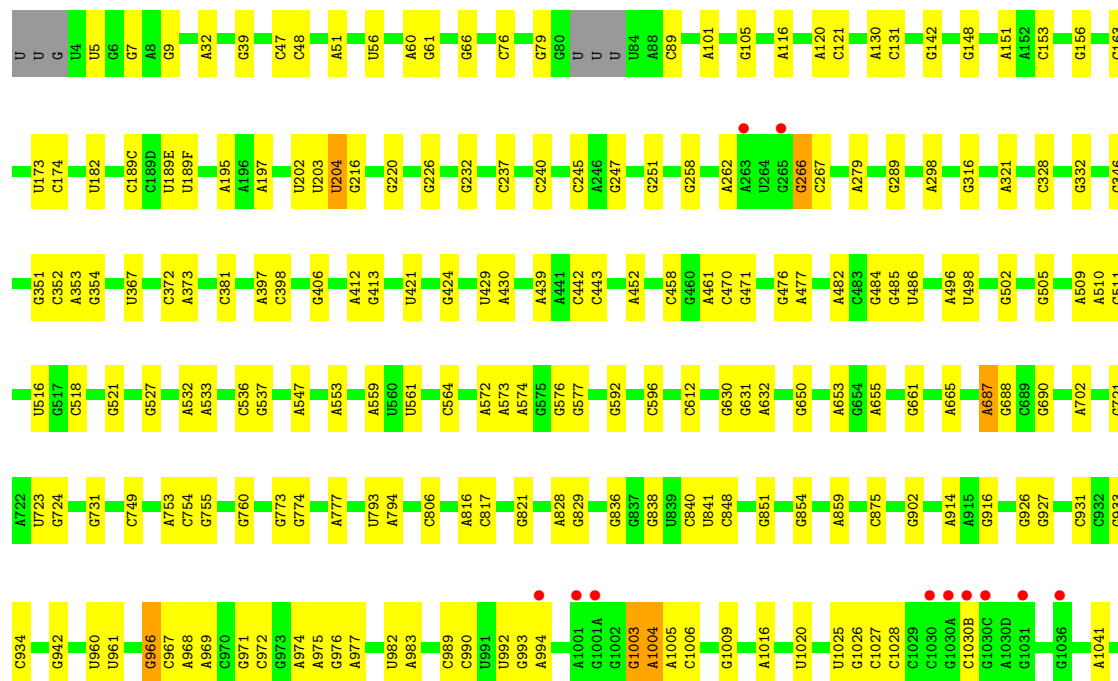
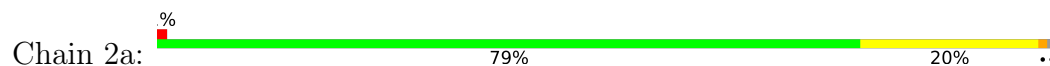
- Molecule 32: 16S Ribosomal RNA

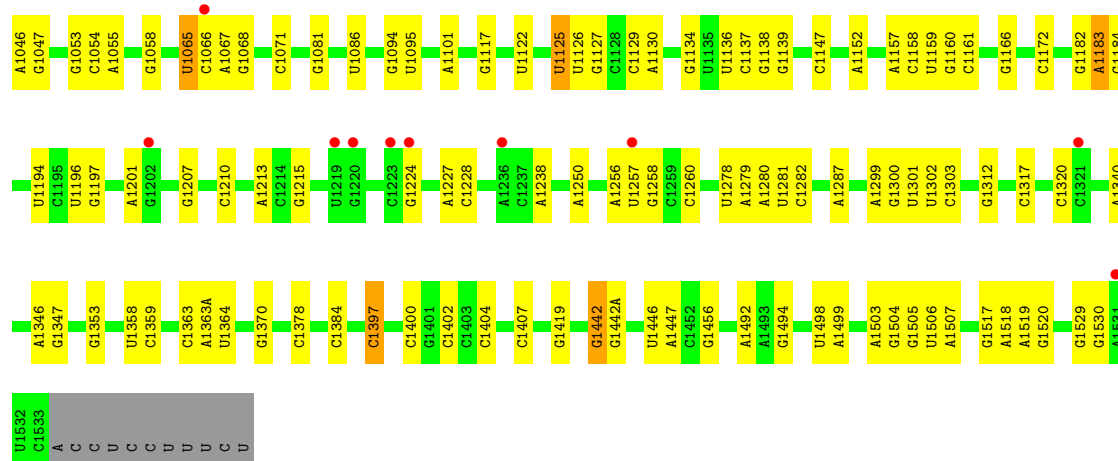




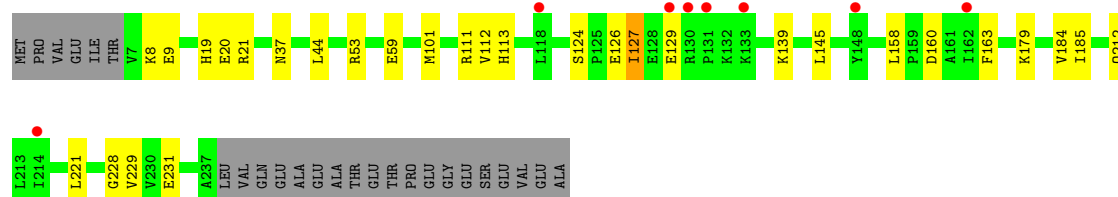
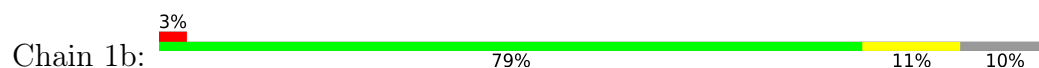


• Molecule 32: 16S Ribosomal RNA

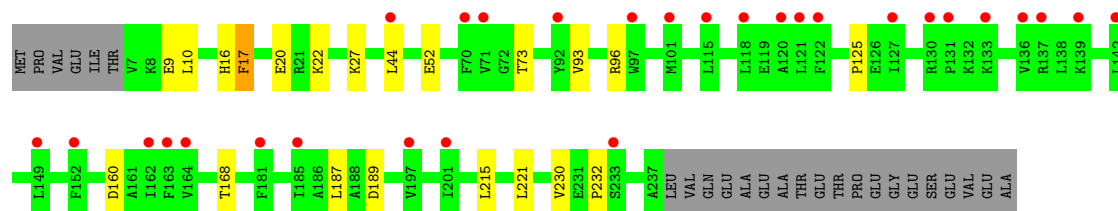
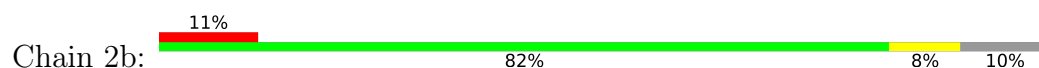




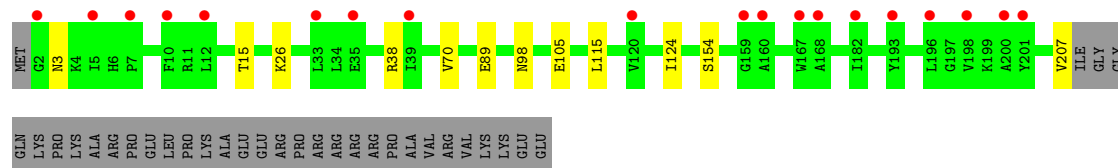
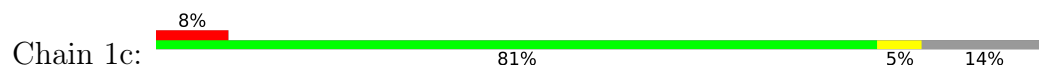
• Molecule 33: 30S ribosomal protein S2



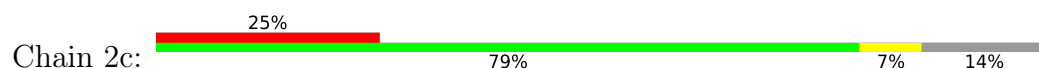
• Molecule 33: 30S ribosomal protein S2

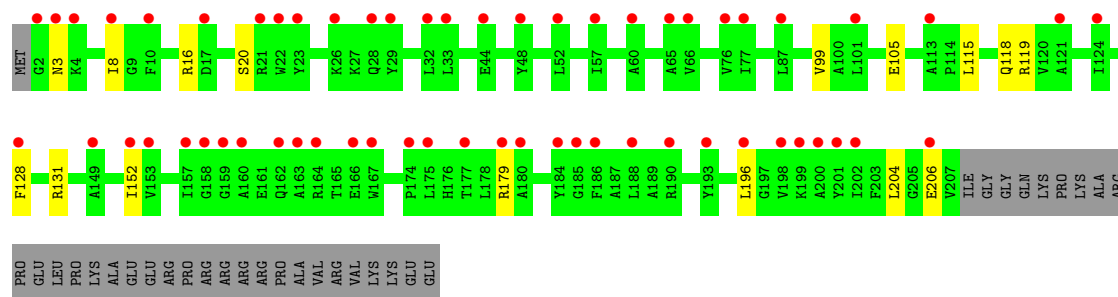


• Molecule 34: 30S ribosomal protein S3

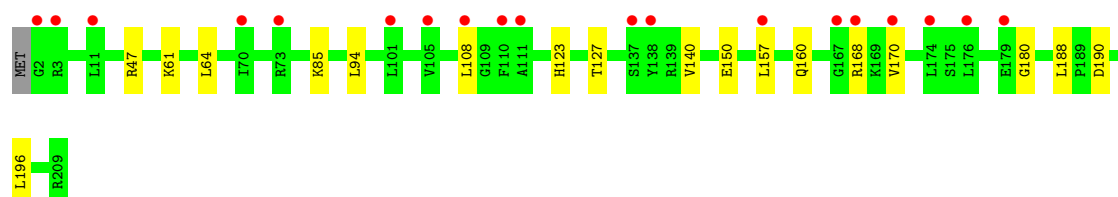
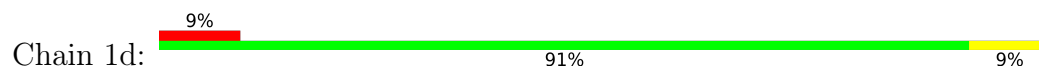


• Molecule 34: 30S ribosomal protein S3

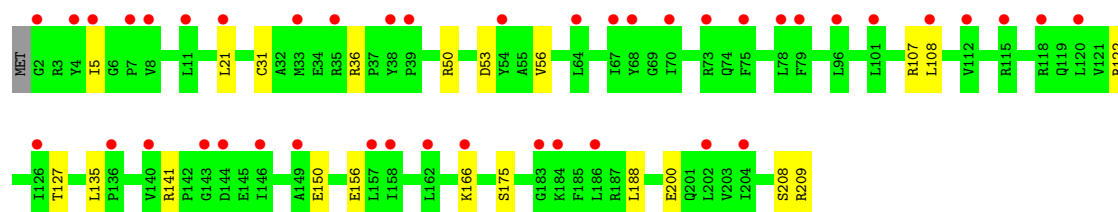
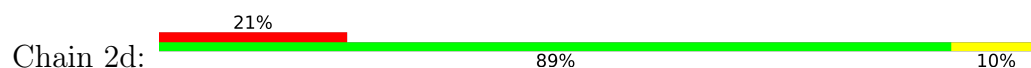




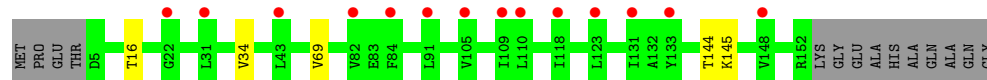
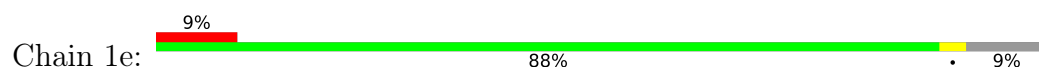
- Molecule 35: 30S ribosomal protein S4



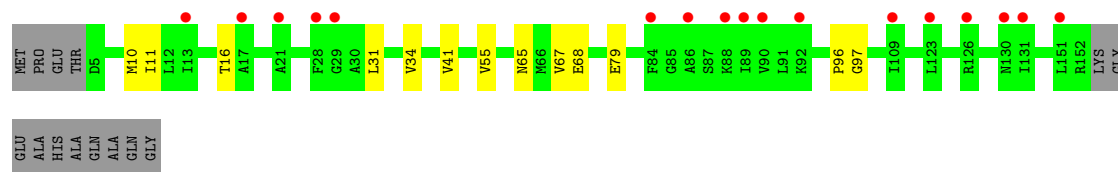
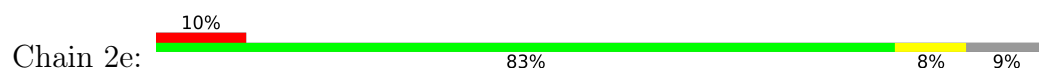
- Molecule 35: 30S ribosomal protein S4



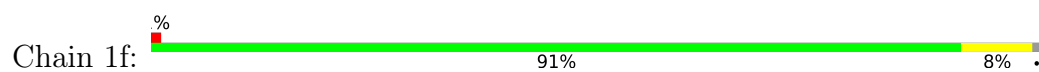
- Molecule 36: 30S ribosomal protein S5



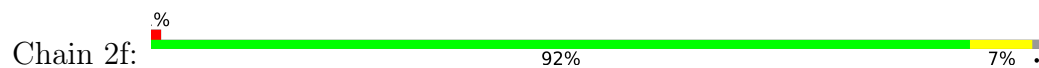
- Molecule 36: 30S ribosomal protein S5



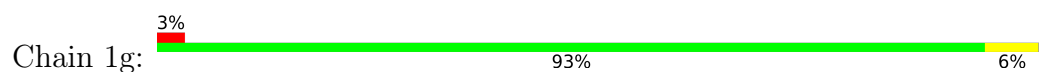
- Molecule 37: 30S ribosomal protein S6



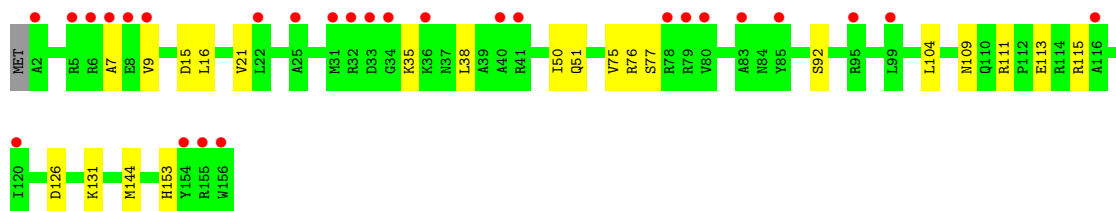
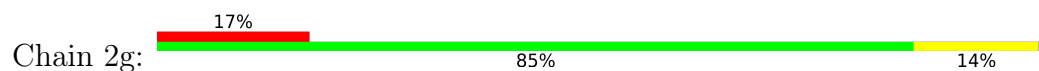
- Molecule 37: 30S ribosomal protein S6



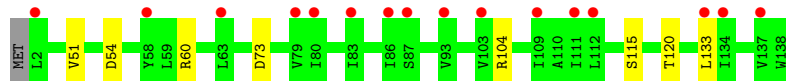
- Molecule 38: 30S ribosomal protein S7



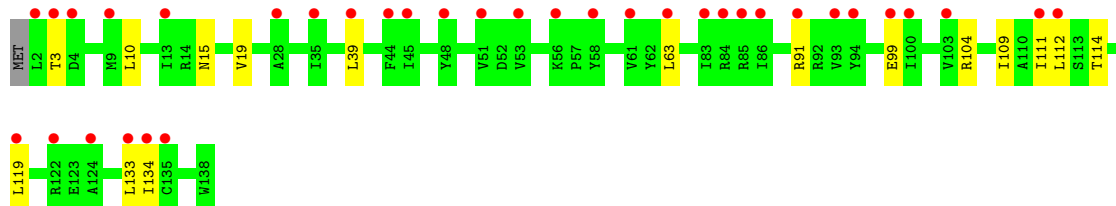
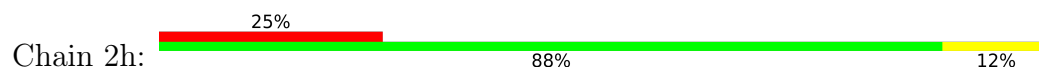
- Molecule 38: 30S ribosomal protein S7



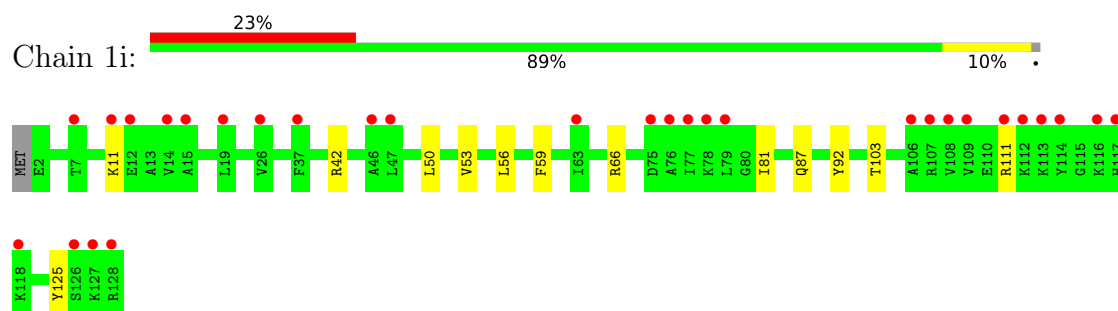
- Molecule 39: 30S ribosomal protein S8



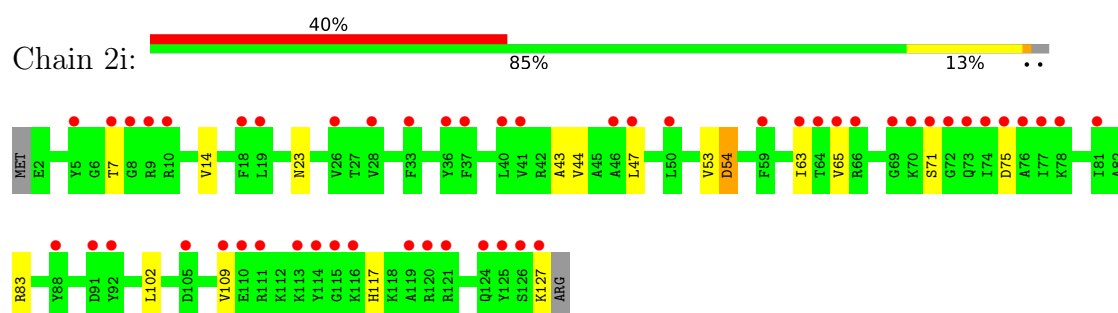
- Molecule 39: 30S ribosomal protein S8



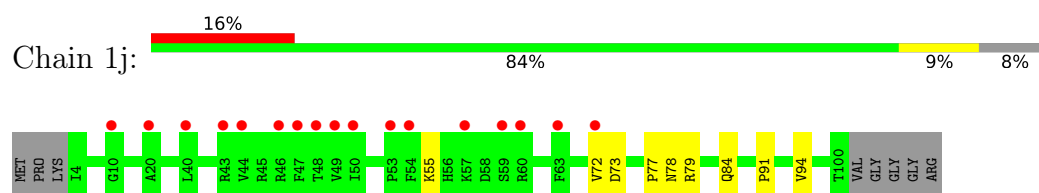
- Molecule 40: 30S ribosomal protein S9



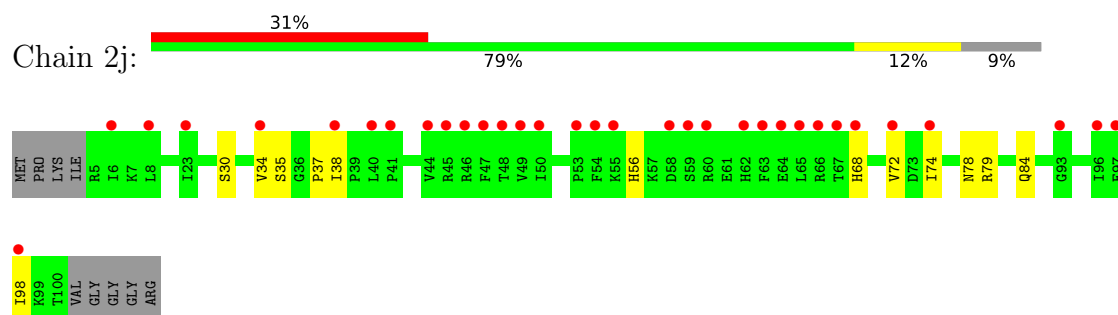
- Molecule 40: 30S ribosomal protein S9



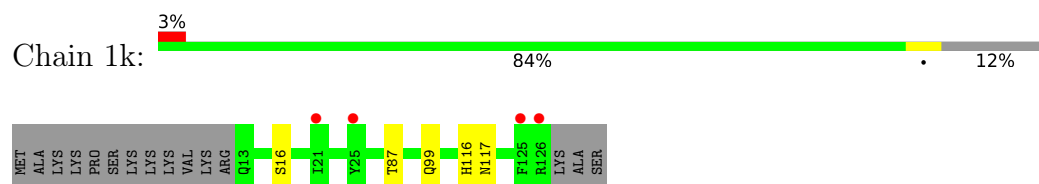
- Molecule 41: 30S ribosomal protein S10



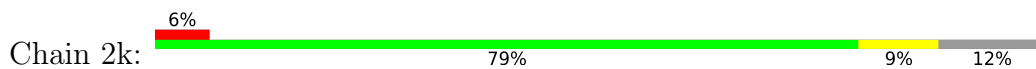
- Molecule 41: 30S ribosomal protein S10



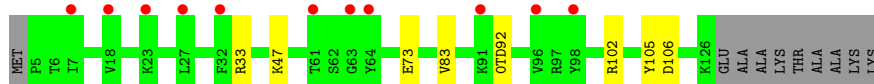
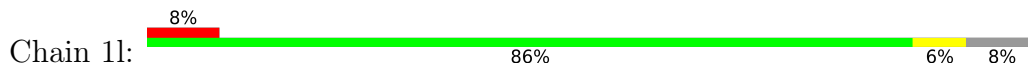
- Molecule 42: 30S ribosomal protein S11



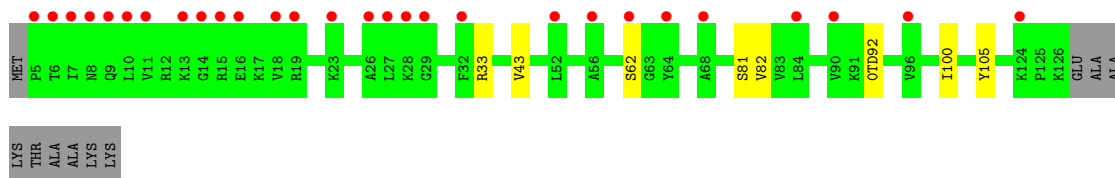
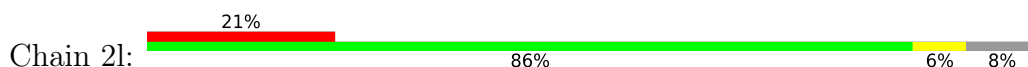
- Molecule 42: 30S ribosomal protein S11



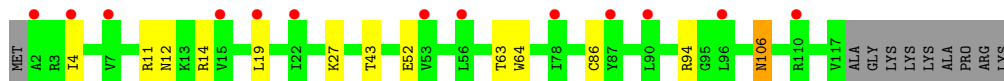
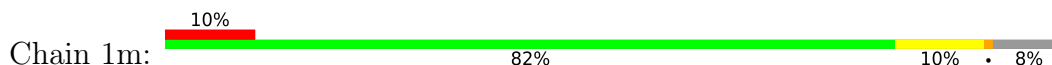
- Molecule 43: 30S ribosomal protein S12



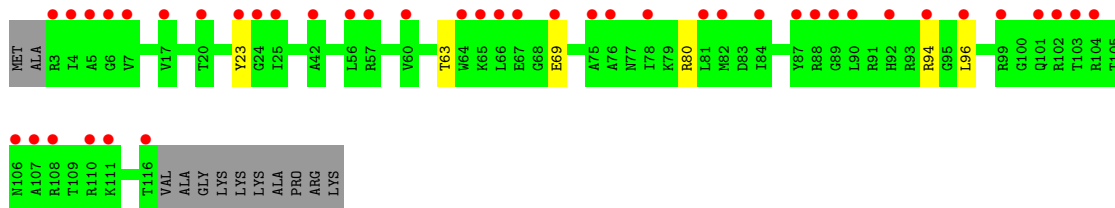
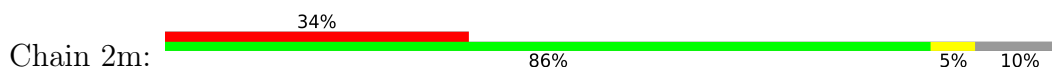
- Molecule 43: 30S ribosomal protein S12



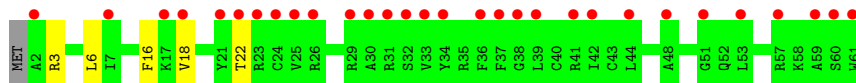
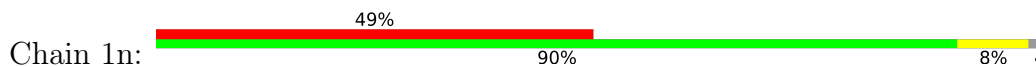
- Molecule 44: 30S ribosomal protein S13



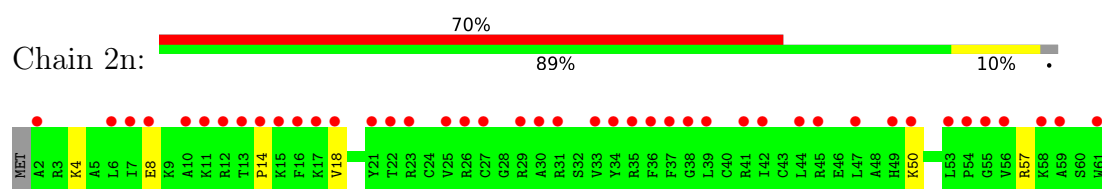
- Molecule 44: 30S ribosomal protein S13



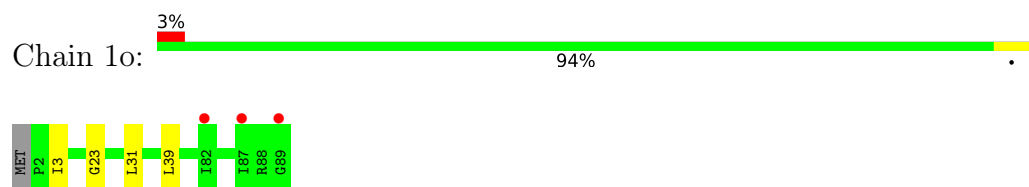
- Molecule 45: 30S ribosomal protein S14 type Z



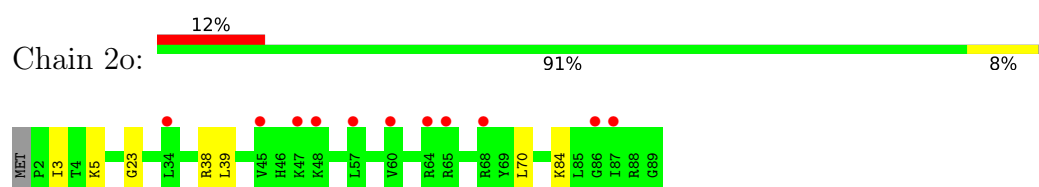
- Molecule 45: 30S ribosomal protein S14 type Z



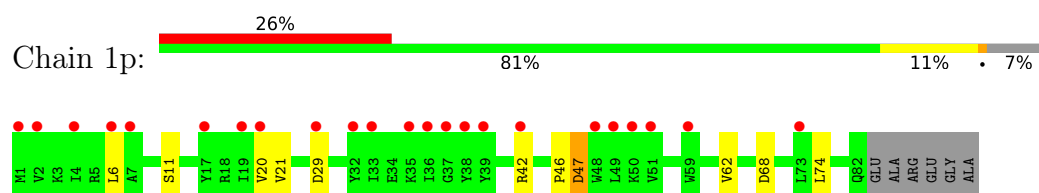
- Molecule 46: 30S ribosomal protein S15



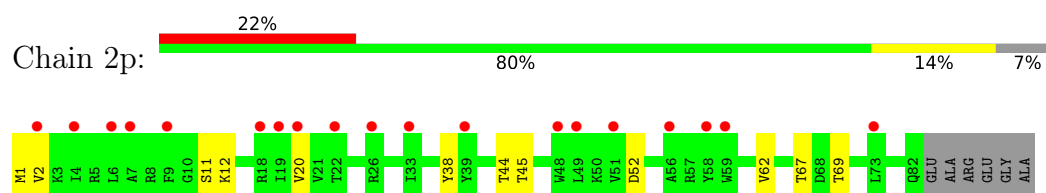
- Molecule 46: 30S ribosomal protein S15



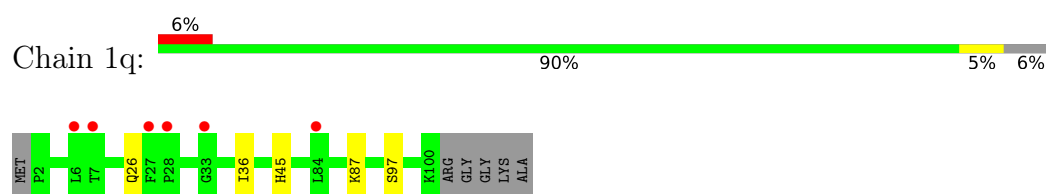
- Molecule 47: 30S ribosomal protein S16



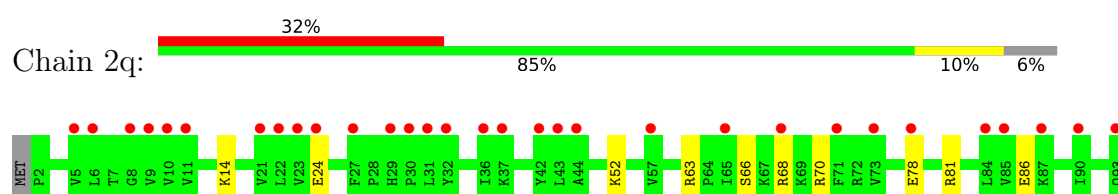
- Molecule 47: 30S ribosomal protein S16

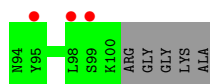


- Molecule 48: 30S ribosomal protein S17

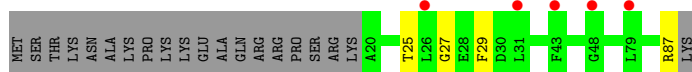
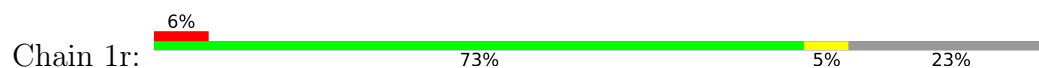


- Molecule 48: 30S ribosomal protein S17

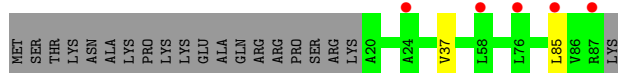
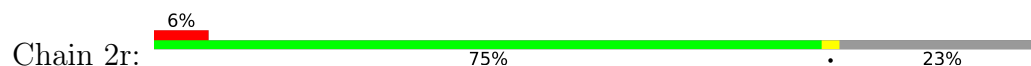




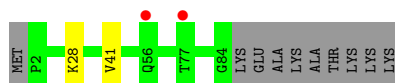
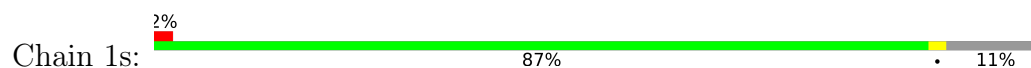
- Molecule 49: 30S ribosomal protein S18



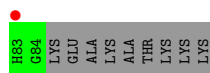
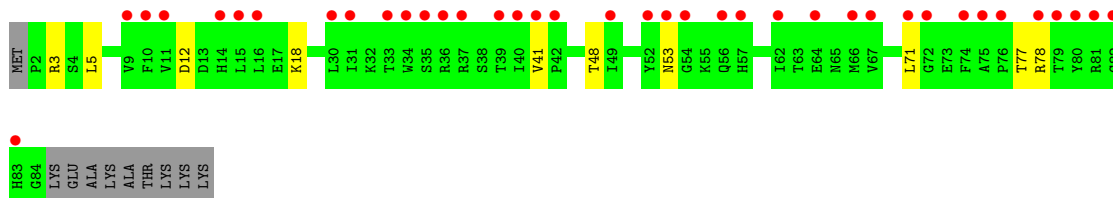
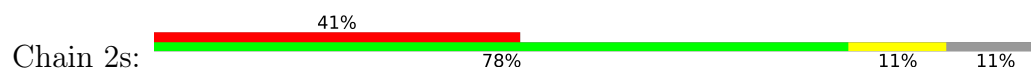
- Molecule 49: 30S ribosomal protein S18



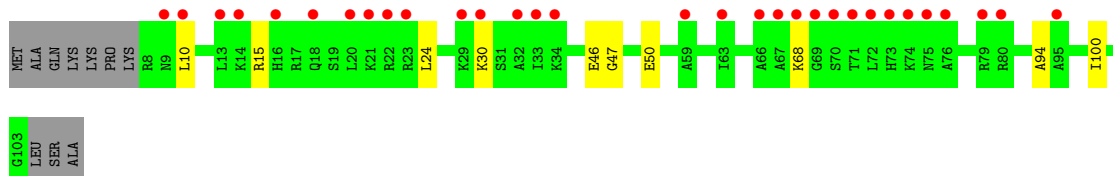
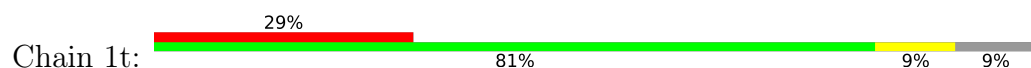
- Molecule 50: 30S ribosomal protein S19



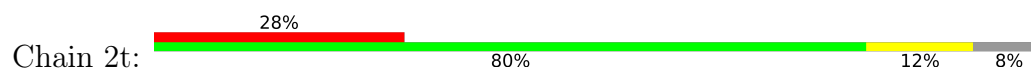
- Molecule 50: 30S ribosomal protein S19



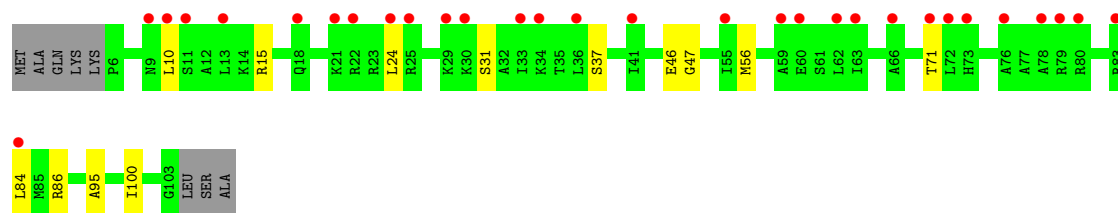
- Molecule 51: 30S ribosomal protein S20



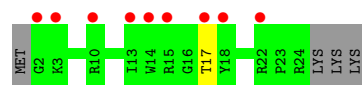
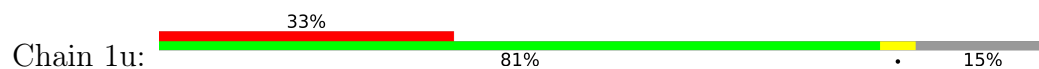
- Molecule 51: 30S ribosomal protein S20



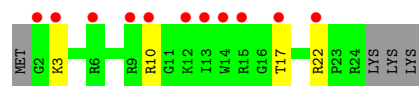
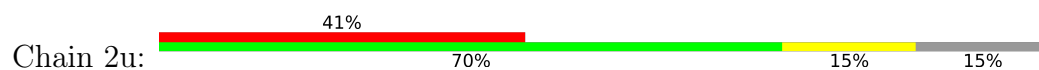




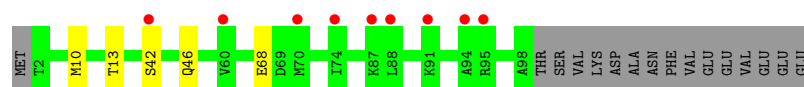
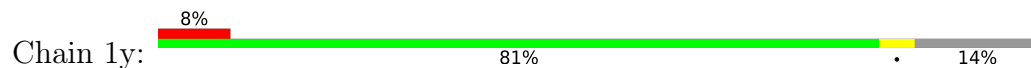
- Molecule 52: 30S ribosomal protein Thx



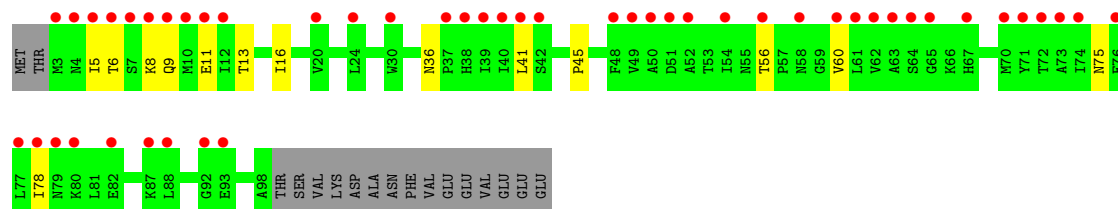
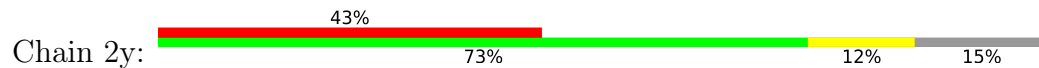
- Molecule 52: 30S ribosomal protein Thx



- Molecule 53: Ribosome-associated inhibitor A



- Molecule 53: Ribosome-associated inhibitor A



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	209.51Å 448.86Å 619.61Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	224.43 – 2.55 254.97 – 2.55	Depositor EDS
% Data completeness (in resolution range)	99.9 (224.43-2.55) 99.9 (254.97-2.55)	Depositor EDS
$R_{merge}$	0.26	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.15 (at 2.55Å)	Xtriage
Refinement program	PHENIX 1.8.2	Depositor
R, $R_{free}$	0.222 , 0.272 0.222 , 0.273	Depositor DCC
$R_{free}$ test set	93828 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	53.8	Xtriage
Anisotropy	0.213	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.28 , 57.8	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.34$ , $\langle L^2 \rangle = 0.17$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.89	EDS
Total number of atoms	296819	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	59.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.59% 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, MG, OMG, 2MU, ZN, SF4, 0TD, MPD, ERY, 2MA, 2MG, 5MC, UR3, MA6, 4OC, M2G, 7MG, 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	0.54	2/69029 (0.0%)	1.02	89/107746 (0.1%)
1	2A	0.43	1/68901 (0.0%)	0.92	63/107544 (0.1%)
2	1B	0.45	0/2876	0.95	0/4486
2	2B	0.36	0/2878	0.87	0/4490
3	1D	0.36	0/2181	0.60	0/2940
3	2D	0.33	0/2186	0.52	0/2944
4	1E	0.36	0/1592	0.56	0/2149
4	2E	0.31	0/1592	0.51	0/2149
5	1F	0.33	0/1619	0.53	0/2193
5	2F	0.30	0/1615	0.52	0/2188
6	1G	0.30	0/1451	0.50	0/1961
6	2G	0.30	0/1449	0.49	0/1957
7	1H	0.33	0/1356	0.51	0/1834
7	2H	0.29	0/1350	0.48	0/1826
8	1I	0.29	0/1109	0.49	0/1512
8	2I	0.28	0/1091	0.50	0/1490
9	1N	0.34	0/1148	0.52	0/1547
9	2N	0.29	0/1144	0.47	0/1543
10	1O	0.40	0/943	0.57	0/1269
10	2O	0.33	0/943	0.53	0/1269
11	1P	0.35	0/1152	0.57	0/1533
11	2P	0.31	0/1152	0.51	0/1533
12	1Q	0.35	0/1143	0.52	0/1527
12	2Q	0.30	0/1143	0.48	0/1527
13	1R	0.34	0/982	0.55	0/1312
13	2R	0.30	0/982	0.51	0/1312
14	1S	0.32	0/887	0.53	0/1180
14	2S	0.29	0/880	0.51	0/1172
15	1T	0.33	0/1105	0.53	0/1477
15	2T	0.31	0/1097	0.49	0/1468
16	1U	0.34	0/977	0.52	0/1301

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
16	2U	0.29	0/977	0.44	0/1301
17	1V	0.35	0/786	0.55	0/1053
17	2V	0.31	0/782	0.55	0/1049
18	1W	0.35	0/897	0.53	0/1205
18	2W	0.31	0/897	0.49	0/1205
19	1X	0.36	0/764	0.58	0/1025
19	2X	0.31	0/764	0.50	0/1025
20	1Y	0.39	0/823	0.55	0/1099
20	2Y	0.32	0/823	0.53	0/1100
21	1Z	0.32	0/1620	0.50	0/2200
21	2Z	0.30	0/1590	0.50	0/2162
22	10	0.37	0/616	0.55	0/821
22	20	0.31	0/616	0.51	0/821
23	11	0.34	0/761	0.52	0/1013
23	21	0.33	0/766	0.52	0/1018
24	12	0.32	0/590	0.56	0/781
24	22	0.29	0/594	0.44	0/785
25	13	0.37	0/474	0.55	0/635
25	23	0.28	0/469	0.52	0/630
26	14	0.30	0/559	0.54	0/754
26	24	0.36	0/549	0.55	0/741
27	15	0.37	0/473	0.60	0/639
27	25	0.29	0/469	0.56	0/635
28	16	0.34	0/460	0.50	0/613
28	26	0.30	0/456	0.49	0/608
29	17	0.37	0/426	0.54	0/561
29	27	0.30	0/426	0.51	0/561
30	18	0.35	0/525	0.53	0/691
30	28	0.30	0/525	0.48	0/691
31	19	0.31	0/310	0.52	0/407
31	29	0.32	0/310	0.52	0/407
32	1a	0.38	0/35795	0.90	12/55864 (0.0%)
32	2a	0.37	0/35890	0.91	32/56012 (0.1%)
33	1b	0.29	0/1876	0.48	0/2533
33	2b	0.31	0/1860	0.51	0/2518
34	1c	0.30	0/1582	0.47	0/2137
34	2c	0.30	0/1566	0.47	0/2119
35	1d	0.29	0/1695	0.50	0/2274
35	2d	0.31	0/1698	0.49	0/2277
36	1e	0.30	0/1149	0.51	0/1548
36	2e	0.31	0/1149	0.48	0/1548
37	1f	0.30	0/827	0.48	0/1120
37	2f	0.29	0/829	0.49	0/1123

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
38	1g	0.28	0/1254	0.43	0/1683
38	2g	0.28	0/1248	0.42	0/1676
39	1h	0.29	0/1118	0.49	0/1506
39	2h	0.28	0/1108	0.48	0/1494
40	1i	0.30	0/1005	0.49	0/1351
40	2i	0.29	0/985	0.47	0/1329
41	1j	0.27	0/732	0.46	0/993
41	2j	0.29	0/723	0.50	0/984
42	1k	0.28	0/849	0.47	0/1150
42	2k	0.28	0/848	0.50	0/1149
43	1l	0.29	0/937	0.50	0/1260
43	2l	0.29	0/937	0.50	0/1260
44	1m	0.28	0/924	0.50	0/1242
44	2m	0.29	0/905	0.50	0/1217
45	1n	0.29	0/501	0.47	0/664
45	2n	0.29	0/501	0.47	0/664
46	1o	0.29	0/739	0.45	0/985
46	2o	0.28	0/739	0.45	0/985
47	1p	0.28	0/697	0.50	0/939
47	2p	0.28	0/693	0.49	0/935
48	1q	0.31	0/836	0.51	0/1117
48	2q	0.29	0/836	0.50	0/1117
49	1r	0.29	0/560	0.49	0/746
49	2r	0.30	0/560	0.49	0/746
50	1s	0.29	0/663	0.50	0/895
50	2s	0.30	0/660	0.49	0/893
51	1t	0.29	0/734	0.46	0/969
51	2t	0.28	0/736	0.43	0/976
52	1u	0.31	0/203	0.46	0/266
52	2u	0.25	0/203	0.51	0/266
53	1y	0.29	0/776	0.47	0/1048
53	2y	0.27	0/761	0.46	0/1030
All	All	0.41	3/309937 (0.0%)	0.85	196/463223 (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
21	2Z	0	1
26	24	0	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
40	1i	0	1
All	All	0	3

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	1A	330	A	N9-C4	-7.27	1.33	1.37
1	1A	330	A	N3-C4	-5.58	1.31	1.34
1	2A	2104	G	N1-C2	-5.16	1.33	1.37

All (196) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	2A	2104	G	C5-C6-O6	12.37	136.02	128.60
1	1A	1042	G	OP1-P-O3'	-12.06	78.67	105.20
1	2A	2104	G	N3-C2-N2	10.78	127.44	119.90
1	1A	588	U	O5'-P-OP2	-10.44	96.31	105.70
1	1A	330	A	C2-N3-C4	-10.23	105.48	110.60
1	2A	2104	G	N1-C2-N2	-10.15	107.07	116.20
1	2A	2185	C	N1-C2-O2	9.19	124.42	118.90
1	1A	512	G	O4'-C1'-N9	9.17	115.53	108.20
1	2A	2185	C	C2-N3-C4	9.10	124.45	119.90
1	1A	330	A	N1-C2-N3	8.95	133.77	129.30
1	1A	1249	U	O5'-P-OP1	-8.91	97.68	105.70
32	2a	1003	G	N3-C4-C5	-8.62	124.29	128.60
1	1A	946	G	O5'-P-OP1	-8.58	97.98	105.70
32	2a	1003	G	C8-N9-C4	-8.57	102.97	106.40
1	1A	1372	U	C5-C4-O4	-8.48	120.81	125.90
1	1A	999	U	O5'-P-OP2	-8.07	98.44	105.70
1	2A	2108	C	C2-N3-C4	8.00	123.90	119.90
1	1A	2430	A	O5'-P-OP2	-7.78	98.70	105.70
32	2a	1003	G	C4-N9-C1'	7.62	136.40	126.50
1	2A	2104	G	C5-C6-N1	-7.58	107.71	111.50
1	1A	948	G	O5'-P-OP1	-7.49	98.96	105.70
1	1A	1043	C	OP1-P-OP2	7.45	130.77	119.60
1	1A	1042	G	OP2-P-O3'	-7.43	88.85	105.20
1	2A	2181	G	C5-C6-O6	7.36	133.02	128.60
1	1A	1372	U	N3-C4-O4	7.34	124.53	119.40
1	2A	1648	C	O5'-P-OP1	-7.33	99.11	105.70
1	1A	2612	C	N1-C2-O2	7.32	123.29	118.90
1	1A	740	U	O5'-P-OP2	-7.31	99.12	105.70
1	1A	1352	U	O5'-P-OP1	-7.24	99.18	105.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1A	1187	G	N1-C6-O6	-7.21	115.58	119.90
1	1A	2103	C	C2-N3-C4	7.17	123.49	119.90
1	1A	31	C	O5'-P-OP1	-7.07	99.34	105.70
32	2a	266	G	P-O3'-C3'	7.04	128.15	119.70
32	2a	1003	G	N7-C8-N9	6.99	116.59	113.10
1	1A	330	A	N3-C4-N9	-6.96	121.83	127.40
1	1A	801	G	O5'-P-OP2	-6.91	99.48	105.70
32	2a	1378	C	C2-N1-C1'	6.91	126.40	118.80
1	1A	226	G	O4'-C1'-N9	6.90	113.72	108.20
1	2A	645	C	C2-N1-C1'	6.83	126.32	118.80
1	1A	2598	A	O5'-P-OP1	-6.83	99.55	105.70
1	2A	2104	G	C6-N1-C2	6.80	129.18	125.10
1	1A	1300	U	P-O3'-C3'	6.78	127.83	119.70
1	1A	1342	A	O5'-P-OP2	-6.75	99.62	105.70
1	2A	2108	C	N1-C2-O2	6.74	122.94	118.90
1	1A	1176	G	OP1-P-O3'	6.71	119.97	105.20
1	1A	1385	G	O4'-C1'-N9	6.70	113.56	108.20
1	1A	2685	G	N1-C6-O6	-6.69	115.89	119.90
32	1a	1030(B)	C	C2-N1-C1'	6.62	126.08	118.80
1	1A	1086	A	N1-C6-N6	-6.60	114.64	118.60
1	1A	2268	A	O5'-P-OP1	-6.43	99.91	105.70
32	1a	1030(B)	C	C6-N1-C2	-6.43	117.73	120.30
1	2A	1313	U	N3-C2-O2	-6.42	117.70	122.20
1	1A	1075	C	N1-C2-O2	6.42	122.75	118.90
1	2A	1076	C	OP1-P-O3'	6.38	119.23	105.20
32	2a	754	C	C2-N1-C1'	6.32	125.75	118.80
32	2a	1158	C	C6-N1-C2	-6.31	117.78	120.30
1	1A	1784	A	O5'-P-OP2	-6.30	100.03	105.70
32	1a	1030(B)	C	N1-C2-O2	6.30	122.68	118.90
1	1A	2249	U	N1-C2-O2	6.28	127.20	122.80
1	2A	2689	U	N3-C2-O2	-6.21	117.86	122.20
1	1A	2319	G	O4'-C1'-N9	6.20	113.16	108.20
1	2A	2181	G	C6-N1-C2	6.15	128.79	125.10
1	1A	748	G	O4'-C1'-N9	6.13	113.10	108.20
1	2A	2185	C	C5-C6-N1	6.07	124.04	121.00
1	2A	2104	G	N1-C6-O6	-6.07	116.26	119.90
1	2A	1092	C	N1-C2-O2	6.07	122.54	118.90
1	1A	2349	G	O5'-P-OP1	-6.06	100.25	105.70
1	2A	512	G	O4'-C1'-N9	6.05	113.04	108.20
1	1A	575	A	O5'-P-OP1	-6.02	100.28	105.70
1	2A	2104	G	C4-N9-C1'	5.99	134.29	126.50
32	1a	1442	G	N3-C4-C5	-5.99	125.60	128.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	2A	2152	G	C6-C5-N7	5.99	133.99	130.40
1	1A	2102	U	N3-C2-O2	-5.96	118.03	122.20
1	1A	787	U	O5'-P-OP1	-5.93	100.37	105.70
32	2a	1004	A	O4'-C1'-N9	5.91	112.93	108.20
32	2a	1158	C	N1-C2-O2	5.91	122.44	118.90
1	1A	2032	G	C5-N7-C8	5.88	107.24	104.30
1	1A	784	A	OP1-P-O3'	5.87	118.12	105.20
1	2A	2183	C	C2-N3-C4	5.87	122.84	119.90
1	1A	195	A	C5-N7-C8	5.83	106.81	103.90
32	2a	1378	C	N1-C2-O2	5.78	122.37	118.90
1	2A	2108	C	N3-C4-C5	-5.78	119.59	121.90
1	2A	2104	G	C8-N9-C1'	-5.78	119.49	127.00
1	2A	2172	U	OP1-P-O3'	5.77	117.89	105.20
1	2A	2152	G	C8-N9-C1'	5.76	134.49	127.00
32	2a	754	C	N1-C2-O2	5.73	122.34	118.90
1	2A	1313	U	C2-N1-C1'	5.72	124.57	117.70
1	2A	2185	C	C5-C4-N4	5.72	124.21	120.20
32	1a	1030(B)	C	N3-C2-O2	-5.71	117.90	121.90
1	2A	2249	U	N3-C4-O4	-5.71	115.41	119.40
1	1A	2103	C	N1-C2-O2	5.70	122.32	118.90
1	1A	392	C	O5'-P-OP1	-5.68	100.59	105.70
1	2A	1313	U	N1-C2-O2	5.66	126.76	122.80
1	2A	2172	U	P-O3'-C3'	5.66	126.49	119.70
1	1A	1985	G	C5-C6-O6	-5.64	125.22	128.60
1	2A	1075	C	N1-C2-O2	5.62	122.27	118.90
32	2a	204	U	C2-N1-C1'	5.62	124.44	117.70
1	1A	1493	C	N1-C2-O2	5.62	122.27	118.90
32	2a	79	G	C5-C6-O6	5.62	131.97	128.60
1	1A	784	A	P-O3'-C3'	5.60	126.42	119.70
32	2a	1126	U	N1-C2-O2	5.60	126.72	122.80
32	2a	1058	G	C5-C6-O6	-5.59	125.25	128.60
1	1A	2249	U	N3-C4-O4	-5.58	115.49	119.40
32	1a	73	G	C5-C6-O6	5.58	131.95	128.60
1	2A	1992	G	P-O3'-C3'	5.55	126.36	119.70
1	2A	2206	G	C4-N9-C1'	-5.55	119.29	126.50
1	2A	383	U	O4'-C1'-N1	5.54	112.64	108.20
32	2a	1183	A	P-O3'-C3'	5.53	126.33	119.70
1	2A	576	U	O5'-P-OP1	-5.52	100.73	105.70
1	1A	2057	A	N1-C6-N6	-5.48	115.31	118.60
1	1A	1647	G	O4'-C1'-N9	-5.45	103.84	108.20
32	2a	1054	C	N1-C2-O2	5.43	122.16	118.90
1	2A	1936	A	O4'-C1'-N9	5.43	112.55	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	2A	2152	G	C4-N9-C1'	-5.43	119.44	126.50
32	2a	1125	U	C2-N1-C1'	5.41	124.19	117.70
1	1A	845	G	O4'-C1'-N9	5.41	112.53	108.20
32	2a	1065	U	P-O3'-C3'	5.41	126.19	119.70
1	1A	674	G	C5-C6-O6	-5.40	125.36	128.60
1	2A	2321	G	C4-N9-C1'	5.40	133.52	126.50
1	1A	847	U	C2-N1-C1'	5.40	124.18	117.70
1	1A	2388	A	O4'-C1'-N9	5.40	112.52	108.20
1	1A	2269	A	O5'-P-OP1	-5.39	100.85	105.70
32	2a	687	A	P-O3'-C3'	5.38	126.16	119.70
1	1A	1297	C	OP1-P-O3'	5.38	117.04	105.20
32	2a	1067	A	P-O3'-C3'	5.38	126.15	119.70
1	1A	2789	C	C2-N1-C1'	-5.37	112.89	118.80
32	2a	1003	G	N3-C4-N9	5.37	129.22	126.00
1	1A	1327	C	N1-C2-O2	-5.36	115.68	118.90
32	1a	266	G	P-O3'-C3'	5.36	126.13	119.70
1	1A	2790	A	C2-N3-C4	5.35	113.28	110.60
1	2A	746	A	O4'-C1'-N9	5.35	112.48	108.20
1	2A	568	U	C5-C4-O4	-5.35	122.69	125.90
1	2A	801	G	O5'-P-OP2	-5.34	100.90	105.70
1	1A	330	A	N3-C4-C5	5.33	130.53	126.80
1	1A	645	C	N1-C2-O2	5.33	122.10	118.90
1	1A	1380	G	O5'-P-OP2	-5.32	100.91	105.70
1	2A	1062	G	C4-N9-C1'	5.31	133.40	126.50
1	2A	574	C	C2-N1-C1'	-5.31	112.96	118.80
1	1A	1385	G	N3-C4-C5	5.30	131.25	128.60
1	2A	1082	U	N3-C2-O2	-5.29	118.50	122.20
1	1A	114	U	C2-N1-C1'	5.29	124.05	117.70
1	1A	570	G	C5-C6-O6	-5.29	125.43	128.60
1	1A	2498	C	O5'-P-OP1	5.28	117.03	110.70
1	2A	195	A	P-O3'-C3'	5.28	126.03	119.70
1	1A	2497	A	OP2-P-O3'	5.28	116.81	105.20
32	2a	1442	G	N3-C4-C5	-5.28	125.96	128.60
1	2A	1639	U	O5'-P-OP2	-5.27	100.95	105.70
32	1a	1065	U	P-O3'-C3'	5.26	126.02	119.70
1	1A	1493	C	C2-N1-C1'	5.26	124.58	118.80
1	2A	1076	C	P-O3'-C3'	5.26	126.01	119.70
1	1A	240	G	C5-C6-O6	-5.25	125.45	128.60
1	1A	750	A	OP1-P-O3'	5.25	116.75	105.20
1	1A	1653	G	P-O3'-C3'	5.23	125.97	119.70
1	1A	180	G	C5-C6-O6	-5.23	125.46	128.60
32	2a	266	G	OP2-P-O3'	5.23	116.70	105.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	2A	12	U	N1-C2-O2	5.22	126.46	122.80
32	2a	1158	C	C2-N1-C1'	5.22	124.54	118.80
32	1a	90	U	C2-N1-C1'	5.21	123.95	117.70
1	2A	1129	A	O4'-C1'-N9	5.20	112.36	108.20
1	1A	2689	U	P-O3'-C3'	5.20	125.94	119.70
32	1a	1028	C	C5-C6-N1	5.19	123.60	121.00
32	2a	1397	C	C2-N1-C1'	5.19	124.51	118.80
1	1A	196	A	OP1-P-O3'	-5.19	93.79	105.20
1	1A	2593	U	N3-C4-O4	-5.18	115.78	119.40
1	2A	2248	C	O5'-P-OP2	-5.17	101.05	105.70
1	2A	2689	U	P-O3'-C3'	5.16	125.89	119.70
1	1A	2441	C	N1-C2-O2	5.12	121.97	118.90
1	2A	12	U	N3-C2-O2	-5.12	118.62	122.20
1	1A	1430	C	N1-C2-O2	5.11	121.97	118.90
32	1a	1442	G	P-O3'-C3'	5.11	125.83	119.70
1	2A	645	C	N1-C2-O2	5.11	121.97	118.90
1	2A	1092	C	C2-N1-C1'	5.11	124.42	118.80
1	1A	1602	U	N3-C4-O4	-5.11	115.83	119.40
1	1A	2441	C	N3-C2-O2	-5.10	118.33	121.90
32	2a	1397	C	N1-C2-O2	5.10	121.96	118.90
1	1A	529	A	N1-C6-N6	5.10	121.66	118.60
1	1A	2102	U	C6-N1-C2	-5.10	117.94	121.00
1	2A	1306	C	N1-C2-O2	5.09	121.96	118.90
32	2a	79	G	C6-N1-C2	5.09	128.16	125.10
1	2A	2185	C	N3-C4-N4	-5.09	114.44	118.00
1	1A	1428	C	C6-N1-C2	5.08	122.33	120.30
1	2A	301	G	C4-N9-C1'	-5.08	119.90	126.50
1	1A	2006	C	O5'-P-OP1	-5.06	101.14	105.70
32	2a	1442	G	N3-C4-N9	5.05	129.03	126.00
1	1A	937	U	N3-C2-O2	5.05	125.73	122.20
1	1A	2690	C	O5'-P-OP1	-5.05	101.16	105.70
32	1a	687	A	P-O3'-C3'	5.04	125.75	119.70
1	1A	2055	C	OP1-P-O3'	5.04	116.29	105.20
32	2a	754	C	N3-C2-O2	-5.04	118.37	121.90
1	1A	1116	C	C2-N1-C1'	5.04	124.34	118.80
1	2A	784	A	O4'-C1'-N9	5.03	112.22	108.20
1	2A	2501	C	C2-N1-C1'	-5.02	113.28	118.80
1	2A	1092	C	C5-C6-N1	5.02	123.51	121.00
1	1A	565	C	C6-N1-C2	-5.01	118.30	120.30
1	2A	2108	C	C5-C4-N4	5.01	123.71	120.20
32	2a	1158	C	N3-C2-O2	-5.01	118.39	121.90

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
40	1i	59	PHE	Peptide
26	24	18	CYS	Peptide
21	2Z	136	PHE	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%)	259 (95%)	14 (5%)	0	100	100
3	2D	273/276 (99%)	252 (92%)	21 (8%)	0	100	100
4	1E	202/206 (98%)	192 (95%)	7 (4%)	3 (2%)	10	14
4	2E	202/206 (98%)	186 (92%)	14 (7%)	2 (1%)	15	22
5	1F	201/210 (96%)	192 (96%)	8 (4%)	1 (0%)	29	40
5	2F	201/210 (96%)	195 (97%)	5 (2%)	1 (0%)	29	40
6	1G	179/182 (98%)	157 (88%)	17 (10%)	5 (3%)	5	4
6	2G	179/182 (98%)	152 (85%)	24 (13%)	3 (2%)	9	11
7	1H	172/180 (96%)	161 (94%)	9 (5%)	2 (1%)	13	17
7	2H	171/180 (95%)	153 (90%)	13 (8%)	5 (3%)	4	4
8	1I	145/148 (98%)	126 (87%)	18 (12%)	1 (1%)	22	30
8	2I	144/148 (97%)	133 (92%)	9 (6%)	2 (1%)	11	15
9	1N	138/140 (99%)	134 (97%)	3 (2%)	1 (1%)	22	30
9	2N	138/140 (99%)	133 (96%)	5 (4%)	0	100	100
10	1O	120/122 (98%)	112 (93%)	7 (6%)	1 (1%)	19	27

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
10	2O	120/122 (98%)	111 (92%)	8 (7%)	1 (1%)	19	27
11	1P	147/150 (98%)	137 (93%)	10 (7%)	0	100	100
11	2P	147/150 (98%)	135 (92%)	10 (7%)	2 (1%)	11	15
12	1Q	139/141 (99%)	134 (96%)	4 (3%)	1 (1%)	22	30
12	2Q	139/141 (99%)	126 (91%)	13 (9%)	0	100	100
13	1R	116/118 (98%)	113 (97%)	3 (3%)	0	100	100
13	2R	116/118 (98%)	112 (97%)	4 (3%)	0	100	100
14	1S	108/112 (96%)	99 (92%)	8 (7%)	1 (1%)	17	24
14	2S	108/112 (96%)	95 (88%)	13 (12%)	0	100	100
15	1T	129/146 (88%)	122 (95%)	7 (5%)	0	100	100
15	2T	129/146 (88%)	119 (92%)	10 (8%)	0	100	100
16	1U	114/118 (97%)	112 (98%)	2 (2%)	0	100	100
16	2U	114/118 (97%)	111 (97%)	3 (3%)	0	100	100
17	1V	99/101 (98%)	94 (95%)	3 (3%)	2 (2%)	7	8
17	2V	99/101 (98%)	94 (95%)	4 (4%)	1 (1%)	15	22
18	1W	110/113 (97%)	108 (98%)	2 (2%)	0	100	100
18	2W	110/113 (97%)	106 (96%)	4 (4%)	0	100	100
19	1X	93/96 (97%)	88 (95%)	4 (4%)	1 (1%)	14	19
19	2X	93/96 (97%)	87 (94%)	5 (5%)	1 (1%)	14	19
20	1Y	105/110 (96%)	97 (92%)	7 (7%)	1 (1%)	15	22
20	2Y	105/110 (96%)	97 (92%)	7 (7%)	1 (1%)	15	22
21	1Z	201/206 (98%)	185 (92%)	15 (8%)	1 (0%)	29	40
21	2Z	199/206 (97%)	177 (89%)	19 (10%)	3 (2%)	10	14
22	10	75/85 (88%)	72 (96%)	3 (4%)	0	100	100
22	20	75/85 (88%)	69 (92%)	6 (8%)	0	100	100
23	11	95/98 (97%)	94 (99%)	1 (1%)	0	100	100
23	21	95/98 (97%)	88 (93%)	6 (6%)	1 (1%)	14	19
24	12	68/72 (94%)	67 (98%)	1 (2%)	0	100	100
24	22	68/72 (94%)	63 (93%)	5 (7%)	0	100	100
25	13	57/60 (95%)	54 (95%)	3 (5%)	0	100	100
25	23	57/60 (95%)	55 (96%)	2 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
26	14	67/71 (94%)	52 (78%)	8 (12%)	7 (10%)	0	0
26	24	67/71 (94%)	44 (66%)	16 (24%)	7 (10%)	0	0
27	15	57/60 (95%)	57 (100%)	0	0	100	100
27	25	57/60 (95%)	55 (96%)	2 (4%)	0	100	100
28	16	51/54 (94%)	49 (96%)	2 (4%)	0	100	100
28	26	51/54 (94%)	47 (92%)	4 (8%)	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%)	62 (100%)	0	0	100	100
30	28	62/65 (95%)	61 (98%)	1 (2%)	0	100	100
31	19	35/37 (95%)	34 (97%)	1 (3%)	0	100	100
31	29	35/37 (95%)	33 (94%)	2 (6%)	0	100	100
33	1b	229/256 (90%)	191 (83%)	28 (12%)	10 (4%)	2	1
33	2b	229/256 (90%)	197 (86%)	27 (12%)	5 (2%)	6	7
34	1c	204/239 (85%)	186 (91%)	18 (9%)	0	100	100
34	2c	204/239 (85%)	175 (86%)	27 (13%)	2 (1%)	15	22
35	1d	206/209 (99%)	193 (94%)	12 (6%)	1 (0%)	29	40
35	2d	206/209 (99%)	186 (90%)	19 (9%)	1 (0%)	29	40
36	1e	146/162 (90%)	140 (96%)	6 (4%)	0	100	100
36	2e	146/162 (90%)	134 (92%)	10 (7%)	2 (1%)	11	15
37	1f	98/101 (97%)	92 (94%)	6 (6%)	0	100	100
37	2f	98/101 (97%)	89 (91%)	9 (9%)	0	100	100
38	1g	153/156 (98%)	143 (94%)	9 (6%)	1 (1%)	22	30
38	2g	153/156 (98%)	131 (86%)	19 (12%)	3 (2%)	7	8
39	1h	135/138 (98%)	128 (95%)	7 (5%)	0	100	100
39	2h	135/138 (98%)	122 (90%)	11 (8%)	2 (2%)	10	14
40	1i	125/128 (98%)	112 (90%)	12 (10%)	1 (1%)	19	27
40	2i	124/128 (97%)	106 (86%)	15 (12%)	3 (2%)	6	5
41	1j	95/105 (90%)	77 (81%)	13 (14%)	5 (5%)	2	0
41	2j	94/105 (90%)	75 (80%)	12 (13%)	7 (7%)	1	0
42	1k	112/129 (87%)	102 (91%)	9 (8%)	1 (1%)	17	24

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
42	2k	112/129 (87%)	102 (91%)	8 (7%)	2 (2%)	8	10
43	1l	119/132 (90%)	109 (92%)	9 (8%)	1 (1%)	19	27
43	2l	119/132 (90%)	107 (90%)	11 (9%)	1 (1%)	19	27
44	1m	114/126 (90%)	100 (88%)	11 (10%)	3 (3%)	5	5
44	2m	112/126 (89%)	95 (85%)	16 (14%)	1 (1%)	17	24
45	1n	58/61 (95%)	56 (97%)	2 (3%)	0	100	100
45	2n	58/61 (95%)	50 (86%)	7 (12%)	1 (2%)	9	11
46	1o	86/89 (97%)	81 (94%)	4 (5%)	1 (1%)	13	17
46	2o	86/89 (97%)	81 (94%)	4 (5%)	1 (1%)	13	17
47	1p	80/88 (91%)	71 (89%)	6 (8%)	3 (4%)	3	2
47	2p	80/88 (91%)	67 (84%)	12 (15%)	1 (1%)	12	16
48	1q	97/105 (92%)	88 (91%)	9 (9%)	0	100	100
48	2q	97/105 (92%)	88 (91%)	8 (8%)	1 (1%)	15	22
49	1r	66/88 (75%)	64 (97%)	1 (2%)	1 (2%)	10	14
49	2r	66/88 (75%)	61 (92%)	5 (8%)	0	100	100
50	1s	81/93 (87%)	71 (88%)	10 (12%)	0	100	100
50	2s	81/93 (87%)	70 (86%)	11 (14%)	0	100	100
51	1t	94/106 (89%)	86 (92%)	6 (6%)	2 (2%)	7	7
51	2t	96/106 (91%)	84 (88%)	9 (9%)	3 (3%)	4	3
52	1u	21/27 (78%)	19 (90%)	2 (10%)	0	100	100
52	2u	21/27 (78%)	16 (76%)	4 (19%)	1 (5%)	2	1
53	1y	95/113 (84%)	93 (98%)	1 (1%)	1 (1%)	14	19
53	2y	94/113 (83%)	88 (94%)	4 (4%)	2 (2%)	7	7
All	All	11629/12354 (94%)	10669 (92%)	832 (7%)	128 (1%)	14	19

All (128) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	1E	71	GLY
6	1G	47	LYS
7	1H	92	ILE
14	1S	59	LYS
26	14	44	THR
26	14	45	GLY

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Mol	Chain	Res	Type
33	1b	37	ASN
33	1b	124	SER
33	1b	127	ILE
41	1j	55	LYS
44	1m	106	ASN
5	2F	130	ALA
33	2b	17	PHE
33	2b	125	PRO
36	2e	96	PRO
36	2e	97	GLY
41	2j	79	ARG
42	2k	106	LYS
51	2t	100	ILE
6	1G	50	ALA
17	1V	43	GLU
19	1X	94	GLY
26	14	39	CYS
33	1b	21	ARG
38	1g	55	GLY
40	1i	11	LYS
51	1t	47	GLY
51	1t	94	ALA
6	2G	126	ASP
8	2I	10	GLU
8	2I	85	GLU
11	2P	36	LYS
17	2V	79	VAL
19	2X	94	GLY
20	2Y	40	GLU
21	2Z	104	PHE
26	24	45	GLY
26	24	65	ASP
35	2d	156	GLU
40	2i	43	ALA
40	2i	54	ASP
41	2j	56	HIS
42	2k	15	ALA
48	2q	68	ARG
5	1F	130	ALA
6	1G	52	ILE
7	1H	159	GLU
10	1O	5	GLN

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Mol	Chain	Res	Type
26	14	49	PHE
41	1j	77	PRO
47	1p	47	ASP
7	2H	65	HIS
7	2H	126	PRO
11	2P	29	LYS
21	2Z	52	SER
21	2Z	120	ILE
23	21	3	LYS
26	24	24	THR
26	24	55	ARG
26	24	62	ARG
33	2b	22	LYS
34	2c	99	VAL
41	2j	78	ASN
43	2l	105	TYR
46	2o	23	GLY
47	2p	52	ASP
52	2u	3	LYS
4	1E	28	ALA
4	1E	52	LEU
20	1Y	90	LEU
26	14	47	GLN
33	1b	20	GLU
33	1b	129	GLU
33	1b	158	LEU
35	1d	180	GLY
42	1k	117	ASN
44	1m	11	ARG
47	1p	46	PRO
53	1y	68	GLU
4	2E	28	ALA
4	2E	52	LEU
6	2G	45	GLU
7	2H	55	PRO
10	2O	5	GLN
34	2c	204	LEU
38	2g	7	ALA
38	2g	109	ASN
39	2h	133	LEU
41	2j	30	SER
51	2t	47	GLY

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Mol	Chain	Res	Type
51	2t	95	ALA
12	1Q	24	GLY
17	1V	79	VAL
26	14	55	ARG
26	14	61	ARG
41	1j	78	ASN
41	1j	79	ARG
43	1l	105	TYR
6	2G	43	LEU
7	2H	174	GLY
33	2b	20	GLU
38	2g	131	LYS
41	2j	34	VAL
44	2m	23	TYR
21	1Z	52	SER
33	1b	9	GLU
33	1b	228	GLY
44	1m	12	ASN
47	1p	68	ASP
7	2H	110	SER
41	2j	84	GLN
45	2n	14	PRO
6	1G	44	GLY
49	1r	27	GLY
33	1b	231	GLU
46	1o	23	GLY
33	2b	232	PRO
40	2i	44	VAL
41	2j	37	PRO
6	1G	179	PRO
8	1I	137	PRO
9	1N	129	PRO
26	24	11	PRO
26	24	56	VAL
39	2h	134	ILE
53	2y	36	ASN
41	1j	91	PRO
53	2y	45	PRO

### 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	214/218 (98%)	197 (92%)	17 (8%)	12	15
3	2D	215/218 (99%)	196 (91%)	19 (9%)	10	12
4	1E	164/166 (99%)	152 (93%)	12 (7%)	14	18
4	2E	164/166 (99%)	155 (94%)	9 (6%)	21	29
5	1F	160/166 (96%)	144 (90%)	16 (10%)	7	8
5	2F	159/166 (96%)	145 (91%)	14 (9%)	10	12
6	1G	144/156 (92%)	135 (94%)	9 (6%)	18	23
6	2G	142/156 (91%)	118 (83%)	24 (17%)	2	2
7	1H	144/148 (97%)	137 (95%)	7 (5%)	25	34
7	2H	143/148 (97%)	123 (86%)	20 (14%)	3	3
8	1I	111/124 (90%)	92 (83%)	19 (17%)	2	2
8	2I	108/124 (87%)	98 (91%)	10 (9%)	9	10
9	1N	119/119 (100%)	111 (93%)	8 (7%)	16	21
9	2N	118/119 (99%)	108 (92%)	10 (8%)	10	13
10	1O	100/100 (100%)	95 (95%)	5 (5%)	24	33
10	2O	100/100 (100%)	92 (92%)	8 (8%)	12	15
11	1P	115/116 (99%)	109 (95%)	6 (5%)	23	30
11	2P	115/116 (99%)	110 (96%)	5 (4%)	29	39
12	1Q	111/111 (100%)	104 (94%)	7 (6%)	18	23
12	2Q	111/111 (100%)	105 (95%)	6 (5%)	22	29
13	1R	101/101 (100%)	92 (91%)	9 (9%)	9	12
13	2R	101/101 (100%)	92 (91%)	9 (9%)	9	12
14	1S	87/88 (99%)	77 (88%)	10 (12%)	5	5
14	2S	85/88 (97%)	75 (88%)	10 (12%)	5	5
15	1T	115/127 (91%)	108 (94%)	7 (6%)	18	24
15	2T	113/127 (89%)	105 (93%)	8 (7%)	14	19

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
16	1U	93/94 (99%)	85 (91%)	8 (9%)	10	13
16	2U	93/94 (99%)	87 (94%)	6 (6%)	17	23
17	1V	81/82 (99%)	74 (91%)	7 (9%)	10	13
17	2V	80/82 (98%)	68 (85%)	12 (15%)	3	2
18	1W	90/92 (98%)	83 (92%)	7 (8%)	12	16
18	2W	90/92 (98%)	87 (97%)	3 (3%)	38	51
19	1X	77/78 (99%)	72 (94%)	5 (6%)	17	23
19	2X	77/78 (99%)	72 (94%)	5 (6%)	17	23
20	1Y	86/91 (94%)	79 (92%)	7 (8%)	11	14
20	2Y	86/91 (94%)	76 (88%)	10 (12%)	5	5
21	1Z	169/179 (94%)	156 (92%)	13 (8%)	13	16
21	2Z	165/179 (92%)	149 (90%)	16 (10%)	8	9
22	10	61/67 (91%)	60 (98%)	1 (2%)	62	77
22	20	61/67 (91%)	58 (95%)	3 (5%)	25	34
23	11	79/83 (95%)	77 (98%)	2 (2%)	47	62
23	21	81/83 (98%)	78 (96%)	3 (4%)	34	46
24	12	65/67 (97%)	59 (91%)	6 (9%)	9	11
24	22	66/67 (98%)	60 (91%)	6 (9%)	9	11
25	13	51/52 (98%)	46 (90%)	5 (10%)	8	9
25	23	50/52 (96%)	44 (88%)	6 (12%)	5	5
26	14	58/63 (92%)	51 (88%)	7 (12%)	5	4
26	24	54/63 (86%)	46 (85%)	8 (15%)	3	2
27	15	51/52 (98%)	47 (92%)	4 (8%)	12	16
27	25	50/52 (96%)	49 (98%)	1 (2%)	55	70
28	16	51/52 (98%)	45 (88%)	6 (12%)	5	5
28	26	50/52 (96%)	46 (92%)	4 (8%)	12	15
29	17	41/42 (98%)	38 (93%)	3 (7%)	14	18
29	27	41/42 (98%)	37 (90%)	4 (10%)	8	9
30	18	54/55 (98%)	49 (91%)	5 (9%)	9	10
30	28	54/55 (98%)	48 (89%)	6 (11%)	6	6
31	19	34/34 (100%)	33 (97%)	1 (3%)	42	57

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
31	29	34/34 (100%)	31 (91%)	3 (9%)	10	12
33	1b	191/220 (87%)	170 (89%)	21 (11%)	6	6
33	2b	187/220 (85%)	170 (91%)	17 (9%)	9	11
34	1c	144/188 (77%)	132 (92%)	12 (8%)	11	14
34	2c	140/188 (74%)	126 (90%)	14 (10%)	7	8
35	1d	171/181 (94%)	154 (90%)	17 (10%)	8	9
35	2d	172/181 (95%)	152 (88%)	20 (12%)	5	5
36	1e	114/123 (93%)	109 (96%)	5 (4%)	28	38
36	2e	114/123 (93%)	103 (90%)	11 (10%)	8	9
37	1f	85/90 (94%)	77 (91%)	8 (9%)	8	10
37	2f	85/90 (94%)	78 (92%)	7 (8%)	11	14
38	1g	120/127 (94%)	111 (92%)	9 (8%)	13	17
38	2g	119/127 (94%)	100 (84%)	19 (16%)	2	2
39	1h	116/119 (98%)	108 (93%)	8 (7%)	15	20
39	2h	114/119 (96%)	100 (88%)	14 (12%)	4	4
40	1i	91/99 (92%)	80 (88%)	11 (12%)	5	4
40	2i	88/99 (89%)	73 (83%)	15 (17%)	2	2
41	1j	68/92 (74%)	64 (94%)	4 (6%)	19	25
41	2j	68/92 (74%)	62 (91%)	6 (9%)	10	12
42	1k	83/99 (84%)	79 (95%)	4 (5%)	25	34
42	2k	83/99 (84%)	73 (88%)	10 (12%)	5	5
43	1l	96/108 (89%)	90 (94%)	6 (6%)	18	23
43	2l	96/108 (89%)	90 (94%)	6 (6%)	18	23
44	1m	90/101 (89%)	79 (88%)	11 (12%)	5	4
44	2m	87/101 (86%)	82 (94%)	5 (6%)	20	27
45	1n	49/50 (98%)	44 (90%)	5 (10%)	7	8
45	2n	49/50 (98%)	44 (90%)	5 (10%)	7	8
46	1o	78/80 (98%)	75 (96%)	3 (4%)	33	45
46	2o	78/80 (98%)	72 (92%)	6 (8%)	13	16
47	1p	69/74 (93%)	60 (87%)	9 (13%)	4	3
47	2p	68/74 (92%)	57 (84%)	11 (16%)	2	2

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
48	1q	94/97 (97%)	89 (95%)	5 (5%)	22	30
48	2q	94/97 (97%)	85 (90%)	9 (10%)	8	9
49	1r	59/77 (77%)	56 (95%)	3 (5%)	24	32
49	2r	59/77 (77%)	57 (97%)	2 (3%)	37	50
50	1s	68/80 (85%)	66 (97%)	2 (3%)	42	57
50	2s	67/80 (84%)	57 (85%)	10 (15%)	3	2
51	1t	71/82 (87%)	63 (89%)	8 (11%)	6	5
51	2t	70/82 (85%)	60 (86%)	10 (14%)	3	3
52	1u	18/22 (82%)	17 (94%)	1 (6%)	21	28
52	2u	18/22 (82%)	15 (83%)	3 (17%)	2	2
53	1y	82/98 (84%)	78 (95%)	4 (5%)	25	34
53	2y	79/98 (81%)	67 (85%)	12 (15%)	3	2
All	All	9524/10260 (93%)	8689 (91%)	835 (9%)	10	12

All (835) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	1D	37	LEU
3	1D	39	LYS
3	1D	61	LEU
3	1D	71	ASP
3	1D	94	LEU
3	1D	99	ASP
3	1D	103	ARG
3	1D	106	ILE
3	1D	115	GLN
3	1D	126	GLN
3	1D	134	ARG
3	1D	155	LEU
3	1D	193	VAL
3	1D	211	ARG
3	1D	229	VAL
3	1D	242	ARG
3	1D	253	GLN
4	1E	7	VAL
4	1E	9	VAL
4	1E	23	VAL
4	1E	38	THR

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Mol	Chain	Res	Type
4	1E	72	VAL
4	1E	73	GLU
4	1E	75	VAL
4	1E	78	LEU
4	1E	93	VAL
4	1E	116	VAL
4	1E	119	ARG
4	1E	195	LEU
5	1F	12	LEU
5	1F	17	ARG
5	1F	18	ARG
5	1F	53	THR
5	1F	57	VAL
5	1F	74	ARG
5	1F	77	ASP
5	1F	88	VAL
5	1F	110	LEU
5	1F	132	VAL
5	1F	154	VAL
5	1F	158	THR
5	1F	162	LEU
5	1F	191	ARG
5	1F	192	LEU
5	1F	197	ASP
6	1G	7	LEU
6	1G	31	VAL
6	1G	52	ILE
6	1G	62	LEU
6	1G	79	ASN
6	1G	82	LEU
6	1G	133	LEU
6	1G	149	VAL
6	1G	175	LEU
7	1H	8	PRO
7	1H	24	VAL
7	1H	52	VAL
7	1H	71	LEU
7	1H	97	ARG
7	1H	105	LEU
7	1H	119	GLU
8	1I	5	LEU
8	1I	11	ASN

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Mol	Chain	Res	Type
8	1I	12	LEU
8	1I	20	ASP
8	1I	38	LEU
8	1I	43	ASN
8	1I	44	LEU
8	1I	47	LEU
8	1I	57	ARG
8	1I	58	LEU
8	1I	66	GLU
8	1I	78	THR
8	1I	87	LYS
8	1I	92	VAL
8	1I	109	ILE
8	1I	117	GLU
8	1I	127	VAL
8	1I	128	LEU
8	1I	140	LEU
9	1N	46	VAL
9	1N	48	MET
9	1N	62	VAL
9	1N	67	LEU
9	1N	87	LEU
9	1N	99	LEU
9	1N	119	ARG
9	1N	121	LYS
10	1O	10	VAL
10	1O	23	ARG
10	1O	24	VAL
10	1O	53	LYS
10	1O	109	LYS
11	1P	15	ARG
11	1P	56	SER
11	1P	133	SER
11	1P	135	LEU
11	1P	147	LEU
11	1P	149	GLU
12	1Q	6	ARG
12	1Q	7	MET
12	1Q	60	ARG
12	1Q	75	THR
12	1Q	109	VAL
12	1Q	112	GLU

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Mol	Chain	Res	Type
12	1Q	129	THR
13	1R	29	LEU
13	1R	33	ARG
13	1R	36	THR
13	1R	54	LEU
13	1R	67	LEU
13	1R	75	LEU
13	1R	96	ARG
13	1R	100	LEU
13	1R	114	VAL
14	1S	3	ARG
14	1S	25	ARG
14	1S	48	LEU
14	1S	50	SER
14	1S	52	SER
14	1S	57	LYS
14	1S	59	LYS
14	1S	64	GLU
14	1S	80	LEU
14	1S	85	VAL
15	1T	18	ASP
15	1T	39	ARG
15	1T	49	VAL
15	1T	53	ARG
15	1T	82	LEU
15	1T	104	ASN
15	1T	107	ASP
16	1U	5	LYS
16	1U	8	VAL
16	1U	31	SER
16	1U	34	LYS
16	1U	36	ARG
16	1U	59	ARG
16	1U	74	LEU
16	1U	104	GLN
17	1V	18	LEU
17	1V	46	VAL
17	1V	51	VAL
17	1V	61	VAL
17	1V	71	LEU
17	1V	72	VAL
17	1V	79	VAL

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Mol	Chain	Res	Type
18	1W	11	ARG
18	1W	15	ARG
18	1W	17	VAL
18	1W	23	LEU
18	1W	67	ASP
18	1W	100	THR
18	1W	107	LEU
19	1X	15	GLU
19	1X	23	GLU
19	1X	66	LEU
19	1X	68	ARG
19	1X	81	VAL
20	1Y	9	LYS
20	1Y	34	LYS
20	1Y	43	ASN
20	1Y	72	VAL
20	1Y	99	CYS
20	1Y	102	CYS
20	1Y	107	ASP
21	1Z	2	GLU
21	1Z	20	ARG
21	1Z	31	ARG
21	1Z	86	VAL
21	1Z	91	LEU
21	1Z	111	VAL
21	1Z	112	ARG
21	1Z	150	LEU
21	1Z	155	LEU
21	1Z	161	VAL
21	1Z	163	LEU
21	1Z	191	VAL
21	1Z	202	GLU
22	10	82	ARG
23	11	21	ARG
23	11	30	VAL
24	12	1	MET
24	12	19	VAL
24	12	32	LEU
24	12	53	LEU
24	12	55	ARG
24	12	70	GLN
25	13	8	LEU

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Mol	Chain	Res	Type
25	13	23	LEU
25	13	44	ARG
25	13	54	VAL
25	13	56	VAL
26	14	1	MET
26	14	3	GLU
26	14	33	VAL
26	14	34	GLU
26	14	49	PHE
26	14	50	VAL
26	14	61	ARG
27	15	6	VAL
27	15	16	ARG
27	15	55	ARG
27	15	58	LEU
28	16	6	ARG
28	16	9	LEU
28	16	14	THR
28	16	44	ARG
28	16	48	VAL
28	16	52	VAL
29	17	43	THR
29	17	47	ARG
29	17	48	LYS
30	18	29	LYS
30	18	30	ARG
30	18	31	HIS
30	18	50	LEU
30	18	58	ILE
31	19	17	ILE
33	1b	8	LYS
33	1b	19	HIS
33	1b	44	LEU
33	1b	53	ARG
33	1b	59	GLU
33	1b	101	MET
33	1b	111	ARG
33	1b	112	VAL
33	1b	113	HIS
33	1b	126	GLU
33	1b	127	ILE
33	1b	139	LYS

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Mol	Chain	Res	Type
33	1b	145	LEU
33	1b	160	ASP
33	1b	163	PHE
33	1b	179	LYS
33	1b	184	VAL
33	1b	185	ILE
33	1b	212	GLN
33	1b	221	LEU
33	1b	229	VAL
34	1c	3	ASN
34	1c	15	THR
34	1c	26	LYS
34	1c	38	ARG
34	1c	70	VAL
34	1c	89	GLU
34	1c	98	ASN
34	1c	105	GLU
34	1c	115	LEU
34	1c	124	ILE
34	1c	154	SER
34	1c	207	VAL
35	1d	47	ARG
35	1d	61	LYS
35	1d	64	LEU
35	1d	85	LYS
35	1d	94	LEU
35	1d	108	LEU
35	1d	123	HIS
35	1d	127	THR
35	1d	140	VAL
35	1d	150	GLU
35	1d	157	LEU
35	1d	160	GLN
35	1d	168	ARG
35	1d	170	VAL
35	1d	188	LEU
35	1d	190	ASP
35	1d	196	LEU
36	1e	16	THR
36	1e	34	VAL
36	1e	69	VAL
36	1e	144	THR

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Mol	Chain	Res	Type
36	1e	145	LYS
37	1f	48	LEU
37	1f	57	GLN
37	1f	63	TYR
37	1f	64	GLN
37	1f	69	GLU
37	1f	73	ASN
37	1f	86	ARG
37	1f	98	LEU
38	1g	6	ARG
38	1g	52	GLU
38	1g	74	GLU
38	1g	75	VAL
38	1g	94	ARG
38	1g	104	LEU
38	1g	113	GLU
38	1g	143	ARG
38	1g	144	MET
39	1h	51	VAL
39	1h	54	ASP
39	1h	60	ARG
39	1h	73	ASP
39	1h	104	ARG
39	1h	115	SER
39	1h	120	THR
39	1h	133	LEU
40	1i	42	ARG
40	1i	50	LEU
40	1i	53	VAL
40	1i	56	LEU
40	1i	66	ARG
40	1i	81	ILE
40	1i	87	GLN
40	1i	92	TYR
40	1i	103	THR
40	1i	111	ARG
40	1i	125	TYR
41	1j	72	VAL
41	1j	73	ASP
41	1j	84	GLN
41	1j	94	VAL
42	1k	16	SER

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Mol	Chain	Res	Type
42	1k	87	THR
42	1k	99	GLN
42	1k	116	HIS
43	1l	33	ARG
43	1l	47	LYS
43	1l	73	GLU
43	1l	83	VAL
43	1l	102	ARG
43	1l	106	ASP
44	1m	4	ILE
44	1m	14	ARG
44	1m	19	LEU
44	1m	27	LYS
44	1m	43	THR
44	1m	52	GLU
44	1m	63	THR
44	1m	64	TRP
44	1m	86	CYS
44	1m	94	ARG
44	1m	106	ASN
45	1n	3	ARG
45	1n	6	LEU
45	1n	16	PHE
45	1n	18	VAL
45	1n	22	THR
46	1o	3	ILE
46	1o	31	LEU
46	1o	39	LEU
47	1p	6	LEU
47	1p	11	SER
47	1p	20	VAL
47	1p	21	VAL
47	1p	29	ASP
47	1p	42	ARG
47	1p	47	ASP
47	1p	62	VAL
47	1p	74	LEU
48	1q	26	GLN
48	1q	36	ILE
48	1q	45	HIS
48	1q	87	LYS
48	1q	97	SER

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Mol	Chain	Res	Type
49	1r	25	THR
49	1r	29	PHE
49	1r	87	ARG
50	1s	28	LYS
50	1s	41	VAL
51	1t	10	LEU
51	1t	15	ARG
51	1t	24	LEU
51	1t	30	LYS
51	1t	46	GLU
51	1t	50	GLU
51	1t	68	LYS
51	1t	100	ILE
52	1u	17	THR
53	1y	10	MET
53	1y	13	THR
53	1y	42	SER
53	1y	46	GLN
3	2D	3	VAL
3	2D	27	THR
3	2D	43	ARG
3	2D	54	ARG
3	2D	61	LEU
3	2D	71	ASP
3	2D	73	VAL
3	2D	75	ILE
3	2D	94	LEU
3	2D	103	ARG
3	2D	155	LEU
3	2D	183	ARG
3	2D	200	ASP
3	2D	211	ARG
3	2D	221	VAL
3	2D	229	VAL
3	2D	242	ARG
3	2D	259	THR
3	2D	276	LYS
4	2E	12	THR
4	2E	23	VAL
4	2E	38	THR
4	2E	75	VAL
4	2E	89	ASP

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Mol	Chain	Res	Type
4	2E	113	PHE
4	2E	116	VAL
4	2E	119	ARG
4	2E	188	VAL
5	2F	15	SER
5	2F	20	LEU
5	2F	27	GLU
5	2F	33	LEU
5	2F	57	VAL
5	2F	62	ARG
5	2F	74	ARG
5	2F	88	VAL
5	2F	126	VAL
5	2F	140	LEU
5	2F	158	THR
5	2F	161	GLU
5	2F	175	THR
5	2F	183	VAL
6	2G	3	LEU
6	2G	7	LEU
6	2G	16	ARG
6	2G	28	VAL
6	2G	47	LYS
6	2G	49	ASP
6	2G	53	LEU
6	2G	62	LEU
6	2G	80	PHE
6	2G	88	ILE
6	2G	92	VAL
6	2G	97	ASP
6	2G	103	LEU
6	2G	113	ARG
6	2G	116	ASP
6	2G	124	SER
6	2G	133	LEU
6	2G	139	LEU
6	2G	149	VAL
6	2G	152	LEU
6	2G	155	MET
6	2G	159	VAL
6	2G	165	THR
6	2G	175	LEU

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Mol	Chain	Res	Type
7	2H	3	ARG
7	2H	11	VAL
7	2H	17	VAL
7	2H	33	LEU
7	2H	34	GLU
7	2H	38	SER
7	2H	43	VAL
7	2H	44	VAL
7	2H	45	VAL
7	2H	47	GLU
7	2H	58	GLU
7	2H	68	THR
7	2H	70	THR
7	2H	80	SER
7	2H	95	ARG
7	2H	129	THR
7	2H	131	VAL
7	2H	133	VAL
7	2H	134	SER
7	2H	139	GLN
8	2I	37	VAL
8	2I	38	LEU
8	2I	43	ASN
8	2I	70	GLU
8	2I	76	THR
8	2I	108	THR
8	2I	127	VAL
8	2I	139	GLN
8	2I	140	LEU
8	2I	142	VAL
9	2N	21	LYS
9	2N	28	THR
9	2N	33	LEU
9	2N	46	VAL
9	2N	68	GLU
9	2N	73	THR
9	2N	87	LEU
9	2N	119	ARG
9	2N	133	GLN
9	2N	140	VAL
10	2O	10	VAL
10	2O	23	ARG

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Mol	Chain	Res	Type
10	2O	24	VAL
10	2O	35	VAL
10	2O	53	LYS
10	2O	94	ARG
10	2O	108	GLU
10	2O	113	LYS
11	2P	4	SER
11	2P	15	ARG
11	2P	71	VAL
11	2P	148	LEU
11	2P	149	GLU
12	2Q	1	MET
12	2Q	7	MET
12	2Q	60	ARG
12	2Q	75	THR
12	2Q	109	VAL
12	2Q	112	GLU
13	2R	29	LEU
13	2R	33	ARG
13	2R	36	THR
13	2R	44	LEU
13	2R	49	ASP
13	2R	75	LEU
13	2R	96	ARG
13	2R	100	LEU
13	2R	111	LEU
14	2S	12	PHE
14	2S	14	VAL
14	2S	27	SER
14	2S	44	LYS
14	2S	49	VAL
14	2S	52	SER
14	2S	64	GLU
14	2S	80	LEU
14	2S	85	VAL
14	2S	110	LEU
15	2T	36	GLU
15	2T	53	ARG
15	2T	85	LYS
15	2T	95	ARG
15	2T	99	LEU
15	2T	106	SER

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Mol	Chain	Res	Type
15	2T	107	ASP
15	2T	109	GLU
16	2U	52	ARG
16	2U	53	ARG
16	2U	74	LEU
16	2U	77	SER
16	2U	104	GLN
16	2U	108	GLU
17	2V	7	THR
17	2V	12	TYR
17	2V	26	ASP
17	2V	32	THR
17	2V	35	LEU
17	2V	39	LEU
17	2V	56	SER
17	2V	62	LEU
17	2V	72	VAL
17	2V	73	SER
17	2V	79	VAL
17	2V	90	PRO
18	2W	11	ARG
18	2W	17	VAL
18	2W	67	ASP
19	2X	15	GLU
19	2X	49	VAL
19	2X	57	LEU
19	2X	81	VAL
19	2X	92	LEU
20	2Y	2	ARG
20	2Y	3	VAL
20	2Y	6	HIS
20	2Y	42	VAL
20	2Y	67	LEU
20	2Y	72	VAL
20	2Y	83	THR
20	2Y	85	VAL
20	2Y	99	CYS
20	2Y	102	CYS
21	2Z	14	LYS
21	2Z	27	VAL
21	2Z	31	ARG
21	2Z	35	ARG

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Mol	Chain	Res	Type
21	2Z	41	LEU
21	2Z	52	SER
21	2Z	72	ARG
21	2Z	86	VAL
21	2Z	91	LEU
21	2Z	94	GLU
21	2Z	107	THR
21	2Z	123	ASP
21	2Z	140	ASP
21	2Z	142	SER
21	2Z	170	THR
21	2Z	185	GLU
22	20	14	ARG
22	20	55	ARG
22	20	68	GLU
23	21	21	ARG
23	21	40	ARG
23	21	65	SER
24	22	14	ARG
24	22	17	SER
24	22	32	LEU
24	22	52	ASP
24	22	53	LEU
24	22	70	GLN
25	23	23	LEU
25	23	31	LEU
25	23	44	ARG
25	23	53	LEU
25	23	54	VAL
25	23	55	ARG
26	24	10	VAL
26	24	15	ILE
26	24	21	VAL
26	24	24	THR
26	24	53	GLU
26	24	58	ARG
26	24	62	ARG
26	24	63	TYR
27	25	15	ARG
28	26	3	SER
28	26	14	THR
28	26	34	LEU

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Mol	Chain	Res	Type
28	26	52	VAL
29	27	1	MET
29	27	24	THR
29	27	41	ARG
29	27	48	LYS
30	28	23	VAL
30	28	30	ARG
30	28	31	HIS
30	28	34	TRP
30	28	46	ARG
30	28	49	VAL
31	29	7	VAL
31	29	17	ILE
31	29	26	ILE
33	2b	9	GLU
33	2b	10	LEU
33	2b	16	HIS
33	2b	17	PHE
33	2b	27	LYS
33	2b	44	LEU
33	2b	52	GLU
33	2b	73	THR
33	2b	93	VAL
33	2b	96	ARG
33	2b	160	ASP
33	2b	168	THR
33	2b	187	LEU
33	2b	189	ASP
33	2b	215	LEU
33	2b	221	LEU
33	2b	230	VAL
34	2c	3	ASN
34	2c	8	ILE
34	2c	16	ARG
34	2c	20	SER
34	2c	105	GLU
34	2c	115	LEU
34	2c	118	GLN
34	2c	119	ARG
34	2c	128	PHE
34	2c	131	ARG
34	2c	152	ILE

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Mol	Chain	Res	Type
34	2c	179	ARG
34	2c	196	LEU
34	2c	206	GLU
35	2d	5	ILE
35	2d	21	LEU
35	2d	31	CYS
35	2d	36	ARG
35	2d	50	ARG
35	2d	53	ASP
35	2d	56	VAL
35	2d	107	ARG
35	2d	108	LEU
35	2d	122	ARG
35	2d	127	THR
35	2d	135	LEU
35	2d	141	ARG
35	2d	150	GLU
35	2d	166	LYS
35	2d	175	SER
35	2d	188	LEU
35	2d	200	GLU
35	2d	208	SER
35	2d	209	ARG
36	2e	10	MET
36	2e	11	ILE
36	2e	16	THR
36	2e	31	LEU
36	2e	34	VAL
36	2e	41	VAL
36	2e	55	VAL
36	2e	65	ASN
36	2e	67	VAL
36	2e	68	GLU
36	2e	79	GLU
37	2f	22	GLU
37	2f	63	TYR
37	2f	70	ASP
37	2f	72	VAL
37	2f	73	ASN
37	2f	81	ILE
37	2f	95	GLU
38	2g	9	VAL

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Mol	Chain	Res	Type
38	2g	15	ASP
38	2g	16	LEU
38	2g	21	VAL
38	2g	35	LYS
38	2g	38	LEU
38	2g	50	ILE
38	2g	51	GLN
38	2g	75	VAL
38	2g	76	ARG
38	2g	77	SER
38	2g	92	SER
38	2g	104	LEU
38	2g	111	ARG
38	2g	113	GLU
38	2g	115	ARG
38	2g	126	ASP
38	2g	144	MET
38	2g	153	HIS
39	2h	3	THR
39	2h	10	LEU
39	2h	15	ASN
39	2h	19	VAL
39	2h	39	LEU
39	2h	63	LEU
39	2h	91	ARG
39	2h	99	GLU
39	2h	104	ARG
39	2h	109	ILE
39	2h	111	ILE
39	2h	112	LEU
39	2h	114	THR
39	2h	119	LEU
40	2i	7	THR
40	2i	14	VAL
40	2i	23	ASN
40	2i	47	LEU
40	2i	53	VAL
40	2i	54	ASP
40	2i	63	ILE
40	2i	65	VAL
40	2i	71	SER
40	2i	75	ASP

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Mol	Chain	Res	Type
40	2i	83	ARG
40	2i	102	LEU
40	2i	109	VAL
40	2i	117	HIS
40	2i	127	LYS
41	2j	35	SER
41	2j	38	ILE
41	2j	68	HIS
41	2j	72	VAL
41	2j	74	ILE
41	2j	98	ILE
42	2k	18	ARG
42	2k	26	ASN
42	2k	28	THR
42	2k	38	ASN
42	2k	53	SER
42	2k	103	LEU
42	2k	104	GLN
42	2k	109	VAL
42	2k	112	THR
42	2k	117	ASN
43	2l	33	ARG
43	2l	43	VAL
43	2l	62	SER
43	2l	81	SER
43	2l	82	VAL
43	2l	100	ILE
44	2m	63	THR
44	2m	69	GLU
44	2m	80	ARG
44	2m	94	ARG
44	2m	96	LEU
45	2n	4	LYS
45	2n	8	GLU
45	2n	18	VAL
45	2n	50	LYS
45	2n	57	ARG
46	2o	3	ILE
46	2o	5	LYS
46	2o	38	ARG
46	2o	39	LEU
46	2o	70	LEU

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Mol	Chain	Res	Type
46	2o	84	LYS
47	2p	1	MET
47	2p	2	VAL
47	2p	11	SER
47	2p	12	LYS
47	2p	20	VAL
47	2p	38	TYR
47	2p	44	THR
47	2p	45	THR
47	2p	62	VAL
47	2p	67	THR
47	2p	69	THR
48	2q	14	LYS
48	2q	24	GLU
48	2q	52	LYS
48	2q	63	ARG
48	2q	66	SER
48	2q	70	ARG
48	2q	78	GLU
48	2q	81	ARG
48	2q	86	GLU
49	2r	37	VAL
49	2r	85	LEU
50	2s	3	ARG
50	2s	5	LEU
50	2s	12	ASP
50	2s	18	LYS
50	2s	41	VAL
50	2s	48	THR
50	2s	53	ASN
50	2s	71	LEU
50	2s	77	THR
50	2s	78	ARG
51	2t	10	LEU
51	2t	15	ARG
51	2t	24	LEU
51	2t	31	SER
51	2t	37	SER
51	2t	46	GLU
51	2t	56	MET
51	2t	71	THR
51	2t	84	LEU

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Mol	Chain	Res	Type
51	2t	86	ARG
52	2u	10	ARG
52	2u	17	THR
52	2u	22	ARG
53	2y	5	ILE
53	2y	6	THR
53	2y	8	LYS
53	2y	9	GLN
53	2y	11	GLU
53	2y	13	THR
53	2y	16	ILE
53	2y	41	LEU
53	2y	56	THR
53	2y	60	VAL
53	2y	75	ASN
53	2y	78	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (126) such sidechains are listed below:

Mol	Chain	Res	Type
3	1D	87	ASN
3	1D	253	GLN
4	1E	48	GLN
5	1F	69	HIS
5	1F	203	GLN
6	1G	26	GLN
6	1G	132	ASN
8	1I	104	GLN
9	1N	69	GLN
9	1N	133	GLN
10	1O	3	GLN
10	1O	5	GLN
10	1O	89	ASN
11	1P	84	ASN
12	1Q	57	HIS
12	1Q	89	ASN
13	1R	71	GLN
14	1S	84	GLN
15	1T	58	ASN
16	1U	104	GLN
19	1X	31	HIS
20	1Y	6	HIS

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Mol	Chain	Res	Type
20	1Y	43	ASN
20	1Y	92	ASN
22	10	35	ASN
23	11	56	GLN
24	12	70	GLN
25	13	32	GLN
33	1b	40	HIS
34	1c	6	HIS
34	1c	37	GLN
34	1c	102	ASN
34	1c	104	GLN
34	1c	123	GLN
35	1d	43	HIS
35	1d	77	ASN
35	1d	103	ASN
35	1d	119	GLN
35	1d	123	HIS
35	1d	125	HIS
35	1d	129	ASN
35	1d	160	GLN
37	1f	73	ASN
38	1g	13	GLN
38	1g	28	ASN
38	1g	64	GLN
38	1g	148	ASN
40	1i	3	GLN
40	1i	34	ASN
40	1i	73	GLN
41	1j	13	HIS
41	1j	56	HIS
42	1k	93	GLN
43	1l	99	HIS
44	1m	92	HIS
44	1m	106	ASN
46	1o	28	GLN
47	1p	13	HIS
47	1p	16	HIS
47	1p	65	GLN
48	1q	26	GLN
48	1q	93	GLN
50	1s	56	GLN
50	1s	83	HIS

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Mol	Chain	Res	Type
51	1t	18	GLN
51	1t	42	GLN
53	1y	38	HIS
3	2D	116	GLN
3	2D	126	GLN
3	2D	253	GLN
4	2E	48	GLN
5	2F	69	HIS
5	2F	75	HIS
5	2F	203	GLN
6	2G	79	ASN
6	2G	121	ASN
6	2G	123	ASN
8	2I	43	ASN
8	2I	139	GLN
10	2O	3	GLN
11	2P	27	HIS
12	2Q	57	HIS
12	2Q	89	ASN
12	2Q	123	HIS
12	2Q	141	GLN
17	2V	64	HIS
18	2W	34	ASN
18	2W	60	ASN
19	2X	31	HIS
19	2X	82	GLN
20	2Y	6	HIS
20	2Y	92	ASN
21	2Z	34	ASN
21	2Z	151	HIS
22	20	50	ASN
23	21	56	GLN
25	23	32	GLN
30	28	35	GLN
33	2b	19	HIS
33	2b	135	GLN
34	2c	6	HIS
34	2c	139	GLN
34	2c	176	HIS
35	2d	42	GLN
35	2d	77	ASN
35	2d	116	GLN

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Mol	Chain	Res	Type
35	2d	125	HIS
35	2d	201	GLN
36	2e	72	GLN
37	2f	100	ASN
38	2g	13	GLN
38	2g	64	GLN
38	2g	86	GLN
40	2i	3	GLN
40	2i	73	GLN
40	2i	117	HIS
41	2j	62	HIS
41	2j	69	ASN
44	2m	62	ASN
44	2m	77	ASN
46	2o	13	GLN
46	2o	28	GLN
47	2p	65	GLN
48	2q	26	GLN
51	2t	90	GLN
53	2y	31	GLN

### 5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	1A	2862/2915 (98%)	434 (15%)	33 (1%)
1	2A	2855/2915 (97%)	485 (16%)	31 (1%)
2	1B	119/121 (98%)	10 (8%)	0
2	2B	119/121 (98%)	16 (13%)	0
32	1a	1494/1521 (98%)	257 (17%)	0
32	2a	1498/1521 (98%)	290 (19%)	0
All	All	8947/9114 (98%)	1492 (16%)	64 (0%)

All (1492) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	1A	12	U
1	1A	14	A
1	1A	15	G
1	1A	34	C
1	1A	45	C
1	1A	61	G

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Mol	Chain	Res	Type
1	1A	71	A
1	1A	74	A
1	1A	75	G
1	1A	118	A
1	1A	119	A
1	1A	120	U
1	1A	125	G
1	1A	140	G
1	1A	141	A
1	1A	154(A)	C
1	1A	196	A
1	1A	199	A
1	1A	205	G
1	1A	216	A
1	1A	222	A
1	1A	229	A
1	1A	233	A
1	1A	248	G
1	1A	271(I)	G
1	1A	271(K)	U
1	1A	271(L)	U
1	1A	271(M)	G
1	1A	271(O)	C
1	1A	272(A)	U
1	1A	272(B)	G
1	1A	272(H)	C
1	1A	272(J)	C
1	1A	275	G
1	1A	279	C
1	1A	280	C
1	1A	283	A
1	1A	311	A
1	1A	324	A
1	1A	330	A
1	1A	352	G
1	1A	360	G
1	1A	363	G
1	1A	363(B)	G
1	1A	363(C)	G
1	1A	386	G
1	1A	396	G
1	1A	407	G

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Mol	Chain	Res	Type
1	1A	411	G
1	1A	412	A
1	1A	421	U
1	1A	428	A
1	1A	448	U
1	1A	456	C
1	1A	457	A
1	1A	481	G
1	1A	505	A
1	1A	509	C
1	1A	527	C
1	1A	528	A
1	1A	530	G
1	1A	531	C
1	1A	532	A
1	1A	533	G
1	1A	545	G
1	1A	549	G
1	1A	563	G
1	1A	573	G
1	1A	575	A
1	1A	586	A
1	1A	603	A
1	1A	604	G
1	1A	607	U
1	1A	614(B)	G
1	1A	615	G
1	1A	616	G
1	1A	627	A
1	1A	637	A
1	1A	645	C
1	1A	646	A
1	1A	652(E)	G
1	1A	652(T)	C
1	1A	652(U)	G
1	1A	654	A
1	1A	668	G
1	1A	669	G
1	1A	686	G
1	1A	714	U
1	1A	730	C
1	1A	740	U

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Mol	Chain	Res	Type
1	1A	746	A
1	1A	747	U
1	1A	762	U
1	1A	775	G
1	1A	776	G
1	1A	782	A
1	1A	784	A
1	1A	785	G
1	1A	790	C
1	1A	792	G
1	1A	793	A
1	1A	805	G
1	1A	812	C
1	1A	827	U
1	1A	828	U
1	1A	859	G
1	1A	866	A
1	1A	879	G
1	1A	885	C
1	1A	886	C
1	1A	888	C
1	1A	889	C
1	1A	890	A
1	1A	896	A
1	1A	899	A
1	1A	907	U
1	1A	910	A
1	1A	932	G
1	1A	945	A
1	1A	946	G
1	1A	958	U
1	1A	959	A
1	1A	961	C
1	1A	974	G
1	1A	975	C
1	1A	979	G
1	1A	983	A
1	1A	996	A
1	1A	1012	U
1	1A	1013	C
1	1A	1022	G
1	1A	1026	U

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Mol	Chain	Res	Type
1	1A	1033	U
1	1A	1039	G
1	1A	1042	G
1	1A	1043	C
1	1A	1044	G
1	1A	1046	A
1	1A	1047	G
1	1A	1048	A
1	1A	1054	A
1	1A	1055	G
1	1A	1060	U
1	1A	1061	U
1	1A	1062	G
1	1A	1065	U
1	1A	1066	U
1	1A	1069	A
1	1A	1070	A
1	1A	1071	G
1	1A	1073	A
1	1A	1076	C
1	1A	1077	A
1	1A	1078	U
1	1A	1080	C
1	1A	1088	A
1	1A	1090	U
1	1A	1096	A
1	1A	1097	U
1	1A	1109	C
1	1A	1110	G
1	1A	1112	G
1	1A	1129	A
1	1A	1130	U
1	1A	1135	C
1	1A	1136	G
1	1A	1144	G
1	1A	1150	C
1	1A	1171	G
1	1A	1173	G
1	1A	1174	A
1	1A	1175	U
1	1A	1176	G
1	1A	1177	A

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Mol	Chain	Res	Type
1	1A	1178	C
1	1A	1180	C
1	1A	1210	A
1	1A	1211	U
1	1A	1218	C
1	1A	1220	A
1	1A	1229	G
1	1A	1236	G
1	1A	1253	A
1	1A	1256	G
1	1A	1271	G
1	1A	1272	A
1	1A	1273	U
1	1A	1300	U
1	1A	1301	A
1	1A	1320	C
1	1A	1321	A
1	1A	1345	C
1	1A	1352	U
1	1A	1359	A
1	1A	1365	A
1	1A	1370	C
1	1A	1380	G
1	1A	1384	A
1	1A	1385	G
1	1A	1395	A
1	1A	1416	G
1	1A	1417	C
1	1A	1420	U
1	1A	1421	G
1	1A	1428	C
1	1A	1437	C
1	1A	1445	A
1	1A	1450	G
1	1A	1452	A
1	1A	1455	G
1	1A	1459	G
1	1A	1460	A
1	1A	1467	C
1	1A	1471	A
1	1A	1482	G
1	1A	1493	C

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Mol	Chain	Res	Type
1	1A	1497	U
1	1A	1506	C
1	1A	1508	A
1	1A	1509	C
1	1A	1509(A)	A
1	1A	1525	G
1	1A	1542	A
1	1A	1543	C
1	1A	1558	A
1	1A	1569	A
1	1A	1578	U
1	1A	1580	A
1	1A	1581	G
1	1A	1584	C
1	1A	1586	A
1	1A	1608	A
1	1A	1609	A
1	1A	1610	A
1	1A	1644	C
1	1A	1647	G
1	1A	1648	C
1	1A	1654	A
1	1A	1664	A
1	1A	1674	G
1	1A	1696	G
1	1A	1700	A
1	1A	1701	A
1	1A	1706	U
1	1A	1722	A
1	1A	1739	U
1	1A	1747	G
1	1A	1756	G
1	1A	1757	U
1	1A	1762	A
1	1A	1763	G
1	1A	1764	G
1	1A	1773	A
1	1A	1780	A
1	1A	1782	C
1	1A	1791	A
1	1A	1800	C
1	1A	1801	G

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Mol	Chain	Res	Type
1	1A	1816	G
1	1A	1828	G
1	1A	1829	A
1	1A	1839	G
1	1A	1847	A
1	1A	1848	A
1	1A	1877	A
1	1A	1878	G
1	1A	1889	A
1	1A	1900	A
1	1A	1906	G
1	1A	1907	G
1	1A	1913	A
1	1A	1914	C
1	1A	1929	G
1	1A	1930	G
1	1A	1934	C
1	1A	1937	A
1	1A	1938	A
1	1A	1941	C
1	1A	1955	U
1	1A	1963	U
1	1A	1965	C
1	1A	1967	C
1	1A	1970	A
1	1A	1971	A
1	1A	1972	A
1	1A	1985	G
1	1A	1993	U
1	1A	1997	G
1	1A	2020	A
1	1A	2023	G
1	1A	2031	A
1	1A	2032	G
1	1A	2033	A
1	1A	2043	C
1	1A	2055	C
1	1A	2056	G
1	1A	2060	A
1	1A	2061	G
1	1A	2069	G
1	1A	2099	U

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Mol	Chain	Res	Type
1	1A	2103	C
1	1A	2104	G
1	1A	2107	C
1	1A	2108	C
1	1A	2112	G
1	1A	2113	U
1	1A	2116	G
1	1A	2117	A
1	1A	2119	A
1	1A	2122	U
1	1A	2123	G
1	1A	2126	A
1	1A	2127	G
1	1A	2131	G
1	1A	2132	U
1	1A	2133	G
1	1A	2134	A
1	1A	2135	A
1	1A	2137	C
1	1A	2139	C
1	1A	2142	C
1	1A	2144	U
1	1A	2146	C
1	1A	2148	G
1	1A	2157	G
1	1A	2158	A
1	1A	2159	G
1	1A	2161	C
1	1A	2162	G
1	1A	2164	C
1	1A	2165	G
1	1A	2173	A
1	1A	2176	A
1	1A	2185	C
1	1A	2186	G
1	1A	2187	G
1	1A	2190	G
1	1A	2192	G
1	1A	2198	A
1	1A	2206	G
1	1A	2207	G
1	1A	2208	A

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Mol	Chain	Res	Type
1	1A	2225	A
1	1A	2238	G
1	1A	2239	G
1	1A	2268	A
1	1A	2280	G
1	1A	2283	C
1	1A	2287	A
1	1A	2289	G
1	1A	2305	A
1	1A	2320	A
1	1A	2325	G
1	1A	2326	C
1	1A	2334	G
1	1A	2336	A
1	1A	2347	C
1	1A	2350	C
1	1A	2383	G
1	1A	2385	C
1	1A	2393	A
1	1A	2396	G
1	1A	2405	G
1	1A	2406	U
1	1A	2422	A
1	1A	2423	U
1	1A	2425	A
1	1A	2428	G
1	1A	2429	G
1	1A	2430	A
1	1A	2435	A
1	1A	2439	A
1	1A	2441	C
1	1A	2448	A
1	1A	2475	C
1	1A	2476	A
1	1A	2478	A
1	1A	2480	C
1	1A	2491	U
1	1A	2492	U
1	1A	2498	C
1	1A	2502	G
1	1A	2505	G
1	1A	2506	U

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Mol	Chain	Res	Type
1	1A	2518	A
1	1A	2529	G
1	1A	2535	G
1	1A	2549	G
1	1A	2554	U
1	1A	2566	A
1	1A	2567	G
1	1A	2573	C
1	1A	2602	A
1	1A	2603	G
1	1A	2608	G
1	1A	2609	U
1	1A	2611	U
1	1A	2612	C
1	1A	2615	U
1	1A	2629	A
1	1A	2630	G
1	1A	2641	G
1	1A	2654	A
1	1A	2662	A
1	1A	2689	U
1	1A	2690	C
1	1A	2702	U
1	1A	2703	C
1	1A	2712(A)	A
1	1A	2713	A
1	1A	2714	G
1	1A	2726	U
1	1A	2733	A
1	1A	2758	A
1	1A	2761	G
1	1A	2765	A
1	1A	2766	G
1	1A	2778	A
1	1A	2790	A
1	1A	2791	C
1	1A	2792	G
1	1A	2793	G
1	1A	2794	C
1	1A	2802	G
1	1A	2818	G
1	1A	2820	A

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Mol	Chain	Res	Type
1	1A	2821	A
1	1A	2833	G
1	1A	2835	A
1	1A	2872	G
1	1A	2874	C
1	1A	2892	A
1	1A	2893	G
1	1A	2894	G
2	1B	2	C
2	1B	7	G
2	1B	13	A
2	1B	30	C
2	1B	45	A
2	1B	53	A
2	1B	56	G
2	1B	73	A
2	1B	84	C
2	1B	110	G
32	1a	9	G
32	1a	32	A
32	1a	39	G
32	1a	47	C
32	1a	48	C
32	1a	51	A
32	1a	53	A
32	1a	61	G
32	1a	78	G
32	1a	79	G
32	1a	91	C
32	1a	96	U
32	1a	101	A
32	1a	116	A
32	1a	120	A
32	1a	121	C
32	1a	131	C
32	1a	141	A
32	1a	156	G
32	1a	163	C
32	1a	173	U
32	1a	174	C
32	1a	182	U
32	1a	189(C)	C

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Mol	Chain	Res	Type
32	1a	189(D)	C
32	1a	189(F)	U
32	1a	195	A
32	1a	202	U
32	1a	203	U
32	1a	204	U
32	1a	216	G
32	1a	220	G
32	1a	236	G
32	1a	240	C
32	1a	247	G
32	1a	251	G
32	1a	254	G
32	1a	258	G
32	1a	266	G
32	1a	267	C
32	1a	289	G
32	1a	301	G
32	1a	306	G
32	1a	321	A
32	1a	327	A
32	1a	328	C
32	1a	329	A
32	1a	332	G
32	1a	352	C
32	1a	353	A
32	1a	354	G
32	1a	356	A
32	1a	367	U
32	1a	372	C
32	1a	373	A
32	1a	397	A
32	1a	398	C
32	1a	406	G
32	1a	412	A
32	1a	413	G
32	1a	414	A
32	1a	422	C
32	1a	423	G
32	1a	424	G
32	1a	429	U
32	1a	430	A

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Mol	Chain	Res	Type
32	1a	439	A
32	1a	441	A
32	1a	444	C
32	1a	452	A
32	1a	461	A
32	1a	470	C
32	1a	485	G
32	1a	496	A
32	1a	498	U
32	1a	505	G
32	1a	509	A
32	1a	510	A
32	1a	511	C
32	1a	518	C
32	1a	532	A
32	1a	547	A
32	1a	559	A
32	1a	561	U
32	1a	564	C
32	1a	572	A
32	1a	573	A
32	1a	576	G
32	1a	577	G
32	1a	607	A
32	1a	619	U
32	1a	630	G
32	1a	632	A
32	1a	650	G
32	1a	653	A
32	1a	660	G
32	1a	665	A
32	1a	671	G
32	1a	687	A
32	1a	688	G
32	1a	693	G
32	1a	697	U
32	1a	702	A
32	1a	723	U
32	1a	728	A
32	1a	731	G
32	1a	734	G
32	1a	752	G

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Mol	Chain	Res	Type
32	1a	755	G
32	1a	759	A
32	1a	767	A
32	1a	774	G
32	1a	777	A
32	1a	786	G
32	1a	793	U
32	1a	794	A
32	1a	815	A
32	1a	817	C
32	1a	821	G
32	1a	828	A
32	1a	829	G
32	1a	838	G
32	1a	839	U
32	1a	840	C
32	1a	841	U
32	1a	848	C
32	1a	851	G
32	1a	872	A
32	1a	902	G
32	1a	914	A
32	1a	926	G
32	1a	927	G
32	1a	934	C
32	1a	935	A
32	1a	960	U
32	1a	961	U
32	1a	968	A
32	1a	969	A
32	1a	971	G
32	1a	975	A
32	1a	976	G
32	1a	977	A
32	1a	991	U
32	1a	992	U
32	1a	993	G
32	1a	994	A
32	1a	998	G
32	1a	999	C
32	1a	1001	A
32	1a	1001(A)	G

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Mol	Chain	Res	Type
32	1a	1004	A
32	1a	1021	G
32	1a	1023	G
32	1a	1024	G
32	1a	1025	U
32	1a	1026	G
32	1a	1027	C
32	1a	1028	C
32	1a	1029	C
32	1a	1030	C
32	1a	1030(A)	G
32	1a	1030(B)	C
32	1a	1030(C)	G
32	1a	1032	G
32	1a	1033	G
32	1a	1037	C
32	1a	1038	C
32	1a	1040	U
32	1a	1044	A
32	1a	1065	U
32	1a	1066	C
32	1a	1067	A
32	1a	1070	U
32	1a	1081	G
32	1a	1085	U
32	1a	1093	A
32	1a	1094	G
32	1a	1095	U
32	1a	1101	A
32	1a	1121	U
32	1a	1123	A
32	1a	1124	G
32	1a	1125	U
32	1a	1126	U
32	1a	1130	A
32	1a	1132	C
32	1a	1134	G
32	1a	1136	U
32	1a	1137	C
32	1a	1139	G
32	1a	1140	C
32	1a	1144	G

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Mol	Chain	Res	Type
32	1a	1146	A
32	1a	1152	A
32	1a	1158	C
32	1a	1159	U
32	1a	1168	A
32	1a	1183	A
32	1a	1184	G
32	1a	1193	G
32	1a	1196	U
32	1a	1197	G
32	1a	1202	G
32	1a	1208	C
32	1a	1213	A
32	1a	1214	C
32	1a	1224	G
32	1a	1227	A
32	1a	1238	A
32	1a	1256	A
32	1a	1257	U
32	1a	1258	G
32	1a	1270	C
32	1a	1277	C
32	1a	1278	U
32	1a	1279	A
32	1a	1280	A
32	1a	1286	A
32	1a	1287	A
32	1a	1293	G
32	1a	1294	G
32	1a	1299	A
32	1a	1300	G
32	1a	1302	U
32	1a	1312	G
32	1a	1320	C
32	1a	1338	G
32	1a	1346	A
32	1a	1347	G
32	1a	1353	G
32	1a	1363	C
32	1a	1370	G
32	1a	1381	U
32	1a	1397	C

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Mol	Chain	Res	Type
32	1a	1398	A
32	1a	1406	U
32	1a	1419	G
32	1a	1429	C
32	1a	1442	G
32	1a	1442(A)	G
32	1a	1442(B)	A
32	1a	1446	U
32	1a	1447	A
32	1a	1452	C
32	1a	1456	G
32	1a	1487	G
32	1a	1492	A
32	1a	1493	A
32	1a	1499	A
32	1a	1504	G
32	1a	1505	G
32	1a	1506	U
32	1a	1517	G
32	1a	1520	G
32	1a	1529	G
32	1a	1530	G
32	1a	1531	A
1	2A	10	G
1	2A	15	G
1	2A	34	C
1	2A	45	C
1	2A	71	A
1	2A	74	A
1	2A	75	G
1	2A	84	A
1	2A	92	A
1	2A	102	G
1	2A	118	A
1	2A	119	A
1	2A	120	U
1	2A	131	G
1	2A	141	A
1	2A	157	U
1	2A	181	A
1	2A	182	A
1	2A	196	A

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Mol	Chain	Res	Type
1	2A	199	A
1	2A	205	G
1	2A	214	G
1	2A	215	G
1	2A	216	A
1	2A	221	A
1	2A	222	A
1	2A	229	A
1	2A	230	U
1	2A	233	A
1	2A	245	G
1	2A	248	G
1	2A	271(K)	U
1	2A	271(L)	U
1	2A	271(M)	G
1	2A	271(N)	U
1	2A	271(O)	C
1	2A	272	G
1	2A	272(A)	U
1	2A	272(B)	G
1	2A	277	C
1	2A	278	A
1	2A	283	A
1	2A	311	A
1	2A	329	G
1	2A	330	A
1	2A	333	G
1	2A	352	G
1	2A	362	U
1	2A	363	G
1	2A	372	G
1	2A	380	U
1	2A	386	G
1	2A	391	G
1	2A	396	G
1	2A	405	U
1	2A	407	G
1	2A	411	G
1	2A	412	A
1	2A	428	A
1	2A	444	C
1	2A	454	A

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Mol	Chain	Res	Type
1	2A	455	C
1	2A	456	C
1	2A	457	A
1	2A	470	A
1	2A	481	G
1	2A	482	A
1	2A	505	A
1	2A	509	C
1	2A	521	G
1	2A	524	U
1	2A	530	G
1	2A	531	C
1	2A	532	A
1	2A	533	G
1	2A	545	G
1	2A	563	G
1	2A	568	U
1	2A	573	G
1	2A	575	A
1	2A	603	A
1	2A	604	G
1	2A	607	U
1	2A	610	G
1	2A	614(B)	G
1	2A	614(C)	A
1	2A	615	G
1	2A	627	A
1	2A	634	C
1	2A	637	A
1	2A	645	C
1	2A	646	A
1	2A	652(B)	A
1	2A	652(C)	G
1	2A	652(U)	G
1	2A	653	A
1	2A	669	G
1	2A	676	A
1	2A	686	G
1	2A	715	G
1	2A	730	C
1	2A	752	A
1	2A	753	C

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Mol	Chain	Res	Type
1	2A	775	G
1	2A	776	G
1	2A	782	A
1	2A	784	A
1	2A	785	G
1	2A	792	G
1	2A	793	A
1	2A	794	G
1	2A	802	A
1	2A	805	G
1	2A	812	C
1	2A	827	U
1	2A	833	U
1	2A	857	C
1	2A	859	G
1	2A	866	A
1	2A	875	G
1	2A	877	U
1	2A	880	G
1	2A	886	C
1	2A	887	A
1	2A	888	C
1	2A	889	C
1	2A	890	A
1	2A	893	C
1	2A	896	A
1	2A	897	C
1	2A	901	A
1	2A	910	A
1	2A	914	C
1	2A	917	A
1	2A	932	G
1	2A	936	C
1	2A	941	A
1	2A	945	A
1	2A	946	G
1	2A	953	A
1	2A	959	A
1	2A	961	C
1	2A	974	G
1	2A	975	C
1	2A	980	A

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Mol	Chain	Res	Type
1	2A	983	A
1	2A	996	A
1	2A	1012	U
1	2A	1013	C
1	2A	1026	U
1	2A	1033	U
1	2A	1038	C
1	2A	1045	A
1	2A	1046	A
1	2A	1047	G
1	2A	1052	C
1	2A	1053	C
1	2A	1054	A
1	2A	1058	G
1	2A	1060	U
1	2A	1063	G
1	2A	1064	C
1	2A	1065	U
1	2A	1066	U
1	2A	1067	A
1	2A	1068	G
1	2A	1069	A
1	2A	1070	A
1	2A	1071	G
1	2A	1073	A
1	2A	1074	G
1	2A	1076	C
1	2A	1077	A
1	2A	1078	U
1	2A	1079	C
1	2A	1082	U
1	2A	1083	U
1	2A	1084	A
1	2A	1085	A
1	2A	1086	A
1	2A	1087	G
1	2A	1088	A
1	2A	1090	U
1	2A	1091	G
1	2A	1092	C
1	2A	1093	G
1	2A	1095	A

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Mol	Chain	Res	Type
1	2A	1096	A
1	2A	1097	U
1	2A	1109	C
1	2A	1111	A
1	2A	1112	G
1	2A	1116	C
1	2A	1117	G
1	2A	1129	A
1	2A	1130	U
1	2A	1135	C
1	2A	1136	G
1	2A	1142(A)	A
1	2A	1171	G
1	2A	1211	U
1	2A	1212	G
1	2A	1236	G
1	2A	1237	A
1	2A	1244	G
1	2A	1248	G
1	2A	1253	A
1	2A	1256	G
1	2A	1271	G
1	2A	1272	A
1	2A	1287	A
1	2A	1300	U
1	2A	1301	A
1	2A	1303	G
1	2A	1314	C
1	2A	1321	A
1	2A	1342	A
1	2A	1349	A
1	2A	1352	U
1	2A	1360	A
1	2A	1365	A
1	2A	1368	G
1	2A	1370	C
1	2A	1384	A
1	2A	1385	G
1	2A	1386	C
1	2A	1416	G
1	2A	1417	C
1	2A	1421	G

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Mol	Chain	Res	Type
1	2A	1427	A
1	2A	1428	C
1	2A	1445	A
1	2A	1450	G
1	2A	1455	G
1	2A	1459	G
1	2A	1467	C
1	2A	1471	A
1	2A	1472	A
1	2A	1482	G
1	2A	1493	C
1	2A	1497	U
1	2A	1508	A
1	2A	1509	C
1	2A	1509(A)	A
1	2A	1510	G
1	2A	1531	C
1	2A	1537	G
1	2A	1542	A
1	2A	1543	C
1	2A	1554	A
1	2A	1555	G
1	2A	1558	A
1	2A	1559	G
1	2A	1566	A
1	2A	1569	A
1	2A	1578	U
1	2A	1580	A
1	2A	1583	A
1	2A	1584	C
1	2A	1586	A
1	2A	1589	C
1	2A	1590	U
1	2A	1608	A
1	2A	1609	A
1	2A	1639	U
1	2A	1640	C
1	2A	1647	G
1	2A	1648	C
1	2A	1664	A
1	2A	1674	G
1	2A	1693	U

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Mol	Chain	Res	Type
1	2A	1696	G
1	2A	1700	A
1	2A	1701	A
1	2A	1703	G
1	2A	1721	G
1	2A	1722	A
1	2A	1740	G
1	2A	1746	G
1	2A	1756	G
1	2A	1763	G
1	2A	1764	G
1	2A	1773	A
1	2A	1780	A
1	2A	1782	C
1	2A	1786	A
1	2A	1791	A
1	2A	1800	C
1	2A	1801	G
1	2A	1816	G
1	2A	1835	G
1	2A	1839	G
1	2A	1847	A
1	2A	1848	A
1	2A	1877	A
1	2A	1878	G
1	2A	1882	C
1	2A	1900	A
1	2A	1914	C
1	2A	1918	A
1	2A	1929	G
1	2A	1930	G
1	2A	1937	A
1	2A	1938	A
1	2A	1955	U
1	2A	1963	U
1	2A	1967	C
1	2A	1970	A
1	2A	1971	A
1	2A	1972	A
1	2A	1993	U
1	2A	1997	G
1	2A	2001	A

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Mol	Chain	Res	Type
1	2A	2020	A
1	2A	2023	G
1	2A	2031	A
1	2A	2033	A
1	2A	2043	C
1	2A	2055	C
1	2A	2056	G
1	2A	2060	A
1	2A	2061	G
1	2A	2069	G
1	2A	2093	G
1	2A	2096	U
1	2A	2098	U
1	2A	2101	G
1	2A	2103	C
1	2A	2105	C
1	2A	2107	C
1	2A	2108	C
1	2A	2109	U
1	2A	2116	G
1	2A	2117	A
1	2A	2118	U
1	2A	2119	A
1	2A	2120	G
1	2A	2121	G
1	2A	2123	G
1	2A	2126	A
1	2A	2127	G
1	2A	2129	C
1	2A	2130	U
1	2A	2132	U
1	2A	2133	G
1	2A	2134	A
1	2A	2135	A
1	2A	2136	C
1	2A	2142	C
1	2A	2145	C
1	2A	2146	C
1	2A	2147	G
1	2A	2148	G
1	2A	2150	U
1	2A	2151	G

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Mol	Chain	Res	Type
1	2A	2158	A
1	2A	2159	G
1	2A	2161	C
1	2A	2163	C
1	2A	2164	C
1	2A	2167	U
1	2A	2168	G
1	2A	2172	U
1	2A	2173	A
1	2A	2174	C
1	2A	2178	C
1	2A	2182	G
1	2A	2184	G
1	2A	2186	G
1	2A	2187	G
1	2A	2189	U
1	2A	2192	G
1	2A	2198	A
1	2A	2206	G
1	2A	2207	G
1	2A	2208	A
1	2A	2218	U
1	2A	2219	G
1	2A	2225	A
1	2A	2268	A
1	2A	2269	A
1	2A	2275	C
1	2A	2278	A
1	2A	2280	G
1	2A	2283	C
1	2A	2287	A
1	2A	2289	G
1	2A	2298	A
1	2A	2300	G
1	2A	2305	A
1	2A	2308	G
1	2A	2309	A
1	2A	2310	A
1	2A	2314	C
1	2A	2319	G
1	2A	2320	A
1	2A	2321	G

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Mol	Chain	Res	Type
1	2A	2322	A
1	2A	2325	G
1	2A	2334	G
1	2A	2335	A
1	2A	2336	A
1	2A	2343	C
1	2A	2347	C
1	2A	2350	C
1	2A	2366	A
1	2A	2379	G
1	2A	2383	G
1	2A	2385	C
1	2A	2391	G
1	2A	2406	U
1	2A	2410	G
1	2A	2414	G
1	2A	2422	A
1	2A	2423	U
1	2A	2425	A
1	2A	2429	G
1	2A	2430	A
1	2A	2432	A
1	2A	2435	A
1	2A	2439	A
1	2A	2441	C
1	2A	2445	G
1	2A	2448	A
1	2A	2470	G
1	2A	2474	C
1	2A	2476	A
1	2A	2480	C
1	2A	2487	G
1	2A	2490	G
1	2A	2502	G
1	2A	2504	U
1	2A	2505	G
1	2A	2506	U
1	2A	2507	C
1	2A	2518	A
1	2A	2520	C
1	2A	2529	G
1	2A	2554	U

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Mol	Chain	Res	Type
1	2A	2555	U
1	2A	2566	A
1	2A	2567	G
1	2A	2573	C
1	2A	2585	U
1	2A	2602	A
1	2A	2603	G
1	2A	2609	U
1	2A	2611	U
1	2A	2612	C
1	2A	2615	U
1	2A	2629	A
1	2A	2630	G
1	2A	2654	A
1	2A	2667	C
1	2A	2682	U
1	2A	2689	U
1	2A	2690	C
1	2A	2702	U
1	2A	2703	C
1	2A	2707	G
1	2A	2712(A)	A
1	2A	2713	A
1	2A	2714	G
1	2A	2718	G
1	2A	2726	U
1	2A	2733	A
1	2A	2750	A
1	2A	2752	C
1	2A	2757	A
1	2A	2758	A
1	2A	2764	A
1	2A	2765	A
1	2A	2778	A
1	2A	2789	C
1	2A	2803	C
1	2A	2818	G
1	2A	2820	A
1	2A	2821	A
1	2A	2833	G
1	2A	2836	U
1	2A	2872	G

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Mol	Chain	Res	Type
1	2A	2880	C
1	2A	2892	A
1	2A	2894	G
1	2A	2897	U
2	2B	2	C
2	2B	8	U
2	2B	9	G
2	2B	12	C
2	2B	13	A
2	2B	24	G
2	2B	30	C
2	2B	33	G
2	2B	35	U
2	2B	56	G
2	2B	73	A
2	2B	84	C
2	2B	106	G
2	2B	109	C
2	2B	110	G
2	2B	118	G
32	2a	5	U
32	2a	7	G
32	2a	9	G
32	2a	32	A
32	2a	39	G
32	2a	47	C
32	2a	48	C
32	2a	51	A
32	2a	60	A
32	2a	61	G
32	2a	66	G
32	2a	76	C
32	2a	89	C
32	2a	101	A
32	2a	105	G
32	2a	116	A
32	2a	120	A
32	2a	121	C
32	2a	130	A
32	2a	131	C
32	2a	142	G
32	2a	148	G

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Mol	Chain	Res	Type
32	2a	151	A
32	2a	153	C
32	2a	156	G
32	2a	163	C
32	2a	173	U
32	2a	174	C
32	2a	182	U
32	2a	189(C)	C
32	2a	189(E)	U
32	2a	189(F)	U
32	2a	195	A
32	2a	197	A
32	2a	202	U
32	2a	203	U
32	2a	204	U
32	2a	216	G
32	2a	220	G
32	2a	226	G
32	2a	232	G
32	2a	237	C
32	2a	240	C
32	2a	245	C
32	2a	247	G
32	2a	251	G
32	2a	258	G
32	2a	262	A
32	2a	266	G
32	2a	267	C
32	2a	279	A
32	2a	289	G
32	2a	298	A
32	2a	316	G
32	2a	321	A
32	2a	328	C
32	2a	332	G
32	2a	346	G
32	2a	351	G
32	2a	352	C
32	2a	353	A
32	2a	354	G
32	2a	367	U
32	2a	372	C

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Mol	Chain	Res	Type
32	2a	373	A
32	2a	381	C
32	2a	397	A
32	2a	398	C
32	2a	406	G
32	2a	412	A
32	2a	413	G
32	2a	421	U
32	2a	424	G
32	2a	429	U
32	2a	430	A
32	2a	439	A
32	2a	442	C
32	2a	443	C
32	2a	452	A
32	2a	458	C
32	2a	461	A
32	2a	470	C
32	2a	471	G
32	2a	476	G
32	2a	477	A
32	2a	482	A
32	2a	484	G
32	2a	485	G
32	2a	486	U
32	2a	496	A
32	2a	498	U
32	2a	502	G
32	2a	505	G
32	2a	509	A
32	2a	510	A
32	2a	511	C
32	2a	518	C
32	2a	521	G
32	2a	532	A
32	2a	533	A
32	2a	536	C
32	2a	537	G
32	2a	547	A
32	2a	553	A
32	2a	559	A
32	2a	561	U

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Mol	Chain	Res	Type
32	2a	564	C
32	2a	572	A
32	2a	573	A
32	2a	574	A
32	2a	576	G
32	2a	577	G
32	2a	592	G
32	2a	596	C
32	2a	612	C
32	2a	630	G
32	2a	631	G
32	2a	632	A
32	2a	650	G
32	2a	653	A
32	2a	655	A
32	2a	661	G
32	2a	665	A
32	2a	687	A
32	2a	688	G
32	2a	690	G
32	2a	702	A
32	2a	721	G
32	2a	723	U
32	2a	724	G
32	2a	731	G
32	2a	749	C
32	2a	753	A
32	2a	755	G
32	2a	760	G
32	2a	773	G
32	2a	774	G
32	2a	777	A
32	2a	793	U
32	2a	794	A
32	2a	806	C
32	2a	816	A
32	2a	817	C
32	2a	821	G
32	2a	828	A
32	2a	829	G
32	2a	836	G
32	2a	838	G

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Mol	Chain	Res	Type
32	2a	840	C
32	2a	841	U
32	2a	848	C
32	2a	851	G
32	2a	854	G
32	2a	859	A
32	2a	875	C
32	2a	902	G
32	2a	914	A
32	2a	916	G
32	2a	926	G
32	2a	927	G
32	2a	931	C
32	2a	933	G
32	2a	934	C
32	2a	942	G
32	2a	960	U
32	2a	961	U
32	2a	966	M2G
32	2a	968	A
32	2a	969	A
32	2a	971	G
32	2a	972	C
32	2a	974	A
32	2a	975	A
32	2a	976	G
32	2a	977	A
32	2a	982	U
32	2a	983	A
32	2a	989	C
32	2a	990	C
32	2a	992	U
32	2a	993	G
32	2a	994	A
32	2a	1003	G
32	2a	1004	A
32	2a	1005	A
32	2a	1006	C
32	2a	1009	G
32	2a	1016	A
32	2a	1020	U
32	2a	1025	U

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Mol	Chain	Res	Type
32	2a	1026	G
32	2a	1027	C
32	2a	1028	C
32	2a	1030(B)	C
32	2a	1041	A
32	2a	1046	A
32	2a	1047	G
32	2a	1053	G
32	2a	1055	A
32	2a	1065	U
32	2a	1066	C
32	2a	1068	G
32	2a	1071	C
32	2a	1081	G
32	2a	1086	U
32	2a	1094	G
32	2a	1095	U
32	2a	1101	A
32	2a	1117	G
32	2a	1122	U
32	2a	1125	U
32	2a	1127	G
32	2a	1129	C
32	2a	1130	A
32	2a	1134	G
32	2a	1136	U
32	2a	1137	C
32	2a	1138	G
32	2a	1139	G
32	2a	1147	C
32	2a	1152	A
32	2a	1157	A
32	2a	1159	U
32	2a	1160	G
32	2a	1161	C
32	2a	1166	G
32	2a	1172	C
32	2a	1182	G
32	2a	1183	A
32	2a	1184	G
32	2a	1194	U
32	2a	1196	U

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Mol	Chain	Res	Type
32	2a	1197	G
32	2a	1201	A
32	2a	1210	C
32	2a	1213	A
32	2a	1215	G
32	2a	1224	G
32	2a	1227	A
32	2a	1228	C
32	2a	1238	A
32	2a	1250	A
32	2a	1256	A
32	2a	1257	U
32	2a	1258	G
32	2a	1260	C
32	2a	1278	U
32	2a	1279	A
32	2a	1280	A
32	2a	1281	U
32	2a	1282	C
32	2a	1287	A
32	2a	1299	A
32	2a	1300	G
32	2a	1301	U
32	2a	1302	U
32	2a	1303	C
32	2a	1312	G
32	2a	1317	C
32	2a	1320	C
32	2a	1340	A
32	2a	1346	A
32	2a	1347	G
32	2a	1353	G
32	2a	1358	U
32	2a	1359	C
32	2a	1363	C
32	2a	1363(A)	A
32	2a	1364	U
32	2a	1370	G
32	2a	1384	C
32	2a	1397	C
32	2a	1419	G
32	2a	1442	G

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Mol	Chain	Res	Type
32	2a	1442(A)	G
32	2a	1446	U
32	2a	1447	A
32	2a	1456	G
32	2a	1492	A
32	2a	1494	G
32	2a	1499	A
32	2a	1503	A
32	2a	1504	G
32	2a	1505	G
32	2a	1506	U
32	2a	1507	A
32	2a	1517	G
32	2a	1520	G
32	2a	1529	G
32	2a	1530	G

All (64) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	1A	266	G
1	1A	278	A
1	1A	573	G
1	1A	685	A
1	1A	746	A
1	1A	764	A
1	1A	774	A
1	1A	839	U
1	1A	840	C
1	1A	888	C
1	1A	895	U
1	1A	974	G
1	1A	1047	G
1	1A	1065	U
1	1A	1089	G
1	1A	1142(A)	A
1	1A	1174	A
1	1A	1175	U
1	1A	1176	G
1	1A	1210	A
1	1A	1300	U
1	1A	1379	A

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Mol	Chain	Res	Type
1	1A	1442	G
1	1A	1608	A
1	1A	1653	G
1	1A	1663	C
1	1A	2111	C
1	1A	2126	A
1	1A	2406	U
1	1A	2422	A
1	1A	2602	A
1	1A	2689	U
1	1A	2893	G
1	2A	195	A
1	2A	196	A
1	2A	266	G
1	2A	271(M)	G
1	2A	277	C
1	2A	752	A
1	2A	764	A
1	2A	774	A
1	2A	827	U
1	2A	840	C
1	2A	856	C
1	2A	900	A
1	2A	1053	C
1	2A	1057	A
1	2A	1065	U
1	2A	1067	A
1	2A	1073	A
1	2A	1076	C
1	2A	1210	A
1	2A	1420	U
1	2A	1442	G
1	2A	1491	G
1	2A	1992	G
1	2A	2126	A
1	2A	2171	A
1	2A	2172	U
1	2A	2321	G
1	2A	2406	U
1	2A	2602	A
1	2A	2689	U
1	2A	2756	U

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
32	4OC	2a	1402	32	16,23,24	0.68	0	17,32,35	1.25	1 (5%)
32	5MC	2a	1404	32	15,22,23	1.34	1 (6%)	19,32,35	1.40	3 (15%)
32	PSU	2a	516	32,54	17,21,22	1.69	3 (17%)	20,30,33	3.07	7 (35%)
1	4OC	2A	1920	1	15,22,24	0.74	0	17,31,35	1.35	1 (5%)
1	2MA	1A	2503	1,54	17,25,26	1.28	2 (11%)	19,37,40	1.90	3 (15%)
1	5MU	2A	1939	1,54	15,22,23	1.13	1 (6%)	16,32,35	1.79	2 (12%)
1	PSU	2A	2605	1	17,21,22	1.83	3 (17%)	20,30,33	3.30	6 (30%)
1	5MU	1A	1939	1	15,22,23	1.17	1 (6%)	16,32,35	1.86	2 (12%)
32	UR3	1a	1498	32	14,22,23	0.71	0	15,32,35	0.66	0
32	2MG	1a	1207	32,54	19,26,27	1.29	2 (10%)	21,38,41	2.68	10 (47%)
32	MA6	1a	1518	32	19,26,27	0.84	0	18,38,41	1.28	2 (11%)
43	0TD	1l	92	43	4,9,10	3.10	1 (25%)	3,11,13	6.44	1 (33%)
32	UR3	2a	1498	32	14,22,23	0.82	1 (7%)	15,32,35	0.78	1 (6%)
32	MA6	2a	1519	32	19,26,27	0.82	0	18,38,41	1.53	2 (11%)
32	5MC	1a	1407	32	15,22,23	1.38	1 (6%)	19,32,35	1.33	1 (5%)
1	5MU	1A	1915	1	15,22,23	1.04	1 (6%)	16,32,35	2.02	1 (6%)
32	MA6	1a	1519	32	19,26,27	0.82	0	18,38,41	1.52	2 (11%)
32	M2G	1a	966	32	20,27,28	1.33	3 (15%)	22,40,43	2.13	5 (22%)
1	PSU	2A	1911	1	17,21,22	1.52	3 (17%)	20,30,33	3.10	6 (30%)
1	4OC	1A	1920	1	15,22,24	0.73	0	17,31,35	1.47	2 (11%)
32	5MC	2a	967	32	15,22,23	1.38	1 (6%)	19,32,35	1.29	2 (10%)
1	OMG	1A	2251	1,54	18,26,27	1.35	2 (11%)	20,38,41	2.33	6 (30%)
32	MA6	2a	1518	32	19,26,27	0.79	0	18,38,41	1.39	2 (11%)
1	2MA	2A	2503	1,54	17,25,26	1.38	2 (11%)	19,37,40	2.04	3 (15%)
32	PSU	1a	516	32,54	17,21,22	1.47	4 (23%)	20,30,33	3.14	6 (30%)
1	PSU	2A	1917	1	17,21,22	1.57	2 (11%)	20,30,33	3.07	6 (30%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
1	5MC	2A	1962	1,54	15,22,23	1.27	1 (6%)	19,32,35	1.52	4 (21%)
32	5MC	2a	1400	32	15,22,23	1.36	1 (6%)	19,32,35	1.36	3 (15%)
1	5MC	1A	1962	1	15,22,23	1.23	1 (6%)	19,32,35	1.18	2 (10%)
1	PSU	1A	2605	1,54	17,21,22	1.63	3 (17%)	20,30,33	3.28	6 (30%)
1	PSU	1A	1911	1	17,21,22	1.56	3 (17%)	20,30,33	3.06	6 (30%)
32	5MC	1a	967	32	15,22,23	1.29	1 (6%)	19,32,35	1.33	3 (15%)
1	2MU	2A	2552	1,54	14,22,24	0.91	0	14,31,36	0.75	1 (7%)
32	7MG	2a	527	32	22,26,27	1.77	4 (18%)	28,39,42	2.68	8 (28%)
32	5MC	2a	1407	32	15,22,23	1.32	1 (6%)	19,32,35	1.35	2 (10%)
1	OMG	2A	2251	1,54	18,26,27	1.21	2 (11%)	20,38,41	2.18	6 (30%)
1	PSU	1A	1917	1	17,21,22	1.50	2 (11%)	20,30,33	3.19	6 (30%)
43	0TD	2l	92	43	4,9,10	3.03	1 (25%)	3,11,13	7.87	1 (33%)
1	5MU	2A	1915	1	15,22,23	1.06	1 (6%)	16,32,35	2.13	1 (6%)
32	7MG	1a	527	32,54	22,26,27	1.73	4 (18%)	28,39,42	2.71	8 (28%)
32	4OC	1a	1402	32	16,23,24	0.64	0	17,32,35	1.22	1 (5%)
32	2MG	2a	1207	32	19,26,27	1.25	2 (10%)	21,38,41	2.17	6 (28%)
1	5MC	2A	1942	1	15,22,23	1.35	1 (6%)	19,32,35	1.37	3 (15%)
32	M2G	2a	966	32	20,27,28	1.49	3 (15%)	22,40,43	2.13	5 (22%)
32	5MC	1a	1400	32	15,22,23	1.37	1 (6%)	19,32,35	1.38	3 (15%)
1	5MC	1A	1942	1	15,22,23	1.32	1 (6%)	19,32,35	1.25	2 (10%)
32	5MC	1a	1404	32	15,22,23	1.33	1 (6%)	19,32,35	1.30	3 (15%)
1	2MU	1A	2552	1,54	14,22,24	0.76	0	14,31,36	0.86	1 (7%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
32	4OC	2a	1402	32	-	2/9/29/30	0/2/2/2
32	5MC	2a	1404	32	-	0/5/25/26	0/2/2/2
32	PSU	2a	516	32,54	-	0/7/25/26	0/2/2/2
1	4OC	2A	1920	1	-	1/7/27/30	0/2/2/2
1	2MA	1A	2503	1,54	-	2/3/25/26	0/3/3/3
1	5MU	2A	1939	1,54	-	0/5/25/26	0/2/2/2
1	PSU	2A	2605	1	-	0/7/25/26	0/2/2/2
1	5MU	1A	1939	1	-	0/5/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
32	UR3	1a	1498	32	-	0/5/25/26	0/2/2/2
32	2MG	1a	1207	32,54	-	2/5/27/28	0/3/3/3
32	MA6	1a	1518	32	-	0/7/29/30	0/3/3/3
43	0TD	1l	92	43	-	1/3/12/14	-
32	UR3	2a	1498	32	-	0/5/25/26	0/2/2/2
32	MA6	2a	1519	32	-	2/7/29/30	0/3/3/3
32	5MC	1a	1407	32	-	0/5/25/26	0/2/2/2
1	5MU	1A	1915	1	-	0/5/25/26	0/2/2/2
32	MA6	1a	1519	32	-	2/7/29/30	0/3/3/3
32	M2G	1a	966	32	-	0/7/29/30	0/3/3/3
1	PSU	2A	1911	1	-	0/7/25/26	0/2/2/2
1	4OC	1A	1920	1	-	1/7/27/30	0/2/2/2
32	5MC	2a	967	32	-	0/5/25/26	0/2/2/2
1	OMG	1A	2251	1,54	-	1/5/27/28	0/3/3/3
32	MA6	2a	1518	32	-	0/7/29/30	0/3/3/3
1	2MA	2A	2503	1,54	-	1/3/25/26	0/3/3/3
32	PSU	1a	516	32,54	-	0/7/25/26	0/2/2/2
1	PSU	2A	1917	1	-	1/7/25/26	0/2/2/2
1	5MC	2A	1962	1,54	-	2/5/25/26	0/2/2/2
32	5MC	2a	1400	32	-	2/5/25/26	0/2/2/2
1	5MC	1A	1962	1	-	2/5/25/26	0/2/2/2
1	PSU	1A	2605	1,54	-	0/7/25/26	0/2/2/2
1	PSU	1A	1911	1	-	0/7/25/26	0/2/2/2
32	5MC	1a	967	32	-	0/5/25/26	0/2/2/2
1	2MU	2A	2552	1,54	-	0/7/27/28	0/2/2/2
32	7MG	2a	527	32	-	2/7/37/38	0/3/3/3
32	5MC	2a	1407	32	-	0/5/25/26	0/2/2/2
1	OMG	2A	2251	1,54	-	1/5/27/28	0/3/3/3
1	PSU	1A	1917	1	-	1/7/25/26	0/2/2/2
43	0TD	2l	92	43	-	1/3/12/14	-
1	5MU	2A	1915	1	-	0/5/25/26	0/2/2/2
32	7MG	1a	527	32,54	-	2/7/37/38	0/3/3/3
32	4OC	1a	1402	32	-	4/9/29/30	0/2/2/2
32	2MG	2a	1207	32	-	2/5/27/28	0/3/3/3
1	5MC	2A	1942	1	-	0/5/25/26	0/2/2/2
32	M2G	2a	966	32	-	0/7/29/30	0/3/3/3
32	5MC	1a	1400	32	-	0/5/25/26	0/2/2/2
1	5MC	1A	1942	1	-	0/5/25/26	0/2/2/2
32	5MC	1a	1404	32	-	0/5/25/26	0/2/2/2
1	2MU	1A	2552	1,54	-	0/7/27/28	0/2/2/2

All (68) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
43	1l	92	0TD	CB-SB	-5.87	1.69	1.84
1	2A	2605	PSU	C5-C1'	-5.79	1.47	1.52
43	2l	92	0TD	CB-SB	-5.78	1.70	1.84
32	2a	967	5MC	C5-C4	5.01	1.49	1.41
32	2a	1400	5MC	C5-C4	4.85	1.48	1.41
32	1a	1407	5MC	C5-C4	4.85	1.48	1.41
32	1a	1400	5MC	C5-C4	4.84	1.48	1.41
32	2a	516	PSU	C5-C1'	-4.84	1.48	1.52
32	2a	1404	5MC	C5-C4	4.79	1.48	1.41
1	2A	1942	5MC	C5-C4	4.79	1.48	1.41
32	1a	1404	5MC	C5-C4	4.78	1.48	1.41
1	1A	1942	5MC	C5-C4	4.73	1.48	1.41
32	2a	1407	5MC	C5-C4	4.68	1.48	1.41
32	2a	527	7MG	C6-C5	4.66	1.47	1.41
32	1a	967	5MC	C5-C4	4.64	1.48	1.41
1	1A	2605	PSU	C5-C1'	-4.60	1.48	1.52
1	2A	2503	2MA	C6-C5	4.59	1.48	1.41
32	2a	966	M2G	C6-C5	4.51	1.49	1.41
1	2A	1962	5MC	C5-C4	4.49	1.48	1.41
32	2a	527	7MG	C5-C4	4.47	1.47	1.39
1	1A	2251	OMG	C6-C5	4.46	1.49	1.41
32	2a	1207	2MG	C6-C5	4.43	1.49	1.41
32	1a	1207	2MG	C6-C5	4.41	1.49	1.41
32	1a	527	7MG	C5-C4	4.38	1.47	1.39
1	1A	1962	5MC	C5-C4	4.35	1.48	1.41
32	1a	527	7MG	C6-C5	4.23	1.47	1.41
1	1A	1911	PSU	C5-C1'	-4.16	1.48	1.52
1	1A	2503	2MA	C6-C5	4.14	1.47	1.41
32	1a	966	M2G	C6-C5	4.08	1.48	1.41
1	2A	2251	OMG	C6-C5	3.97	1.48	1.41
1	2A	1917	PSU	C5-C1'	-3.84	1.49	1.52
1	2A	1917	PSU	C4-C5	3.79	1.49	1.41
1	1A	1939	5MU	C4-C5	3.67	1.49	1.41
1	2A	1911	PSU	C4-C5	3.64	1.49	1.41
1	2A	1939	5MU	C4-C5	3.63	1.49	1.41
1	1A	1917	PSU	C4-C5	3.62	1.49	1.41
1	2A	1911	PSU	C5-C1'	-3.61	1.49	1.52
32	2a	516	PSU	C4-C5	3.59	1.49	1.41
1	1A	1917	PSU	C5-C1'	-3.57	1.49	1.52
32	1a	527	7MG	C5-N7	-3.56	1.33	1.39
32	2a	527	7MG	C5-N7	-3.46	1.33	1.39
32	2a	966	M2G	C2-N2	3.46	1.40	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	1A	1911	PSU	C4-C5	3.44	1.48	1.41
32	1a	516	PSU	C5-C1'	-3.41	1.49	1.52
32	1a	516	PSU	C4-C5	3.33	1.48	1.41
1	1A	1915	5MU	C4-C5	3.31	1.48	1.41
1	2A	1915	5MU	C4-C5	3.20	1.48	1.41
32	1a	966	M2G	C2-N2	3.13	1.40	1.34
1	1A	2605	PSU	C4-C5	2.89	1.47	1.41
1	2A	2605	PSU	C4-C5	2.73	1.47	1.41
32	2a	966	M2G	C5-C4	2.71	1.48	1.40
1	2A	2251	OMG	C5-C4	2.56	1.47	1.40
1	1A	2605	PSU	C2-N3	-2.53	1.33	1.38
32	2a	1207	2MG	C5-C4	2.51	1.47	1.40
1	1A	2251	OMG	C5-C4	2.51	1.47	1.40
32	1a	527	7MG	C4-N9	-2.47	1.33	1.38
32	2a	527	7MG	C4-N9	-2.46	1.33	1.38
1	2A	2605	PSU	C2-N3	-2.44	1.33	1.38
32	1a	966	M2G	C5-C4	2.42	1.47	1.40
1	1A	2503	2MA	C5-C4	2.31	1.47	1.40
1	2A	2503	2MA	C5-C4	2.26	1.46	1.40
32	2a	1498	UR3	C4-N3	2.26	1.41	1.38
32	1a	1207	2MG	C5-C4	2.23	1.46	1.40
32	1a	516	PSU	O4'-C1'	-2.19	1.41	1.44
32	2a	516	PSU	O4'-C1'	-2.16	1.41	1.44
1	2A	1911	PSU	C2-N3	-2.04	1.34	1.38
1	1A	1911	PSU	O4'-C1'	-2.02	1.41	1.44
32	1a	516	PSU	C2-N3	-2.01	1.34	1.38

All (164) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
43	2l	92	0TD	CSB-SB-CB	-13.56	75.19	101.85
43	1l	92	0TD	CSB-SB-CB	-11.08	80.06	101.85
1	1A	2605	PSU	N1-C2-N3	-8.96	121.31	128.43
1	1A	1917	PSU	N1-C2-N3	-8.86	121.39	128.43
32	1a	516	PSU	N1-C2-N3	-8.85	121.39	128.43
32	1a	527	7MG	N3-C4-N9	8.84	138.27	126.91
1	2A	2605	PSU	N1-C2-N3	-8.57	121.62	128.43
32	2a	527	7MG	N3-C4-N9	8.55	137.89	126.91
1	2A	1911	PSU	N1-C2-N3	-8.35	121.79	128.43
1	2A	1917	PSU	N1-C2-N3	-8.28	121.85	128.43
1	1A	1911	PSU	N1-C2-N3	-8.00	122.07	128.43
32	2a	516	PSU	N1-C2-N3	-7.84	122.20	128.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	2A	1915	5MU	C4-N3-C2	7.72	121.66	115.14
1	1A	1915	5MU	C4-N3-C2	7.42	121.41	115.14
1	1A	1911	PSU	C4-N3-C2	6.98	121.04	115.14
1	1A	1917	PSU	C4-N3-C2	6.94	121.00	115.14
32	1a	516	PSU	C4-N3-C2	6.72	120.82	115.14
1	2A	1911	PSU	C4-N3-C2	6.70	120.80	115.14
1	2A	1917	PSU	C4-N3-C2	6.57	120.69	115.14
1	1A	2605	PSU	C4-N3-C2	6.55	120.67	115.14
1	1A	1939	5MU	C4-N3-C2	6.51	120.64	115.14
1	2A	2503	2MA	C2-N3-C4	6.37	120.70	115.52
1	2A	1939	5MU	C4-N3-C2	6.28	120.45	115.14
32	2a	516	PSU	C4-N3-C2	6.24	120.41	115.14
1	2A	2605	PSU	C4-N3-C2	6.18	120.36	115.14
1	1A	2503	2MA	C2-N3-C4	5.85	120.28	115.52
32	2a	516	PSU	C5-C4-N3	-5.80	117.89	125.36
1	1A	1911	PSU	C5-C4-N3	-5.74	117.97	125.36
1	2A	2605	PSU	C5-C6-N1	-5.39	117.81	124.44
1	2A	1917	PSU	C5-C4-N3	-5.33	118.49	125.36
1	1A	2251	OMG	C2-N3-C4	5.31	121.42	115.36
32	2a	966	M2G	C6-N1-C2	5.29	122.47	116.18
32	1a	527	7MG	N7-C8-N9	-5.27	95.85	103.38
1	1A	1917	PSU	C5-C4-N3	-5.23	118.62	125.36
32	1a	516	PSU	C5-C4-N3	-5.20	118.66	125.36
32	1a	966	M2G	C6-N1-C2	5.16	122.33	116.18
32	2a	527	7MG	N7-C8-N9	-5.13	96.03	103.38
1	2A	1911	PSU	C5-C4-N3	-5.06	118.84	125.36
1	2A	2605	PSU	C5-C4-N3	-5.02	118.90	125.36
32	2a	966	M2G	C2-N3-C4	5.00	120.95	115.28
32	1a	1207	2MG	C2-N3-C4	4.96	120.91	115.28
32	2a	527	7MG	C5-C4-N3	-4.85	118.57	126.49
32	2a	1519	MA6	N3-C2-N1	-4.81	121.16	128.68
32	1a	966	M2G	C2-N3-C4	4.77	120.70	115.28
32	1a	527	7MG	C6-N1-C2	4.74	123.47	115.93
32	2a	527	7MG	C6-N1-C2	4.74	123.45	115.93
32	1a	1519	MA6	N3-C2-N1	-4.70	121.33	128.68
1	2A	2251	OMG	C2-N3-C4	4.70	120.73	115.36
1	1A	2605	PSU	C5-C1'-C2'	-4.67	106.99	115.32
1	1A	2605	PSU	C5-C6-N1	-4.66	118.71	124.44
32	1a	1207	2MG	C6-C5-C4	-4.65	116.36	120.80
32	2a	516	PSU	C5-C6-N1	-4.64	118.74	124.44
32	1a	527	7MG	C5-C4-N3	-4.62	118.94	126.49
1	2A	2605	PSU	C6-N1-C2	4.61	122.96	115.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	2a	1518	MA6	N3-C2-N1	-4.60	121.48	128.68
1	1A	2605	PSU	C5-C4-N3	-4.58	119.45	125.36
32	2a	1207	2MG	C2-N3-C4	4.50	120.39	115.28
1	1A	2605	PSU	C6-N1-C2	4.49	122.76	115.36
1	2A	2503	2MA	C5-C6-N1	-4.48	118.36	123.06
1	1A	2503	2MA	C5-C6-N1	-4.48	118.36	123.06
32	1a	1518	MA6	N3-C2-N1	-4.42	121.77	128.68
1	1A	1920	4OC	C2-N3-C4	4.41	120.81	116.34
1	1A	2251	OMG	C6-N1-C2	4.41	122.93	115.93
32	2a	1207	2MG	C5-C6-N1	-4.39	117.43	123.43
32	1a	516	PSU	C6-N1-C2	4.39	122.59	115.36
1	2A	2605	PSU	C5-C1'-C2'	-4.33	107.59	115.32
1	2A	1920	4OC	C2-N3-C4	4.31	120.71	116.34
1	2A	2251	OMG	C5-C6-N1	-4.29	117.56	123.43
1	2A	2251	OMG	C6-N1-C2	4.29	122.75	115.93
32	2a	966	M2G	C5-C6-N1	-4.29	117.57	123.43
1	1A	2251	OMG	C5-C6-N1	-4.23	117.64	123.43
1	1A	1917	PSU	C6-N1-C2	4.21	122.30	115.36
32	1a	516	PSU	C5-C6-N1	-4.20	119.28	124.44
32	2a	516	PSU	C6-N1-C2	4.19	122.27	115.36
32	1a	1207	2MG	CM2-N2-C2	-4.16	118.58	123.59
1	2A	1917	PSU	C6-N1-C2	4.14	122.19	115.36
32	1a	966	M2G	C5-C6-N1	-4.13	117.78	123.43
32	2a	527	7MG	C6-C5-C4	4.13	119.63	115.20
1	2A	1911	PSU	C6-N1-C2	4.11	122.14	115.36
1	2A	1911	PSU	C5-C6-N1	-4.00	119.53	124.44
32	1a	1207	2MG	C6-N1-C2	3.98	122.30	115.18
32	1a	527	7MG	C6-C5-C4	3.96	119.45	115.20
32	1a	1402	4OC	CM4-N4-C4	-3.96	119.57	122.97
32	2a	1207	2MG	C6-N1-C2	3.95	122.25	115.18
32	1a	1207	2MG	C5-C6-N1	-3.92	118.08	123.43
32	2a	527	7MG	C5-C6-N1	-3.88	115.18	123.14
1	1A	1917	PSU	C5-C6-N1	-3.85	119.71	124.44
1	2A	1917	PSU	C5-C6-N1	-3.84	119.72	124.44
32	2a	967	5MC	C2-N3-C4	3.82	120.63	116.02
32	1a	527	7MG	C5-C6-N1	-3.78	115.37	123.14
32	2a	1404	5MC	C2-N3-C4	3.75	120.55	116.02
32	1a	1407	5MC	C2-N3-C4	3.73	120.52	116.02
1	1A	2251	OMG	N3-C2-N1	-3.72	122.27	127.22
1	1A	1911	PSU	C6-N1-C2	3.71	121.47	115.36
32	1a	1400	5MC	C2-N3-C4	3.70	120.48	116.02
1	1A	1911	PSU	C5-C6-N1	-3.69	119.90	124.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	2a	1407	5MC	C2-N3-C4	3.67	120.45	116.02
32	2a	1207	2MG	C6-C5-C4	-3.67	117.30	120.80
32	1a	966	M2G	C6-C5-C4	-3.66	117.31	120.80
32	1a	967	5MC	C2-N3-C4	3.63	120.40	116.02
1	1A	2251	OMG	C6-C5-C4	-3.61	117.35	120.80
32	1a	1207	2MG	C1'-N9-C4	-3.58	120.35	126.64
1	2A	1962	5MC	N4-C4-N3	3.58	122.09	117.03
1	2A	2251	OMG	C6-C5-C4	-3.57	117.39	120.80
32	1a	1207	2MG	C4-C5-N7	-3.44	105.81	109.40
32	1a	1404	5MC	C2-N3-C4	3.42	120.15	116.02
1	1A	1962	5MC	C2-N3-C4	3.39	120.11	116.02
1	2A	1962	5MC	C2-N3-C4	3.37	120.08	116.02
1	2A	1942	5MC	C2-N3-C4	3.36	120.07	116.02
32	2a	1519	MA6	C4-C5-N7	-3.36	105.90	109.40
1	1A	1942	5MC	C2-N3-C4	3.35	120.06	116.02
1	2A	1911	PSU	C5-C1'-C2'	-3.31	109.41	115.32
32	1a	1207	2MG	N2-C2-N1	3.30	120.13	116.96
1	2A	2251	OMG	N3-C2-N1	-3.28	122.85	127.22
1	1A	2251	OMG	C4-C5-N7	-3.26	106.00	109.40
32	2a	966	M2G	C6-C5-C4	-3.26	117.69	120.80
32	2a	1207	2MG	CM2-N2-C2	-3.24	119.68	123.59
32	2a	1400	5MC	C2-N3-C4	3.20	119.88	116.02
32	1a	1519	MA6	C4-C5-N7	-3.19	106.08	109.40
1	2A	2503	2MA	C4-C5-N7	-3.09	106.17	109.40
32	2a	1207	2MG	C4-C5-N7	-3.06	106.21	109.40
32	2a	1400	5MC	C5-C6-N1	-3.01	118.95	122.19
1	2A	1942	5MC	N4-C4-N3	2.98	121.25	117.03
1	1A	1917	PSU	C5-C1'-C2'	-2.92	110.11	115.32
32	2a	1402	4OC	CM4-N4-C4	-2.90	120.47	122.97
32	2a	1518	MA6	C4-C5-N7	-2.87	106.41	109.40
1	1A	1939	5MU	C5-C6-N1	-2.77	119.21	122.19
1	2A	2251	OMG	C4-C5-N7	-2.74	106.54	109.40
32	2a	516	PSU	C5-C1'-C2'	-2.74	110.43	115.32
32	1a	1400	5MC	N4-C4-N3	2.74	120.90	117.03
32	2a	966	M2G	C4-C5-N7	-2.73	106.56	109.40
32	2a	1404	5MC	N4-C4-N3	2.72	120.87	117.03
32	2a	967	5MC	N4-C4-N3	2.67	120.81	117.03
32	2a	1407	5MC	N4-C4-N3	2.66	120.79	117.03
32	2a	527	7MG	C8-N7-C5	2.63	115.78	108.94
32	1a	966	M2G	C4-C5-N7	-2.62	106.67	109.40
1	1A	1911	PSU	C5-C1'-C2'	-2.61	110.66	115.32
32	1a	527	7MG	C5-C4-N9	-2.61	102.79	106.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	1a	1400	5MC	C5-C6-N1	-2.57	119.42	122.19
1	2A	1942	5MC	C5-C6-N1	-2.55	119.45	122.19
32	1a	527	7MG	C8-N7-C5	2.52	115.50	108.94
1	1A	2503	2MA	C4-C5-N7	-2.51	106.78	109.40
1	1A	1942	5MC	C5-C6-N1	-2.49	119.51	122.19
1	1A	2552	2MU	C5-C4-N3	-2.44	117.93	123.31
32	1a	967	5MC	C5-C6-N1	-2.41	119.59	122.19
1	1A	1962	5MC	C5-C6-N1	-2.40	119.61	122.19
32	1a	967	5MC	N4-C4-N3	2.38	120.40	117.03
32	1a	1404	5MC	N4-C4-N3	2.36	120.37	117.03
1	2A	1962	5MC	CM5-C5-C4	-2.36	119.33	121.72
1	1A	1920	4OC	N4-C4-N3	2.35	120.20	116.49
32	1a	516	PSU	O4'-C1'-C2'	2.29	108.37	104.66
32	1a	1404	5MC	C5-C6-N1	-2.29	119.73	122.19
1	2A	1917	PSU	C5-C1'-C2'	-2.20	111.39	115.32
32	2a	1498	UR3	C3U-N3-C4	2.18	121.01	118.12
1	2A	1939	5MU	C5-C6-N1	-2.18	119.84	122.19
32	2a	1400	5MC	N4-C4-N3	2.17	120.10	117.03
32	1a	1207	2MG	N3-C2-N1	-2.17	122.80	126.23
32	2a	516	PSU	O4'-C1'-C2'	2.15	108.14	104.66
32	2a	1404	5MC	C5-C6-N1	-2.10	119.93	122.19
32	2a	527	7MG	C5-C4-N9	-2.09	103.52	106.44
1	2A	2552	2MU	C5-C4-N3	-2.08	118.73	123.31
1	2A	1962	5MC	C5-C6-N1	-2.06	119.97	122.19
32	1a	1518	MA6	C4-C5-N7	-2.04	107.27	109.40
32	1a	1207	2MG	O3'-C3'-C2'	2.01	118.33	111.82

There are no chirality outliers.

All (35) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
32	2a	1402	4OC	N3-C4-N4-CM4
32	2a	1402	4OC	C5-C4-N4-CM4
1	2A	1920	4OC	O4'-C1'-N1-C6
32	1a	1207	2MG	N1-C2-N2-CM2
32	1a	1207	2MG	N3-C2-N2-CM2
1	1A	1920	4OC	C2'-C1'-N1-C6
1	2A	1962	5MC	O4'-C1'-N1-C6
1	2A	1962	5MC	C2'-C1'-N1-C6
32	2a	1400	5MC	O4'-C1'-N1-C6
32	2a	1400	5MC	C2'-C1'-N1-C6
1	1A	1962	5MC	O4'-C1'-N1-C6

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Mol	Chain	Res	Type	Atoms
1	1A	1962	5MC	C2'-C1'-N1-C6
1	2A	2251	OMG	C1'-C2'-O2'-CM2
32	1a	1402	4OC	N3-C4-N4-CM4
32	1a	1402	4OC	C5-C4-N4-CM4
32	2a	1207	2MG	N1-C2-N2-CM2
32	2a	1519	MA6	O4'-C4'-C5'-O5'
32	1a	1519	MA6	O4'-C4'-C5'-O5'
32	1a	1519	MA6	C3'-C4'-C5'-O5'
32	2a	1519	MA6	C3'-C4'-C5'-O5'
32	1a	527	7MG	C3'-C4'-C5'-O5'
32	1a	527	7MG	O4'-C4'-C5'-O5'
32	2a	1207	2MG	N3-C2-N2-CM2
32	2a	527	7MG	C3'-C4'-C5'-O5'
32	1a	1402	4OC	O4'-C4'-C5'-O5'
1	1A	2251	OMG	C4'-C5'-O5'-P
1	1A	2503	2MA	C4'-C5'-O5'-P
1	2A	1917	PSU	C2'-C1'-C5-C6
1	1A	1917	PSU	C2'-C1'-C5-C6
32	2a	527	7MG	O4'-C4'-C5'-O5'
1	2A	2503	2MA	O4'-C4'-C5'-O5'
32	1a	1402	4OC	C3'-C4'-C5'-O5'
43	1l	92	0TD	CG-CB-SB-CSB
43	2l	92	0TD	CG-CB-SB-CSB
1	1A	2503	2MA	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 2499 ligands modelled in this entry, 2486 are monoatomic - leaving 13 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	$\# Z  > 2$
56	MPD	2A	3735	-	7,7,7	0.26	0	9,10,10	0.22	0
59	SF4	2d	501	35	0,12,12	0.00	-	-		
56	MPD	1T	204	-	7,7,7	0.31	0	9,10,10	0.26	0
56	MPD	2A	3736	-	7,7,7	0.31	0	9,10,10	0.32	0
55	ERY	2A	3734	-	53,53,53	0.91	2 (3%)	82,82,82	1.58	13 (15%)
59	SF4	1d	306	35	0,12,12	0.00	-	-		
57	ARG	1B	233	54	7,11,11	0.24	0	6,13,13	0.27	0
57	ARG	1F	319	54	7,11,11	0.34	0	6,13,13	0.37	0
56	MPD	1a	1875	-	7,7,7	0.37	0	9,10,10	0.44	0
55	ERY	1A	4021	-	53,53,53	0.91	2 (3%)	82,82,82	1.44	13 (15%)
56	MPD	2B	219	-	7,7,7	0.29	0	9,10,10	0.28	0
56	MPD	1A	4022	54	7,7,7	0.27	0	9,10,10	0.57	0
56	MPD	18	103	-	7,7,7	0.31	0	9,10,10	0.49	0

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
56	MPD	2A	3735	-	-	2/5/5/5	-
57	ARG	1B	233	54	-	2/7/11/11	-
56	MPD	1T	204	-	-	4/5/5/5	-
56	MPD	2A	3736	-	-	2/5/5/5	-
55	ERY	2A	3734	-	-	7/72/107/107	0/3/3/3
59	SF4	2d	501	35	-	-	0/6/5/5
56	MPD	18	103	-	-	2/5/5/5	-
57	ARG	1F	319	54	-	0/7/11/11	-
56	MPD	1a	1875	-	-	3/5/5/5	-
55	ERY	1A	4021	-	-	7/72/107/107	0/3/3/3
59	SF4	1d	306	35	-	-	0/6/5/5
56	MPD	2B	219	-	-	2/5/5/5	-
56	MPD	1A	4022	54	-	3/5/5/5	-

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
55	2A	3734	ERY	O2-C1	4.77	1.45	1.34
55	1A	4021	ERY	O2-C1	4.66	1.45	1.34
55	1A	4021	ERY	O2-C13	-2.52	1.42	1.46
55	2A	3734	ERY	O2-C13	-2.02	1.42	1.46

All (26) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
55	2A	3734	ERY	O5-C16-C17	4.33	110.22	103.81
55	2A	3734	ERY	C13-O2-C1	-4.14	110.81	118.18
55	1A	4021	ERY	O7-C5-C4	-3.83	105.80	111.54
55	2A	3734	ERY	C6-C5-C4	-3.82	108.64	114.05
55	2A	3734	ERY	O5-C16-C15	-3.57	107.24	112.96
55	2A	3734	ERY	O4-C18-C17	3.41	116.12	110.03
55	2A	3734	ERY	O2-C1-C2	3.39	119.00	111.56
55	1A	4021	ERY	O5-C16-C15	-3.31	107.66	112.96
55	1A	4021	ERY	C15-C16-C17	3.13	113.28	107.67
55	1A	4021	ERY	O7-C5-C6	3.12	110.23	106.39
55	1A	4021	ERY	C32-C6-C5	3.10	115.57	110.12
55	1A	4021	ERY	C6-C5-C4	-3.09	109.68	114.05
55	2A	3734	ERY	C20-O5-C16	3.04	123.89	117.55
55	1A	4021	ERY	C13-O2-C1	-3.03	112.79	118.18
55	1A	4021	ERY	O3-C3-C4	2.94	111.76	108.22
55	2A	3734	ERY	O7-C5-C4	-2.92	107.17	111.54
55	1A	4021	ERY	O2-C1-C2	2.68	117.44	111.56
55	2A	3734	ERY	C16-C17-C18	2.47	114.92	111.14
55	1A	4021	ERY	C16-C17-C18	2.35	114.74	111.14
55	2A	3734	ERY	C2-C3-C4	-2.27	106.47	113.05
55	2A	3734	ERY	C36-C13-C12	-2.27	110.89	115.20
55	2A	3734	ERY	O2-C1-O1	-2.25	119.73	123.94
55	2A	3734	ERY	O7-C5-C6	2.22	109.13	106.39
55	1A	4021	ERY	O6-C17-C16	-2.22	106.97	111.12
55	1A	4021	ERY	C2-C3-C4	-2.07	107.07	113.05
55	1A	4021	ERY	O4-C18-C17	2.04	113.68	110.03

There are no chirality outliers.

All (34) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
56	1A	4022	MPD	C1-C2-C3-C4
56	1A	4022	MPD	O2-C2-C3-C4
55	2A	3734	ERY	C32-C6-C7-C8

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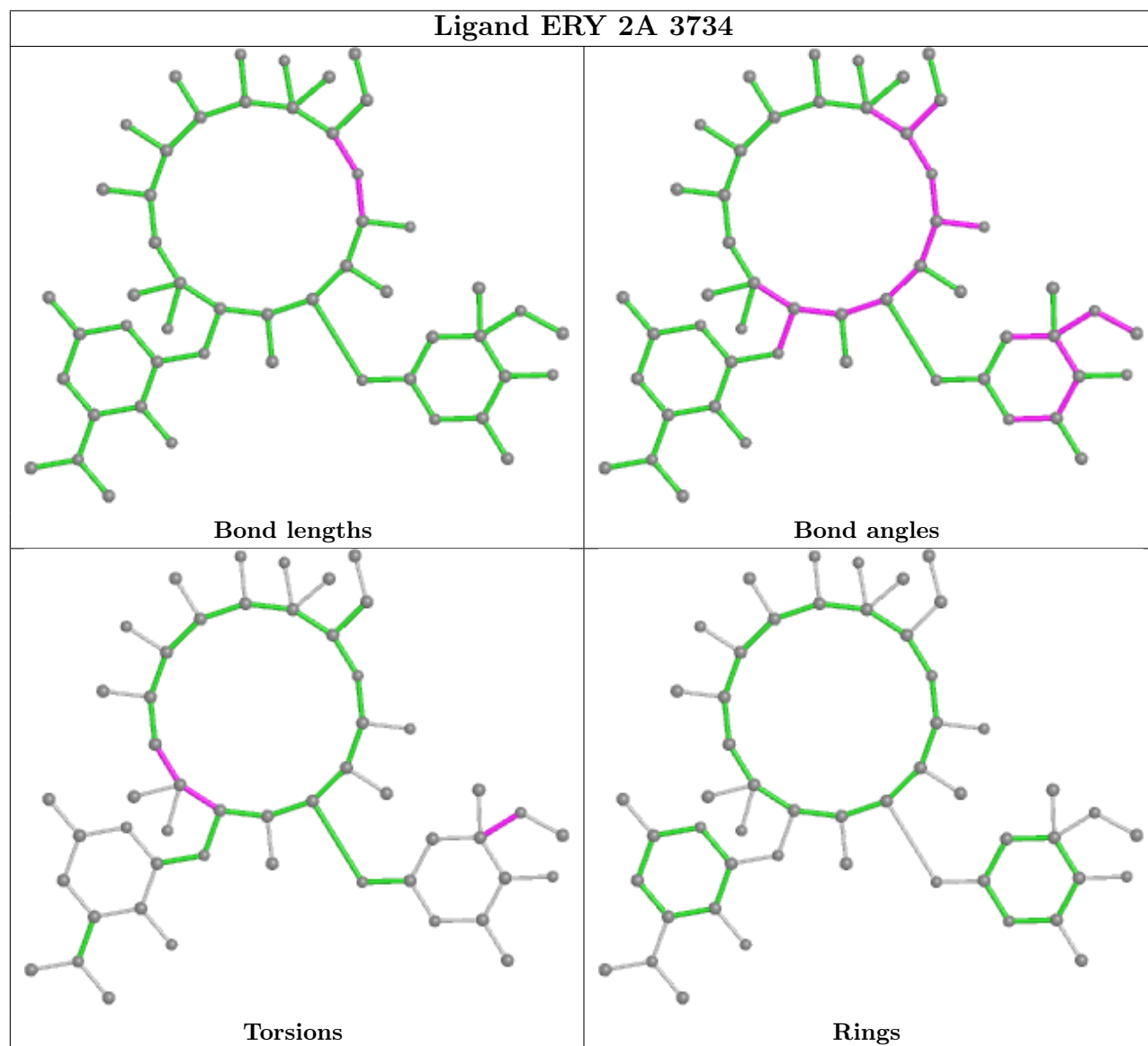
Mol	Chain	Res	Type	Atoms
55	2A	3734	ERY	C15-C16-O5-C20
55	2A	3734	ERY	C17-C16-O5-C20
55	2A	3734	ERY	C19-C16-O5-C20
56	2A	3736	MPD	C2-C3-C4-O4
56	1a	1875	MPD	C2-C3-C4-O4
55	1A	4021	ERY	C15-C16-O5-C20
55	1A	4021	ERY	C17-C16-O5-C20
55	1A	4021	ERY	C19-C16-O5-C20
57	1B	233	ARG	NE-CD-CG-CB
57	1B	233	ARG	CA-CB-CG-CD
55	2A	3734	ERY	O10-C6-C7-C8
55	2A	3734	ERY	C4-C5-C6-O10
55	1A	4021	ERY	C4-C5-C6-O10
56	2B	219	MPD	C2-C3-C4-C5
56	1a	1875	MPD	C2-C3-C4-C5
56	2B	219	MPD	C2-C3-C4-O4
56	1A	4022	MPD	CM-C2-C3-C4
56	1T	204	MPD	CM-C2-C3-C4
56	2A	3736	MPD	C1-C2-C3-C4
56	2A	3735	MPD	CM-C2-C3-C4
55	1A	4021	ERY	O7-C5-C6-C7
55	2A	3734	ERY	C4-C5-C6-C32
55	1A	4021	ERY	C30-C2-C3-C4
55	1A	4021	ERY	C32-C6-C7-C8
56	1T	204	MPD	O2-C2-C3-C4
56	1a	1875	MPD	O2-C2-C3-C4
56	2A	3735	MPD	O2-C2-C3-C4
56	1T	204	MPD	C2-C3-C4-C5
56	18	103	MPD	C2-C3-C4-C5
56	1T	204	MPD	C2-C3-C4-O4
56	18	103	MPD	C2-C3-C4-O4

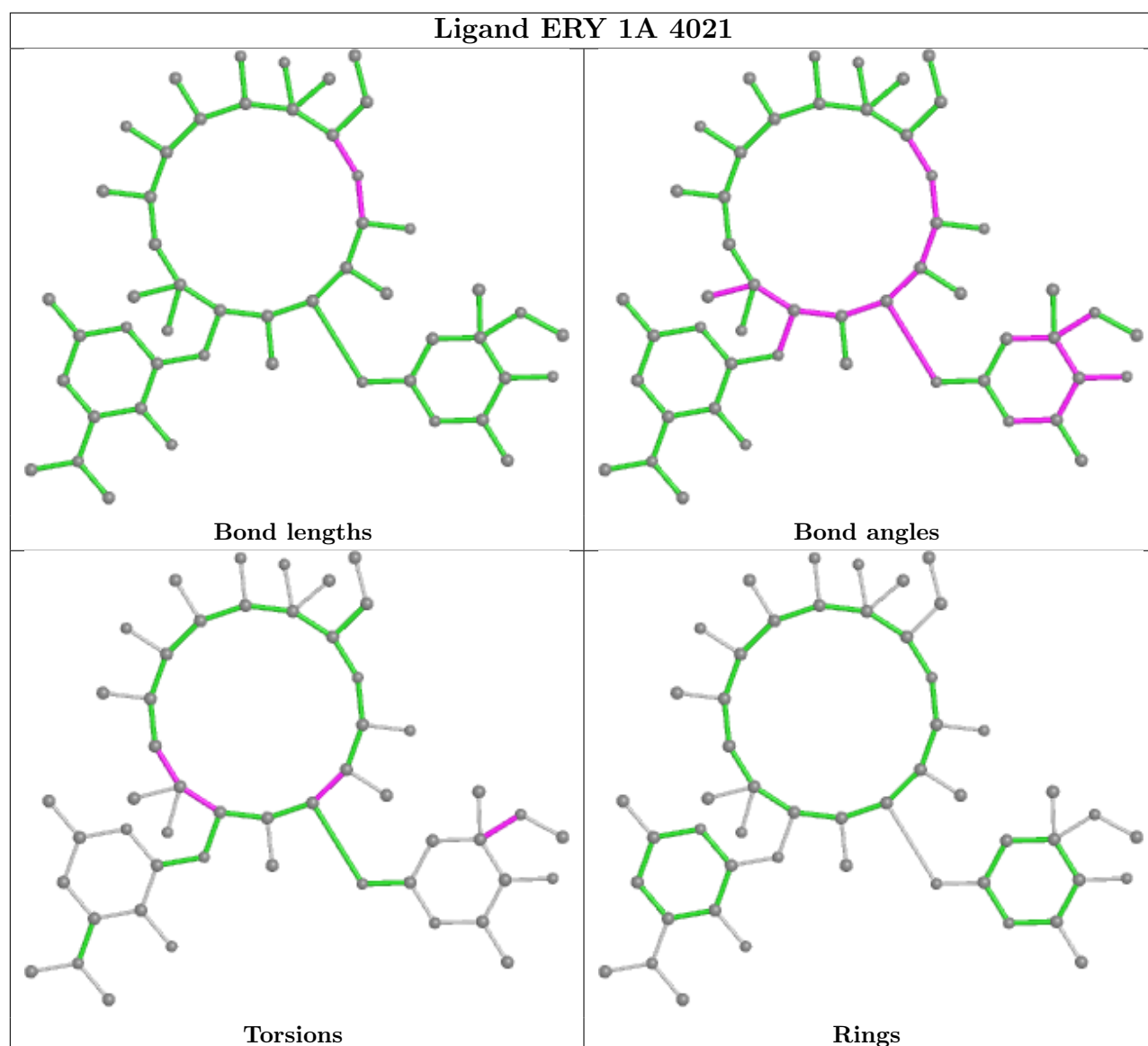
There are no ring outliers.

No monomer is involved in short contacts.

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the

average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.





## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.



## 6 Fit of model and data ⓘ

### 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	2861/2915 (98%)	0.27	42 (1%) 73 79	22, 39, 89, 104	0
1	2A	2856/2915 (97%)	0.04	33 (1%) 79 84	35, 58, 91, 103	0
2	1B	120/121 (99%)	-0.01	0 100 100	30, 52, 65, 78	0
2	2B	120/121 (99%)	-0.34	0 100 100	60, 75, 83, 87	0
3	1D	275/276 (99%)	0.70	8 (2%) 51 59	25, 41, 54, 72	0
3	2D	275/276 (99%)	1.08	44 (16%) 1 2	36, 53, 65, 78	0
4	1E	204/206 (99%)	0.64	3 (1%) 73 79	23, 44, 60, 70	0
4	2E	204/206 (99%)	0.53	9 (4%) 34 41	32, 58, 73, 81	0
5	1F	203/210 (96%)	0.50	1 (0%) 91 94	22, 46, 68, 84	0
5	2F	203/210 (96%)	0.54	10 (4%) 29 35	36, 65, 77, 83	0
6	1G	181/182 (99%)	0.34	6 (3%) 46 53	47, 63, 74, 79	0
6	2G	181/182 (99%)	1.60	59 (32%) 0 0	70, 79, 86, 89	0
7	1H	174/180 (96%)	0.38	1 (0%) 89 92	38, 55, 66, 74	0
7	2H	173/180 (96%)	1.56	58 (33%) 0 0	66, 77, 83, 87	0
8	1I	147/148 (99%)	0.22	6 (4%) 37 44	46, 71, 79, 82	0
8	2I	146/148 (98%)	0.70	23 (15%) 2 2	60, 72, 81, 85	0
9	1N	140/140 (100%)	0.56	0 100 100	29, 42, 62, 79	0
9	2N	140/140 (100%)	0.79	9 (6%) 19 22	45, 62, 74, 80	0
10	1O	122/122 (100%)	0.55	0 100 100	32, 44, 58, 64	0
10	2O	122/122 (100%)	0.62	5 (4%) 37 44	49, 58, 68, 77	0
11	1P	149/150 (99%)	0.44	1 (0%) 87 90	23, 48, 66, 76	0
11	2P	149/150 (99%)	0.74	15 (10%) 7 8	39, 65, 77, 83	0
12	1Q	141/141 (100%)	0.55	1 (0%) 87 90	30, 44, 54, 65	0
12	2Q	141/141 (100%)	0.94	13 (9%) 9 10	47, 62, 72, 76	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
13	1R	118/118 (100%)	0.59	1 (0%) 86 89	30, 39, 53, 62	0
13	2R	118/118 (100%)	0.79	10 (8%) 10 12	42, 54, 63, 72	0
14	1S	110/112 (98%)	0.34	0 100 100	39, 51, 64, 69	0
14	2S	110/112 (98%)	0.75	16 (14%) 2 3	63, 70, 76, 79	0
15	1T	131/146 (89%)	0.54	2 (1%) 73 79	34, 48, 66, 80	0
15	2T	131/146 (89%)	0.58	8 (6%) 21 25	49, 60, 73, 78	0
16	1U	116/118 (98%)	0.85	4 (3%) 45 52	24, 35, 49, 67	0
16	2U	116/118 (98%)	0.88	16 (13%) 2 3	41, 59, 71, 76	0
17	1V	101/101 (100%)	0.64	1 (0%) 82 86	27, 44, 60, 67	0
17	2V	101/101 (100%)	0.43	6 (5%) 22 26	44, 65, 73, 78	0
18	1W	112/113 (99%)	0.60	0 100 100	26, 34, 55, 80	0
18	2W	112/113 (99%)	0.84	9 (8%) 12 15	39, 50, 65, 88	0
19	1X	95/96 (98%)	0.65	3 (3%) 47 55	30, 39, 60, 69	0
19	2X	95/96 (98%)	1.18	17 (17%) 1 1	48, 60, 71, 76	0
20	1Y	107/110 (97%)	0.43	0 100 100	35, 50, 65, 70	0
20	2Y	107/110 (97%)	1.11	17 (15%) 1 2	57, 67, 76, 81	0
21	1Z	203/206 (98%)	0.31	0 100 100	41, 58, 71, 80	0
21	2Z	201/206 (97%)	0.63	20 (9%) 7 9	65, 73, 79, 84	0
22	10	77/85 (90%)	0.60	1 (1%) 77 82	31, 40, 56, 60	0
22	20	77/85 (90%)	1.49	23 (29%) 0 0	50, 62, 70, 74	0
23	11	97/98 (98%)	1.05	11 (11%) 5 6	31, 46, 65, 72	0
23	21	97/98 (98%)	1.27	19 (19%) 1 1	43, 58, 72, 75	0
24	12	70/72 (97%)	0.49	0 100 100	36, 50, 61, 76	0
24	22	70/72 (97%)	0.70	6 (8%) 10 12	57, 66, 73, 76	0
25	13	59/60 (98%)	0.48	0 100 100	30, 40, 60, 65	0
25	23	59/60 (98%)	1.42	19 (32%) 0 0	50, 61, 75, 80	0
26	14	69/71 (97%)	0.24	5 (7%) 15 18	55, 77, 87, 90	0
26	24	69/71 (97%)	1.38	21 (30%) 0 0	74, 84, 89, 94	0
27	15	59/60 (98%)	0.58	0 100 100	23, 38, 56, 63	0
27	25	59/60 (98%)	0.50	0 100 100	37, 52, 66, 70	0
28	16	53/54 (98%)	0.40	0 100 100	35, 46, 59, 64	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
28	26	53/54 (98%)	0.47	2 (3%) 40 47	52, 60, 68, 71	0
29	17	48/49 (97%)	0.81	4 (8%) 11 13	23, 31, 55, 62	0
29	27	48/49 (97%)	0.93	4 (8%) 11 13	34, 43, 63, 68	0
30	18	64/65 (98%)	0.73	2 (3%) 49 56	30, 37, 45, 60	0
30	28	64/65 (98%)	1.55	18 (28%) 0 0	44, 56, 64, 70	0
31	19	37/37 (100%)	1.01	3 (8%) 12 15	35, 46, 62, 63	0
31	29	37/37 (100%)	1.76	13 (35%) 0 0	57, 64, 76, 80	0
32	1a	1488/1521 (97%)	-0.09	9 (0%) 89 92	42, 69, 88, 101	0
32	2a	1492/1521 (98%)	-0.01	21 (1%) 75 81	55, 76, 91, 100	0
33	1b	231/256 (90%)	0.28	8 (3%) 44 51	66, 75, 82, 88	0
33	2b	231/256 (90%)	0.61	29 (12%) 3 4	71, 80, 86, 89	0
34	1c	206/239 (86%)	0.62	19 (9%) 9 10	57, 71, 78, 84	0
34	2c	206/239 (86%)	1.34	59 (28%) 0 0	72, 80, 86, 90	0
35	1d	208/209 (99%)	0.67	19 (9%) 9 11	58, 70, 77, 86	0
35	2d	208/209 (99%)	1.12	43 (20%) 1 0	64, 72, 79, 81	0
36	1e	148/162 (91%)	0.86	14 (9%) 8 10	56, 65, 73, 80	0
36	2e	148/162 (91%)	0.63	17 (11%) 4 6	63, 73, 80, 85	0
37	1f	100/101 (99%)	0.19	1 (1%) 82 86	58, 65, 73, 77	0
37	2f	100/101 (99%)	0.14	1 (1%) 82 86	59, 70, 76, 79	0
38	1g	155/156 (99%)	0.26	5 (3%) 47 55	61, 70, 77, 87	0
38	2g	155/156 (99%)	0.95	27 (17%) 1 1	69, 78, 83, 87	0
39	1h	137/138 (99%)	0.82	16 (11%) 4 6	59, 68, 74, 77	0
39	2h	137/138 (99%)	1.27	35 (25%) 0 0	65, 73, 78, 87	0
40	1i	127/128 (99%)	1.20	30 (23%) 0 0	58, 75, 81, 84	0
40	2i	126/128 (98%)	1.95	51 (40%) 0 0	74, 80, 84, 89	0
41	1j	97/105 (92%)	0.74	17 (17%) 1 1	64, 73, 83, 85	0
41	2j	96/105 (91%)	1.52	33 (34%) 0 0	71, 81, 86, 88	0
42	1k	114/129 (88%)	0.41	4 (3%) 44 51	44, 64, 71, 76	0
42	2k	114/129 (88%)	0.68	8 (7%) 16 19	61, 72, 79, 84	0
43	1l	121/132 (91%)	0.76	11 (9%) 9 11	53, 60, 69, 74	0
43	2l	121/132 (91%)	1.21	28 (23%) 0 0	59, 68, 76, 79	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
44	1m	116/126 (92%)	0.70	13 (11%) 5 7	58, 72, 78, 84	0
44	2m	114/126 (90%)	1.80	43 (37%) 0 0	74, 80, 84, 85	0
45	1n	60/61 (98%)	2.25	30 (50%) 0 0	63, 69, 75, 75	0
45	2n	60/61 (98%)	3.24	43 (71%) 0 0	73, 80, 85, 87	0
46	1o	88/89 (98%)	0.45	3 (3%) 45 52	50, 65, 75, 78	0
46	2o	88/89 (98%)	0.85	11 (12%) 3 5	65, 73, 78, 84	0
47	1p	82/88 (93%)	1.56	23 (28%) 0 0	61, 70, 77, 81	0
47	2p	82/88 (93%)	1.25	19 (23%) 0 0	63, 71, 75, 80	0
48	1q	99/105 (94%)	0.85	6 (6%) 21 25	58, 66, 75, 77	0
48	2q	99/105 (94%)	1.61	34 (34%) 0 0	61, 70, 77, 82	0
49	1r	68/88 (77%)	0.54	5 (7%) 14 18	58, 65, 74, 80	0
49	2r	68/88 (77%)	0.60	5 (7%) 14 18	65, 73, 80, 82	0
50	1s	83/93 (89%)	0.37	2 (2%) 59 65	65, 73, 80, 83	0
50	2s	83/93 (89%)	1.76	38 (45%) 0 0	71, 81, 86, 88	0
51	1t	96/106 (90%)	1.36	31 (32%) 0 0	62, 69, 79, 84	0
51	2t	98/106 (92%)	1.39	30 (30%) 0 0	59, 69, 76, 81	0
52	1u	23/27 (85%)	1.82	9 (39%) 0 0	67, 72, 78, 79	0
52	2u	23/27 (85%)	2.12	11 (47%) 0 0	74, 78, 82, 83	0
53	1y	97/113 (85%)	0.75	9 (9%) 8 10	54, 63, 73, 75	0
53	2y	96/113 (84%)	2.28	49 (51%) 0 0	67, 76, 82, 84	0
All	All	20766/21468 (96%)	0.51	1547 (7%) 14 18	22, 64, 84, 104	0

All (1547) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
45	2n	2	ALA	10.8
1	1A	1087	G	8.2
8	2I	3	VAL	8.0
1	1A	1090	U	7.9
40	2i	115	GLY	7.8
33	2b	118	LEU	7.8
7	2H	165	ALA	7.5
34	2c	124	ILE	7.5
40	2i	109	VAL	7.3
26	24	49	PHE	7.1

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Mol	Chain	Res	Type	RSRZ
41	2j	96	ILE	7.1
45	2n	42	ILE	6.9
6	2G	140	ILE	6.8
39	2h	2	LEU	6.8
45	2n	61	TRP	6.7
35	2d	158	ILE	6.7
6	2G	152	LEU	6.6
7	2H	115	VAL	6.5
19	2X	92	LEU	6.3
44	2m	102	ARG	6.3
6	2G	139	LEU	6.3
6	2G	39	ILE	6.3
52	2u	14	TRP	6.2
44	1m	56	LEU	6.2
40	2i	126	SER	6.2
47	1p	19	ILE	6.1
45	2n	6	LEU	6.1
40	2i	114	TYR	6.1
40	1i	106	ALA	6.1
41	2j	44	VAL	5.9
6	2G	92	VAL	5.9
23	2l	2	SER	5.9
41	2j	67	THR	5.8
12	2Q	104	PHE	5.8
41	2j	63	PHE	5.8
3	1D	276	LYS	5.8
45	1n	25	VAL	5.8
7	2H	145	ALA	5.8
7	2H	21	PRO	5.8
44	1m	2	ALA	5.7
1	1A	1091	G	5.7
44	2m	65	LYS	5.7
45	2n	12	ARG	5.7
41	1j	50	ILE	5.7
8	2I	19	VAL	5.7
45	2n	34	TYR	5.7
40	1i	109	VAL	5.6
35	1d	167	GLY	5.6
43	2l	7	ILE	5.6
44	2m	5	ALA	5.6
45	1n	33	VAL	5.6
52	1u	14	TRP	5.5

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Mol	Chain	Res	Type	RSRZ
53	2y	49	VAL	5.5
48	2q	98	LEU	5.5
45	2n	18	VAL	5.5
40	2i	75	ASP	5.4
6	2G	157	ILE	5.4
53	2y	40	ILE	5.4
44	2m	7	VAL	5.4
44	2m	66	LEU	5.4
38	2g	154	TYR	5.4
50	2s	15	LEU	5.4
53	2y	41	LEU	5.4
41	2j	62	HIS	5.3
40	2i	7	THR	5.3
6	2G	135	LEU	5.3
40	2i	8	GLY	5.3
43	2l	18	VAL	5.3
1	1A	1076	C	5.3
53	2y	50	ALA	5.3
53	2y	73	ALA	5.2
6	2G	136	ARG	5.2
21	2Z	191	VAL	5.2
44	2m	64	TRP	5.2
45	2n	36	PHE	5.2
7	2H	166	GLY	5.2
40	2i	127	LYS	5.2
50	2s	34	TRP	5.2
45	2n	21	TYR	5.2
51	1t	72	LEU	5.1
45	2n	29	ARG	5.1
7	2H	123	PHE	5.1
45	2n	38	GLY	5.1
41	1j	47	PHE	5.1
40	1i	113	LYS	5.1
50	2s	75	ALA	5.1
53	2y	78	ILE	5.1
41	2j	65	LEU	5.0
20	2Y	1	MET	5.0
26	24	50	VAL	5.0
6	2G	155	MET	5.0
44	2m	87	TYR	5.0
20	2Y	44	ILE	5.0
34	2c	157	ILE	5.0

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Mol	Chain	Res	Type	RSRZ
33	2b	122	PHE	4.9
41	2j	47	PHE	4.9
1	2A	2146	C	4.9
48	2q	36	ILE	4.9
25	23	26	LEU	4.9
50	2s	62	ILE	4.9
32	2a	1030(B)	C	4.9
34	2c	33	LEU	4.9
53	2y	51	ASP	4.9
38	2g	156	TRP	4.9
41	2j	48	THR	4.8
29	27	48	LYS	4.8
45	2n	7	ILE	4.8
43	2l	28	LYS	4.8
52	2u	2	GLY	4.8
1	2A	2139	C	4.8
36	2e	123	LEU	4.7
41	2j	54	PHE	4.7
45	2n	30	ALA	4.7
6	2G	3	LEU	4.7
43	1l	64	TYR	4.7
22	20	76	GLY	4.7
1	1A	1103	A	4.7
34	2c	186	PHE	4.7
18	2W	112	GLY	4.7
34	2c	152	ILE	4.6
29	27	1	MET	4.6
51	2t	62	LEU	4.6
45	1n	61	TRP	4.6
6	2G	41	GLN	4.6
41	2j	46	ARG	4.6
44	2m	6	GLY	4.6
41	1j	49	VAL	4.6
43	2l	19	ARG	4.6
40	2i	76	ALA	4.6
34	2c	163	ALA	4.5
48	2q	99	SER	4.5
52	2u	13	ILE	4.5
26	24	56	VAL	4.5
53	2y	48	PHE	4.5
32	2a	1030(A)	G	4.5
6	2G	133	LEU	4.5

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Mol	Chain	Res	Type	RSRZ
22	20	75	LEU	4.5
43	2l	64	TYR	4.4
1	1A	2147	G	4.4
42	2k	25	TYR	4.4
12	2Q	65	PHE	4.4
45	2n	16	PHE	4.4
45	2n	13	THR	4.4
1	1A	1089	G	4.4
6	2G	43	LEU	4.4
26	14	49	PHE	4.4
45	2n	15	LYS	4.4
51	2t	30	LYS	4.4
21	2Z	197	ILE	4.4
51	1t	18	GLN	4.4
35	2d	146	ILE	4.3
8	2I	30	LEU	4.3
13	2R	18	LEU	4.3
38	1g	16	LEU	4.3
6	2G	137	GLU	4.3
32	2a	1001(A)	G	4.3
32	2a	1257	U	4.3
51	1t	67	ALA	4.3
53	2y	7	SER	4.3
43	2l	13	LYS	4.3
45	1n	39	LEU	4.3
53	2y	77	LEU	4.3
1	2A	2602	A	4.3
47	2p	19	ILE	4.3
53	2y	12	ILE	4.3
22	20	9	SER	4.3
47	1p	49	LEU	4.3
50	2s	71	LEU	4.3
6	2G	146	TYR	4.3
36	2e	13	ILE	4.2
6	2G	90	LEU	4.2
49	1r	43	PHE	4.2
35	2d	4	TYR	4.2
19	2X	89	ILE	4.2
50	2s	52	TYR	4.2
1	1A	2143	C	4.2
26	24	51	ASP	4.2
7	2H	76	VAL	4.2

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Mol	Chain	Res	Type	RSRZ
7	2H	9	ILE	4.2
8	2I	20	ASP	4.2
38	2g	33	ASP	4.2
23	11	2	SER	4.2
47	1p	32	TYR	4.2
21	2Z	155	LEU	4.1
29	27	47	ARG	4.1
35	1d	2	GLY	4.1
8	2I	2	LYS	4.1
12	2Q	100	GLY	4.1
53	2y	10	MET	4.1
1	2A	1064	C	4.1
53	2y	52	ALA	4.1
48	2q	32	TYR	4.1
51	2t	10	LEU	4.1
40	2i	110	GLU	4.1
20	2Y	31	LEU	4.1
43	2l	5	PRO	4.1
45	1n	34	TYR	4.1
47	1p	59	TRP	4.1
19	2X	33	LYS	4.0
7	2H	24	VAL	4.0
50	2s	9	VAL	4.0
36	1e	84	PHE	4.0
26	24	45	GLY	4.0
29	27	46	VAL	4.0
45	2n	35	ARG	4.0
33	2b	115	LEU	4.0
7	2H	35	VAL	4.0
45	2n	37	PHE	4.0
39	2h	134	ILE	4.0
40	2i	63	ILE	4.0
53	2y	58	ASN	4.0
53	2y	42	SER	4.0
32	2a	1202	G	4.0
43	2l	10	LEU	4.0
32	1a	1257	U	4.0
7	2H	164	TYR	4.0
44	2m	24	GLY	4.0
21	2Z	196	VAL	3.9
52	1u	2	GLY	3.9
40	1i	108	VAL	3.9

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Mol	Chain	Res	Type	RSRZ
43	2l	32	PHE	3.9
47	2p	9	PHE	3.9
51	1t	71	THR	3.9
6	2G	62	LEU	3.9
7	2H	105	LEU	3.9
48	2q	71	PHE	3.9
6	2G	72	ARG	3.9
3	2D	221	VAL	3.9
23	1l	98	LEU	3.9
41	1j	48	THR	3.9
53	2y	74	ILE	3.9
45	1n	59	ALA	3.9
47	2p	7	ALA	3.9
1	2A	2145	C	3.9
3	2D	37	LEU	3.9
45	2n	22	THR	3.8
1	1A	2141	G	3.8
35	1d	138	TYR	3.8
22	20	8	GLY	3.8
34	2c	160	ALA	3.8
47	1p	1	MET	3.8
45	2n	25	VAL	3.8
9	2N	116	LEU	3.8
1	1A	1102	C	3.8
45	1n	36	PHE	3.8
6	2G	87	PRO	3.8
33	2b	201	ILE	3.8
51	1t	66	ALA	3.8
51	2t	76	ALA	3.8
34	2c	162	GLN	3.8
17	2V	72	VAL	3.8
40	1i	111	ARG	3.8
32	2a	1036	G	3.8
7	2H	82	GLY	3.8
51	2t	71	THR	3.8
40	2i	36	TYR	3.8
45	1n	21	TYR	3.8
45	1n	30	ALA	3.8
53	2y	62	VAL	3.8
7	2H	129	THR	3.8
34	2c	149	ALA	3.7
47	1p	7	ALA	3.7

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Mol	Chain	Res	Type	RSRZ
53	2y	63	ALA	3.7
32	1a	1030(B)	C	3.7
32	2a	1030	C	3.7
35	2d	64	LEU	3.7
7	2H	121	ILE	3.7
17	2V	71	LEU	3.7
8	2I	1	MET	3.7
46	2o	87	ILE	3.7
50	2s	49	ILE	3.7
51	1t	73	HIS	3.7
22	20	52	GLY	3.7
53	2y	72	THR	3.7
51	2t	59	ALA	3.7
44	1m	87	TYR	3.7
45	2n	41	ARG	3.7
33	1b	118	LEU	3.7
39	1h	2	LEU	3.7
53	2y	61	LEU	3.7
23	21	70	VAL	3.7
31	29	13	LYS	3.7
40	2i	72	GLY	3.7
40	2i	33	PHE	3.7
7	2H	89	ILE	3.7
34	2c	174	PRO	3.7
53	2y	88	LEU	3.7
8	1I	3	VAL	3.7
31	29	16	VAL	3.7
39	1h	137	VAL	3.7
45	1n	18	VAL	3.7
26	24	40	HIS	3.7
50	2s	80	TYR	3.7
39	2h	135	CYS	3.7
40	2i	69	GLY	3.7
30	28	60	LEU	3.7
40	2i	120	ARG	3.7
11	2P	71	VAL	3.7
20	2Y	42	VAL	3.7
45	2n	10	ALA	3.7
30	28	58	ILE	3.6
47	2p	33	ILE	3.6
7	2H	101	ARG	3.6
20	2Y	35	TYR	3.6

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Mol	Chain	Res	Type	RSRZ
40	1i	114	TYR	3.6
7	2H	103	LEU	3.6
6	2G	149	VAL	3.6
40	2i	46	ALA	3.6
44	2m	4	ILE	3.6
38	2g	78	ARG	3.6
40	1i	126	SER	3.6
34	2c	57	ILE	3.6
44	2m	111	LYS	3.6
53	2y	8	LYS	3.6
40	2i	88	TYR	3.6
34	2c	190	ARG	3.6
34	1c	2	GLY	3.6
19	2X	39	ILE	3.6
1	1A	1064	C	3.6
1	1A	2142	C	3.6
40	2i	125	TYR	3.6
45	2n	23	ARG	3.6
22	20	10	THR	3.6
24	22	25	VAL	3.6
39	1h	93	VAL	3.6
1	2A	1067	A	3.6
3	2D	106	ILE	3.6
14	2S	82	ILE	3.6
3	2D	276	LYS	3.6
25	23	6	VAL	3.6
34	2c	159	GLY	3.6
41	1j	44	VAL	3.6
21	2Z	199	LYS	3.6
15	2T	105	LEU	3.6
30	28	24	ALA	3.6
40	1i	46	ALA	3.6
51	1t	80	ARG	3.5
3	2D	225	ALA	3.5
25	23	54	VAL	3.5
48	2q	23	VAL	3.5
45	2n	39	LEU	3.5
22	20	74	ARG	3.5
1	2A	1075	C	3.5
7	2H	107	VAL	3.5
34	2c	184	TYR	3.5
30	28	21	LYS	3.5

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Mol	Chain	Res	Type	RSRZ
41	2j	50	ILE	3.5
47	1p	48	TRP	3.5
53	2y	39	ILE	3.5
13	2R	68	ARG	3.5
34	2c	87	LEU	3.5
35	2d	101	LEU	3.5
41	2j	49	VAL	3.5
35	1d	101	LEU	3.5
49	2r	85	LEU	3.5
48	2q	10	VAL	3.5
26	24	55	ARG	3.5
39	2h	83	ILE	3.5
47	2p	6	LEU	3.5
38	2g	7	ALA	3.5
33	2b	131	PRO	3.5
51	2t	79	ARG	3.5
35	2d	5	ILE	3.5
50	2s	79	THR	3.5
42	2k	126	ARG	3.5
50	2s	56	GLN	3.5
35	2d	2	GLY	3.5
43	2l	96	VAL	3.5
44	2m	60	VAL	3.5
44	2m	106	ASN	3.5
47	1p	35	LYS	3.5
22	20	78	TYR	3.4
45	2n	8	GLU	3.4
7	2H	84	SER	3.4
1	2A	2147	G	3.4
34	2c	8	ILE	3.4
1	2A	2138	C	3.4
34	2c	32	LEU	3.4
45	2n	44	LEU	3.4
22	20	46	LYS	3.4
29	17	48	LYS	3.4
20	2Y	5	MET	3.4
50	2s	11	VAL	3.4
18	2W	92	ARG	3.4
51	2t	34	LYS	3.4
35	1d	157	LEU	3.4
44	2m	96	LEU	3.4
21	2Z	192	ALA	3.4

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Mol	Chain	Res	Type	RSRZ
14	2S	12	PHE	3.4
35	2d	96	LEU	3.4
39	2h	133	LEU	3.4
44	2m	81	LEU	3.4
45	1n	29	ARG	3.4
4	2E	134	ILE	3.4
35	2d	70	ILE	3.4
8	2I	38	LEU	3.4
34	2c	200	ALA	3.4
1	1A	1077	A	3.4
47	1p	51	VAL	3.4
40	1i	107	ARG	3.4
43	1l	63	GLY	3.4
40	2i	50	LEU	3.4
40	2i	71	SER	3.4
44	2m	90	LEU	3.4
51	1t	76	ALA	3.4
6	2G	154	GLY	3.3
23	2l	26	ARG	3.3
39	2h	85	ARG	3.3
44	2m	88	ARG	3.3
50	2s	41	VAL	3.3
42	2k	13	GLN	3.3
1	2A	2153	G	3.3
32	1a	1036	G	3.3
50	2s	35	SER	3.3
6	2G	144	ILE	3.3
25	23	31	LEU	3.3
14	2S	33	LYS	3.3
25	23	17	LYS	3.3
40	2i	119	ALA	3.3
51	2t	78	ALA	3.3
41	2j	64	GLU	3.3
45	2n	27	CYS	3.3
6	2G	112	PRO	3.3
8	1I	38	LEU	3.3
44	1m	90	LEU	3.3
3	2D	2	ALA	3.3
23	2l	71	TYR	3.3
45	1n	38	GLY	3.3
16	2U	90	VAL	3.3
41	2j	34	VAL	3.3

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Mol	Chain	Res	Type	RSRZ
25	23	12	PRO	3.3
35	2d	75	PHE	3.3
40	2i	66	ARG	3.3
45	1n	26	ARG	3.3
45	1n	7	ILE	3.3
51	2t	84	LEU	3.3
1	2A	1026	U	3.3
7	2H	85	LYS	3.3
42	2k	109	VAL	3.3
6	2G	106	LEU	3.3
44	2m	84	ILE	3.3
34	2c	185	GLY	3.3
40	1i	112	LYS	3.3
38	2g	40	ALA	3.3
41	1j	54	PHE	3.3
52	1u	18	TYR	3.3
35	2d	8	VAL	3.3
39	1h	133	LEU	3.2
51	1t	20	LEU	3.2
51	2t	72	LEU	3.2
40	1i	76	ALA	3.2
44	2m	75	ALA	3.2
45	1n	22	THR	3.2
53	2y	5	ILE	3.2
22	20	77	ARG	3.2
33	2b	92	TYR	3.2
35	2d	38	TYR	3.2
53	2y	76	GLU	3.2
48	2q	84	LEU	3.2
40	2i	18	PHE	3.2
45	1n	2	ALA	3.2
34	1c	193	TYR	3.2
42	1k	25	TYR	3.2
8	2I	37	VAL	3.2
23	11	70	VAL	3.2
13	2R	10	LEU	3.2
43	1l	91	LYS	3.2
51	1t	68	LYS	3.2
44	2m	42	ALA	3.2
34	1c	39	ILE	3.2
1	1A	1075	C	3.2
36	1e	133	TYR	3.2

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Mol	Chain	Res	Type	RSRZ
23	2l	4	VAL	3.2
39	2h	53	VAL	3.2
34	2c	60	ALA	3.2
8	2I	4	ILE	3.2
34	1c	10	PHE	3.2
50	2s	31	ILE	3.2
3	2D	35	LYS	3.2
50	2s	57	HIS	3.2
53	2y	38	HIS	3.2
20	2Y	45	VAL	3.2
34	2c	66	VAL	3.2
40	2i	5	TYR	3.2
34	2c	196	LEU	3.2
33	2b	133	LYS	3.2
45	2n	11	LYS	3.2
48	2q	27	PHE	3.2
43	2l	15	ARG	3.2
47	2p	59	TRP	3.2
1	1A	2116	G	3.2
7	2H	87	LEU	3.2
41	1j	57	LYS	3.2
50	2s	30	LEU	3.2
39	2h	84	ARG	3.2
40	2i	111	ARG	3.2
47	2p	26	ARG	3.2
41	2j	23	ILE	3.2
41	2j	74	ILE	3.2
43	2l	8	ASN	3.2
40	2i	113	LYS	3.2
6	2G	131	TYR	3.1
45	2n	53	LEU	3.2
1	1A	1092	C	3.1
31	29	17	ILE	3.1
7	1H	2	SER	3.1
38	2g	32	ARG	3.1
34	2c	153	VAL	3.1
6	2G	158	ALA	3.1
6	2G	85	GLY	3.1
29	17	1	MET	3.1
1	2A	2169	A	3.1
45	2n	31	ARG	3.1
6	2G	151	ALA	3.1

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Mol	Chain	Res	Type	RSRZ
7	2H	25	LYS	3.1
11	2P	59	LEU	3.1
31	29	15	LYS	3.1
35	2d	166	LYS	3.1
51	2t	29	LYS	3.1
45	2n	55	GLY	3.1
1	2A	1076	C	3.1
30	28	61	LEU	3.1
34	2c	167	TRP	3.1
38	2g	116	ALA	3.1
48	2q	73	VAL	3.1
38	2g	41	ARG	3.1
46	2o	64	ARG	3.1
3	2D	6	PHE	3.1
51	2t	33	ILE	3.1
3	1D	275	LYS	3.1
19	2X	66	LEU	3.1
3	2D	34	VAL	3.1
7	2H	169	VAL	3.1
10	2O	57	VAL	3.1
26	24	44	THR	3.1
43	2l	6	THR	3.1
44	2m	116	THR	3.1
49	1r	79	LEU	3.1
16	2U	40	PHE	3.1
40	2i	92	TYR	3.1
53	2y	71	TYR	3.1
1	2A	2140	C	3.1
21	2Z	125	LEU	3.1
26	24	52	THR	3.1
35	2d	157	LEU	3.1
46	2o	48	LYS	3.1
1	2A	2144	U	3.1
34	2c	48	TYR	3.1
39	2h	35	ILE	3.1
40	2i	73	GLN	3.1
44	2m	104	ARG	3.1
39	2h	56	LYS	3.1
43	1l	23	LYS	3.1
7	2H	88	LEU	3.1
15	1T	114	LEU	3.1
51	1t	59	ALA	3.1

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Mol	Chain	Res	Type	RSRZ
33	1b	131	PRO	3.0
23	2l	61	ARG	3.0
14	2S	73	LEU	3.0
52	2u	15	ARG	3.0
5	2F	82	ILE	3.0
35	2d	204	ILE	3.0
36	1e	131	ILE	3.0
39	2h	45	ILE	3.0
48	1q	27	PHE	3.0
50	2s	53	ASN	3.0
50	2s	82	GLY	3.0
44	2m	69	GLU	3.0
22	20	55	ARG	3.0
52	2u	10	ARG	3.0
6	2G	74	LYS	3.0
23	2l	62	VAL	3.0
1	1A	1066	U	3.0
44	1m	22	ILE	3.0
11	2P	15	ARG	3.0
39	2h	4	ASP	3.0
40	1i	116	LYS	3.0
48	2q	37	LYS	3.0
51	1t	22	ARG	3.0
52	2u	6	ARG	3.0
34	1c	33	LEU	3.0
48	2q	31	LEU	3.0
9	2N	46	VAL	3.0
35	2d	67	ILE	3.0
26	24	43	TYR	3.0
16	2U	48	ALA	3.0
40	1i	15	ALA	3.0
43	2l	26	ALA	3.0
47	1p	6	LEU	3.0
48	2q	30	PRO	3.0
1	2A	2174	C	3.0
34	2c	199	LYS	3.0
23	2l	7	ILE	3.0
34	2c	77	ILE	3.0
19	2X	69	TYR	3.0
41	1j	59	SER	3.0
35	2d	202	LEU	3.0
36	1e	123	LEU	3.0

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Mol	Chain	Res	Type	RSRZ
51	2t	21	LYS	3.0
34	2c	164	ARG	3.0
41	2j	93	GLY	3.0
1	2A	2116	G	3.0
1	2A	2154	G	3.0
53	2y	3	MET	3.0
21	2Z	53	ILE	3.0
39	1h	109	ILE	3.0
41	1j	63	PHE	3.0
46	1o	87	ILE	3.0
6	2G	173	LEU	3.0
8	2I	5	LEU	3.0
41	2j	45	ARG	3.0
51	2t	83	ARG	3.0
7	2H	141	VAL	2.9
12	2Q	68	ILE	2.9
45	1n	31	ARG	2.9
51	2t	66	ALA	2.9
51	2t	80	ARG	2.9
25	23	9	VAL	2.9
20	2Y	75	ILE	2.9
39	2h	111	ILE	2.9
47	2p	4	ILE	2.9
45	1n	32	SER	2.9
25	23	30	ARG	2.9
26	24	36	CYS	2.9
1	1A	888	C	2.9
23	11	71	TYR	2.9
23	21	68	PRO	2.9
23	21	73	LEU	2.9
34	2c	65	ALA	2.9
50	1s	77	THR	2.9
6	2G	58	GLN	2.9
40	2i	10	ARG	2.9
13	2R	83	ILE	2.9
33	2b	162	ILE	2.9
39	1h	86	ILE	2.9
30	28	38	GLY	2.9
34	1c	159	GLY	2.9
7	2H	27	LYS	2.9
7	2H	71	LEU	2.9
18	2W	82	LEU	2.9

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Mol	Chain	Res	Type	RSRZ
38	1g	12	LEU	2.9
51	1t	21	LYS	2.9
53	1y	88	LEU	2.9
1	1A	2159	G	2.9
44	2m	92	HIS	2.9
39	2h	103	VAL	2.9
50	2s	67	VAL	2.9
52	2u	9	ARG	2.9
53	1y	95	ARG	2.9
1	1A	2602	A	2.9
51	1t	70	SER	2.9
17	2V	75	PHE	2.9
40	1i	37	PHE	2.9
51	2t	55	ILE	2.9
34	2c	2	GLY	2.9
40	2i	116	LYS	2.9
51	1t	69	GLY	2.9
34	2c	188	LEU	2.9
36	1e	43	LEU	2.9
43	2l	62	SER	2.9
3	2D	271	ILE	2.9
46	1o	89	GLY	2.9
7	2H	167	GLU	2.9
8	2I	12	LEU	2.9
30	28	50	LEU	2.9
35	1d	179	GLU	2.9
39	2h	112	LEU	2.9
41	2j	40	LEU	2.9
45	1n	23	ARG	2.9
51	1t	32	ALA	2.9
53	2y	67	HIS	2.9
4	2E	151	TYR	2.9
7	2H	94	TYR	2.9
3	2D	51	VAL	2.9
6	2G	159	VAL	2.9
8	2I	18	VAL	2.9
8	2I	21	VAL	2.9
47	2p	20	VAL	2.9
51	2t	9	ASN	2.9
22	20	69	PHE	2.9
50	2s	74	PHE	2.9
52	1u	10	ARG	2.9

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Mol	Chain	Res	Type	RSRZ
3	2D	155	LEU	2.9
23	21	46	LEU	2.9
25	23	53	LEU	2.9
50	2s	16	LEU	2.9
7	2H	131	VAL	2.8
53	2y	70	MET	2.8
18	2W	51	LEU	2.8
32	1a	1001	A	2.8
34	2c	175	LEU	2.8
50	2s	64	GLU	2.8
8	2I	25	TYR	2.8
33	2b	137	ARG	2.8
42	2k	75	TYR	2.8
48	2q	42	TYR	2.8
16	2U	17	ILE	2.8
50	2s	76	PRO	2.8
51	1t	29	LYS	2.8
36	1e	105	VAL	2.8
35	1d	70	ILE	2.8
39	2h	119	LEU	2.8
19	2X	68	ARG	2.8
46	2o	47	LYS	2.8
53	1y	91	LYS	2.8
45	1n	60	SER	2.8
3	2D	16	MET	2.8
39	2h	93	VAL	2.8
30	28	64	TYR	2.8
39	2h	58	TYR	2.8
16	2U	41	ALA	2.8
22	20	72	ARG	2.8
38	2g	6	ARG	2.8
51	2t	22	ARG	2.8
22	20	21	LEU	2.8
40	1i	79	LEU	2.8
40	1i	78	LYS	2.8
52	1u	3	LYS	2.8
7	2H	130	ARG	2.8
38	2g	85	TYR	2.8
41	2j	60	ARG	2.8
36	2e	86	ALA	2.8
23	11	46	LEU	2.8
45	1n	53	LEU	2.8

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Mol	Chain	Res	Type	RSRZ
43	2l	23	LYS	2.8
31	29	1	MET	2.8
35	2d	140	VAL	2.8
40	2i	41	VAL	2.8
7	2H	102	ALA	2.8
39	2h	3	THR	2.8
53	2y	4	ASN	2.8
21	2Z	76	LEU	2.8
51	1t	13	LEU	2.8
7	2H	29	PRO	2.8
44	2m	17	VAL	2.7
36	2e	109	ILE	2.7
40	1i	11	LYS	2.7
35	1d	110	PHE	2.7
40	2i	74	ILE	2.7
48	2q	90	ILE	2.7
16	2U	39	LEU	2.7
35	2d	11	LEU	2.7
45	1n	57	ARG	2.7
1	2A	2162	G	2.7
7	2H	116	GLU	2.7
35	2d	184	LYS	2.7
40	1i	26	VAL	2.7
41	2j	72	VAL	2.7
1	1A	2132	U	2.7
23	2l	60	PHE	2.7
38	2g	120	ILE	2.7
39	2h	86	ILE	2.7
44	2m	94	ARG	2.7
45	1n	24	CYS	2.7
47	1p	17	TYR	2.7
34	2c	22	TRP	2.7
50	2s	40	ILE	2.7
35	1d	176	LEU	2.7
36	2e	92	LYS	2.7
1	1A	2107	C	2.7
40	1i	14	VAL	2.7
16	2U	46	ALA	2.7
44	2m	20	THR	2.7
48	2q	24	GLU	2.7
25	23	23	LEU	2.7
25	23	28	LEU	2.7

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Mol	Chain	Res	Type	RSRZ
35	2d	78	LEU	2.7
9	2N	104	LYS	2.7
45	2n	58	LYS	2.7
45	1n	51	GLY	2.7
4	2E	116	VAL	2.7
40	2i	26	VAL	2.7
45	2n	33	VAL	2.7
6	2G	73	ALA	2.7
34	2c	4	LYS	2.7
45	1n	17	LYS	2.7
22	20	45	PHE	2.7
30	28	48	PHE	2.7
45	1n	37	PHE	2.7
47	1p	38	TYR	2.7
6	2G	29	TRP	2.7
5	2F	76	GLY	2.7
25	23	29	ARG	2.7
32	2a	1001	A	2.7
41	1j	60	ARG	2.7
53	2y	87	LYS	2.7
43	2l	9	GLN	2.7
33	2b	70	PHE	2.7
25	23	15	TYR	2.7
7	2H	128	PRO	2.7
41	1j	10	GLY	2.7
51	1t	9	ASN	2.7
13	2R	69	ASP	2.7
40	2i	64	THR	2.7
53	2y	93	GLU	2.7
3	2D	204	ILE	2.7
44	1m	110	ARG	2.7
11	2P	109	GLY	2.7
8	1I	20	ASP	2.7
25	23	25	ALA	2.6
36	2e	21	ALA	2.6
1	2A	2506	U	2.6
17	2V	74	LYS	2.6
40	1i	7	THR	2.6
44	2m	103	THR	2.6
7	2H	171	LEU	2.6
35	2d	120	LEU	2.6
48	2q	29	HIS	2.6

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Mol	Chain	Res	Type	RSRZ
16	2U	43	GLY	2.6
40	2i	59	PHE	2.6
33	1b	133	LYS	2.6
33	2b	130	ARG	2.6
48	2q	68	ARG	2.6
39	2h	61	VAL	2.6
6	2G	88	ILE	2.6
31	19	17	ILE	2.6
35	2d	21	LEU	2.6
40	1i	63	ILE	2.6
45	1n	44	LEU	2.6
47	1p	36	ILE	2.6
1	2A	34	C	2.6
32	1a	63	C	2.6
34	1c	7	PRO	2.6
21	2Z	179	ASP	2.6
7	2H	163	TYR	2.6
16	2U	45	TYR	2.6
50	2s	66	MET	2.6
32	1a	309	G	2.6
5	2F	49	ALA	2.6
22	10	8	GLY	2.6
34	2c	177	THR	2.6
35	2d	149	ALA	2.6
51	1t	95	ALA	2.6
8	2I	140	LEU	2.6
44	1m	19	LEU	2.6
6	2G	150	ASP	2.6
14	2S	3	ARG	2.6
35	2d	73	ARG	2.6
51	1t	23	ARG	2.6
7	2H	83	TYR	2.6
23	2l	8	SER	2.6
3	2D	166	GLN	2.6
5	2F	89	VAL	2.6
48	2q	5	VAL	2.6
53	1y	60	VAL	2.6
53	2y	9	GLN	2.6
50	2s	33	THR	2.6
8	2I	35	LEU	2.6
33	2b	142	LEU	2.6
34	2c	101	LEU	2.6

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Mol	Chain	Res	Type	RSRZ
39	1h	63	LEU	2.6
48	1q	84	LEU	2.6
21	2Z	146	ILE	2.6
36	1e	118	ILE	2.6
1	2A	2142	C	2.6
35	2d	54	TYR	2.6
43	1l	98	TYR	2.6
23	21	48	LYS	2.6
25	23	20	LYS	2.6
40	1i	118	LYS	2.6
19	2X	83	VAL	2.6
21	2Z	188	ALA	2.6
30	28	23	VAL	2.6
31	29	7	VAL	2.6
31	29	12	ASP	2.6
38	2g	2	ALA	2.6
38	2g	25	ALA	2.6
43	1l	96	VAL	2.6
45	1n	41	ARG	2.6
19	2X	13	LEU	2.6
30	18	60	LEU	2.6
48	2q	22	LEU	2.6
33	2b	181	PHE	2.6
52	1u	13	ILE	2.6
40	1i	127	LYS	2.6
44	2m	82	MET	2.6
38	2g	34	GLY	2.6
51	2t	73	HIS	2.6
8	2I	26	ALA	2.6
39	2h	28	ALA	2.6
39	2h	51	VAL	2.6
34	1c	12	LEU	2.6
35	2d	136	PRO	2.6
43	2l	84	LEU	2.6
6	2G	23	PHE	2.6
24	22	41	ILE	2.6
40	1i	77	ILE	2.6
44	2m	101	GLN	2.6
3	2D	170	GLY	2.6
32	2a	994	A	2.6
32	2a	1321	C	2.6
40	2i	65	VAL	2.5

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Mol	Chain	Res	Type	RSRZ
48	1q	7	THR	2.5
7	2H	33	LEU	2.5
22	20	59	LEU	2.5
44	2m	56	LEU	2.5
9	2N	16	ILE	2.5
44	2m	108	ARG	2.5
45	2n	49	HIS	2.5
44	2m	107	ALA	2.5
45	2n	50	LYS	2.5
3	2D	40	THR	2.5
23	21	49	VAL	2.5
35	2d	112	VAL	2.5
38	2g	80	VAL	2.5
41	2j	8	LEU	2.5
45	2n	56	VAL	2.5
35	2d	118	ARG	2.5
38	2g	95	ARG	2.5
39	1h	134	ILE	2.5
39	2h	100	ILE	2.5
34	2c	201	TYR	2.5
6	2G	160	VAL	2.5
16	1U	9	VAL	2.5
23	21	30	VAL	2.5
33	2b	71	VAL	2.5
32	2a	1223	C	2.5
34	1c	196	LEU	2.5
45	2n	45	ARG	2.5
43	2l	16	GLU	2.5
48	2q	43	LEU	2.5
48	2q	78	GLU	2.5
23	11	60	PHE	2.5
38	1g	43	PHE	2.5
40	2i	81	ILE	2.5
48	2q	65	ILE	2.5
9	2N	74	ARG	2.5
45	2n	59	ALA	2.5
50	2s	36	ARG	2.5
52	1u	15	ARG	2.5
50	2s	39	THR	2.5
53	2y	11	GLU	2.5
35	2d	68	TYR	2.5
3	2D	182	LEU	2.5

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Mol	Chain	Res	Type	RSRZ
8	1I	19	VAL	2.5
33	2b	121	LEU	2.5
35	2d	162	LEU	2.5
40	1i	47	LEU	2.5
40	1i	75	ASP	2.5
40	2i	47	LEU	2.5
41	2j	58	ASP	2.5
30	28	9	GLY	2.5
36	2e	29	GLY	2.5
16	1U	117	GLN	2.5
38	2g	8	GLU	2.5
7	2H	140	LYS	2.5
39	2h	124	ALA	2.5
52	2u	17	THR	2.5
8	2I	47	LEU	2.5
13	1R	10	LEU	2.5
29	17	31	LEU	2.5
31	29	37	GLY	2.5
34	2c	193	TYR	2.5
35	1d	108	LEU	2.5
1	2A	1046	A	2.5
1	2A	2173	A	2.5
9	2N	51	PHE	2.5
53	2y	64	SER	2.5
32	2a	1224	G	2.5
51	1t	30	LYS	2.5
5	1F	166	ALA	2.5
34	1c	200	ALA	2.5
33	1b	148	TYR	2.5
37	1f	6	VAL	2.5
38	2g	9	VAL	2.5
1	1A	2506	U	2.5
15	2T	108	ARG	2.5
47	1p	4	ILE	2.5
6	1G	73	ALA	2.5
36	1e	22	GLY	2.5
42	2k	89	ALA	2.5
53	2y	92	GLY	2.5
40	2i	40	LEU	2.4
44	2m	99	ARG	2.4
48	2q	6	LEU	2.4
49	2r	58	LEU	2.4

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Mol	Chain	Res	Type	RSRZ
51	1t	34	LYS	2.4
52	2u	22	ARG	2.4
31	29	24	TYR	2.4
46	2o	60	VAL	2.4
48	2q	21	VAL	2.4
33	2b	97	TRP	2.4
15	2T	102	ILE	2.4
46	1o	82	ILE	2.4
35	2d	144	ASP	2.4
7	2H	170	ARG	2.4
12	2Q	59	ARG	2.4
16	2U	113	ALA	2.4
20	2Y	36	ALA	2.4
34	1c	168	ALA	2.4
44	2m	76	ALA	2.4
41	2j	68	HIS	2.4
49	2r	87	ARG	2.4
19	1X	66	LEU	2.4
43	2l	52	LEU	2.4
33	2b	164	VAL	2.4
48	2q	95	TYR	2.4
9	2N	85	ILE	2.4
26	14	59	PHE	2.4
26	24	15	ILE	2.4
7	2H	132	ARG	2.4
22	20	73	GLY	2.4
34	2c	3	ASN	2.4
48	2q	93	GLN	2.4
52	1u	17	THR	2.4
6	2G	103	LEU	2.4
8	1I	9	LEU	2.4
51	2t	24	LEU	2.4
5	2F	97	TYR	2.4
32	2a	1030(C)	G	2.4
6	2G	141	PHE	2.4
33	1b	214	ILE	2.4
40	2i	78	LYS	2.4
41	2j	38	ILE	2.4
51	2t	41	ILE	2.4
45	2n	26	ARG	2.4
50	2s	81	ARG	2.4
44	2m	89	GLY	2.4

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Mol	Chain	Res	Type	RSRZ
3	2D	259	THR	2.4
35	1d	111	ALA	2.4
43	2l	68	ALA	2.4
34	2c	166	GLU	2.4
34	2c	206	GLU	2.4
38	2g	99	LEU	2.4
53	2y	24	LEU	2.4
7	2H	114	VAL	2.4
14	2S	57	LYS	2.4
23	2l	51	VAL	2.4
31	29	25	VAL	2.4
34	1c	120	VAL	2.4
26	24	46	GLN	2.4
34	2c	28	GLN	2.4
41	1j	46	ARG	2.4
41	2j	6	ILE	2.4
33	2b	152	PHE	2.4
20	2Y	29	GLU	2.4
26	24	57	GLU	2.4
30	28	7	HIS	2.4
44	2m	67	GLU	2.4
41	2j	55	LYS	2.4
53	2y	80	LYS	2.4
1	1A	1088	A	2.4
3	2D	215	LEU	2.4
6	2G	175	LEU	2.4
9	2N	23	LEU	2.4
14	2S	32	LEU	2.4
16	2U	27	LEU	2.4
20	2Y	106	LEU	2.4
45	2n	47	LEU	2.4
3	2D	127	VAL	2.4
16	2U	63	VAL	2.4
22	20	51	VAL	2.4
6	2G	42	GLY	2.4
7	2H	148	ILE	2.4
34	2c	23	TYR	2.4
26	24	7	PRO	2.4
50	2s	10	PHE	2.4
4	2E	131	ALA	2.4
15	2T	90	GLN	2.4
15	2T	106	SER	2.4

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Mol	Chain	Res	Type	RSRZ
44	2m	110	ARG	2.4
15	2T	114	LEU	2.4
46	2o	34	LEU	2.4
40	2i	28	VAL	2.4
53	1y	87	LYS	2.4
7	2H	154	PRO	2.4
14	2S	92	TYR	2.4
19	1X	1	MET	2.4
28	26	54	ILE	2.4
45	2n	54	PRO	2.4
35	2d	115	ARG	2.4
40	2i	9	ARG	2.4
47	2p	18	ARG	2.4
47	2p	56	ALA	2.4
51	2t	11	SER	2.4
28	26	11	LEU	2.4
39	1h	112	LEU	2.4
11	2P	37	GLY	2.3
22	20	42	GLY	2.3
40	2i	70	LYS	2.3
46	2o	86	GLY	2.3
50	2s	72	GLY	2.3
39	1h	103	VAL	2.3
48	2q	57	VAL	2.3
53	2y	60	VAL	2.3
32	2a	1531	A	2.3
48	1q	28	PRO	2.3
3	2D	217	ARG	2.3
6	2G	80	PHE	2.3
8	2I	14	ASP	2.3
10	2O	81	ASP	2.3
36	2e	84	PHE	2.3
40	1i	128	ARG	2.3
12	2Q	9	TYR	2.3
8	2I	36	ALA	2.3
13	2R	51	LEU	2.3
1	1A	2115	G	2.3
8	2I	107	VAL	2.3
33	2b	127	ILE	2.3
42	2k	104	GLN	2.3
44	2m	78	ILE	2.3
3	2D	159	ALA	2.3

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Mol	Chain	Res	Type	RSRZ
23	11	91	LYS	2.3
29	17	45	ALA	2.3
30	28	59	LYS	2.3
39	2h	94	TYR	2.3
51	1t	14	LYS	2.3
41	2j	59	SER	2.3
5	2F	41	LEU	2.3
6	1G	82	LEU	2.3
17	1V	71	LEU	2.3
43	2l	27	LEU	2.3
48	1q	6	LEU	2.3
31	29	19	ARG	2.3
34	1c	35	GLU	2.3
13	2R	39	PRO	2.3
17	2V	47	VAL	2.3
53	2y	37	PRO	2.3
3	2D	5	LYS	2.3
5	2F	64	ILE	2.3
9	2N	71	ILE	2.3
25	23	13	ILE	2.3
1	1A	2145	C	2.3
3	2D	15	PHE	2.3
1	2A	229	A	2.3
41	1j	20	ALA	2.3
3	1D	243	GLY	2.3
12	1Q	100	GLY	2.3
14	2S	22	GLY	2.3
48	1q	33	GLY	2.3
22	20	11	ARG	2.3
33	2b	44	LEU	2.3
34	2c	179	ARG	2.3
38	2g	22	LEU	2.3
47	1p	73	LEU	2.3
36	2e	88	LYS	2.3
21	2Z	161	VAL	2.3
34	1c	167	TRP	2.3
41	2j	53	PRO	2.3
7	2H	41	MET	2.3
53	1y	70	MET	2.3
22	20	36	ILE	2.3
42	1k	21	ILE	2.3
44	1m	4	ILE	2.3

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Mol	Chain	Res	Type	RSRZ
44	2m	25	ILE	2.3
53	2y	54	ILE	2.3
6	2G	134	GLY	2.3
6	2G	161	THR	2.3
32	2a	1220	G	2.3
34	2c	29	TYR	2.3
39	2h	122	ARG	2.3
47	2p	22	THR	2.3
3	2D	147	LEU	2.3
6	2G	7	LEU	2.3
10	2O	8	LEU	2.3
12	2Q	118	LEU	2.3
40	2i	19	LEU	2.3
50	2s	83	HIS	2.3
5	2F	81	PRO	2.3
7	2H	99	VAL	2.3
12	2Q	97	VAL	2.3
26	24	5	ILE	2.3
30	28	16	ILE	2.3
39	2h	13	ILE	2.3
47	1p	37	GLY	2.3
50	2s	78	ARG	2.3
3	2D	153	ALA	2.3
34	1c	201	TYR	2.3
3	2D	61	LEU	2.3
40	1i	19	LEU	2.3
44	1m	96	LEU	2.3
47	2p	73	LEU	2.3
7	2H	32	GLU	2.3
41	2j	97	GLU	2.3
21	2Z	180	VAL	2.3
33	2b	197	VAL	2.3
1	1A	2144	U	2.3
6	1G	136	ARG	2.3
41	2j	66	ARG	2.3
6	2G	75	LYS	2.3
7	2H	30	LYS	2.3
13	2R	1	MET	2.3
12	2Q	117	ALA	2.3
13	2R	109	ALA	2.3
16	2U	25	TRP	2.3
36	2e	17	ALA	2.3

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Mol	Chain	Res	Type	RSRZ
51	2t	18	GLN	2.3
40	1i	117	HIS	2.3
50	2s	14	HIS	2.3
6	1G	25	TYR	2.3
1	1A	2108	C	2.3
6	2G	34	LEU	2.3
19	1X	70	LEU	2.3
36	2e	151	LEU	2.3
41	1j	40	LEU	2.3
35	1d	73	ARG	2.2
39	2h	91	ARG	2.2
47	1p	50	LYS	2.2
51	2t	25	ARG	2.2
1	1A	2155	G	2.2
1	2A	2148	G	2.2
4	2E	150	VAL	2.2
19	2X	54	VAL	2.2
20	2Y	15	VAL	2.2
33	2b	136	VAL	2.2
43	1l	18	VAL	2.2
43	2l	90	VAL	2.2
53	2y	65	GLY	2.2
34	2c	17	ASP	2.2
19	2X	80	ILE	2.2
34	1c	160	ALA	2.2
47	2p	48	TRP	2.2
4	1E	195	LEU	2.2
11	2P	79	ARG	2.2
18	2W	19	LEU	2.2
23	1l	95	LEU	2.2
35	1d	11	LEU	2.2
35	1d	174	LEU	2.2
35	2d	108	LEU	2.2
44	2m	3	ARG	2.2
52	1u	22	ARG	2.2
1	1A	2117	A	2.2
7	2H	144	VAL	2.2
32	2a	1031	G	2.2
53	2y	82	GLU	2.2
15	2T	110	ILE	2.2
20	2Y	61	ILE	2.2
36	1e	109	ILE	2.2

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Mol	Chain	Res	Type	RSRZ
42	1k	126	ARG	2.2
47	1p	42	ARG	2.2
51	1t	79	ARG	2.2
10	2O	25	LEU	2.2
14	2S	56	LEU	2.2
33	2b	149	LEU	2.2
35	2d	186	LEU	2.2
39	2h	48	TYR	2.2
47	1p	39	TYR	2.2
35	2d	183	GLY	2.2
49	1r	48	GLY	2.2
1	1A	2114	A	2.2
22	20	53	MET	2.2
26	14	50	VAL	2.2
47	1p	2	VAL	2.2
48	2q	9	VAL	2.2
32	2a	1236	A	2.2
4	1E	4	ILE	2.2
4	2E	149	ARG	2.2
7	2H	95	ARG	2.2
33	1b	130	ARG	2.2
33	2b	120	ALA	2.2
35	2d	35	ARG	2.2
38	2g	5	ARG	2.2
7	2H	117	PRO	2.2
15	2T	99	LEU	2.2
40	2i	124	GLN	2.2
47	1p	29	ASP	2.2
11	2P	110	TYR	2.2
38	2g	36	LYS	2.2
39	1h	58	TYR	2.2
48	2q	87	LYS	2.2
33	2b	233	SER	2.2
1	1A	2161	C	2.2
1	2A	2585	U	2.2
1	2A	2804	C	2.2
6	2G	15	VAL	2.2
23	11	4	VAL	2.2
24	22	1	MET	2.2
33	2b	101	MET	2.2
48	2q	11	VAL	2.2
4	2E	114	ALA	2.2

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Mol	Chain	Res	Type	RSRZ
10	2O	41	ALA	2.2
12	2Q	121	ALA	2.2
3	2D	17	THR	2.2
3	2D	50	THR	2.2
31	19	26	ILE	2.2
36	2e	89	ILE	2.2
43	1l	7	ILE	2.2
14	2S	29	PHE	2.2
34	2c	10	PHE	2.2
6	2G	94	LEU	2.2
33	2b	139	LYS	2.2
34	2c	26	LYS	2.2
35	2d	143	GLY	2.2
41	2j	41	PRO	2.2
51	1t	10	LEU	2.2
52	2u	12	LYS	2.2
26	24	63	TYR	2.2
44	2m	23	TYR	2.2
46	2o	68	ARG	2.2
39	1h	87	SER	2.2
30	28	25	MET	2.2
30	28	49	VAL	2.2
47	2p	51	VAL	2.2
53	2y	20	VAL	2.2
3	2D	254	THR	2.2
39	1h	80	ILE	2.2
16	1U	40	PHE	2.2
40	2i	37	PHE	2.2
53	2y	79	ASN	2.2
21	2Z	18	LEU	2.2
21	2Z	83	PRO	2.2
23	11	94	LEU	2.2
1	2A	614(B)	G	2.2
7	2H	159	GLU	2.2
26	24	67	TYR	2.2
38	1g	156	TRP	2.2
6	2G	138	GLN	2.2
35	2d	33	MET	2.2
16	2U	30	LYS	2.2
51	1t	74	LYS	2.2
49	2r	24	ALA	2.2
33	2b	185	ILE	2.2

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Mol	Chain	Res	Type	RSRZ
19	2X	47	PHE	2.2
33	2b	163	PHE	2.2
30	28	2	PRO	2.2
35	2d	7	PRO	2.2
6	2G	111	LEU	2.2
14	2S	58	LEU	2.2
16	1U	39	LEU	2.2
26	14	53	GLU	2.2
39	2h	99	GLU	2.2
42	2k	123	LYS	2.1
47	2p	39	TYR	2.1
47	2p	58	TYR	2.1
1	2A	2106	G	2.1
11	1P	71	VAL	2.1
20	2Y	7	VAL	2.1
31	19	23	VAL	2.1
35	1d	170	VAL	2.1
36	2e	90	VAL	2.1
41	1j	72	VAL	2.1
47	1p	20	VAL	2.1
47	2p	2	VAL	2.1
48	2q	85	VAL	2.1
23	2l	63	ALA	2.1
38	2g	83	ALA	2.1
48	2q	44	ALA	2.1
37	2f	46	ARG	2.1
51	1t	75	ASN	2.1
11	2P	24	GLY	2.1
12	2Q	47	ILE	2.1
51	2t	63	ILE	2.1
1	2A	1509	C	2.1
11	2P	51	PHE	2.1
40	1i	12	GLU	2.1
45	2n	14	PRO	2.1
3	2D	175	LEU	2.1
39	2h	39	LEU	2.1
11	2P	68	GLN	2.1
6	2G	86	MET	2.1
36	1e	148	VAL	2.1
36	2e	126	ARG	2.1
39	2h	9	MET	2.1
40	2i	91	ASP	2.1

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Mol	Chain	Res	Type	RSRZ
1	1A	1026	U	2.1
3	1D	221	VAL	2.1
3	2D	3	VAL	2.1
19	2X	81	VAL	2.1
44	1m	53	VAL	2.1
53	1y	94	ALA	2.1
1	1A	2153	G	2.1
11	2P	46	LYS	2.1
12	2Q	64	ILE	2.1
4	2E	113	PHE	2.1
32	2a	265	G	2.1
43	2l	124	LYS	2.1
51	1t	63	ILE	2.1
47	2p	49	LEU	2.1
51	2t	36	LEU	2.1
32	2a	1066	C	2.1
6	2G	51	ARG	2.1
30	28	46	ARG	2.1
35	1d	3	ARG	2.1
38	2g	155	ARG	2.1
36	2e	130	ASN	2.1
3	2D	202	LYS	2.1
43	2l	14	GLY	2.1
1	1A	1065	U	2.1
1	1A	2150	U	2.1
3	1D	240	ALA	2.1
4	1E	116	VAL	2.1
23	11	74	VAL	2.1
32	2a	1219	U	2.1
45	1n	48	ALA	2.1
6	2G	68	PRO	2.1
25	23	16	PRO	2.1
26	24	41	PRO	2.1
39	1h	111	ILE	2.1
51	1t	33	ILE	2.1
6	2G	102	PHE	2.1
35	2d	79	PHE	2.1
8	2I	123	LEU	2.1
36	1e	31	LEU	2.1
39	2h	63	LEU	2.1
49	1r	31	LEU	2.1
1	2A	2124	G	2.1

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	1A	1080	C	2.1
20	2Y	97	ARG	2.1
32	1a	1001(A)	G	2.1
12	2Q	30	GLY	2.1
26	14	45	GLY	2.1
32	1a	915	A	2.1
38	2g	31	MET	2.1
19	2X	42	ALA	2.1
24	22	63	VAL	2.1
34	2c	76	VAL	2.1
34	2c	121	ALA	2.1
46	2o	45	VAL	2.1
43	1l	61	THR	2.1
34	1c	182	ILE	2.1
35	2d	126	ILE	2.1
38	1g	27	ILE	2.1
39	1h	83	ILE	2.1
44	1m	78	ILE	2.1
34	2c	21	ARG	2.1
41	1j	43	ARG	2.1
46	2o	65	ARG	2.1
35	1d	137	SER	2.1
40	2i	105	ASP	2.1
1	1A	2129	C	2.1
1	1A	2139	C	2.1
1	1A	2109	U	2.1
7	2H	37	VAL	2.1
5	2F	72	ARG	2.1
19	2X	3	THR	2.1
21	2Z	175	VAL	2.1
34	2c	180	ALA	2.1
21	2Z	176	PRO	2.1
32	1a	975	A	2.1
34	2c	198	VAL	2.1
36	1e	82	VAL	2.1
50	2s	42	PRO	2.1
44	2m	57	ARG	2.1
50	2s	37	ARG	2.1
6	2G	49	ASP	2.1
14	2S	35	ILE	2.1
16	2U	56	ASP	2.1
34	2c	202	ILE	2.1

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Mol	Chain	Res	Type	RSRZ
41	2j	98	ILE	2.1
18	2W	13	SER	2.1
19	2X	9	LEU	2.1
20	2Y	60	PHE	2.1
36	2e	28	PHE	2.1
42	1k	125	PHE	2.1
46	2o	57	LEU	2.1
11	2P	66	GLY	2.1
15	1T	37	GLY	2.1
50	1s	56	GLN	2.1
1	2A	2155	G	2.1
16	2U	35	ALA	2.1
1	1A	2130	U	2.1
11	2P	32	THR	2.1
18	2W	47	VAL	2.1
35	2d	39	PRO	2.1
44	1m	15	VAL	2.1
53	2y	6	THR	2.1
23	2l	13	ILE	2.1
36	2e	131	ILE	2.1
5	2F	162	LEU	2.1
6	1G	133	LEU	2.1
13	2R	70	LEU	2.1
36	1e	91	LEU	2.1
49	1r	26	LEU	2.1
49	2r	76	LEU	2.1
53	1y	42	SER	2.1
34	2c	44	GLU	2.1
43	2l	29	GLY	2.1
3	2D	275	LYS	2.1
21	2Z	201	LYS	2.1
3	1D	225	ALA	2.0
11	2P	48	PRO	2.0
18	2W	74	ALA	2.0
30	18	2	PRO	2.0
3	1D	10	THR	2.0
8	2I	40	THR	2.0
19	2X	12	VAL	2.0
39	1h	79	VAL	2.0
8	1I	29	TYR	2.0
18	2W	75	TYR	2.0
3	1D	253	GLN	2.0

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Mol	Chain	Res	Type	RSRZ
3	2D	105	ILE	2.0
33	1b	162	ILE	2.0
40	2i	77	ILE	2.0
21	2Z	150	LEU	2.0
4	2E	139	GLY	2.0
26	24	54	GLY	2.0
34	2c	128	PHE	2.0
36	1e	110	LEU	2.0
39	2h	44	PHE	2.0
43	1l	27	LEU	2.0
51	2t	13	LEU	2.0
45	2n	17	LYS	2.0
35	1d	168	ARG	2.0
53	2y	30	TRP	2.0
6	2G	32	PRO	2.0
34	2c	113	ALA	2.0
43	2l	56	ALA	2.0
3	2D	185	VAL	2.0
44	1m	7	VAL	2.0
53	2y	56	THR	2.0
3	2D	24	ILE	2.0
7	2H	162	ILE	2.0
14	2S	40	ILE	2.0
22	20	22	GLY	2.0
24	22	57	ILE	2.0
34	1c	5	ILE	2.0
45	1n	42	ILE	2.0
52	2u	3	LYS	2.0
34	2c	158	GLY	2.0
50	2s	54	GLY	2.0
3	2D	53	PHE	2.0
3	2D	67	PHE	2.0
3	2D	176	ARG	2.0
31	29	18	ARG	2.0
43	1l	32	PHE	2.0
32	2a	263	A	2.0
25	23	18	ASP	2.0
3	2D	28	GLU	2.0
7	2H	34	GLU	2.0
51	2t	60	GLU	2.0
25	23	19	GLN	2.0
26	24	39	CYS	2.0

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Mol	Chain	Res	Type	RSRZ
31	29	5	ALA	2.0
51	1t	16	HIS	2.0
1	1A	2167	U	2.0
7	2H	113	VAL	2.0
34	1c	198	VAL	2.0
35	1d	105	VAL	2.0
43	2l	11	VAL	2.0
14	2S	9	ARG	2.0
20	2Y	73	ARG	2.0
38	2g	79	ARG	2.0
40	2i	121	ARG	2.0
48	2q	8	GLY	2.0
6	2G	120	LEU	2.0
11	2P	62	LEU	2.0
24	22	24	LEU	2.0
34	2c	52	LEU	2.0
47	1p	33	ILE	2.0
53	1y	74	ILE	2.0
3	2D	135	PHE	2.0
6	1G	146	TYR	2.0
17	2V	81	TYR	2.0
33	1b	129	GLU	2.0
3	2D	4	LYS	2.0
14	2S	11	LYS	2.0
41	1j	53	PRO	2.0

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

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
32	5MC	2a	967	21/22	0.91	0.20	71,76,81,84	0
43	0TD	2l	92	10/11	0.91	0.21	67,70,73,81	0
32	M2G	2a	966	25/26	0.91	0.20	69,76,86,98	0
1	5MU	2A	1915	21/22	0.92	0.11	80,84,88,102	0
1	PSU	2A	1917	20/21	0.92	0.12	73,79,95,99	0
32	4OC	2a	1402	22/23	0.93	0.18	62,69,73,81	0
32	PSU	2a	516	20/21	0.93	0.12	76,79,84,89	0
1	4OC	2A	1920	21/23	0.93	0.16	67,70,73,76	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
32	2MG	1a	1207	24/25	0.93	0.14	63,72,76,80	0
32	2MG	2a	1207	24/25	0.93	0.13	77,85,88,97	0
1	PSU	2A	1911	20/21	0.93	0.11	68,74,86,88	0
32	5MC	2a	1404	21/22	0.94	0.19	63,68,70,73	0
43	0TD	1l	92	10/11	0.94	0.17	51,59,63,68	0
1	5MU	1A	1915	21/22	0.94	0.12	68,75,80,84	0
1	PSU	1A	1911	20/21	0.94	0.14	61,69,76,82	0
1	PSU	1A	1917	20/21	0.95	0.13	65,72,76,79	0
32	M2G	1a	966	25/26	0.96	0.20	54,65,71,77	0
32	5MC	1a	967	21/22	0.96	0.21	65,71,75,80	0
32	7MG	2a	527	24/25	0.96	0.15	64,69,71,76	0
32	5MC	2a	1407	21/22	0.96	0.16	60,68,72,78	0
32	MA6	2a	1519	24/25	0.96	0.21	62,67,71,76	0
32	5MC	1a	1407	21/22	0.96	0.19	46,56,62,67	0
32	MA6	2a	1518	24/25	0.96	0.23	63,70,73,75	0
32	7MG	1a	527	24/25	0.96	0.17	50,57,62,62	0
32	PSU	1a	516	20/21	0.96	0.14	61,67,71,77	0
32	UR3	2a	1498	21/22	0.96	0.17	57,64,70,75	0
1	OMG	2A	2251	24/25	0.97	0.21	42,46,51,51	0
1	4OC	1A	1920	21/23	0.97	0.18	47,62,69,73	0
32	5MC	2a	1400	21/22	0.97	0.26	67,74,78,81	0
32	MA6	1a	1519	24/25	0.97	0.21	48,54,58,62	0
32	MA6	1a	1518	24/25	0.97	0.23	44,53,57,60	0
32	4OC	1a	1402	22/23	0.97	0.19	50,55,61,64	0
1	2MA	2A	2503	23/24	0.97	0.22	31,37,43,44	0
1	PSU	2A	2605	20/21	0.97	0.23	37,41,48,49	0
32	5MC	1a	1400	21/22	0.97	0.21	43,56,64,66	0
32	5MC	1a	1404	21/22	0.97	0.17	49,54,59,61	0
1	5MU	2A	1939	21/22	0.98	0.19	39,48,50,53	0
1	2MU	2A	2552	21/23	0.98	0.18	40,46,51,53	0
1	5MC	2A	1962	21/22	0.98	0.16	44,53,56,59	0
1	5MU	1A	1939	21/22	0.98	0.17	29,34,38,40	0
1	5MC	2A	1942	21/22	0.98	0.16	43,57,62,67	0
1	5MC	1A	1962	21/22	0.98	0.18	30,39,45,47	0
1	PSU	1A	2605	20/21	0.98	0.18	30,33,38,39	0
32	UR3	1a	1498	21/22	0.98	0.18	49,55,59,65	0
1	2MU	1A	2552	21/23	0.98	0.20	30,35,38,43	0
1	5MC	1A	1942	21/22	0.99	0.16	35,42,48,56	0
1	OMG	1A	2251	24/25	0.99	0.20	24,29,33,33	0
1	2MA	1A	2503	23/24	0.99	0.21	20,25,30,32	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
54	MG	2a	3056	1/1	0.38	0.18	74,74,74,74	0
54	MG	2A	3244	1/1	0.45	0.16	69,69,69,69	0
54	MG	2A	3651	1/1	0.46	0.19	81,81,81,81	0
54	MG	2A	3577	1/1	0.48	0.17	58,58,58,58	0
54	MG	2a	3170	1/1	0.49	0.33	70,70,70,70	0
54	MG	2A	3667	1/1	0.52	0.12	79,79,79,79	0
54	MG	1A	3945	1/1	0.52	0.18	65,65,65,65	0
54	MG	2A	3630	1/1	0.55	0.26	61,61,61,61	0
54	MG	2A	3436	1/1	0.55	0.16	77,77,77,77	0
54	MG	1A	3557	1/1	0.56	0.10	59,59,59,59	0
54	MG	2A	3695	1/1	0.56	0.09	66,66,66,66	0
54	MG	2a	3115	1/1	0.56	0.23	82,82,82,82	0
54	MG	1A	3285	1/1	0.57	0.24	79,79,79,79	0
54	MG	1A	3965	1/1	0.62	0.22	59,59,59,59	0
54	MG	1A	3622	1/1	0.63	0.15	30,30,30,30	0
54	MG	2A	3539	1/1	0.64	0.07	76,76,76,76	0
54	MG	2A	3604	1/1	0.65	0.12	52,52,52,52	0
54	MG	1A	3593	1/1	0.65	0.20	57,57,57,57	0
54	MG	1A	4010	1/1	0.66	0.09	48,48,48,48	0
54	MG	1A	3109	1/1	0.66	0.32	61,61,61,61	0
54	MG	1A	3917	1/1	0.67	0.16	35,35,35,35	0
54	MG	2A	3613	1/1	0.67	0.15	47,47,47,47	0
54	MG	2A	3721	1/1	0.68	0.19	73,73,73,73	0
54	MG	1A	3870	1/1	0.69	0.13	51,51,51,51	0
54	MG	1a	1800	1/1	0.69	0.14	74,74,74,74	0
54	MG	1a	1604	1/1	0.69	0.12	69,69,69,69	0
54	MG	2a	3069	1/1	0.70	0.16	77,77,77,77	0
54	MG	2A	3486	1/1	0.70	0.19	61,61,61,61	0
54	MG	2A	3219	1/1	0.71	0.12	70,70,70,70	0
54	MG	2A	3512	1/1	0.71	0.09	62,62,62,62	0
54	MG	2A	3525	1/1	0.71	0.09	68,68,68,68	0
54	MG	2A	3044	1/1	0.71	0.11	79,79,79,79	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
54	MG	1A	3986	1/1	0.71	0.14	70,70,70,70	0
54	MG	2F	303	1/1	0.72	0.14	67,67,67,67	0
54	MG	2A	3475	1/1	0.72	0.18	46,46,46,46	0
54	MG	2A	3185	1/1	0.72	0.14	67,67,67,67	0
54	MG	2a	3150	1/1	0.72	0.15	66,66,66,66	0
54	MG	1a	1786	1/1	0.72	0.15	62,62,62,62	0
54	MG	1A	3883	1/1	0.72	0.08	49,49,49,49	0
54	MG	2A	3566	1/1	0.72	0.14	40,40,40,40	0
54	MG	1a	1760	1/1	0.72	0.17	66,66,66,66	0
54	MG	2a	3009	1/1	0.73	0.23	68,68,68,68	0
54	MG	1a	1775	1/1	0.73	0.26	79,79,79,79	0
54	MG	1a	1756	1/1	0.73	0.23	59,59,59,59	0
54	MG	1A	3385	1/1	0.73	0.20	33,33,33,33	0
54	MG	2a	3105	1/1	0.73	0.18	71,71,71,71	0
54	MG	2B	217	1/1	0.73	0.07	72,72,72,72	0
54	MG	2A	3598	1/1	0.74	0.11	42,42,42,42	0
54	MG	2A	3254	1/1	0.74	0.32	64,64,64,64	0
54	MG	1a	1766	1/1	0.74	0.08	69,69,69,69	0
54	MG	2A	3106	1/1	0.74	0.18	56,56,56,56	0
54	MG	1a	1810	1/1	0.74	0.09	76,76,76,76	0
54	MG	1A	3693	1/1	0.74	0.16	63,63,63,63	0
54	MG	2A	3196	1/1	0.74	0.19	67,67,67,67	0
54	MG	18	102	1/1	0.74	0.12	58,58,58,58	0
54	MG	1a	1742	1/1	0.74	0.17	59,59,59,59	0
54	MG	1a	1859	1/1	0.75	0.14	68,68,68,68	0
54	MG	2A	3040	1/1	0.75	0.13	70,70,70,70	0
54	MG	1A	3582	1/1	0.75	0.14	46,46,46,46	0
54	MG	2A	3285	1/1	0.75	0.10	47,47,47,47	0
54	MG	1A	3521	1/1	0.75	0.16	56,56,56,56	0
54	MG	2A	3732	1/1	0.75	0.11	66,66,66,66	0
54	MG	1a	1825	1/1	0.75	0.10	71,71,71,71	0
54	MG	2O	202	1/1	0.75	0.19	80,80,80,80	0
54	MG	1a	1844	1/1	0.76	0.18	69,69,69,69	0
54	MG	1A	3989	1/1	0.76	0.69	47,47,47,47	0
54	MG	1A	3321	1/1	0.76	0.13	63,63,63,63	0
54	MG	1D	312	1/1	0.76	0.16	66,66,66,66	0
54	MG	1A	3014	1/1	0.76	0.21	57,57,57,57	0
54	MG	1A	3591	1/1	0.76	0.12	51,51,51,51	0
54	MG	1a	1774	1/1	0.76	0.20	70,70,70,70	0
54	MG	2a	3085	1/1	0.76	0.12	67,67,67,67	0
54	MG	1A	3586	1/1	0.76	0.17	67,67,67,67	0
54	MG	1A	3036	1/1	0.76	0.19	37,37,37,37	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
54	MG	2A	3233	1/1	0.76	0.18	54,54,54,54	0
54	MG	1A	3660	1/1	0.76	0.07	54,54,54,54	0
54	MG	2A	3619	1/1	0.77	0.16	45,45,45,45	0
54	MG	2A	3024	1/1	0.77	0.47	67,67,67,67	0
54	MG	2a	3025	1/1	0.77	0.19	79,79,79,79	0
54	MG	1A	3215	1/1	0.77	0.11	64,64,64,64	0
54	MG	2A	3048	1/1	0.77	0.12	63,63,63,63	0
54	MG	2a	3106	1/1	0.77	0.24	70,70,70,70	0
54	MG	2A	3547	1/1	0.77	0.08	70,70,70,70	0
54	MG	1a	1693	1/1	0.77	0.17	70,70,70,70	0
54	MG	1A	3288	1/1	0.77	0.18	60,60,60,60	0
54	MG	2a	3065	1/1	0.77	0.10	76,76,76,76	0
54	MG	2A	3618	1/1	0.77	0.14	39,39,39,39	0
54	MG	1G	203	1/1	0.77	0.19	74,74,74,74	0
54	MG	2A	3093	1/1	0.77	0.11	67,67,67,67	0
54	MG	2A	3295	1/1	0.77	0.14	56,56,56,56	0
54	MG	2A	3222	1/1	0.77	0.12	58,58,58,58	0
54	MG	1a	1746	1/1	0.77	0.15	71,71,71,71	0
54	MG	1A	3473	1/1	0.77	0.12	33,33,33,33	0
54	MG	2A	3676	1/1	0.78	0.12	69,69,69,69	0
54	MG	1A	3707	1/1	0.78	0.14	70,70,70,70	0
54	MG	1A	3915	1/1	0.78	0.08	50,50,50,50	0
54	MG	2a	3141	1/1	0.78	0.13	57,57,57,57	0
54	MG	2A	3679	1/1	0.78	0.11	72,72,72,72	0
54	MG	2A	3179	1/1	0.78	0.12	60,60,60,60	0
54	MG	1Y	202	1/1	0.78	0.13	55,55,55,55	0
54	MG	2A	3062	1/1	0.78	0.11	57,57,57,57	0
54	MG	2a	3172	1/1	0.78	0.08	76,76,76,76	0
54	MG	2A	3126	1/1	0.78	0.08	65,65,65,65	0
54	MG	1b	301	1/1	0.78	0.12	80,80,80,80	0
54	MG	2A	3420	1/1	0.78	0.24	73,73,73,73	0
54	MG	1A	4016	1/1	0.78	0.11	60,60,60,60	0
54	MG	2B	201	1/1	0.78	0.11	75,75,75,75	0
54	MG	2a	3037	1/1	0.78	0.19	65,65,65,65	0
54	MG	2A	3255	1/1	0.78	0.35	64,64,64,64	0
54	MG	1a	1688	1/1	0.78	0.14	60,60,60,60	0
54	MG	1A	3449	1/1	0.78	0.14	49,49,49,49	0
54	MG	1A	3923	1/1	0.78	0.16	51,51,51,51	0
54	MG	2A	3345	1/1	0.78	0.10	41,41,41,41	0
54	MG	1a	1715	1/1	0.78	0.14	69,69,69,69	0
54	MG	1a	1757	1/1	0.78	0.21	64,64,64,64	0
54	MG	2a	3004	1/1	0.78	0.13	72,72,72,72	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
54	MG	2A	3311	1/1	0.78	0.12	58,58,58,58	0
54	MG	1a	1706	1/1	0.78	0.18	57,57,57,57	0
54	MG	2A	3625	1/1	0.79	0.07	82,82,82,82	0
54	MG	2A	3491	1/1	0.79	0.12	64,64,64,64	0
54	MG	2A	3675	1/1	0.79	0.17	74,74,74,74	0
54	MG	1A	3231	1/1	0.79	0.16	49,49,49,49	0
54	MG	20	102	1/1	0.79	0.17	73,73,73,73	0
54	MG	2A	3529	1/1	0.79	0.34	64,64,64,64	0
54	MG	2a	3017	1/1	0.79	0.17	61,61,61,61	0
54	MG	2A	3480	1/1	0.79	0.14	45,45,45,45	0
54	MG	1A	3406	1/1	0.79	0.15	64,64,64,64	0
54	MG	1A	3997	1/1	0.79	0.10	74,74,74,74	0
54	MG	1A	3220	1/1	0.79	0.19	66,66,66,66	0
54	MG	1h	202	1/1	0.79	0.12	79,79,79,79	0
54	MG	1a	1641	1/1	0.79	0.13	65,65,65,65	0
54	MG	2A	3481	1/1	0.80	0.12	59,59,59,59	0
54	MG	2a	3134	1/1	0.80	0.10	65,65,65,65	0
54	MG	1a	1608	1/1	0.80	0.09	63,63,63,63	0
54	MG	2A	3210	1/1	0.80	0.15	56,56,56,56	0
58	ZN	2Y	501	1/1	0.80	0.15	84,84,84,84	0
54	MG	1a	1621	1/1	0.80	0.11	61,61,61,61	0
54	MG	1A	3287	1/1	0.80	0.13	69,69,69,69	0
54	MG	2a	3019	1/1	0.80	0.18	67,67,67,67	0
54	MG	2A	3638	1/1	0.80	0.07	79,79,79,79	0
54	MG	1a	1865	1/1	0.80	0.06	74,74,74,74	0
54	MG	1A	3529	1/1	0.80	0.11	51,51,51,51	0
54	MG	1A	3580	1/1	0.80	0.20	70,70,70,70	0
54	MG	1A	3283	1/1	0.80	0.14	58,58,58,58	0
54	MG	1A	3611	1/1	0.80	0.50	58,58,58,58	0
54	MG	2A	3473	1/1	0.80	0.13	75,75,75,75	0
54	MG	1a	1848	1/1	0.80	0.11	70,70,70,70	0
54	MG	1a	1674	1/1	0.80	0.16	56,56,56,56	0
54	MG	2A	3121	1/1	0.80	0.25	72,72,72,72	0
54	MG	1A	3589	1/1	0.80	0.11	63,63,63,63	0
54	MG	2A	3328	1/1	0.80	0.21	52,52,52,52	0
54	MG	2A	3091	1/1	0.80	0.12	54,54,54,54	0
54	MG	2A	3378	1/1	0.80	0.11	39,39,39,39	0
54	MG	2G	201	1/1	0.80	0.23	78,78,78,78	0
54	MG	1a	1816	1/1	0.80	0.09	92,92,92,92	0
54	MG	2A	3640	1/1	0.81	0.06	47,47,47,47	0
54	MG	1a	1798	1/1	0.81	0.19	60,60,60,60	0
54	MG	2A	3151	1/1	0.81	0.13	57,57,57,57	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
54	MG	2A	3063	1/1	0.81	0.45	54,54,54,54	0
54	MG	1a	1753	1/1	0.81	0.25	73,73,73,73	0
54	MG	2A	3519	1/1	0.81	0.17	64,64,64,64	0
54	MG	2a	3119	1/1	0.81	0.13	72,72,72,72	0
54	MG	1A	3633	1/1	0.81	0.65	45,45,45,45	0
54	MG	2a	3072	1/1	0.81	0.14	72,72,72,72	0
57	ARG	1F	319	12/12	0.81	0.16	55,65,74,77	0
54	MG	2A	3186	1/1	0.81	0.35	72,72,72,72	0
54	MG	1a	1624	1/1	0.81	0.16	59,59,59,59	0
54	MG	1a	1682	1/1	0.81	0.26	75,75,75,75	0
54	MG	2A	3161	1/1	0.81	0.12	70,70,70,70	0
54	MG	2A	3172	1/1	0.81	0.21	63,63,63,63	0
54	MG	1a	1777	1/1	0.81	0.10	66,66,66,66	0
54	MG	2A	3183	1/1	0.81	0.37	54,54,54,54	0
54	MG	1G	202	1/1	0.81	0.13	55,55,55,55	0
54	MG	2A	3588	1/1	0.81	0.17	54,54,54,54	0
54	MG	2A	3722	1/1	0.81	0.30	73,73,73,73	0
54	MG	2a	3054	1/1	0.81	0.10	70,70,70,70	0
54	MG	2a	3020	1/1	0.81	0.08	63,63,63,63	0
54	MG	1a	1813	1/1	0.81	0.09	56,56,56,56	0
54	MG	1a	1849	1/1	0.81	0.21	85,85,85,85	0
54	MG	2A	3401	1/1	0.82	0.17	59,59,59,59	0
54	MG	2a	3060	1/1	0.82	0.13	77,77,77,77	0
54	MG	1A	3413	1/1	0.82	0.14	31,31,31,31	0
54	MG	1A	3588	1/1	0.82	0.27	50,50,50,50	0
54	MG	2A	3435	1/1	0.82	0.09	59,59,59,59	0
54	MG	1A	3990	1/1	0.82	0.17	43,43,43,43	0
54	MG	2A	3356	1/1	0.82	0.10	73,73,73,73	0
54	MG	2A	3363	1/1	0.82	0.29	61,61,61,61	0
54	MG	1a	1696	1/1	0.82	0.13	71,71,71,71	0
54	MG	2A	3235	1/1	0.82	0.31	62,62,62,62	0
54	MG	1A	3944	1/1	0.82	0.22	49,49,49,49	0
54	MG	2A	3042	1/1	0.82	0.13	48,48,48,48	0
54	MG	1a	1689	1/1	0.82	0.10	73,73,73,73	0
54	MG	1A	3464	1/1	0.82	0.07	46,46,46,46	0
54	MG	1a	1857	1/1	0.82	0.11	65,65,65,65	0
54	MG	2a	3062	1/1	0.82	0.11	79,79,79,79	0
54	MG	1a	1668	1/1	0.82	0.21	64,64,64,64	0
54	MG	11	103	1/1	0.82	0.19	56,56,56,56	0
54	MG	2A	3301	1/1	0.82	0.23	71,71,71,71	0
54	MG	1A	3654	1/1	0.82	0.13	34,34,34,34	0
54	MG	2A	3187	1/1	0.82	0.15	66,66,66,66	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
54	MG	2B	214	1/1	0.82	0.11	74,74,74,74	0
54	MG	2A	3562	1/1	0.82	0.12	37,37,37,37	0
54	MG	2A	3032	1/1	0.83	0.13	56,56,56,56	0
54	MG	1A	3922	1/1	0.83	0.09	43,43,43,43	0
54	MG	2a	3090	1/1	0.83	0.09	76,76,76,76	0
54	MG	1a	1828	1/1	0.83	0.13	65,65,65,65	0
54	MG	2a	3166	1/1	0.83	0.09	66,66,66,66	0
54	MG	2f	201	1/1	0.83	0.11	61,61,61,61	0
54	MG	1a	1665	1/1	0.83	0.15	71,71,71,71	0
54	MG	10	105	1/1	0.83	0.10	60,60,60,60	0
54	MG	2A	3469	1/1	0.83	0.25	63,63,63,63	0
54	MG	2A	3230	1/1	0.83	0.26	56,56,56,56	0
54	MG	2A	3494	1/1	0.83	0.09	63,63,63,63	0
54	MG	1a	1645	1/1	0.83	0.13	57,57,57,57	0
54	MG	1A	3457	1/1	0.83	0.14	36,36,36,36	0
54	MG	1A	3072	1/1	0.83	0.28	47,47,47,47	0
54	MG	2A	3133	1/1	0.83	0.09	59,59,59,59	0
54	MG	2A	3424	1/1	0.83	0.12	57,57,57,57	0
54	MG	2A	3272	1/1	0.83	0.08	58,58,58,58	0
54	MG	1A	3722	1/1	0.83	0.08	65,65,65,65	0
54	MG	1A	3131	1/1	0.83	0.21	51,51,51,51	0
54	MG	1a	1874	1/1	0.83	0.12	71,71,71,71	0
54	MG	2A	3557	1/1	0.83	0.07	69,69,69,69	0
54	MG	2A	3059	1/1	0.83	0.37	54,54,54,54	0
54	MG	2A	3511	1/1	0.83	0.17	38,38,38,38	0
54	MG	2a	3089	1/1	0.83	0.15	71,71,71,71	0
54	MG	1a	1603	1/1	0.83	0.19	75,75,75,75	0
54	MG	2A	3528	1/1	0.83	0.20	80,80,80,80	0
54	MG	2A	3001	1/1	0.83	0.22	64,64,64,64	0
54	MG	1A	3817	1/1	0.83	0.28	41,41,41,41	0
54	MG	1a	1695	1/1	0.83	0.09	54,54,54,54	0
54	MG	1A	3187	1/1	0.83	0.17	54,54,54,54	0
54	MG	1B	222	1/1	0.83	0.22	54,54,54,54	0
54	MG	2A	3523	1/1	0.83	0.12	71,71,71,71	0
54	MG	2A	3628	1/1	0.84	0.23	64,64,64,64	0
54	MG	2A	3456	1/1	0.84	0.15	61,61,61,61	0
54	MG	2a	3015	1/1	0.84	0.14	63,63,63,63	0
54	MG	1A	3221	1/1	0.84	0.13	61,61,61,61	0
54	MG	1A	3895	1/1	0.84	0.12	27,27,27,27	0
54	MG	2a	3058	1/1	0.84	0.19	74,74,74,74	0
54	MG	1A	4014	1/1	0.84	0.17	39,39,39,39	0
54	MG	1A	3002	1/1	0.84	0.47	56,56,56,56	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
54	MG	1A	3832	1/1	0.84	0.08	59,59,59,59	0
54	MG	1A	3830	1/1	0.84	0.14	50,50,50,50	0
54	MG	1A	3971	1/1	0.84	0.19	45,45,45,45	0
54	MG	2A	3190	1/1	0.84	0.27	47,47,47,47	0
54	MG	2A	3034	1/1	0.84	0.17	57,57,57,57	0
54	MG	1a	1870	1/1	0.84	0.12	68,68,68,68	0
54	MG	1A	3615	1/1	0.84	0.11	51,51,51,51	0
54	MG	2E	304	1/1	0.84	0.14	40,40,40,40	0
54	MG	1a	1661	1/1	0.84	0.80	74,74,74,74	0
54	MG	1d	302	1/1	0.84	0.12	71,71,71,71	0
54	MG	2A	3216	1/1	0.84	0.30	59,59,59,59	0
54	MG	1A	3510	1/1	0.84	0.13	55,55,55,55	0
54	MG	2a	3061	1/1	0.84	0.15	64,64,64,64	0
54	MG	1A	3425	1/1	0.84	0.20	40,40,40,40	0
54	MG	1a	1811	1/1	0.84	0.13	66,66,66,66	0
54	MG	1A	3787	1/1	0.84	0.16	43,43,43,43	0
54	MG	2A	3465	1/1	0.84	0.13	55,55,55,55	0
54	MG	2A	3227	1/1	0.84	0.40	67,67,67,67	0
54	MG	1A	3030	1/1	0.84	0.12	34,34,34,34	0
54	MG	2a	3040	1/1	0.84	0.10	75,75,75,75	0
54	MG	1A	3935	1/1	0.84	0.10	50,50,50,50	0
54	MG	1A	3925	1/1	0.84	0.14	66,66,66,66	0
54	MG	1A	3590	1/1	0.84	0.12	39,39,39,39	0
54	MG	2A	3012	1/1	0.84	0.64	66,66,66,66	0
54	MG	1a	1714	1/1	0.84	0.11	77,77,77,77	0
54	MG	19	101	1/1	0.85	0.14	69,69,69,69	0
54	MG	1a	1657	1/1	0.85	0.28	67,67,67,67	0
54	MG	1A	3856	1/1	0.85	0.12	54,54,54,54	0
54	MG	2A	3003	1/1	0.85	0.10	51,51,51,51	0
54	MG	1A	3292	1/1	0.85	0.17	44,44,44,44	0
54	MG	2A	3047	1/1	0.85	0.28	60,60,60,60	0
54	MG	2A	3417	1/1	0.85	0.08	72,72,72,72	0
54	MG	1a	1671	1/1	0.85	0.06	79,79,79,79	0
54	MG	2A	3443	1/1	0.85	0.14	60,60,60,60	0
54	MG	1A	3721	1/1	0.85	0.14	42,42,42,42	0
54	MG	1a	1808	1/1	0.85	0.15	56,56,56,56	0
54	MG	1A	3640	1/1	0.85	0.27	61,61,61,61	0
54	MG	1A	3835	1/1	0.85	0.15	49,49,49,49	0
54	MG	1V	206	1/1	0.85	0.20	47,47,47,47	0
54	MG	2A	3587	1/1	0.85	0.09	48,48,48,48	0
54	MG	2A	3278	1/1	0.85	0.15	44,44,44,44	0
54	MG	1A	3303	1/1	0.85	0.12	67,67,67,67	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
54	MG	2A	3704	1/1	0.85	0.13	52,52,52,52	0
54	MG	2a	3007	1/1	0.85	0.15	72,72,72,72	0
54	MG	2a	3070	1/1	0.85	0.12	78,78,78,78	0
54	MG	1A	3772	1/1	0.85	0.11	34,34,34,34	0
54	MG	1A	3672	1/1	0.85	0.11	53,53,53,53	0
54	MG	2a	3023	1/1	0.85	0.09	69,69,69,69	0
54	MG	1A	3819	1/1	0.85	0.44	39,39,39,39	0
54	MG	1a	1801	1/1	0.85	0.05	65,65,65,65	0
54	MG	2a	3117	1/1	0.85	0.11	66,66,66,66	0
54	MG	2A	3731	1/1	0.85	0.25	62,62,62,62	0
54	MG	1a	1797	1/1	0.85	0.13	65,65,65,65	0
54	MG	1A	3383	1/1	0.85	0.14	50,50,50,50	0
54	MG	1A	3789	1/1	0.85	0.31	66,66,66,66	0
54	MG	2a	3057	1/1	0.85	0.23	64,64,64,64	0
54	MG	1F	317	1/1	0.85	0.09	51,51,51,51	0
54	MG	2A	3080	1/1	0.85	0.10	73,73,73,73	0
54	MG	2A	3296	1/1	0.85	0.07	46,46,46,46	0
54	MG	1a	1685	1/1	0.85	0.32	58,58,58,58	0
54	MG	2A	3602	1/1	0.85	0.06	70,70,70,70	0
54	MG	1a	1660	1/1	0.85	0.31	56,56,56,56	0
54	MG	1A	3748	1/1	0.85	0.18	21,21,21,21	0
54	MG	1T	202	1/1	0.85	0.14	77,77,77,77	0
54	MG	1H	202	1/1	0.85	0.13	46,46,46,46	0
54	MG	2A	3035	1/1	0.85	0.11	59,59,59,59	0
54	MG	2A	3054	1/1	0.85	0.13	70,70,70,70	0
54	MG	1a	1731	1/1	0.85	0.10	56,56,56,56	0
54	MG	1P	204	1/1	0.85	0.58	57,57,57,57	0
54	MG	2A	3723	1/1	0.86	0.10	35,35,35,35	0
54	MG	2A	3180	1/1	0.86	0.09	66,66,66,66	0
54	MG	1A	3327	1/1	0.86	0.14	39,39,39,39	0
54	MG	2A	3110	1/1	0.86	0.26	57,57,57,57	0
54	MG	2A	3089	1/1	0.86	0.15	72,72,72,72	0
54	MG	1A	3857	1/1	0.86	0.26	51,51,51,51	0
54	MG	2A	3585	1/1	0.86	0.15	60,60,60,60	0
54	MG	1A	3276	1/1	0.86	0.20	48,48,48,48	0
54	MG	1A	3865	1/1	0.86	0.13	65,65,65,65	0
54	MG	1A	3571	1/1	0.86	0.15	23,23,23,23	0
54	MG	1A	3097	1/1	0.86	0.23	66,66,66,66	0
54	MG	1a	1732	1/1	0.86	0.10	79,79,79,79	0
54	MG	1a	1802	1/1	0.86	0.17	72,72,72,72	0
54	MG	2A	3711	1/1	0.86	0.26	64,64,64,64	0
54	MG	1A	3183	1/1	0.86	0.10	52,52,52,52	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
54	MG	2A	3055	1/1	0.86	0.12	72,72,72,72	0
54	MG	2A	3458	1/1	0.86	0.11	74,74,74,74	0
54	MG	1a	1618	1/1	0.86	0.10	62,62,62,62	0
54	MG	2A	3368	1/1	0.86	0.12	37,37,37,37	0
54	MG	2A	3177	1/1	0.86	0.47	48,48,48,48	0
54	MG	2a	3024	1/1	0.86	0.18	63,63,63,63	0
54	MG	1A	3022	1/1	0.86	0.25	49,49,49,49	0
54	MG	1n	102	1/1	0.86	0.16	58,58,58,58	0
54	MG	1A	3210	1/1	0.86	0.50	46,46,46,46	0
54	MG	15	106	1/1	0.86	0.23	68,68,68,68	0
54	MG	1A	3983	1/1	0.86	0.10	46,46,46,46	0
54	MG	2G	203	1/1	0.86	0.07	70,70,70,70	0
58	ZN	24	501	1/1	0.86	0.04	122,122,122,122	0
54	MG	2A	3306	1/1	0.86	0.11	67,67,67,67	0
54	MG	2A	3582	1/1	0.86	0.10	83,83,83,83	0
54	MG	1a	1652	1/1	0.86	0.32	69,69,69,69	0
54	MG	2A	3361	1/1	0.86	0.21	56,56,56,56	0
54	MG	1A	3193	1/1	0.86	0.12	57,57,57,57	0
54	MG	1a	1752	1/1	0.86	0.14	61,61,61,61	0
54	MG	2A	3418	1/1	0.86	0.44	47,47,47,47	0
54	MG	1A	3994	1/1	0.86	0.41	48,48,48,48	0
54	MG	1E	306	1/1	0.86	0.12	45,45,45,45	0
54	MG	1A	3699	1/1	0.86	0.34	48,48,48,48	0
54	MG	1A	3612	1/1	0.86	0.21	39,39,39,39	0
54	MG	1a	1826	1/1	0.86	0.10	72,72,72,72	0
54	MG	1A	3301	1/1	0.86	0.19	43,43,43,43	0
54	MG	2A	3271	1/1	0.86	0.10	64,64,64,64	0
54	MG	2A	3131	1/1	0.86	0.12	51,51,51,51	0
54	MG	1A	3150	1/1	0.86	0.08	70,70,70,70	0
54	MG	2A	3701	1/1	0.86	0.13	50,50,50,50	0
54	MG	2A	3639	1/1	0.86	0.25	73,73,73,73	0
54	MG	2A	3114	1/1	0.86	0.24	69,69,69,69	0
54	MG	1A	3755	1/1	0.86	0.23	77,77,77,77	0
54	MG	1a	1821	1/1	0.86	0.10	68,68,68,68	0
54	MG	2A	3514	1/1	0.86	0.10	34,34,34,34	0
54	MG	1B	209	1/1	0.87	0.34	60,60,60,60	0
54	MG	1A	3907	1/1	0.87	0.07	37,37,37,37	0
54	MG	1t	201	1/1	0.87	0.13	56,56,56,56	0
54	MG	2A	3371	1/1	0.87	0.08	53,53,53,53	0
54	MG	2A	3498	1/1	0.87	0.10	66,66,66,66	0
54	MG	2A	3382	1/1	0.87	0.27	54,54,54,54	0
54	MG	1A	4003	1/1	0.87	0.15	90,90,90,90	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MPD	2B	219	8/8	0.87	0.16	61,71,72,75	0
54	MG	1A	3694	1/1	0.87	0.26	52,52,52,52	0
54	MG	1A	4001	1/1	0.87	0.25	62,62,62,62	0
54	MG	2a	3022	1/1	0.87	0.16	64,64,64,64	0
54	MG	2A	3412	1/1	0.87	0.11	72,72,72,72	0
54	MG	2A	3463	1/1	0.87	0.15	64,64,64,64	0
54	MG	2a	3033	1/1	0.87	0.14	68,68,68,68	0
54	MG	1B	207	1/1	0.87	0.10	50,50,50,50	0
54	MG	2A	3671	1/1	0.87	0.11	67,67,67,67	0
54	MG	2A	3428	1/1	0.87	0.24	69,69,69,69	0
54	MG	1A	3705	1/1	0.87	0.24	55,55,55,55	0
54	MG	2e	201	1/1	0.87	0.26	68,68,68,68	0
54	MG	2A	3231	1/1	0.87	0.28	55,55,55,55	0
54	MG	1A	3196	1/1	0.87	0.26	62,62,62,62	0
54	MG	2A	3245	1/1	0.87	0.12	68,68,68,68	0
54	MG	2A	3016	1/1	0.87	0.19	69,69,69,69	0
54	MG	1a	1719	1/1	0.87	0.16	76,76,76,76	0
54	MG	1A	3569	1/1	0.87	0.12	70,70,70,70	0
54	MG	1a	1672	1/1	0.87	0.28	62,62,62,62	0
54	MG	1A	3454	1/1	0.87	0.12	39,39,39,39	0
54	MG	1y	201	1/1	0.87	0.09	56,56,56,56	0
54	MG	2A	3354	1/1	0.87	0.19	63,63,63,63	0
54	MG	2T	3301	1/1	0.87	0.18	56,56,56,56	0
54	MG	2A	3342	1/1	0.87	0.14	48,48,48,48	0
54	MG	1A	3616	1/1	0.87	0.18	34,34,34,34	0
54	MG	2A	3169	1/1	0.87	0.31	67,67,67,67	0
54	MG	1A	3479	1/1	0.87	0.16	22,22,22,22	0
54	MG	2A	3550	1/1	0.87	0.13	63,63,63,63	0
54	MG	1A	3543	1/1	0.87	0.10	55,55,55,55	0
54	MG	1A	3188	1/1	0.87	0.17	71,71,71,71	0
54	MG	1A	3522	1/1	0.87	0.19	41,41,41,41	0
54	MG	2A	3634	1/1	0.87	0.29	75,75,75,75	0
54	MG	2a	3128	1/1	0.87	0.14	67,67,67,67	0
54	MG	2A	3240	1/1	0.87	0.20	64,64,64,64	0
54	MG	1a	1678	1/1	0.87	0.10	59,59,59,59	0
54	MG	1a	1784	1/1	0.87	0.14	69,69,69,69	0
54	MG	1A	3881	1/1	0.87	0.13	29,29,29,29	0
54	MG	1a	1707	1/1	0.87	0.10	62,62,62,62	0
54	MG	1A	3354	1/1	0.87	0.17	36,36,36,36	0
54	MG	2A	3484	1/1	0.87	0.14	49,49,49,49	0
54	MG	2a	3027	1/1	0.88	0.26	70,70,70,70	0
54	MG	1a	1680	1/1	0.88	0.19	52,52,52,52	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
54	MG	2A	3253	1/1	0.88	0.07	73,73,73,73	0
54	MG	1a	1794	1/1	0.88	0.43	86,86,86,86	0
54	MG	1B	228	1/1	0.88	0.14	65,65,65,65	0
54	MG	2A	3209	1/1	0.88	0.09	66,66,66,66	0
54	MG	1A	3823	1/1	0.88	0.17	34,34,34,34	0
54	MG	1A	3826	1/1	0.88	0.11	43,43,43,43	0
54	MG	2A	3336	1/1	0.88	0.10	41,41,41,41	0
54	MG	1A	3487	1/1	0.88	0.17	41,41,41,41	0
54	MG	1a	1647	1/1	0.88	0.12	63,63,63,63	0
54	MG	1A	3631	1/1	0.88	0.16	42,42,42,42	0
54	MG	2A	3260	1/1	0.88	0.16	59,59,59,59	0
54	MG	1A	4002	1/1	0.88	0.15	50,50,50,50	0
54	MG	1A	3080	1/1	0.88	0.26	42,42,42,42	0
54	MG	1A	3063	1/1	0.88	0.15	45,45,45,45	0
54	MG	1a	1763	1/1	0.88	0.20	64,64,64,64	0
54	MG	1A	3745	1/1	0.88	0.17	54,54,54,54	0
54	MG	2A	3221	1/1	0.88	0.16	52,52,52,52	0
54	MG	1A	3234	1/1	0.88	0.55	42,42,42,42	0
54	MG	1A	3927	1/1	0.88	0.17	56,56,56,56	0
54	MG	1a	1819	1/1	0.88	0.16	75,75,75,75	0
54	MG	2a	3133	1/1	0.88	0.11	75,75,75,75	0
54	MG	2A	3309	1/1	0.88	0.12	54,54,54,54	0
54	MG	2A	3125	1/1	0.88	0.14	54,54,54,54	0
54	MG	2A	3533	1/1	0.88	0.12	37,37,37,37	0
54	MG	2A	3220	1/1	0.88	0.21	64,64,64,64	0
54	MG	2a	3175	1/1	0.88	0.13	71,71,71,71	0
54	MG	2A	3534	1/1	0.88	0.10	43,43,43,43	0
54	MG	1A	3642	1/1	0.88	0.30	70,70,70,70	0
54	MG	1A	3882	1/1	0.88	0.13	52,52,52,52	0
54	MG	2A	3198	1/1	0.88	0.48	62,62,62,62	0
54	MG	1A	3951	1/1	0.88	0.17	44,44,44,44	0
54	MG	2A	3718	1/1	0.88	0.15	56,56,56,56	0
54	MG	1A	3388	1/1	0.88	0.23	31,31,31,31	0
54	MG	1A	3827	1/1	0.88	0.26	42,42,42,42	0
54	MG	1A	3057	1/1	0.88	0.18	53,53,53,53	0
54	MG	1A	3261	1/1	0.88	0.10	40,40,40,40	0
54	MG	1A	3578	1/1	0.88	0.10	51,51,51,51	0
54	MG	2A	3516	1/1	0.88	0.36	56,56,56,56	0
54	MG	2a	3028	1/1	0.88	0.08	81,81,81,81	0
54	MG	1A	3924	1/1	0.88	0.09	51,51,51,51	0
54	MG	1A	3728	1/1	0.88	0.16	28,28,28,28	0
54	MG	2A	3373	1/1	0.88	0.19	59,59,59,59	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
54	MG	1a	1610	1/1	0.88	0.30	65,65,65,65	0
54	MG	1A	3904	1/1	0.88	0.18	37,37,37,37	0
54	MG	2F	302	1/1	0.88	0.12	39,39,39,39	0
54	MG	2A	3708	1/1	0.88	0.08	60,60,60,60	0
54	MG	2A	3405	1/1	0.88	0.09	41,41,41,41	0
54	MG	2A	3346	1/1	0.88	0.14	66,66,66,66	0
54	MG	2A	3423	1/1	0.88	0.40	77,77,77,77	0
54	MG	1B	220	1/1	0.88	0.16	37,37,37,37	0
54	MG	2A	3575	1/1	0.88	0.12	50,50,50,50	0
54	MG	2A	3531	1/1	0.88	0.09	65,65,65,65	0
54	MG	2a	3136	1/1	0.88	0.35	84,84,84,84	0
54	MG	1A	3779	1/1	0.88	0.15	45,45,45,45	0
54	MG	2A	3507	1/1	0.88	0.09	73,73,73,73	0
54	MG	1A	3138	1/1	0.88	0.16	45,45,45,45	0
54	MG	2A	3660	1/1	0.88	0.12	81,81,81,81	0
54	MG	2a	3012	1/1	0.88	0.14	62,62,62,62	0
54	MG	1A	3451	1/1	0.88	0.14	61,61,61,61	0
54	MG	2a	3180	1/1	0.88	0.07	57,57,57,57	0
54	MG	1a	1700	1/1	0.88	0.11	54,54,54,54	0
54	MG	2a	3174	1/1	0.88	0.13	75,75,75,75	0
54	MG	1A	3955	1/1	0.88	0.07	71,71,71,71	0
54	MG	1A	3858	1/1	0.88	0.12	52,52,52,52	0
54	MG	2A	3073	1/1	0.88	0.32	49,49,49,49	0
54	MG	1R	205	1/1	0.88	0.17	47,47,47,47	0
54	MG	2A	3386	1/1	0.88	0.15	56,56,56,56	0
54	MG	2A	3259	1/1	0.88	0.14	55,55,55,55	0
54	MG	1B	211	1/1	0.88	0.14	54,54,54,54	0
54	MG	1A	3336	1/1	0.88	0.16	48,48,48,48	0
54	MG	1A	3662	1/1	0.89	0.27	33,33,33,33	0
54	MG	1a	1690	1/1	0.89	0.11	60,60,60,60	0
54	MG	2A	3226	1/1	0.89	0.16	43,43,43,43	0
54	MG	2A	3573	1/1	0.89	0.19	67,67,67,67	0
54	MG	1A	3969	1/1	0.89	0.12	55,55,55,55	0
54	MG	1A	3206	1/1	0.89	0.14	70,70,70,70	0
54	MG	2A	3211	1/1	0.89	0.11	48,48,48,48	0
54	MG	1A	3677	1/1	0.89	0.14	55,55,55,55	0
54	MG	2A	3450	1/1	0.89	0.22	57,57,57,57	0
54	MG	2A	3017	1/1	0.89	0.22	56,56,56,56	0
54	MG	2a	3130	1/1	0.89	0.07	64,64,64,64	0
54	MG	1A	3918	1/1	0.89	0.27	55,55,55,55	0
54	MG	2O	201	1/1	0.89	0.10	58,58,58,58	0
54	MG	2A	3320	1/1	0.89	0.18	41,41,41,41	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
54	MG	1B	232	1/1	0.89	0.17	68,68,68,68	0
54	MG	2A	3112	1/1	0.89	0.12	71,71,71,71	0
54	MG	2a	3049	1/1	0.89	0.24	59,59,59,59	0
54	MG	2A	3256	1/1	0.89	0.14	59,59,59,59	0
54	MG	1A	3314	1/1	0.89	0.20	57,57,57,57	0
54	MG	2B	202	1/1	0.89	0.08	71,71,71,71	0
54	MG	1a	1669	1/1	0.89	0.13	61,61,61,61	0
54	MG	2A	3165	1/1	0.89	0.70	52,52,52,52	0
54	MG	2A	3090	1/1	0.89	0.20	68,68,68,68	0
54	MG	1A	3777	1/1	0.89	0.21	44,44,44,44	0
54	MG	1A	3379	1/1	0.89	0.20	30,30,30,30	0
54	MG	1A	3104	1/1	0.89	0.80	43,43,43,43	0
54	MG	1V	205	1/1	0.89	0.40	60,60,60,60	0
54	MG	2A	3570	1/1	0.89	0.12	53,53,53,53	0
54	MG	1a	1663	1/1	0.89	0.10	66,66,66,66	0
54	MG	1A	3807	1/1	0.89	0.22	44,44,44,44	0
54	MG	1A	3302	1/1	0.89	0.28	64,64,64,64	0
54	MG	1l	104	1/1	0.89	0.09	45,45,45,45	0
54	MG	2A	3459	1/1	0.89	0.11	59,59,59,59	0
54	MG	2A	3524	1/1	0.89	0.09	59,59,59,59	0
54	MG	1A	3255	1/1	0.89	0.13	51,51,51,51	0
54	MG	1B	203	1/1	0.89	0.18	61,61,61,61	0
54	MG	1a	1662	1/1	0.89	0.14	74,74,74,74	0
54	MG	1A	3898	1/1	0.89	0.15	61,61,61,61	0
56	MPD	2A	3735	8/8	0.89	0.41	50,57,60,64	0
54	MG	2A	3364	1/1	0.89	0.16	62,62,62,62	0
54	MG	2A	3444	1/1	0.89	0.11	73,73,73,73	0
54	MG	1A	3467	1/1	0.89	0.18	56,56,56,56	0
54	MG	2A	3168	1/1	0.89	0.20	58,58,58,58	0
54	MG	1A	3786	1/1	0.89	0.19	26,26,26,26	0
54	MG	1A	3440	1/1	0.89	0.13	74,74,74,74	0
54	MG	2A	3584	1/1	0.89	0.07	46,46,46,46	0
54	MG	2A	3683	1/1	0.89	0.10	65,65,65,65	0
54	MG	1A	3941	1/1	0.89	0.21	55,55,55,55	0
54	MG	2A	3058	1/1	0.89	0.22	41,41,41,41	0
54	MG	1E	305	1/1	0.89	0.06	44,44,44,44	0
54	MG	1A	3575	1/1	0.89	0.18	59,59,59,59	0
54	MG	2A	3552	1/1	0.89	0.09	39,39,39,39	0
54	MG	2a	3046	1/1	0.89	0.12	67,67,67,67	0
54	MG	1A	3113	1/1	0.89	0.27	40,40,40,40	0
54	MG	1a	1631	1/1	0.89	0.21	51,51,51,51	0
54	MG	2a	3031	1/1	0.89	0.11	59,59,59,59	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
54	MG	1A	3920	1/1	0.89	0.07	48,48,48,48	0
54	MG	1A	3012	1/1	0.89	0.21	39,39,39,39	0
54	MG	1a	1803	1/1	0.89	0.22	62,62,62,62	0
54	MG	2A	3056	1/1	0.89	0.16	62,62,62,62	0
54	MG	2a	3086	1/1	0.89	0.08	60,60,60,60	0
54	MG	2A	3583	1/1	0.89	0.08	55,55,55,55	0
54	MG	1A	3050	1/1	0.89	0.41	46,46,46,46	0
54	MG	1B	210	1/1	0.89	0.11	46,46,46,46	0
54	MG	1A	3244	1/1	0.89	0.30	39,39,39,39	0
54	MG	1P	205	1/1	0.89	0.09	65,65,65,65	0
54	MG	1A	3514	1/1	0.89	0.20	39,39,39,39	0
54	MG	1A	3548	1/1	0.89	0.30	43,43,43,43	0
54	MG	1A	3892	1/1	0.89	0.21	42,42,42,42	0
54	MG	2A	3348	1/1	0.89	0.12	53,53,53,53	0
54	MG	1a	1767	1/1	0.89	0.16	66,66,66,66	0
54	MG	2A	3477	1/1	0.89	0.27	54,54,54,54	0
54	MG	2A	3064	1/1	0.89	0.16	48,48,48,48	0
54	MG	2a	3081	1/1	0.89	0.21	64,64,64,64	0
54	MG	1A	3698	1/1	0.89	0.55	47,47,47,47	0
54	MG	2A	3261	1/1	0.89	0.14	55,55,55,55	0
54	MG	1A	3770	1/1	0.89	0.15	32,32,32,32	0
54	MG	1a	1720	1/1	0.89	0.17	63,63,63,63	0
54	MG	2A	3238	1/1	0.89	0.12	61,61,61,61	0
54	MG	2A	3501	1/1	0.89	0.12	66,66,66,66	0
54	MG	1A	3664	1/1	0.89	0.18	52,52,52,52	0
54	MG	1a	1636	1/1	0.89	0.19	58,58,58,58	0
54	MG	1A	3802	1/1	0.89	0.13	56,56,56,56	0
54	MG	2A	3053	1/1	0.89	0.08	49,49,49,49	0
54	MG	2a	3043	1/1	0.89	0.20	54,54,54,54	0
54	MG	2A	3389	1/1	0.89	0.12	70,70,70,70	0
54	MG	1A	3781	1/1	0.90	0.07	33,33,33,33	0
54	MG	1y	203	1/1	0.90	0.18	75,75,75,75	0
54	MG	1a	1697	1/1	0.90	0.10	71,71,71,71	0
54	MG	1A	3708	1/1	0.90	0.08	52,52,52,52	0
54	MG	1A	3956	1/1	0.90	0.12	50,50,50,50	0
54	MG	2A	3470	1/1	0.90	0.10	67,67,67,67	0
54	MG	1A	3324	1/1	0.90	0.23	49,49,49,49	0
54	MG	1B	223	1/1	0.90	0.17	55,55,55,55	0
54	MG	2A	3281	1/1	0.90	0.15	51,51,51,51	0
54	MG	1a	1842	1/1	0.90	0.10	63,63,63,63	0
54	MG	1A	3981	1/1	0.90	0.16	46,46,46,46	0
54	MG	2a	3124	1/1	0.90	0.13	56,56,56,56	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
54	MG	1B	226	1/1	0.90	0.19	54,54,54,54	0
54	MG	2A	3002	1/1	0.90	0.10	52,52,52,52	0
54	MG	2A	3005	1/1	0.90	0.14	56,56,56,56	0
54	MG	1A	3723	1/1	0.90	0.12	42,42,42,42	0
54	MG	2A	3194	1/1	0.90	0.26	62,62,62,62	0
54	MG	2A	3098	1/1	0.90	0.09	57,57,57,57	0
54	MG	1B	224	1/1	0.90	0.06	53,53,53,53	0
54	MG	2A	3505	1/1	0.90	0.13	61,61,61,61	0
54	MG	2E	307	1/1	0.90	0.17	63,63,63,63	0
54	MG	1D	309	1/1	0.90	0.59	55,55,55,55	0
54	MG	2A	3041	1/1	0.90	0.16	56,56,56,56	0
54	MG	2A	3440	1/1	0.90	0.14	71,71,71,71	0
54	MG	2A	3712	1/1	0.90	0.22	57,57,57,57	0
54	MG	1a	1643	1/1	0.90	0.27	63,63,63,63	0
54	MG	1A	3475	1/1	0.90	0.15	46,46,46,46	0
54	MG	1A	3476	1/1	0.90	0.17	35,35,35,35	0
54	MG	1A	3439	1/1	0.90	0.11	51,51,51,51	0
54	MG	2A	3331	1/1	0.90	0.12	59,59,59,59	0
54	MG	1A	3767	1/1	0.90	0.15	28,28,28,28	0
54	MG	2P	201	1/1	0.90	0.34	45,45,45,45	0
54	MG	2a	3094	1/1	0.90	0.10	82,82,82,82	0
54	MG	1a	1837	1/1	0.90	0.08	57,57,57,57	0
54	MG	2A	3467	1/1	0.90	0.07	60,60,60,60	0
54	MG	2a	3144	1/1	0.90	0.15	66,66,66,66	0
54	MG	2A	3335	1/1	0.90	0.13	61,61,61,61	0
54	MG	1A	3087	1/1	0.90	0.20	32,32,32,32	0
54	MG	2A	3069	1/1	0.90	0.37	63,63,63,63	0
54	MG	1A	3293	1/1	0.90	0.16	48,48,48,48	0
54	MG	1a	1781	1/1	0.90	0.13	74,74,74,74	0
54	MG	1A	3304	1/1	0.90	0.07	84,84,84,84	0
54	MG	2A	3153	1/1	0.90	0.11	45,45,45,45	0
54	MG	1a	1716	1/1	0.90	0.32	75,75,75,75	0
54	MG	2a	3142	1/1	0.90	0.09	57,57,57,57	0
54	MG	2a	3013	1/1	0.90	0.07	73,73,73,73	0
54	MG	1A	3576	1/1	0.90	0.48	44,44,44,44	0
54	MG	1a	1824	1/1	0.90	0.14	64,64,64,64	0
54	MG	1A	3804	1/1	0.90	0.15	51,51,51,51	0
54	MG	1f	201	1/1	0.90	0.20	55,55,55,55	0
54	MG	1A	3572	1/1	0.90	0.09	44,44,44,44	0
54	MG	1A	3861	1/1	0.90	0.13	57,57,57,57	0
54	MG	1A	3092	1/1	0.90	0.39	36,36,36,36	0
54	MG	1A	3135	1/1	0.90	0.12	49,49,49,49	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
54	MG	1a	1634	1/1	0.90	0.13	44,44,44,44	0
54	MG	1A	3714	1/1	0.90	0.58	53,53,53,53	0
54	MG	2a	3084	1/1	0.90	0.14	59,59,59,59	0
54	MG	2a	3016	1/1	0.90	0.09	52,52,52,52	0
54	MG	2A	3670	1/1	0.90	0.10	68,68,68,68	0
54	MG	1A	3821	1/1	0.90	0.13	71,71,71,71	0
54	MG	1A	3348	1/1	0.90	0.15	39,39,39,39	0
54	MG	1A	3453	1/1	0.90	0.22	23,23,23,23	0
54	MG	2a	3055	1/1	0.90	0.09	65,65,65,65	0
54	MG	1A	3410	1/1	0.90	0.18	25,25,25,25	0
54	MG	2A	3623	1/1	0.90	0.10	52,52,52,52	0
54	MG	1a	1850	1/1	0.90	0.23	64,64,64,64	0
54	MG	1A	3194	1/1	0.90	0.21	43,43,43,43	0
54	MG	1A	3377	1/1	0.90	0.16	42,42,42,42	0
54	MG	1A	3934	1/1	0.90	0.10	48,48,48,48	0
54	MG	2A	3181	1/1	0.90	0.24	55,55,55,55	0
54	MG	1a	1771	1/1	0.90	0.11	80,80,80,80	0
54	MG	1A	3395	1/1	0.90	0.15	24,24,24,24	0
54	MG	1B	230	1/1	0.90	0.13	55,55,55,55	0
54	MG	2A	3150	1/1	0.90	0.39	53,53,53,53	0
54	MG	1A	3149	1/1	0.90	0.16	46,46,46,46	0
54	MG	1A	4019	1/1	0.90	0.39	58,58,58,58	0
54	MG	1a	1780	1/1	0.90	0.14	63,63,63,63	0
54	MG	1A	3246	1/1	0.90	0.16	48,48,48,48	0
54	MG	1A	3893	1/1	0.90	0.14	46,46,46,46	0
54	MG	2a	3160	1/1	0.90	0.12	74,74,74,74	0
54	MG	1A	3996	1/1	0.90	0.16	36,36,36,36	0
54	MG	1A	3987	1/1	0.90	0.10	55,55,55,55	0
54	MG	2N	201	1/1	0.90	0.27	76,76,76,76	0
54	MG	1G	204	1/1	0.90	0.14	58,58,58,58	0
54	MG	2A	3620	1/1	0.90	0.14	50,50,50,50	0
54	MG	1A	3626	1/1	0.90	0.17	34,34,34,34	0
54	MG	2A	3563	1/1	0.90	0.13	44,44,44,44	0
54	MG	1a	1867	1/1	0.90	0.10	80,80,80,80	0
54	MG	1A	3011	1/1	0.90	0.17	43,43,43,43	0
54	MG	2A	3109	1/1	0.90	0.24	51,51,51,51	0
54	MG	2A	3248	1/1	0.90	0.15	65,65,65,65	0
54	MG	2a	3018	1/1	0.90	0.20	73,73,73,73	0
54	MG	1A	3027	1/1	0.90	0.09	69,69,69,69	0
54	MG	1A	3280	1/1	0.90	0.27	49,49,49,49	0
54	MG	1A	3625	1/1	0.90	0.12	33,33,33,33	0
54	MG	1F	312	1/1	0.90	0.15	41,41,41,41	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
54	MG	1A	3275	1/1	0.90	0.16	56,56,56,56	0
56	MPD	1T	204	8/8	0.90	0.17	61,65,73,74	0
54	MG	1A	3107	1/1	0.90	0.15	44,44,44,44	0
54	MG	1a	1625	1/1	0.90	0.13	53,53,53,53	0
54	MG	2A	3349	1/1	0.90	0.10	39,39,39,39	0
54	MG	1a	1843	1/1	0.90	0.23	79,79,79,79	0
54	MG	2A	3595	1/1	0.90	0.10	47,47,47,47	0
54	MG	2A	3160	1/1	0.90	0.41	50,50,50,50	0
54	MG	1A	3416	1/1	0.90	0.15	31,31,31,31	0
54	MG	2A	3201	1/1	0.90	0.16	63,63,63,63	0
54	MG	1A	3539	1/1	0.90	0.16	41,41,41,41	0
54	MG	1A	3533	1/1	0.90	0.16	49,49,49,49	0
54	MG	2a	3001	1/1	0.90	0.28	56,56,56,56	0
54	MG	2j	201	1/1	0.90	0.11	73,73,73,73	0
54	MG	1A	3962	1/1	0.90	0.24	68,68,68,68	0
54	MG	1A	3035	1/1	0.90	0.21	43,43,43,43	0
54	MG	2B	208	1/1	0.90	0.12	63,63,63,63	0
54	MG	1A	3535	1/1	0.90	0.18	43,43,43,43	0
54	MG	1a	1853	1/1	0.90	0.06	55,55,55,55	0
54	MG	1A	3757	1/1	0.91	0.19	37,37,37,37	0
54	MG	2A	3733	1/1	0.91	0.10	52,52,52,52	0
54	MG	1A	3224	1/1	0.91	0.31	35,35,35,35	0
54	MG	2A	3369	1/1	0.91	0.11	68,68,68,68	0
54	MG	2A	3127	1/1	0.91	0.41	47,47,47,47	0
54	MG	2A	3659	1/1	0.91	0.11	56,56,56,56	0
54	MG	1A	3556	1/1	0.91	0.18	58,58,58,58	0
54	MG	2A	3495	1/1	0.91	0.12	59,59,59,59	0
54	MG	1A	3366	1/1	0.91	0.21	39,39,39,39	0
54	MG	2A	3399	1/1	0.91	0.10	59,59,59,59	0
54	MG	1a	1725	1/1	0.91	0.14	66,66,66,66	0
54	MG	1a	1639	1/1	0.91	0.22	75,75,75,75	0
54	MG	1a	1675	1/1	0.91	0.15	64,64,64,64	0
54	MG	1A	3266	1/1	0.91	0.18	66,66,66,66	0
54	MG	1A	3236	1/1	0.91	0.41	43,43,43,43	0
54	MG	25	101	1/1	0.91	0.50	44,44,44,44	0
54	MG	1A	3137	1/1	0.91	0.13	54,54,54,54	0
54	MG	2A	3025	1/1	0.91	0.17	56,56,56,56	0
54	MG	1a	1664	1/1	0.91	0.39	67,67,67,67	0
54	MG	1A	3191	1/1	0.91	0.17	40,40,40,40	0
54	MG	10	101	1/1	0.91	0.21	42,42,42,42	0
54	MG	2A	3171	1/1	0.91	0.46	70,70,70,70	0
54	MG	1A	3528	1/1	0.91	0.18	45,45,45,45	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
54	MG	2B	203	1/1	0.91	0.09	83,83,83,83	0
54	MG	1A	3565	1/1	0.91	0.12	62,62,62,62	0
54	MG	2A	3617	1/1	0.91	0.23	77,77,77,77	0
54	MG	1A	3067	1/1	0.91	0.12	50,50,50,50	0
54	MG	1A	3209	1/1	0.91	0.22	64,64,64,64	0
54	MG	1A	3192	1/1	0.91	0.14	64,64,64,64	0
54	MG	2a	3100	1/1	0.91	0.17	69,69,69,69	0
54	MG	1a	1609	1/1	0.91	0.11	67,67,67,67	0
54	MG	1A	3429	1/1	0.91	0.11	52,52,52,52	0
54	MG	2A	3313	1/1	0.91	0.15	55,55,55,55	0
54	MG	1A	3599	1/1	0.91	0.10	55,55,55,55	0
54	MG	1A	3850	1/1	0.91	0.10	35,35,35,35	0
54	MG	1A	3307	1/1	0.91	0.15	38,38,38,38	0
54	MG	1B	214	1/1	0.91	0.20	45,45,45,45	0
54	MG	2A	3189	1/1	0.91	0.10	53,53,53,53	0
54	MG	2a	3109	1/1	0.91	0.06	81,81,81,81	0
54	MG	1A	3618	1/1	0.91	0.23	32,32,32,32	0
54	MG	1A	3628	1/1	0.91	0.10	68,68,68,68	0
54	MG	2A	3499	1/1	0.91	0.16	46,46,46,46	0
54	MG	2A	3086	1/1	0.91	0.21	48,48,48,48	0
54	MG	1A	3614	1/1	0.91	0.14	64,64,64,64	0
54	MG	1A	3436	1/1	0.91	0.13	54,54,54,54	0
54	MG	1A	3037	1/1	0.91	0.22	43,43,43,43	0
54	MG	2a	3146	1/1	0.91	0.19	67,67,67,67	0
54	MG	2a	3178	1/1	0.91	0.11	65,65,65,65	0
54	MG	2A	3655	1/1	0.91	0.16	73,73,73,73	0
54	MG	1A	3375	1/1	0.91	0.14	45,45,45,45	0
54	MG	1a	1686	1/1	0.91	0.15	59,59,59,59	0
54	MG	2A	3390	1/1	0.91	0.23	69,69,69,69	0
54	MG	1a	1638	1/1	0.91	0.10	49,49,49,49	0
54	MG	2A	3257	1/1	0.91	0.10	57,57,57,57	0
54	MG	1a	1782	1/1	0.91	0.14	82,82,82,82	0
54	MG	2A	3462	1/1	0.91	0.21	70,70,70,70	0
54	MG	1A	3066	1/1	0.91	0.13	59,59,59,59	0
54	MG	2a	3118	1/1	0.91	0.23	68,68,68,68	0
54	MG	2A	3429	1/1	0.91	0.57	63,63,63,63	0
54	MG	2a	3091	1/1	0.91	0.11	71,71,71,71	0
54	MG	1A	3592	1/1	0.91	0.17	51,51,51,51	0
54	MG	1A	3638	1/1	0.91	0.14	60,60,60,60	0
54	MG	1A	3538	1/1	0.91	0.10	34,34,34,34	0
54	MG	1a	1721	1/1	0.91	0.32	80,80,80,80	0
54	MG	1a	1772	1/1	0.91	0.10	62,62,62,62	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
54	MG	2A	3358	1/1	0.91	0.10	58,58,58,58	0
54	MG	1A	3166	1/1	0.91	0.16	54,54,54,54	0
54	MG	2A	3203	1/1	0.91	0.14	53,53,53,53	0
54	MG	2A	3273	1/1	0.91	0.09	63,63,63,63	0
54	MG	1a	1869	1/1	0.91	0.12	64,64,64,64	0
54	MG	2A	3104	1/1	0.91	0.21	54,54,54,54	0
54	MG	1A	3679	1/1	0.91	0.11	76,76,76,76	0
54	MG	1A	3979	1/1	0.91	0.13	65,65,65,65	0
54	MG	2A	3134	1/1	0.91	0.15	62,62,62,62	0
54	MG	1A	3688	1/1	0.91	0.20	58,58,58,58	0
54	MG	1F	307	1/1	0.91	0.14	39,39,39,39	0
54	MG	1A	3794	1/1	0.91	0.07	78,78,78,78	0
54	MG	2A	3489	1/1	0.91	0.08	68,68,68,68	0
54	MG	2A	3288	1/1	0.91	0.10	52,52,52,52	0
54	MG	1A	3353	1/1	0.91	0.14	49,49,49,49	0
54	MG	1a	1834	1/1	0.91	0.12	50,50,50,50	0
54	MG	1A	3909	1/1	0.91	0.53	48,48,48,48	0
54	MG	1A	3585	1/1	0.91	0.13	55,55,55,55	0
54	MG	1a	1795	1/1	0.91	0.14	60,60,60,60	0
54	MG	1A	3678	1/1	0.91	0.13	76,76,76,76	0
54	MG	2a	3116	1/1	0.91	0.22	59,59,59,59	0
54	MG	2A	3606	1/1	0.91	0.35	62,62,62,62	0
54	MG	1A	3977	1/1	0.91	0.16	63,63,63,63	0
54	MG	1A	3549	1/1	0.91	0.10	44,44,44,44	0
54	MG	2A	3633	1/1	0.91	0.07	66,66,66,66	0
54	MG	2D	307	1/1	0.91	0.29	42,42,42,42	0
54	MG	2A	3648	1/1	0.91	0.10	67,67,67,67	0
54	MG	2A	3545	1/1	0.91	0.12	71,71,71,71	0
54	MG	1A	3498	1/1	0.91	0.12	45,45,45,45	0
54	MG	1A	3581	1/1	0.91	0.12	38,38,38,38	0
54	MG	1A	3809	1/1	0.91	0.22	57,57,57,57	0
54	MG	1A	3954	1/1	0.91	0.05	65,65,65,65	0
54	MG	1A	3685	1/1	0.91	0.06	45,45,45,45	0
54	MG	1A	3060	1/1	0.91	0.22	49,49,49,49	0
54	MG	2a	3129	1/1	0.91	0.23	77,77,77,77	0
54	MG	1A	3609	1/1	0.91	0.41	42,42,42,42	0
54	MG	1A	3950	1/1	0.91	0.10	48,48,48,48	0
54	MG	1B	208	1/1	0.91	0.21	47,47,47,47	0
54	MG	2a	3162	1/1	0.91	0.07	61,61,61,61	0
54	MG	1a	1778	1/1	0.91	0.12	71,71,71,71	0
54	MG	1A	3937	1/1	0.91	0.08	69,69,69,69	0
54	MG	1A	3162	1/1	0.91	0.27	35,35,35,35	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
54	MG	2A	3200	1/1	0.91	0.10	68,68,68,68	0
54	MG	1A	3758	1/1	0.91	0.08	53,53,53,53	0
54	MG	1A	3852	1/1	0.91	0.15	27,27,27,27	0
54	MG	1A	3634	1/1	0.91	0.20	59,59,59,59	0
54	MG	1A	3921	1/1	0.91	0.12	67,67,67,67	0
54	MG	1G	201	1/1	0.91	0.10	61,61,61,61	0
54	MG	1a	1796	1/1	0.91	0.22	71,71,71,71	0
54	MG	17	104	1/1	0.91	0.17	35,35,35,35	0
54	MG	2A	3074	1/1	0.91	0.07	65,65,65,65	0
54	MG	1A	3808	1/1	0.91	0.21	40,40,40,40	0
54	MG	2A	3215	1/1	0.91	0.15	56,56,56,56	0
54	MG	2A	3352	1/1	0.91	0.15	69,69,69,69	0
54	MG	1A	3976	1/1	0.91	0.09	52,52,52,52	0
54	MG	1A	3879	1/1	0.91	0.15	27,27,27,27	0
54	MG	2A	3572	1/1	0.91	0.16	75,75,75,75	0
54	MG	1A	3766	1/1	0.91	0.17	47,47,47,47	0
54	MG	2a	3177	1/1	0.91	0.09	74,74,74,74	0
54	MG	2a	3053	1/1	0.91	0.14	66,66,66,66	0
54	MG	2a	3103	1/1	0.91	0.09	85,85,85,85	0
54	MG	1A	3849	1/1	0.91	0.14	42,42,42,42	0
54	MG	2A	3438	1/1	0.91	0.09	54,54,54,54	0
54	MG	2a	3044	1/1	0.91	0.07	69,69,69,69	0
54	MG	1A	3647	1/1	0.91	0.15	33,33,33,33	0
54	MG	1A	3877	1/1	0.91	0.08	71,71,71,71	0
54	MG	1A	3059	1/1	0.91	0.18	45,45,45,45	0
54	MG	1A	3389	1/1	0.91	0.10	36,36,36,36	0
54	MG	1A	3524	1/1	0.91	0.11	51,51,51,51	0
54	MG	1A	3373	1/1	0.91	0.18	54,54,54,54	0
54	MG	2A	3520	1/1	0.91	0.15	57,57,57,57	0
54	MG	1a	1761	1/1	0.91	0.14	84,84,84,84	0
54	MG	1D	313	1/1	0.91	0.11	57,57,57,57	0
54	MG	1a	1629	1/1	0.91	0.13	63,63,63,63	0
54	MG	1A	3394	1/1	0.91	0.18	22,22,22,22	0
54	MG	2A	3154	1/1	0.91	0.26	65,65,65,65	0
54	MG	2a	3121	1/1	0.91	0.14	68,68,68,68	0
54	MG	2A	3503	1/1	0.91	0.10	77,77,77,77	0
54	MG	1A	3186	1/1	0.91	0.10	46,46,46,46	0
54	MG	1O	201	1/1	0.91	0.32	50,50,50,50	0
54	MG	1a	1666	1/1	0.92	0.45	56,56,56,56	0
54	MG	1A	3932	1/1	0.92	0.08	61,61,61,61	0
54	MG	2A	3324	1/1	0.92	0.13	53,53,53,53	0
54	MG	2A	3559	1/1	0.92	0.19	69,69,69,69	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
54	MG	1A	3641	1/1	0.92	0.21	41,41,41,41	0
54	MG	2A	3325	1/1	0.92	0.16	39,39,39,39	0
54	MG	2A	3277	1/1	0.92	0.10	73,73,73,73	0
57	ARG	1B	233	12/12	0.92	0.20	36,52,59,62	0
54	MG	1A	3412	1/1	0.92	0.07	73,73,73,73	0
54	MG	1A	3872	1/1	0.92	0.19	35,35,35,35	0
54	MG	2D	305	1/1	0.92	0.21	38,38,38,38	0
54	MG	1g	202	1/1	0.92	0.12	59,59,59,59	0
54	MG	2a	3148	1/1	0.92	0.12	69,69,69,69	0
54	MG	2A	3558	1/1	0.92	0.12	65,65,65,65	0
54	MG	1a	1726	1/1	0.92	0.21	56,56,56,56	0
54	MG	1A	3632	1/1	0.92	0.16	39,39,39,39	0
54	MG	1a	1807	1/1	0.92	0.12	68,68,68,68	0
54	MG	1A	3384	1/1	0.92	0.15	32,32,32,32	0
54	MG	2a	3158	1/1	0.92	0.23	69,69,69,69	0
54	MG	2a	3083	1/1	0.92	0.23	52,52,52,52	0
54	MG	1A	3905	1/1	0.92	0.10	54,54,54,54	0
54	MG	2A	3208	1/1	0.92	0.52	59,59,59,59	0
54	MG	1N	204	1/1	0.92	0.06	65,65,65,65	0
54	MG	2a	3079	1/1	0.92	0.13	59,59,59,59	0
54	MG	2A	3658	1/1	0.92	0.08	53,53,53,53	0
54	MG	1A	3527	1/1	0.92	0.26	49,49,49,49	0
54	MG	1A	3197	1/1	0.92	0.42	44,44,44,44	0
54	MG	1A	3942	1/1	0.92	0.16	42,42,42,42	0
54	MG	2A	3472	1/1	0.92	0.07	54,54,54,54	0
54	MG	1A	3906	1/1	0.92	0.16	30,30,30,30	0
54	MG	2A	3362	1/1	0.92	0.22	53,53,53,53	0
54	MG	2a	3153	1/1	0.92	0.09	58,58,58,58	0
54	MG	1a	1872	1/1	0.92	0.14	65,65,65,65	0
54	MG	1a	1617	1/1	0.92	0.06	73,73,73,73	0
54	MG	1B	225	1/1	0.92	0.07	49,49,49,49	0
54	MG	2A	3287	1/1	0.92	0.10	60,60,60,60	0
54	MG	2R	202	1/1	0.92	0.21	52,52,52,52	0
54	MG	2A	3163	1/1	0.92	0.21	56,56,56,56	0
54	MG	2A	3141	1/1	0.92	0.18	66,66,66,66	0
54	MG	1A	3853	1/1	0.92	0.11	59,59,59,59	0
54	MG	2A	3689	1/1	0.92	0.10	40,40,40,40	0
54	MG	1d	305	1/1	0.92	0.08	79,79,79,79	0
54	MG	2A	3102	1/1	0.92	0.11	51,51,51,51	0
54	MG	2A	3592	1/1	0.92	0.06	65,65,65,65	0
54	MG	2A	3607	1/1	0.92	0.06	57,57,57,57	0
54	MG	2a	3077	1/1	0.92	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
54	MG	2a	3034	1/1	0.92	0.08	58,58,58,58	0
54	MG	2a	3088	1/1	0.92	0.10	68,68,68,68	0
54	MG	1a	1724	1/1	0.92	0.14	40,40,40,40	0
54	MG	2a	3026	1/1	0.92	0.11	63,63,63,63	0
54	MG	1A	3218	1/1	0.92	0.22	30,30,30,30	0
54	MG	2A	3663	1/1	0.92	0.14	33,33,33,33	0
54	MG	1a	1846	1/1	0.92	0.13	48,48,48,48	0
54	MG	1A	3369	1/1	0.92	0.15	70,70,70,70	0
54	MG	2A	3457	1/1	0.92	0.17	74,74,74,74	0
54	MG	2A	3715	1/1	0.92	0.15	64,64,64,64	0
54	MG	10	104	1/1	0.92	0.09	47,47,47,47	0
54	MG	1A	3242	1/1	0.92	0.36	55,55,55,55	0
54	MG	1a	1622	1/1	0.92	0.14	48,48,48,48	0
54	MG	1A	3551	1/1	0.92	0.10	49,49,49,49	0
54	MG	2A	3391	1/1	0.92	0.08	39,39,39,39	0
54	MG	1A	3899	1/1	0.92	0.09	42,42,42,42	0
54	MG	1A	4006	1/1	0.92	0.29	57,57,57,57	0
54	MG	1e	202	1/1	0.92	0.24	55,55,55,55	0
54	MG	2A	3249	1/1	0.92	0.44	44,44,44,44	0
54	MG	2a	3078	1/1	0.92	0.08	57,57,57,57	0
54	MG	1a	1858	1/1	0.92	0.20	62,62,62,62	0
54	MG	1A	3810	1/1	0.92	0.27	46,46,46,46	0
54	MG	1A	3560	1/1	0.92	0.12	49,49,49,49	0
54	MG	1a	1692	1/1	0.92	0.17	63,63,63,63	0
54	MG	2A	3724	1/1	0.92	0.37	48,48,48,48	0
54	MG	1a	1851	1/1	0.92	0.12	53,53,53,53	0
54	MG	1A	3696	1/1	0.92	0.21	44,44,44,44	0
54	MG	1A	3102	1/1	0.92	0.17	54,54,54,54	0
54	MG	2A	3300	1/1	0.92	0.27	59,59,59,59	0
54	MG	2A	3697	1/1	0.92	0.10	40,40,40,40	0
54	MG	1A	3797	1/1	0.92	0.09	41,41,41,41	0
54	MG	1A	3661	1/1	0.92	0.11	47,47,47,47	0
54	MG	10	102	1/1	0.92	0.26	37,37,37,37	0
54	MG	1a	1814	1/1	0.92	0.08	72,72,72,72	0
54	MG	1a	1601	1/1	0.92	0.13	50,50,50,50	0
54	MG	1A	3426	1/1	0.92	0.10	40,40,40,40	0
54	MG	2a	3052	1/1	0.92	0.10	57,57,57,57	0
54	MG	2A	3714	1/1	0.92	0.06	78,78,78,78	0
54	MG	1A	3583	1/1	0.92	0.18	42,42,42,42	0
54	MG	2a	3063	1/1	0.92	0.09	59,59,59,59	0
54	MG	1A	3251	1/1	0.92	0.35	42,42,42,42	0
54	MG	1A	3471	1/1	0.92	0.17	27,27,27,27	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
54	MG	1A	3803	1/1	0.92	0.14	38,38,38,38	0
54	MG	2A	3343	1/1	0.92	0.15	42,42,42,42	0
54	MG	2A	3170	1/1	0.92	0.15	76,76,76,76	0
54	MG	1A	3241	1/1	0.92	0.23	67,67,67,67	0
54	MG	1B	217	1/1	0.92	0.25	50,50,50,50	0
54	MG	1A	3788	1/1	0.92	0.18	42,42,42,42	0
54	MG	1A	3008	1/1	0.92	0.20	42,42,42,42	0
54	MG	1W	201	1/1	0.92	0.32	51,51,51,51	0
54	MG	2A	3653	1/1	0.92	0.10	51,51,51,51	0
54	MG	1A	3785	1/1	0.92	0.24	45,45,45,45	0
54	MG	1A	3799	1/1	0.92	0.08	40,40,40,40	0
54	MG	1A	3765	1/1	0.92	0.19	62,62,62,62	0
54	MG	1a	1602	1/1	0.92	0.19	55,55,55,55	0
54	MG	1A	3993	1/1	0.92	0.09	65,65,65,65	0
54	MG	2A	3087	1/1	0.92	0.07	80,80,80,80	0
54	MG	2A	3527	1/1	0.92	0.14	45,45,45,45	0
54	MG	1A	3031	1/1	0.92	0.14	19,19,19,19	0
54	MG	2a	3127	1/1	0.92	0.12	63,63,63,63	0
54	MG	1a	1790	1/1	0.92	0.08	80,80,80,80	0
54	MG	1D	307	1/1	0.92	0.14	49,49,49,49	0
54	MG	1a	1701	1/1	0.92	0.15	72,72,72,72	0
54	MG	1A	3715	1/1	0.92	0.71	46,46,46,46	0
54	MG	1A	3505	1/1	0.92	0.16	26,26,26,26	0
54	MG	1A	3959	1/1	0.92	0.17	54,54,54,54	0
54	MG	2A	3224	1/1	0.92	0.21	48,48,48,48	0
54	MG	1B	216	1/1	0.92	0.11	56,56,56,56	0
54	MG	1P	203	1/1	0.92	0.50	36,36,36,36	0
54	MG	1B	231	1/1	0.92	0.18	71,71,71,71	0
54	MG	2A	3669	1/1	0.92	0.07	71,71,71,71	0
54	MG	2a	3042	1/1	0.92	0.09	76,76,76,76	0
54	MG	1a	1768	1/1	0.92	0.10	60,60,60,60	0
54	MG	2A	3393	1/1	0.92	0.12	69,69,69,69	0
54	MG	1A	3448	1/1	0.92	0.12	49,49,49,49	0
54	MG	1A	3171	1/1	0.92	0.11	49,49,49,49	0
54	MG	2A	3223	1/1	0.92	0.21	70,70,70,70	0
54	MG	2A	3077	1/1	0.92	0.25	44,44,44,44	0
54	MG	2A	3596	1/1	0.92	0.07	34,34,34,34	0
54	MG	1a	1860	1/1	0.92	0.11	57,57,57,57	0
54	MG	1A	3768	1/1	0.92	0.12	46,46,46,46	0
54	MG	2A	3340	1/1	0.92	0.11	44,44,44,44	0
54	MG	2A	3650	1/1	0.92	0.10	53,53,53,53	0
54	MG	1A	3952	1/1	0.92	0.11	47,47,47,47	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
54	MG	2A	3447	1/1	0.92	0.13	63,63,63,63	0
54	MG	2A	3705	1/1	0.92	0.07	56,56,56,56	0
54	MG	1A	3469	1/1	0.92	0.16	43,43,43,43	0
54	MG	2A	3656	1/1	0.92	0.11	51,51,51,51	0
54	MG	2A	3199	1/1	0.92	0.20	50,50,50,50	0
54	MG	1A	4007	1/1	0.92	0.10	50,50,50,50	0
54	MG	2A	3542	1/1	0.92	0.07	56,56,56,56	0
54	MG	1a	1847	1/1	0.92	0.13	68,68,68,68	0
56	MPD	1a	1875	8/8	0.92	0.21	60,64,68,69	0
54	MG	2A	3615	1/1	0.93	0.12	68,68,68,68	0
54	MG	1a	1736	1/1	0.93	0.24	62,62,62,62	0
54	MG	1F	316	1/1	0.93	0.17	42,42,42,42	0
54	MG	1A	3257	1/1	0.93	0.16	46,46,46,46	0
54	MG	2A	3426	1/1	0.93	0.15	49,49,49,49	0
54	MG	2A	3014	1/1	0.93	0.23	55,55,55,55	0
54	MG	2A	3026	1/1	0.93	0.08	42,42,42,42	0
54	MG	1A	3128	1/1	0.93	0.10	62,62,62,62	0
54	MG	1A	3065	1/1	0.93	0.08	55,55,55,55	0
54	MG	1a	1754	1/1	0.93	0.10	55,55,55,55	0
54	MG	1A	3930	1/1	0.93	0.04	39,39,39,39	0
54	MG	2A	3626	1/1	0.93	0.14	57,57,57,57	0
54	MG	1a	1632	1/1	0.93	0.09	55,55,55,55	0
54	MG	2a	3114	1/1	0.93	0.13	70,70,70,70	0
54	MG	2A	3195	1/1	0.93	0.10	54,54,54,54	0
54	MG	2A	3727	1/1	0.93	0.28	65,65,65,65	0
54	MG	2A	3674	1/1	0.93	0.18	51,51,51,51	0
54	MG	1A	3033	1/1	0.93	0.23	37,37,37,37	0
54	MG	2A	3146	1/1	0.93	0.39	34,34,34,34	0
54	MG	1a	1856	1/1	0.93	0.12	53,53,53,53	0
54	MG	2A	3509	1/1	0.93	0.30	63,63,63,63	0
54	MG	1D	315	1/1	0.93	0.16	49,49,49,49	0
54	MG	1a	1619	1/1	0.93	0.13	55,55,55,55	0
54	MG	2A	3377	1/1	0.93	0.11	34,34,34,34	0
54	MG	1A	3643	1/1	0.93	0.21	46,46,46,46	0
54	MG	1A	3749	1/1	0.93	0.10	35,35,35,35	0
54	MG	2A	3270	1/1	0.93	0.56	51,51,51,51	0
54	MG	1A	3339	1/1	0.93	0.17	61,61,61,61	0
54	MG	1A	4018	1/1	0.93	0.12	46,46,46,46	0
54	MG	2A	3322	1/1	0.93	0.12	64,64,64,64	0
54	MG	2A	3006	1/1	0.93	0.13	54,54,54,54	0
54	MG	2A	3242	1/1	0.93	0.19	59,59,59,59	0
54	MG	2A	3425	1/1	0.93	0.16	48,48,48,48	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
54	MG	2A	3316	1/1	0.93	0.11	39,39,39,39	0
54	MG	1A	3840	1/1	0.93	0.17	54,54,54,54	0
54	MG	1A	3126	1/1	0.93	0.10	46,46,46,46	0
54	MG	1A	3495	1/1	0.93	0.14	61,61,61,61	0
54	MG	1a	1687	1/1	0.93	0.14	53,53,53,53	0
54	MG	2a	3108	1/1	0.93	0.19	79,79,79,79	0
54	MG	13	103	1/1	0.93	0.10	45,45,45,45	0
54	MG	1A	3864	1/1	0.93	0.13	41,41,41,41	0
54	MG	2A	3088	1/1	0.93	0.27	39,39,39,39	0
54	MG	1A	3671	1/1	0.93	0.09	64,64,64,64	0
54	MG	2A	3124	1/1	0.93	0.12	39,39,39,39	0
54	MG	2A	3407	1/1	0.93	0.20	61,61,61,61	0
54	MG	2A	3142	1/1	0.93	0.19	46,46,46,46	0
54	MG	1a	1642	1/1	0.93	0.12	67,67,67,67	0
54	MG	2a	3036	1/1	0.93	0.10	61,61,61,61	0
54	MG	1A	3980	1/1	0.93	0.07	55,55,55,55	0
54	MG	2A	3568	1/1	0.93	0.06	33,33,33,33	0
54	MG	2A	3197	1/1	0.93	0.19	58,58,58,58	0
54	MG	2A	3276	1/1	0.93	0.17	56,56,56,56	0
54	MG	1A	3341	1/1	0.93	0.09	40,40,40,40	0
54	MG	1A	3801	1/1	0.93	0.12	44,44,44,44	0
54	MG	1B	206	1/1	0.93	0.33	43,43,43,43	0
54	MG	1a	1673	1/1	0.93	0.14	66,66,66,66	0
54	MG	17	103	1/1	0.93	0.34	40,40,40,40	0
54	MG	2A	3478	1/1	0.93	0.20	56,56,56,56	0
54	MG	1A	3431	1/1	0.93	0.16	67,67,67,67	0
54	MG	1A	3886	1/1	0.93	0.15	51,51,51,51	0
54	MG	2A	3247	1/1	0.93	0.37	61,61,61,61	0
54	MG	2A	3071	1/1	0.93	0.72	57,57,57,57	0
54	MG	1d	304	1/1	0.93	0.25	60,60,60,60	0
54	MG	1A	3203	1/1	0.93	0.21	72,72,72,72	0
54	MG	2A	3700	1/1	0.93	0.15	62,62,62,62	0
54	MG	1A	3648	1/1	0.93	0.13	49,49,49,49	0
54	MG	1A	3596	1/1	0.93	0.07	53,53,53,53	0
54	MG	2B	207	1/1	0.93	0.18	63,63,63,63	0
54	MG	2a	3082	1/1	0.93	0.18	61,61,61,61	0
54	MG	2A	3214	1/1	0.93	0.17	57,57,57,57	0
54	MG	1A	3125	1/1	0.93	0.21	56,56,56,56	0
54	MG	2a	3030	1/1	0.93	0.22	59,59,59,59	0
54	MG	1A	3838	1/1	0.93	0.14	44,44,44,44	0
54	MG	1A	3158	1/1	0.93	0.47	37,37,37,37	0
54	MG	2a	3048	1/1	0.93	0.25	69,69,69,69	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
54	MG	2A	3720	1/1	0.93	0.08	69,69,69,69	0
54	MG	1l	202	1/1	0.93	0.12	70,70,70,70	0
54	MG	2A	3096	1/1	0.93	0.11	46,46,46,46	0
54	MG	1A	3584	1/1	0.93	0.10	56,56,56,56	0
54	MG	1a	1627	1/1	0.93	0.12	62,62,62,62	0
54	MG	2A	3729	1/1	0.93	0.12	54,54,54,54	0
54	MG	1A	3961	1/1	0.93	0.11	57,57,57,57	0
54	MG	2A	3395	1/1	0.93	0.08	36,36,36,36	0
54	MG	2A	3687	1/1	0.93	0.12	69,69,69,69	0
54	MG	2A	3698	1/1	0.93	0.08	50,50,50,50	0
54	MG	1A	3903	1/1	0.93	0.17	28,28,28,28	0
54	MG	2A	3213	1/1	0.93	0.14	55,55,55,55	0
54	MG	1A	3704	1/1	0.93	0.35	50,50,50,50	0
54	MG	2A	3380	1/1	0.93	0.14	68,68,68,68	0
54	MG	2A	3033	1/1	0.93	0.66	57,57,57,57	0
54	MG	2A	3432	1/1	0.93	0.05	48,48,48,48	0
54	MG	1A	3600	1/1	0.93	0.18	32,32,32,32	0
54	MG	1A	3264	1/1	0.93	0.28	27,27,27,27	0
54	MG	1n	103	1/1	0.93	0.15	63,63,63,63	0
54	MG	1F	302	1/1	0.93	0.62	33,33,33,33	0
54	MG	1A	3145	1/1	0.93	0.25	68,68,68,68	0
54	MG	1A	3546	1/1	0.93	0.19	37,37,37,37	0
54	MG	1A	3400	1/1	0.93	0.14	32,32,32,32	0
54	MG	1A	3277	1/1	0.93	0.13	41,41,41,41	0
54	MG	1A	3466	1/1	0.93	0.16	42,42,42,42	0
54	MG	1A	3659	1/1	0.93	0.16	22,22,22,22	0
54	MG	1A	3083	1/1	0.93	0.14	35,35,35,35	0
54	MG	1A	3594	1/1	0.93	0.17	41,41,41,41	0
54	MG	1a	1635	1/1	0.93	0.16	50,50,50,50	0
54	MG	1A	3386	1/1	0.93	0.15	29,29,29,29	0
54	MG	1A	3998	1/1	0.93	0.27	48,48,48,48	0
54	MG	2A	3217	1/1	0.93	0.19	54,54,54,54	0
54	MG	2A	3556	1/1	0.93	0.18	58,58,58,58	0
54	MG	2A	3553	1/1	0.93	0.06	63,63,63,63	0
54	MG	1A	3676	1/1	0.93	0.15	60,60,60,60	0
54	MG	1A	3427	1/1	0.93	0.09	37,37,37,37	0
54	MG	2A	3140	1/1	0.93	0.31	46,46,46,46	0
54	MG	1a	1873	1/1	0.93	0.10	59,59,59,59	0
54	MG	1a	1630	1/1	0.93	0.07	57,57,57,57	0
54	MG	2A	3050	1/1	0.93	0.14	71,71,71,71	0
54	MG	2A	3624	1/1	0.93	0.10	68,68,68,68	0
54	MG	2a	3165	1/1	0.93	0.11	68,68,68,68	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
54	MG	1A	3978	1/1	0.93	0.07	60,60,60,60	0
54	MG	2A	3065	1/1	0.93	0.18	44,44,44,44	0
54	MG	2D	309	1/1	0.93	0.15	51,51,51,51	0
54	MG	1a	1841	1/1	0.93	0.21	61,61,61,61	0
54	MG	1t	202	1/1	0.93	0.18	62,62,62,62	0
54	MG	2a	3006	1/1	0.93	0.17	63,63,63,63	0
54	MG	1A	3831	1/1	0.93	0.15	37,37,37,37	0
54	MG	1A	3776	1/1	0.93	0.17	30,30,30,30	0
54	MG	1A	3342	1/1	0.93	0.09	57,57,57,57	0
54	MG	1U	204	1/1	0.93	0.48	33,33,33,33	0
54	MG	2A	3175	1/1	0.93	0.22	57,57,57,57	0
54	MG	1A	3684	1/1	0.93	0.09	46,46,46,46	0
54	MG	2A	3173	1/1	0.93	0.24	45,45,45,45	0
54	MG	1A	3357	1/1	0.93	0.18	21,21,21,21	0
54	MG	1N	203	1/1	0.93	0.10	53,53,53,53	0
54	MG	2A	3101	1/1	0.93	0.09	61,61,61,61	0
54	MG	1a	1605	1/1	0.93	0.18	73,73,73,73	0
54	MG	2A	3661	1/1	0.93	0.18	58,58,58,58	0
54	MG	1A	3597	1/1	0.93	0.11	36,36,36,36	0
54	MG	1g	201	1/1	0.93	0.18	62,62,62,62	0
54	MG	1A	3142	1/1	0.93	0.17	37,37,37,37	0
54	MG	1A	3670	1/1	0.93	0.13	38,38,38,38	0
54	MG	1A	3088	1/1	0.93	0.10	35,35,35,35	0
54	MG	2X	101	1/1	0.93	0.10	57,57,57,57	0
54	MG	1B	227	1/1	0.93	0.10	42,42,42,42	0
54	MG	1A	3313	1/1	0.93	0.15	51,51,51,51	0
54	MG	2A	3157	1/1	0.93	0.12	47,47,47,47	0
54	MG	1A	3507	1/1	0.93	0.18	43,43,43,43	0
54	MG	1d	301	1/1	0.93	0.12	69,69,69,69	0
54	MG	2A	3204	1/1	0.93	0.13	57,57,57,57	0
54	MG	1A	3619	1/1	0.93	0.20	38,38,38,38	0
54	MG	2A	3474	1/1	0.93	0.13	59,59,59,59	0
54	MG	1A	3437	1/1	0.93	0.09	33,33,33,33	0
54	MG	1A	3525	1/1	0.93	0.14	59,59,59,59	0
54	MG	2A	3677	1/1	0.93	0.14	49,49,49,49	0
54	MG	1A	3068	1/1	0.93	0.17	33,33,33,33	0
54	MG	1A	3271	1/1	0.93	0.16	51,51,51,51	0
54	MG	1A	3601	1/1	0.93	0.27	32,32,32,32	0
54	MG	1a	1738	1/1	0.93	0.15	52,52,52,52	0
54	MG	1A	3686	1/1	0.93	0.20	56,56,56,56	0
54	MG	1A	3608	1/1	0.93	0.12	31,31,31,31	0
54	MG	2A	3709	1/1	0.93	0.06	57,57,57,57	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
54	MG	1A	3773	1/1	0.93	0.24	21,21,21,21	0
54	MG	1a	1791	1/1	0.93	0.11	68,68,68,68	0
54	MG	1a	1863	1/1	0.93	0.11	61,61,61,61	0
54	MG	1A	3848	1/1	0.93	0.10	45,45,45,45	0
54	MG	1a	1812	1/1	0.93	0.09	66,66,66,66	0
54	MG	2A	3068	1/1	0.93	0.10	54,54,54,54	0
54	MG	1A	3182	1/1	0.93	0.54	42,42,42,42	0
54	MG	2A	3291	1/1	0.93	0.14	57,57,57,57	0
54	MG	1A	3055	1/1	0.93	0.22	41,41,41,41	0
54	MG	1A	3474	1/1	0.93	0.21	26,26,26,26	0
54	MG	1A	3262	1/1	0.93	0.14	55,55,55,55	0
54	MG	1A	3975	1/1	0.93	0.13	52,52,52,52	0
54	MG	2A	3518	1/1	0.93	0.08	65,65,65,65	0
54	MG	2A	3603	1/1	0.93	0.18	60,60,60,60	0
54	MG	1A	3691	1/1	0.93	0.09	48,48,48,48	0
54	MG	2A	3448	1/1	0.93	0.11	49,49,49,49	0
54	MG	2A	3662	1/1	0.93	0.15	38,38,38,38	0
54	MG	1A	3933	1/1	0.93	0.23	55,55,55,55	0
54	MG	2A	3649	1/1	0.93	0.09	46,46,46,46	0
54	MG	1A	3133	1/1	0.93	0.42	37,37,37,37	0
54	MG	1a	1681	1/1	0.93	0.28	52,52,52,52	0
54	MG	1A	3957	1/1	0.93	0.09	59,59,59,59	0
54	MG	1a	1644	1/1	0.93	0.13	64,64,64,64	0
54	MG	2A	3202	1/1	0.93	0.16	50,50,50,50	0
54	MG	2A	3143	1/1	0.93	0.17	71,71,71,71	0
54	MG	1A	3199	1/1	0.93	0.29	52,52,52,52	0
54	MG	1A	3995	1/1	0.93	0.04	52,52,52,52	0
54	MG	1A	3916	1/1	0.93	0.08	41,41,41,41	0
54	MG	1A	3674	1/1	0.93	0.12	76,76,76,76	0
54	MG	2A	3394	1/1	0.94	0.07	59,59,59,59	0
54	MG	1A	3356	1/1	0.94	0.12	45,45,45,45	0
54	MG	2A	3267	1/1	0.94	0.25	53,53,53,53	0
54	MG	10	107	1/1	0.94	0.17	51,51,51,51	0
54	MG	2A	3383	1/1	0.94	0.13	46,46,46,46	0
54	MG	2A	3571	1/1	0.94	0.07	67,67,67,67	0
54	MG	1A	3496	1/1	0.94	0.14	39,39,39,39	0
54	MG	2A	3250	1/1	0.94	0.11	52,52,52,52	0
54	MG	2a	3159	1/1	0.94	0.12	66,66,66,66	0
54	MG	1l	201	1/1	0.94	0.16	70,70,70,70	0
54	MG	1A	3939	1/1	0.94	0.12	30,30,30,30	0
54	MG	2A	3299	1/1	0.94	0.15	68,68,68,68	0
54	MG	1A	3074	1/1	0.94	0.16	42,42,42,42	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
54	MG	2a	3126	1/1	0.94	0.14	66,66,66,66	0
54	MG	1A	3335	1/1	0.94	0.16	35,35,35,35	0
54	MG	1a	1835	1/1	0.94	0.08	75,75,75,75	0
54	MG	2a	3120	1/1	0.94	0.16	68,68,68,68	0
54	MG	13	101	1/1	0.94	0.16	39,39,39,39	0
54	MG	2A	3084	1/1	0.94	0.22	45,45,45,45	0
54	MG	1A	3701	1/1	0.94	0.17	53,53,53,53	0
54	MG	1A	3300	1/1	0.94	0.31	37,37,37,37	0
54	MG	2A	3605	1/1	0.94	0.11	40,40,40,40	0
54	MG	1A	3703	1/1	0.94	0.09	33,33,33,33	0
54	MG	1A	3719	1/1	0.94	0.12	47,47,47,47	0
54	MG	1A	3579	1/1	0.94	0.10	36,36,36,36	0
54	MG	1a	1822	1/1	0.94	0.14	67,67,67,67	0
54	MG	2A	3408	1/1	0.94	0.16	55,55,55,55	0
54	MG	1A	3402	1/1	0.94	0.18	17,17,17,17	0
54	MG	2A	3404	1/1	0.94	0.15	60,60,60,60	0
54	MG	2A	3280	1/1	0.94	0.10	32,32,32,32	0
54	MG	2A	3616	1/1	0.94	0.15	49,49,49,49	0
54	MG	2A	3590	1/1	0.94	0.09	59,59,59,59	0
54	MG	2A	3546	1/1	0.94	0.18	44,44,44,44	0
54	MG	2Q	201	1/1	0.94	0.08	63,63,63,63	0
54	MG	1A	3010	1/1	0.94	0.15	60,60,60,60	0
54	MG	2A	3289	1/1	0.94	0.14	33,33,33,33	0
54	MG	2A	3636	1/1	0.94	0.09	62,62,62,62	0
54	MG	2A	3029	1/1	0.94	0.12	54,54,54,54	0
54	MG	2A	3241	1/1	0.94	0.36	48,48,48,48	0
54	MG	1A	4013	1/1	0.94	0.16	42,42,42,42	0
54	MG	1A	3999	1/1	0.94	0.09	51,51,51,51	0
54	MG	1U	201	1/1	0.94	0.32	36,36,36,36	0
54	MG	1A	3860	1/1	0.94	0.17	37,37,37,37	0
54	MG	1A	3484	1/1	0.94	0.09	56,56,56,56	0
54	MG	1A	3683	1/1	0.94	0.20	35,35,35,35	0
54	MG	20	101	1/1	0.94	0.50	63,63,63,63	0
54	MG	1A	3433	1/1	0.94	0.17	62,62,62,62	0
54	MG	1A	3370	1/1	0.94	0.30	61,61,61,61	0
54	MG	2A	3360	1/1	0.94	0.07	44,44,44,44	0
54	MG	1A	3747	1/1	0.94	0.23	34,34,34,34	0
54	MG	2A	3699	1/1	0.94	0.20	54,54,54,54	0
54	MG	1A	3482	1/1	0.94	0.17	27,27,27,27	0
54	MG	1A	3706	1/1	0.94	0.10	41,41,41,41	0
54	MG	1A	3958	1/1	0.94	0.16	47,47,47,47	0
54	MG	1A	3839	1/1	0.94	0.26	41,41,41,41	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
54	MG	2A	3264	1/1	0.94	0.09	55,55,55,55	0
54	MG	1A	3263	1/1	0.94	0.19	40,40,40,40	0
54	MG	1A	3682	1/1	0.94	0.10	49,49,49,49	0
54	MG	1A	3093	1/1	0.94	0.18	41,41,41,41	0
54	MG	1F	314	1/1	0.94	0.45	43,43,43,43	0
54	MG	2A	3159	1/1	0.94	0.28	61,61,61,61	0
54	MG	1A	3279	1/1	0.94	0.20	42,42,42,42	0
54	MG	1H	201	1/1	0.94	0.21	56,56,56,56	0
54	MG	1A	3908	1/1	0.94	0.17	21,21,21,21	0
54	MG	1a	1653	1/1	0.94	0.12	62,62,62,62	0
54	MG	1A	3761	1/1	0.94	0.09	28,28,28,28	0
54	MG	2a	3064	1/1	0.94	0.08	69,69,69,69	0
54	MG	1A	3645	1/1	0.94	0.25	59,59,59,59	0
54	MG	2A	3526	1/1	0.94	0.11	47,47,47,47	0
54	MG	1A	3249	1/1	0.94	0.68	43,43,43,43	0
54	MG	1A	3103	1/1	0.94	0.16	31,31,31,31	0
54	MG	1A	3323	1/1	0.94	0.16	30,30,30,30	0
54	MG	1A	3009	1/1	0.94	0.11	26,26,26,26	0
54	MG	1A	3418	1/1	0.94	0.20	43,43,43,43	0
54	MG	2A	3123	1/1	0.94	0.16	44,44,44,44	0
54	MG	2A	3019	1/1	0.94	0.50	44,44,44,44	0
54	MG	2A	3431	1/1	0.94	0.64	51,51,51,51	0
54	MG	2A	3693	1/1	0.94	0.20	54,54,54,54	0
54	MG	1A	3837	1/1	0.94	0.16	35,35,35,35	0
54	MG	1B	202	1/1	0.94	0.23	50,50,50,50	0
54	MG	1B	201	1/1	0.94	0.27	51,51,51,51	0
54	MG	1Z	301	1/1	0.94	0.22	54,54,54,54	0
54	MG	2A	3567	1/1	0.94	0.11	53,53,53,53	0
54	MG	1A	3081	1/1	0.94	0.26	41,41,41,41	0
54	MG	2a	3035	1/1	0.94	0.18	74,74,74,74	0
54	MG	2A	3668	1/1	0.94	0.15	44,44,44,44	0
54	MG	1A	3542	1/1	0.94	0.19	40,40,40,40	0
54	MG	2I	201	1/1	0.94	0.16	59,59,59,59	0
54	MG	2A	3366	1/1	0.94	0.05	79,79,79,79	0
54	MG	1A	3833	1/1	0.94	0.19	34,34,34,34	0
54	MG	2a	3008	1/1	0.94	0.11	78,78,78,78	0
54	MG	2A	3228	1/1	0.94	0.11	47,47,47,47	0
54	MG	1A	3736	1/1	0.94	0.14	51,51,51,51	0
54	MG	1A	3322	1/1	0.94	0.15	29,29,29,29	0
54	MG	1a	1817	1/1	0.94	0.11	67,67,67,67	0
54	MG	2a	3002	1/1	0.94	0.16	56,56,56,56	0
54	MG	1A	3415	1/1	0.94	0.23	28,28,28,28	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
54	MG	1A	3417	1/1	0.94	0.11	46,46,46,46	0
54	MG	1A	3658	1/1	0.94	0.15	51,51,51,51	0
54	MG	1A	3034	1/1	0.94	0.21	69,69,69,69	0
54	MG	1A	3724	1/1	0.94	0.12	42,42,42,42	0
54	MG	2A	3541	1/1	0.94	0.06	63,63,63,63	0
54	MG	2A	3341	1/1	0.94	0.08	47,47,47,47	0
54	MG	1A	3700	1/1	0.94	0.26	35,35,35,35	0
54	MG	1A	3492	1/1	0.94	0.13	44,44,44,44	0
54	MG	1a	1628	1/1	0.94	0.33	58,58,58,58	0
54	MG	1A	3459	1/1	0.94	0.14	55,55,55,55	0
54	MG	1A	3657	1/1	0.94	0.15	16,16,16,16	0
54	MG	2a	3151	1/1	0.94	0.10	68,68,68,68	0
54	MG	1A	3710	1/1	0.94	0.10	33,33,33,33	0
54	MG	1A	3156	1/1	0.94	0.42	39,39,39,39	0
54	MG	1A	4015	1/1	0.94	0.18	40,40,40,40	0
54	MG	1A	3076	1/1	0.94	0.27	43,43,43,43	0
54	MG	1A	3173	1/1	0.94	0.18	49,49,49,49	0
54	MG	2A	3269	1/1	0.94	0.32	48,48,48,48	0
54	MG	1A	3610	1/1	0.94	0.24	49,49,49,49	0
54	MG	25	102	1/1	0.94	0.51	42,42,42,42	0
54	MG	2a	3092	1/1	0.94	0.13	67,67,67,67	0
54	MG	2A	3680	1/1	0.94	0.24	60,60,60,60	0
54	MG	2a	3132	1/1	0.94	0.07	65,65,65,65	0
54	MG	2A	3321	1/1	0.94	0.12	48,48,48,48	0
54	MG	2E	305	1/1	0.94	0.09	50,50,50,50	0
54	MG	1A	3470	1/1	0.94	0.16	23,23,23,23	0
54	MG	2T	3303	1/1	0.94	0.09	65,65,65,65	0
54	MG	2A	3206	1/1	0.94	0.19	64,64,64,64	0
54	MG	1A	3274	1/1	0.94	0.09	61,61,61,61	0
54	MG	1A	3984	1/1	0.94	0.07	73,73,73,73	0
54	MG	1A	3119	1/1	0.94	0.28	33,33,33,33	0
54	MG	1a	1762	1/1	0.94	0.20	72,72,72,72	0
54	MG	1A	3885	1/1	0.94	0.16	56,56,56,56	0
54	MG	2A	3381	1/1	0.94	0.14	53,53,53,53	0
54	MG	1A	3117	1/1	0.94	0.12	33,33,33,33	0
54	MG	1A	3491	1/1	0.94	0.12	56,56,56,56	0
54	MG	1A	3463	1/1	0.94	0.07	38,38,38,38	0
54	MG	1T	201	1/1	0.94	0.07	64,64,64,64	0
54	MG	2A	3703	1/1	0.94	0.07	67,67,67,67	0
54	MG	1A	3602	1/1	0.94	0.07	67,67,67,67	0
54	MG	1A	3230	1/1	0.94	0.24	36,36,36,36	0
54	MG	2A	3039	1/1	0.94	0.13	51,51,51,51	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
54	MG	1A	3184	1/1	0.94	0.19	41,41,41,41	0
54	MG	1A	3889	1/1	0.94	0.14	40,40,40,40	0
54	MG	1A	3843	1/1	0.94	0.10	55,55,55,55	0
54	MG	2A	3333	1/1	0.94	0.10	51,51,51,51	0
56	MPD	2A	3736	8/8	0.94	0.26	52,56,60,62	0
54	MG	2B	218	1/1	0.94	0.11	68,68,68,68	0
54	MG	1A	3919	1/1	0.94	0.13	62,62,62,62	0
54	MG	1A	3940	1/1	0.94	0.18	36,36,36,36	0
54	MG	2a	3101	1/1	0.94	0.18	62,62,62,62	0
54	MG	2A	3130	1/1	0.94	0.56	75,75,75,75	0
54	MG	1A	3480	1/1	0.94	0.08	51,51,51,51	0
54	MG	1A	3208	1/1	0.94	0.47	45,45,45,45	0
54	MG	1A	3368	1/1	0.94	0.16	39,39,39,39	0
54	MG	1A	3869	1/1	0.94	0.15	30,30,30,30	0
54	MG	2A	3038	1/1	0.94	0.09	68,68,68,68	0
54	MG	1A	3046	1/1	0.94	0.20	50,50,50,50	0
54	MG	2A	3452	1/1	0.94	0.10	69,69,69,69	0
54	MG	2a	3051	1/1	0.94	0.12	55,55,55,55	0
54	MG	1A	3435	1/1	0.94	0.13	49,49,49,49	0
54	MG	1A	3744	1/1	0.94	0.21	65,65,65,65	0
54	MG	1a	1831	1/1	0.94	0.15	69,69,69,69	0
54	MG	1E	301	1/1	0.94	0.33	40,40,40,40	0
54	MG	1A	3310	1/1	0.94	0.82	53,53,53,53	0
54	MG	1A	3968	1/1	0.94	0.10	40,40,40,40	0
54	MG	1A	3099	1/1	0.94	0.15	44,44,44,44	0
54	MG	1A	3319	1/1	0.94	0.19	58,58,58,58	0
54	MG	2A	3593	1/1	0.94	0.07	50,50,50,50	0
54	MG	1A	3202	1/1	0.94	0.23	52,52,52,52	0
54	MG	2B	206	1/1	0.94	0.09	63,63,63,63	0
54	MG	1A	3741	1/1	0.94	0.24	44,44,44,44	0
54	MG	2A	3461	1/1	0.94	0.07	56,56,56,56	0
54	MG	1a	1691	1/1	0.94	0.15	55,55,55,55	0
54	MG	2A	3158	1/1	0.94	0.14	59,59,59,59	0
54	MG	2A	3591	1/1	0.94	0.07	59,59,59,59	0
54	MG	2A	3083	1/1	0.94	0.41	71,71,71,71	0
54	MG	1a	1613	1/1	0.94	0.08	74,74,74,74	0
54	MG	1A	3029	1/1	0.94	0.21	39,39,39,39	0
54	MG	2A	3023	1/1	0.94	0.20	58,58,58,58	0
54	MG	1A	3115	1/1	0.94	0.29	36,36,36,36	0
54	MG	1A	3798	1/1	0.94	0.14	47,47,47,47	0
54	MG	2a	3041	1/1	0.94	0.10	73,73,73,73	0
54	MG	1T	203	1/1	0.94	0.17	57,57,57,57	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
54	MG	2W	202	1/1	0.94	0.67	61,61,61,61	0
54	MG	2n	101	1/1	0.94	0.11	69,69,69,69	0
54	MG	1A	3605	1/1	0.94	0.30	38,38,38,38	0
54	MG	2A	3274	1/1	0.94	0.13	56,56,56,56	0
54	MG	1A	3312	1/1	0.94	0.40	58,58,58,58	0
54	MG	1A	3154	1/1	0.94	0.16	57,57,57,57	0
54	MG	1A	3399	1/1	0.94	0.13	45,45,45,45	0
54	MG	2A	3297	1/1	0.94	0.12	36,36,36,36	0
54	MG	1A	3461	1/1	0.94	0.14	53,53,53,53	0
54	MG	2A	3212	1/1	0.94	0.11	55,55,55,55	0
54	MG	2A	3654	1/1	0.94	0.13	54,54,54,54	0
54	MG	1A	3190	1/1	0.94	0.27	39,39,39,39	0
54	MG	2A	3176	1/1	0.94	0.10	42,42,42,42	0
54	MG	2A	3066	1/1	0.94	0.10	51,51,51,51	0
54	MG	1A	3146	1/1	0.94	0.11	30,30,30,30	0
54	MG	1A	3795	1/1	0.94	0.09	41,41,41,41	0
54	MG	2A	3207	1/1	0.94	0.21	60,60,60,60	0
54	MG	1A	3595	1/1	0.94	0.11	44,44,44,44	0
54	MG	2a	3045	1/1	0.94	0.24	59,59,59,59	0
54	MG	2A	3144	1/1	0.94	0.28	41,41,41,41	0
54	MG	2T	3302	1/1	0.94	0.16	53,53,53,53	0
54	MG	2A	3323	1/1	0.94	0.07	46,46,46,46	0
54	MG	1a	1651	1/1	0.94	0.17	53,53,53,53	0
54	MG	1A	3195	1/1	0.94	0.12	55,55,55,55	0
54	MG	1a	1830	1/1	0.94	0.13	66,66,66,66	0
54	MG	1e	203	1/1	0.94	0.11	70,70,70,70	0
54	MG	1A	3666	1/1	0.94	0.14	47,47,47,47	0
54	MG	2A	3107	1/1	0.94	0.17	38,38,38,38	0
54	MG	1A	3455	1/1	0.94	0.17	59,59,59,59	0
54	MG	1A	3884	1/1	0.94	0.27	46,46,46,46	0
54	MG	1A	3100	1/1	0.94	0.55	38,38,38,38	0
54	MG	1A	3468	1/1	0.94	0.16	26,26,26,26	0
54	MG	2A	3334	1/1	0.94	0.17	50,50,50,50	0
54	MG	2A	3414	1/1	0.94	0.76	52,52,52,52	0
54	MG	1A	3949	1/1	0.94	0.12	33,33,33,33	0
54	MG	2A	3688	1/1	0.94	0.09	71,71,71,71	0
54	MG	1A	3790	1/1	0.94	0.15	49,49,49,49	0
54	MG	1D	311	1/1	0.94	0.27	39,39,39,39	0
54	MG	1g	203	1/1	0.94	0.14	51,51,51,51	0
54	MG	1A	3075	1/1	0.94	0.11	44,44,44,44	0
54	MG	2a	3156	1/1	0.94	0.09	62,62,62,62	0
54	MG	2A	3307	1/1	0.94	0.19	57,57,57,57	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
54	MG	28	102	1/1	0.94	0.12	56,56,56,56	0
54	MG	2A	3521	1/1	0.94	0.12	64,64,64,64	0
54	MG	1A	3938	1/1	0.94	0.12	45,45,45,45	0
54	MG	1A	3815	1/1	0.95	0.14	53,53,53,53	0
54	MG	2A	3726	1/1	0.95	0.11	57,57,57,57	0
54	MG	2P	202	1/1	0.95	0.12	61,61,61,61	0
54	MG	1A	3751	1/1	0.95	0.18	51,51,51,51	0
54	MG	1A	3259	1/1	0.95	0.10	41,41,41,41	0
54	MG	1a	1871	1/1	0.95	0.10	62,62,62,62	0
54	MG	2a	3167	1/1	0.95	0.22	76,76,76,76	0
54	MG	1A	3216	1/1	0.95	0.27	37,37,37,37	0
54	MG	2a	3107	1/1	0.95	0.14	66,66,66,66	0
54	MG	1A	3687	1/1	0.95	0.16	58,58,58,58	0
54	MG	1A	3982	1/1	0.95	0.15	32,32,32,32	0
54	MG	2A	3332	1/1	0.95	0.12	33,33,33,33	0
54	MG	1a	1614	1/1	0.95	0.22	38,38,38,38	0
54	MG	1A	3349	1/1	0.95	0.17	25,25,25,25	0
54	MG	1A	3750	1/1	0.95	0.10	56,56,56,56	0
54	MG	2A	3193	1/1	0.95	0.10	57,57,57,57	0
54	MG	1A	3223	1/1	0.95	0.18	41,41,41,41	0
54	MG	1A	3733	1/1	0.95	0.12	49,49,49,49	0
54	MG	2a	3157	1/1	0.95	0.15	73,73,73,73	0
54	MG	1A	3258	1/1	0.95	0.28	32,32,32,32	0
54	MG	2A	3682	1/1	0.95	0.09	67,67,67,67	0
54	MG	1A	3778	1/1	0.95	0.22	45,45,45,45	0
54	MG	2A	3251	1/1	0.95	0.13	58,58,58,58	0
54	MG	1A	3170	1/1	0.95	0.17	48,48,48,48	0
54	MG	1a	1755	1/1	0.95	0.14	61,61,61,61	0
54	MG	2A	3162	1/1	0.95	0.19	56,56,56,56	0
54	MG	2a	3080	1/1	0.95	0.13	57,57,57,57	0
54	MG	1a	1737	1/1	0.95	0.12	59,59,59,59	0
54	MG	1A	3534	1/1	0.95	0.10	25,25,25,25	0
54	MG	1a	1836	1/1	0.95	0.06	55,55,55,55	0
54	MG	2a	3161	1/1	0.95	0.08	69,69,69,69	0
54	MG	1A	3896	1/1	0.95	0.12	46,46,46,46	0
54	MG	1A	3106	1/1	0.95	0.27	39,39,39,39	0
54	MG	1A	3735	1/1	0.95	0.14	37,37,37,37	0
54	MG	1a	1839	1/1	0.95	0.08	63,63,63,63	0
54	MG	1A	3621	1/1	0.95	0.14	54,54,54,54	0
54	MG	1A	3253	1/1	0.95	0.19	37,37,37,37	0
54	MG	1a	1718	1/1	0.95	0.09	60,60,60,60	0
54	MG	1A	3970	1/1	0.95	0.11	34,34,34,34	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
54	MG	2A	3445	1/1	0.95	0.25	64,64,64,64	0
54	MG	1A	3140	1/1	0.95	0.18	43,43,43,43	0
54	MG	1A	3442	1/1	0.95	0.09	46,46,46,46	0
54	MG	2A	3205	1/1	0.95	0.12	43,43,43,43	0
54	MG	1A	3680	1/1	0.95	0.24	28,28,28,28	0
54	MG	1A	3168	1/1	0.95	0.05	58,58,58,58	0
54	MG	1a	1730	1/1	0.95	0.33	63,63,63,63	0
54	MG	1A	3812	1/1	0.95	0.12	45,45,45,45	0
54	MG	15	101	1/1	0.95	0.47	42,42,42,42	0
54	MG	2A	3565	1/1	0.95	0.10	41,41,41,41	0
54	MG	28	101	1/1	0.95	0.12	44,44,44,44	0
54	MG	1A	3617	1/1	0.95	0.20	23,23,23,23	0
54	MG	1B	219	1/1	0.95	0.16	52,52,52,52	0
54	MG	2a	3095	1/1	0.95	0.06	65,65,65,65	0
54	MG	1A	3256	1/1	0.95	0.10	64,64,64,64	0
54	MG	1A	3523	1/1	0.95	0.11	25,25,25,25	0
54	MG	1A	3712	1/1	0.95	0.43	36,36,36,36	0
54	MG	2A	3409	1/1	0.95	0.15	47,47,47,47	0
54	MG	1A	3697	1/1	0.95	0.15	48,48,48,48	0
54	MG	2A	3719	1/1	0.95	0.19	48,48,48,48	0
54	MG	1a	1646	1/1	0.95	0.19	51,51,51,51	0
54	MG	2a	3066	1/1	0.95	0.18	63,63,63,63	0
54	MG	2A	3631	1/1	0.95	0.14	51,51,51,51	0
54	MG	1A	3873	1/1	0.95	0.10	50,50,50,50	0
54	MG	1A	3562	1/1	0.95	0.24	43,43,43,43	0
54	MG	2a	3068	1/1	0.95	0.23	60,60,60,60	0
54	MG	1A	3398	1/1	0.95	0.17	48,48,48,48	0
54	MG	1a	1773	1/1	0.95	0.17	68,68,68,68	0
54	MG	1A	3064	1/1	0.95	0.15	31,31,31,31	0
54	MG	2A	3094	1/1	0.95	0.10	76,76,76,76	0
54	MG	2l	201	1/1	0.95	0.13	63,63,63,63	0
54	MG	1A	3663	1/1	0.95	0.14	54,54,54,54	0
54	MG	1a	1633	1/1	0.95	0.14	66,66,66,66	0
54	MG	1A	3269	1/1	0.95	0.43	35,35,35,35	0
54	MG	2A	3555	1/1	0.95	0.11	48,48,48,48	0
54	MG	2A	3152	1/1	0.95	0.15	67,67,67,67	0
54	MG	1A	3563	1/1	0.95	0.17	21,21,21,21	0
54	MG	2A	3292	1/1	0.95	0.08	57,57,57,57	0
54	MG	2A	3027	1/1	0.95	0.28	59,59,59,59	0
54	MG	1A	3780	1/1	0.95	0.19	40,40,40,40	0
54	MG	1E	302	1/1	0.95	0.58	38,38,38,38	0
54	MG	2A	3580	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
54	MG	2A	3433	1/1	0.95	0.08	47,47,47,47	0
54	MG	1A	3229	1/1	0.95	0.45	42,42,42,42	0
54	MG	2A	3312	1/1	0.95	0.14	50,50,50,50	0
54	MG	1B	218	1/1	0.95	0.46	63,63,63,63	0
54	MG	1V	204	1/1	0.95	0.20	52,52,52,52	0
54	MG	1A	3854	1/1	0.95	0.14	39,39,39,39	0
54	MG	1A	3178	1/1	0.95	0.22	48,48,48,48	0
54	MG	2G	202	1/1	0.95	0.05	76,76,76,76	0
54	MG	2A	3147	1/1	0.95	0.62	60,60,60,60	0
54	MG	1A	3254	1/1	0.95	0.18	53,53,53,53	0
54	MG	1A	3238	1/1	0.95	0.31	39,39,39,39	0
54	MG	2a	3073	1/1	0.95	0.15	55,55,55,55	0
54	MG	2A	3283	1/1	0.95	0.10	66,66,66,66	0
54	MG	2A	3564	1/1	0.95	0.09	58,58,58,58	0
54	MG	2A	3339	1/1	0.95	0.19	59,59,59,59	0
54	MG	1A	3082	1/1	0.95	0.36	34,34,34,34	0
54	MG	2B	204	1/1	0.95	0.18	66,66,66,66	0
54	MG	2A	3517	1/1	0.95	0.35	63,63,63,63	0
54	MG	2A	3279	1/1	0.95	0.08	53,53,53,53	0
54	MG	1A	3326	1/1	0.95	0.16	31,31,31,31	0
54	MG	2A	3419	1/1	0.95	0.15	57,57,57,57	0
54	MG	1a	1854	1/1	0.95	0.11	61,61,61,61	0
54	MG	1A	3518	1/1	0.95	0.07	44,44,44,44	0
54	MG	1A	3363	1/1	0.95	0.17	34,34,34,34	0
54	MG	1A	3673	1/1	0.95	0.21	41,41,41,41	0
54	MG	2A	3225	1/1	0.95	0.08	60,60,60,60	0
54	MG	1A	3086	1/1	0.95	0.23	56,56,56,56	0
54	MG	1A	3079	1/1	0.95	0.19	40,40,40,40	0
54	MG	1A	3225	1/1	0.95	0.14	36,36,36,36	0
54	MG	1A	3912	1/1	0.95	0.13	20,20,20,20	0
54	MG	2a	3135	1/1	0.95	0.07	67,67,67,67	0
54	MG	1A	3401	1/1	0.95	0.15	68,68,68,68	0
54	MG	1a	1654	1/1	0.95	0.08	50,50,50,50	0
54	MG	2A	3560	1/1	0.95	0.05	65,65,65,65	0
54	MG	2a	3087	1/1	0.95	0.17	76,76,76,76	0
54	MG	1A	3695	1/1	0.95	0.36	33,33,33,33	0
54	MG	1d	303	1/1	0.95	0.11	56,56,56,56	0
54	MG	2a	3123	1/1	0.95	0.10	58,58,58,58	0
54	MG	1A	3118	1/1	0.95	0.28	35,35,35,35	0
54	MG	1A	3020	1/1	0.95	0.40	39,39,39,39	0
54	MG	1R	204	1/1	0.95	0.12	44,44,44,44	0
54	MG	1A	3007	1/1	0.95	0.13	38,38,38,38	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
54	MG	1A	3992	1/1	0.95	0.16	52,52,52,52	0
54	MG	1A	3483	1/1	0.95	0.16	35,35,35,35	0
54	MG	2A	3367	1/1	0.95	0.16	59,59,59,59	0
54	MG	2A	3691	1/1	0.95	0.19	57,57,57,57	0
54	MG	2a	3179	1/1	0.95	0.09	62,62,62,62	0
54	MG	1A	3725	1/1	0.95	0.14	49,49,49,49	0
54	MG	2a	3003	1/1	0.95	0.12	64,64,64,64	0
54	MG	1a	1792	1/1	0.95	0.11	57,57,57,57	0
54	MG	1a	1684	1/1	0.95	0.29	53,53,53,53	0
54	MG	10	103	1/1	0.95	0.10	40,40,40,40	0
54	MG	1B	204	1/1	0.95	0.34	52,52,52,52	0
54	MG	1E	304	1/1	0.95	0.11	24,24,24,24	0
54	MG	2a	3021	1/1	0.95	0.08	41,41,41,41	0
54	MG	1A	3148	1/1	0.95	0.11	51,51,51,51	0
54	MG	2a	3149	1/1	0.95	0.08	71,71,71,71	0
54	MG	1y	202	1/1	0.95	0.13	53,53,53,53	0
54	MG	1A	3361	1/1	0.95	0.11	27,27,27,27	0
54	MG	17	101	1/1	0.95	0.12	28,28,28,28	0
54	MG	2A	3293	1/1	0.95	0.15	62,62,62,62	0
54	MG	2A	3052	1/1	0.95	0.11	45,45,45,45	0
54	MG	1a	1626	1/1	0.95	0.09	49,49,49,49	0
54	MG	1A	3329	1/1	0.95	0.18	38,38,38,38	0
54	MG	1A	3378	1/1	0.95	0.13	36,36,36,36	0
54	MG	2A	3479	1/1	0.95	0.15	31,31,31,31	0
54	MG	2a	3096	1/1	0.95	0.15	49,49,49,49	0
54	MG	1A	3311	1/1	0.95	0.24	36,36,36,36	0
54	MG	1A	3635	1/1	0.95	0.37	34,34,34,34	0
54	MG	2a	3010	1/1	0.95	0.12	56,56,56,56	0
54	MG	1A	3742	1/1	0.95	0.13	58,58,58,58	0
54	MG	1A	3544	1/1	0.95	0.23	45,45,45,45	0
54	MG	1A	3272	1/1	0.95	0.23	43,43,43,43	0
54	MG	1A	3910	1/1	0.95	0.22	31,31,31,31	0
54	MG	2A	3468	1/1	0.95	0.09	33,33,33,33	0
54	MG	1a	1739	1/1	0.95	0.17	53,53,53,53	0
54	MG	1A	3738	1/1	0.95	0.11	39,39,39,39	0
54	MG	1A	3891	1/1	0.95	0.11	52,52,52,52	0
54	MG	2A	3167	1/1	0.95	0.65	67,67,67,67	0
54	MG	1A	3718	1/1	0.95	0.12	30,30,30,30	0
54	MG	2A	3536	1/1	0.95	0.11	38,38,38,38	0
54	MG	1A	3846	1/1	0.95	0.08	36,36,36,36	0
54	MG	2A	3290	1/1	0.95	0.12	48,48,48,48	0
54	MG	1A	3775	1/1	0.95	0.19	34,34,34,34	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
54	MG	2a	3074	1/1	0.95	0.20	58,58,58,58	0
54	MG	1A	3769	1/1	0.95	0.09	40,40,40,40	0
54	MG	1a	1679	1/1	0.95	0.24	56,56,56,56	0
54	MG	2A	3403	1/1	0.95	0.07	69,69,69,69	0
54	MG	2A	3013	1/1	0.95	0.12	33,33,33,33	0
54	MG	1a	1750	1/1	0.95	0.09	67,67,67,67	0
54	MG	1A	3656	1/1	0.95	0.11	55,55,55,55	0
54	MG	2A	3608	1/1	0.95	0.07	45,45,45,45	0
54	MG	1A	3213	1/1	0.95	0.30	43,43,43,43	0
54	MG	2a	3075	1/1	0.95	0.21	61,61,61,61	0
54	MG	1A	3318	1/1	0.95	0.18	40,40,40,40	0
54	MG	1A	3624	1/1	0.95	0.08	57,57,57,57	0
54	MG	2A	3095	1/1	0.95	0.16	53,53,53,53	0
54	MG	1m	201	1/1	0.95	0.10	68,68,68,68	0
56	MPD	18	103	8/8	0.95	0.31	33,41,46,48	0
54	MG	2A	3045	1/1	0.95	0.12	52,52,52,52	0
54	MG	1a	1637	1/1	0.95	0.12	60,60,60,60	0
54	MG	1A	3281	1/1	0.95	0.34	36,36,36,36	0
54	MG	1A	3127	1/1	0.95	0.27	56,56,56,56	0
54	MG	1P	202	1/1	0.95	0.37	29,29,29,29	0
54	MG	1D	314	1/1	0.95	0.09	63,63,63,63	0
54	MG	1A	3430	1/1	0.95	0.14	51,51,51,51	0
54	MG	1a	1789	1/1	0.95	0.10	56,56,56,56	0
54	MG	1A	3553	1/1	0.95	0.14	54,54,54,54	0
54	MG	2D	308	1/1	0.95	0.42	46,46,46,46	0
54	MG	1A	3232	1/1	0.95	0.28	30,30,30,30	0
54	MG	1a	1741	1/1	0.95	0.17	52,52,52,52	0
54	MG	1A	3669	1/1	0.95	0.12	61,61,61,61	0
54	MG	2A	3009	1/1	0.95	0.22	43,43,43,43	0
54	MG	1A	3732	1/1	0.95	0.13	32,32,32,32	0
54	MG	1a	1615	1/1	0.95	0.18	60,60,60,60	0
54	MG	1A	3270	1/1	0.95	0.14	53,53,53,53	0
54	MG	2A	3239	1/1	0.95	0.09	51,51,51,51	0
54	MG	1A	3613	1/1	0.95	0.10	34,34,34,34	0
54	MG	2A	3430	1/1	0.95	0.08	36,36,36,36	0
54	MG	2A	3350	1/1	0.95	0.10	32,32,32,32	0
54	MG	1W	202	1/1	0.95	0.23	52,52,52,52	0
54	MG	2A	3579	1/1	0.95	0.27	54,54,54,54	0
54	MG	2A	3330	1/1	0.95	0.05	56,56,56,56	0
54	MG	1a	1655	1/1	0.95	0.18	58,58,58,58	0
56	MPD	1A	4022	8/8	0.95	0.14	46,53,56,59	0
54	MG	2B	209	1/1	0.95	0.18	72,72,72,72	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
54	MG	2a	3183	1/1	0.95	0.14	86,86,86,86	0
54	MG	2a	3039	1/1	0.95	0.16	56,56,56,56	0
54	MG	1a	1868	1/1	0.95	0.11	63,63,63,63	0
54	MG	1A	3039	1/1	0.95	0.09	41,41,41,41	0
54	MG	1A	3991	1/1	0.95	0.14	43,43,43,43	0
54	MG	1A	3515	1/1	0.95	0.11	56,56,56,56	0
54	MG	1A	4009	1/1	0.95	0.12	47,47,47,47	0
54	MG	2A	3115	1/1	0.95	0.22	48,48,48,48	0
54	MG	2A	3388	1/1	0.95	0.12	46,46,46,46	0
54	MG	1a	1640	1/1	0.95	0.10	72,72,72,72	0
54	MG	1A	3947	1/1	0.95	0.16	39,39,39,39	0
54	MG	2A	3612	1/1	0.95	0.08	62,62,62,62	0
54	MG	2A	3043	1/1	0.95	0.14	30,30,30,30	0
54	MG	2A	3627	1/1	0.95	0.16	68,68,68,68	0
54	MG	1F	318	1/1	0.95	0.11	60,60,60,60	0
54	MG	1A	3201	1/1	0.95	0.08	40,40,40,40	0
54	MG	1a	1820	1/1	0.95	0.12	64,64,64,64	0
54	MG	1D	303	1/1	0.95	0.11	33,33,33,33	0
54	MG	2A	3252	1/1	0.95	0.32	46,46,46,46	0
54	MG	1A	3316	1/1	0.95	0.16	35,35,35,35	0
54	MG	1A	3816	1/1	0.95	0.12	27,27,27,27	0
54	MG	2A	3561	1/1	0.95	0.12	54,54,54,54	0
54	MG	1A	3291	1/1	0.95	0.47	44,44,44,44	0
54	MG	1A	3652	1/1	0.95	0.55	47,47,47,47	0
54	MG	2A	3122	1/1	0.95	0.16	43,43,43,43	0
54	MG	2A	3672	1/1	0.95	0.07	62,62,62,62	0
54	MG	1A	3019	1/1	0.95	0.37	28,28,28,28	0
54	MG	1A	3153	1/1	0.95	0.18	30,30,30,30	0
54	MG	2A	3351	1/1	0.95	0.15	47,47,47,47	0
54	MG	1a	1699	1/1	0.95	0.19	60,60,60,60	0
54	MG	1A	3564	1/1	0.95	0.18	39,39,39,39	0
54	MG	2A	3060	1/1	0.95	0.14	46,46,46,46	0
54	MG	2A	3645	1/1	0.95	0.17	40,40,40,40	0
54	MG	2A	3145	1/1	0.95	0.30	49,49,49,49	0
54	MG	2A	3586	1/1	0.95	0.08	53,53,53,53	0
54	MG	2A	3549	1/1	0.95	0.08	59,59,59,59	0
54	MG	1f	202	1/1	0.95	0.14	39,39,39,39	0
54	MG	1a	1740	1/1	0.95	0.11	76,76,76,76	0
54	MG	10	106	1/1	0.95	0.10	63,63,63,63	0
54	MG	1A	3139	1/1	0.95	0.25	42,42,42,42	0
54	MG	2A	3120	1/1	0.95	0.59	54,54,54,54	0
54	MG	1a	1606	1/1	0.95	0.12	49,49,49,49	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
54	MG	1a	1805	1/1	0.95	0.16	56,56,56,56	0
54	MG	1a	1799	1/1	0.95	0.10	71,71,71,71	0
54	MG	1A	3305	1/1	0.95	0.16	48,48,48,48	0
54	MG	1A	3811	1/1	0.95	0.08	30,30,30,30	0
54	MG	1A	3791	1/1	0.95	0.12	53,53,53,53	0
54	MG	2A	3622	1/1	0.95	0.12	66,66,66,66	0
54	MG	1A	3541	1/1	0.95	0.11	47,47,47,47	0
54	MG	2A	3372	1/1	0.95	0.18	63,63,63,63	0
54	MG	1i	201	1/1	0.95	0.14	59,59,59,59	0
54	MG	1A	3929	1/1	0.95	0.10	38,38,38,38	0
54	MG	1a	1818	1/1	0.95	0.11	76,76,76,76	0
54	MG	1A	3759	1/1	0.95	0.43	59,59,59,59	0
54	MG	1Q	204	1/1	0.95	0.13	47,47,47,47	0
54	MG	2a	3071	1/1	0.96	0.07	58,58,58,58	0
54	MG	2a	3076	1/1	0.96	0.06	68,68,68,68	0
54	MG	1A	3867	1/1	0.96	0.14	37,37,37,37	0
54	MG	1A	3343	1/1	0.96	0.12	29,29,29,29	0
54	MG	1A	3477	1/1	0.96	0.19	33,33,33,33	0
54	MG	1a	1751	1/1	0.96	0.12	58,58,58,58	0
54	MG	2A	3544	1/1	0.96	0.11	56,56,56,56	0
54	MG	2A	3359	1/1	0.96	0.13	38,38,38,38	0
54	MG	2a	3139	1/1	0.96	0.12	70,70,70,70	0
54	MG	2A	3092	1/1	0.96	0.15	46,46,46,46	0
54	MG	1a	1815	1/1	0.96	0.10	53,53,53,53	0
54	MG	1A	3408	1/1	0.96	0.09	42,42,42,42	0
54	MG	1A	3988	1/1	0.96	0.13	21,21,21,21	0
54	MG	2A	3710	1/1	0.96	0.23	48,48,48,48	0
54	MG	2A	3061	1/1	0.96	0.11	48,48,48,48	0
54	MG	2A	3007	1/1	0.96	0.45	50,50,50,50	0
54	MG	1A	3048	1/1	0.96	0.28	47,47,47,47	0
54	MG	1a	1733	1/1	0.96	0.12	43,43,43,43	0
54	MG	1A	3345	1/1	0.96	0.15	59,59,59,59	0
54	MG	1A	3644	1/1	0.96	0.14	41,41,41,41	0
54	MG	1A	3428	1/1	0.96	0.10	50,50,50,50	0
54	MG	1A	3091	1/1	0.96	0.14	28,28,28,28	0
54	MG	1A	3876	1/1	0.96	0.17	30,30,30,30	0
58	ZN	29	501	1/1	0.96	0.11	81,81,81,81	0
54	MG	1Y	201	1/1	0.96	0.14	57,57,57,57	0
54	MG	2A	3135	1/1	0.96	0.29	54,54,54,54	0
54	MG	2A	3488	1/1	0.96	0.08	54,54,54,54	0
54	MG	2A	3578	1/1	0.96	0.17	54,54,54,54	0
54	MG	2V	202	1/1	0.96	0.47	53,53,53,53	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
54	MG	1A	3260	1/1	0.96	0.15	75,75,75,75	0
54	MG	2A	3319	1/1	0.96	0.17	51,51,51,51	0
54	MG	1A	3222	1/1	0.96	0.44	37,37,37,37	0
54	MG	1A	3228	1/1	0.96	0.61	42,42,42,42	0
54	MG	1A	3637	1/1	0.96	0.20	27,27,27,27	0
54	MG	1A	3362	1/1	0.96	0.18	27,27,27,27	0
54	MG	1A	3946	1/1	0.96	0.08	24,24,24,24	0
54	MG	2A	3129	1/1	0.96	0.10	70,70,70,70	0
54	MG	1A	3502	1/1	0.96	0.12	50,50,50,50	0
54	MG	2A	3028	1/1	0.96	0.07	36,36,36,36	0
54	MG	2A	3537	1/1	0.96	0.10	47,47,47,47	0
54	MG	2a	3154	1/1	0.96	0.18	57,57,57,57	0
54	MG	1A	3771	1/1	0.96	0.09	44,44,44,44	0
54	MG	2A	3178	1/1	0.96	0.12	43,43,43,43	0
54	MG	1A	3372	1/1	0.96	0.11	44,44,44,44	0
54	MG	1A	3452	1/1	0.96	0.20	46,46,46,46	0
54	MG	2A	3376	1/1	0.96	0.09	53,53,53,53	0
54	MG	2A	3182	1/1	0.96	0.14	43,43,43,43	0
54	MG	1a	1683	1/1	0.96	0.10	79,79,79,79	0
54	MG	2A	3298	1/1	0.96	0.15	44,44,44,44	0
54	MG	2A	3601	1/1	0.96	0.04	63,63,63,63	0
54	MG	1A	3124	1/1	0.96	0.18	60,60,60,60	0
54	MG	2A	3646	1/1	0.96	0.06	69,69,69,69	0
54	MG	1a	1717	1/1	0.96	0.11	54,54,54,54	0
54	MG	1R	202	1/1	0.96	0.13	41,41,41,41	0
54	MG	1A	3297	1/1	0.96	0.08	48,48,48,48	0
54	MG	1A	4004	1/1	0.96	0.38	41,41,41,41	0
54	MG	1A	3914	1/1	0.96	0.33	33,33,33,33	0
54	MG	1A	3235	1/1	0.96	0.38	36,36,36,36	0
54	MG	1a	1759	1/1	0.96	0.10	60,60,60,60	0
54	MG	1A	3382	1/1	0.96	0.15	31,31,31,31	0
54	MG	1U	207	1/1	0.96	0.75	40,40,40,40	0
54	MG	1A	3793	1/1	0.96	0.23	61,61,61,61	0
54	MG	2a	3138	1/1	0.96	0.14	65,65,65,65	0
54	MG	1a	1779	1/1	0.96	0.23	57,57,57,57	0
54	MG	1A	3636	1/1	0.96	0.16	34,34,34,34	0
54	MG	2A	3265	1/1	0.96	0.10	32,32,32,32	0
54	MG	2A	3455	1/1	0.96	0.12	48,48,48,48	0
54	MG	2a	3099	1/1	0.96	0.13	69,69,69,69	0
54	MG	2A	3441	1/1	0.96	0.17	57,57,57,57	0
54	MG	1A	3547	1/1	0.96	0.24	58,58,58,58	0
54	MG	1A	3445	1/1	0.96	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
54	MG	2A	3326	1/1	0.96	0.13	36,36,36,36	0
54	MG	1A	3960	1/1	0.96	0.09	52,52,52,52	0
54	MG	2a	3032	1/1	0.96	0.16	49,49,49,49	0
54	MG	1A	3568	1/1	0.96	0.12	31,31,31,31	0
54	MG	2A	3155	1/1	0.96	0.12	45,45,45,45	0
54	MG	2A	3422	1/1	0.96	0.14	60,60,60,60	0
54	MG	1A	3084	1/1	0.96	0.13	43,43,43,43	0
54	MG	1a	1785	1/1	0.96	0.13	68,68,68,68	0
54	MG	1a	1852	1/1	0.96	0.11	57,57,57,57	0
54	MG	2A	3437	1/1	0.96	0.10	58,58,58,58	0
54	MG	1A	3245	1/1	0.96	0.40	36,36,36,36	0
54	MG	1A	3818	1/1	0.96	0.18	39,39,39,39	0
54	MG	1a	1743	1/1	0.96	0.08	52,52,52,52	0
54	MG	1a	1788	1/1	0.96	0.09	75,75,75,75	0
54	MG	1A	3090	1/1	0.96	0.15	37,37,37,37	0
54	MG	1a	1748	1/1	0.96	0.19	67,67,67,67	0
54	MG	2a	3182	1/1	0.96	0.13	79,79,79,79	0
54	MG	2A	3266	1/1	0.96	0.65	42,42,42,42	0
54	MG	1A	3200	1/1	0.96	0.22	53,53,53,53	0
54	MG	2A	3647	1/1	0.96	0.10	53,53,53,53	0
54	MG	2A	3482	1/1	0.96	0.09	48,48,48,48	0
54	MG	1a	1670	1/1	0.96	0.52	58,58,58,58	0
54	MG	2A	3031	1/1	0.96	0.09	37,37,37,37	0
54	MG	2A	3502	1/1	0.96	0.17	49,49,49,49	0
54	MG	1a	1694	1/1	0.96	0.17	49,49,49,49	0
54	MG	1a	1729	1/1	0.96	0.06	62,62,62,62	0
54	MG	2A	3421	1/1	0.96	0.10	36,36,36,36	0
54	MG	1n	101	1/1	0.96	0.17	72,72,72,72	0
54	MG	27	101	1/1	0.96	0.23	39,39,39,39	0
54	MG	1A	3743	1/1	0.96	0.18	53,53,53,53	0
54	MG	2A	3664	1/1	0.96	0.06	42,42,42,42	0
54	MG	2A	3082	1/1	0.96	0.08	49,49,49,49	0
54	MG	2A	3466	1/1	0.96	0.05	48,48,48,48	0
54	MG	2A	3344	1/1	0.96	0.07	75,75,75,75	0
54	MG	1A	3265	1/1	0.96	0.21	26,26,26,26	0
54	MG	1A	3049	1/1	0.96	0.29	39,39,39,39	0
54	MG	2D	302	1/1	0.96	0.84	43,43,43,43	0
54	MG	2A	3657	1/1	0.96	0.14	44,44,44,44	0
54	MG	2A	3543	1/1	0.96	0.16	69,69,69,69	0
54	MG	2A	3569	1/1	0.96	0.14	61,61,61,61	0
54	MG	1A	3900	1/1	0.96	0.14	54,54,54,54	0
54	MG	1a	1827	1/1	0.96	0.10	57,57,57,57	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
54	MG	1A	3497	1/1	0.96	0.12	40,40,40,40	0
54	MG	1A	3096	1/1	0.96	0.17	48,48,48,48	0
54	MG	1A	3376	1/1	0.96	0.11	52,52,52,52	0
54	MG	2A	3504	1/1	0.96	0.12	67,67,67,67	0
54	MG	2A	3610	1/1	0.96	0.17	38,38,38,38	0
54	MG	2A	3192	1/1	0.96	0.13	60,60,60,60	0
58	ZN	14	501	1/1	0.96	0.07	110,110,110,110	0
54	MG	1a	1829	1/1	0.96	0.23	82,82,82,82	0
54	MG	1A	3456	1/1	0.96	0.14	45,45,45,45	0
54	MG	1F	308	1/1	0.96	0.18	24,24,24,24	0
54	MG	2B	213	1/1	0.96	0.16	60,60,60,60	0
54	MG	1a	1776	1/1	0.96	0.21	68,68,68,68	0
54	MG	2A	3232	1/1	0.96	0.18	54,54,54,54	0
54	MG	1A	3690	1/1	0.96	0.10	47,47,47,47	0
54	MG	1a	1749	1/1	0.96	0.14	70,70,70,70	0
54	MG	1A	3390	1/1	0.96	0.15	30,30,30,30	0
54	MG	2A	3243	1/1	0.96	0.30	67,67,67,67	0
54	MG	1a	1806	1/1	0.96	0.10	69,69,69,69	0
54	MG	1B	205	1/1	0.96	0.11	41,41,41,41	0
54	MG	2I	101	1/1	0.96	0.11	75,75,75,75	0
54	MG	1A	3558	1/1	0.96	0.11	56,56,56,56	0
54	MG	1a	1727	1/1	0.96	0.12	65,65,65,65	0
54	MG	2a	3181	1/1	0.96	0.12	72,72,72,72	0
54	MG	1A	3782	1/1	0.96	0.11	46,46,46,46	0
54	MG	2A	3497	1/1	0.96	0.07	64,64,64,64	0
54	MG	1A	3639	1/1	0.96	0.30	69,69,69,69	0
54	MG	2F	301	1/1	0.96	0.44	47,47,47,47	0
54	MG	2A	3548	1/1	0.96	0.16	45,45,45,45	0
54	MG	2A	3702	1/1	0.96	0.07	48,48,48,48	0
54	MG	1A	3774	1/1	0.96	0.21	38,38,38,38	0
54	MG	1A	3650	1/1	0.96	0.13	55,55,55,55	0
54	MG	1A	3813	1/1	0.96	0.12	48,48,48,48	0
54	MG	1A	3038	1/1	0.96	0.12	38,38,38,38	0
54	MG	1A	3754	1/1	0.96	0.17	37,37,37,37	0
54	MG	2a	3131	1/1	0.96	0.13	61,61,61,61	0
54	MG	1V	207	1/1	0.96	0.13	67,67,67,67	0
54	MG	1A	3016	1/1	0.96	0.51	36,36,36,36	0
54	MG	2A	3022	1/1	0.96	0.51	54,54,54,54	0
54	MG	2A	3673	1/1	0.96	0.06	51,51,51,51	0
54	MG	2A	3355	1/1	0.96	0.10	47,47,47,47	0
54	MG	1A	3129	1/1	0.96	0.12	34,34,34,34	0
54	MG	1A	3472	1/1	0.96	0.13	25,25,25,25	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
54	MG	2A	3678	1/1	0.96	0.13	39,39,39,39	0
54	MG	1A	3478	1/1	0.96	0.19	28,28,28,28	0
54	MG	1A	3868	1/1	0.96	0.18	45,45,45,45	0
54	MG	1a	1728	1/1	0.96	0.07	54,54,54,54	0
54	MG	1A	3111	1/1	0.96	0.26	36,36,36,36	0
54	MG	1a	1616	1/1	0.96	0.09	56,56,56,56	0
54	MG	2A	3156	1/1	0.96	0.25	58,58,58,58	0
54	MG	2B	216	1/1	0.96	0.11	59,59,59,59	0
54	MG	1A	3655	1/1	0.96	0.13	31,31,31,31	0
54	MG	1A	3559	1/1	0.96	0.12	40,40,40,40	0
54	MG	1A	3711	1/1	0.96	0.07	20,20,20,20	0
54	MG	2A	3067	1/1	0.96	0.17	48,48,48,48	0
54	MG	2A	3149	1/1	0.96	0.27	60,60,60,60	0
54	MG	1A	3015	1/1	0.96	0.20	33,33,33,33	0
54	MG	1A	3756	1/1	0.96	0.16	32,32,32,32	0
54	MG	1a	1745	1/1	0.96	0.08	57,57,57,57	0
54	MG	2A	3132	1/1	0.96	0.15	60,60,60,60	0
54	MG	1a	1623	1/1	0.96	0.26	60,60,60,60	0
54	MG	1A	3393	1/1	0.96	0.18	20,20,20,20	0
54	MG	1A	3511	1/1	0.96	0.08	52,52,52,52	0
54	MG	1A	3240	1/1	0.96	0.19	25,25,25,25	0
54	MG	1A	3911	1/1	0.96	0.08	49,49,49,49	0
54	MG	1a	1864	1/1	0.96	0.12	47,47,47,47	0
54	MG	1a	1723	1/1	0.96	0.10	63,63,63,63	0
54	MG	2A	3485	1/1	0.96	0.08	37,37,37,37	0
54	MG	2A	3609	1/1	0.96	0.11	39,39,39,39	0
54	MG	2A	3406	1/1	0.96	0.05	51,51,51,51	0
54	MG	2A	3416	1/1	0.96	0.17	50,50,50,50	0
54	MG	2A	3684	1/1	0.96	0.09	55,55,55,55	0
54	MG	2A	3286	1/1	0.96	0.08	48,48,48,48	0
54	MG	1A	3875	1/1	0.96	0.17	39,39,39,39	0
54	MG	2A	3148	1/1	0.96	0.08	64,64,64,64	0
54	MG	1A	3404	1/1	0.96	0.25	55,55,55,55	0
54	MG	1A	3508	1/1	0.96	0.09	50,50,50,50	0
54	MG	2A	3011	1/1	0.96	0.12	35,35,35,35	0
54	MG	1a	1607	1/1	0.96	0.11	51,51,51,51	0
54	MG	2A	3492	1/1	0.96	0.06	40,40,40,40	0
54	MG	2a	3038	1/1	0.96	0.16	66,66,66,66	0
54	MG	1A	3762	1/1	0.96	0.16	54,54,54,54	0
54	MG	1A	3792	1/1	0.96	0.17	58,58,58,58	0
54	MG	1A	3053	1/1	0.96	0.43	37,37,37,37	0
54	MG	2A	3471	1/1	0.96	0.08	67,67,67,67	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
54	MG	1A	3897	1/1	0.96	0.05	47,47,47,47	0
54	MG	1a	1744	1/1	0.96	0.15	65,65,65,65	0
54	MG	1A	3407	1/1	0.96	0.16	35,35,35,35	0
54	MG	1A	3446	1/1	0.96	0.20	57,57,57,57	0
54	MG	2a	3122	1/1	0.96	0.20	74,74,74,74	0
54	MG	2B	215	1/1	0.96	0.13	67,67,67,67	0
54	MG	1A	3101	1/1	0.96	0.37	33,33,33,33	0
54	MG	2o	101	1/1	0.96	0.08	65,65,65,65	0
54	MG	2a	3140	1/1	0.96	0.16	67,67,67,67	0
54	MG	1a	1705	1/1	0.96	0.08	59,59,59,59	0
54	MG	2A	3692	1/1	0.96	0.15	51,51,51,51	0
54	MG	1A	3734	1/1	0.96	0.13	40,40,40,40	0
54	MG	1A	3021	1/1	0.96	0.43	43,43,43,43	0
54	MG	1A	3414	1/1	0.96	0.07	63,63,63,63	0
54	MG	1B	215	1/1	0.96	0.14	39,39,39,39	0
54	MG	1A	3163	1/1	0.96	0.13	52,52,52,52	0
54	MG	1A	3298	1/1	0.96	0.21	49,49,49,49	0
54	MG	1A	3842	1/1	0.96	0.14	44,44,44,44	0
54	MG	1A	3315	1/1	0.96	0.15	27,27,27,27	0
54	MG	2A	3375	1/1	0.96	0.13	57,57,57,57	0
54	MG	2A	3574	1/1	0.96	0.15	53,53,53,53	0
54	MG	1A	3783	1/1	0.96	0.21	50,50,50,50	0
54	MG	1A	3004	1/1	0.96	0.08	45,45,45,45	0
54	MG	1a	1667	1/1	0.96	0.22	63,63,63,63	0
54	MG	1A	3894	1/1	0.96	0.16	39,39,39,39	0
54	MG	1A	3204	1/1	0.96	0.17	38,38,38,38	0
54	MG	1A	3462	1/1	0.96	0.25	47,47,47,47	0
54	MG	2A	3442	1/1	0.96	0.10	64,64,64,64	0
54	MG	1A	3665	1/1	0.96	0.15	63,63,63,63	0
54	MG	1A	3871	1/1	0.96	0.14	28,28,28,28	0
54	MG	2D	304	1/1	0.96	0.61	44,44,44,44	0
54	MG	2R	201	1/1	0.96	0.19	46,46,46,46	0
54	MG	1A	3729	1/1	0.96	0.26	34,34,34,34	0
54	MG	2A	3716	1/1	0.96	0.06	65,65,65,65	0
54	MG	1a	1713	1/1	0.96	0.10	48,48,48,48	0
54	MG	2a	3145	1/1	0.96	0.07	60,60,60,60	0
54	MG	2a	3014	1/1	0.96	0.10	64,64,64,64	0
54	MG	2A	3644	1/1	0.96	0.14	38,38,38,38	0
54	MG	1A	3108	1/1	0.96	0.24	34,34,34,34	0
54	MG	2a	3005	1/1	0.96	0.15	65,65,65,65	0
54	MG	1A	3653	1/1	0.96	0.09	31,31,31,31	0
54	MG	1A	3306	1/1	0.96	0.17	28,28,28,28	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
54	MG	1A	3320	1/1	0.96	0.18	29,29,29,29	0
54	MG	1A	3374	1/1	0.96	0.09	48,48,48,48	0
54	MG	1A	3513	1/1	0.96	0.16	21,21,21,21	0
54	MG	1F	309	1/1	0.96	0.31	34,34,34,34	0
54	MG	1A	4011	1/1	0.96	0.13	58,58,58,58	0
54	MG	2A	3327	1/1	0.96	0.13	42,42,42,42	0
54	MG	1A	3764	1/1	0.96	0.09	30,30,30,30	0
54	MG	1A	3268	1/1	0.96	0.44	34,34,34,34	0
54	MG	1A	3964	1/1	0.96	0.17	51,51,51,51	0
54	MG	1A	3077	1/1	0.96	0.20	30,30,30,30	0
54	MG	2A	3057	1/1	0.96	0.14	52,52,52,52	0
54	MG	1A	3026	1/1	0.96	0.35	34,34,34,34	0
54	MG	1A	3567	1/1	0.96	0.14	45,45,45,45	0
54	MG	2A	3128	1/1	0.96	0.42	43,43,43,43	0
54	MG	1A	3554	1/1	0.96	0.11	40,40,40,40	0
54	MG	2A	3500	1/1	0.96	0.11	60,60,60,60	0
54	MG	2A	3427	1/1	0.96	0.12	38,38,38,38	0
54	MG	1A	3973	1/1	0.96	0.11	26,26,26,26	0
54	MG	1A	3874	1/1	0.96	0.17	39,39,39,39	0
54	MG	2A	3075	1/1	0.96	0.16	37,37,37,37	0
54	MG	2A	3078	1/1	0.96	0.07	42,42,42,42	0
54	MG	1A	3396	1/1	0.96	0.10	28,28,28,28	0
54	MG	1A	3966	1/1	0.96	0.10	43,43,43,43	0
54	MG	18	101	1/1	0.96	0.22	34,34,34,34	0
54	MG	1A	3561	1/1	0.96	0.05	43,43,43,43	0
54	MG	1A	3006	1/1	0.96	0.17	25,25,25,25	0
54	MG	1A	3880	1/1	0.96	0.16	62,62,62,62	0
54	MG	1A	3506	1/1	0.96	0.17	20,20,20,20	0
54	MG	2A	3103	1/1	0.96	0.10	66,66,66,66	0
54	MG	2A	3184	1/1	0.96	0.28	60,60,60,60	0
54	MG	2A	3392	1/1	0.96	0.14	37,37,37,37	0
54	MG	2A	3021	1/1	0.96	0.18	50,50,50,50	0
54	MG	2A	3685	1/1	0.96	0.12	39,39,39,39	0
54	MG	1A	3392	1/1	0.96	0.17	24,24,24,24	0
54	MG	1A	3250	1/1	0.96	0.24	34,34,34,34	0
54	MG	1A	3296	1/1	0.96	0.11	40,40,40,40	0
54	MG	1A	3134	1/1	0.96	0.23	36,36,36,36	0
54	MG	2A	3105	1/1	0.96	0.09	69,69,69,69	0
54	MG	1A	3247	1/1	0.96	0.41	40,40,40,40	0
54	MG	2A	3515	1/1	0.96	0.22	49,49,49,49	0
54	MG	2A	3713	1/1	0.96	0.41	47,47,47,47	0
54	MG	2A	3554	1/1	0.97	0.10	28,28,28,28	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
54	MG	1A	3023	1/1	0.97	0.16	26,26,26,26	0
54	MG	1A	3859	1/1	0.97	0.11	48,48,48,48	0
54	MG	2a	3111	1/1	0.97	0.06	57,57,57,57	0
54	MG	1A	3003	1/1	0.97	0.16	36,36,36,36	0
54	MG	1A	3931	1/1	0.97	0.11	56,56,56,56	0
54	MG	1A	3890	1/1	0.97	0.13	32,32,32,32	0
54	MG	1A	3878	1/1	0.97	0.19	49,49,49,49	0
54	MG	1A	3219	1/1	0.97	0.15	27,27,27,27	0
54	MG	1A	3598	1/1	0.97	0.14	41,41,41,41	0
54	MG	2A	3506	1/1	0.97	0.15	39,39,39,39	0
54	MG	1A	3630	1/1	0.97	0.06	40,40,40,40	0
54	MG	2B	212	1/1	0.97	0.12	80,80,80,80	0
54	MG	2E	303	1/1	0.97	0.10	57,57,57,57	0
54	MG	2A	3337	1/1	0.97	0.07	36,36,36,36	0
54	MG	1E	309	1/1	0.97	0.14	52,52,52,52	0
54	MG	1A	3252	1/1	0.97	0.19	36,36,36,36	0
54	MG	1E	310	1/1	0.97	0.09	58,58,58,58	0
54	MG	2E	306	1/1	0.97	0.13	30,30,30,30	0
54	MG	1A	3863	1/1	0.97	0.15	35,35,35,35	0
54	MG	1A	3123	1/1	0.97	0.31	32,32,32,32	0
54	MG	1a	1709	1/1	0.97	0.16	35,35,35,35	0
54	MG	1D	301	1/1	0.97	0.41	40,40,40,40	0
54	MG	1A	3403	1/1	0.97	0.09	33,33,33,33	0
54	MG	1A	3689	1/1	0.97	0.14	39,39,39,39	0
54	MG	2A	3310	1/1	0.97	0.14	43,43,43,43	0
54	MG	1A	3121	1/1	0.97	0.20	35,35,35,35	0
54	MG	2a	3112	1/1	0.97	0.12	64,64,64,64	0
54	MG	1A	3248	1/1	0.97	0.15	39,39,39,39	0
54	MG	13	102	1/1	0.97	0.15	41,41,41,41	0
54	MG	2A	3411	1/1	0.97	0.15	53,53,53,53	0
54	MG	2A	3085	1/1	0.97	0.44	50,50,50,50	0
54	MG	2a	3125	1/1	0.97	0.08	64,64,64,64	0
54	MG	1A	3574	1/1	0.97	0.20	33,33,33,33	0
54	MG	1W	204	1/1	0.97	0.31	54,54,54,54	0
54	MG	2A	3036	1/1	0.97	0.17	48,48,48,48	0
54	MG	1A	3052	1/1	0.97	0.23	43,43,43,43	0
54	MG	1A	3062	1/1	0.97	0.14	32,32,32,32	0
54	MG	2A	3413	1/1	0.97	0.06	62,62,62,62	0
54	MG	2A	3621	1/1	0.97	0.10	52,52,52,52	0
54	MG	1A	3070	1/1	0.97	0.28	27,27,27,27	0
54	MG	1a	1649	1/1	0.97	0.13	50,50,50,50	0
54	MG	1A	3159	1/1	0.97	0.13	29,29,29,29	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
54	MG	2B	205	1/1	0.97	0.12	51,51,51,51	0
54	MG	2A	3237	1/1	0.97	0.33	52,52,52,52	0
54	MG	2A	3008	1/1	0.97	0.51	49,49,49,49	0
54	MG	1A	3490	1/1	0.97	0.19	30,30,30,30	0
54	MG	1A	3606	1/1	0.97	0.37	35,35,35,35	0
54	MG	2A	3113	1/1	0.97	0.09	56,56,56,56	0
54	MG	2A	3665	1/1	0.97	0.14	40,40,40,40	0
54	MG	2A	3681	1/1	0.97	0.12	55,55,55,55	0
54	MG	1A	3577	1/1	0.97	0.17	39,39,39,39	0
54	MG	2A	3268	1/1	0.97	0.14	29,29,29,29	0
54	MG	1A	3040	1/1	0.97	0.06	52,52,52,52	0
54	MG	2A	3513	1/1	0.97	0.17	47,47,47,47	0
54	MG	1A	3499	1/1	0.97	0.14	25,25,25,25	0
54	MG	1A	3550	1/1	0.97	0.17	43,43,43,43	0
54	MG	2a	3147	1/1	0.97	0.12	62,62,62,62	0
54	MG	1a	1677	1/1	0.97	0.21	58,58,58,58	0
54	MG	2A	3236	1/1	0.97	0.24	45,45,45,45	0
54	MG	1A	3531	1/1	0.97	0.11	47,47,47,47	0
54	MG	2A	3347	1/1	0.97	0.14	35,35,35,35	0
54	MG	2D	301	1/1	0.97	0.51	45,45,45,45	0
54	MG	2A	3049	1/1	0.97	0.09	64,64,64,64	0
54	MG	2A	3379	1/1	0.97	0.07	45,45,45,45	0
54	MG	2A	3329	1/1	0.97	0.12	36,36,36,36	0
54	MG	2A	3398	1/1	0.97	0.13	42,42,42,42	0
54	MG	2A	3117	1/1	0.97	0.17	43,43,43,43	0
54	MG	1A	3820	1/1	0.97	0.46	27,27,27,27	0
54	MG	1a	1787	1/1	0.97	0.10	70,70,70,70	0
54	MG	2A	3483	1/1	0.97	0.11	43,43,43,43	0
54	MG	1A	3675	1/1	0.97	0.21	57,57,57,57	0
54	MG	1a	1866	1/1	0.97	0.06	44,44,44,44	0
54	MG	1F	313	1/1	0.97	0.52	48,48,48,48	0
54	MG	1A	3061	1/1	0.97	0.26	38,38,38,38	0
54	MG	1A	3355	1/1	0.97	0.13	18,18,18,18	0
54	MG	1A	3098	1/1	0.97	0.19	31,31,31,31	0
54	MG	1A	3411	1/1	0.97	0.22	25,25,25,25	0
54	MG	1B	213	1/1	0.97	0.10	48,48,48,48	0
54	MG	2A	3508	1/1	0.97	0.12	46,46,46,46	0
54	MG	17	105	1/1	0.97	0.22	42,42,42,42	0
54	MG	1A	3913	1/1	0.97	0.06	36,36,36,36	0
54	MG	2A	3496	1/1	0.97	0.09	56,56,56,56	0
54	MG	1a	1832	1/1	0.97	0.27	52,52,52,52	0
54	MG	1U	205	1/1	0.97	0.28	36,36,36,36	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
54	MG	1a	1704	1/1	0.97	0.14	42,42,42,42	0
54	MG	1A	3211	1/1	0.97	0.30	46,46,46,46	0
54	MG	2a	3113	1/1	0.97	0.08	55,55,55,55	0
54	MG	1A	3017	1/1	0.97	0.20	36,36,36,36	0
54	MG	2a	3163	1/1	0.97	0.13	58,58,58,58	0
54	MG	1A	3845	1/1	0.97	0.08	52,52,52,52	0
54	MG	1A	3520	1/1	0.97	0.37	32,32,32,32	0
54	MG	1A	3752	1/1	0.97	0.13	40,40,40,40	0
54	MG	1A	3299	1/1	0.97	0.26	38,38,38,38	0
54	MG	2a	3097	1/1	0.97	0.12	61,61,61,61	0
54	MG	1A	3094	1/1	0.97	0.18	31,31,31,31	0
54	MG	1A	3649	1/1	0.97	0.29	40,40,40,40	0
55	ERY	2A	3734	51/51	0.97	0.31	32,46,59,66	0
54	MG	2A	3010	1/1	0.97	0.19	60,60,60,60	0
54	MG	15	102	1/1	0.97	0.24	25,25,25,25	0
54	MG	2a	3059	1/1	0.97	0.11	61,61,61,61	0
54	MG	1A	3155	1/1	0.97	0.28	43,43,43,43	0
54	MG	2A	3635	1/1	0.97	0.12	72,72,72,72	0
54	MG	1A	3095	1/1	0.97	0.14	18,18,18,18	0
54	MG	2A	3020	1/1	0.97	0.35	45,45,45,45	0
54	MG	1A	3243	1/1	0.97	0.27	56,56,56,56	0
54	MG	2A	3629	1/1	0.97	0.15	46,46,46,46	0
54	MG	2E	301	1/1	0.97	0.44	43,43,43,43	0
54	MG	1A	3151	1/1	0.97	0.20	46,46,46,46	0
54	MG	2A	3464	1/1	0.97	0.11	57,57,57,57	0
54	MG	2a	3067	1/1	0.97	0.14	61,61,61,61	0
54	MG	1a	1698	1/1	0.97	0.10	54,54,54,54	0
54	MG	2a	3176	1/1	0.97	0.15	60,60,60,60	0
54	MG	1a	1658	1/1	0.97	0.06	64,64,64,64	0
54	MG	1A	3566	1/1	0.97	0.14	38,38,38,38	0
54	MG	2A	3099	1/1	0.97	0.14	42,42,42,42	0
54	MG	2V	203	1/1	0.97	0.12	47,47,47,47	0
54	MG	2Q	202	1/1	0.97	0.11	57,57,57,57	0
54	MG	2A	3611	1/1	0.97	0.09	33,33,33,33	0
54	MG	1A	3347	1/1	0.97	0.17	31,31,31,31	0
54	MG	2A	3453	1/1	0.97	0.08	36,36,36,36	0
54	MG	1A	3024	1/1	0.97	0.16	19,19,19,19	0
54	MG	1A	3112	1/1	0.97	0.15	39,39,39,39	0
54	MG	2a	3171	1/1	0.97	0.07	63,63,63,63	0
54	MG	1A	3866	1/1	0.97	0.11	45,45,45,45	0
54	MG	1A	3078	1/1	0.97	0.21	34,34,34,34	0
54	MG	2A	3046	1/1	0.97	0.17	51,51,51,51	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
54	MG	1a	1793	1/1	0.97	0.09	52,52,52,52	0
54	MG	1A	3073	1/1	0.97	0.10	29,29,29,29	0
54	MG	1A	3438	1/1	0.97	0.16	44,44,44,44	0
54	MG	1a	1758	1/1	0.97	0.08	68,68,68,68	0
54	MG	2A	3652	1/1	0.97	0.16	51,51,51,51	0
54	MG	2A	3308	1/1	0.97	0.19	39,39,39,39	0
54	MG	1A	3746	1/1	0.97	0.10	34,34,34,34	0
54	MG	1A	3164	1/1	0.97	0.14	48,48,48,48	0
54	MG	1A	3176	1/1	0.97	0.17	48,48,48,48	0
54	MG	1A	3114	1/1	0.97	0.18	28,28,28,28	0
54	MG	1A	3836	1/1	0.97	0.08	30,30,30,30	0
54	MG	1B	229	1/1	0.97	0.08	45,45,45,45	0
54	MG	2A	3396	1/1	0.97	0.17	47,47,47,47	0
58	ZN	1n	104	1/1	0.97	0.12	68,68,68,68	0
54	MG	1A	3481	1/1	0.97	0.16	27,27,27,27	0
54	MG	1a	1770	1/1	0.97	0.09	69,69,69,69	0
54	MG	1U	203	1/1	0.97	0.21	34,34,34,34	0
54	MG	2A	3072	1/1	0.97	0.15	30,30,30,30	0
54	MG	1A	3157	1/1	0.97	0.20	48,48,48,48	0
54	MG	1A	3740	1/1	0.97	0.20	45,45,45,45	0
54	MG	1a	1809	1/1	0.97	0.15	71,71,71,71	0
54	MG	2A	3037	1/1	0.97	0.34	57,57,57,57	0
54	MG	1A	3570	1/1	0.97	0.09	49,49,49,49	0
54	MG	1A	3517	1/1	0.97	0.17	53,53,53,53	0
54	MG	1N	201	1/1	0.97	0.14	36,36,36,36	0
54	MG	1A	3974	1/1	0.97	0.13	52,52,52,52	0
54	MG	1V	202	1/1	0.97	0.33	32,32,32,32	0
54	MG	1A	3730	1/1	0.97	0.12	57,57,57,57	0
54	MG	1a	1620	1/1	0.97	0.20	48,48,48,48	0
54	MG	1A	3391	1/1	0.97	0.17	18,18,18,18	0
54	MG	2A	3402	1/1	0.97	0.15	37,37,37,37	0
54	MG	1A	3174	1/1	0.97	0.27	31,31,31,31	0
54	MG	1A	3189	1/1	0.97	0.19	36,36,36,36	0
54	MG	1A	3308	1/1	0.97	0.14	23,23,23,23	0
54	MG	1e	201	1/1	0.97	0.22	48,48,48,48	0
54	MG	1A	4017	1/1	0.97	0.26	43,43,43,43	0
54	MG	1A	3668	1/1	0.97	0.10	44,44,44,44	0
54	MG	2A	3070	1/1	0.97	0.16	43,43,43,43	0
54	MG	2A	3353	1/1	0.97	0.08	65,65,65,65	0
54	MG	1A	3214	1/1	0.97	0.71	47,47,47,47	0
54	MG	2A	3449	1/1	0.97	0.09	53,53,53,53	0
54	MG	1A	3753	1/1	0.97	0.08	51,51,51,51	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
54	MG	1A	3530	1/1	0.97	0.11	52,52,52,52	0
54	MG	1a	1769	1/1	0.97	0.21	63,63,63,63	0
54	MG	1A	3537	1/1	0.97	0.13	40,40,40,40	0
54	MG	1P	201	1/1	0.97	0.61	36,36,36,36	0
54	MG	1a	1711	1/1	0.97	0.15	66,66,66,66	0
54	MG	1A	3160	1/1	0.97	0.67	36,36,36,36	0
54	MG	2a	3029	1/1	0.97	0.12	59,59,59,59	0
54	MG	2A	3686	1/1	0.97	0.12	56,56,56,56	0
54	MG	2A	3111	1/1	0.97	0.13	51,51,51,51	0
54	MG	1A	3217	1/1	0.97	0.10	38,38,38,38	0
54	MG	2B	210	1/1	0.97	0.07	64,64,64,64	0
54	MG	1A	3552	1/1	0.97	0.07	51,51,51,51	0
55	ERY	1A	4021	51/51	0.97	0.28	23,35,44,46	0
54	MG	2A	3138	1/1	0.97	0.12	53,53,53,53	0
54	MG	2A	3643	1/1	0.97	0.12	56,56,56,56	0
54	MG	2A	3136	1/1	0.97	0.14	42,42,42,42	0
54	MG	2A	3535	1/1	0.97	0.13	34,34,34,34	0
54	MG	1A	3737	1/1	0.97	0.16	28,28,28,28	0
54	MG	1a	1656	1/1	0.97	0.19	51,51,51,51	0
54	MG	1A	3185	1/1	0.97	0.23	44,44,44,44	0
54	MG	1R	203	1/1	0.97	0.26	38,38,38,38	0
54	MG	1A	3181	1/1	0.97	0.29	35,35,35,35	0
54	MG	1A	3147	1/1	0.97	0.37	32,32,32,32	0
54	MG	1D	305	1/1	0.97	0.14	40,40,40,40	0
54	MG	2A	3576	1/1	0.97	0.60	65,65,65,65	0
54	MG	1A	3458	1/1	0.97	0.06	52,52,52,52	0
54	MG	2A	3487	1/1	0.97	0.09	56,56,56,56	0
54	MG	1h	201	1/1	0.97	0.16	57,57,57,57	0
54	MG	1a	1855	1/1	0.97	0.15	63,63,63,63	0
54	MG	2A	3397	1/1	0.97	0.10	55,55,55,55	0
54	MG	2A	3522	1/1	0.97	0.18	63,63,63,63	0
54	MG	2A	3174	1/1	0.97	0.19	45,45,45,45	0
54	MG	2a	3011	1/1	0.97	0.16	59,59,59,59	0
54	MG	2A	3284	1/1	0.97	0.11	41,41,41,41	0
54	MG	2A	3164	1/1	0.97	0.23	48,48,48,48	0
54	MG	2D	310	1/1	0.97	0.33	60,60,60,60	0
54	MG	2A	3725	1/1	0.97	0.10	42,42,42,42	0
54	MG	1A	3352	1/1	0.97	0.12	46,46,46,46	0
54	MG	2A	3139	1/1	0.97	0.14	46,46,46,46	0
54	MG	1A	3888	1/1	0.97	0.54	38,38,38,38	0
54	MG	2a	3169	1/1	0.97	0.17	64,64,64,64	0
54	MG	1A	3130	1/1	0.97	0.17	30,30,30,30	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
54	MG	1A	3503	1/1	0.97	0.13	19,19,19,19	0
54	MG	2A	3370	1/1	0.97	0.20	51,51,51,51	0
54	MG	1A	3834	1/1	0.97	0.16	39,39,39,39	0
54	MG	2A	3294	1/1	0.97	0.06	33,33,33,33	0
54	MG	2A	3581	1/1	0.97	0.10	53,53,53,53	0
54	MG	1A	3953	1/1	0.97	0.13	58,58,58,58	0
54	MG	2A	3599	1/1	0.97	0.14	51,51,51,51	0
54	MG	2A	3118	1/1	0.97	0.22	56,56,56,56	0
54	MG	1E	307	1/1	0.97	0.18	23,23,23,23	0
54	MG	1B	221	1/1	0.97	0.18	31,31,31,31	0
54	MG	2A	3632	1/1	0.97	0.08	58,58,58,58	0
54	MG	1A	3512	1/1	0.97	0.10	46,46,46,46	0
54	MG	1a	1845	1/1	0.97	0.29	64,64,64,64	0
54	MG	1A	3948	1/1	0.97	0.12	27,27,27,27	0
54	MG	1D	308	1/1	0.97	0.25	33,33,33,33	0
54	MG	1A	3450	1/1	0.97	0.15	45,45,45,45	0
54	MG	2B	211	1/1	0.97	0.13	59,59,59,59	0
54	MG	2V	201	1/1	0.97	0.20	62,62,62,62	0
54	MG	1A	3420	1/1	0.97	0.19	28,28,28,28	0
54	MG	2A	3079	1/1	0.97	0.15	54,54,54,54	0
54	MG	2A	3540	1/1	0.97	0.05	60,60,60,60	0
54	MG	1A	3364	1/1	0.97	0.12	50,50,50,50	0
54	MG	1A	3294	1/1	0.97	0.16	29,29,29,29	0
54	MG	2a	3050	1/1	0.97	0.18	54,54,54,54	0
54	MG	2A	3717	1/1	0.97	0.16	64,64,64,64	0
54	MG	1A	3284	1/1	0.97	0.32	49,49,49,49	0
54	MG	1A	3239	1/1	0.97	0.34	32,32,32,32	0
54	MG	2A	3365	1/1	0.97	0.10	61,61,61,61	0
54	MG	2A	3191	1/1	0.97	0.21	49,49,49,49	0
54	MG	1A	3212	1/1	0.97	0.30	39,39,39,39	0
54	MG	2A	3314	1/1	0.97	0.14	62,62,62,62	0
54	MG	1A	3177	1/1	0.97	0.29	37,37,37,37	0
54	MG	1A	3381	1/1	0.97	0.14	31,31,31,31	0
54	MG	1a	1703	1/1	0.97	0.18	52,52,52,52	0
54	MG	1A	3340	1/1	0.97	0.20	28,28,28,28	0
54	MG	1D	302	1/1	0.97	0.17	50,50,50,50	0
54	MG	1F	311	1/1	0.97	0.12	39,39,39,39	0
54	MG	2A	3706	1/1	0.97	0.07	52,52,52,52	0
54	MG	1a	1702	1/1	0.97	0.09	63,63,63,63	0
54	MG	1A	3179	1/1	0.97	0.34	35,35,35,35	0
54	MG	1A	3295	1/1	0.97	0.19	45,45,45,45	0
54	MG	2A	3614	1/1	0.97	0.14	51,51,51,51	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
54	MG	2A	3385	1/1	0.97	0.12	53,53,53,53	0
54	MG	2A	3694	1/1	0.97	0.13	66,66,66,66	0
54	MG	2A	3415	1/1	0.97	0.10	50,50,50,50	0
54	MG	1A	3516	1/1	0.97	0.18	22,22,22,22	0
54	MG	1A	3805	1/1	0.97	0.17	73,73,73,73	0
54	MG	1A	3717	1/1	0.97	0.18	34,34,34,34	0
54	MG	1A	3198	1/1	0.97	0.26	34,34,34,34	0
54	MG	2A	3275	1/1	0.97	0.12	48,48,48,48	0
54	MG	2a	3155	1/1	0.97	0.10	70,70,70,70	0
54	MG	1A	3681	1/1	0.97	0.45	62,62,62,62	0
54	MG	1A	3855	1/1	0.97	0.13	47,47,47,47	0
54	MG	1F	304	1/1	0.97	0.34	38,38,38,38	0
54	MG	2A	3454	1/1	0.97	0.07	59,59,59,59	0
54	MG	2A	3410	1/1	0.97	0.12	58,58,58,58	0
54	MG	1V	203	1/1	0.97	0.15	45,45,45,45	0
54	MG	1B	212	1/1	0.97	0.29	61,61,61,61	0
54	MG	2A	3589	1/1	0.97	0.10	42,42,42,42	0
54	MG	1A	3405	1/1	0.97	0.14	29,29,29,29	0
54	MG	2A	3051	1/1	0.97	0.12	56,56,56,56	0
54	MG	2A	3317	1/1	0.97	0.17	31,31,31,31	0
54	MG	1A	3360	1/1	0.97	0.12	32,32,32,32	0
54	MG	1F	310	1/1	0.97	0.11	56,56,56,56	0
54	MG	1A	3013	1/1	0.97	0.16	22,22,22,22	0
54	MG	1A	3692	1/1	0.98	0.15	43,43,43,43	0
54	MG	1A	3043	1/1	0.98	0.15	28,28,28,28	0
54	MG	1F	301	1/1	0.98	0.14	29,29,29,29	0
54	MG	1A	3071	1/1	0.98	0.25	30,30,30,30	0
54	MG	1A	3486	1/1	0.98	0.13	30,30,30,30	0
54	MG	2A	3318	1/1	0.98	0.13	50,50,50,50	0
54	MG	2a	3104	1/1	0.98	0.19	68,68,68,68	0
54	MG	2a	3102	1/1	0.98	0.04	70,70,70,70	0
54	MG	1Q	203	1/1	0.98	0.14	41,41,41,41	0
54	MG	1a	1710	1/1	0.98	0.19	49,49,49,49	0
54	MG	1E	308	1/1	0.98	0.10	25,25,25,25	0
54	MG	1A	4008	1/1	0.98	0.12	38,38,38,38	0
54	MG	1A	3290	1/1	0.98	0.17	21,21,21,21	0
54	MG	2A	3166	1/1	0.98	0.22	38,38,38,38	0
54	MG	1A	3397	1/1	0.98	0.20	22,22,22,22	0
54	MG	1A	3371	1/1	0.98	0.09	31,31,31,31	0
54	MG	2a	3093	1/1	0.98	0.15	49,49,49,49	0
54	MG	2a	3152	1/1	0.98	0.10	71,71,71,71	0
54	MG	2a	3047	1/1	0.98	0.18	61,61,61,61	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
54	MG	1A	3085	1/1	0.98	0.27	41,41,41,41	0
54	MG	1A	3620	1/1	0.98	0.14	52,52,52,52	0
54	MG	1a	1862	1/1	0.98	0.11	35,35,35,35	0
54	MG	1A	3443	1/1	0.98	0.18	48,48,48,48	0
54	MG	1A	3331	1/1	0.98	0.13	47,47,47,47	0
54	MG	2A	3076	1/1	0.98	0.51	54,54,54,54	0
54	MG	1U	206	1/1	0.98	0.40	33,33,33,33	0
54	MG	1A	3165	1/1	0.98	0.21	35,35,35,35	0
54	MG	2A	3304	1/1	0.98	0.10	32,32,32,32	0
54	MG	2A	3707	1/1	0.98	0.19	59,59,59,59	0
54	MG	1A	3233	1/1	0.98	0.52	34,34,34,34	0
54	MG	1A	3226	1/1	0.98	0.30	42,42,42,42	0
54	MG	1A	3806	1/1	0.98	0.14	30,30,30,30	0
54	MG	1A	3143	1/1	0.98	0.17	36,36,36,36	0
54	MG	1A	3069	1/1	0.98	0.33	36,36,36,36	0
54	MG	1A	3152	1/1	0.98	0.45	36,36,36,36	0
54	MG	1a	1804	1/1	0.98	0.09	47,47,47,47	0
54	MG	1N	202	1/1	0.98	0.15	41,41,41,41	0
54	MG	1A	3936	1/1	0.98	0.08	59,59,59,59	0
54	MG	1A	3847	1/1	0.98	0.15	39,39,39,39	0
54	MG	2t	201	1/1	0.98	0.08	42,42,42,42	0
54	MG	1a	1708	1/1	0.98	0.10	47,47,47,47	0
54	MG	1F	315	1/1	0.98	0.11	41,41,41,41	0
54	MG	2A	3357	1/1	0.98	0.17	47,47,47,47	0
54	MG	1A	3540	1/1	0.98	0.17	34,34,34,34	0
54	MG	13	104	1/1	0.98	0.13	40,40,40,40	0
54	MG	1F	306	1/1	0.98	0.30	34,34,34,34	0
54	MG	2A	3338	1/1	0.98	0.10	37,37,37,37	0
54	MG	1A	3739	1/1	0.98	0.13	42,42,42,42	0
54	MG	2A	3018	1/1	0.98	0.44	41,41,41,41	0
54	MG	1Q	202	1/1	0.98	0.13	29,29,29,29	0
54	MG	2A	3597	1/1	0.98	0.10	50,50,50,50	0
54	MG	2a	3164	1/1	0.98	0.03	74,74,74,74	0
54	MG	1A	4005	1/1	0.98	0.14	15,15,15,15	0
54	MG	1A	3460	1/1	0.98	0.12	41,41,41,41	0
54	MG	1A	3555	1/1	0.98	0.17	33,33,33,33	0
54	MG	1A	3338	1/1	0.98	0.11	49,49,49,49	0
54	MG	1A	3727	1/1	0.98	0.14	54,54,54,54	0
54	MG	1A	3841	1/1	0.98	0.10	23,23,23,23	0
54	MG	1A	3367	1/1	0.98	0.09	26,26,26,26	0
54	MG	2A	3551	1/1	0.98	0.07	44,44,44,44	0
58	ZN	25	103	1/1	0.98	0.19	57,57,57,57	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
54	MG	1A	3926	1/1	0.98	0.16	32,32,32,32	0
54	MG	1A	3604	1/1	0.98	0.25	39,39,39,39	0
54	MG	1A	3227	1/1	0.98	0.20	31,31,31,31	0
54	MG	2D	303	1/1	0.98	0.38	51,51,51,51	0
54	MG	1A	3493	1/1	0.98	0.15	36,36,36,36	0
54	MG	1A	3282	1/1	0.98	0.43	45,45,45,45	0
54	MG	1A	3365	1/1	0.98	0.14	44,44,44,44	0
54	MG	1A	3350	1/1	0.98	0.16	32,32,32,32	0
54	MG	2a	3168	1/1	0.98	0.10	50,50,50,50	0
54	MG	1l	102	1/1	0.98	0.13	35,35,35,35	0
54	MG	1A	3545	1/1	0.98	0.22	32,32,32,32	0
54	MG	2A	3387	1/1	0.98	0.15	59,59,59,59	0
54	MG	1A	3629	1/1	0.98	0.12	39,39,39,39	0
54	MG	1A	3180	1/1	0.98	0.10	30,30,30,30	0
54	MG	2A	3262	1/1	0.98	0.38	41,41,41,41	0
54	MG	1A	3025	1/1	0.98	0.33	40,40,40,40	0
54	MG	1a	1764	1/1	0.98	0.17	39,39,39,39	0
54	MG	2a	3110	1/1	0.98	0.14	61,61,61,61	0
54	MG	2A	3400	1/1	0.98	0.11	47,47,47,47	0
54	MG	1A	3519	1/1	0.98	0.11	26,26,26,26	0
54	MG	1A	3465	1/1	0.98	0.12	47,47,47,47	0
54	MG	1A	3972	1/1	0.98	0.14	19,19,19,19	0
54	MG	2A	3600	1/1	0.98	0.07	40,40,40,40	0
54	MG	2A	3218	1/1	0.98	0.52	45,45,45,45	0
54	MG	1a	1838	1/1	0.98	0.12	67,67,67,67	0
54	MG	1A	3796	1/1	0.98	0.18	32,32,32,32	0
54	MG	1a	1833	1/1	0.98	0.19	45,45,45,45	0
54	MG	1A	3603	1/1	0.98	0.18	51,51,51,51	0
54	MG	1A	3344	1/1	0.98	0.13	53,53,53,53	0
54	MG	1A	3132	1/1	0.98	0.57	37,37,37,37	0
54	MG	1A	3844	1/1	0.98	0.09	35,35,35,35	0
54	MG	1A	3409	1/1	0.98	0.15	27,27,27,27	0
54	MG	1A	3032	1/1	0.98	0.10	42,42,42,42	0
54	MG	1A	3800	1/1	0.98	0.22	41,41,41,41	0
54	MG	1A	3237	1/1	0.98	0.21	34,34,34,34	0
54	MG	2A	3594	1/1	0.98	0.19	54,54,54,54	0
54	MG	1A	3504	1/1	0.98	0.13	22,22,22,22	0
54	MG	2a	3098	1/1	0.98	0.14	60,60,60,60	0
54	MG	1A	3501	1/1	0.98	0.11	53,53,53,53	0
54	MG	2A	3374	1/1	0.98	0.11	56,56,56,56	0
54	MG	1A	3489	1/1	0.98	0.11	46,46,46,46	0
54	MG	1A	3573	1/1	0.98	0.19	29,29,29,29	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
54	MG	2A	3229	1/1	0.98	0.21	56,56,56,56	0
54	MG	1A	3423	1/1	0.98	0.20	41,41,41,41	0
54	MG	15	103	1/1	0.98	0.31	36,36,36,36	0
54	MG	1A	3122	1/1	0.98	0.19	37,37,37,37	0
54	MG	1A	3646	1/1	0.98	0.05	73,73,73,73	0
58	ZN	15	107	1/1	0.98	0.20	47,47,47,47	0
54	MG	1A	3042	1/1	0.98	0.14	24,24,24,24	0
54	MG	1a	1765	1/1	0.98	0.17	65,65,65,65	0
54	MG	2A	3666	1/1	0.98	0.12	33,33,33,33	0
54	MG	2A	3081	1/1	0.98	0.15	57,57,57,57	0
54	MG	1A	3726	1/1	0.98	0.17	24,24,24,24	0
54	MG	1A	3424	1/1	0.98	0.12	51,51,51,51	0
54	MG	1A	3054	1/1	0.98	0.26	24,24,24,24	0
54	MG	2A	3451	1/1	0.98	0.14	68,68,68,68	0
54	MG	15	104	1/1	0.98	0.14	25,25,25,25	0
54	MG	1A	3289	1/1	0.98	0.18	25,25,25,25	0
54	MG	1a	1676	1/1	0.98	0.24	68,68,68,68	0
54	MG	1U	202	1/1	0.98	0.27	32,32,32,32	0
54	MG	2A	3538	1/1	0.98	0.09	44,44,44,44	0
54	MG	1A	3494	1/1	0.98	0.11	48,48,48,48	0
54	MG	1A	3784	1/1	0.98	0.10	29,29,29,29	0
54	MG	2a	3173	1/1	0.98	0.08	65,65,65,65	0
54	MG	1a	1823	1/1	0.98	0.08	52,52,52,52	0
54	MG	1A	3731	1/1	0.98	0.15	49,49,49,49	0
54	MG	1A	3432	1/1	0.98	0.12	18,18,18,18	0
54	MG	1A	3120	1/1	0.98	0.22	26,26,26,26	0
54	MG	1A	3488	1/1	0.98	0.10	49,49,49,49	0
54	MG	1A	4020	1/1	0.98	0.12	44,44,44,44	0
54	MG	1A	3207	1/1	0.98	0.33	41,41,41,41	0
54	MG	1A	3500	1/1	0.98	0.14	59,59,59,59	0
54	MG	1A	3967	1/1	0.98	0.09	27,27,27,27	0
54	MG	17	102	1/1	0.98	0.14	33,33,33,33	0
54	MG	1A	3359	1/1	0.98	0.18	55,55,55,55	0
54	MG	2A	3510	1/1	0.98	0.13	54,54,54,54	0
54	MG	1A	3380	1/1	0.98	0.15	19,19,19,19	0
54	MG	1A	3105	1/1	0.98	0.18	38,38,38,38	0
54	MG	2A	3188	1/1	0.98	0.11	54,54,54,54	0
54	MG	2A	3728	1/1	0.98	0.07	46,46,46,46	0
54	MG	1A	3824	1/1	0.98	0.17	33,33,33,33	0
54	MG	1a	1747	1/1	0.98	0.18	50,50,50,50	0
54	MG	1A	3814	1/1	0.98	0.09	43,43,43,43	0
54	MG	1A	3526	1/1	0.98	0.15	31,31,31,31	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
54	MG	1A	3169	1/1	0.98	0.46	38,38,38,38	0
54	MG	1A	3044	1/1	0.98	0.18	32,32,32,32	0
54	MG	1A	3346	1/1	0.98	0.16	36,36,36,36	0
54	MG	1A	3702	1/1	0.98	0.35	41,41,41,41	0
54	MG	1A	3317	1/1	0.98	0.16	34,34,34,34	0
54	MG	1A	3485	1/1	0.98	0.11	36,36,36,36	0
54	MG	1a	1650	1/1	0.98	0.18	55,55,55,55	0
54	MG	15	105	1/1	0.98	0.11	49,49,49,49	0
54	MG	1A	3051	1/1	0.98	0.49	42,42,42,42	0
54	MG	2A	3446	1/1	0.98	0.06	60,60,60,60	0
54	MG	1A	3985	1/1	0.98	0.20	39,39,39,39	0
54	MG	1A	3278	1/1	0.98	0.21	42,42,42,42	0
54	MG	1A	3447	1/1	0.98	0.11	55,55,55,55	0
54	MG	1A	3041	1/1	0.98	0.21	30,30,30,30	0
54	MG	2A	3258	1/1	0.98	0.15	60,60,60,60	0
54	MG	1A	3387	1/1	0.98	0.21	24,24,24,24	0
54	MG	1F	303	1/1	0.98	0.27	28,28,28,28	0
54	MG	1A	3309	1/1	0.98	0.23	35,35,35,35	0
54	MG	1F	305	1/1	0.98	0.26	35,35,35,35	0
54	MG	2A	3460	1/1	0.98	0.15	45,45,45,45	0
54	MG	2A	3690	1/1	0.98	0.16	38,38,38,38	0
54	MG	1a	1712	1/1	0.98	0.15	44,44,44,44	0
54	MG	1A	3716	1/1	0.98	0.24	38,38,38,38	0
54	MG	2A	3097	1/1	0.98	0.07	62,62,62,62	0
54	MG	2A	3637	1/1	0.98	0.05	72,72,72,72	0
54	MG	1A	3422	1/1	0.98	0.10	20,20,20,20	0
54	MG	1P	206	1/1	0.98	0.08	30,30,30,30	0
54	MG	1A	3334	1/1	0.98	0.10	33,33,33,33	0
54	MG	2A	3696	1/1	0.98	0.10	55,55,55,55	0
54	MG	1a	1612	1/1	0.98	0.15	43,43,43,43	0
54	MG	1A	3536	1/1	0.98	0.12	28,28,28,28	0
54	MG	1A	3862	1/1	0.98	0.14	28,28,28,28	0
54	MG	1A	3509	1/1	0.98	0.20	23,23,23,23	0
54	MG	2A	3532	1/1	0.98	0.20	50,50,50,50	0
58	ZN	1Y	203	1/1	0.98	0.18	56,56,56,56	0
54	MG	1A	3172	1/1	0.98	0.13	30,30,30,30	0
54	MG	1A	3651	1/1	0.98	0.32	56,56,56,56	0
54	MG	2A	3305	1/1	0.98	0.16	60,60,60,60	0
54	MG	1A	3205	1/1	0.98	0.12	49,49,49,49	0
54	MG	2A	3108	1/1	0.98	0.13	60,60,60,60	0
54	MG	1A	3328	1/1	0.98	0.16	15,15,15,15	0
54	MG	11	101	1/1	0.98	0.20	38,38,38,38	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
54	MG	1A	3047	1/1	0.98	0.16	29,29,29,29	0
54	MG	1A	3110	1/1	0.98	0.31	31,31,31,31	0
58	ZN	2n	102	1/1	0.98	0.07	93,93,93,93	0
54	MG	1a	1783	1/1	0.98	0.23	63,63,63,63	0
54	MG	1A	3167	1/1	0.98	0.16	27,27,27,27	0
54	MG	1A	3623	1/1	0.98	0.12	43,43,43,43	0
54	MG	1Q	201	1/1	0.98	0.15	40,40,40,40	0
54	MG	1A	3444	1/1	0.98	0.16	29,29,29,29	0
54	MG	1A	3161	1/1	0.98	0.16	31,31,31,31	0
54	MG	2A	3263	1/1	0.98	0.09	52,52,52,52	0
54	MG	1A	3332	1/1	0.98	0.16	33,33,33,33	0
54	MG	1a	1659	1/1	0.98	0.27	42,42,42,42	0
54	MG	1A	3337	1/1	0.98	0.13	46,46,46,46	0
54	MG	2A	3116	1/1	0.98	0.16	50,50,50,50	0
54	MG	1D	316	1/1	0.98	0.24	32,32,32,32	0
54	MG	1D	304	1/1	0.98	0.09	36,36,36,36	0
54	MG	2A	3642	1/1	0.98	0.10	48,48,48,48	0
54	MG	1A	3928	1/1	0.98	0.22	54,54,54,54	0
54	MG	2W	201	1/1	0.98	0.27	45,45,45,45	0
54	MG	1A	3421	1/1	0.98	0.16	30,30,30,30	0
54	MG	2W	203	1/1	0.98	0.09	61,61,61,61	0
54	MG	1U	208	1/1	0.98	0.35	41,41,41,41	0
54	MG	1A	3587	1/1	0.98	0.15	25,25,25,25	0
54	MG	1o	101	1/1	0.98	0.10	53,53,53,53	0
54	MG	1A	3286	1/1	0.98	0.12	37,37,37,37	0
54	MG	2a	3143	1/1	0.98	0.14	64,64,64,64	0
54	MG	2A	3303	1/1	0.98	0.11	51,51,51,51	0
54	MG	2A	3730	1/1	0.98	0.11	56,56,56,56	0
54	MG	1a	1840	1/1	0.98	0.14	42,42,42,42	0
54	MG	1A	3358	1/1	0.98	0.11	20,20,20,20	0
54	MG	1A	3963	1/1	0.98	0.17	51,51,51,51	0
54	MG	1A	3441	1/1	0.98	0.15	43,43,43,43	0
54	MG	1A	3763	1/1	0.98	0.20	56,56,56,56	0
54	MG	2A	3119	1/1	0.98	0.19	52,52,52,52	0
54	MG	2A	3434	1/1	0.98	0.12	60,60,60,60	0
54	MG	1A	3273	1/1	0.98	0.23	26,26,26,26	0
54	MG	2A	3030	1/1	0.98	0.19	48,48,48,48	0
54	MG	2A	3439	1/1	0.98	0.12	61,61,61,61	0
54	MG	1A	4012	1/1	0.99	0.12	43,43,43,43	0
54	MG	1A	3018	1/1	0.99	0.21	27,27,27,27	0
54	MG	1A	3828	1/1	0.99	0.19	46,46,46,46	0
54	MG	1A	3144	1/1	0.99	0.20	30,30,30,30	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
54	MG	2A	3004	1/1	0.99	0.12	40,40,40,40	0
54	MG	2e	202	1/1	0.99	0.13	64,64,64,64	0
54	MG	1A	3709	1/1	0.99	0.11	37,37,37,37	0
54	MG	1A	3902	1/1	0.99	0.10	31,31,31,31	0
54	MG	1V	201	1/1	0.99	0.45	29,29,29,29	0
54	MG	1a	1861	1/1	0.99	0.13	54,54,54,54	0
54	MG	1A	3141	1/1	0.99	0.15	31,31,31,31	0
54	MG	1A	3419	1/1	0.99	0.24	25,25,25,25	0
54	MG	1A	3943	1/1	0.99	0.08	41,41,41,41	0
54	MG	1A	3136	1/1	0.99	0.21	25,25,25,25	0
54	MG	1A	3267	1/1	0.99	0.23	33,33,33,33	0
54	MG	2A	3246	1/1	0.99	0.27	60,60,60,60	0
54	MG	1A	3005	1/1	0.99	0.20	22,22,22,22	0
54	MG	1a	1735	1/1	0.99	0.11	54,54,54,54	0
54	MG	23	101	1/1	0.99	0.46	54,54,54,54	0
54	MG	1A	3760	1/1	0.99	0.26	33,33,33,33	0
54	MG	1a	1648	1/1	0.99	0.21	61,61,61,61	0
54	MG	1R	201	1/1	0.99	0.20	29,29,29,29	0
54	MG	1D	306	1/1	0.99	0.12	16,16,16,16	0
54	MG	1A	3901	1/1	0.99	0.18	32,32,32,32	0
54	MG	2A	3490	1/1	0.99	0.14	29,29,29,29	0
54	MG	2A	3137	1/1	0.99	0.13	60,60,60,60	0
54	MG	1A	3607	1/1	0.99	0.17	28,28,28,28	0
54	MG	1A	3887	1/1	0.99	0.20	37,37,37,37	0
59	SF4	2d	501	8/8	0.99	0.14	70,71,85,85	0
54	MG	1A	3713	1/1	0.99	0.16	32,32,32,32	0
54	MG	1A	3825	1/1	0.99	0.13	18,18,18,18	0
54	MG	1a	1611	1/1	0.99	0.17	48,48,48,48	0
54	MG	2a	3137	1/1	0.99	0.17	59,59,59,59	0
54	MG	2A	3100	1/1	0.99	0.10	39,39,39,39	0
54	MG	1A	3325	1/1	0.99	0.14	25,25,25,25	0
54	MG	2E	302	1/1	0.99	0.09	45,45,45,45	0
54	MG	1A	3330	1/1	0.99	0.19	34,34,34,34	0
54	MG	1A	4000	1/1	0.99	0.11	60,60,60,60	0
54	MG	1A	3627	1/1	0.99	0.16	23,23,23,23	0
54	MG	2A	3282	1/1	0.99	0.10	21,21,21,21	0
54	MG	2A	3530	1/1	0.99	0.09	51,51,51,51	0
59	SF4	1d	306	8/8	0.99	0.17	61,69,73,74	0
54	MG	1A	3851	1/1	0.99	0.25	46,46,46,46	0
58	ZN	26	501	1/1	0.99	0.20	60,60,60,60	0
54	MG	1A	3001	1/1	0.99	0.11	33,33,33,33	0
54	MG	1D	310	1/1	0.99	0.29	33,33,33,33	0

*Continued on next page...*

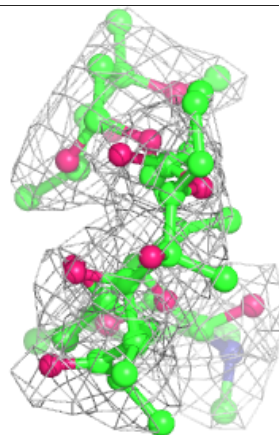
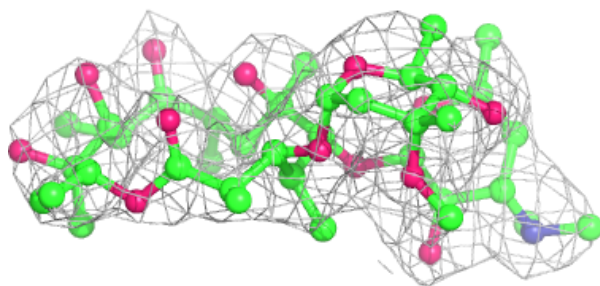
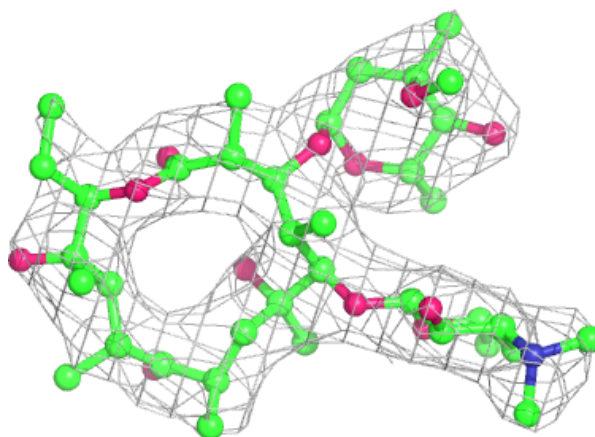
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
54	MG	2A	3384	1/1	0.99	0.16	47,47,47,47	0
54	MG	2A	3315	1/1	0.99	0.14	49,49,49,49	0
54	MG	1A	3058	1/1	0.99	0.17	24,24,24,24	0
58	ZN	16	501	1/1	0.99	0.24	46,46,46,46	0
54	MG	1W	203	1/1	0.99	0.10	28,28,28,28	0
54	MG	1E	303	1/1	0.99	0.21	36,36,36,36	0
54	MG	1A	3333	1/1	0.99	0.14	48,48,48,48	0
54	MG	1A	3667	1/1	0.99	0.25	37,37,37,37	0
54	MG	1A	3056	1/1	0.99	0.15	41,41,41,41	0
54	MG	1A	3822	1/1	0.99	0.12	19,19,19,19	0
54	MG	1A	3829	1/1	0.99	0.16	45,45,45,45	0
54	MG	1A	3351	1/1	0.99	0.11	22,22,22,22	0
54	MG	2A	3234	1/1	0.99	0.44	39,39,39,39	0
54	MG	1A	3434	1/1	0.99	0.15	35,35,35,35	0
54	MG	2F	304	1/1	0.99	0.22	42,42,42,42	0
54	MG	1a	1722	1/1	0.99	0.13	43,43,43,43	0
54	MG	1A	3045	1/1	0.99	0.17	14,14,14,14	0
54	MG	2D	306	1/1	0.99	0.36	49,49,49,49	0
54	MG	2A	3641	1/1	0.99	0.16	65,65,65,65	0
54	MG	2A	3302	1/1	0.99	0.18	57,57,57,57	0
54	MG	1A	3116	1/1	0.99	0.25	41,41,41,41	0
54	MG	2A	3493	1/1	0.99	0.09	47,47,47,47	0
54	MG	2A	3015	1/1	0.99	0.17	38,38,38,38	0
54	MG	1a	1734	1/1	0.99	0.10	60,60,60,60	0
54	MG	1A	3720	1/1	0.99	0.14	32,32,32,32	0
54	MG	1A	3175	1/1	0.99	0.17	22,22,22,22	0
54	MG	1A	3089	1/1	0.99	0.15	38,38,38,38	0
54	MG	1A	3028	1/1	0.99	0.32	25,25,25,25	0
54	MG	1A	3532	1/1	0.99	0.60	35,35,35,35	0
54	MG	2A	3476	1/1	0.99	0.09	42,42,42,42	0
58	ZN	19	102	1/1	1.00	0.21	49,49,49,49	0

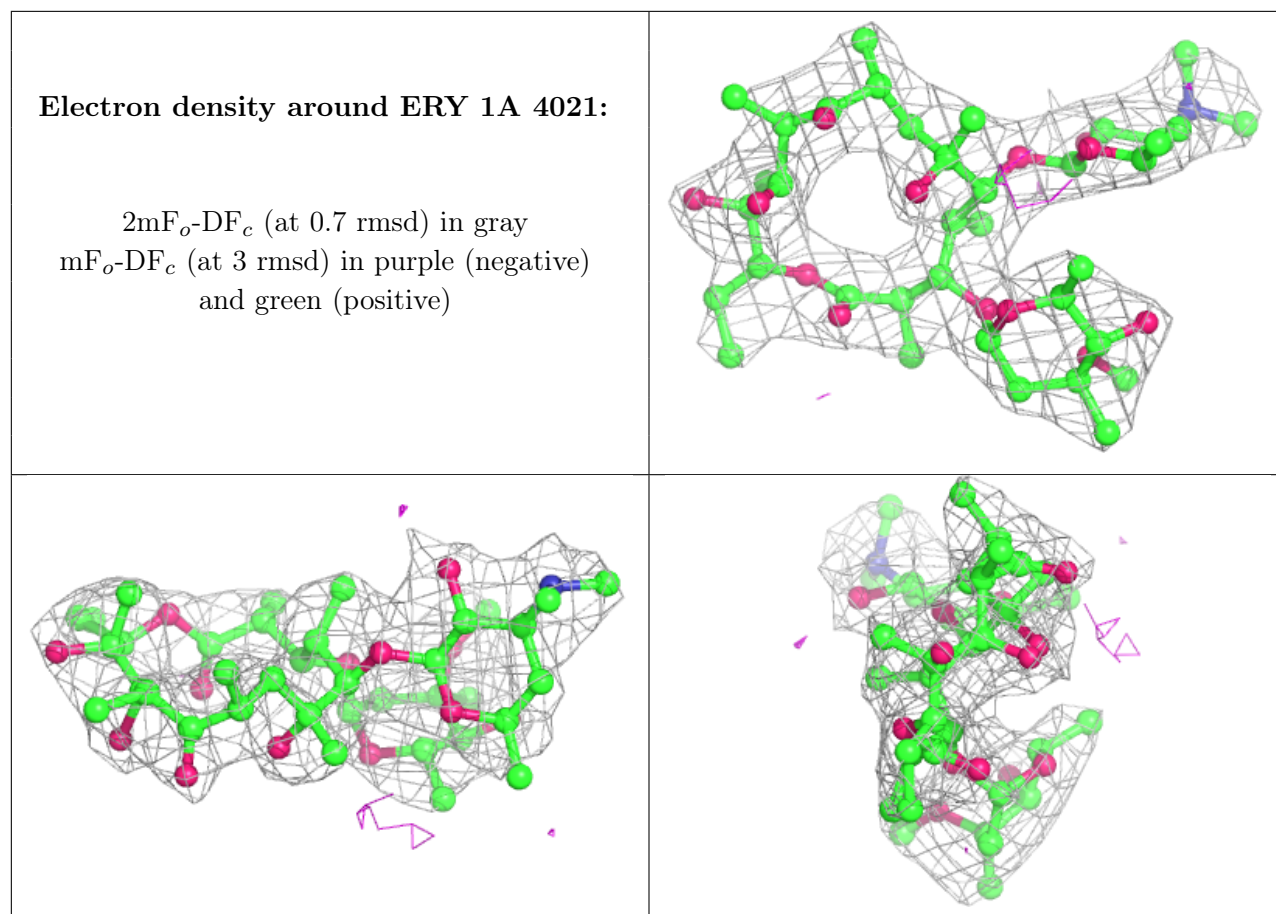
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

**Electron density around ERY 2A 3734:**

$2mF_o - DF_c$  (at 0.7 rmsd) in gray  
 $mF_o - DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)







## 6.5 Other polymers [i](#)

There are no such residues in this entry.