



Full wwPDB X-ray Structure Validation Report ⓘ

Dec 11, 2022 – 11:15 PM EST

PDB ID : 8EKB
Title : Crystal structure of the *Thermus thermophilus* 70S ribosome in complex with mRNA, deacylated P-site tRNA^{met}, and thermorubin at 2.70Å resolution
Authors : Paranjpe, M.N.; Polikanov, Y.S.
Deposited on : 2022-09-20
Resolution : 2.70 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.31.2
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.2

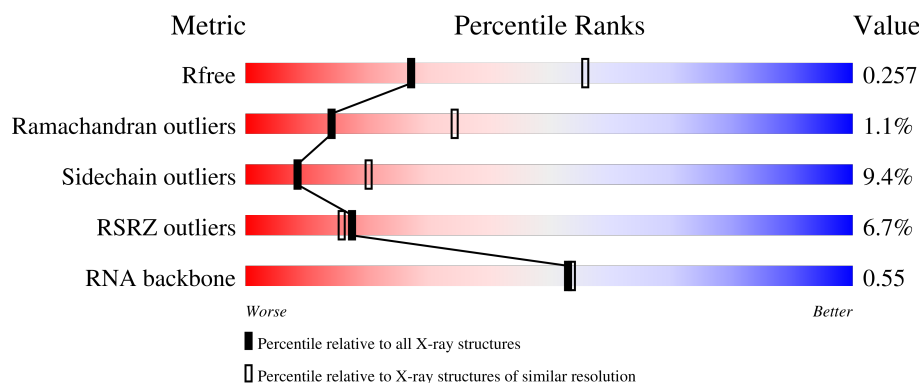
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.70 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.



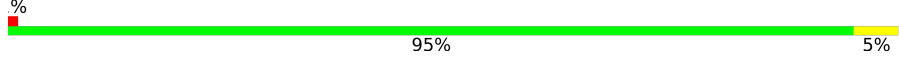

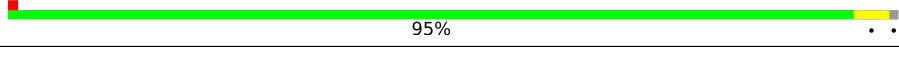

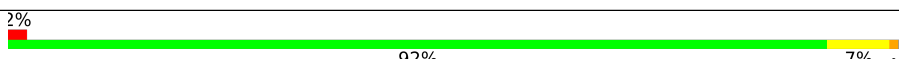

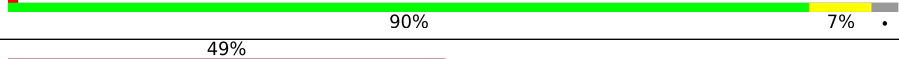

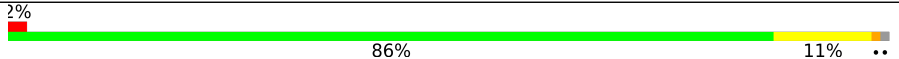
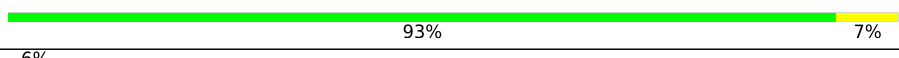
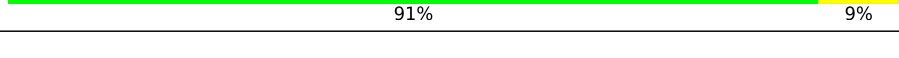
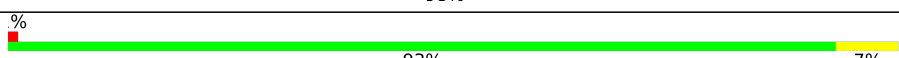
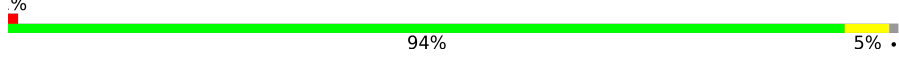
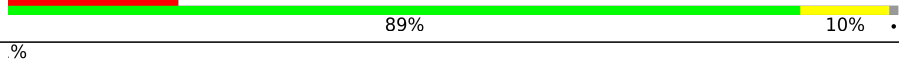
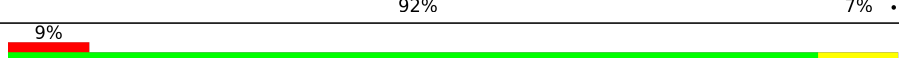
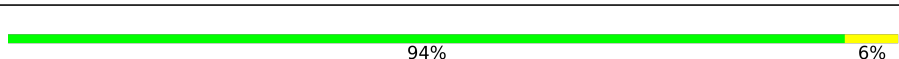
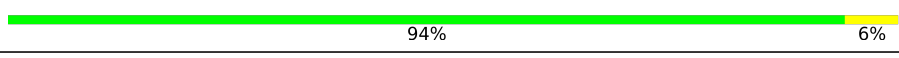
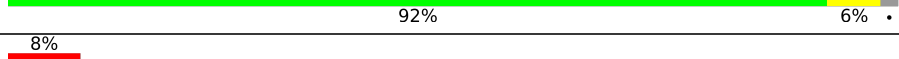





Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	2808 (2.70-2.70)
Ramachandran outliers	138981	3069 (2.70-2.70)
Sidechain outliers	138945	3069 (2.70-2.70)
RSRZ outliers	127900	2737 (2.70-2.70)
RNA backbone	3102	1159 (3.00-2.40)

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

Mol	Chain	Length	Quality of chain
1	1A	2915	<div> <div>3%</div> <div>82%</div> <div>16%</div> <div>..</div> </div>
1	2A	2915	<div> <div>3%</div> <div>80%</div> <div>15%</div> <div>..</div> </div>
2	1B	121	<div> <div>92%</div> <div>7%</div> <div>.</div> </div>
2	2B	121	<div> <div>75%</div> <div>24%</div> <div>.</div> </div>
3	1D	276	<div> <div>%</div> <div>92%</div> <div>8%</div> </div>

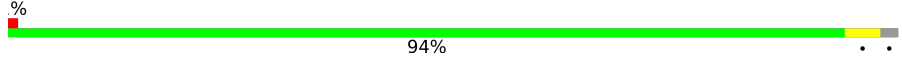
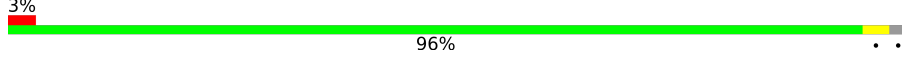
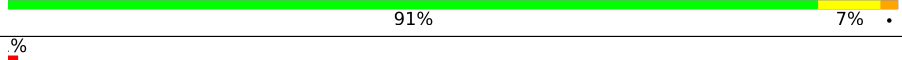
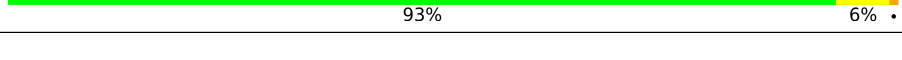
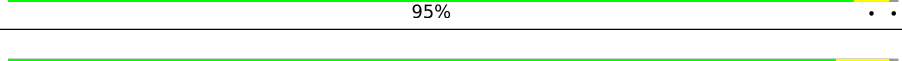
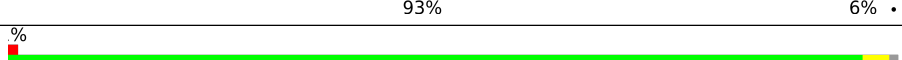
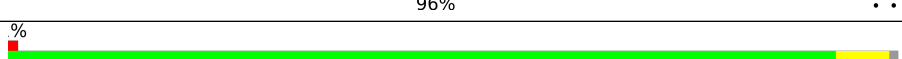
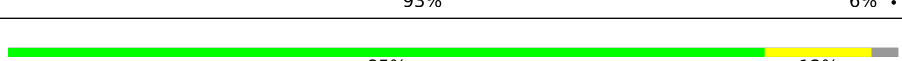

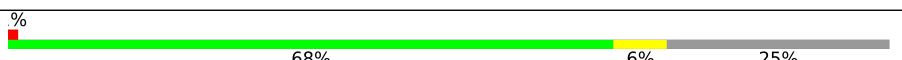
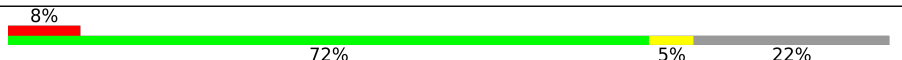
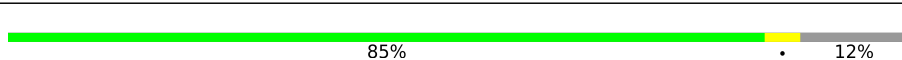

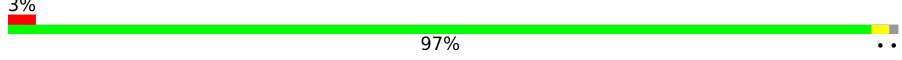
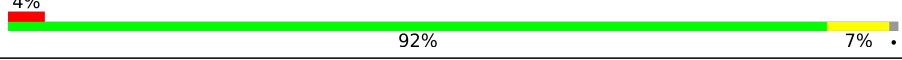
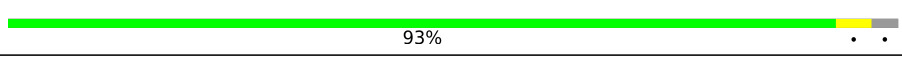
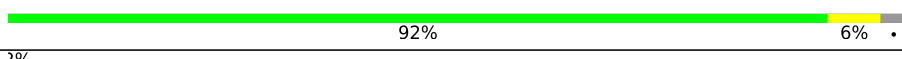
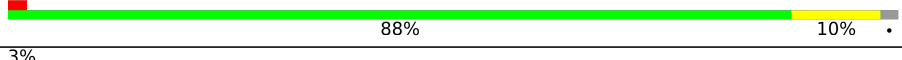



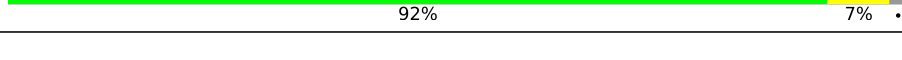
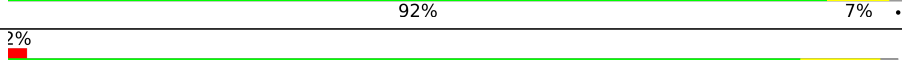
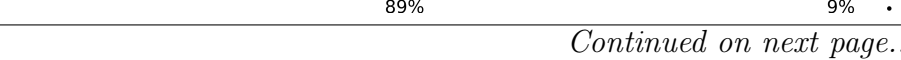

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Mol	Chain	Length	Quality of chain
3	2D	276	
4	1E	206	
4	2E	206	
5	1F	210	
5	2F	210	
6	1G	182	
6	2G	182	
7	1H	180	
7	2H	180	
8	1I	148	
8	2I	148	
9	1N	140	
9	2N	140	
10	1O	122	
10	2O	122	
11	1P	150	
11	2P	150	
12	1Q	141	
12	2Q	141	
13	1R	118	
13	2R	118	
14	1S	112	
14	2S	112	
15	1T	146	
15	2T	146	

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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	<div> <div>39%</div> <div>80%</div> <div>12%</div> <div>8%</div> </div>
41	2j	105	<div> <div>51%</div> <div>81%</div> <div>10%</div> <div>9%</div> </div>
42	1k	129	<div> <div>5%</div> <div>81%</div> <div>8%</div> <div>12%</div> </div>
42	2k	129	<div> <div>7%</div> <div>81%</div> <div>7%</div> <div>12%</div> </div>
43	1l	132	<div> <div>2%</div> <div>87%</div> <div>5%</div> <div>8%</div> </div>
43	2l	132	<div> <div>5%</div> <div>84%</div> <div>8%</div> <div>8%</div> </div>
44	1m	126	<div> <div>21%</div> <div>87%</div> <div>10%</div> <div>..</div> </div>
44	2m	126	<div> <div>26%</div> <div>84%</div> <div>13%</div> <div>.</div> </div>
45	1n	61	<div> <div>43%</div> <div>90%</div> <div>8%</div> <div>.</div> </div>
45	2n	61	<div> <div>80%</div> <div>87%</div> <div>11%</div> <div>.</div> </div>
46	1o	89	<div> <div>%</div> <div>97%</div> <div>..</div> </div>
46	2o	89	<div> <div>94%</div> <div>..</div> </div>
47	1p	88	<div> <div>17%</div> <div>84%</div> <div>9%</div> <div>7%</div> </div>
47	2p	88	<div> <div>5%</div> <div>82%</div> <div>11%</div> <div>7%</div> </div>
48	1q	105	<div> <div>2%</div> <div>88%</div> <div>7%</div> <div>6%</div> </div>
48	2q	105	<div> <div>%</div> <div>90%</div> <div>5%</div> <div>6%</div> </div>
49	1r	88	<div> <div>3%</div> <div>69%</div> <div>8%</div> <div>23%</div> </div>
49	2r	88	<div> <div>%</div> <div>68%</div> <div>9%</div> <div>23%</div> </div>
50	1s	93	<div> <div>8%</div> <div>84%</div> <div>5%</div> <div>11%</div> </div>
50	2s	93	<div> <div>18%</div> <div>80%</div> <div>10%</div> <div>11%</div> </div>
51	1t	106	<div> <div>18%</div> <div>84%</div> <div>6%</div> <div>9%</div> </div>
51	2t	106	<div> <div>12%</div> <div>85%</div> <div>6%</div> <div>9%</div> </div>
52	1u	27	<div> <div>48%</div> <div>81%</div> <div>.</div> <div>15%</div> </div>
52	2u	27	<div> <div>44%</div> <div>81%</div> <div>.</div> <div>15%</div> </div>
53	1v	21	<div> <div>24%</div> <div>76%</div> </div>

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Mol	Chain	Length	Quality of chain
53	2v	21	
54	1x	77	
54	2x	77	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
55	MG	18	108	-	-	-	X
55	MG	1A	3282	-	-	-	X
55	MG	1A	3284	-	-	-	X
55	MG	1A	3356	-	-	-	X
55	MG	1A	3359	-	-	-	X
55	MG	1A	3371	-	-	-	X
55	MG	1A	3387	-	-	-	X
55	MG	1A	3392	-	-	-	X
55	MG	1A	3394	-	-	-	X
55	MG	1A	3401	-	-	-	X
55	MG	1A	3405	-	-	-	X
55	MG	1A	3462	-	-	-	X
55	MG	1A	3514	-	-	-	X
55	MG	1A	3908	-	-	-	X
55	MG	1A	3969	-	-	-	X
55	MG	1A	3991	-	-	-	X
55	MG	1A	4041	-	-	-	X
55	MG	1E	311	-	-	-	X
55	MG	1F	307	-	-	-	X
55	MG	1W	207	-	-	-	X
55	MG	1a	1797	-	-	-	X
55	MG	2A	3148	-	-	-	X
55	MG	2A	3219	-	-	-	X
55	MG	2A	3228	-	-	-	X
55	MG	2A	3256	-	-	-	X
55	MG	2A	3262	-	-	-	X
55	MG	2A	3433	-	-	-	X
55	MG	2A	3460	-	-	-	X
55	MG	2A	3487	-	-	-	X
55	MG	2A	3609	-	-	-	X
55	MG	2B	204	-	-	-	X
55	MG	2D	306	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
55	MG	2a	1778	-	-	-	X

2 Entry composition [i](#)

There are 60 unique types of molecules in this entry. The entry contains 292790 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	2871	Total	C	N	O	P	0	0	0
			61852	27531	11572	19878	2871			
1	2A	2800	Total	C	N	O	P	0	0	0
			60322	26848	11284	19390	2800			

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	1P	149	Total	C	N	O	S	0	0	0
			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
			873	550	174	149			
14	2S	110	Total	C	N	O	0	0	0
			870	549	173	148			

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
22	10	75	Total	C	N	O	S	0	0	0
			598	370	127	100	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
			755	475	148	131	1			
23	21	97	Total	C	N	O	S	0	0	0
			755	475	148	131	1			

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

- 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
			1846	1179	331	331	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
			1548	973	301	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
			1655	1038	326	284	7			
35	2d	208	Total	C	N	O	S	0	0	0
			1674	1050	333	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
			1129	714	213	198	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
			810	514	144	149	3			
37	2f	100	Total	C	N	O	S	0	0	0
			816	516	146	151	3			

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

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

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

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

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

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

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

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

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

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

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
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	123	Total	C	N	O	S	0	0	0
			958	592	198	166	2			
44	2m	122	Total	C	N	O	S	0	0	0
			950	586	197	165	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
			652	417	120	113	2			
50	2s	83	Total	C	N	O	S	0	0	0
			646	412	119	113	2			

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

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

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

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

- Molecule 53 is a RNA chain called M-Stop-mRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
53	1v	5	Total	C	N	O	P	0	0	0
			109	49	22	33	5			
53	2v	5	Total	C	N	O	P	0	0	0
			109	49	22	33	5			

- Molecule 54 is a RNA chain called P-site deacylated tRNA^{met}.

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

- Molecule 55 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
55	1A	1052	Total	Mg	0	0
			1052	1052		
55	1B	38	Total	Mg	0	0
			38	38		
55	1D	11	Total	Mg	0	0
			11	11		
55	1E	13	Total	Mg	0	0
			13	13		
55	1F	11	Total	Mg	0	0
			11	11		
55	1G	5	Total	Mg	0	0
			5	5		
55	1I	1	Total	Mg	0	0
			1	1		
55	1N	6	Total	Mg	0	0
			6	6		
55	1O	5	Total	Mg	0	0
			5	5		
55	1P	6	Total	Mg	0	0
			6	6		
55	1Q	7	Total	Mg	0	0
			7	7		
55	1R	5	Total	Mg	0	0
			5	5		
55	1S	3	Total	Mg	0	0
			3	3		
55	1T	2	Total	Mg	0	0
			2	2		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
55	1U	13	Total 13	Mg 13	0	0
55	1V	8	Total 8	Mg 8	0	0
55	1W	7	Total 7	Mg 7	0	0
55	1X	6	Total 6	Mg 6	0	0
55	1Y	2	Total 2	Mg 2	0	0
55	1Z	3	Total 3	Mg 3	0	0
55	10	7	Total 7	Mg 7	0	0
55	11	4	Total 4	Mg 4	0	0
55	12	2	Total 2	Mg 2	0	0
55	13	3	Total 3	Mg 3	0	0
55	14	1	Total 1	Mg 1	0	0
55	15	7	Total 7	Mg 7	0	0
55	16	1	Total 1	Mg 1	0	0
55	17	6	Total 6	Mg 6	0	0
55	18	8	Total 8	Mg 8	0	0
55	1a	198	Total 198	Mg 198	0	0
55	1b	1	Total 1	Mg 1	0	0
55	1d	1	Total 1	Mg 1	0	0
55	1e	1	Total 1	Mg 1	0	0
55	1f	1	Total 1	Mg 1	0	0
55	1l	2	Total 2	Mg 2	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
55	1m	2	Total Mg 2 2	0	0
55	1n	1	Total Mg 1 1	0	0
55	1p	1	Total Mg 1 1	0	0
55	1r	1	Total Mg 1 1	0	0
55	1t	1	Total Mg 1 1	0	0
55	1v	1	Total Mg 1 1	0	0
55	1x	15	Total Mg 15 15	0	0
55	2A	716	Total Mg 716 716	0	0
55	2B	17	Total Mg 17 17	0	0
55	2D	7	Total Mg 7 7	0	0
55	2E	6	Total Mg 6 6	0	0
55	2F	3	Total Mg 3 3	0	0
55	2G	1	Total Mg 1 1	0	0
55	2N	1	Total Mg 1 1	0	0
55	2O	1	Total Mg 1 1	0	0
55	2P	1	Total Mg 1 1	0	0
55	2Q	4	Total Mg 4 4	0	0
55	2R	2	Total Mg 2 2	0	0
55	2T	2	Total Mg 2 2	0	0
55	2U	1	Total Mg 1 1	0	0
55	2V	2	Total Mg 2 2	0	0

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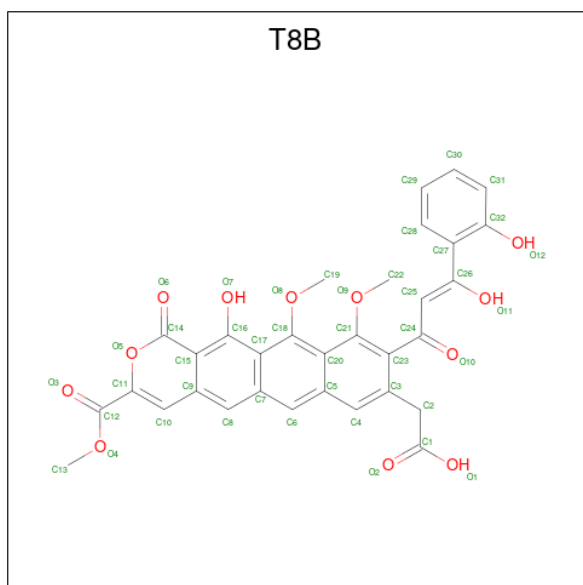
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
55	2W	3	Total 3	Mg 3	0	0
55	2Y	1	Total 1	Mg 1	0	0
55	2Z	1	Total 1	Mg 1	0	0
55	20	1	Total 1	Mg 1	0	0
55	21	1	Total 1	Mg 1	0	0
55	23	1	Total 1	Mg 1	0	0
55	25	1	Total 1	Mg 1	0	0
55	27	3	Total 3	Mg 3	0	0
55	28	3	Total 3	Mg 3	0	0
55	2a	197	Total 197	Mg 197	0	0
55	2e	1	Total 1	Mg 1	0	0
55	2f	2	Total 2	Mg 2	0	0
55	2j	1	Total 1	Mg 1	0	0
55	2k	1	Total 1	Mg 1	0	0
55	2l	4	Total 4	Mg 4	0	0
55	2q	2	Total 2	Mg 2	0	0
55	2r	1	Total 1	Mg 1	0	0
55	2t	1	Total 1	Mg 1	0	0
55	2x	5	Total 5	Mg 5	0	0

- Molecule 56 is POTASSIUM ION (three-letter code: K) (formula: K).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
56	1A	1	Total K 1 1	0	0
56	2A	1	Total K 1 1	0	0

- Molecule 57 is Thermorubin (three-letter code: T8B) (formula: C₃₂H₂₄O₁₂) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
57	1A	1	Total C O 44 32 12	0	0
57	2A	1	Total C O 44 32 12	0	0

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

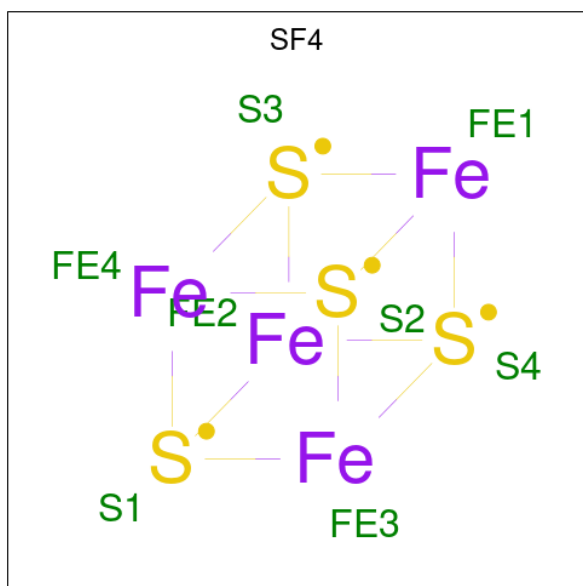
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
58	1Y	1	Total Zn 1 1	0	0
58	14	1	Total Zn 1 1	0	0
58	15	1	Total Zn 1 1	0	0
58	16	1	Total Zn 1 1	0	0
58	19	1	Total Zn 1 1	0	0

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

- Molecule 59 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe_4S_4).



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	2039	Total 2039	O 2039	0	0
60	1B	63	Total 63	O 63	0	0
60	1D	24	Total 24	O 24	0	0
60	1E	27	Total 27	O 27	0	0
60	1F	14	Total 14	O 14	0	0
60	1G	2	Total 2	O 2	0	0
60	1H	3	Total 3	O 3	0	0
60	1I	1	Total 1	O 1	0	0
60	1N	5	Total 5	O 5	0	0
60	1O	5	Total 5	O 5	0	0
60	1P	21	Total 21	O 21	0	0
60	1Q	7	Total 7	O 7	0	0
60	1R	13	Total 13	O 13	0	0
60	1S	4	Total 4	O 4	0	0
60	1T	7	Total 7	O 7	0	0
60	1U	13	Total 13	O 13	0	0
60	1V	8	Total 8	O 8	0	0
60	1W	8	Total 8	O 8	0	0
60	1X	5	Total 5	O 5	0	0
60	1Y	2	Total 2	O 2	0	0
60	1Z	1	Total 1	O 1	0	0
60	10	11	Total 11	O 11	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
60	11	12	Total 12	O 12	0	0
60	12	4	Total 4	O 4	0	0
60	13	5	Total 5	O 5	0	0
60	14	1	Total 1	O 1	0	0
60	15	6	Total 6	O 6	0	0
60	16	2	Total 2	O 2	0	0
60	17	11	Total 11	O 11	0	0
60	18	10	Total 10	O 10	0	0
60	1a	297	Total 297	O 297	0	0
60	1d	1	Total 1	O 1	0	0
60	1e	1	Total 1	O 1	0	0
60	1f	1	Total 1	O 1	0	0
60	1g	1	Total 1	O 1	0	0
60	1l	8	Total 8	O 8	0	0
60	1m	1	Total 1	O 1	0	0
60	1o	2	Total 2	O 2	0	0
60	1p	1	Total 1	O 1	0	0
60	1q	2	Total 2	O 2	0	0
60	1v	3	Total 3	O 3	0	0
60	1x	15	Total 15	O 15	0	0
60	2A	971	Total 971	O 971	0	0

Continued on next page...

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
60	2B	15	Total 15	O 15	0	0
60	2D	18	Total 18	O 18	0	0
60	2E	10	Total 10	O 10	0	0
60	2F	11	Total 11	O 11	0	0
60	2N	3	Total 3	O 3	0	0
60	2O	2	Total 2	O 2	0	0
60	2P	11	Total 11	O 11	0	0
60	2Q	2	Total 2	O 2	0	0
60	2R	3	Total 3	O 3	0	0
60	2T	3	Total 3	O 3	0	0
60	2U	2	Total 2	O 2	0	0
60	2V	1	Total 1	O 1	0	0
60	2W	3	Total 3	O 3	0	0
60	2X	4	Total 4	O 4	0	0
60	2Z	1	Total 1	O 1	0	0
60	20	4	Total 4	O 4	0	0
60	21	3	Total 3	O 3	0	0
60	23	2	Total 2	O 2	0	0
60	26	1	Total 1	O 1	0	0
60	27	2	Total 2	O 2	0	0
60	28	3	Total 3	O 3	0	0

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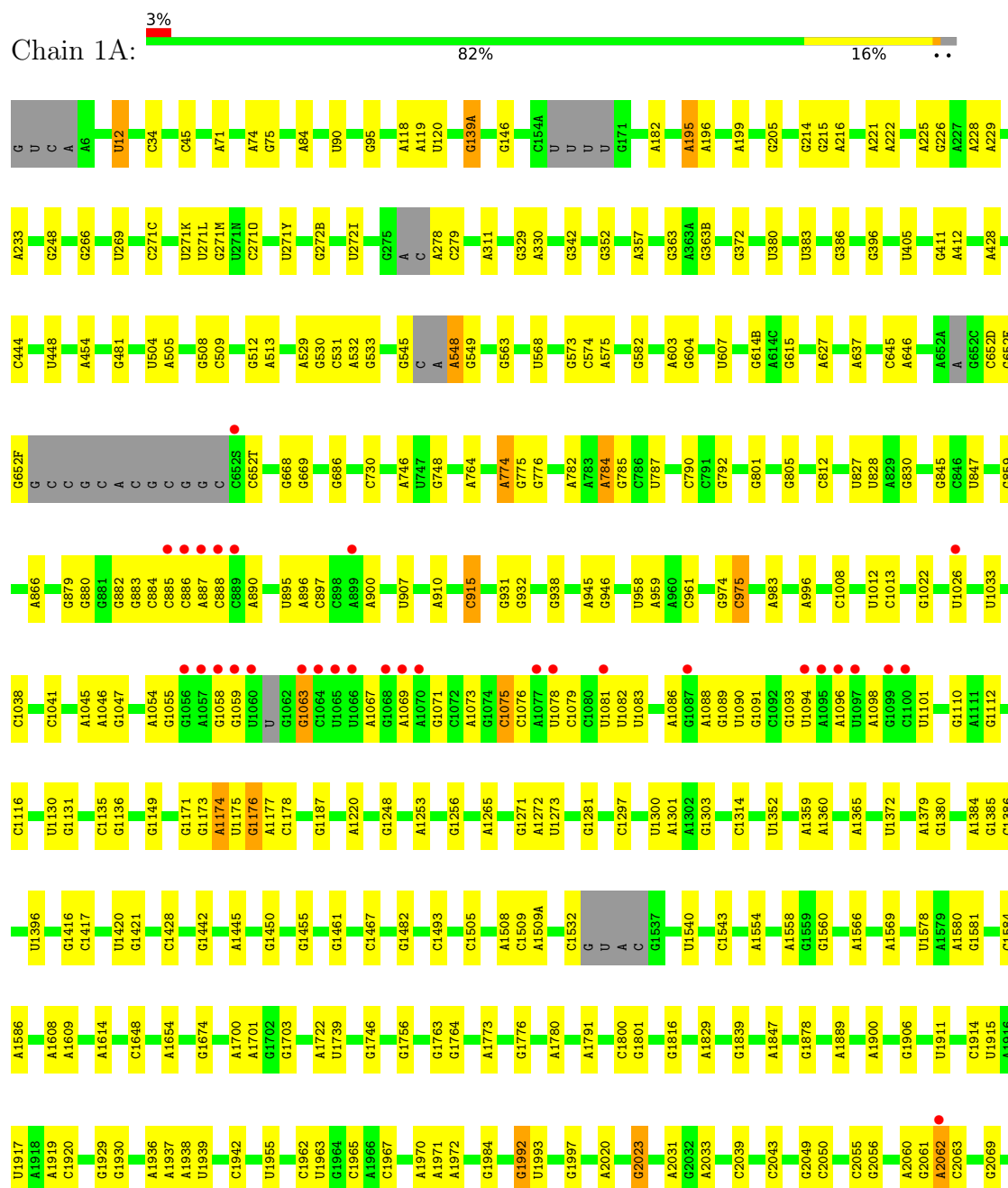
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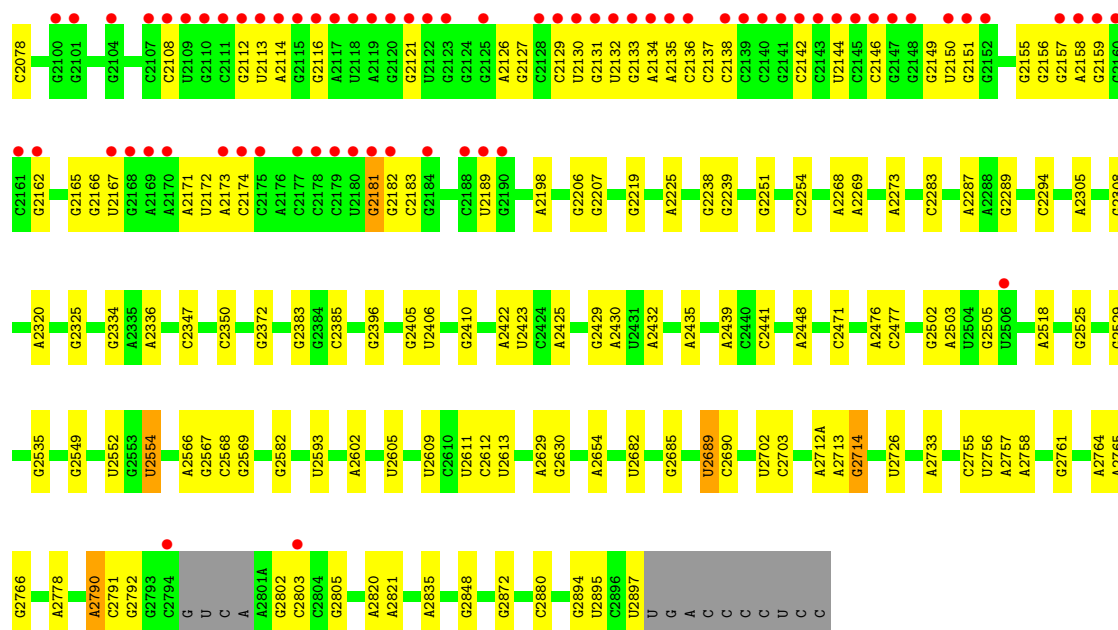
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
60	29	1	Total 1	O 1	0	0
60	2a	176	Total 176	O 176	0	0
60	2c	1	Total 1	O 1	0	0
60	2d	1	Total 1	O 1	0	0
60	2e	1	Total 1	O 1	0	0
60	2f	1	Total 1	O 1	0	0
60	2j	2	Total 2	O 2	0	0
60	2l	2	Total 2	O 2	0	0
60	2n	1	Total 1	O 1	0	0
60	2p	3	Total 3	O 3	0	0
60	2q	2	Total 2	O 2	0	0
60	2r	3	Total 3	O 3	0	0
60	2t	6	Total 6	O 6	0	0
60	2v	1	Total 1	O 1	0	0
60	2x	3	Total 3	O 3	0	0

3 Residue-property plots

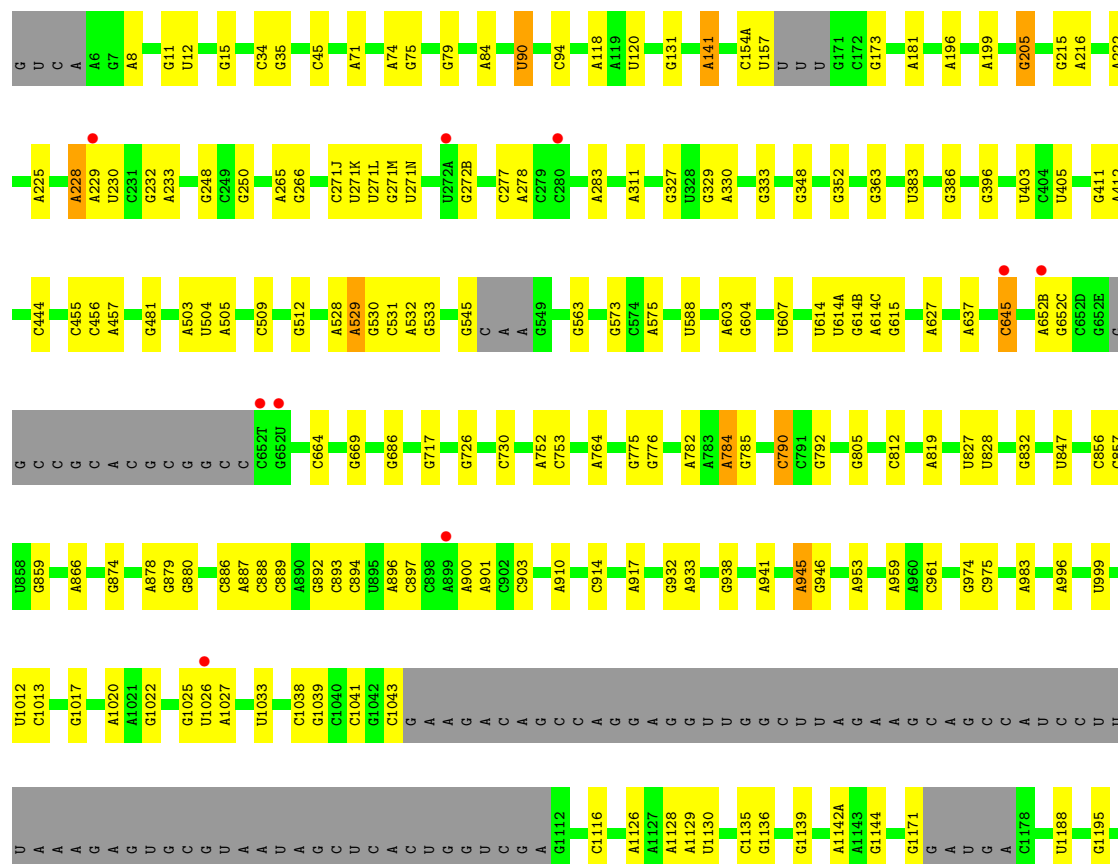
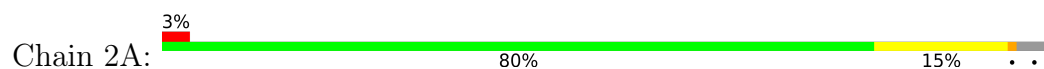
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

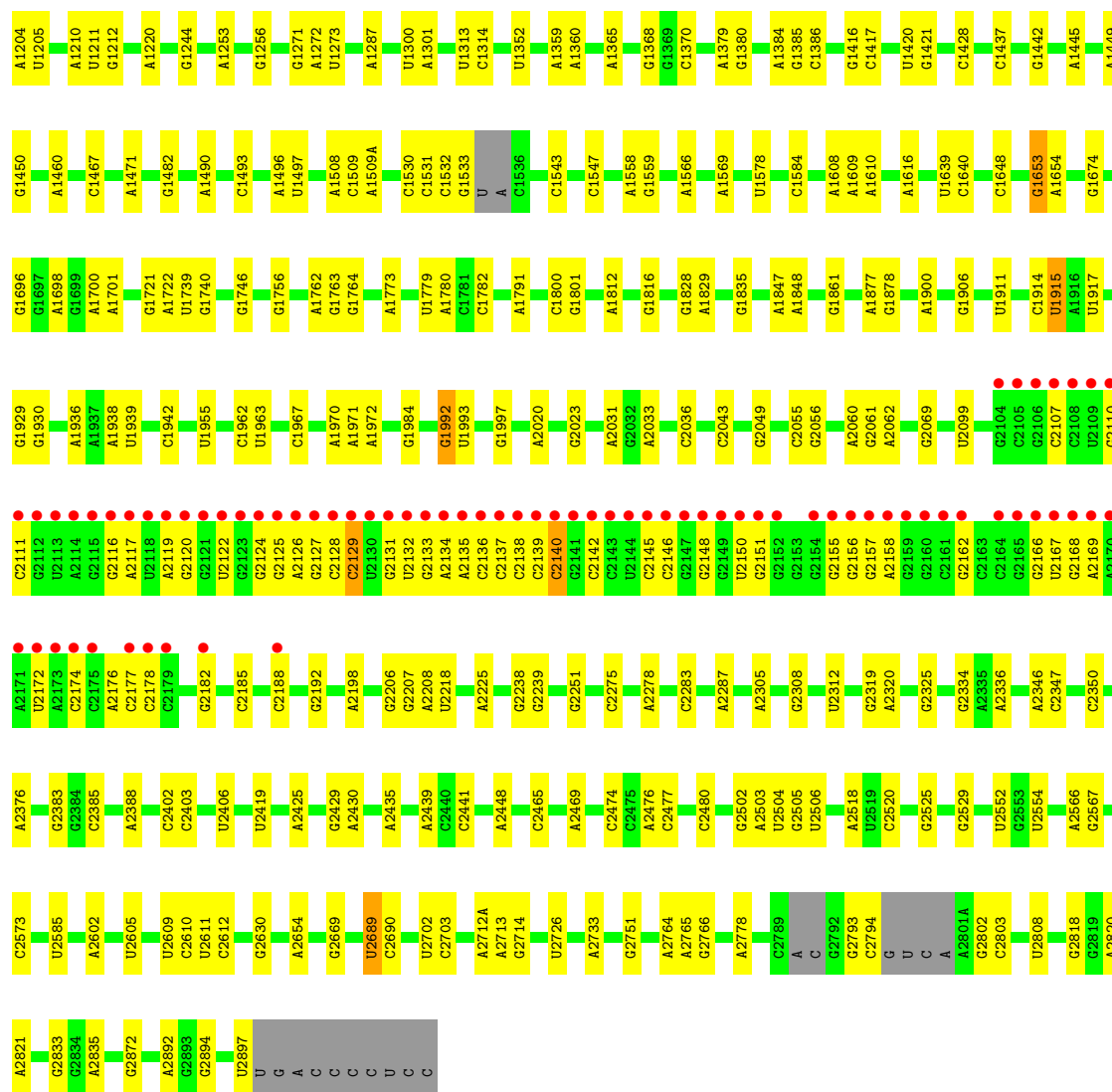
• Molecule 1: 23S Ribosomal RNA





- Molecule 1: 23S Ribosomal RNA





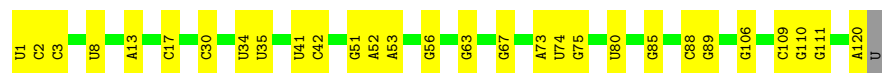
- Molecule 2: 5S Ribosomal RNA

Chain 1B: 92% 7%



- Molecule 2: 5S Ribosomal RNA

Chain 2B: 75% 24%



- Molecule 3: 50S ribosomal protein L2

Chain 1D: 92% 8%



- Molecule 3: 50S ribosomal protein L2



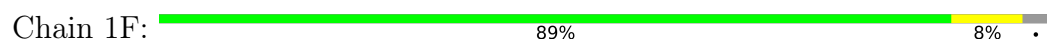
- Molecule 4: 50S ribosomal protein L3



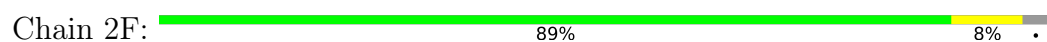
- Molecule 4: 50S ribosomal protein L3



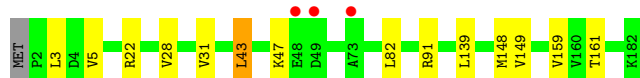
- Molecule 5: 50S ribosomal protein L4



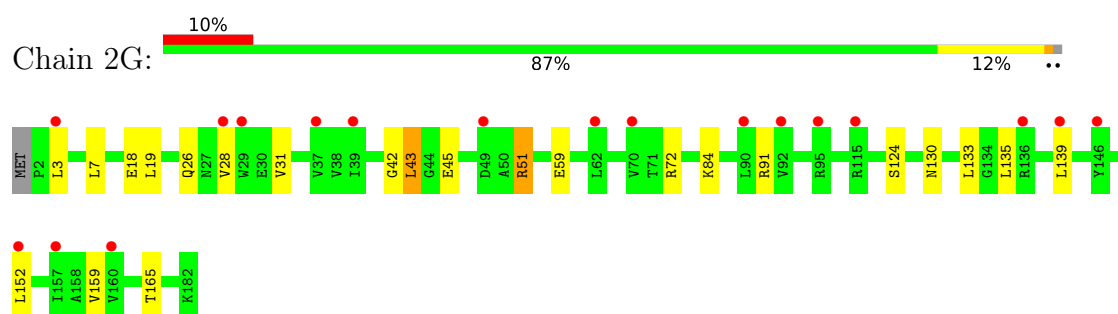
- Molecule 5: 50S ribosomal protein L4



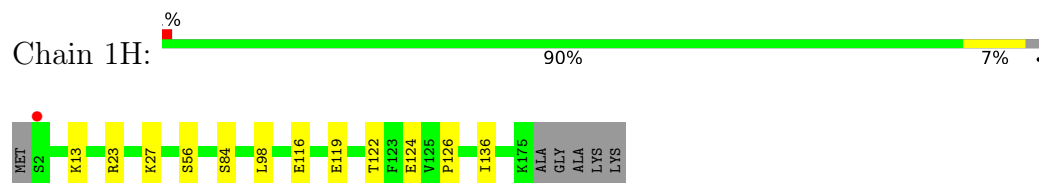
- Molecule 6: 50S ribosomal protein L5



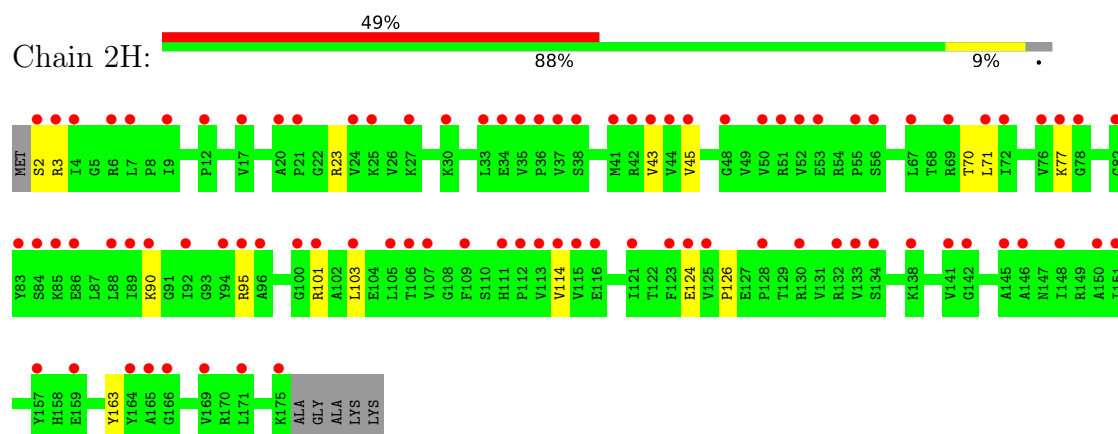
- Molecule 6: 50S ribosomal protein L5



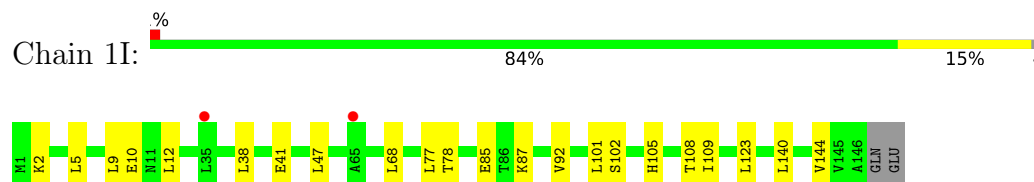
- Molecule 7: 50S ribosomal protein L6



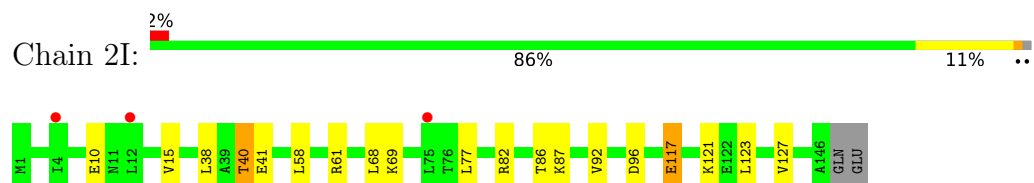
- Molecule 7: 50S ribosomal protein L6



- Molecule 8: 50S ribosomal protein L9

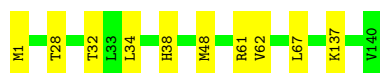


- Molecule 8: 50S ribosomal protein L9

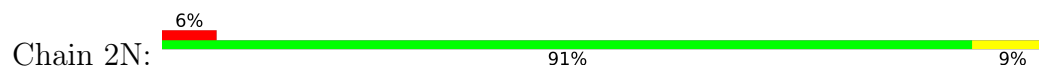


- Molecule 9: 50S ribosomal protein L13





- Molecule 9: 50S ribosomal protein L13



- Molecule 10: 50S ribosomal protein L14



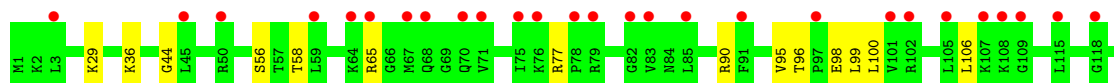
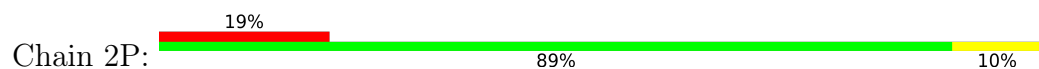
- Molecule 10: 50S ribosomal protein L14



- Molecule 11: 50S ribosomal protein L15



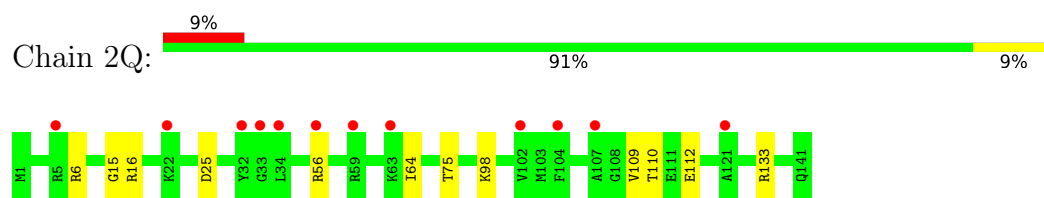
- Molecule 11: 50S ribosomal protein L15



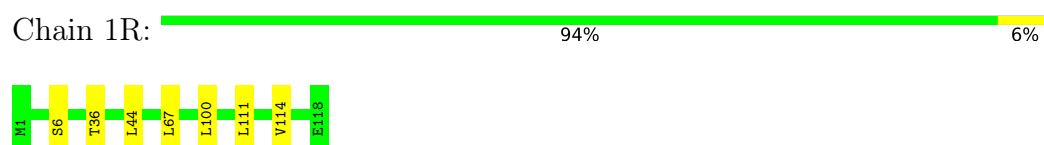
- Molecule 12: 50S ribosomal protein L16



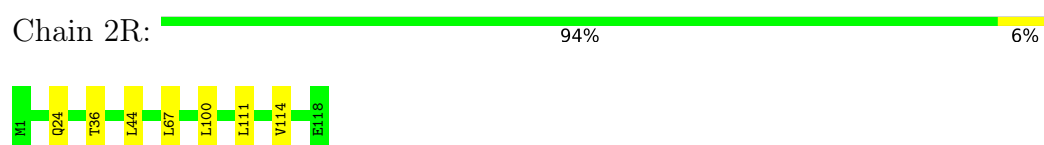
- Molecule 12: 50S ribosomal protein L16



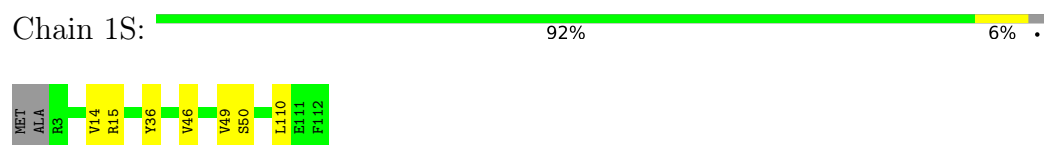
- Molecule 13: 50S ribosomal protein L17



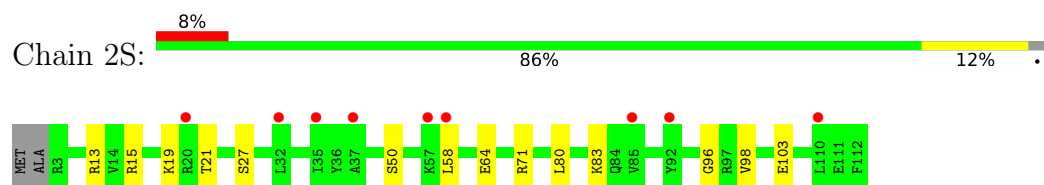
- Molecule 13: 50S ribosomal protein L17



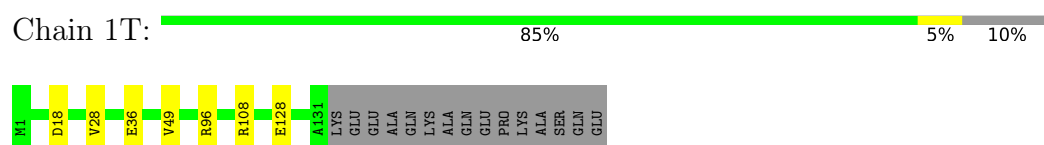
- Molecule 14: 50S ribosomal protein L18



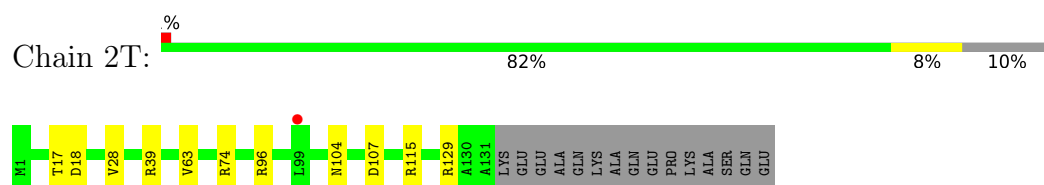
- Molecule 14: 50S ribosomal protein L18



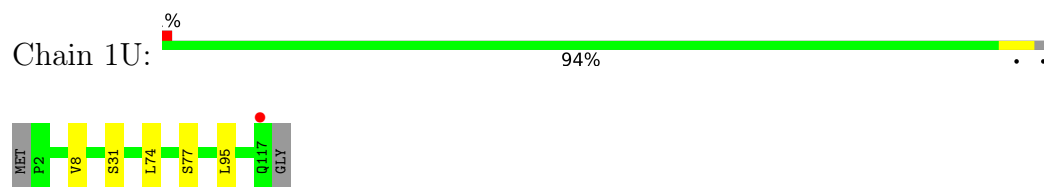
- Molecule 15: 50S ribosomal protein L19



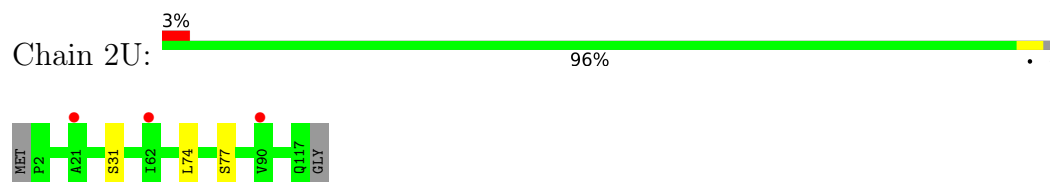
- Molecule 15: 50S ribosomal protein L19



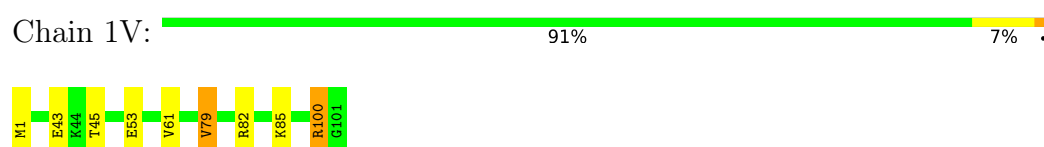
- Molecule 16: 50S ribosomal protein L20



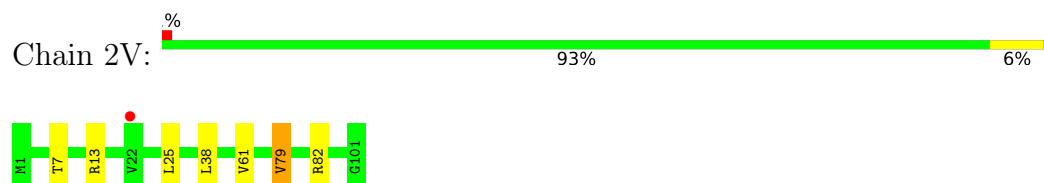
- Molecule 16: 50S ribosomal protein L20



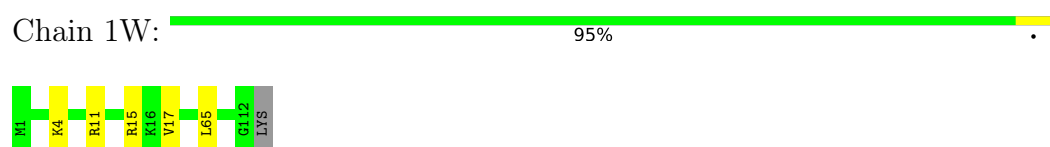
- Molecule 17: 50S ribosomal protein L21



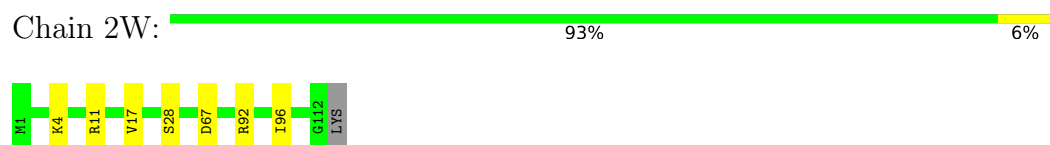
- Molecule 17: 50S ribosomal protein L21



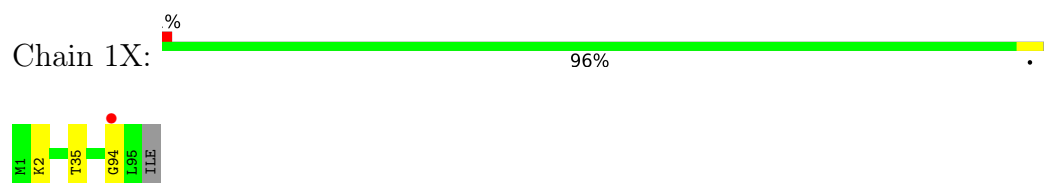
- Molecule 18: 50S ribosomal protein L22



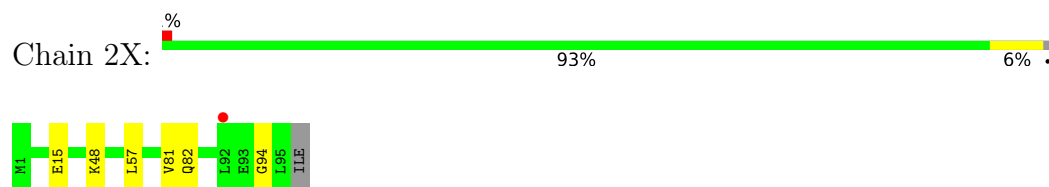
- Molecule 18: 50S ribosomal protein L22



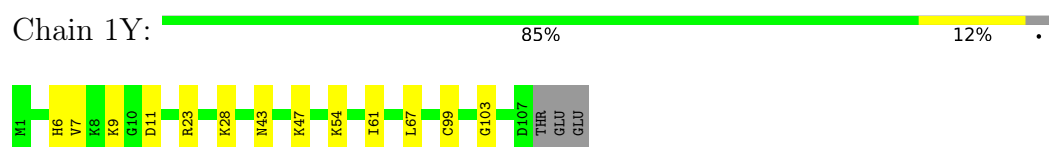
- Molecule 19: 50S ribosomal protein L23



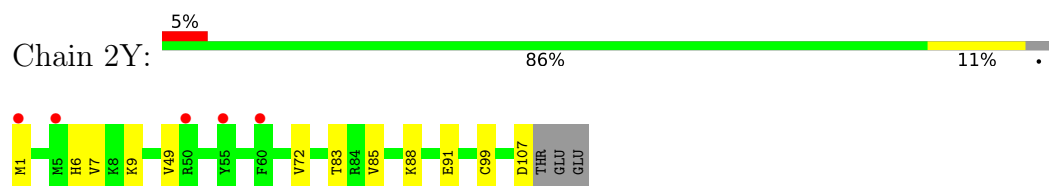
- Molecule 19: 50S ribosomal protein L23



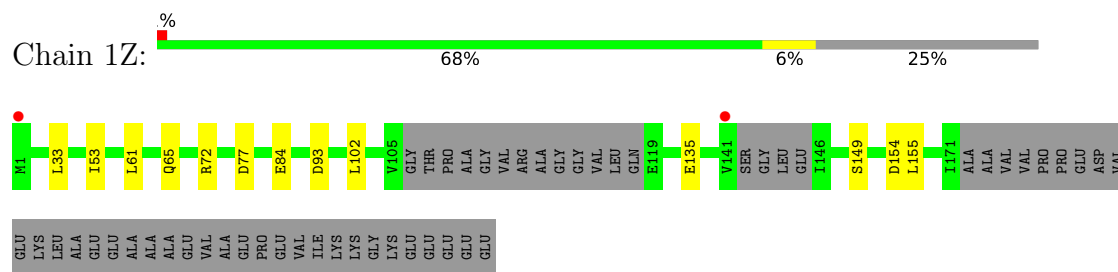
- Molecule 20: 50S ribosomal protein L24



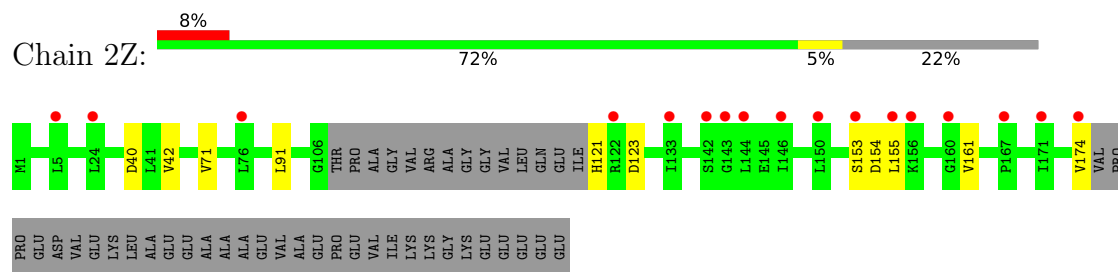
- Molecule 20: 50S ribosomal protein L24



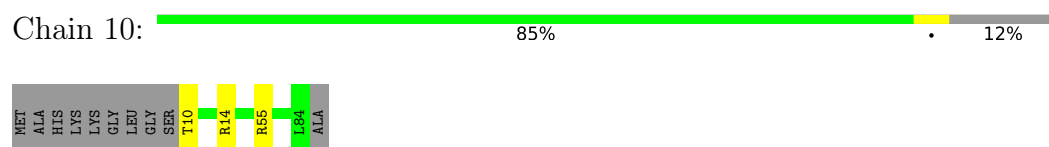
- Molecule 21: 50S ribosomal protein L25



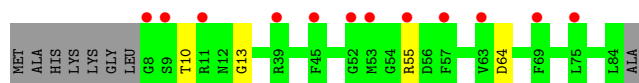
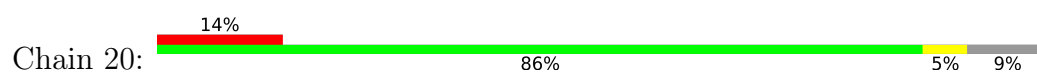
- Molecule 21: 50S ribosomal protein L25



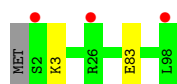
- Molecule 22: 50S ribosomal protein L27



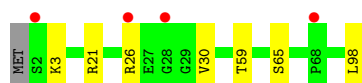
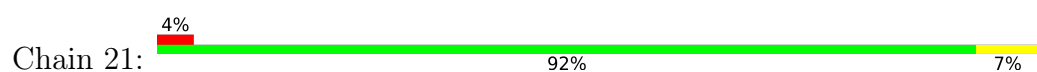
- Molecule 22: 50S ribosomal protein L27



- Molecule 23: 50S ribosomal protein L28



- Molecule 23: 50S ribosomal protein L28



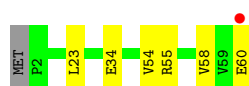
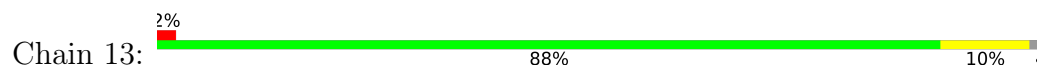
- Molecule 24: 50S ribosomal protein L29



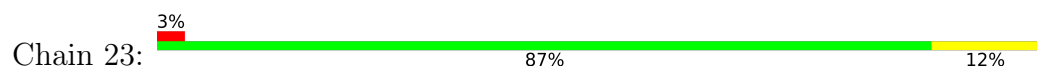
- Molecule 24: 50S ribosomal protein L29



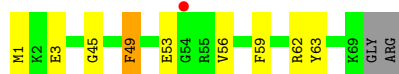
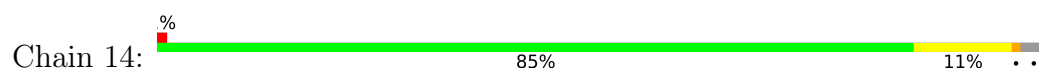
- Molecule 25: 50S ribosomal protein L30



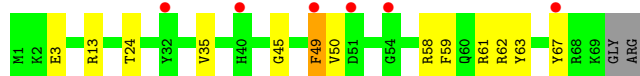
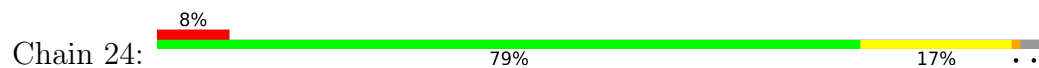
- Molecule 25: 50S ribosomal protein L30



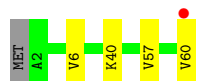
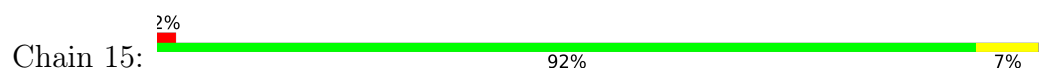
- Molecule 26: 50S ribosomal protein L31



- Molecule 26: 50S ribosomal protein L31



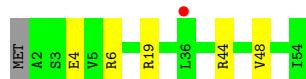
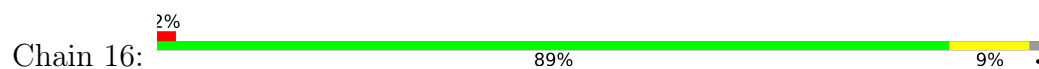
- Molecule 27: 50S ribosomal protein L32



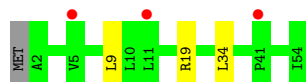
- Molecule 27: 50S ribosomal protein L32



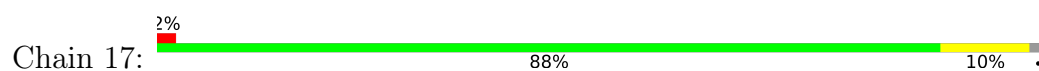
- Molecule 28: 50S ribosomal protein L33



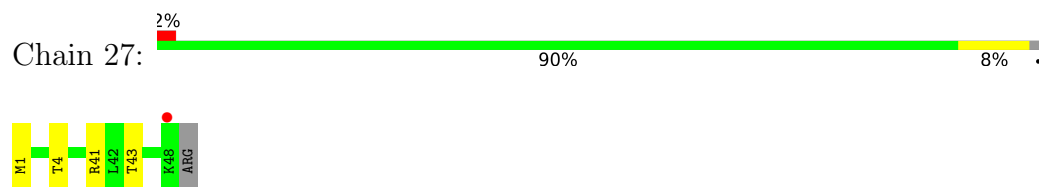
- Molecule 28: 50S ribosomal protein L33



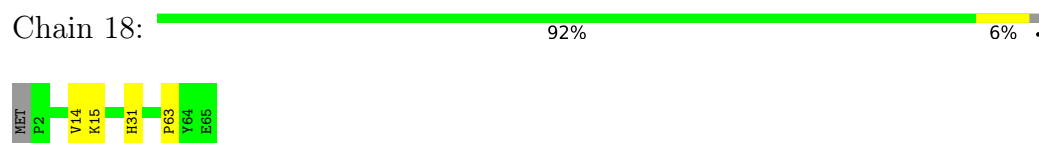
- Molecule 29: 50S ribosomal protein L34



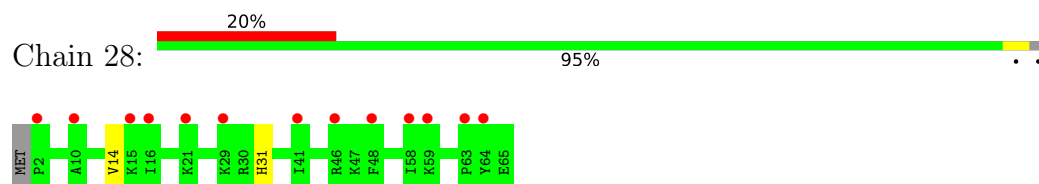
- Molecule 29: 50S ribosomal protein L34



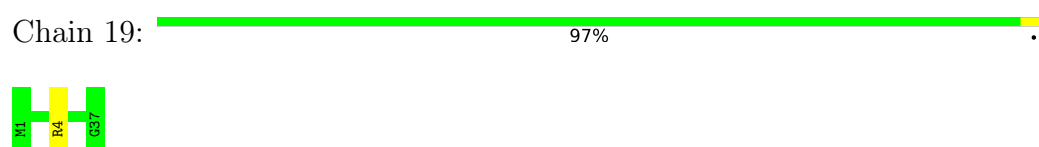
- Molecule 30: 50S ribosomal protein L35



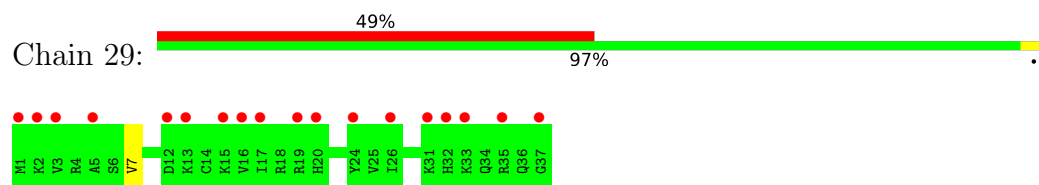
- Molecule 30: 50S ribosomal protein L35



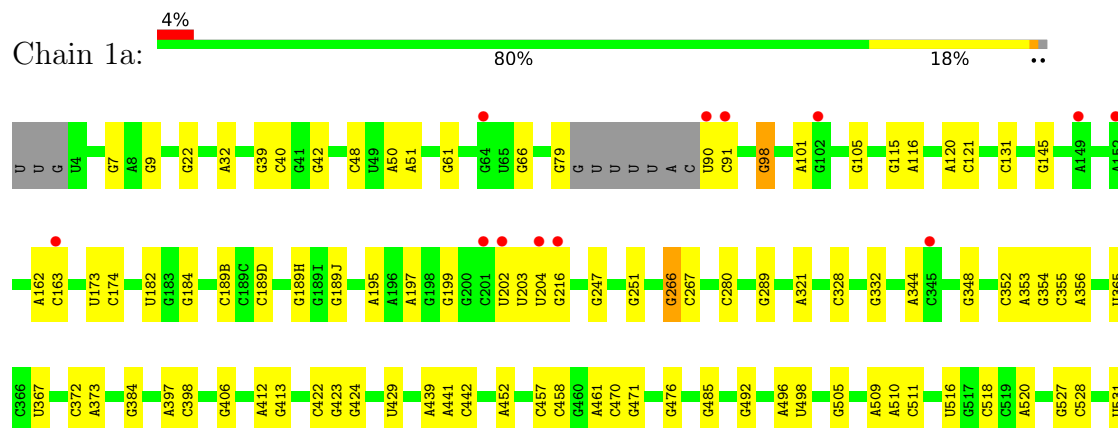
- Molecule 31: 50S ribosomal protein L36

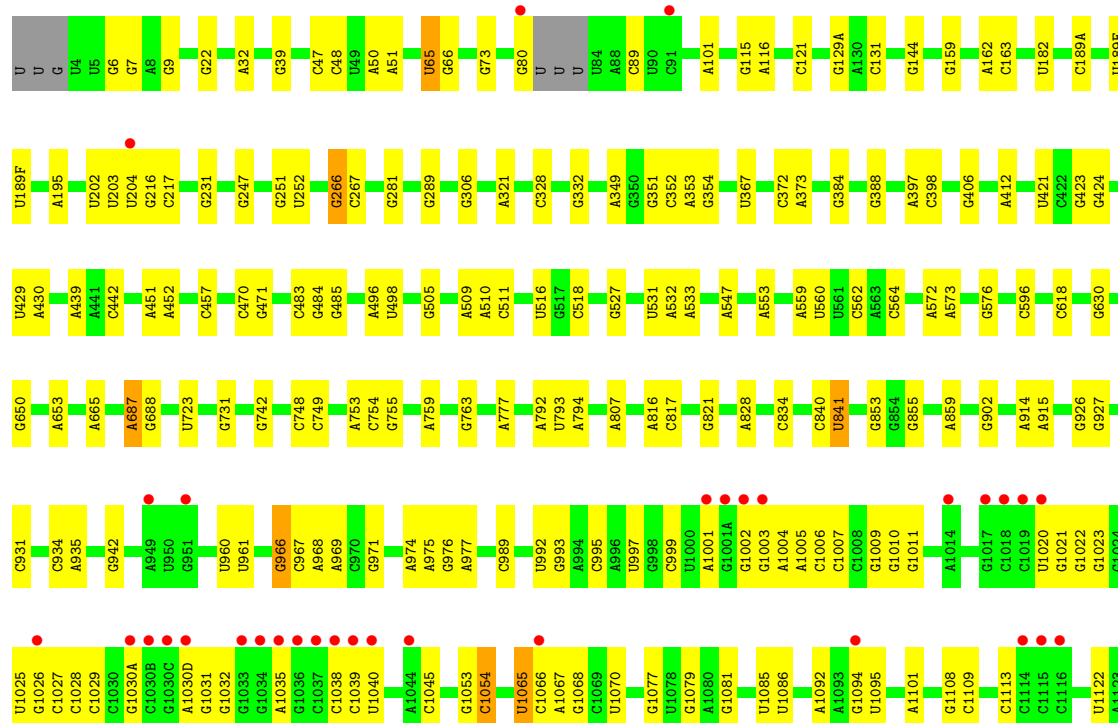


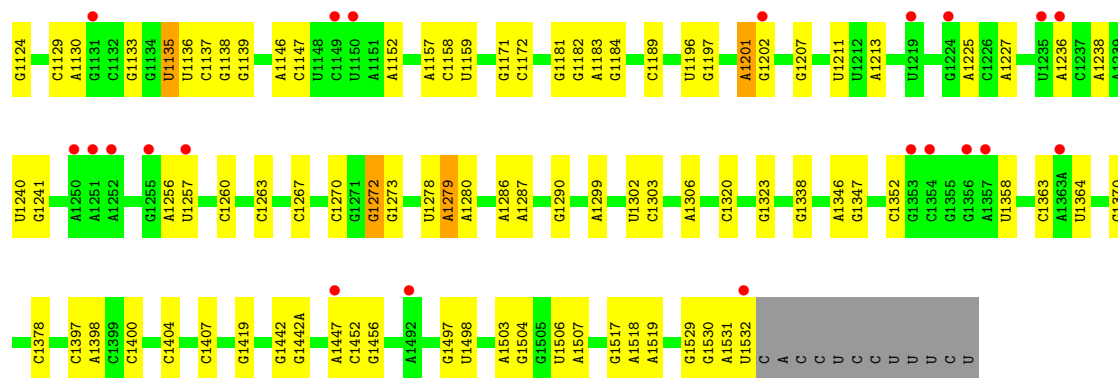
- Molecule 31: 50S ribosomal protein L36



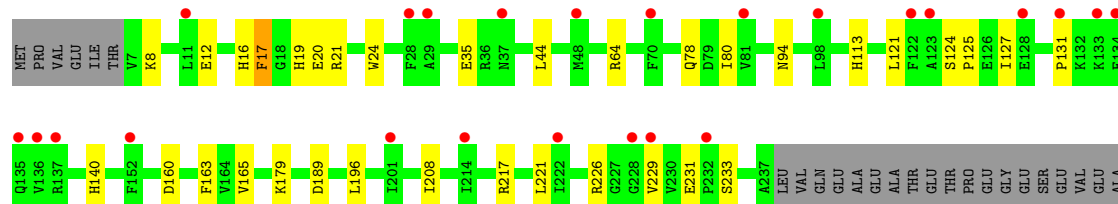
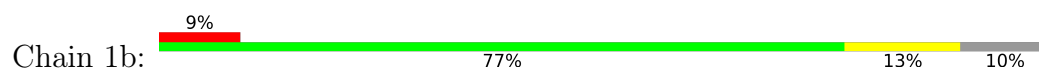
- Molecule 32: 16S Ribosomal RNA



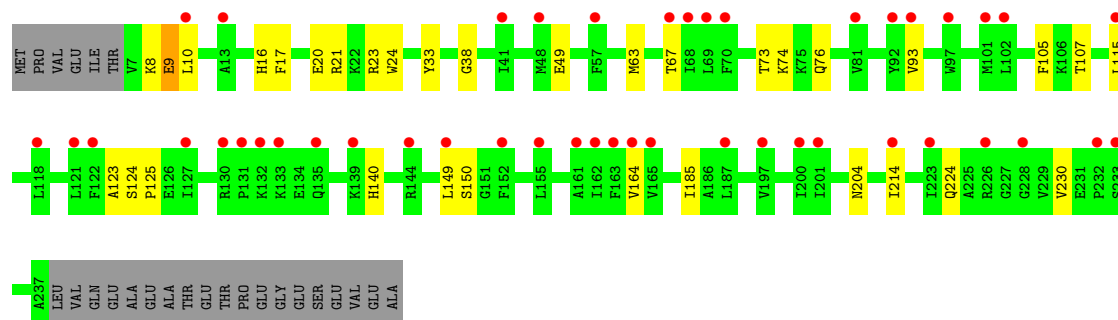
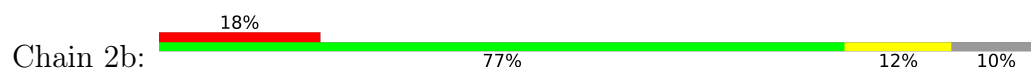




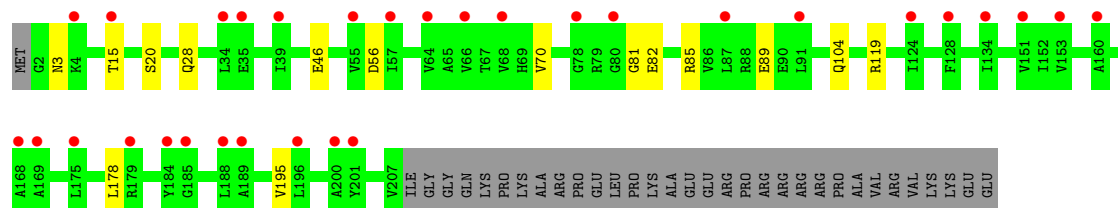
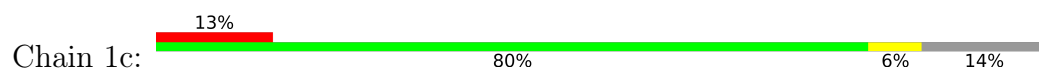
• Molecule 33: 30S ribosomal protein S2



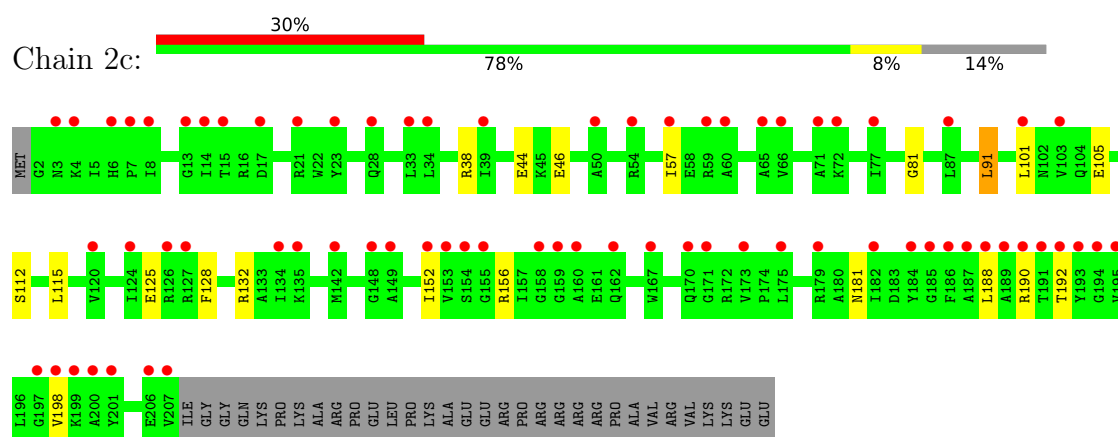
• Molecule 33: 30S ribosomal protein S2



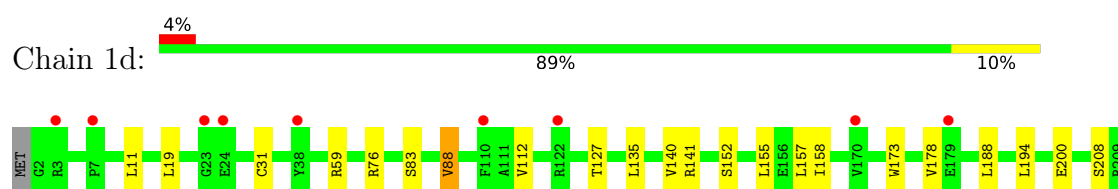
• Molecule 34: 30S ribosomal protein S3



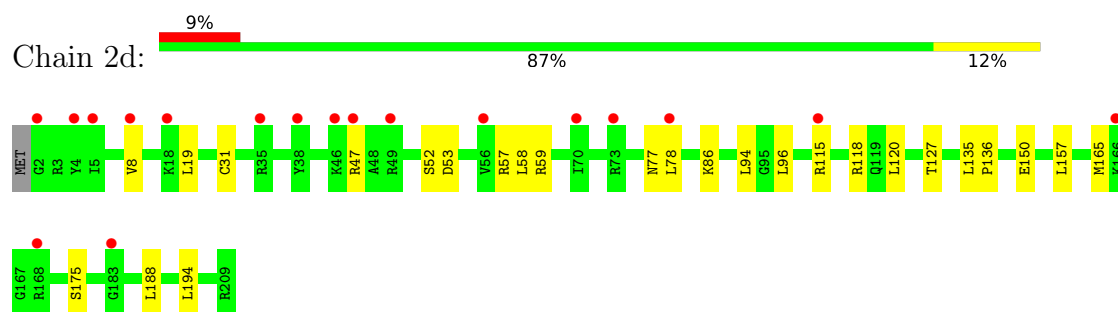
• Molecule 34: 30S ribosomal protein S3



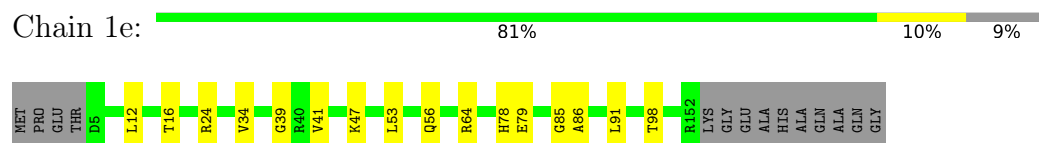
- Molecule 35: 30S ribosomal protein S4



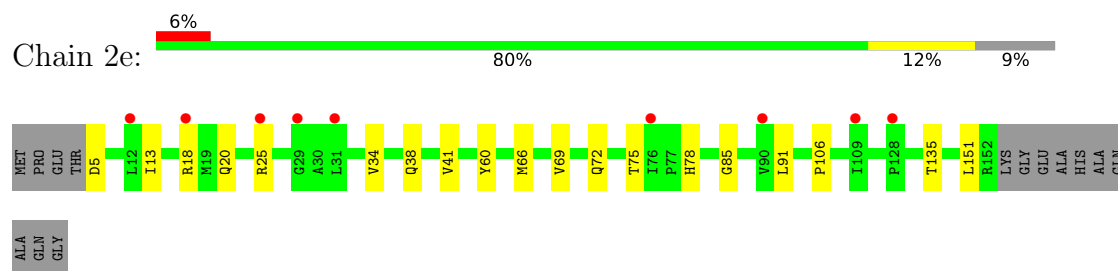
- Molecule 35: 30S ribosomal protein S4



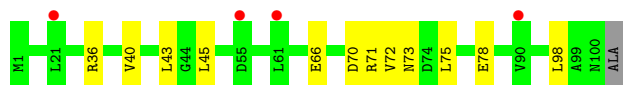
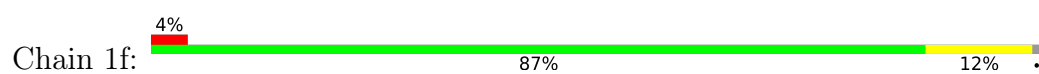
- Molecule 36: 30S ribosomal protein S5



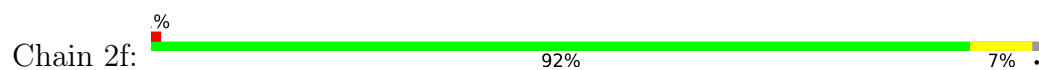
- Molecule 36: 30S ribosomal protein S5



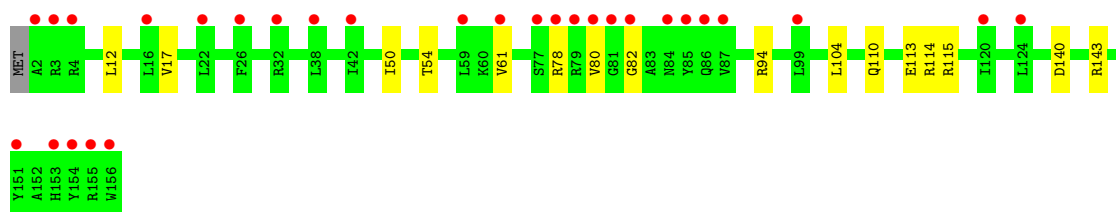
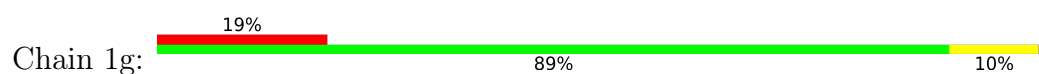
- Molecule 37: 30S ribosomal protein S6



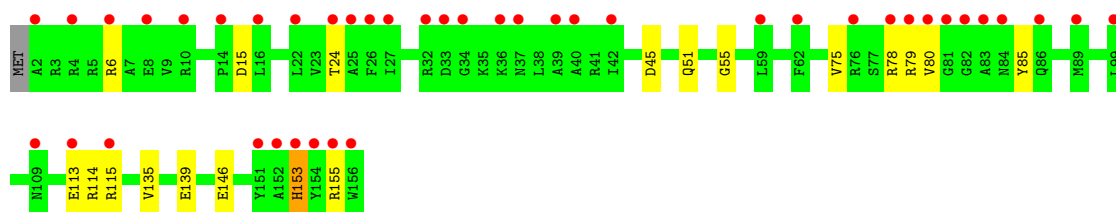
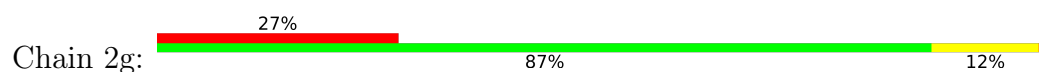
- Molecule 37: 30S ribosomal protein S6



- Molecule 38: 30S ribosomal protein S7



- Molecule 38: 30S ribosomal protein S7



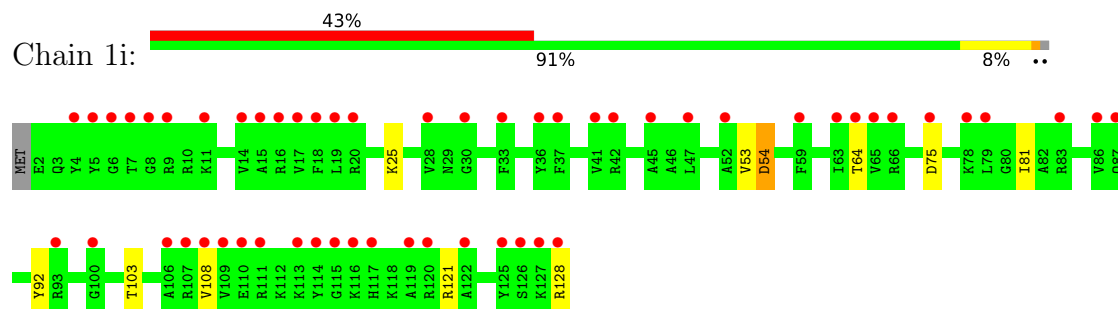
- Molecule 39: 30S ribosomal protein S8



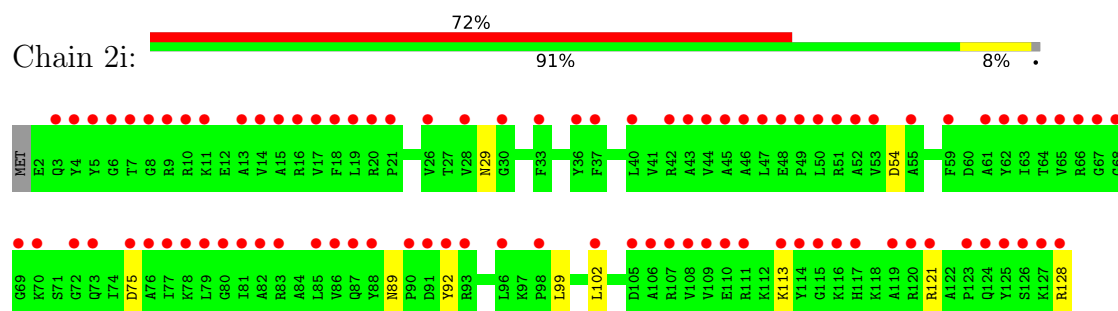
- Molecule 39: 30S ribosomal protein S8



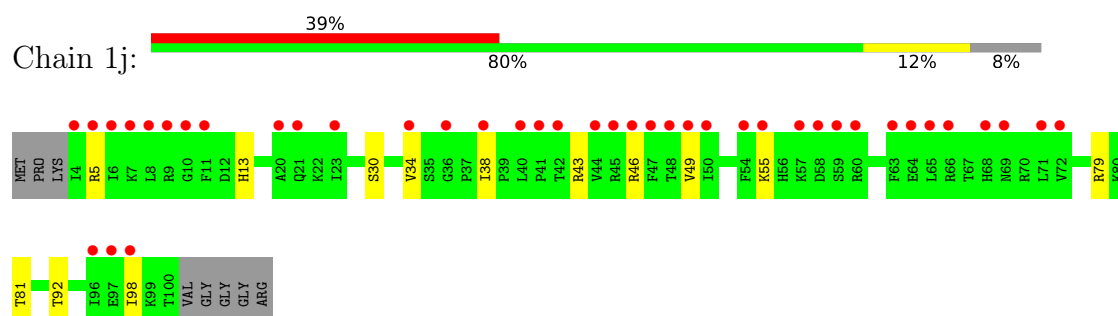
- Molecule 40: 30S ribosomal protein S9



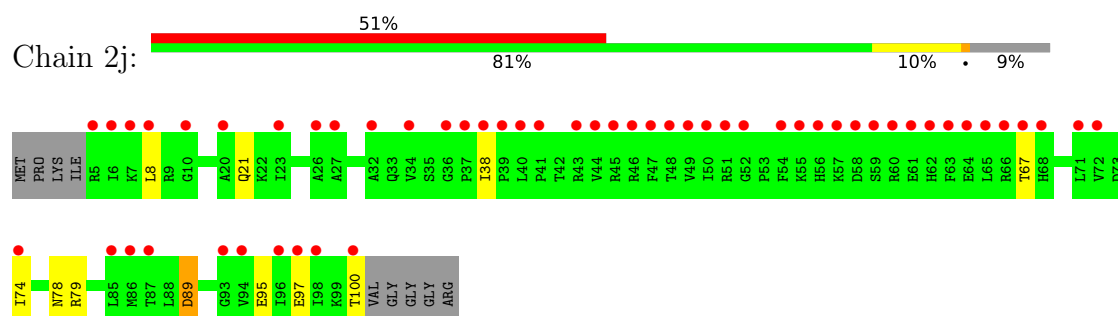
- Molecule 40: 30S ribosomal protein S9



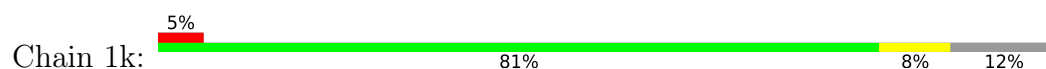
- Molecule 41: 30S ribosomal protein S10

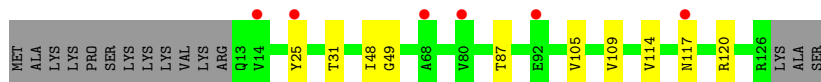


- Molecule 41: 30S ribosomal protein S10

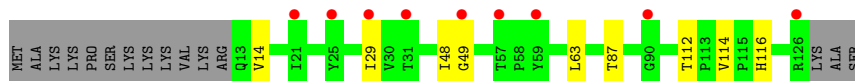
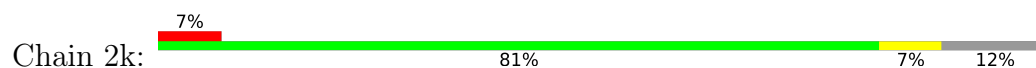


- Molecule 42: 30S ribosomal protein S11

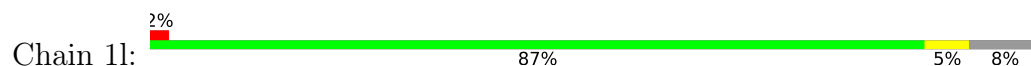




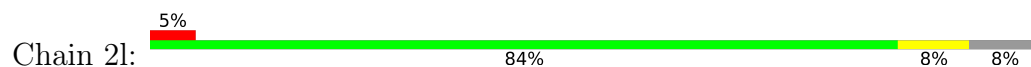
- Molecule 42: 30S ribosomal protein S11



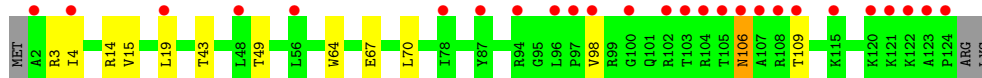
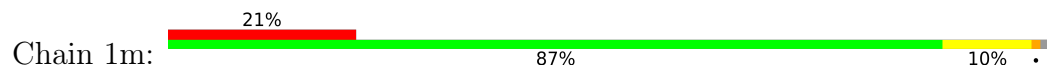
- Molecule 43: 30S ribosomal protein S12



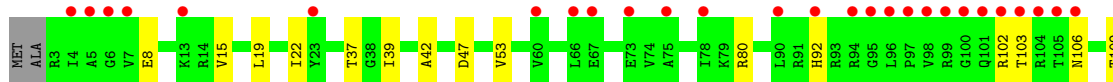
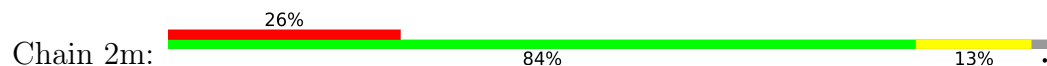
- Molecule 43: 30S ribosomal protein S12



- Molecule 44: 30S ribosomal protein S13

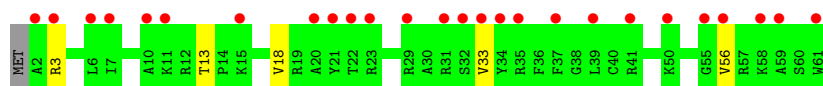


- Molecule 44: 30S ribosomal protein S13

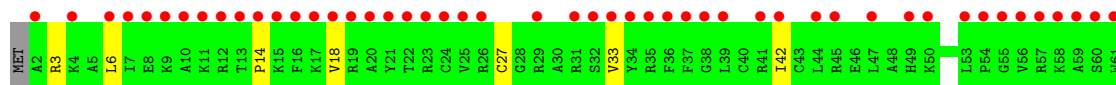
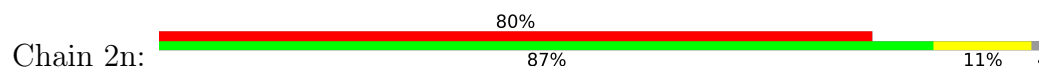


- Molecule 45: 30S ribosomal protein S14 type Z





- Molecule 45: 30S ribosomal protein S14 type Z



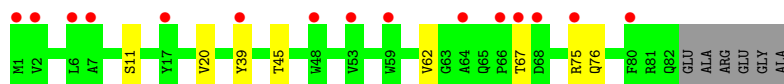
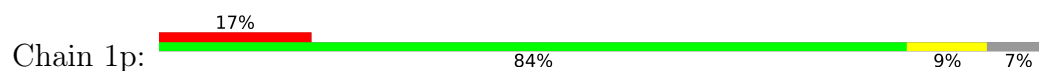
- Molecule 46: 30S ribosomal protein S15



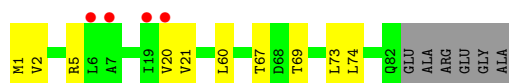
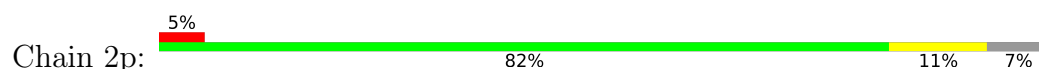
- Molecule 46: 30S ribosomal protein S15



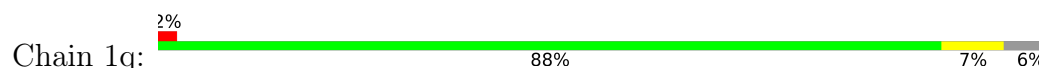
- Molecule 47: 30S ribosomal protein S16



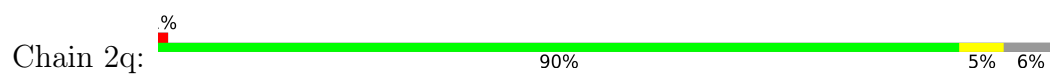
- Molecule 47: 30S ribosomal protein S16



- Molecule 48: 30S ribosomal protein S17



- Molecule 48: 30S ribosomal protein S17



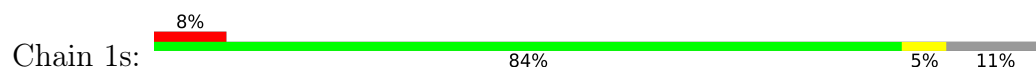
- Molecule 49: 30S ribosomal protein S18



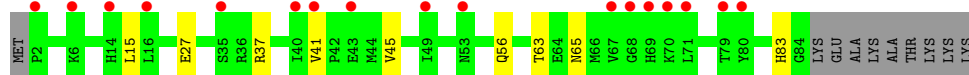
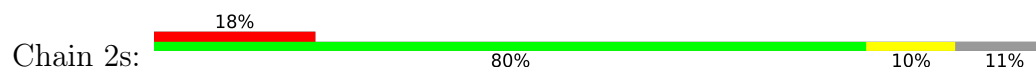
- Molecule 49: 30S ribosomal protein S18



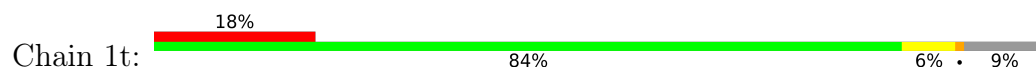
- Molecule 50: 30S ribosomal protein S19



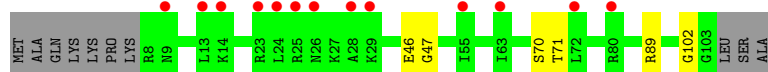
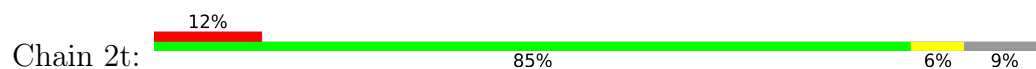
- Molecule 50: 30S ribosomal protein S19



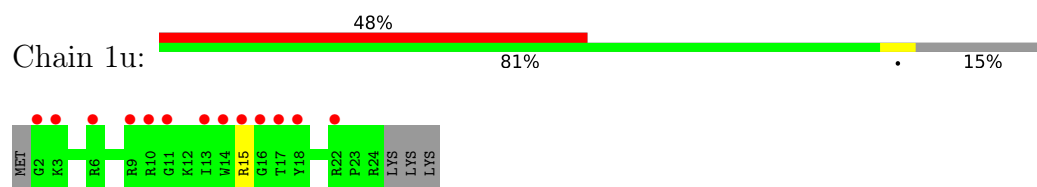
- Molecule 51: 30S ribosomal protein S20



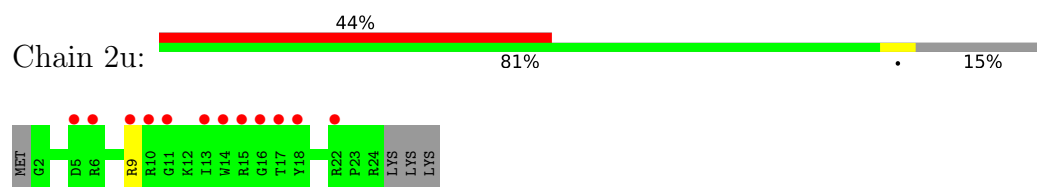
- Molecule 51: 30S ribosomal protein S20



- Molecule 52: 30S ribosomal protein Thx



- Molecule 52: 30S ribosomal protein Thx



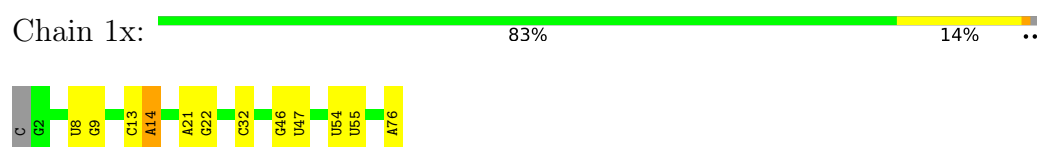
- Molecule 53: M-Stop-mRNA



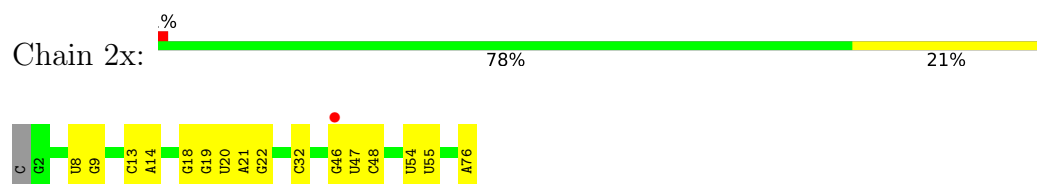
- Molecule 53: M-Stop-mRNA



- Molecule 54: P-site deacylated tRNAmet



- Molecule 54: P-site deacylated tRNAmet



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	209.51Å 449.73Å 622.15Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	155.54 – 2.70 181.64 – 2.70	Depositor EDS
% Data completeness (in resolution range)	96.8 (155.54-2.70) 96.8 (181.64-2.70)	Depositor EDS
R_{merge}	0.17	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.18 (at 2.69Å)	Xtriage
Refinement program	PHENIX 1.17.1	Depositor
R, R_{free}	0.209 , 0.257 0.209 , 0.257	Depositor DCC
R_{free} test set	77099 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å ²)	56.8	Xtriage
Anisotropy	0.175	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 57.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.44$, $\langle L^2 \rangle = 0.26$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	292790	wwPDB-VP
Average B, all atoms (Å ²)	57.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.73% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: 2MA, ZN, 2MG, M2G, OMU, K, 5MU, 4SU, MA6, MG, 0TD, OMG, G7M, T8B, 5MC, PSU, OMC, SF4, UR3, 4OC

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	0.53	0/69011	0.97	80/107720 (0.1%)
1	2A	0.41	0/67295	0.88	36/105042 (0.0%)
2	1B	0.44	1/2882 (0.0%)	0.85	0/4494
2	2B	0.43	1/2879 (0.0%)	0.86	1/4487 (0.0%)
3	1D	0.38	0/2186	0.56	0/2944
3	2D	0.33	0/2186	0.53	0/2944
4	1E	0.35	0/1592	0.54	0/2149
4	2E	0.31	0/1592	0.52	0/2149
5	1F	0.35	0/1619	0.54	0/2193
5	2F	0.30	0/1615	0.51	0/2188
6	1G	0.30	0/1448	0.49	0/1957
6	2G	0.30	0/1453	0.47	0/1963
7	1H	0.32	0/1356	0.51	0/1834
7	2H	0.29	0/1356	0.47	0/1834
8	1I	0.29	0/1112	0.50	0/1514
8	2I	0.28	0/1079	0.50	0/1475
9	1N	0.33	0/1144	0.51	0/1543
9	2N	0.33	0/1144	0.45	0/1543
10	1O	0.35	0/943	0.53	0/1269
10	2O	0.33	0/943	0.53	0/1269
11	1P	0.33	0/1152	0.55	0/1533
11	2P	0.32	0/1152	0.57	0/1533
12	1Q	0.36	0/1143	0.54	0/1527
12	2Q	0.31	0/1143	0.49	0/1527
13	1R	0.32	0/982	0.54	0/1312
13	2R	0.27	0/982	0.50	0/1312
14	1S	0.31	0/883	0.50	0/1176
14	2S	0.32	0/880	0.50	0/1172
15	1T	0.32	0/1105	0.53	1/1477 (0.1%)
15	2T	0.30	0/1097	0.49	0/1468
16	1U	0.38	0/977	0.50	0/1301

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
16	2U	0.29	0/977	0.45	0/1301
17	1V	0.34	0/782	0.55	0/1049
17	2V	0.29	0/782	0.49	0/1049
18	1W	0.33	0/897	0.53	0/1205
18	2W	0.31	0/897	0.48	0/1205
19	1X	0.36	0/764	0.55	0/1025
19	2X	0.31	0/764	0.52	0/1025
20	1Y	0.33	0/819	0.51	0/1095
20	2Y	0.31	0/819	0.52	0/1095
21	1Z	0.32	0/1267	0.52	0/1717
21	2Z	0.32	0/1299	0.50	0/1763
22	10	0.36	0/606	0.57	0/808
22	20	0.32	0/616	0.51	0/821
23	11	0.36	0/762	0.53	0/1014
23	21	0.32	0/762	0.50	0/1014
24	12	0.32	0/590	0.46	0/781
24	22	0.30	0/590	0.38	0/781
25	13	0.33	0/474	0.55	0/635
25	23	0.27	0/469	0.45	0/630
26	14	0.34	0/565	0.53	0/761
26	24	0.31	0/545	0.51	0/737
27	15	0.32	0/469	0.54	0/635
27	25	0.31	0/469	0.50	0/635
28	16	0.35	0/460	0.53	0/613
28	26	0.31	0/456	0.49	0/608
29	17	0.38	0/426	0.54	0/561
29	27	0.30	0/426	0.49	0/561
30	18	0.35	0/525	0.56	0/691
30	28	0.30	0/525	0.51	0/691
31	19	0.35	0/310	0.52	0/407
31	29	0.30	0/310	0.54	0/407
32	1a	0.38	0/35795	0.87	25/55864 (0.0%)
32	2a	0.37	2/35886 (0.0%)	0.88	38/56005 (0.1%)
33	1b	0.30	0/1881	0.49	0/2542
33	2b	0.33	0/1860	0.50	0/2518
34	1c	0.29	0/1572	0.46	0/2126
34	2c	0.31	0/1566	0.48	0/2119
35	1d	0.29	0/1685	0.49	0/2262
35	2d	0.29	0/1704	0.47	0/2284
36	1e	0.29	0/1145	0.50	0/1543
36	2e	0.30	0/1149	0.49	0/1548
37	1f	0.30	0/823	0.49	0/1115
37	2f	0.31	0/829	0.48	0/1123

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
38	1g	0.29	0/1250	0.43	0/1679
38	2g	0.29	0/1254	0.44	0/1683
39	1h	0.28	0/1108	0.47	0/1494
39	2h	0.28	0/1108	0.47	0/1494
40	1i	0.31	0/1002	0.51	0/1346
40	2i	0.31	0/997	0.49	0/1343
41	1j	0.30	0/722	0.49	0/982
41	2j	0.30	0/727	0.50	0/988
42	1k	0.29	0/844	0.49	0/1145
42	2k	0.29	0/848	0.47	0/1149
43	1l	0.30	0/937	0.49	0/1260
43	2l	0.29	0/937	0.49	0/1260
44	1m	0.28	0/969	0.48	0/1302
44	2m	0.30	0/961	0.47	0/1291
45	1n	0.31	0/501	0.50	0/664
45	2n	0.31	0/501	0.45	0/664
46	1o	0.28	0/739	0.45	0/985
46	2o	0.28	0/739	0.45	0/985
47	1p	0.29	0/697	0.51	0/939
47	2p	0.29	0/693	0.51	0/935
48	1q	0.30	0/836	0.48	0/1117
48	2q	0.28	0/836	0.46	0/1117
49	1r	0.29	0/560	0.49	0/746
49	2r	0.30	0/560	0.45	0/746
50	1s	0.29	0/667	0.52	0/900
50	2s	0.31	0/661	0.55	0/893
51	1t	0.28	0/730	0.46	0/965
51	2t	0.27	0/729	0.43	0/965
52	1u	0.29	0/203	0.48	0/266
52	2u	0.28	0/203	0.47	0/266
53	1v	0.55	0/122	0.98	0/188
53	2v	0.47	0/122	0.96	0/188
54	1x	0.55	3/1725 (0.2%)	1.12	18/2689 (0.7%)
54	2x	0.46	0/1725	1.05	11/2689 (0.4%)
All	All	0.41	7/309861 (0.0%)	0.82	210/463541 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
26	24	0	1

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	1B	1	U	OP3-P	-10.21	1.48	1.61
2	2B	1	U	OP3-P	-10.13	1.49	1.61
54	1x	22	G	N7-C5	6.85	1.43	1.39
32	2a	1272	G	N1-C2	-6.70	1.32	1.37
32	2a	1272	G	C6-N1	-5.91	1.35	1.39
54	1x	14	A	C8-N7	-5.26	1.27	1.31
54	1x	46	G	C6-N1	5.17	1.43	1.39

All (210) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	2a	1263	C	N1-C2-O2	19.39	130.53	118.90
32	2a	1272	G	N3-C2-N2	17.69	132.28	119.90
32	2a	1272	G	N1-C2-N2	-14.94	102.75	116.20
32	2a	1272	G	C5-C6-O6	14.02	137.01	128.60
1	1A	1075	C	N1-C2-O2	12.06	126.14	118.90
54	1x	46	G	C6-N1-C2	-11.36	118.29	125.10
1	1A	2554	U	O5'-P-OP1	-10.92	95.87	105.70
32	2a	1263	C	C2-N3-C4	10.62	125.21	119.90
32	2a	1272	G	C6-N1-C2	10.31	131.28	125.10
1	1A	1075	C	C2-N3-C4	10.07	124.93	119.90
32	2a	1272	G	C5-C6-N1	-10.06	106.47	111.50
32	2a	1263	C	N3-C2-O2	-9.96	114.92	121.90
1	1A	1063	G	C5-C6-O6	9.33	134.20	128.60
32	2a	1263	C	C5-C6-N1	9.18	125.59	121.00
32	2a	1272	G	C4-N9-C1'	9.02	138.23	126.50
54	1x	22	G	C5-N7-C8	-9.00	99.80	104.30
32	2a	1272	G	C8-N9-C1'	-8.77	115.60	127.00
54	2x	46	G	C6-N1-C2	-8.67	119.90	125.10
1	1A	2129	C	N1-C2-O2	8.55	124.03	118.90
54	1x	14	A	C4-C5-C6	8.46	121.23	117.00
1	2A	2136	C	N1-C2-O2	8.39	123.93	118.90
1	1A	2167	U	C2-N1-C1'	8.14	127.47	117.70
1	1A	1086	A	N1-C6-N6	-8.12	113.73	118.60
32	1a	841	U	C2-N1-C1'	8.03	127.34	117.70
54	2x	14	A	C4-C5-C6	7.97	120.98	117.00
2	2B	80	U	O4'-C1'-N1	7.96	114.57	108.20
1	1A	1063	G	N3-C2-N2	7.93	125.45	119.90
54	1x	22	G	C4-C5-C6	-7.86	114.08	118.80
1	1A	1063	G	C6-N1-C2	7.86	129.81	125.10
1	1A	512	G	O4'-C1'-N9	7.85	114.48	108.20
54	2x	14	A	C5-N7-C8	7.77	107.78	103.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	1x	14	A	C5-N7-C8	7.67	107.74	103.90
1	1A	2129	C	C2-N1-C1'	7.60	127.16	118.80
54	1x	22	G	N3-C4-N9	-7.59	121.45	126.00
1	1A	2167	U	N3-C2-O2	-7.41	117.01	122.20
1	1A	1614	A	O5'-P-OP1	-7.40	99.04	105.70
1	1A	1075	C	N3-C2-O2	-7.38	116.73	121.90
32	2a	1225	A	N1-C6-N6	-7.33	114.20	118.60
32	2a	1263	C	C2-N1-C1'	7.27	126.80	118.80
32	2a	1263	C	C4-C5-C6	-7.22	113.79	117.40
1	1A	801	G	O5'-P-OP2	-7.16	99.25	105.70
1	1A	2167	U	N1-C2-O2	7.10	127.77	122.80
1	1A	226	G	O4'-C1'-N9	7.05	113.84	108.20
32	2a	1054	C	C2-N1-C1'	6.93	126.42	118.80
32	1a	90	U	C2-N1-C1'	6.84	125.91	117.70
54	1x	22	G	N1-C6-O6	-6.74	115.86	119.90
1	1A	568	U	C5-C4-O4	-6.73	121.86	125.90
32	2a	1263	C	N1-C2-N3	-6.69	114.52	119.20
32	2a	1225	A	C5-C6-N6	6.69	129.05	123.70
1	1A	582	G	N1-C6-O6	-6.67	115.90	119.90
54	1x	46	G	C5-C6-N1	6.64	114.82	111.50
1	1A	845	G	O4'-C1'-N9	6.61	113.49	108.20
54	2x	22	G	C5-N7-C8	-6.59	101.00	104.30
32	1a	1029	C	C2-N3-C4	6.56	123.18	119.90
32	1a	1034	G	C6-N1-C2	6.53	129.02	125.10
54	1x	14	A	C5-C6-N1	-6.47	114.46	117.70
54	1x	46	G	C5-C6-O6	-6.42	124.75	128.60
32	1a	841	U	C5-C6-N1	6.41	125.90	122.70
1	1A	2682	U	O5'-P-OP2	-6.39	99.95	105.70
32	1a	90	U	N1-C2-O2	6.37	127.26	122.80
1	2A	1313	U	C2-N1-C1'	6.36	125.33	117.70
1	1A	1075	C	C5-C4-N4	6.32	124.62	120.20
54	1x	22	G	N7-C8-N9	6.24	116.22	113.10
1	2A	141	A	N7-C8-N9	6.24	116.92	113.80
32	1a	266	G	P-O3'-C3'	6.24	127.18	119.70
1	1A	847	U	C2-N1-C1'	6.22	125.16	117.70
32	2a	1272	G	C2-N3-C4	-6.21	108.79	111.90
1	1A	975	C	N1-C2-O2	-6.20	115.18	118.90
54	1x	46	G	N1-C2-N3	6.18	127.61	123.90
32	1a	1029	C	N1-C2-O2	6.17	122.60	118.90
1	1A	2593	U	N3-C4-O4	-6.15	115.09	119.40
1	1A	774	A	C8-N9-C4	-6.15	103.34	105.80
32	1a	841	U	N1-C2-O2	6.14	127.10	122.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	2a	266	G	P-O3'-C3'	6.13	127.06	119.70
54	1x	22	G	C8-N9-C1'	6.12	134.96	127.00
32	1a	90	U	N3-C2-O2	-6.11	117.92	122.20
1	1A	2167	U	C6-N1-C2	-6.11	117.34	121.00
32	2a	1272	G	N3-C4-N9	6.10	129.66	126.00
54	2x	46	G	N3-C2-N2	-6.09	115.63	119.90
1	1A	1776	G	O5'-P-OP2	-6.09	100.22	105.70
1	1A	582	G	C5-C6-O6	6.08	132.25	128.60
1	1A	2167	U	C5-C6-N1	6.06	125.73	122.70
32	1a	841	U	N3-C2-O2	-6.04	117.97	122.20
1	2A	1653	G	P-O3'-C3'	6.04	126.94	119.70
1	1A	1992	G	P-O3'-C3'	6.00	126.90	119.70
1	2A	1639	U	O5'-P-OP2	-5.94	100.35	105.70
32	1a	1030	C	N1-C2-O2	5.92	122.45	118.90
1	2A	1204	A	O4'-C1'-N9	5.91	112.93	108.20
32	1a	365	U	O4'-C1'-N1	5.91	112.92	108.20
1	1A	271(Y)	U	O4'-C1'-N1	5.87	112.90	108.20
1	1A	1063	G	N1-C6-O6	-5.85	116.39	119.90
32	2a	1135	U	O4'-C1'-N1	5.82	112.86	108.20
32	2a	1029	C	N1-C2-O2	5.77	122.36	118.90
1	1A	2129	C	C6-N1-C1'	-5.75	113.89	120.80
1	1A	2078	C	N3-C2-O2	-5.75	117.88	121.90
1	1A	1176	G	OP1-P-O3'	5.75	117.85	105.20
1	1A	2023	G	O5'-P-OP1	-5.75	100.53	105.70
1	1A	372	G	O4'-C1'-N9	5.74	112.79	108.20
1	1A	2050	C	N1-C2-O2	-5.74	115.46	118.90
1	1A	1075	C	C6-N1-C2	-5.74	118.00	120.30
1	1A	787	U	O5'-P-OP1	-5.73	100.54	105.70
1	1A	2062	A	P-O3'-C3'	5.73	126.58	119.70
1	2A	2140	C	C2-N1-C1'	5.70	125.07	118.80
32	1a	1034	G	C5-C6-O6	5.69	132.02	128.60
54	1x	22	G	N3-C4-C5	5.69	131.45	128.60
32	2a	1272	G	N1-C6-O6	-5.68	116.49	119.90
32	1a	1197	G	N3-C4-N9	5.67	129.41	126.00
1	2A	512	G	O4'-C1'-N9	5.66	112.73	108.20
1	2A	2129	C	N1-C2-O2	5.66	122.30	118.90
1	2A	1698	A	O4'-C1'-N9	5.65	112.72	108.20
32	2a	841	U	C5-C6-N1	5.64	125.52	122.70
54	1x	22	G	C6-C5-N7	5.62	133.77	130.40
32	1a	1442	G	C2-N3-C4	5.62	114.71	111.90
1	1A	2129	C	C2-N3-C4	5.61	122.71	119.90
1	1A	2714	G	O5'-P-OP2	-5.60	100.66	105.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1A	1372	U	N3-C4-O4	5.59	123.31	119.40
15	1T	18	ASP	C-N-CA	-5.58	107.76	121.70
1	1A	1936	A	O4'-C1'-N9	5.57	112.66	108.20
1	1A	2685	G	N1-C6-O6	-5.55	116.57	119.90
1	1A	1075	C	N3-C4-C5	-5.54	119.68	121.90
1	2A	790	C	O5'-P-OP2	-5.54	100.72	105.70
1	2A	1779	U	O4'-C1'-N1	5.53	112.62	108.20
1	2A	90	U	N3-C2-O2	-5.53	118.33	122.20
54	2x	22	G	C4-C5-C6	-5.53	115.48	118.80
54	2x	22	G	N1-C6-O6	-5.52	116.58	119.90
1	1A	2254	C	N1-C2-O2	-5.51	115.59	118.90
32	2a	754	C	C2-N1-C1'	5.51	124.86	118.80
32	1a	841	U	C6-N1-C2	-5.50	117.70	121.00
54	2x	14	A	C5-C6-N1	-5.50	114.95	117.70
1	2A	141	A	O4'-C1'-N9	5.49	112.59	108.20
1	2A	1992	G	P-O3'-C3'	5.46	126.26	119.70
32	2a	1065	U	P-O3'-C3'	5.46	126.25	119.70
1	1A	2848	G	O4'-C1'-N9	5.46	112.57	108.20
32	1a	115	G	P-O3'-C3'	5.46	126.25	119.70
1	1A	1174	A	P-O3'-C3'	5.45	126.24	119.70
1	2A	141	A	C8-N9-C4	-5.45	103.62	105.80
1	1A	12	U	N3-C2-O2	-5.45	118.39	122.20
1	1A	548	A	P-O3'-C3'	5.45	126.24	119.70
54	2x	22	G	C8-N9-C1'	5.43	134.06	127.00
32	1a	1030	C	N3-C2-O2	-5.41	118.11	121.90
1	1A	1314	C	C2-N1-C1'	5.41	124.75	118.80
32	1a	1442	G	N3-C4-C5	-5.40	125.90	128.60
1	1A	1075	C	C5-C6-N1	5.38	123.69	121.00
1	2A	2136	C	N3-C2-O2	-5.38	118.14	121.90
32	2a	1279	A	N7-C8-N9	5.36	116.48	113.80
1	2A	383	U	O4'-C1'-N1	5.36	112.49	108.20
32	1a	1025	U	N1-C2-O2	5.36	126.55	122.80
1	1A	1075	C	C2-N1-C1'	5.35	124.69	118.80
1	2A	2155	G	C6-N1-C2	5.35	128.31	125.10
1	2A	228	A	P-O3'-C3'	5.34	126.11	119.70
1	1A	784	A	O4'-C1'-N9	5.33	112.47	108.20
1	1A	1297	C	OP1-P-O3'	5.33	116.92	105.20
32	2a	65	U	P-O3'-C3'	5.33	126.09	119.70
1	2A	265	A	O4'-C1'-N9	5.32	112.45	108.20
1	2A	645	C	N1-C2-O2	5.31	122.09	118.90
1	2A	1698	A	C6-C5-N7	-5.31	128.58	132.30
1	1A	748	G	C4-N9-C1'	-5.30	119.61	126.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	2a	115	G	P-O3'-C3'	5.29	126.05	119.70
1	2A	614	U	N3-C2-O2	-5.27	118.51	122.20
1	1A	915	C	N1-C2-O2	5.26	122.06	118.90
1	1A	2689	U	P-O3'-C3'	5.26	126.02	119.70
32	2a	1272	G	C6-C5-N7	-5.25	127.25	130.40
54	2x	46	G	C5-C6-N1	5.25	114.12	111.50
1	1A	1187	G	N1-C6-O6	-5.25	116.75	119.90
1	2A	945	A	O4'-C1'-N9	5.25	112.40	108.20
32	2a	1067	A	P-O3'-C3'	5.24	125.98	119.70
1	1A	139(A)	G	N3-C4-N9	5.23	129.14	126.00
1	2A	847	U	C2-N1-C1'	5.23	123.98	117.70
32	1a	1067	A	P-O3'-C3'	5.23	125.97	119.70
32	1a	98	G	N3-C4-N9	5.22	129.13	126.00
1	1A	2181	G	C4-N9-C1'	5.21	133.28	126.50
1	1A	2078	C	N1-C2-O2	5.21	122.03	118.90
1	1A	2129	C	C5-C6-N1	5.21	123.60	121.00
1	1A	2790	A	C2-N3-C4	5.21	113.20	110.60
1	1A	784	A	P-O3'-C3'	5.20	125.94	119.70
1	2A	2689	U	P-O3'-C3'	5.19	125.92	119.70
1	1A	784	A	OP1-P-O3'	5.18	116.61	105.20
1	2A	784	A	O4'-C1'-N9	5.18	112.35	108.20
1	1A	195	A	P-O3'-C3'	5.17	125.90	119.70
1	2A	645	C	C2-N1-C1'	5.17	124.48	118.80
1	2A	141	A	C5-N7-C8	-5.16	101.32	103.90
1	1A	1265	A	O5'-P-OP2	-5.15	101.06	105.70
32	2a	687	A	P-O3'-C3'	5.13	125.85	119.70
32	2a	1054	C	C6-N1-C1'	-5.13	114.65	120.80
32	1a	365	U	C2-N1-C1'	5.12	123.85	117.70
1	1A	146	G	N1-C6-O6	-5.12	116.83	119.90
1	1A	2568	C	OP2-P-O3'	5.12	116.47	105.20
32	2a	1201	A	P-O3'-C3'	5.12	125.84	119.70
1	1A	1082	U	N3-C4-O4	-5.12	115.82	119.40
1	1A	774	A	N7-C8-N9	5.12	116.36	113.80
54	1x	14	A	C4-N9-C1'	5.12	135.51	126.30
32	2a	1263	C	C6-N1-C1'	-5.10	114.69	120.80
1	1A	1174	A	OP1-P-O3'	5.09	116.40	105.20
1	1A	383	U	C2-N1-C1'	-5.09	111.59	117.70
32	1a	98	G	C4-N9-C1'	5.09	133.11	126.50
32	2a	1263	C	N3-C4-N4	-5.08	114.44	118.00
1	2A	529	A	O5'-P-OP1	-5.08	101.13	105.70
1	2A	784	A	OP1-P-O3'	5.08	116.37	105.20
1	1A	1372	U	C5-C4-O4	-5.07	122.86	125.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	2A	2136	C	C2-N3-C4	5.07	122.43	119.90
32	2a	1279	A	OP1-P-O3'	5.06	116.33	105.20
1	1A	1131	G	O4'-C1'-N9	5.05	112.24	108.20
54	1x	22	G	C5-C6-N1	5.04	114.02	111.50
54	1x	14	A	C8-N9-C1'	-5.04	118.64	127.70
1	2A	205	G	O5'-P-OP2	-5.04	101.17	105.70
54	2x	46	G	C5-C6-O6	-5.03	125.58	128.60
1	2A	1828	G	O5'-P-OP1	-5.03	101.18	105.70
32	2a	1054	C	N1-C2-O2	5.02	121.91	118.90
1	2A	228	A	OP1-P-O3'	5.02	116.24	105.20
1	1A	748	G	C8-N9-C1'	5.01	133.51	127.00

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
26	24	61	ARG	Peptide

5.2 Too-close contacts [i](#)

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

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	1D	273/276 (99%)	257 (94%)	16 (6%)	0	100	100
3	2D	273/276 (99%)	257 (94%)	16 (6%)	0	100	100
4	1E	202/206 (98%)	189 (94%)	12 (6%)	1 (0%)	29	54
4	2E	202/206 (98%)	191 (95%)	10 (5%)	1 (0%)	29	54
5	1F	201/210 (96%)	198 (98%)	2 (1%)	1 (0%)	29	54

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
5	2F	201/210 (96%)	187 (93%)	13 (6%)	1 (0%)	29	54
6	1G	179/182 (98%)	167 (93%)	10 (6%)	2 (1%)	14	34
6	2G	179/182 (98%)	152 (85%)	22 (12%)	5 (3%)	5	11
7	1H	172/180 (96%)	161 (94%)	10 (6%)	1 (1%)	25	50
7	2H	172/180 (96%)	149 (87%)	22 (13%)	1 (1%)	25	50
8	1I	144/148 (97%)	130 (90%)	14 (10%)	0	100	100
8	2I	144/148 (97%)	118 (82%)	22 (15%)	4 (3%)	5	11
9	1N	138/140 (99%)	133 (96%)	5 (4%)	0	100	100
9	2N	138/140 (99%)	129 (94%)	8 (6%)	1 (1%)	22	46
10	1O	120/122 (98%)	115 (96%)	5 (4%)	0	100	100
10	2O	120/122 (98%)	110 (92%)	9 (8%)	1 (1%)	19	43
11	1P	147/150 (98%)	132 (90%)	15 (10%)	0	100	100
11	2P	147/150 (98%)	129 (88%)	15 (10%)	3 (2%)	7	19
12	1Q	139/141 (99%)	131 (94%)	6 (4%)	2 (1%)	11	28
12	2Q	139/141 (99%)	127 (91%)	10 (7%)	2 (1%)	11	28
13	1R	116/118 (98%)	110 (95%)	6 (5%)	0	100	100
13	2R	116/118 (98%)	112 (97%)	4 (3%)	0	100	100
14	1S	108/112 (96%)	104 (96%)	4 (4%)	0	100	100
14	2S	108/112 (96%)	100 (93%)	7 (6%)	1 (1%)	17	40
15	1T	129/146 (88%)	120 (93%)	9 (7%)	0	100	100
15	2T	129/146 (88%)	123 (95%)	6 (5%)	0	100	100
16	1U	114/118 (97%)	112 (98%)	2 (2%)	0	100	100
16	2U	114/118 (97%)	109 (96%)	5 (4%)	0	100	100
17	1V	99/101 (98%)	93 (94%)	2 (2%)	4 (4%)	3	6
17	2V	99/101 (98%)	91 (92%)	7 (7%)	1 (1%)	15	37
18	1W	110/113 (97%)	109 (99%)	1 (1%)	0	100	100
18	2W	110/113 (97%)	107 (97%)	3 (3%)	0	100	100
19	1X	93/96 (97%)	90 (97%)	1 (1%)	2 (2%)	6	17
19	2X	93/96 (97%)	87 (94%)	3 (3%)	3 (3%)	4	9
20	1Y	105/110 (96%)	93 (89%)	10 (10%)	2 (2%)	8	20
20	2Y	105/110 (96%)	97 (92%)	8 (8%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
21	1Z	148/206 (72%)	131 (88%)	15 (10%)	2 (1%)	11	28
21	2Z	156/206 (76%)	129 (83%)	26 (17%)	1 (1%)	25	50
22	10	73/85 (86%)	69 (94%)	4 (6%)	0	100	100
22	20	75/85 (88%)	67 (89%)	7 (9%)	1 (1%)	12	30
23	11	95/98 (97%)	92 (97%)	2 (2%)	1 (1%)	14	34
23	21	95/98 (97%)	94 (99%)	0	1 (1%)	14	34
24	12	68/72 (94%)	66 (97%)	2 (3%)	0	100	100
24	22	68/72 (94%)	64 (94%)	4 (6%)	0	100	100
25	13	57/60 (95%)	54 (95%)	3 (5%)	0	100	100
25	23	57/60 (95%)	51 (90%)	5 (9%)	1 (2%)	8	21
26	14	67/71 (94%)	49 (73%)	15 (22%)	3 (4%)	2	5
26	24	67/71 (94%)	54 (81%)	11 (16%)	2 (3%)	4	10
27	15	57/60 (95%)	55 (96%)	2 (4%)	0	100	100
27	25	57/60 (95%)	55 (96%)	2 (4%)	0	100	100
28	16	51/54 (94%)	50 (98%)	1 (2%)	0	100	100
28	26	51/54 (94%)	48 (94%)	3 (6%)	0	100	100
29	17	46/49 (94%)	44 (96%)	2 (4%)	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%)	62 (100%)	0	0	100	100
31	19	35/37 (95%)	35 (100%)	0	0	100	100
31	29	35/37 (95%)	34 (97%)	1 (3%)	0	100	100
33	1b	229/256 (90%)	195 (85%)	27 (12%)	7 (3%)	4	9
33	2b	229/256 (90%)	176 (77%)	42 (18%)	11 (5%)	2	4
34	1c	204/239 (85%)	184 (90%)	19 (9%)	1 (0%)	29	54
34	2c	204/239 (85%)	167 (82%)	32 (16%)	5 (2%)	5	14
35	1d	206/209 (99%)	184 (89%)	19 (9%)	3 (2%)	10	26
35	2d	206/209 (99%)	186 (90%)	19 (9%)	1 (0%)	29	54
36	1e	146/162 (90%)	130 (89%)	13 (9%)	3 (2%)	7	18
36	2e	146/162 (90%)	133 (91%)	11 (8%)	2 (1%)	11	28
37	1f	98/101 (97%)	87 (89%)	8 (8%)	3 (3%)	4	9

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
37	2f	98/101 (97%)	94 (96%)	4 (4%)	0	100	100
38	1g	153/156 (98%)	139 (91%)	10 (6%)	4 (3%)	5	13
38	2g	153/156 (98%)	137 (90%)	13 (8%)	3 (2%)	7	19
39	1h	135/138 (98%)	125 (93%)	9 (7%)	1 (1%)	22	46
39	2h	135/138 (98%)	124 (92%)	11 (8%)	0	100	100
40	1i	125/128 (98%)	106 (85%)	18 (14%)	1 (1%)	19	43
40	2i	125/128 (98%)	103 (82%)	21 (17%)	1 (1%)	19	43
41	1j	95/105 (90%)	83 (87%)	10 (10%)	2 (2%)	7	18
41	2j	94/105 (90%)	79 (84%)	12 (13%)	3 (3%)	4	9
42	1k	112/129 (87%)	102 (91%)	8 (7%)	2 (2%)	8	21
42	2k	112/129 (87%)	98 (88%)	13 (12%)	1 (1%)	17	40
43	1l	119/132 (90%)	113 (95%)	4 (3%)	2 (2%)	9	23
43	2l	119/132 (90%)	112 (94%)	7 (6%)	0	100	100
44	1m	121/126 (96%)	107 (88%)	12 (10%)	2 (2%)	9	23
44	2m	120/126 (95%)	94 (78%)	24 (20%)	2 (2%)	9	23
45	1n	58/61 (95%)	54 (93%)	4 (7%)	0	100	100
45	2n	58/61 (95%)	55 (95%)	1 (2%)	2 (3%)	3	8
46	1o	86/89 (97%)	78 (91%)	8 (9%)	0	100	100
46	2o	86/89 (97%)	80 (93%)	6 (7%)	0	100	100
47	1p	80/88 (91%)	70 (88%)	9 (11%)	1 (1%)	12	30
47	2p	80/88 (91%)	69 (86%)	11 (14%)	0	100	100
48	1q	97/105 (92%)	89 (92%)	7 (7%)	1 (1%)	15	37
48	2q	97/105 (92%)	88 (91%)	8 (8%)	1 (1%)	15	37
49	1r	66/88 (75%)	59 (89%)	6 (9%)	1 (2%)	10	26
49	2r	66/88 (75%)	64 (97%)	2 (3%)	0	100	100
50	1s	81/93 (87%)	68 (84%)	12 (15%)	1 (1%)	13	32
50	2s	81/93 (87%)	59 (73%)	21 (26%)	1 (1%)	13	32
51	1t	94/106 (89%)	87 (93%)	3 (3%)	4 (4%)	2	5
51	2t	94/106 (89%)	86 (92%)	6 (6%)	2 (2%)	7	18
52	1u	21/27 (78%)	18 (86%)	3 (14%)	0	100	100
52	2u	21/27 (78%)	19 (90%)	2 (10%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	11356/12128 (94%)	10330 (91%)	901 (8%)	125 (1%)	14	34

All (125) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
5	1F	130	ALA
7	1H	126	PRO
12	1Q	60	ARG
17	1V	100	ARG
21	1Z	53	ILE
21	1Z	93	ASP
23	11	3	LYS
26	14	45	GLY
26	14	49	PHE
26	14	62	ARG
33	1b	17	PHE
33	1b	125	PRO
38	1g	80	VAL
40	1i	54	ASP
41	1j	79	ARG
42	1k	105	VAL
43	1l	91	LYS
44	1m	67	GLU
44	1m	106	ASN
50	1s	81	ARG
6	2G	51	ARG
6	2G	84	LYS
7	2H	126	PRO
10	2O	5	GLN
11	2P	29	LYS
11	2P	36	LYS
33	2b	16	HIS
33	2b	17	PHE
42	2k	49	GLY
35	1d	173	TRP
36	1e	85	GLY
48	1q	68	ARG
5	2F	130	ALA
6	2G	42	GLY
8	2I	10	GLU
8	2I	40	THR
8	2I	41	GLU

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Mol	Chain	Res	Type
11	2P	44	GLY
17	2V	79	VAL
19	2X	94	GLY
26	24	45	GLY
33	2b	20	GLU
33	2b	123	ALA
38	2g	55	GLY
38	2g	80	VAL
40	2i	121	ARG
44	2m	8	GLU
48	2q	68	ARG
51	2t	47	GLY
6	1G	47	LYS
17	1V	79	VAL
19	1X	94	GLY
33	1b	8	LYS
37	1f	71	ARG
41	1j	30	SER
42	1k	49	GLY
47	1p	39	TYR
51	1t	47	GLY
12	2Q	16	ARG
26	24	49	PHE
33	2b	10	LEU
33	2b	21	ARG
34	2c	91	LEU
34	2c	156	ARG
34	2c	181	ASN
34	2c	188	LEU
38	2g	153	HIS
4	1E	52	LEU
17	1V	43	GLU
19	1X	2	LYS
20	1Y	54	LYS
33	1b	16	HIS
33	1b	20	GLU
38	1g	54	THR
49	1r	25	THR
51	1t	102	GLY
4	2E	52	LEU
6	2G	43	LEU
6	2G	72	ARG

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Mol	Chain	Res	Type
8	2I	117	GLU
19	2X	15	GLU
21	2Z	153	SER
33	2b	38	GLY
33	2b	74	LYS
33	2b	105	PHE
33	2b	125	PRO
34	2c	81	GLY
41	2j	79	ARG
45	2n	27	CYS
50	2s	65	ASN
6	1G	43	LEU
12	1Q	59	ARG
17	1V	53	GLU
33	1b	131	PRO
35	1d	88	VAL
37	1f	70	ASP
51	1t	100	ILE
9	2N	2	LYS
23	2I	3	LYS
25	23	38	GLU
33	2b	9	GLU
36	2e	69	VAL
41	2j	78	ASN
44	2m	42	ALA
45	2n	14	PRO
33	1b	231	GLU
34	1c	81	GLY
36	1e	86	ALA
38	1g	17	VAL
43	1l	105	TYR
51	1t	96	GLY
19	2X	48	LYS
41	2j	89	ASP
37	1f	40	VAL
22	20	13	GLY
36	2e	85	GLY
20	1Y	103	GLY
38	1g	82	GLY
35	2d	136	PRO
39	1h	73	ASP
12	2Q	15	GLY

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Mol	Chain	Res	Type
51	2t	102	GLY
35	1d	178	VAL
14	2S	96	GLY
36	1e	39	GLY

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	1D	215/218 (99%)	194 (90%)	21 (10%)	8	18
3	2D	215/218 (99%)	201 (94%)	14 (6%)	17	38
4	1E	164/166 (99%)	146 (89%)	18 (11%)	6	14
4	2E	164/166 (99%)	156 (95%)	8 (5%)	25	52
5	1F	160/166 (96%)	145 (91%)	15 (9%)	8	20
5	2F	159/166 (96%)	143 (90%)	16 (10%)	7	17
6	1G	143/156 (92%)	130 (91%)	13 (9%)	9	21
6	2G	143/156 (92%)	123 (86%)	20 (14%)	3	8
7	1H	144/148 (97%)	133 (92%)	11 (8%)	13	30
7	2H	144/148 (97%)	129 (90%)	15 (10%)	7	16
8	1I	113/124 (91%)	91 (80%)	22 (20%)	1	3
8	2I	105/124 (85%)	88 (84%)	17 (16%)	2	6
9	1N	118/119 (99%)	108 (92%)	10 (8%)	10	24
9	2N	118/119 (99%)	107 (91%)	11 (9%)	9	21
10	1O	100/100 (100%)	97 (97%)	3 (3%)	41	70
10	2O	100/100 (100%)	92 (92%)	8 (8%)	12	27
11	1P	115/116 (99%)	107 (93%)	8 (7%)	15	35
11	2P	115/116 (99%)	103 (90%)	12 (10%)	7	16
12	1Q	111/111 (100%)	101 (91%)	10 (9%)	9	22
12	2Q	111/111 (100%)	101 (91%)	10 (9%)	9	22

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
13	1R	101/101 (100%)	94 (93%)	7 (7%)	15	35
13	2R	101/101 (100%)	94 (93%)	7 (7%)	15	35
14	1S	86/88 (98%)	79 (92%)	7 (8%)	11	27
14	2S	85/88 (97%)	72 (85%)	13 (15%)	2	7
15	1T	115/127 (91%)	109 (95%)	6 (5%)	23	49
15	2T	113/127 (89%)	102 (90%)	11 (10%)	8	19
16	1U	93/94 (99%)	88 (95%)	5 (5%)	22	47
16	2U	93/94 (99%)	90 (97%)	3 (3%)	39	68
17	1V	80/82 (98%)	73 (91%)	7 (9%)	10	23
17	2V	80/82 (98%)	73 (91%)	7 (9%)	10	23
18	1W	90/92 (98%)	85 (94%)	5 (6%)	21	45
18	2W	90/92 (98%)	83 (92%)	7 (8%)	12	29
19	1X	77/78 (99%)	76 (99%)	1 (1%)	69	87
19	2X	77/78 (99%)	74 (96%)	3 (4%)	32	61
20	1Y	85/91 (93%)	74 (87%)	11 (13%)	4	10
20	2Y	85/91 (93%)	73 (86%)	12 (14%)	3	8
21	1Z	135/179 (75%)	124 (92%)	11 (8%)	11	27
21	2Z	137/179 (76%)	127 (93%)	10 (7%)	14	33
22	10	60/67 (90%)	57 (95%)	3 (5%)	24	51
22	20	61/67 (91%)	58 (95%)	3 (5%)	25	52
23	11	80/83 (96%)	79 (99%)	1 (1%)	69	87
23	21	80/83 (96%)	74 (92%)	6 (8%)	13	31
24	12	65/67 (97%)	62 (95%)	3 (5%)	27	54
24	22	65/67 (97%)	61 (94%)	4 (6%)	18	40
25	13	51/52 (98%)	45 (88%)	6 (12%)	5	12
25	23	50/52 (96%)	44 (88%)	6 (12%)	5	11
26	14	59/63 (94%)	52 (88%)	7 (12%)	5	12
26	24	53/63 (84%)	42 (79%)	11 (21%)	1	3
27	15	50/52 (96%)	46 (92%)	4 (8%)	12	27
27	25	50/52 (96%)	46 (92%)	4 (8%)	12	27
28	16	51/52 (98%)	46 (90%)	5 (10%)	8	18

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
28	26	50/52 (96%)	47 (94%)	3 (6%)	19	42
29	17	41/42 (98%)	36 (88%)	5 (12%)	5	11
29	27	41/42 (98%)	37 (90%)	4 (10%)	8	18
30	18	54/55 (98%)	50 (93%)	4 (7%)	13	32
30	28	54/55 (98%)	52 (96%)	2 (4%)	34	63
31	19	34/34 (100%)	33 (97%)	1 (3%)	42	71
31	29	34/34 (100%)	33 (97%)	1 (3%)	42	71
33	1b	192/220 (87%)	164 (85%)	28 (15%)	3	7
33	2b	187/220 (85%)	164 (88%)	23 (12%)	4	11
34	1c	142/188 (76%)	128 (90%)	14 (10%)	8	18
34	2c	140/188 (74%)	124 (89%)	16 (11%)	5	13
35	1d	169/181 (93%)	149 (88%)	20 (12%)	5	12
35	2d	173/181 (96%)	148 (86%)	25 (14%)	3	8
36	1e	113/123 (92%)	100 (88%)	13 (12%)	5	13
36	2e	114/123 (93%)	97 (85%)	17 (15%)	3	7
37	1f	84/90 (93%)	75 (89%)	9 (11%)	6	15
37	2f	85/90 (94%)	78 (92%)	7 (8%)	11	26
38	1g	119/127 (94%)	107 (90%)	12 (10%)	7	17
38	2g	120/127 (94%)	103 (86%)	17 (14%)	3	8
39	1h	114/119 (96%)	106 (93%)	8 (7%)	15	35
39	2h	114/119 (96%)	107 (94%)	7 (6%)	18	41
40	1i	90/99 (91%)	79 (88%)	11 (12%)	5	11
40	2i	89/99 (90%)	80 (90%)	9 (10%)	7	17
41	1j	66/92 (72%)	55 (83%)	11 (17%)	2	5
41	2j	69/92 (75%)	60 (87%)	9 (13%)	4	10
42	1k	82/99 (83%)	74 (90%)	8 (10%)	8	18
42	2k	83/99 (84%)	75 (90%)	8 (10%)	8	19
43	1l	96/108 (89%)	92 (96%)	4 (4%)	30	58
43	2l	96/108 (89%)	86 (90%)	10 (10%)	7	16
44	1m	93/101 (92%)	81 (87%)	12 (13%)	4	10
44	2m	92/101 (91%)	78 (85%)	14 (15%)	3	7

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
45	1n	49/50 (98%)	44 (90%)	5 (10%)	7	17
45	2n	49/50 (98%)	44 (90%)	5 (10%)	7	17
46	1o	78/80 (98%)	76 (97%)	2 (3%)	46	75
46	2o	78/80 (98%)	74 (95%)	4 (5%)	24	50
47	1p	69/74 (93%)	62 (90%)	7 (10%)	7	17
47	2p	68/74 (92%)	58 (85%)	10 (15%)	3	7
48	1q	94/97 (97%)	88 (94%)	6 (6%)	17	39
48	2q	94/97 (97%)	90 (96%)	4 (4%)	29	57
49	1r	59/77 (77%)	53 (90%)	6 (10%)	7	17
49	2r	59/77 (77%)	51 (86%)	8 (14%)	3	8
50	1s	69/80 (86%)	65 (94%)	4 (6%)	20	43
50	2s	67/80 (84%)	59 (88%)	8 (12%)	5	12
51	1t	70/82 (85%)	66 (94%)	4 (6%)	20	44
51	2t	70/82 (85%)	66 (94%)	4 (6%)	20	44
52	1u	18/22 (82%)	17 (94%)	1 (6%)	21	45
52	2u	18/22 (82%)	17 (94%)	1 (6%)	21	45
All	All	9294/10064 (92%)	8425 (91%)	869 (9%)	8	20

All (869) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	1D	3	VAL
3	1D	14	ARG
3	1D	16	MET
3	1D	18	VAL
3	1D	32	SER
3	1D	34	VAL
3	1D	38	LYS
3	1D	61	LEU
3	1D	71	ASP
3	1D	99	ASP
3	1D	112	GLN
3	1D	142	VAL
3	1D	155	LEU
3	1D	200	ASP
3	1D	211	ARG

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Mol	Chain	Res	Type
3	1D	221	VAL
3	1D	229	VAL
3	1D	242	ARG
3	1D	253	GLN
3	1D	259	THR
3	1D	273	ARG
4	1E	7	VAL
4	1E	9	VAL
4	1E	12	THR
4	1E	21	VAL
4	1E	33	VAL
4	1E	34	VAL
4	1E	45	THR
4	1E	47	VAL
4	1E	49	LEU
4	1E	59	VAL
4	1E	73	GLU
4	1E	78	LEU
4	1E	97	LYS
4	1E	116	VAL
4	1E	127	ASP
4	1E	173	VAL
4	1E	181	LEU
4	1E	184	VAL
5	1F	24	LEU
5	1F	32	LEU
5	1F	33	LEU
5	1F	53	THR
5	1F	70	THR
5	1F	72	ARG
5	1F	74	ARG
5	1F	88	VAL
5	1F	106	ARG
5	1F	132	VAL
5	1F	140	LEU
5	1F	162	LEU
5	1F	168	ARG
5	1F	192	LEU
5	1F	203	GLN
6	1G	3	LEU
6	1G	5	VAL
6	1G	22	ARG

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Mol	Chain	Res	Type
6	1G	28	VAL
6	1G	31	VAL
6	1G	43	LEU
6	1G	82	LEU
6	1G	91	ARG
6	1G	139	LEU
6	1G	148	MET
6	1G	149	VAL
6	1G	159	VAL
6	1G	161	THR
7	1H	13	LYS
7	1H	23	ARG
7	1H	27	LYS
7	1H	56	SER
7	1H	84	SER
7	1H	98	LEU
7	1H	116	GLU
7	1H	119	GLU
7	1H	122	THR
7	1H	124	GLU
7	1H	136	ILE
8	1I	2	LYS
8	1I	5	LEU
8	1I	9	LEU
8	1I	10	GLU
8	1I	12	LEU
8	1I	38	LEU
8	1I	41	GLU
8	1I	47	LEU
8	1I	68	LEU
8	1I	77	LEU
8	1I	78	THR
8	1I	85	GLU
8	1I	87	LYS
8	1I	92	VAL
8	1I	101	LEU
8	1I	102	SER
8	1I	105	HIS
8	1I	108	THR
8	1I	109	ILE
8	1I	123	LEU
8	1I	140	LEU

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Mol	Chain	Res	Type
8	1I	144	VAL
9	1N	1	MET
9	1N	28	THR
9	1N	32	THR
9	1N	34	LEU
9	1N	38	HIS
9	1N	48	MET
9	1N	61	ARG
9	1N	62	VAL
9	1N	67	LEU
9	1N	137	LYS
10	1O	21	CYS
10	1O	69	ILE
10	1O	98	VAL
11	1P	7	ARG
11	1P	45	LEU
11	1P	56	SER
11	1P	95	VAL
11	1P	98	GLU
11	1P	101	VAL
11	1P	125	VAL
11	1P	148	LEU
12	1Q	7	MET
12	1Q	8	LYS
12	1Q	12	GLN
12	1Q	16	ARG
12	1Q	56	ARG
12	1Q	60	ARG
12	1Q	63	LYS
12	1Q	75	THR
12	1Q	109	VAL
12	1Q	110	THR
13	1R	6	SER
13	1R	36	THR
13	1R	44	LEU
13	1R	67	LEU
13	1R	100	LEU
13	1R	111	LEU
13	1R	114	VAL
14	1S	14	VAL
14	1S	15	ARG
14	1S	36	TYR

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Mol	Chain	Res	Type
14	1S	46	VAL
14	1S	49	VAL
14	1S	50	SER
14	1S	110	LEU
15	1T	28	VAL
15	1T	36	GLU
15	1T	49	VAL
15	1T	96	ARG
15	1T	108	ARG
15	1T	128	GLU
16	1U	8	VAL
16	1U	31	SER
16	1U	74	LEU
16	1U	77	SER
16	1U	95	LEU
17	1V	1	MET
17	1V	45	THR
17	1V	61	VAL
17	1V	79	VAL
17	1V	82	ARG
17	1V	85	LYS
17	1V	100	ARG
18	1W	4	LYS
18	1W	11	ARG
18	1W	15	ARG
18	1W	17	VAL
18	1W	65	LEU
19	1X	35	THR
20	1Y	6	HIS
20	1Y	7	VAL
20	1Y	9	LYS
20	1Y	11	ASP
20	1Y	23	ARG
20	1Y	28	LYS
20	1Y	43	ASN
20	1Y	47	LYS
20	1Y	61	ILE
20	1Y	67	LEU
20	1Y	99	CYS
21	1Z	33	LEU
21	1Z	61	LEU
21	1Z	65	GLN

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Mol	Chain	Res	Type
21	1Z	72	ARG
21	1Z	77	ASP
21	1Z	84	GLU
21	1Z	102	LEU
21	1Z	135	GLU
21	1Z	149	SER
21	1Z	154	ASP
21	1Z	155	LEU
22	10	10	THR
22	10	14	ARG
22	10	55	ARG
23	11	83	GLU
24	12	3	LEU
24	12	53	LEU
24	12	65	ASN
25	13	23	LEU
25	13	34	GLU
25	13	54	VAL
25	13	55	ARG
25	13	58	VAL
25	13	60	GLU
26	14	1	MET
26	14	3	GLU
26	14	49	PHE
26	14	53	GLU
26	14	56	VAL
26	14	59	PHE
26	14	63	TYR
27	15	6	VAL
27	15	40	LYS
27	15	57	VAL
27	15	60	VAL
28	16	4	GLU
28	16	6	ARG
28	16	19	ARG
28	16	44	ARG
28	16	48	VAL
29	17	1	MET
29	17	4	THR
29	17	24	THR
29	17	41	ARG
29	17	43	THR

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Mol	Chain	Res	Type
30	18	14	VAL
30	18	15	LYS
30	18	31	HIS
30	18	63	PRO
31	19	4	ARG
33	1b	12	GLU
33	1b	17	PHE
33	1b	19	HIS
33	1b	21	ARG
33	1b	24	TRP
33	1b	35	GLU
33	1b	44	LEU
33	1b	64	ARG
33	1b	78	GLN
33	1b	80	ILE
33	1b	94	ASN
33	1b	113	HIS
33	1b	121	LEU
33	1b	124	SER
33	1b	127	ILE
33	1b	140	HIS
33	1b	160	ASP
33	1b	163	PHE
33	1b	165	VAL
33	1b	179	LYS
33	1b	189	ASP
33	1b	196	LEU
33	1b	208	ILE
33	1b	217	ARG
33	1b	221	LEU
33	1b	226	ARG
33	1b	229	VAL
33	1b	233	SER
34	1c	3	ASN
34	1c	15	THR
34	1c	20	SER
34	1c	28	GLN
34	1c	46	GLU
34	1c	56	ASP
34	1c	70	VAL
34	1c	82	GLU
34	1c	85	ARG

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Mol	Chain	Res	Type
34	1c	89	GLU
34	1c	104	GLN
34	1c	119	ARG
34	1c	178	LEU
34	1c	195	VAL
35	1d	11	LEU
35	1d	19	LEU
35	1d	31	CYS
35	1d	59	ARG
35	1d	76	ARG
35	1d	83	SER
35	1d	88	VAL
35	1d	112	VAL
35	1d	127	THR
35	1d	135	LEU
35	1d	140	VAL
35	1d	141	ARG
35	1d	152	SER
35	1d	155	LEU
35	1d	157	LEU
35	1d	158	ILE
35	1d	188	LEU
35	1d	194	LEU
35	1d	200	GLU
35	1d	208	SER
36	1e	12	LEU
36	1e	16	THR
36	1e	24	ARG
36	1e	34	VAL
36	1e	41	VAL
36	1e	47	LYS
36	1e	53	LEU
36	1e	56	GLN
36	1e	64	ARG
36	1e	78	HIS
36	1e	79	GLU
36	1e	91	LEU
36	1e	98	THR
37	1f	36	ARG
37	1f	43	LEU
37	1f	45	LEU
37	1f	66	GLU

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Mol	Chain	Res	Type
37	1f	72	VAL
37	1f	73	ASN
37	1f	75	LEU
37	1f	78	GLU
37	1f	98	LEU
38	1g	12	LEU
38	1g	50	ILE
38	1g	61	VAL
38	1g	78	ARG
38	1g	94	ARG
38	1g	104	LEU
38	1g	110	GLN
38	1g	113	GLU
38	1g	114	ARG
38	1g	115	ARG
38	1g	140	ASP
38	1g	143	ARG
39	1h	29	SER
39	1h	49	GLU
39	1h	51	VAL
39	1h	112	LEU
39	1h	115	SER
39	1h	121	ASP
39	1h	122	ARG
39	1h	133	LEU
40	1i	25	LYS
40	1i	53	VAL
40	1i	54	ASP
40	1i	64	THR
40	1i	75	ASP
40	1i	81	ILE
40	1i	92	TYR
40	1i	103	THR
40	1i	108	VAL
40	1i	121	ARG
40	1i	128	ARG
41	1j	5	ARG
41	1j	13	HIS
41	1j	34	VAL
41	1j	38	ILE
41	1j	43	ARG
41	1j	46	ARG

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Mol	Chain	Res	Type
41	1j	49	VAL
41	1j	55	LYS
41	1j	81	THR
41	1j	92	THR
41	1j	98	ILE
42	1k	25	TYR
42	1k	31	THR
42	1k	48	ILE
42	1k	87	THR
42	1k	109	VAL
42	1k	114	VAL
42	1k	117	ASN
42	1k	120	ARG
43	1l	33	ARG
43	1l	83	VAL
43	1l	86	ARG
43	1l	124	LYS
44	1m	3	ARG
44	1m	4	ILE
44	1m	14	ARG
44	1m	15	VAL
44	1m	19	LEU
44	1m	43	THR
44	1m	49	THR
44	1m	64	TRP
44	1m	70	LEU
44	1m	98	VAL
44	1m	106	ASN
44	1m	109	THR
45	1n	3	ARG
45	1n	13	THR
45	1n	18	VAL
45	1n	33	VAL
45	1n	56	VAL
46	1o	39	LEU
46	1o	84	LYS
47	1p	11	SER
47	1p	20	VAL
47	1p	45	THR
47	1p	62	VAL
47	1p	67	THR
47	1p	75	ARG

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Mol	Chain	Res	Type
47	1p	76	GLN
48	1q	11	VAL
48	1q	19	VAL
48	1q	45	HIS
48	1q	52	LYS
48	1q	53	LEU
48	1q	63	ARG
49	1r	35	ARG
49	1r	37	VAL
49	1r	42	ARG
49	1r	46	GLU
49	1r	58	LEU
49	1r	84	LYS
50	1s	28	LYS
50	1s	37	ARG
50	1s	48	THR
50	1s	63	THR
51	1t	10	LEU
51	1t	24	LEU
51	1t	84	LEU
51	1t	100	ILE
52	1u	15	ARG
3	2D	3	VAL
3	2D	32	SER
3	2D	37	LEU
3	2D	38	LYS
3	2D	71	ASP
3	2D	116	GLN
3	2D	141	VAL
3	2D	142	VAL
3	2D	221	VAL
3	2D	229	VAL
3	2D	242	ARG
3	2D	259	THR
3	2D	260	ARG
3	2D	275	LYS
4	2E	21	VAL
4	2E	34	VAL
4	2E	38	THR
4	2E	73	GLU
4	2E	78	LEU
4	2E	113	PHE

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Mol	Chain	Res	Type
4	2E	116	VAL
4	2E	184	VAL
5	2F	20	LEU
5	2F	33	LEU
5	2F	43	LYS
5	2F	70	THR
5	2F	74	ARG
5	2F	106	ARG
5	2F	133	ASN
5	2F	135	LYS
5	2F	145	GLU
5	2F	153	SER
5	2F	158	THR
5	2F	162	LEU
5	2F	165	ARG
5	2F	183	VAL
5	2F	192	LEU
5	2F	201	VAL
6	2G	3	LEU
6	2G	7	LEU
6	2G	18	GLU
6	2G	19	LEU
6	2G	26	GLN
6	2G	28	VAL
6	2G	31	VAL
6	2G	43	LEU
6	2G	45	GLU
6	2G	51	ARG
6	2G	59	GLU
6	2G	91	ARG
6	2G	124	SER
6	2G	130	ASN
6	2G	133	LEU
6	2G	135	LEU
6	2G	139	LEU
6	2G	152	LEU
6	2G	159	VAL
6	2G	165	THR
7	2H	2	SER
7	2H	3	ARG
7	2H	23	ARG
7	2H	43	VAL

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Mol	Chain	Res	Type
7	2H	45	VAL
7	2H	70	THR
7	2H	71	LEU
7	2H	77	LYS
7	2H	90	LYS
7	2H	95	ARG
7	2H	101	ARG
7	2H	103	LEU
7	2H	114	VAL
7	2H	124	GLU
7	2H	163	TYR
8	2I	15	VAL
8	2I	38	LEU
8	2I	40	THR
8	2I	58	LEU
8	2I	61	ARG
8	2I	68	LEU
8	2I	69	LYS
8	2I	77	LEU
8	2I	82	ARG
8	2I	86	THR
8	2I	87	LYS
8	2I	92	VAL
8	2I	96	ASP
8	2I	117	GLU
8	2I	121	LYS
8	2I	123	LEU
8	2I	127	VAL
9	2N	1	MET
9	2N	5	VAL
9	2N	14	VAL
9	2N	28	THR
9	2N	34	LEU
9	2N	38	HIS
9	2N	61	ARG
9	2N	68	GLU
9	2N	83	LYS
9	2N	99	LEU
9	2N	131	GLN
10	2O	1	MET
10	2O	21	CYS
10	2O	28	SER

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Mol	Chain	Res	Type
10	2O	52	VAL
10	2O	53	LYS
10	2O	69	ILE
10	2O	78	ARG
10	2O	98	VAL
11	2P	56	SER
11	2P	58	THR
11	2P	65	ARG
11	2P	77	ARG
11	2P	90	ARG
11	2P	95	VAL
11	2P	96	THR
11	2P	98	GLU
11	2P	99	LEU
11	2P	100	LEU
11	2P	106	LEU
11	2P	125	VAL
12	2Q	6	ARG
12	2Q	25	ASP
12	2Q	56	ARG
12	2Q	64	ILE
12	2Q	75	THR
12	2Q	98	LYS
12	2Q	109	VAL
12	2Q	110	THR
12	2Q	112	GLU
12	2Q	133	ARG
13	2R	24	GLN
13	2R	36	THR
13	2R	44	LEU
13	2R	67	LEU
13	2R	100	LEU
13	2R	111	LEU
13	2R	114	VAL
14	2S	13	ARG
14	2S	15	ARG
14	2S	19	LYS
14	2S	21	THR
14	2S	27	SER
14	2S	50	SER
14	2S	58	LEU
14	2S	64	GLU

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Mol	Chain	Res	Type
14	2S	71	ARG
14	2S	80	LEU
14	2S	83	LYS
14	2S	98	VAL
14	2S	103	GLU
15	2T	17	THR
15	2T	18	ASP
15	2T	28	VAL
15	2T	39	ARG
15	2T	63	VAL
15	2T	74	ARG
15	2T	96	ARG
15	2T	104	ASN
15	2T	107	ASP
15	2T	115	ARG
15	2T	129	ARG
16	2U	31	SER
16	2U	74	LEU
16	2U	77	SER
17	2V	7	THR
17	2V	13	ARG
17	2V	25	LEU
17	2V	38	LEU
17	2V	61	VAL
17	2V	79	VAL
17	2V	82	ARG
18	2W	4	LYS
18	2W	11	ARG
18	2W	17	VAL
18	2W	28	SER
18	2W	67	ASP
18	2W	92	ARG
18	2W	96	ILE
19	2X	57	LEU
19	2X	81	VAL
19	2X	82	GLN
20	2Y	1	MET
20	2Y	6	HIS
20	2Y	7	VAL
20	2Y	9	LYS
20	2Y	49	VAL
20	2Y	72	VAL

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Mol	Chain	Res	Type
20	2Y	83	THR
20	2Y	85	VAL
20	2Y	88	LYS
20	2Y	91	GLU
20	2Y	99	CYS
20	2Y	107	ASP
21	2Z	40	ASP
21	2Z	42	VAL
21	2Z	71	VAL
21	2Z	91	LEU
21	2Z	121	HIS
21	2Z	123	ASP
21	2Z	154	ASP
21	2Z	155	LEU
21	2Z	161	VAL
21	2Z	174	VAL
22	20	10	THR
22	20	55	ARG
22	20	64	ASP
23	21	21	ARG
23	21	26	ARG
23	21	30	VAL
23	21	59	THR
23	21	65	SER
23	21	98	LEU
24	22	30	ARG
24	22	35	LEU
24	22	59	ARG
24	22	62	THR
25	23	3	ARG
25	23	5	LYS
25	23	23	LEU
25	23	31	LEU
25	23	54	VAL
25	23	59	VAL
26	24	3	GLU
26	24	13	ARG
26	24	24	THR
26	24	35	VAL
26	24	49	PHE
26	24	50	VAL
26	24	58	ARG

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Mol	Chain	Res	Type
26	24	59	PHE
26	24	62	ARG
26	24	63	TYR
26	24	67	TYR
27	25	6	VAL
27	25	15	ARG
27	25	58	LEU
27	25	59	GLU
28	26	9	LEU
28	26	19	ARG
28	26	34	LEU
29	27	1	MET
29	27	4	THR
29	27	41	ARG
29	27	43	THR
30	28	14	VAL
30	28	31	HIS
31	29	7	VAL
33	2b	8	LYS
33	2b	9	GLU
33	2b	23	ARG
33	2b	24	TRP
33	2b	33	TYR
33	2b	49	GLU
33	2b	63	MET
33	2b	67	THR
33	2b	73	THR
33	2b	76	GLN
33	2b	93	VAL
33	2b	107	THR
33	2b	115	LEU
33	2b	124	SER
33	2b	140	HIS
33	2b	149	LEU
33	2b	150	SER
33	2b	164	VAL
33	2b	185	ILE
33	2b	204	ASN
33	2b	214	ILE
33	2b	224	GLN
33	2b	230	VAL
34	2c	38	ARG

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Mol	Chain	Res	Type
34	2c	44	GLU
34	2c	46	GLU
34	2c	57	ILE
34	2c	91	LEU
34	2c	101	LEU
34	2c	105	GLU
34	2c	112	SER
34	2c	115	LEU
34	2c	125	GLU
34	2c	128	PHE
34	2c	132	ARG
34	2c	152	ILE
34	2c	190	ARG
34	2c	192	THR
34	2c	198	VAL
35	2d	8	VAL
35	2d	19	LEU
35	2d	31	CYS
35	2d	47	ARG
35	2d	52	SER
35	2d	53	ASP
35	2d	57	ARG
35	2d	58	LEU
35	2d	59	ARG
35	2d	77	ASN
35	2d	78	LEU
35	2d	86	LYS
35	2d	94	LEU
35	2d	96	LEU
35	2d	115	ARG
35	2d	118	ARG
35	2d	120	LEU
35	2d	127	THR
35	2d	135	LEU
35	2d	150	GLU
35	2d	157	LEU
35	2d	165	MET
35	2d	175	SER
35	2d	188	LEU
35	2d	194	LEU
36	2e	5	ASP
36	2e	13	ILE

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Mol	Chain	Res	Type
36	2e	18	ARG
36	2e	20	GLN
36	2e	25	ARG
36	2e	34	VAL
36	2e	38	GLN
36	2e	41	VAL
36	2e	60	TYR
36	2e	66	MET
36	2e	72	GLN
36	2e	75	THR
36	2e	78	HIS
36	2e	91	LEU
36	2e	106	PRO
36	2e	135	THR
36	2e	151	LEU
37	2f	21	LEU
37	2f	31	GLU
37	2f	63	TYR
37	2f	64	GLN
37	2f	69	GLU
37	2f	92	LYS
37	2f	95	GLU
38	2g	6	ARG
38	2g	15	ASP
38	2g	24	THR
38	2g	45	ASP
38	2g	51	GLN
38	2g	75	VAL
38	2g	78	ARG
38	2g	79	ARG
38	2g	85	TYR
38	2g	113	GLU
38	2g	114	ARG
38	2g	115	ARG
38	2g	135	VAL
38	2g	139	GLU
38	2g	146	GLU
38	2g	153	HIS
38	2g	155	ARG
39	2h	25	ASP
39	2h	26	VAL
39	2h	37	ARG

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Mol	Chain	Res	Type
39	2h	39	LEU
39	2h	51	VAL
39	2h	112	LEU
39	2h	115	SER
40	2i	29	ASN
40	2i	54	ASP
40	2i	75	ASP
40	2i	89	ASN
40	2i	92	TYR
40	2i	99	LEU
40	2i	102	LEU
40	2i	113	LYS
40	2i	128	ARG
41	2j	8	LEU
41	2j	21	GLN
41	2j	38	ILE
41	2j	67	THR
41	2j	74	ILE
41	2j	89	ASP
41	2j	95	GLU
41	2j	97	GLU
41	2j	100	THR
42	2k	14	VAL
42	2k	29	ILE
42	2k	48	ILE
42	2k	63	LEU
42	2k	87	THR
42	2k	112	THR
42	2k	114	VAL
42	2k	116	HIS
43	2l	33	ARG
43	2l	55	VAL
43	2l	57	LYS
43	2l	67	THR
43	2l	79	GLU
43	2l	83	VAL
43	2l	89	ARG
43	2l	97	ARG
43	2l	102	ARG
43	2l	123	LYS
44	2m	15	VAL
44	2m	19	LEU

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Mol	Chain	Res	Type
44	2m	22	ILE
44	2m	37	THR
44	2m	39	ILE
44	2m	47	ASP
44	2m	53	VAL
44	2m	80	ARG
44	2m	92	HIS
44	2m	102	ARG
44	2m	103	THR
44	2m	106	ASN
44	2m	109	THR
44	2m	116	THR
45	2n	3	ARG
45	2n	6	LEU
45	2n	18	VAL
45	2n	33	VAL
45	2n	42	ILE
46	2o	3	ILE
46	2o	5	LYS
46	2o	26	GLU
46	2o	39	LEU
47	2p	1	MET
47	2p	2	VAL
47	2p	5	ARG
47	2p	20	VAL
47	2p	21	VAL
47	2p	60	LEU
47	2p	67	THR
47	2p	69	THR
47	2p	73	LEU
47	2p	74	LEU
48	2q	60	ILE
48	2q	63	ARG
48	2q	70	ARG
48	2q	99	SER
49	2r	25	THR
49	2r	31	LEU
49	2r	37	VAL
49	2r	44	LEU
49	2r	45	SER
49	2r	46	GLU
49	2r	76	LEU

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Mol	Chain	Res	Type
49	2r	82	THR
50	2s	15	LEU
50	2s	27	GLU
50	2s	37	ARG
50	2s	41	VAL
50	2s	45	VAL
50	2s	56	GLN
50	2s	63	THR
50	2s	83	HIS
51	2t	46	GLU
51	2t	70	SER
51	2t	71	THR
51	2t	89	ARG
52	2u	9	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (117) such sidechains are listed below:

Mol	Chain	Res	Type
3	1D	87	ASN
3	1D	116	GLN
3	1D	126	GLN
3	1D	164	GLN
4	1E	48	GLN
4	1E	121	ASN
5	1F	69	HIS
5	1F	204	ASN
6	1G	26	GLN
6	1G	108	ASN
9	1N	8	GLN
10	1O	3	GLN
12	1Q	123	HIS
13	1R	71	GLN
14	1S	95	HIS
16	1U	94	ASN
19	1X	31	HIS
19	1X	82	GLN
21	1Z	54	HIS
21	1Z	65	GLN
21	1Z	73	GLN
21	1Z	151	HIS
23	11	56	GLN
25	13	32	GLN

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Mol	Chain	Res	Type
33	1b	16	HIS
33	1b	40	HIS
33	1b	94	ASN
34	1c	6	HIS
34	1c	69	HIS
35	1d	42	GLN
35	1d	45	GLN
35	1d	116	GLN
35	1d	123	HIS
35	1d	125	HIS
35	1d	161	ASN
36	1e	20	GLN
36	1e	78	HIS
37	1f	57	GLN
37	1f	73	ASN
37	1f	100	ASN
38	1g	13	GLN
38	1g	28	ASN
40	1i	3	GLN
40	1i	31	GLN
40	1i	34	ASN
40	1i	73	GLN
40	1i	124	GLN
41	1j	56	HIS
43	1l	99	HIS
44	1m	92	HIS
46	1o	9	GLN
47	1p	76	GLN
50	1s	57	HIS
50	1s	83	HIS
51	1t	16	HIS
3	2D	87	ASN
4	2E	48	GLN
5	2F	31	HIS
6	2G	58	GLN
6	2G	121	ASN
6	2G	123	ASN
7	2H	139	GLN
8	2I	139	GLN
10	2O	3	GLN
10	2O	5	GLN
12	2Q	12	GLN

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Mol	Chain	Res	Type
12	2Q	123	HIS
14	2S	38	GLN
14	2S	68	GLN
15	2T	58	ASN
18	2W	60	ASN
19	2X	31	HIS
19	2X	55	ASN
19	2X	82	GLN
21	2Z	34	ASN
21	2Z	55	HIS
21	2Z	73	GLN
23	21	56	GLN
26	24	46	GLN
33	2b	76	GLN
33	2b	94	ASN
33	2b	135	GLN
33	2b	224	GLN
34	2c	98	ASN
35	2d	77	ASN
35	2d	116	GLN
35	2d	119	GLN
35	2d	123	HIS
35	2d	125	HIS
36	2e	20	GLN
36	2e	72	GLN
36	2e	141	GLN
37	2f	64	GLN
37	2f	73	ASN
38	2g	28	ASN
38	2g	86	GLN
38	2g	148	ASN
40	2i	3	GLN
40	2i	58	HIS
40	2i	89	ASN
40	2i	117	HIS
41	2j	13	HIS
41	2j	62	HIS
42	2k	104	GLN
42	2k	117	ASN
43	2l	80	HIS
44	2m	40	ASN
45	2n	49	HIS

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Mol	Chain	Res	Type
46	2o	62	GLN
49	2r	63	GLN
50	2s	23	ASN
50	2s	47	HIS
50	2s	69	HIS
50	2s	83	HIS
51	2t	16	HIS
51	2t	75	ASN
51	2t	90	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	1A	2863/2915 (98%)	417 (14%)	30 (1%)
1	2A	2790/2915 (95%)	433 (15%)	23 (0%)
2	1B	119/121 (98%)	8 (6%)	0
2	2B	118/121 (97%)	27 (22%)	0
32	1a	1494/1521 (98%)	263 (17%)	0
32	2a	1498/1521 (98%)	276 (18%)	0
53	1v	4/21 (19%)	0	0
53	2v	4/21 (19%)	1 (25%)	0
54	1x	75/77 (97%)	6 (8%)	0
54	2x	75/77 (97%)	9 (12%)	0
All	All	9040/9310 (97%)	1440 (15%)	53 (0%)

All (1440) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	1A	12	U
1	1A	34	C
1	1A	45	C
1	1A	71	A
1	1A	74	A
1	1A	75	G
1	1A	84	A
1	1A	95	G
1	1A	118	A
1	1A	119	A
1	1A	120	U
1	1A	139(A)	G
1	1A	182	A

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Mol	Chain	Res	Type
1	1A	196	A
1	1A	199	A
1	1A	205	G
1	1A	214	G
1	1A	215	G
1	1A	216	A
1	1A	221	A
1	1A	222	A
1	1A	225	A
1	1A	228	A
1	1A	229	A
1	1A	233	A
1	1A	248	G
1	1A	269	U
1	1A	271(C)	C
1	1A	271(K)	U
1	1A	271(L)	U
1	1A	271(M)	G
1	1A	271(O)	C
1	1A	272(B)	G
1	1A	272(I)	U
1	1A	279	C
1	1A	311	A
1	1A	329	G
1	1A	330	A
1	1A	342	G
1	1A	352	G
1	1A	357	A
1	1A	363	G
1	1A	363(B)	G
1	1A	380	U
1	1A	386	G
1	1A	396	G
1	1A	405	U
1	1A	411	G
1	1A	412	A
1	1A	428	A
1	1A	444	C
1	1A	448	U
1	1A	454	A
1	1A	481	G
1	1A	504	U

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Mol	Chain	Res	Type
1	1A	505	A
1	1A	508	G
1	1A	509	C
1	1A	513	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	574	C
1	1A	575	A
1	1A	603	A
1	1A	604	G
1	1A	607	U
1	1A	614(B)	G
1	1A	615	G
1	1A	627	A
1	1A	637	A
1	1A	645	C
1	1A	646	A
1	1A	652(D)	C
1	1A	652(E)	G
1	1A	652(F)	G
1	1A	652(T)	C
1	1A	668	G
1	1A	669	G
1	1A	686	G
1	1A	730	C
1	1A	764	A
1	1A	774	A
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	805	G
1	1A	812	C

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Mol	Chain	Res	Type
1	1A	827	U
1	1A	828	U
1	1A	830	G
1	1A	859	G
1	1A	866	A
1	1A	879	G
1	1A	880	G
1	1A	882	G
1	1A	883	G
1	1A	884	C
1	1A	885	C
1	1A	886	C
1	1A	887	A
1	1A	888	C
1	1A	890	A
1	1A	895	U
1	1A	896	A
1	1A	897	C
1	1A	900	A
1	1A	907	U
1	1A	910	A
1	1A	915	C
1	1A	931	G
1	1A	932	G
1	1A	938	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	983	A
1	1A	996	A
1	1A	1008	C
1	1A	1012	U
1	1A	1013	C
1	1A	1022	G
1	1A	1026	U
1	1A	1033	U
1	1A	1038	C
1	1A	1041	C

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Mol	Chain	Res	Type
1	1A	1045	A
1	1A	1046	A
1	1A	1047	G
1	1A	1054	A
1	1A	1055	G
1	1A	1058	G
1	1A	1059	G
1	1A	1063	G
1	1A	1069	A
1	1A	1071	G
1	1A	1073	A
1	1A	1075	C
1	1A	1076	C
1	1A	1078	U
1	1A	1079	C
1	1A	1081	U
1	1A	1083	U
1	1A	1088	A
1	1A	1089	G
1	1A	1090	U
1	1A	1091	G
1	1A	1093	G
1	1A	1094	U
1	1A	1096	A
1	1A	1098	A
1	1A	1101	U
1	1A	1110	G
1	1A	1112	G
1	1A	1116	C
1	1A	1130	U
1	1A	1135	C
1	1A	1136	G
1	1A	1149	G
1	1A	1171	G
1	1A	1173	G
1	1A	1174	A
1	1A	1175	U
1	1A	1176	G
1	1A	1177	A
1	1A	1178	C
1	1A	1220	A
1	1A	1248	G

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Mol	Chain	Res	Type
1	1A	1253	A
1	1A	1256	G
1	1A	1271	G
1	1A	1272	A
1	1A	1273	U
1	1A	1281	G
1	1A	1300	U
1	1A	1301	A
1	1A	1303	G
1	1A	1352	U
1	1A	1359	A
1	1A	1360	A
1	1A	1365	A
1	1A	1380	G
1	1A	1384	A
1	1A	1385	G
1	1A	1386	C
1	1A	1396	U
1	1A	1416	G
1	1A	1417	C
1	1A	1420	U
1	1A	1421	G
1	1A	1428	C
1	1A	1445	A
1	1A	1450	G
1	1A	1455	G
1	1A	1461	G
1	1A	1467	C
1	1A	1482	G
1	1A	1493	C
1	1A	1505	C
1	1A	1508	A
1	1A	1509	C
1	1A	1509(A)	A
1	1A	1532	C
1	1A	1540	U
1	1A	1543	C
1	1A	1554	A
1	1A	1558	A
1	1A	1560	G
1	1A	1566	A
1	1A	1569	A

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Mol	Chain	Res	Type
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	1648	C
1	1A	1654	A
1	1A	1674	G
1	1A	1700	A
1	1A	1701	A
1	1A	1703	G
1	1A	1722	A
1	1A	1739	U
1	1A	1746	G
1	1A	1756	G
1	1A	1763	G
1	1A	1764	G
1	1A	1773	A
1	1A	1780	A
1	1A	1791	A
1	1A	1800	C
1	1A	1801	G
1	1A	1816	G
1	1A	1829	A
1	1A	1839	G
1	1A	1847	A
1	1A	1878	G
1	1A	1889	A
1	1A	1900	A
1	1A	1906	G
1	1A	1914	C
1	1A	1919	A
1	1A	1929	G
1	1A	1930	G
1	1A	1937	A
1	1A	1938	A
1	1A	1955	U
1	1A	1963	U
1	1A	1965	C
1	1A	1967	C

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Mol	Chain	Res	Type
1	1A	1970	A
1	1A	1971	A
1	1A	1972	A
1	1A	1984	G
1	1A	1992	G
1	1A	1993	U
1	1A	1997	G
1	1A	2020	A
1	1A	2023	G
1	1A	2031	A
1	1A	2033	A
1	1A	2039	C
1	1A	2043	C
1	1A	2049	G
1	1A	2055	C
1	1A	2056	G
1	1A	2060	A
1	1A	2061	G
1	1A	2062	A
1	1A	2063	C
1	1A	2069	G
1	1A	2108	C
1	1A	2112	G
1	1A	2113	U
1	1A	2114	A
1	1A	2116	G
1	1A	2121	G
1	1A	2127	G
1	1A	2130	U
1	1A	2131	G
1	1A	2132	U
1	1A	2133	G
1	1A	2134	A
1	1A	2135	A
1	1A	2136	C
1	1A	2137	C
1	1A	2138	C
1	1A	2142	C
1	1A	2144	U
1	1A	2146	C
1	1A	2149	G
1	1A	2150	U

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Mol	Chain	Res	Type
1	1A	2151	G
1	1A	2155	G
1	1A	2156	G
1	1A	2157	G
1	1A	2158	A
1	1A	2159	G
1	1A	2162	G
1	1A	2165	G
1	1A	2166	G
1	1A	2171	A
1	1A	2172	U
1	1A	2173	A
1	1A	2174	C
1	1A	2181	G
1	1A	2182	G
1	1A	2183	C
1	1A	2189	U
1	1A	2198	A
1	1A	2206	G
1	1A	2207	G
1	1A	2219	G
1	1A	2225	A
1	1A	2238	G
1	1A	2239	G
1	1A	2268	A
1	1A	2269	A
1	1A	2273	A
1	1A	2283	C
1	1A	2287	A
1	1A	2289	G
1	1A	2294	C
1	1A	2305	A
1	1A	2308	G
1	1A	2320	A
1	1A	2325	G
1	1A	2334	G
1	1A	2336	A
1	1A	2347	C
1	1A	2350	C
1	1A	2372	G
1	1A	2383	G
1	1A	2385	C

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Mol	Chain	Res	Type
1	1A	2396	G
1	1A	2405	G
1	1A	2406	U
1	1A	2410	G
1	1A	2422	A
1	1A	2423	U
1	1A	2425	A
1	1A	2429	G
1	1A	2430	A
1	1A	2432	A
1	1A	2435	A
1	1A	2439	A
1	1A	2441	C
1	1A	2448	A
1	1A	2471	C
1	1A	2476	A
1	1A	2477	C
1	1A	2502	G
1	1A	2505	G
1	1A	2518	A
1	1A	2525	G
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	2569	G
1	1A	2582	G
1	1A	2602	A
1	1A	2609	U
1	1A	2611	U
1	1A	2612	C
1	1A	2613	U
1	1A	2629	A
1	1A	2630	G
1	1A	2654	A
1	1A	2689	U
1	1A	2690	C
1	1A	2702	U
1	1A	2703	C
1	1A	2712(A)	A

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Mol	Chain	Res	Type
1	1A	2713	A
1	1A	2714	G
1	1A	2726	U
1	1A	2733	A
1	1A	2755	C
1	1A	2757	A
1	1A	2758	A
1	1A	2761	G
1	1A	2764	A
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	2802	G
1	1A	2803	C
1	1A	2805	G
1	1A	2820	A
1	1A	2821	A
1	1A	2835	A
1	1A	2872	G
1	1A	2880	C
1	1A	2894	G
1	1A	2895	U
1	1A	2897	U
2	1B	2	C
2	1B	13	A
2	1B	25	A
2	1B	56	G
2	1B	73	A
2	1B	85	G
2	1B	106	G
2	1B	110	G
32	1a	7	G
32	1a	9	G
32	1a	22	G
32	1a	32	A
32	1a	39	G
32	1a	40	C
32	1a	42	G
32	1a	48	C

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Mol	Chain	Res	Type
32	1a	50	A
32	1a	51	A
32	1a	61	G
32	1a	66	G
32	1a	79	G
32	1a	91	C
32	1a	98	G
32	1a	101	A
32	1a	105	G
32	1a	116	A
32	1a	120	A
32	1a	121	C
32	1a	131	C
32	1a	145	G
32	1a	162	A
32	1a	163	C
32	1a	173	U
32	1a	174	C
32	1a	182	U
32	1a	184	G
32	1a	189(B)	C
32	1a	189(D)	C
32	1a	189(H)	G
32	1a	189(J)	G
32	1a	195	A
32	1a	197	A
32	1a	199	G
32	1a	202	U
32	1a	203	U
32	1a	204	U
32	1a	216	G
32	1a	247	G
32	1a	251	G
32	1a	266	G
32	1a	267	C
32	1a	280	C
32	1a	289	G
32	1a	321	A
32	1a	328	C
32	1a	332	G
32	1a	344	A
32	1a	348	G

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Mol	Chain	Res	Type
32	1a	352	C
32	1a	353	A
32	1a	354	G
32	1a	355	C
32	1a	356	A
32	1a	367	U
32	1a	372	C
32	1a	373	A
32	1a	384	G
32	1a	397	A
32	1a	398	C
32	1a	406	G
32	1a	412	A
32	1a	413	G
32	1a	422	C
32	1a	423	G
32	1a	424	G
32	1a	429	U
32	1a	439	A
32	1a	441	A
32	1a	442	C
32	1a	452	A
32	1a	457	C
32	1a	458	C
32	1a	461	A
32	1a	470	C
32	1a	471	G
32	1a	476	G
32	1a	485	G
32	1a	492	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	520	A
32	1a	528	C
32	1a	531	U
32	1a	532	A
32	1a	534	U

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Mol	Chain	Res	Type
32	1a	536	C
32	1a	547	A
32	1a	559	A
32	1a	561	U
32	1a	562	C
32	1a	564	C
32	1a	568	G
32	1a	572	A
32	1a	573	A
32	1a	576	G
32	1a	577	G
32	1a	596	C
32	1a	630	G
32	1a	631	G
32	1a	639	G
32	1a	640	A
32	1a	653	A
32	1a	665	A
32	1a	687	A
32	1a	688	G
32	1a	693	G
32	1a	695	A
32	1a	717	C
32	1a	722	A
32	1a	723	U
32	1a	724	G
32	1a	731	G
32	1a	749	C
32	1a	752	G
32	1a	755	G
32	1a	760	G
32	1a	766	A
32	1a	770	C
32	1a	777	A
32	1a	793	U
32	1a	794	A
32	1a	817	C
32	1a	821	G
32	1a	827	U
32	1a	828	A
32	1a	840	C
32	1a	841	U

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Mol	Chain	Res	Type
32	1a	851	G
32	1a	864	A
32	1a	872	A
32	1a	874	G
32	1a	902	G
32	1a	914	A
32	1a	926	G
32	1a	927	G
32	1a	934	C
32	1a	935	A
32	1a	936	C
32	1a	942	G
32	1a	960	U
32	1a	961	U
32	1a	968	A
32	1a	969	A
32	1a	971	G
32	1a	972	C
32	1a	974	A
32	1a	975	A
32	1a	976	G
32	1a	977	A
32	1a	982	U
32	1a	992	U
32	1a	993	G
32	1a	997	U
32	1a	1000	U
32	1a	1003	G
32	1a	1005	A
32	1a	1006	C
32	1a	1009	G
32	1a	1011	G
32	1a	1020	U
32	1a	1022	G
32	1a	1023	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

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Mol	Chain	Res	Type
32	1a	1030(C)	G
32	1a	1031	G
32	1a	1033	G
32	1a	1039	C
32	1a	1043	C
32	1a	1044	A
32	1a	1045	C
32	1a	1051	C
32	1a	1052	U
32	1a	1054	C
32	1a	1068	G
32	1a	1081	G
32	1a	1094	G
32	1a	1095	U
32	1a	1101	A
32	1a	1108	G
32	1a	1121	U
32	1a	1123	A
32	1a	1124	G
32	1a	1125	U
32	1a	1132	C
32	1a	1134	G
32	1a	1137	C
32	1a	1138	G
32	1a	1139	G
32	1a	1146	A
32	1a	1152	A
32	1a	1159	U
32	1a	1176	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	1227	A
32	1a	1236	A
32	1a	1238	A
32	1a	1246	C

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Mol	Chain	Res	Type
32	1a	1253	G
32	1a	1256	A
32	1a	1257	U
32	1a	1258	G
32	1a	1260	C
32	1a	1270	C
32	1a	1275	A
32	1a	1278	U
32	1a	1279	A
32	1a	1280	A
32	1a	1286	A
32	1a	1287	A
32	1a	1299	A
32	1a	1300	G
32	1a	1302	U
32	1a	1305	G
32	1a	1312	G
32	1a	1323	G
32	1a	1338	G
32	1a	1346	A
32	1a	1347	G
32	1a	1353	G
32	1a	1363	C
32	1a	1363(A)	A
32	1a	1364	U
32	1a	1370	G
32	1a	1394	A
32	1a	1397	C
32	1a	1419	G
32	1a	1442	G
32	1a	1442(A)	G
32	1a	1446	U
32	1a	1447	A
32	1a	1452	C
32	1a	1456	G
32	1a	1469	G
32	1a	1487	G
32	1a	1492	A
32	1a	1497	G
32	1a	1503	A
32	1a	1504	G
32	1a	1506	U

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Mol	Chain	Res	Type
32	1a	1517	G
32	1a	1529	G
32	1a	1530	G
54	1x	9	G
54	1x	13	C
54	1x	14	A
54	1x	21	A
54	1x	47	U
54	1x	76	A
1	2A	8	A
1	2A	11	G
1	2A	12	U
1	2A	15	G
1	2A	34	C
1	2A	35	G
1	2A	45	C
1	2A	71	A
1	2A	74	A
1	2A	75	G
1	2A	79	G
1	2A	84	A
1	2A	90	U
1	2A	94	C
1	2A	118	A
1	2A	120	U
1	2A	131	G
1	2A	141	A
1	2A	154(A)	C
1	2A	157	U
1	2A	173	G
1	2A	181	A
1	2A	196	A
1	2A	199	A
1	2A	205	G
1	2A	215	G
1	2A	216	A
1	2A	222	A
1	2A	225	A
1	2A	228	A
1	2A	229	A
1	2A	230	U
1	2A	232	G

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Mol	Chain	Res	Type
1	2A	233	A
1	2A	248	G
1	2A	250	G
1	2A	271(J)	C
1	2A	271(K)	U
1	2A	271(L)	U
1	2A	271(M)	G
1	2A	271(N)	U
1	2A	272(B)	G
1	2A	277	C
1	2A	278	A
1	2A	283	A
1	2A	311	A
1	2A	327	G
1	2A	329	G
1	2A	330	A
1	2A	333	G
1	2A	348	G
1	2A	352	G
1	2A	363	G
1	2A	386	G
1	2A	396	G
1	2A	403	U
1	2A	405	U
1	2A	411	G
1	2A	412	A
1	2A	444	C
1	2A	455	C
1	2A	456	C
1	2A	457	A
1	2A	481	G
1	2A	503	A
1	2A	504	U
1	2A	505	A
1	2A	509	C
1	2A	529	A
1	2A	530	G
1	2A	531	C
1	2A	532	A
1	2A	533	G
1	2A	545	G
1	2A	563	G

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Mol	Chain	Res	Type
1	2A	573	G
1	2A	575	A
1	2A	588	U
1	2A	603	A
1	2A	604	G
1	2A	607	U
1	2A	614(A)	U
1	2A	614(B)	G
1	2A	614(C)	A
1	2A	615	G
1	2A	627	A
1	2A	637	A
1	2A	645	C
1	2A	652(B)	A
1	2A	652(C)	G
1	2A	664	C
1	2A	669	G
1	2A	686	G
1	2A	717	G
1	2A	726	G
1	2A	730	C
1	2A	752	A
1	2A	753	C
1	2A	764	A
1	2A	775	G
1	2A	776	G
1	2A	782	A
1	2A	784	A
1	2A	785	G
1	2A	790	C
1	2A	792	G
1	2A	805	G
1	2A	812	C
1	2A	819	A
1	2A	827	U
1	2A	828	U
1	2A	832	G
1	2A	857	C
1	2A	859	G
1	2A	866	A
1	2A	874	G
1	2A	878	A

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Mol	Chain	Res	Type
1	2A	879	G
1	2A	880	G
1	2A	886	C
1	2A	887	A
1	2A	888	C
1	2A	889	C
1	2A	892	G
1	2A	893	C
1	2A	894	C
1	2A	896	A
1	2A	897	C
1	2A	900	A
1	2A	901	A
1	2A	903	C
1	2A	910	A
1	2A	914	C
1	2A	917	A
1	2A	932	G
1	2A	933	A
1	2A	938	G
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	983	A
1	2A	996	A
1	2A	999	U
1	2A	1012	U
1	2A	1013	C
1	2A	1017	G
1	2A	1020	A
1	2A	1022	G
1	2A	1025	G
1	2A	1027	A
1	2A	1033	U
1	2A	1038	C
1	2A	1039	G
1	2A	1041	C

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Mol	Chain	Res	Type
1	2A	1043	C
1	2A	1116	C
1	2A	1126	A
1	2A	1128	A
1	2A	1129	A
1	2A	1130	U
1	2A	1135	C
1	2A	1136	G
1	2A	1139	G
1	2A	1142(A)	A
1	2A	1144	G
1	2A	1171	G
1	2A	1188	U
1	2A	1195	G
1	2A	1205	U
1	2A	1210	A
1	2A	1211	U
1	2A	1212	G
1	2A	1220	A
1	2A	1244	G
1	2A	1253	A
1	2A	1256	G
1	2A	1271	G
1	2A	1272	A
1	2A	1273	U
1	2A	1287	A
1	2A	1300	U
1	2A	1301	A
1	2A	1314	C
1	2A	1352	U
1	2A	1359	A
1	2A	1360	A
1	2A	1365	A
1	2A	1368	G
1	2A	1370	C
1	2A	1380	G
1	2A	1384	A
1	2A	1385	G
1	2A	1386	C
1	2A	1416	G
1	2A	1417	C
1	2A	1420	U

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Mol	Chain	Res	Type
1	2A	1421	G
1	2A	1428	C
1	2A	1437	C
1	2A	1445	A
1	2A	1449	A
1	2A	1450	G
1	2A	1460	A
1	2A	1467	C
1	2A	1471	A
1	2A	1482	G
1	2A	1490	A
1	2A	1493	C
1	2A	1496	A
1	2A	1497	U
1	2A	1508	A
1	2A	1509	C
1	2A	1509(A)	A
1	2A	1531	C
1	2A	1532	C
1	2A	1533	G
1	2A	1543	C
1	2A	1547	C
1	2A	1558	A
1	2A	1559	G
1	2A	1566	A
1	2A	1569	A
1	2A	1578	U
1	2A	1584	C
1	2A	1608	A
1	2A	1609	A
1	2A	1610	A
1	2A	1616	A
1	2A	1640	C
1	2A	1648	C
1	2A	1654	A
1	2A	1674	G
1	2A	1696	G
1	2A	1700	A
1	2A	1701	A
1	2A	1721	G
1	2A	1722	A
1	2A	1739	U

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Mol	Chain	Res	Type
1	2A	1740	G
1	2A	1746	G
1	2A	1756	G
1	2A	1762	A
1	2A	1763	G
1	2A	1764	G
1	2A	1773	A
1	2A	1780	A
1	2A	1782	C
1	2A	1791	A
1	2A	1800	C
1	2A	1801	G
1	2A	1812	A
1	2A	1816	G
1	2A	1829	A
1	2A	1835	G
1	2A	1847	A
1	2A	1848	A
1	2A	1861	G
1	2A	1877	A
1	2A	1878	G
1	2A	1900	A
1	2A	1906	G
1	2A	1914	C
1	2A	1915	5MU
1	2A	1929	G
1	2A	1930	G
1	2A	1936	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	1984	G
1	2A	1993	U
1	2A	1997	G
1	2A	2020	A
1	2A	2023	G
1	2A	2031	A
1	2A	2033	A

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Mol	Chain	Res	Type
1	2A	2036	C
1	2A	2043	C
1	2A	2049	G
1	2A	2055	C
1	2A	2056	G
1	2A	2060	A
1	2A	2061	G
1	2A	2062	A
1	2A	2069	G
1	2A	2099	U
1	2A	2107	C
1	2A	2110	G
1	2A	2111	C
1	2A	2116	G
1	2A	2117	A
1	2A	2120	G
1	2A	2122	U
1	2A	2124	G
1	2A	2125	G
1	2A	2126	A
1	2A	2127	G
1	2A	2128	C
1	2A	2129	C
1	2A	2131	G
1	2A	2132	U
1	2A	2133	G
1	2A	2134	A
1	2A	2135	A
1	2A	2137	C
1	2A	2138	C
1	2A	2139	C
1	2A	2140	C
1	2A	2142	C
1	2A	2145	C
1	2A	2146	C
1	2A	2148	G
1	2A	2150	U
1	2A	2151	G
1	2A	2156	G
1	2A	2157	G
1	2A	2158	A
1	2A	2162	G

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Mol	Chain	Res	Type
1	2A	2166	G
1	2A	2167	U
1	2A	2168	G
1	2A	2169	A
1	2A	2172	U
1	2A	2174	C
1	2A	2176	A
1	2A	2177	C
1	2A	2178	C
1	2A	2182	G
1	2A	2185	C
1	2A	2188	C
1	2A	2192	G
1	2A	2198	A
1	2A	2206	G
1	2A	2207	G
1	2A	2208	A
1	2A	2218	U
1	2A	2225	A
1	2A	2238	G
1	2A	2239	G
1	2A	2275	C
1	2A	2278	A
1	2A	2283	C
1	2A	2287	A
1	2A	2305	A
1	2A	2308	G
1	2A	2312	U
1	2A	2319	G
1	2A	2320	A
1	2A	2325	G
1	2A	2334	G
1	2A	2336	A
1	2A	2346	A
1	2A	2347	C
1	2A	2350	C
1	2A	2376	A
1	2A	2383	G
1	2A	2385	C
1	2A	2388	A
1	2A	2402	C
1	2A	2403	C

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Mol	Chain	Res	Type
1	2A	2406	U
1	2A	2419	U
1	2A	2425	A
1	2A	2429	G
1	2A	2430	A
1	2A	2435	A
1	2A	2439	A
1	2A	2441	C
1	2A	2448	A
1	2A	2465	C
1	2A	2469	A
1	2A	2474	C
1	2A	2476	A
1	2A	2477	C
1	2A	2480	C
1	2A	2502	G
1	2A	2504	U
1	2A	2505	G
1	2A	2506	U
1	2A	2518	A
1	2A	2520	C
1	2A	2525	G
1	2A	2529	G
1	2A	2554	U
1	2A	2566	A
1	2A	2567	G
1	2A	2573	C
1	2A	2585	U
1	2A	2602	A
1	2A	2609	U
1	2A	2610	C
1	2A	2611	U
1	2A	2612	C
1	2A	2630	G
1	2A	2654	A
1	2A	2669	G
1	2A	2689	U
1	2A	2690	C
1	2A	2702	U
1	2A	2703	C
1	2A	2712(A)	A
1	2A	2713	A

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Mol	Chain	Res	Type
1	2A	2714	G
1	2A	2726	U
1	2A	2733	A
1	2A	2751	G
1	2A	2764	A
1	2A	2765	A
1	2A	2766	G
1	2A	2778	A
1	2A	2793	G
1	2A	2794	C
1	2A	2802	G
1	2A	2803	C
1	2A	2808	U
1	2A	2818	G
1	2A	2820	A
1	2A	2821	A
1	2A	2833	G
1	2A	2835	A
1	2A	2872	G
1	2A	2892	A
1	2A	2894	G
1	2A	2897	U
2	2B	2	C
2	2B	3	C
2	2B	8	U
2	2B	13	A
2	2B	17	C
2	2B	30	C
2	2B	34	U
2	2B	35	U
2	2B	41	U
2	2B	42	C
2	2B	51	G
2	2B	52	A
2	2B	53	A
2	2B	56	G
2	2B	63	G
2	2B	67	G
2	2B	73	A
2	2B	74	U
2	2B	75	G
2	2B	85	G

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Mol	Chain	Res	Type
2	2B	88	C
2	2B	89	G
2	2B	106	G
2	2B	109	C
2	2B	110	G
2	2B	111	G
2	2B	120	A
32	2a	6	G
32	2a	7	G
32	2a	9	G
32	2a	22	G
32	2a	32	A
32	2a	39	G
32	2a	47	C
32	2a	48	C
32	2a	50	A
32	2a	51	A
32	2a	65	U
32	2a	66	G
32	2a	73	G
32	2a	80	G
32	2a	89	C
32	2a	101	A
32	2a	116	A
32	2a	121	C
32	2a	129(A)	G
32	2a	131	C
32	2a	144	G
32	2a	159	G
32	2a	162	A
32	2a	163	C
32	2a	182	U
32	2a	189(A)	C
32	2a	189(E)	U
32	2a	189(F)	U
32	2a	195	A
32	2a	202	U
32	2a	203	U
32	2a	204	U
32	2a	216	G
32	2a	217	C
32	2a	231	G

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Mol	Chain	Res	Type
32	2a	247	G
32	2a	251	G
32	2a	252	U
32	2a	266	G
32	2a	267	C
32	2a	281	G
32	2a	289	G
32	2a	306	G
32	2a	321	A
32	2a	328	C
32	2a	332	G
32	2a	349	A
32	2a	351	G
32	2a	352	C
32	2a	353	A
32	2a	354	G
32	2a	367	U
32	2a	372	C
32	2a	373	A
32	2a	384	G
32	2a	388	G
32	2a	397	A
32	2a	398	C
32	2a	406	G
32	2a	412	A
32	2a	421	U
32	2a	423	G
32	2a	424	G
32	2a	429	U
32	2a	430	A
32	2a	439	A
32	2a	442	C
32	2a	451	A
32	2a	452	A
32	2a	457	C
32	2a	470	C
32	2a	471	G
32	2a	483	C
32	2a	484	G
32	2a	485	G
32	2a	496	A
32	2a	498	U

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Mol	Chain	Res	Type
32	2a	505	G
32	2a	509	A
32	2a	510	A
32	2a	511	C
32	2a	518	C
32	2a	531	U
32	2a	532	A
32	2a	533	A
32	2a	547	A
32	2a	553	A
32	2a	559	A
32	2a	560	U
32	2a	562	C
32	2a	564	C
32	2a	572	A
32	2a	573	A
32	2a	576	G
32	2a	596	C
32	2a	618	C
32	2a	630	G
32	2a	650	G
32	2a	653	A
32	2a	665	A
32	2a	687	A
32	2a	688	G
32	2a	723	U
32	2a	731	G
32	2a	742	G
32	2a	748	C
32	2a	749	C
32	2a	753	A
32	2a	755	G
32	2a	759	A
32	2a	763	G
32	2a	777	A
32	2a	792	A
32	2a	793	U
32	2a	794	A
32	2a	807	A
32	2a	816	A
32	2a	817	C
32	2a	821	G

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Mol	Chain	Res	Type
32	2a	828	A
32	2a	834	C
32	2a	840	C
32	2a	841	U
32	2a	853	G
32	2a	855	G
32	2a	859	A
32	2a	902	G
32	2a	914	A
32	2a	915	A
32	2a	926	G
32	2a	927	G
32	2a	931	C
32	2a	934	C
32	2a	935	A
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	974	A
32	2a	975	A
32	2a	976	G
32	2a	977	A
32	2a	989	C
32	2a	992	U
32	2a	993	G
32	2a	995	C
32	2a	997	U
32	2a	999	C
32	2a	1001	A
32	2a	1002	G
32	2a	1003	G
32	2a	1004	A
32	2a	1005	A
32	2a	1006	C
32	2a	1007	C
32	2a	1009	G
32	2a	1010	G
32	2a	1011	G

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Mol	Chain	Res	Type
32	2a	1020	U
32	2a	1021	G
32	2a	1022	G
32	2a	1023	G
32	2a	1025	U
32	2a	1026	G
32	2a	1027	C
32	2a	1028	C
32	2a	1030(A)	G
32	2a	1030(D)	A
32	2a	1031	G
32	2a	1032	G
32	2a	1035	A
32	2a	1038	C
32	2a	1039	C
32	2a	1040	U
32	2a	1045	C
32	2a	1053	G
32	2a	1054	C
32	2a	1065	U
32	2a	1066	C
32	2a	1068	G
32	2a	1070	U
32	2a	1077	G
32	2a	1079	G
32	2a	1081	G
32	2a	1085	U
32	2a	1086	U
32	2a	1092	A
32	2a	1094	G
32	2a	1095	U
32	2a	1101	A
32	2a	1108	G
32	2a	1109	C
32	2a	1113	C
32	2a	1122	U
32	2a	1124	G
32	2a	1129	C
32	2a	1130	A
32	2a	1133	G
32	2a	1135	U
32	2a	1136	U

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Mol	Chain	Res	Type
32	2a	1137	C
32	2a	1138	G
32	2a	1139	G
32	2a	1146	A
32	2a	1147	C
32	2a	1152	A
32	2a	1157	A
32	2a	1158	C
32	2a	1159	U
32	2a	1171	G
32	2a	1172	C
32	2a	1181	G
32	2a	1182	G
32	2a	1183	A
32	2a	1184	G
32	2a	1189	C
32	2a	1196	U
32	2a	1197	G
32	2a	1201	A
32	2a	1202	G
32	2a	1211	U
32	2a	1213	A
32	2a	1227	A
32	2a	1236	A
32	2a	1238	A
32	2a	1240	U
32	2a	1241	G
32	2a	1256	A
32	2a	1257	U
32	2a	1260	C
32	2a	1267	C
32	2a	1270	C
32	2a	1272	G
32	2a	1273	G
32	2a	1278	U
32	2a	1279	A
32	2a	1280	A
32	2a	1286	A
32	2a	1287	A
32	2a	1290	G
32	2a	1299	A
32	2a	1302	U

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Mol	Chain	Res	Type
32	2a	1303	C
32	2a	1306	A
32	2a	1320	C
32	2a	1323	G
32	2a	1338	G
32	2a	1346	A
32	2a	1347	G
32	2a	1352	C
32	2a	1358	U
32	2a	1363	C
32	2a	1364	U
32	2a	1370	G
32	2a	1378	C
32	2a	1397	C
32	2a	1398	A
32	2a	1419	G
32	2a	1442	G
32	2a	1442(A)	G
32	2a	1447	A
32	2a	1452	C
32	2a	1456	G
32	2a	1497	G
32	2a	1503	A
32	2a	1504	G
32	2a	1506	U
32	2a	1507	A
32	2a	1517	G
32	2a	1529	G
32	2a	1530	G
32	2a	1531	A
32	2a	1532	U
53	2v	15	A
54	2x	9	G
54	2x	13	C
54	2x	18	G
54	2x	19	G
54	2x	20	U
54	2x	21	A
54	2x	47	U
54	2x	48	C
54	2x	76	A

All (53) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	1A	90	U
1	1A	195	A
1	1A	196	A
1	1A	266	G
1	1A	278	A
1	1A	529	A
1	1A	548	A
1	1A	746	A
1	1A	764	A
1	1A	774	A
1	1A	827	U
1	1A	958	U
1	1A	974	G
1	1A	1067	A
1	1A	1174	A
1	1A	1176	G
1	1A	1379	A
1	1A	1442	G
1	1A	1508	A
1	1A	1608	A
1	1A	1992	G
1	1A	2062	A
1	1A	2126	A
1	1A	2134	A
1	1A	2406	U
1	1A	2422	A
1	1A	2430	A
1	1A	2439	A
1	1A	2689	U
1	1A	2756	U
1	2A	196	A
1	2A	228	A
1	2A	266	G
1	2A	271(K)	U
1	2A	271(M)	G
1	2A	277	C
1	2A	528	A
1	2A	752	A
1	2A	856	C
1	2A	896	A
1	2A	900	A
1	2A	974	G
1	2A	1026	U

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Mol	Chain	Res	Type
1	2A	1210	A
1	2A	1379	A
1	2A	1420	U
1	2A	1442	G
1	2A	1530	C
1	2A	1653	G
1	2A	1992	G
1	2A	2119	A
1	2A	2126	A
1	2A	2689	U

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
32	2MG	1a	1207	32	18,26,27	0.92	1 (5%)	16,38,41	1.16	2 (12%)
32	PSU	2a	516	32	18,21,22	1.31	2 (11%)	22,30,33	1.79	4 (18%)
43	0TD	1l	92	43	7,9,10	4.57	1 (14%)	6,11,13	10.05	3 (50%)
32	5MC	2a	1404	32	18,22,23	0.91	1 (5%)	26,32,35	1.09	2 (7%)
1	PSU	1A	1917	1	18,21,22	1.42	3 (16%)	22,30,33	1.90	3 (13%)
1	5MC	2A	1942	1	18,22,23	0.95	2 (11%)	26,32,35	1.13	2 (7%)
32	5MC	2a	1407	32	18,22,23	0.98	2 (11%)	26,32,35	1.17	2 (7%)
54	PSU	2x	55	54	18,21,22	1.34	2 (11%)	22,30,33	1.86	3 (13%)
54	5MU	2x	54	54	19,22,23	1.43	5 (26%)	28,32,35	1.87	6 (21%)
32	MA6	2a	1518	32	19,26,27	0.78	0	18,38,41	1.38	2 (11%)
32	G7M	2a	527	32,55	20,26,27	1.27	2 (10%)	17,39,42	0.63	0
1	OMG	2A	2251	54,1	18,26,27	0.85	1 (5%)	19,38,41	1.10	3 (15%)
1	PSU	2A	2605	1	18,21,22	1.32	2 (11%)	22,30,33	1.86	4 (18%)
1	5MC	1A	1962	1	18,22,23	0.91	2 (11%)	26,32,35	1.11	3 (11%)
1	2MA	1A	2503	1,55	17,25,26	1.00	1 (5%)	17,37,40	0.94	2 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	5MU	1A	1939	1,55	19,22,23	1.47	4 (21%)	28,32,35	2.21	6 (21%)
1	OMG	1A	2251	54,1,55	18,26,27	0.95	1 (5%)	19,38,41	1.12	3 (15%)
43	0TD	2l	92	43	7,9,10	4.86	1 (14%)	6,11,13	2.32	3 (50%)
32	MA6	2a	1519	32	19,26,27	0.82	0	18,38,41	1.55	2 (11%)
32	M2G	2a	966	32	20,27,28	1.58	4 (20%)	22,40,43	0.93	2 (9%)
54	5MU	1x	54	54	19,22,23	1.47	5 (26%)	28,32,35	1.69	5 (17%)
1	PSU	2A	1917	1	18,21,22	1.39	2 (11%)	22,30,33	1.96	3 (13%)
1	5MC	2A	1962	1,55	18,22,23	0.98	2 (11%)	26,32,35	1.18	2 (7%)
1	5MU	2A	1915	57,1	19,22,23	1.52	5 (26%)	28,32,35	2.08	6 (21%)
32	MA6	1a	1518	32	19,26,27	0.80	0	18,38,41	1.44	2 (11%)
32	G7M	1a	527	32,55	20,26,27	1.27	2 (10%)	17,39,42	0.56	0
32	5MC	2a	1400	32	18,22,23	0.94	2 (11%)	26,32,35	1.16	2 (7%)
1	5MU	1A	1915	57,1	19,22,23	1.49	4 (21%)	28,32,35	2.23	6 (21%)
32	4OC	1a	1402	32	20,23,24	0.72	0	26,32,35	1.01	3 (11%)
1	OMC	1A	1920	1	19,22,23	0.80	0	26,31,34	0.96	1 (3%)
32	5MC	1a	1407	32	18,22,23	0.88	2 (11%)	26,32,35	1.16	4 (15%)
54	5MC	2x	32	54	18,22,23	1.03	2 (11%)	26,32,35	1.27	3 (11%)
32	2MG	2a	1207	32	18,26,27	0.93	1 (5%)	16,38,41	0.97	1 (6%)
54	4SU	2x	8	54	18,21,22	1.88	5 (27%)	26,30,33	1.41	3 (11%)
1	OMU	1A	2552	1,55	19,22,23	1.17	2 (10%)	26,31,34	1.82	6 (23%)
32	5MC	1a	967	32	18,22,23	0.93	2 (11%)	26,32,35	1.07	2 (7%)
32	MA6	1a	1519	32	19,26,27	0.85	0	18,38,41	1.57	2 (11%)
1	5MC	1A	1942	1,55	18,22,23	0.96	2 (11%)	26,32,35	1.18	2 (7%)
54	5MC	1x	32	54	18,22,23	1.04	2 (11%)	26,32,35	1.39	3 (11%)
32	5MC	2a	967	32	18,22,23	0.93	2 (11%)	26,32,35	1.13	2 (7%)
54	4SU	1x	8	54	18,21,22	2.01	5 (27%)	26,30,33	1.40	5 (19%)
32	4OC	2a	1402	32	20,23,24	0.76	0	26,32,35	1.06	0
32	UR3	1a	1498	32	19,22,23	1.08	1 (5%)	26,32,35	1.54	3 (11%)
1	OMU	2A	2552	1,55	19,22,23	1.23	2 (10%)	26,31,34	1.88	6 (23%)
1	PSU	2A	1911	1	18,21,22	1.43	2 (11%)	22,30,33	1.75	4 (18%)
32	PSU	1a	516	32	18,21,22	1.36	2 (11%)	22,30,33	1.80	3 (13%)
32	UR3	2a	1498	32	19,22,23	1.02	2 (10%)	26,32,35	1.41	2 (7%)
54	PSU	1x	55	54	18,21,22	1.36	2 (11%)	22,30,33	1.87	3 (13%)
1	PSU	1A	1911	1	18,21,22	1.31	2 (11%)	22,30,33	1.89	3 (13%)
1	5MU	2A	1939	1	19,22,23	1.48	5 (26%)	28,32,35	2.18	6 (21%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
32	M2G	1a	966	32	20,27,28	1.44	3 (15%)	22,40,43	1.01	3 (13%)
32	5MC	1a	1404	32	18,22,23	1.05	2 (11%)	26,32,35	1.13	3 (11%)
32	5MC	1a	1400	32	18,22,23	0.98	2 (11%)	26,32,35	1.25	3 (11%)
1	OMC	2A	1920	1	19,22,23	0.79	0	26,31,34	0.92	0
1	2MA	2A	2503	1,55	17,25,26	1.07	2 (11%)	17,37,40	1.01	2 (11%)
1	PSU	1A	2605	1,55	18,21,22	1.42	3 (16%)	22,30,33	1.86	4 (18%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
32	2MG	1a	1207	32	-	0/5/27/28	0/3/3/3
32	PSU	2a	516	32	-	0/7/25/26	0/2/2/2
43	0TD	1l	92	43	-	3/7/12/14	-
32	5MC	2a	1404	32	-	0/7/25/26	0/2/2/2
1	PSU	1A	1917	1	-	0/7/25/26	0/2/2/2
1	5MC	2A	1942	1	-	0/7/25/26	0/2/2/2
32	5MC	2a	1407	32	-	0/7/25/26	0/2/2/2
54	PSU	2x	55	54	-	0/7/25/26	0/2/2/2
54	5MU	2x	54	54	-	0/7/25/26	0/2/2/2
32	MA6	2a	1518	32	-	0/7/29/30	0/3/3/3
32	G7M	2a	527	32,55	-	2/3/25/26	0/3/3/3
1	OMG	2A	2251	54,1	-	0/5/27/28	0/3/3/3
1	PSU	2A	2605	1	-	0/7/25/26	0/2/2/2
1	5MC	1A	1962	1	-	3/7/25/26	0/2/2/2
1	2MA	1A	2503	1,55	-	1/3/25/26	0/3/3/3
1	5MU	1A	1939	1,55	-	0/7/25/26	0/2/2/2
1	OMG	1A	2251	54,1,55	-	1/5/27/28	0/3/3/3
43	0TD	2l	92	43	-	1/7/12/14	-
32	MA6	2a	1519	32	-	3/7/29/30	0/3/3/3
32	M2G	2a	966	32	-	0/7/29/30	0/3/3/3
54	5MU	1x	54	54	-	0/7/25/26	0/2/2/2
1	PSU	2A	1917	1	-	0/7/25/26	0/2/2/2
1	5MC	2A	1962	1,55	-	0/7/25/26	0/2/2/2
1	5MU	2A	1915	57,1	-	0/7/25/26	0/2/2/2
32	MA6	1a	1518	32	-	0/7/29/30	0/3/3/3
32	G7M	1a	527	32,55	-	2/3/25/26	0/3/3/3
32	5MC	2a	1400	32	-	0/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	5MU	1A	1915	57,1	-	0/7/25/26	0/2/2/2
32	4OC	1a	1402	32	-	1/9/29/30	0/2/2/2
1	OMC	1A	1920	1	-	1/9/27/28	0/2/2/2
32	5MC	1a	1407	32	-	0/7/25/26	0/2/2/2
54	5MC	2x	32	54	-	1/7/25/26	0/2/2/2
32	2MG	2a	1207	32	-	0/5/27/28	0/3/3/3
54	4SU	2x	8	54	-	0/7/25/26	0/2/2/2
1	OMU	1A	2552	1,55	-	0/9/27/28	0/2/2/2
32	5MC	1a	967	32	-	2/7/25/26	0/2/2/2
32	MA6	1a	1519	32	-	3/7/29/30	0/3/3/3
1	5MC	1A	1942	1,55	-	0/7/25/26	0/2/2/2
54	5MC	1x	32	54	-	0/7/25/26	0/2/2/2
32	5MC	2a	967	32	-	1/7/25/26	0/2/2/2
54	4SU	1x	8	54	-	0/7/25/26	0/2/2/2
32	4OC	2a	1402	32	-	3/9/29/30	0/2/2/2
32	UR3	1a	1498	32	-	0/7/25/26	0/2/2/2
1	OMU	2A	2552	1,55	-	0/9/27/28	0/2/2/2
1	PSU	2A	1911	1	-	2/7/25/26	0/2/2/2
32	PSU	1a	516	32	-	0/7/25/26	0/2/2/2
32	UR3	2a	1498	32	-	0/7/25/26	0/2/2/2
54	PSU	1x	55	54	-	0/7/25/26	0/2/2/2
1	PSU	1A	1911	1	-	0/7/25/26	0/2/2/2
1	5MU	2A	1939	1	-	0/7/25/26	0/2/2/2
32	M2G	1a	966	32	-	0/7/29/30	0/3/3/3
32	5MC	1a	1404	32	-	0/7/25/26	0/2/2/2
32	5MC	1a	1400	32	-	0/7/25/26	0/2/2/2
1	OMC	2A	1920	1	-	1/9/27/28	0/2/2/2
1	2MA	2A	2503	1,55	-	1/3/25/26	0/3/3/3
1	PSU	1A	2605	1,55	-	0/7/25/26	0/2/2/2

All (114) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
43	2l	92	0TD	CB-SB	-12.54	1.69	1.82
43	1l	92	0TD	CB-SB	-11.75	1.70	1.82
32	2a	966	M2G	C2-N3	5.25	1.37	1.30
54	1x	8	4SU	C4-N3	-4.80	1.32	1.37
32	1a	966	M2G	C2-N3	4.61	1.36	1.30
54	2x	8	4SU	C4-N3	-4.30	1.33	1.37
54	2x	8	4SU	C4-S4	-3.91	1.61	1.68
32	1a	527	G7M	C5-C4	3.87	1.46	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
54	1x	8	4SU	C2-N3	-3.86	1.31	1.38
32	2a	527	G7M	C5-C4	3.82	1.46	1.39
54	1x	8	4SU	C4-S4	-3.61	1.61	1.68
1	1A	1939	5MU	C4-N3	-3.51	1.32	1.38
1	2A	2605	PSU	C6-C5	3.46	1.39	1.35
54	2x	55	PSU	C6-C5	3.44	1.39	1.35
54	1x	55	PSU	C6-C5	3.43	1.39	1.35
1	2A	1915	5MU	C6-C5	3.40	1.40	1.34
1	2A	1911	PSU	C6-C5	3.35	1.39	1.35
1	2A	1917	PSU	C6-C5	3.35	1.39	1.35
32	1a	516	PSU	C6-C5	3.29	1.39	1.35
1	1A	1917	PSU	C6-C5	3.28	1.39	1.35
54	1x	32	5MC	C6-C5	3.22	1.39	1.34
1	1A	1915	5MU	C6-C5	3.14	1.39	1.34
32	1a	1404	5MC	C6-C5	3.13	1.39	1.34
1	1A	2605	PSU	C4-N3	-3.06	1.33	1.38
54	1x	8	4SU	C5-C4	-3.05	1.38	1.42
54	1x	54	5MU	C6-C5	3.02	1.39	1.34
1	1A	1911	PSU	C6-C5	3.02	1.38	1.35
54	1x	54	5MU	C4-N3	-3.00	1.33	1.38
32	2a	516	PSU	C6-C5	2.98	1.38	1.35
1	1A	1917	PSU	C4-N3	-2.95	1.33	1.38
54	2x	54	5MU	C6-C5	2.95	1.39	1.34
1	2A	1939	5MU	C4-N3	-2.92	1.33	1.38
54	2x	32	5MC	C6-C5	2.91	1.39	1.34
1	1A	1939	5MU	C2-N3	-2.91	1.32	1.38
54	2x	8	4SU	C5-C4	-2.88	1.38	1.42
1	2A	1915	5MU	C4-N3	-2.87	1.33	1.38
1	2A	1911	PSU	C4-N3	-2.87	1.33	1.38
1	2A	1939	5MU	C6-C5	2.84	1.39	1.34
54	2x	54	5MU	C4-N3	-2.81	1.33	1.38
1	2A	1962	5MC	C6-C5	2.80	1.39	1.34
32	2a	966	M2G	C2-N2	2.79	1.40	1.35
32	1a	966	M2G	C2-N2	2.76	1.40	1.35
32	2a	1404	5MC	C6-C5	2.76	1.39	1.34
1	1A	1939	5MU	C6-C5	2.75	1.39	1.34
1	2A	1942	5MC	C6-C5	2.73	1.39	1.34
1	2A	1939	5MU	C6-N1	-2.70	1.33	1.38
32	2a	1400	5MC	C6-C5	2.70	1.39	1.34
1	1A	2251	OMG	C6-N1	-2.68	1.33	1.37
1	1A	1962	5MC	C6-C5	2.68	1.39	1.34
1	1A	2552	OMU	C4-N3	-2.67	1.33	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	1A	1942	5MC	C6-C5	2.67	1.39	1.34
1	1A	1915	5MU	C2-N1	2.66	1.42	1.38
32	2a	967	5MC	C6-C5	2.66	1.39	1.34
32	1a	1400	5MC	C6-C5	2.66	1.39	1.34
32	2a	1407	5MC	C6-C5	2.63	1.38	1.34
54	2x	8	4SU	C2-N3	-2.63	1.33	1.38
1	1A	1915	5MU	C4-C5	2.62	1.49	1.44
32	1a	967	5MC	C6-C5	2.62	1.38	1.34
1	2A	2552	OMU	C4-N3	-2.61	1.33	1.38
32	2a	966	M2G	C6-N1	-2.60	1.34	1.37
1	1A	1915	5MU	C4-N3	-2.59	1.34	1.38
1	2A	1915	5MU	C4-C5	2.58	1.49	1.44
1	1A	1911	PSU	C4-N3	-2.57	1.34	1.38
32	1a	516	PSU	C4-N3	-2.56	1.34	1.38
1	1A	2552	OMU	C2-N3	-2.56	1.33	1.38
32	1a	1207	2MG	C6-N1	-2.55	1.34	1.37
1	2A	1939	5MU	C4-C5	2.54	1.49	1.44
32	2a	516	PSU	C4-N3	-2.54	1.34	1.38
1	1A	2605	PSU	C6-C5	2.54	1.38	1.35
1	1A	1942	5MC	C6-N1	-2.52	1.33	1.38
54	2x	55	PSU	C4-N3	-2.51	1.34	1.38
1	2A	1917	PSU	C4-N3	-2.48	1.34	1.38
32	1a	527	G7M	C6-N1	-2.46	1.34	1.37
32	1a	1400	5MC	C6-N1	-2.40	1.34	1.38
1	2A	2605	PSU	C4-N3	-2.38	1.34	1.38
54	1x	55	PSU	C4-N3	-2.34	1.34	1.38
32	1a	1407	5MC	C6-C5	2.33	1.38	1.34
32	1a	1498	UR3	C2-N1	2.32	1.41	1.38
32	2a	527	G7M	C6-N1	-2.32	1.34	1.37
1	1A	2605	PSU	C2-N3	-2.32	1.33	1.37
1	2A	1962	5MC	C6-N1	-2.32	1.34	1.38
32	2a	1207	2MG	C6-N1	-2.31	1.34	1.37
54	2x	54	5MU	C4-C5	2.31	1.48	1.44
1	1A	1939	5MU	C6-N1	-2.30	1.34	1.38
1	2A	2503	2MA	C2-N3	2.30	1.36	1.31
1	2A	2251	OMG	C6-N1	-2.30	1.34	1.37
54	1x	32	5MC	C6-N1	-2.26	1.34	1.38
32	1a	967	5MC	C6-N1	-2.26	1.34	1.38
32	1a	966	M2G	C6-N1	-2.26	1.34	1.37
32	2a	1407	5MC	C6-N1	-2.24	1.34	1.38
54	1x	54	5MU	C2-N3	-2.24	1.34	1.38
1	1A	1962	5MC	C6-N1	-2.21	1.34	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	2a	1400	5MC	C6-N1	-2.21	1.34	1.38
32	1a	1404	5MC	C6-N1	-2.20	1.34	1.38
1	2A	2552	OMU	C5-C4	2.20	1.48	1.43
1	2A	1942	5MC	C6-N1	-2.18	1.34	1.38
54	1x	54	5MU	C4-C5	2.18	1.48	1.44
1	2A	1915	5MU	C2-N1	2.18	1.41	1.38
1	1A	2503	2MA	C2-N3	2.15	1.35	1.31
54	1x	8	4SU	C6-C5	2.14	1.40	1.35
1	2A	1915	5MU	C2-N3	-2.14	1.34	1.38
1	1A	1917	PSU	C2-N3	-2.13	1.33	1.37
1	2A	2503	2MA	C6-N1	-2.11	1.33	1.38
54	2x	8	4SU	O2-C2	2.10	1.26	1.23
32	2a	1498	UR3	C6-C5	2.10	1.39	1.35
32	1a	1407	5MC	C6-N1	-2.10	1.34	1.38
32	2a	967	5MC	C6-N1	-2.06	1.34	1.38
32	2a	1498	UR3	C2-N1	2.06	1.41	1.38
54	2x	54	5MU	C2-N3	-2.05	1.34	1.38
54	1x	54	5MU	C2-N1	2.05	1.41	1.38
1	2A	1939	5MU	C2-N3	-2.05	1.34	1.38
54	2x	54	5MU	C6-N1	-2.04	1.34	1.38
54	2x	32	5MC	C6-N1	-2.04	1.34	1.38
32	2a	966	M2G	C5-C4	2.02	1.48	1.43

All (165) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
43	1l	92	0TD	CSB-SB-CB	24.19	146.21	102.44
1	2A	1917	PSU	N1-C2-N3	6.41	122.39	115.13
1	1A	1917	PSU	N1-C2-N3	6.12	122.06	115.13
1	1A	2605	PSU	N1-C2-N3	6.06	122.00	115.13
54	1x	55	PSU	N1-C2-N3	6.00	121.93	115.13
54	2x	55	PSU	N1-C2-N3	5.97	121.90	115.13
1	1A	1911	PSU	N1-C2-N3	5.95	121.87	115.13
32	1a	516	PSU	N1-C2-N3	5.80	121.70	115.13
1	1A	1915	5MU	C4-N3-C2	-5.72	119.94	127.35
1	2A	1915	5MU	N3-C2-N1	5.71	122.47	114.89
32	1a	1498	UR3	C4-N3-C2	-5.69	119.21	124.56
32	2a	1498	UR3	C4-N3-C2	-5.67	119.22	124.56
1	2A	1939	5MU	C4-N3-C2	-5.64	120.05	127.35
1	1A	1915	5MU	C5-C4-N3	5.63	120.11	115.31
1	2A	1939	5MU	N3-C2-N1	5.62	122.35	114.89
32	2a	516	PSU	N1-C2-N3	5.54	121.41	115.13

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1A	1939	5MU	C5-C4-N3	5.54	120.04	115.31
1	2A	2605	PSU	N1-C2-N3	5.53	121.39	115.13
1	2A	1911	PSU	N1-C2-N3	5.47	121.33	115.13
1	1A	1915	5MU	N3-C2-N1	5.31	121.94	114.89
1	1A	1939	5MU	C4-N3-C2	-5.18	120.65	127.35
1	2A	2552	OMU	N3-C2-N1	5.14	121.72	114.89
32	1a	1519	MA6	N3-C2-N1	-5.14	120.64	128.68
1	2A	1915	5MU	C4-N3-C2	-5.14	120.70	127.35
1	1A	2552	OMU	N3-C2-N1	4.93	121.43	114.89
1	2A	2552	OMU	C4-N3-C2	-4.80	120.25	126.58
1	1A	1939	5MU	O4-C4-C5	-4.79	119.35	124.90
54	2x	54	5MU	N3-C2-N1	4.77	121.23	114.89
32	2a	1519	MA6	N3-C2-N1	-4.74	121.28	128.68
54	1x	32	5MC	C5-C6-N1	-4.73	118.48	123.34
32	1a	1518	MA6	N3-C2-N1	-4.69	121.34	128.68
1	1A	1939	5MU	C5-C6-N1	-4.69	118.52	123.34
1	1A	1939	5MU	N3-C2-N1	4.68	121.11	114.89
54	2x	54	5MU	C4-N3-C2	-4.50	121.52	127.35
1	2A	1939	5MU	C5-C6-N1	-4.38	118.83	123.34
32	2a	1518	MA6	N3-C2-N1	-4.36	121.86	128.68
1	1A	2552	OMU	C4-N3-C2	-4.28	120.93	126.58
1	2A	1915	5MU	C5-C4-N3	4.25	118.94	115.31
54	1x	54	5MU	N3-C2-N1	4.22	120.50	114.89
1	2A	2605	PSU	C4-N3-C2	-4.07	120.47	126.34
1	2A	1939	5MU	C5-C4-N3	4.06	118.78	115.31
1	1A	1911	PSU	C4-N3-C2	-4.00	120.57	126.34
1	1A	1942	5MC	C5-C6-N1	-3.96	119.27	123.34
1	1A	1917	PSU	C4-N3-C2	-3.94	120.66	126.34
1	1A	1915	5MU	O4-C4-C5	-3.92	120.36	124.90
32	2a	1400	5MC	C5-C6-N1	-3.92	119.31	123.34
1	2A	1962	5MC	C5-C6-N1	-3.88	119.35	123.34
54	2x	54	5MU	C5-C4-N3	3.85	118.60	115.31
54	1x	54	5MU	C4-N3-C2	-3.85	122.37	127.35
54	2x	55	PSU	C4-N3-C2	-3.83	120.83	126.34
32	2a	516	PSU	C4-N3-C2	-3.80	120.86	126.34
32	1a	1404	5MC	C5-C6-N1	-3.78	119.45	123.34
1	2A	1917	PSU	O2-C2-N1	-3.75	118.66	122.79
1	2A	1917	PSU	C4-N3-C2	-3.75	120.93	126.34
1	1A	1915	5MU	C5-C6-N1	-3.74	119.50	123.34
54	1x	54	5MU	C5-C4-N3	3.68	118.45	115.31
54	2x	8	4SU	C1'-N1-C2	3.68	124.24	117.57
1	2A	2552	OMU	O2-C2-N1	-3.65	117.94	122.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1A	2605	PSU	C4-N3-C2	-3.64	121.10	126.34
54	1x	8	4SU	C6-C5-C4	-3.63	116.81	119.95
32	2a	1519	MA6	C4-C5-N7	-3.55	105.70	109.40
54	1x	55	PSU	C4-N3-C2	-3.54	121.24	126.34
32	1a	516	PSU	C4-N3-C2	-3.52	121.26	126.34
1	2A	1915	5MU	C5-C6-N1	-3.50	119.73	123.34
32	1a	967	5MC	C5-C6-N1	-3.50	119.74	123.34
1	2A	1942	5MC	C5-C6-N1	-3.48	119.75	123.34
1	1A	1962	5MC	C5-C6-N1	-3.48	119.76	123.34
32	2a	967	5MC	C5-C6-N1	-3.46	119.78	123.34
43	1l	92	0TD	OD2-CG-CB	3.45	120.61	113.15
32	1a	1400	5MC	C5-C6-N1	-3.43	119.81	123.34
43	2l	92	0TD	CSB-SB-CB	-3.41	96.27	102.44
54	2x	54	5MU	C5-C6-N1	-3.38	119.86	123.34
54	2x	32	5MC	C5-C6-N1	-3.38	119.86	123.34
43	2l	92	0TD	OD2-CG-CB	3.37	120.42	113.15
54	1x	54	5MU	C5-C6-N1	-3.33	119.92	123.34
32	2a	1404	5MC	C5-C6-N1	-3.30	119.94	123.34
1	2A	1911	PSU	C4-N3-C2	-3.28	121.62	126.34
1	1A	2552	OMU	O2-C2-N1	-3.27	118.44	122.79
1	1A	1911	PSU	O2-C2-N1	-3.25	119.21	122.79
54	2x	8	4SU	C6-C5-C4	-3.24	117.14	119.95
54	2x	54	5MU	O4-C4-C5	-3.22	121.17	124.90
54	2x	8	4SU	C5-C4-N3	3.22	117.68	114.69
1	2A	1915	5MU	O4-C4-C5	-3.17	121.23	124.90
1	2A	1911	PSU	O2-C2-N1	-3.16	119.31	122.79
54	1x	55	PSU	O2-C2-N1	-3.16	119.32	122.79
54	2x	32	5MC	O2-C2-N3	-3.13	117.23	122.33
1	2A	1939	5MU	O4-C4-C5	-3.13	121.28	124.90
1	2A	1939	5MU	O2-C2-N1	-3.12	118.64	122.79
32	2a	1518	MA6	C4-C5-N7	-3.12	106.15	109.40
54	1x	54	5MU	O4-C4-C5	-3.10	121.31	124.90
32	2a	1407	5MC	C5-C6-N1	-3.07	120.18	123.34
32	1a	1518	MA6	C4-C5-N7	-3.04	106.23	109.40
32	1a	516	PSU	O2-C2-N1	-3.02	119.46	122.79
32	2a	516	PSU	O2-C2-N1	-3.01	119.47	122.79
54	1x	8	4SU	O2-C2-N1	3.00	126.78	122.79
54	2x	55	PSU	O2-C2-N1	-2.98	119.52	122.79
1	1A	2552	OMU	O4-C4-C5	-2.97	119.94	125.16
1	1A	1917	PSU	O2-C2-N1	-2.92	119.57	122.79
32	1a	1407	5MC	C5-C4-N3	-2.91	118.53	121.67
54	1x	32	5MC	C5-C4-N3	-2.90	118.55	121.67

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1A	2552	OMU	C5-C4-N3	2.90	119.17	114.84
1	2A	2552	OMU	C5-C4-N3	2.88	119.14	114.84
32	2a	1407	5MC	C5-C4-N3	-2.77	118.68	121.67
32	1a	1519	MA6	C4-C5-N7	-2.74	106.55	109.40
32	1a	1400	5MC	C5-C4-N3	-2.73	118.73	121.67
1	1A	2251	OMG	C5-C6-N1	2.70	118.72	113.95
1	2A	1915	5MU	O2-C2-N1	-2.68	119.22	122.79
1	1A	1962	5MC	CM5-C5-C6	-2.66	119.30	122.85
32	1a	1207	2MG	C8-N7-C5	2.66	108.05	102.99
1	2A	2552	OMU	O4-C4-C5	-2.64	120.51	125.16
1	1A	2552	OMU	C2'-C1'-N1	-2.64	109.10	114.22
1	2A	2605	PSU	O2-C2-N1	-2.63	119.89	122.79
32	2a	1498	UR3	C3U-N3-C4	2.61	121.61	117.89
1	1A	2605	PSU	O2-C2-N1	-2.60	119.92	122.79
32	1a	1498	UR3	C3U-N3-C4	2.60	121.60	117.89
1	2A	2503	2MA	C5-C6-N1	2.57	118.45	114.02
1	1A	1915	5MU	O2-C2-N1	-2.56	119.38	122.79
32	2a	1404	5MC	C5-C4-N3	-2.55	118.92	121.67
32	1a	967	5MC	C5-C4-N3	-2.52	118.95	121.67
43	2l	92	0TD	OD1-CG-CB	-2.52	117.17	122.44
54	1x	8	4SU	S4-C4-N3	-2.50	117.75	120.21
1	2A	2503	2MA	C8-N7-C5	2.47	107.69	102.99
1	2A	1962	5MC	C5-C4-N3	-2.42	119.06	121.67
32	1a	1498	UR3	C1'-N1-C2	2.42	121.08	116.99
1	1A	1942	5MC	C5-C4-N3	-2.40	119.08	121.67
32	1a	1207	2MG	C5-C6-N1	2.37	118.14	113.95
54	2x	32	5MC	C5-C4-N3	-2.37	119.11	121.67
1	1A	1920	OMC	O2-C2-N3	-2.37	118.47	122.33
54	2x	54	5MU	O2-C2-N1	-2.37	119.64	122.79
43	1l	92	0TD	OD1-CG-CB	-2.36	117.51	122.44
1	2A	2251	OMG	C5-C6-N1	2.35	118.10	113.95
32	1a	1402	4OC	C6-C5-C4	2.34	119.83	116.96
1	2A	2552	OMU	C2'-C1'-N1	-2.33	109.70	114.22
1	1A	2503	2MA	C8-N7-C5	2.29	107.36	102.99
32	1a	1407	5MC	CM5-C5-C6	-2.29	119.79	122.85
1	1A	2251	OMG	C8-N7-C5	2.29	107.35	102.99
1	2A	1942	5MC	C5-C4-N3	-2.28	119.21	121.67
1	2A	2251	OMG	C8-N7-C5	2.28	107.34	102.99
32	2a	966	M2G	C8-N7-C5	2.26	107.30	102.99
32	2a	1207	2MG	C8-N7-C5	2.26	107.29	102.99
1	1A	2251	OMG	O6-C6-C5	-2.26	119.97	124.37
32	2a	1400	5MC	C5-C4-N3	-2.25	119.25	121.67

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	1a	1407	5MC	C5-C6-N1	-2.24	121.03	123.34
32	1a	1404	5MC	C5-C4-N3	-2.23	119.27	121.67
32	1a	1400	5MC	O2-C2-N3	-2.18	118.78	122.33
32	1a	966	M2G	C8-N7-C5	2.18	107.14	102.99
54	1x	8	4SU	C4-N3-C2	2.15	129.43	127.34
1	1A	2503	2MA	C5-C6-N1	2.15	117.72	114.02
32	1a	1407	5MC	O2-C2-N3	-2.14	118.85	122.33
1	2A	2251	OMG	O6-C6-C5	-2.14	120.20	124.37
32	2a	967	5MC	C5-C4-N3	-2.13	119.37	121.67
1	2A	1911	PSU	C6-C5-C4	-2.13	116.71	118.20
32	1a	966	M2G	O6-C6-C5	-2.13	120.21	124.37
32	2a	966	M2G	C5-C6-N1	2.12	117.70	113.95
54	1x	32	5MC	O2-C2-N3	-2.11	118.90	122.33
1	1A	1962	5MC	C5-C4-N3	-2.10	119.40	121.67
54	1x	8	4SU	C5-C4-N3	2.10	116.64	114.69
32	1a	966	M2G	C5-C6-N1	2.08	117.62	113.95
1	2A	2605	PSU	C5-C6-N1	-2.07	119.01	122.11
32	1a	1402	4OC	CM4-N4-C4	-2.06	118.42	122.45
1	1A	2605	PSU	C5-C6-N1	-2.06	119.02	122.11
32	2a	516	PSU	O4'-C1'-C2'	2.06	108.05	105.14
32	1a	1404	5MC	O2-C2-N3	-2.03	119.03	122.33
32	1a	1402	4OC	C5-C6-N1	-2.03	118.41	121.81
1	1A	1939	5MU	O2-C2-N3	-2.02	117.75	121.50

There are no chirality outliers.

All (32) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	1A	2251	OMG	C1'-C2'-O2'-CM2
43	1l	92	0TD	SB-CB-CG-OD2
32	2a	1402	4OC	O4'-C4'-C5'-O5'
32	2a	1519	MA6	O4'-C4'-C5'-O5'
32	1a	1519	MA6	O4'-C4'-C5'-O5'
32	2a	1402	4OC	C3'-C4'-C5'-O5'
32	2a	1519	MA6	C3'-C4'-C5'-O5'
32	1a	527	G7M	C3'-C4'-C5'-O5'
32	1a	1519	MA6	C3'-C4'-C5'-O5'
1	2A	1911	PSU	O4'-C4'-C5'-O5'
32	2a	527	G7M	C3'-C4'-C5'-O5'
32	1a	527	G7M	O4'-C4'-C5'-O5'
43	1l	92	0TD	CG-CB-SB-CSB
43	2l	92	0TD	CG-CB-SB-CSB

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Mol	Chain	Res	Type	Atoms
32	1a	967	5MC	O4'-C4'-C5'-O5'
32	2a	527	G7M	O4'-C4'-C5'-O5'
32	1a	1519	MA6	C4'-C5'-O5'-P
32	2a	1519	MA6	C4'-C5'-O5'-P
1	2A	1911	PSU	C3'-C4'-C5'-O5'
1	1A	1962	5MC	C2'-C1'-N1-C6
1	1A	1962	5MC	O4'-C1'-N1-C6
32	1a	1402	4OC	O4'-C4'-C5'-O5'
32	2a	1402	4OC	C2'-C1'-N1-C2
32	2a	967	5MC	O4'-C4'-C5'-O5'
1	2A	1920	OMC	C2'-C1'-N1-C2
54	2x	32	5MC	C2'-C1'-N1-C2
43	1l	92	0TD	SB-CB-CG-OD1
1	1A	1920	OMC	C2'-C1'-N1-C2
1	1A	2503	2MA	O4'-C4'-C5'-O5'
32	1a	967	5MC	C3'-C4'-C5'-O5'
1	2A	2503	2MA	O4'-C4'-C5'-O5'
1	1A	1962	5MC	C2'-C1'-N1-C2

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 2481 ligands modelled in this entry, 2477 are monoatomic - leaving 4 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
59	SF4	1d	3202	35	0,12,12	-	-	-		
59	SF4	2d	501	35	0,12,12	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
57	T8B	2A	3717	1,55	48,48,48	2.52	11 (22%)	63,71,71	1.76	14 (22%)
57	T8B	1A	4052	1,55	48,48,48	2.51	11 (22%)	63,71,71	1.65	11 (17%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
59	SF4	1d	3202	35	-	-	0/6/5/5
59	SF4	2d	501	35	-	-	0/6/5/5
57	T8B	2A	3717	1,55	-	1/26/26/26	0/5/5/5
57	T8B	1A	4052	1,55	-	3/26/26/26	0/5/5/5

All (22) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
57	2A	3717	T8B	C27-C26	-9.13	1.40	1.48
57	1A	4052	T8B	C27-C26	-8.99	1.40	1.48
57	2A	3717	T8B	C25-C26	8.34	1.53	1.38
57	1A	4052	T8B	C25-C26	7.93	1.53	1.38
57	1A	4052	T8B	C2-C3	-7.48	1.40	1.51
57	2A	3717	T8B	C2-C3	-7.29	1.40	1.51
57	2A	3717	T8B	C10-C11	4.35	1.38	1.34
57	1A	4052	T8B	C10-C11	4.24	1.38	1.34
57	1A	4052	T8B	C11-C12	-4.16	1.39	1.48
57	2A	3717	T8B	C23-C24	-3.78	1.40	1.49
57	1A	4052	T8B	C23-C24	-3.74	1.40	1.49
57	2A	3717	T8B	C11-C12	-3.55	1.40	1.48
57	2A	3717	T8B	C25-C24	3.12	1.53	1.43
57	1A	4052	T8B	C25-C24	3.05	1.53	1.43
57	1A	4052	T8B	C9-C10	-2.73	1.38	1.43
57	2A	3717	T8B	C9-C10	-2.54	1.38	1.43
57	1A	4052	T8B	C15-C14	-2.47	1.40	1.46
57	2A	3717	T8B	C15-C14	-2.43	1.40	1.46
57	2A	3717	T8B	C15-C9	-2.29	1.38	1.42
57	1A	4052	T8B	C15-C9	-2.28	1.38	1.42
57	2A	3717	T8B	O11-C26	2.26	1.36	1.32
57	1A	4052	T8B	O11-C26	2.24	1.36	1.32

All (25) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
57	2A	3717	T8B	C26-C25-C24	-4.81	113.52	120.84
57	2A	3717	T8B	O5-C14-O6	4.57	122.06	116.44
57	1A	4052	T8B	C21-C23-C24	-4.55	119.73	125.03
57	2A	3717	T8B	C21-C23-C24	-4.45	119.84	125.03
57	2A	3717	T8B	C13-O4-C12	-4.34	107.66	115.86
57	1A	4052	T8B	C26-C25-C24	-3.98	114.78	120.84
57	1A	4052	T8B	O5-C14-O6	3.91	121.25	116.44
57	1A	4052	T8B	C13-O4-C12	-3.73	108.80	115.86
57	1A	4052	T8B	O11-C26-C27	3.22	118.78	114.03
57	2A	3717	T8B	O4-C12-C11	3.03	116.17	111.76
57	2A	3717	T8B	O5-C11-C12	2.83	117.81	112.25
57	2A	3717	T8B	O11-C26-C27	2.83	118.21	114.03
57	2A	3717	T8B	C32-C27-C26	2.65	126.83	121.82
57	1A	4052	T8B	O10-C24-C23	2.64	123.09	119.37
57	1A	4052	T8B	C4-C5-C6	-2.60	117.73	122.18
57	2A	3717	T8B	O2-C1-C2	-2.41	116.16	123.04
57	1A	4052	T8B	C32-C27-C26	2.41	126.38	121.82
57	1A	4052	T8B	C11-O5-C14	-2.40	118.98	121.12
57	2A	3717	T8B	C15-C16-C17	2.40	122.99	121.09
57	1A	4052	T8B	C15-C16-C17	2.34	122.95	121.09
57	2A	3717	T8B	O11-C26-C25	-2.30	117.87	121.09
57	2A	3717	T8B	C4-C5-C6	-2.21	118.40	122.18
57	2A	3717	T8B	O10-C24-C23	2.20	122.48	119.37
57	2A	3717	T8B	C19-O8-C18	-2.06	109.25	113.89
57	1A	4052	T8B	O11-C26-C25	-2.04	118.24	121.09

There are no chirality outliers.

All (4) torsion outliers are listed below:

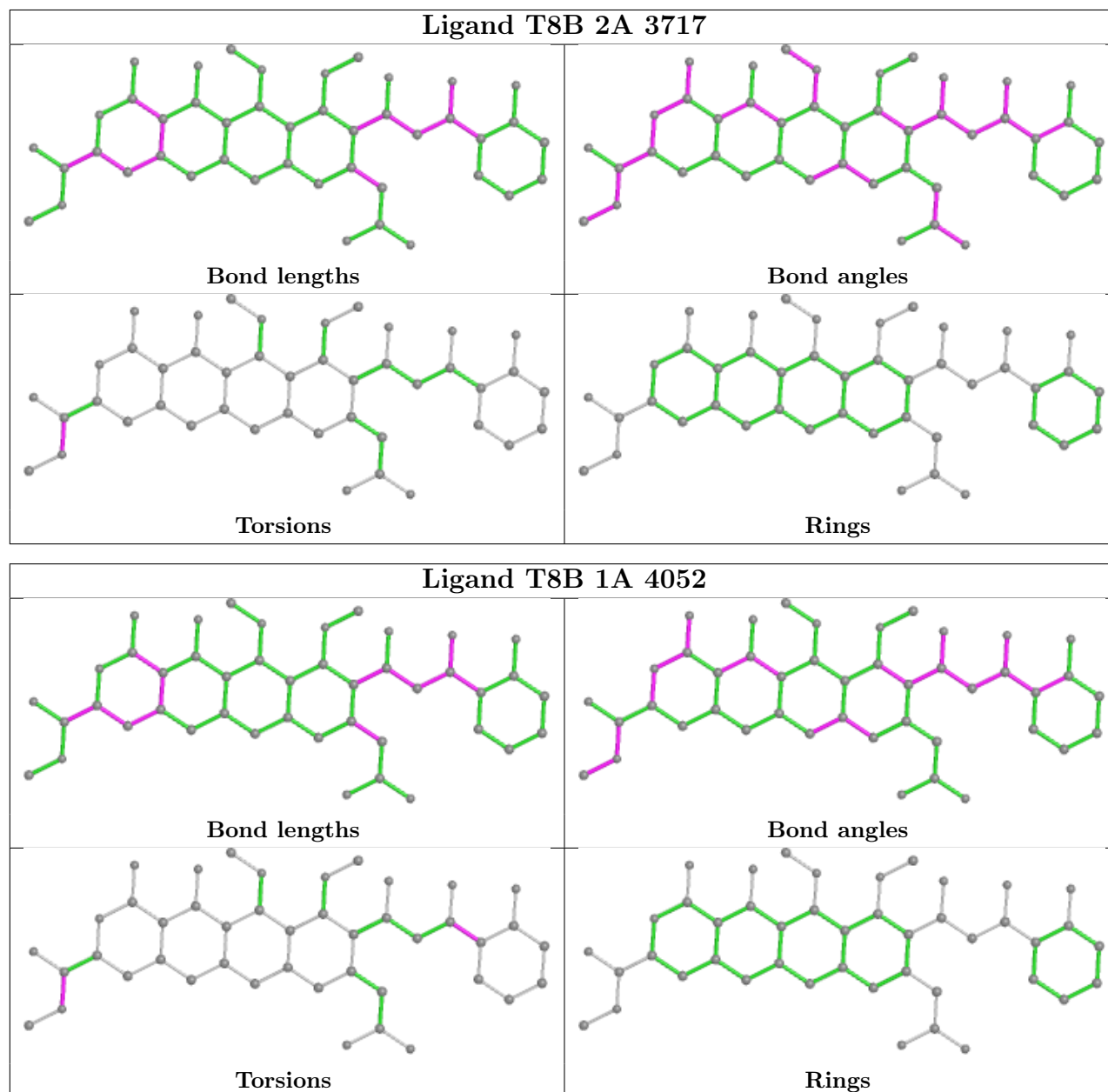
Mol	Chain	Res	Type	Atoms
57	1A	4052	T8B	C11-C12-O4-C13
57	1A	4052	T8B	O3-C12-O4-C13
57	2A	3717	T8B	C11-C12-O4-C13
57	1A	4052	T8B	C25-C26-C27-C28

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 ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

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, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	1A	2860/2915 (98%)	0.15	101 (3%) 44 44	18, 34, 94, 109	0
1	2A	2789/2915 (95%)	0.08	84 (3%) 50 51	29, 54, 92, 108	0
2	1B	120/121 (99%)	-0.31	0 100 100	27, 48, 64, 86	0
2	2B	120/121 (99%)	-0.46	0 100 100	57, 80, 90, 94	0
3	1D	275/276 (99%)	0.27	2 (0%) 87 89	18, 33, 49, 78	0
3	2D	275/276 (99%)	0.39	2 (0%) 87 89	27, 46, 58, 75	0
4	1E	204/206 (99%)	0.19	0 100 100	16, 38, 60, 81	0
4	2E	204/206 (99%)	0.34	2 (0%) 82 83	29, 55, 68, 79	0
5	1F	203/210 (96%)	0.19	1 (0%) 91 92	16, 40, 66, 87	0
5	2F	203/210 (96%)	0.31	1 (0%) 91 92	32, 64, 78, 85	0
6	1G	181/182 (99%)	0.03	3 (1%) 70 72	38, 55, 73, 87	0
6	2G	181/182 (99%)	0.60	18 (9%) 7 5	64, 79, 86, 92	0
7	1H	174/180 (96%)	-0.06	1 (0%) 89 91	38, 53, 66, 70	0
7	2H	174/180 (96%)	2.26	89 (51%) 0 0	66, 80, 88, 94	0
8	1I	146/148 (98%)	0.22	2 (1%) 75 77	41, 68, 79, 84	0
8	2I	146/148 (98%)	0.13	3 (2%) 63 65	50, 72, 81, 89	0
9	1N	140/140 (100%)	0.12	0 100 100	26, 39, 59, 73	0
9	2N	140/140 (100%)	0.53	8 (5%) 23 22	41, 62, 77, 84	0
10	1O	122/122 (100%)	0.29	0 100 100	25, 39, 56, 64	0
10	2O	122/122 (100%)	0.30	1 (0%) 86 87	41, 52, 64, 72	0
11	1P	149/150 (99%)	0.26	1 (0%) 87 89	19, 42, 65, 74	0
11	2P	149/150 (99%)	1.28	29 (19%) 1 0	33, 64, 80, 91	0
12	1Q	141/141 (100%)	0.29	1 (0%) 87 89	24, 38, 52, 67	0
12	2Q	141/141 (100%)	0.67	12 (8%) 10 9	41, 60, 72, 78	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
13	1R	118/118 (100%)	0.20	0 100 100	22, 34, 50, 57	0
13	2R	118/118 (100%)	0.24	0 100 100	37, 49, 59, 69	0
14	1S	110/112 (98%)	0.02	0 100 100	34, 47, 59, 64	0
14	2S	110/112 (98%)	0.71	9 (8%) 11 9	60, 74, 82, 88	0
15	1T	131/146 (89%)	0.10	0 100 100	31, 43, 68, 74	0
15	2T	131/146 (89%)	0.33	1 (0%) 86 87	47, 56, 73, 80	0
16	1U	116/118 (98%)	0.23	1 (0%) 84 85	20, 31, 50, 68	0
16	2U	116/118 (98%)	0.43	3 (2%) 56 57	40, 57, 71, 79	0
17	1V	101/101 (100%)	-0.02	0 100 100	21, 41, 57, 66	0
17	2V	101/101 (100%)	0.21	1 (0%) 82 83	40, 68, 75, 79	0
18	1W	112/113 (99%)	0.15	0 100 100	21, 31, 52, 80	0
18	2W	112/113 (99%)	0.32	0 100 100	37, 48, 67, 83	0
19	1X	95/96 (98%)	0.24	1 (1%) 80 82	24, 36, 60, 78	0
19	2X	95/96 (98%)	0.27	1 (1%) 80 82	45, 58, 74, 85	0
20	1Y	107/110 (97%)	0.09	0 100 100	37, 50, 71, 78	0
20	2Y	107/110 (97%)	0.46	5 (4%) 31 30	54, 70, 80, 90	0
21	1Z	154/206 (74%)	0.21	2 (1%) 77 78	39, 58, 75, 81	0
21	2Z	160/206 (77%)	0.68	17 (10%) 6 4	65, 77, 87, 91	0
22	10	75/85 (88%)	0.25	0 100 100	24, 36, 54, 62	0
22	20	77/85 (90%)	1.18	12 (15%) 2 1	41, 60, 72, 73	0
23	11	97/98 (98%)	0.40	3 (3%) 49 49	23, 42, 68, 72	0
23	21	97/98 (98%)	0.59	4 (4%) 37 36	39, 53, 74, 78	0
24	12	70/72 (97%)	0.18	0 100 100	31, 46, 58, 72	0
24	22	70/72 (97%)	-0.04	0 100 100	57, 68, 74, 76	0
25	13	59/60 (98%)	0.06	1 (1%) 70 72	24, 36, 56, 68	0
25	23	59/60 (98%)	0.64	2 (3%) 45 45	47, 60, 77, 83	0
26	14	69/71 (97%)	0.04	1 (1%) 75 77	53, 74, 88, 91	0
26	24	69/71 (97%)	0.59	6 (8%) 10 8	79, 86, 93, 95	0
27	15	59/60 (98%)	0.19	1 (1%) 70 72	20, 34, 60, 64	0
27	25	59/60 (98%)	0.09	0 100 100	33, 51, 66, 84	0
28	16	53/54 (98%)	0.10	1 (1%) 66 69	29, 39, 56, 58	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
28	26	53/54 (98%)	0.63	3 (5%) 23 22	46, 58, 67, 73	0
29	17	48/49 (97%)	0.38	1 (2%) 63 65	20, 24, 49, 57	0
29	27	48/49 (97%)	0.48	1 (2%) 63 65	30, 38, 63, 69	0
30	18	64/65 (98%)	0.30	0 100 100	25, 31, 41, 47	0
30	28	64/65 (98%)	1.35	13 (20%) 1 0	43, 52, 59, 63	0
31	19	37/37 (100%)	0.37	0 100 100	29, 40, 56, 60	0
31	29	37/37 (100%)	2.24	18 (48%) 0 0	56, 63, 74, 78	0
32	1a	1488/1521 (97%)	0.10	62 (4%) 36 35	33, 68, 94, 106	0
32	2a	1491/1521 (98%)	0.11	54 (3%) 42 42	40, 75, 95, 107	0
33	1b	231/256 (90%)	0.73	24 (10%) 6 4	64, 79, 88, 91	0
33	2b	231/256 (90%)	1.06	45 (19%) 1 0	69, 83, 89, 95	0
34	1c	206/239 (86%)	0.95	31 (15%) 2 1	61, 75, 83, 87	0
34	2c	206/239 (86%)	1.64	71 (34%) 0 0	73, 82, 88, 90	0
35	1d	208/209 (99%)	0.25	9 (4%) 35 33	56, 70, 82, 86	0
35	2d	208/209 (99%)	0.72	18 (8%) 10 8	60, 71, 79, 89	0
36	1e	148/162 (91%)	0.21	0 100 100	50, 63, 74, 82	0
36	2e	148/162 (91%)	0.61	9 (6%) 21 20	59, 72, 79, 86	0
37	1f	100/101 (99%)	0.22	4 (4%) 38 37	57, 68, 76, 80	0
37	2f	100/101 (99%)	-0.01	1 (1%) 82 83	58, 69, 77, 80	0
38	1g	155/156 (99%)	1.13	29 (18%) 1 0	60, 71, 85, 93	0
38	2g	155/156 (99%)	1.42	42 (27%) 0 0	70, 78, 87, 92	0
39	1h	137/138 (99%)	0.19	1 (0%) 87 89	53, 66, 73, 78	0
39	2h	137/138 (99%)	0.18	1 (0%) 87 89	63, 72, 78, 83	0
40	1i	127/128 (99%)	1.77	55 (43%) 0 0	56, 78, 85, 87	0
40	2i	127/128 (99%)	2.95	92 (72%) 0 0	69, 84, 90, 93	0
41	1j	97/105 (92%)	1.84	41 (42%) 0 0	59, 80, 85, 89	0
41	2j	96/105 (91%)	2.42	54 (56%) 0 0	72, 85, 90, 91	0
42	1k	114/129 (88%)	0.64	6 (5%) 26 25	42, 65, 76, 80	0
42	2k	114/129 (88%)	0.51	9 (7%) 12 10	53, 71, 80, 85	0
43	1l	121/132 (91%)	0.22	3 (2%) 57 59	45, 55, 68, 72	0
43	2l	121/132 (91%)	0.53	7 (5%) 23 22	54, 62, 70, 77	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
44	1m	123/126 (97%)	1.17	26 (21%) 1 0	56, 73, 81, 98	0
44	2m	122/126 (96%)	1.50	33 (27%) 0 0	71, 84, 90, 95	0
45	1n	60/61 (98%)	1.87	26 (43%) 0 0	61, 71, 78, 80	0
45	2n	60/61 (98%)	3.48	49 (81%) 0 0	74, 82, 86, 89	0
46	1o	88/89 (98%)	0.14	1 (1%) 80 82	47, 64, 75, 79	0
46	2o	88/89 (98%)	-0.00	0 100 100	57, 68, 76, 83	0
47	1p	82/88 (93%)	1.17	15 (18%) 1 1	58, 71, 81, 86	0
47	2p	82/88 (93%)	0.52	4 (4%) 29 28	59, 67, 77, 80	0
48	1q	99/105 (94%)	0.43	2 (2%) 65 67	54, 65, 74, 77	0
48	2q	99/105 (94%)	0.27	1 (1%) 82 83	58, 69, 76, 81	0
49	1r	68/88 (77%)	0.44	3 (4%) 34 33	56, 68, 77, 80	0
49	2r	68/88 (77%)	0.34	1 (1%) 73 76	62, 69, 79, 83	0
50	1s	83/93 (89%)	0.73	7 (8%) 11 9	66, 76, 84, 87	0
50	2s	83/93 (89%)	1.21	17 (20%) 1 0	78, 86, 92, 94	0
51	1t	96/106 (90%)	0.88	19 (19%) 1 0	61, 70, 77, 84	0
51	2t	96/106 (90%)	0.80	13 (13%) 3 2	58, 67, 78, 83	0
52	1u	23/27 (85%)	2.48	13 (56%) 0 0	64, 68, 75, 78	0
52	2u	23/27 (85%)	2.19	12 (52%) 0 0	74, 81, 84, 86	0
53	1v	5/21 (23%)	1.02	0 100 100	46, 49, 75, 81	0
53	2v	5/21 (23%)	0.87	1 (20%) 1 0	64, 70, 86, 93	0
54	1x	72/77 (93%)	-0.03	0 100 100	32, 55, 74, 86	0
54	2x	72/77 (93%)	-0.22	1 (1%) 75 77	46, 74, 84, 96	0
All	All	20580/21438 (95%)	0.38	1381 (6%) 17 16	16, 61, 87, 109	0

All (1381) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
44	2m	124	PRO	27.0
44	1m	123	ALA	14.4
44	1m	124	PRO	14.2
44	2m	123	ALA	14.2
38	2g	82	GLY	9.5
44	2m	102	ARG	8.7
44	1m	122	LYS	8.4

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Mol	Chain	Res	Type	RSRZ
44	2m	122	LYS	8.2
40	2i	66	ARG	8.0
38	2g	81	GLY	7.7
40	2i	14	VAL	7.5
41	1j	98	ILE	7.3
40	2i	5	TYR	7.2
45	2n	39	LEU	7.1
20	2Y	1	MET	7.0
38	1g	85	TYR	7.0
33	2b	165	VAL	7.0
38	2g	156	TRP	7.0
40	2i	115	GLY	7.0
38	1g	156	TRP	7.0
38	2g	154	TYR	6.9
45	2n	59	ALA	6.9
7	2H	115	VAL	6.9
38	1g	80	VAL	6.8
38	2g	16	LEU	6.8
45	2n	34	TYR	6.7
41	2j	55	LYS	6.7
7	2H	52	VAL	6.7
45	1n	2	ALA	6.6
1	1A	2115	G	6.6
31	29	37	GLY	6.6
40	1i	106	ALA	6.6
38	1g	154	TYR	6.5
1	2A	2133	G	6.5
40	2i	36	TYR	6.4
1	2A	2111	C	6.4
41	2j	47	PHE	6.4
34	2c	87	LEU	6.4
41	2j	46	ARG	6.3
44	2m	121	LYS	6.3
45	2n	35	ARG	6.3
45	2n	29	ARG	6.2
40	2i	106	ALA	6.2
1	1A	2117	A	6.2
38	1g	79	ARG	6.2
52	2u	14	TRP	6.2
1	1A	2121	G	6.2
7	2H	35	VAL	6.2
1	1A	2178	C	6.1

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Mol	Chain	Res	Type	RSRZ
44	1m	96	LEU	6.1
1	1A	1065	U	6.1
45	2n	25	VAL	6.0
1	1A	2145	C	6.0
40	2i	7	THR	6.0
1	2A	2113	U	6.0
40	2i	125	TYR	6.0
7	2H	107	VAL	6.0
32	2a	1035	A	6.0
1	2A	2160	G	5.9
41	2j	65	LEU	5.9
44	2m	120	LYS	5.9
44	2m	6	GLY	5.9
44	1m	102	ARG	5.9
33	1b	133	LYS	5.9
1	1A	1064	C	5.9
3	1D	276	LYS	5.8
7	2H	24	VAL	5.8
41	2j	50	ILE	5.8
1	2A	2147	G	5.8
40	2i	127	LYS	5.8
38	1g	78	ARG	5.7
1	2A	2170	A	5.7
45	2n	53	LEU	5.7
45	2n	2	ALA	5.7
38	2g	79	ARG	5.7
41	2j	6	ILE	5.6
1	1A	1095	A	5.6
32	2a	1036	G	5.6
1	1A	1096	A	5.6
40	1i	19	LEU	5.6
45	2n	38	GLY	5.6
1	2A	2117	A	5.5
1	1A	2159	G	5.5
1	2A	2112	G	5.5
38	2g	80	VAL	5.4
1	2A	2159	G	5.4
33	2b	48	MET	5.4
34	2c	160	ALA	5.3
32	2a	1257	U	5.3
22	20	8	GLY	5.3
45	2n	10	ALA	5.3

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Mol	Chain	Res	Type	RSRZ
45	2n	22	THR	5.3
45	2n	61	TRP	5.3
7	2H	37	VAL	5.3
1	2A	2128	C	5.3
1	2A	2145	C	5.3
41	1j	10	GLY	5.3
44	2m	4	ILE	5.2
41	1j	8	LEU	5.2
41	2j	49	VAL	5.2
32	2a	1030(B)	C	5.2
33	2b	101	MET	5.2
52	1u	13	ILE	5.2
45	2n	12	ARG	5.2
1	1A	2119	A	5.2
7	2H	71	LEU	5.2
41	2j	34	VAL	5.1
1	2A	2174	C	5.1
40	1i	8	GLY	5.1
26	24	49	PHE	5.1
1	1A	2120	G	5.1
1	2A	2127	G	5.1
45	2n	31	ARG	5.1
41	1j	7	LYS	5.1
7	2H	44	VAL	5.1
40	2i	53	VAL	5.1
40	2i	63	ILE	5.0
50	1s	39	THR	5.0
1	2A	2132	U	5.0
32	1a	204	U	5.0
45	2n	41	ARG	5.0
23	21	2	SER	5.0
1	1A	2110	G	5.0
1	1A	2170	A	5.0
1	1A	2140	C	5.0
40	2i	123	PRO	5.0
34	1c	201	TYR	4.9
1	1A	2109	U	4.9
45	2n	58	LYS	4.9
1	2A	2155	G	4.9
11	2P	79	ARG	4.9
1	2A	2110	G	4.9
47	1p	68	ASP	4.9

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Mol	Chain	Res	Type	RSRZ
32	1a	1030(B)	C	4.9
40	1i	5	TYR	4.9
1	1A	1094	U	4.8
1	1A	2113	U	4.8
52	1u	15	ARG	4.8
40	2i	19	LEU	4.8
44	2m	90	LEU	4.8
45	2n	11	LYS	4.8
1	1A	2112	G	4.8
32	1a	1447	A	4.8
38	1g	153	HIS	4.8
41	2j	44	VAL	4.8
52	1u	6	ARG	4.8
38	2g	27	ILE	4.8
41	2j	85	LEU	4.8
32	1a	1257	U	4.8
11	2P	109	GLY	4.7
45	2n	42	ILE	4.7
1	1A	2146	C	4.7
41	1j	71	LEU	4.7
40	1i	109	VAL	4.7
45	2n	44	LEU	4.7
40	2i	110	GLU	4.7
38	1g	155	ARG	4.7
40	2i	9	ARG	4.7
1	2A	2116	G	4.7
1	2A	2115	G	4.7
44	1m	105	THR	4.7
45	2n	37	PHE	4.7
40	1i	65	VAL	4.7
40	2i	28	VAL	4.7
1	2A	2125	G	4.6
35	2d	49	ARG	4.6
1	2A	2108	C	4.6
31	29	16	VAL	4.6
34	2c	4	LYS	4.6
44	1m	2	ALA	4.6
1	1A	2174	C	4.6
7	2H	43	VAL	4.6
1	2A	2104	G	4.6
33	1b	214	ILE	4.6
7	2H	2	SER	4.6

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Mol	Chain	Res	Type	RSRZ
33	2b	232	PRO	4.6
52	1u	14	TRP	4.6
40	2i	15	ALA	4.6
45	2n	57	ARG	4.5
7	2H	94	TYR	4.5
11	2P	68	GLN	4.5
34	2c	198	VAL	4.5
45	2n	56	VAL	4.5
34	2c	57	ILE	4.5
1	1A	2141	G	4.5
32	1a	1026	G	4.5
41	1j	60	ARG	4.5
1	1A	2114	A	4.5
40	2i	46	ALA	4.5
41	1j	47	PHE	4.5
51	2t	24	LEU	4.5
1	2A	2166	G	4.5
1	2A	2138	C	4.5
40	2i	117	HIS	4.5
40	2i	81	ILE	4.5
1	2A	2118	U	4.5
21	2Z	174	VAL	4.5
7	2H	6	ARG	4.4
26	24	40	HIS	4.4
34	2c	167	TRP	4.4
40	2i	18	PHE	4.4
40	2i	26	VAL	4.4
1	2A	2175	C	4.4
40	1i	126	SER	4.4
40	2i	79	LEU	4.4
7	2H	123	PHE	4.4
34	2c	190	ARG	4.4
41	2j	48	THR	4.4
1	1A	1087	G	4.4
40	2i	92	TYR	4.4
34	1c	87	LEU	4.4
41	2j	62	HIS	4.4
40	2i	21	PRO	4.4
1	1A	2169	A	4.4
1	2A	2114	A	4.4
7	2H	133	VAL	4.3
40	1i	4	TYR	4.3

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Mol	Chain	Res	Type	RSRZ
34	2c	187	ALA	4.3
32	1a	1001(A)	G	4.3
38	1g	84	ASN	4.3
1	1A	2125	G	4.3
40	2i	65	VAL	4.3
40	2i	59	PHE	4.3
52	2u	13	ILE	4.3
50	2s	41	VAL	4.3
45	1n	33	VAL	4.3
45	2n	33	VAL	4.3
16	1U	117	GLN	4.3
40	1i	114	TYR	4.3
7	2H	42	ARG	4.2
1	2A	2158	A	4.2
1	2A	2168	G	4.2
40	2i	109	VAL	4.2
1	2A	2146	C	4.2
31	29	19	ARG	4.2
22	20	9	SER	4.2
7	2H	96	ALA	4.2
21	2Z	143	GLY	4.2
47	1p	80	PHE	4.2
1	2A	2157	G	4.1
38	2g	78	ARG	4.1
41	2j	96	ILE	4.1
7	2H	113	VAL	4.1
40	2i	105	ASP	4.1
44	1m	87	TYR	4.1
33	1b	222	ILE	4.1
12	2Q	121	ALA	4.1
47	1p	7	ALA	4.1
41	1j	65	LEU	4.1
45	1n	32	SER	4.1
52	2u	16	GLY	4.1
7	2H	111	HIS	4.1
40	2i	121	ARG	4.1
1	1A	2147	G	4.1
41	1j	45	ARG	4.1
32	2a	1034	G	4.1
34	2c	124	ILE	4.0
38	2g	32	ARG	4.0
33	2b	69	LEU	4.0

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Mol	Chain	Res	Type	RSRZ
40	2i	47	LEU	4.0
21	2Z	153	SER	4.0
1	2A	2122	U	4.0
7	2H	103	LEU	4.0
1	2A	2131	G	4.0
11	2P	78	PRO	4.0
1	1A	1078	U	4.0
41	2j	63	PHE	4.0
38	1g	81	GLY	4.0
41	1j	72	VAL	4.0
52	1u	3	LYS	4.0
40	1i	7	THR	4.0
6	1G	48	GLU	4.0
40	2i	10	ARG	4.0
40	2i	83	ARG	4.0
47	1p	1	MET	4.0
50	2s	71	LEU	4.0
21	2Z	171	ILE	4.0
42	1k	25	TYR	4.0
41	1j	46	ARG	4.0
1	2A	2109	U	4.0
1	1A	2111	C	4.0
33	2b	152	PHE	4.0
40	2i	72	GLY	3.9
42	2k	126	ARG	3.9
51	2t	25	ARG	3.9
41	2j	58	ASP	3.9
32	2a	1131	G	3.9
40	1i	59	PHE	3.9
45	1n	29	ARG	3.9
7	2H	128	PRO	3.9
31	29	13	LYS	3.9
1	1A	1066	U	3.9
1	1A	2122	U	3.9
40	2i	45	ALA	3.9
7	2H	106	THR	3.9
33	2b	187	LEU	3.9
26	24	51	ASP	3.9
7	2H	141	VAL	3.9
40	2i	64	THR	3.9
7	2H	89	ILE	3.9
32	2a	1357	A	3.9

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Mol	Chain	Res	Type	RSRZ
41	2j	98	ILE	3.9
1	1A	2151	G	3.9
1	2A	2123	G	3.9
22	20	55	ARG	3.9
41	1j	66	ARG	3.9
40	2i	4	TYR	3.9
7	2H	9	ILE	3.9
33	2b	122	PHE	3.9
38	1g	151	TYR	3.8
50	2s	80	TYR	3.8
38	1g	2	ALA	3.8
1	2A	2164	C	3.8
32	1a	1001	A	3.8
41	2j	64	GLU	3.8
41	1j	50	ILE	3.8
44	2m	103	THR	3.8
41	2j	60	ARG	3.8
45	2n	23	ARG	3.8
1	1A	899	A	3.8
40	2i	77	ILE	3.8
44	1m	104	ARG	3.8
33	2b	70	PHE	3.8
1	1A	2133	G	3.8
34	2c	60	ALA	3.8
1	2A	652(B)	A	3.8
14	2S	32	LEU	3.7
23	1l	98	LEU	3.7
44	2m	104	ARG	3.7
51	1t	14	LYS	3.7
32	1a	1002	G	3.7
38	1g	124	LEU	3.7
26	24	32	TYR	3.7
33	2b	127	ILE	3.7
34	1c	184	TYR	3.7
41	2j	43	ARG	3.7
1	1A	2128	C	3.7
52	2u	22	ARG	3.7
34	2c	159	GLY	3.7
1	1A	886	C	3.7
1	1A	2179	C	3.7
34	2c	171	GLY	3.7
41	2j	10	GLY	3.7

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Mol	Chain	Res	Type	RSRZ
34	2c	71	ALA	3.7
32	1a	1028	C	3.7
44	2m	78	ILE	3.7
40	1i	30	GLY	3.7
34	2c	186	PHE	3.7
44	2m	98	VAL	3.7
1	1A	2175	C	3.7
11	2P	65	ARG	3.6
40	2i	76	ALA	3.6
36	2e	90	VAL	3.6
52	1u	17	THR	3.6
1	2A	2129	C	3.6
32	1a	1027	C	3.6
7	2H	101	ARG	3.6
34	2c	54	ARG	3.6
45	2n	36	PHE	3.6
32	2a	1002	G	3.6
41	2j	56	HIS	3.6
31	29	15	LYS	3.6
1	2A	2169	A	3.6
1	1A	2132	U	3.6
1	1A	2142	C	3.6
45	2n	15	LYS	3.6
52	1u	16	GLY	3.6
1	1A	2116	G	3.6
32	1a	1036	G	3.6
1	2A	2135	A	3.6
32	2a	1363(A)	A	3.6
40	1i	120	ARG	3.6
39	1h	2	LEU	3.6
41	2j	8	LEU	3.6
44	2m	60	VAL	3.6
1	1A	1099	G	3.6
44	2m	106	ASN	3.6
51	1t	72	LEU	3.6
7	2H	145	ALA	3.6
40	2i	82	ALA	3.6
22	20	45	PHE	3.6
1	1A	2130	U	3.6
7	2H	88	LEU	3.6
22	20	52	GLY	3.6
43	1l	91	LYS	3.6

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Mol	Chain	Res	Type	RSRZ
38	1g	16	LEU	3.6
38	2g	4	ARG	3.5
40	1i	9	ARG	3.5
50	2s	49	ILE	3.5
41	2j	40	LEU	3.5
1	1A	2180	U	3.5
32	2a	1532	U	3.5
6	2G	92	VAL	3.5
7	2H	7	LEU	3.5
7	2H	105	LEU	3.5
1	2A	2121	G	3.5
34	2c	149	ALA	3.5
38	2g	2	ALA	3.5
32	1a	1532	U	3.5
34	1c	39	ILE	3.5
34	2c	155	GLY	3.5
34	2c	182	ILE	3.5
21	2Z	144	LEU	3.5
44	1m	48	LEU	3.5
44	1m	121	LYS	3.5
45	1n	37	PHE	3.5
45	2n	50	LYS	3.5
44	1m	107	ALA	3.5
7	2H	84	SER	3.5
35	2d	168	ARG	3.5
1	1A	2177	C	3.5
41	1j	34	VAL	3.5
1	1A	2189	U	3.5
41	1j	54	PHE	3.5
1	2A	2143	C	3.5
6	2G	136	ARG	3.5
11	2P	85	LEU	3.5
32	1a	1039	C	3.5
40	2i	40	LEU	3.5
1	2A	2150	U	3.4
40	1i	15	ALA	3.4
1	2A	2165	G	3.4
33	2b	197	VAL	3.4
40	2i	20	ARG	3.4
1	1A	2129	C	3.4
44	1m	120	LYS	3.4
51	2t	9	ASN	3.4

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Mol	Chain	Res	Type	RSRZ
40	1i	37	PHE	3.4
11	2P	108	LYS	3.4
51	1t	18	GLN	3.4
1	1A	2138	C	3.4
41	2j	54	PHE	3.4
7	2H	95	ARG	3.4
34	2c	189	ALA	3.4
38	1g	4	ARG	3.4
38	2g	151	TYR	3.4
45	2n	45	ARG	3.4
1	1A	1081	U	3.4
32	1a	1040	U	3.4
40	2i	17	VAL	3.4
34	2c	134	ILE	3.4
44	2m	119	GLY	3.4
1	2A	2120	G	3.4
32	2a	1202	G	3.4
40	2i	88	TYR	3.4
40	2i	108	VAL	3.4
51	1t	55	ILE	3.4
32	2a	1116	C	3.4
38	2g	83	ALA	3.4
44	2m	75	ALA	3.4
11	2P	45	LEU	3.4
7	2H	69	ARG	3.4
38	2g	40	ALA	3.4
41	1j	57	LYS	3.4
1	2A	2107	C	3.4
43	2l	64	TYR	3.4
33	2b	149	LEU	3.4
34	2c	158	GLY	3.4
7	2H	45	VAL	3.4
3	2D	276	LYS	3.3
32	2a	1001(A)	G	3.3
41	2j	74	ILE	3.3
50	2s	40	ILE	3.3
45	2n	6	LEU	3.3
1	1A	2158	A	3.3
34	2c	14	ILE	3.3
1	2A	2148	G	3.3
45	1n	59	ALA	3.3
40	1i	110	GLU	3.3

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Mol	Chain	Res	Type	RSRZ
7	2H	36	PRO	3.3
35	2d	73	ARG	3.3
41	2j	41	PRO	3.3
7	2H	83	TYR	3.3
11	1P	105	LEU	3.3
33	2b	118	LEU	3.3
32	2a	1149	C	3.3
34	2c	39	ILE	3.3
1	1A	2135	A	3.3
1	1A	2173	A	3.3
1	2A	2134	A	3.3
40	2i	70	LYS	3.3
31	29	12	ASP	3.3
38	2g	153	HIS	3.3
41	1j	63	PHE	3.3
7	2H	3	ARG	3.3
34	1c	168	ALA	3.3
41	2j	52	GLY	3.3
52	2u	11	GLY	3.3
1	1A	2167	U	3.3
36	2e	12	LEU	3.3
40	1i	14	VAL	3.3
32	2a	1030(A)	G	3.3
31	29	17	ILE	3.3
40	1i	11	LYS	3.3
52	2u	15	ARG	3.3
1	1A	2108	C	3.3
44	2m	5	ALA	3.3
38	2g	89	MET	3.3
41	1j	68	HIS	3.3
41	2j	38	ILE	3.3
1	2A	2162	G	3.3
41	1j	40	LEU	3.3
1	1A	1060	U	3.3
9	2N	9	VAL	3.3
40	2i	43	ALA	3.3
7	2H	112	PRO	3.3
1	1A	2101	G	3.3
11	2P	70	GLN	3.3
32	1a	1029	C	3.2
32	2a	1040	U	3.2
21	2Z	146	ILE	3.2

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Mol	Chain	Res	Type	RSRZ
34	2c	8	ILE	3.2
33	1b	123	ALA	3.2
44	1m	97	PRO	3.2
47	1p	6	LEU	3.2
7	2H	82	GLY	3.2
33	1b	122	PHE	3.2
45	1n	15	LYS	3.2
1	2A	1026	U	3.2
7	2H	166	GLY	3.2
34	1c	124	ILE	3.2
34	2c	77	ILE	3.2
1	2A	2106	G	3.2
34	1c	200	ALA	3.2
34	2c	59	ARG	3.2
7	2H	25	LYS	3.2
45	1n	50	LYS	3.2
40	1i	66	ARG	3.2
40	2i	124	GLN	3.2
1	2A	2136	C	3.2
1	2A	2167	U	3.2
6	2G	152	LEU	3.2
34	2c	21	ARG	3.2
45	1n	21	TYR	3.2
1	2A	2139	C	3.2
36	2e	18	ARG	3.2
43	1l	89	ARG	3.2
7	2H	169	VAL	3.2
34	2c	66	VAL	3.2
33	2b	200	ILE	3.2
1	1A	1057	A	3.2
1	1A	2143	C	3.2
11	2P	71	VAL	3.2
1	1A	2181	G	3.2
40	2i	119	ALA	3.2
1	2A	2144	U	3.1
1	2A	2173	A	3.1
34	2c	191	THR	3.1
34	2c	192	THR	3.1
40	1i	18	PHE	3.1
34	2c	65	ALA	3.1
40	2i	61	ALA	3.1
1	1A	1058	G	3.1

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Mol	Chain	Res	Type	RSRZ
6	2G	115	ARG	3.1
33	2b	155	LEU	3.1
32	2a	1026	G	3.1
33	2b	133	LYS	3.1
41	1j	55	LYS	3.1
32	1a	1035	A	3.1
38	2g	76	ARG	3.1
40	1i	115	GLY	3.1
40	2i	51	ARG	3.1
22	20	75	LEU	3.1
50	1s	38	SER	3.1
45	2n	8	GLU	3.1
32	1a	202	U	3.1
41	2j	66	ARG	3.1
7	2H	33	LEU	3.1
33	2b	201	ILE	3.1
7	2H	159	GLU	3.1
40	1i	6	GLY	3.1
34	2c	3	ASN	3.1
41	1j	69	ASN	3.1
34	1c	196	LEU	3.1
35	2d	78	LEU	3.1
38	2g	42	ILE	3.1
1	2A	229	A	3.1
51	1t	80	ARG	3.1
41	2j	67	THR	3.1
6	2G	157	ILE	3.1
11	2P	105	LEU	3.1
40	1i	63	ILE	3.1
1	1A	1068	G	3.1
1	1A	2100	G	3.1
32	2a	1224	G	3.1
40	2i	90	PRO	3.1
35	1d	3	ARG	3.1
38	2g	115	ARG	3.1
34	1c	55	VAL	3.1
38	2g	37	ASN	3.1
19	2X	92	LEU	3.1
31	29	5	ALA	3.1
7	2H	72	ILE	3.1
40	2i	62	TYR	3.1
45	1n	3	ARG	3.1

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Mol	Chain	Res	Type	RSRZ
52	2u	6	ARG	3.1
33	2b	163	PHE	3.1
1	2A	652(T)	C	3.1
32	1a	1531	A	3.1
12	2Q	22	LYS	3.1
41	2j	45	ARG	3.1
40	2i	114	TYR	3.0
42	2k	25	TYR	3.0
22	20	69	PHE	3.0
44	1m	103	THR	3.0
6	2G	95	ARG	3.0
7	2H	85	LYS	3.0
45	1n	39	LEU	3.0
45	1n	41	ARG	3.0
41	1j	49	VAL	3.0
45	1n	31	ARG	3.0
30	28	41	ILE	3.0
1	1A	1100	C	3.0
34	1c	185	GLY	3.0
6	2G	146	TYR	3.0
38	2g	155	ARG	3.0
44	2m	105	THR	3.0
1	1A	2118	U	3.0
34	2c	154	SER	3.0
7	2H	67	LEU	3.0
33	2b	131	PRO	3.0
45	1n	34	TYR	3.0
1	1A	885	C	3.0
32	2a	1019	C	3.0
41	2j	59	SER	3.0
6	2G	62	LEU	3.0
7	2H	165	ALA	3.0
14	2S	35	ILE	3.0
7	2H	53	GLU	3.0
41	2j	68	HIS	3.0
51	1t	25	ARG	3.0
1	1A	2131	G	3.0
1	1A	2160	G	3.0
27	15	60	VAL	3.0
32	1a	1037	C	3.0
45	2n	54	PRO	3.0
31	29	26	ILE	3.0

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Mol	Chain	Res	Type	RSRZ
45	2n	7	ILE	3.0
41	1j	5	ARG	3.0
41	1j	9	ARG	3.0
44	1m	108	ARG	3.0
44	2m	66	LEU	3.0
34	2c	7	PRO	3.0
1	2A	2130	U	3.0
33	2b	130	ARG	3.0
33	2b	92	TYR	3.0
33	1b	98	LEU	3.0
51	2t	13	LEU	3.0
1	2A	2137	C	2.9
38	1g	120	ILE	2.9
32	1a	1003	G	2.9
9	2N	10	GLU	2.9
45	2n	13	THR	2.9
33	1b	232	PRO	2.9
40	2i	116	LYS	2.9
51	1t	74	LYS	2.9
41	2j	23	ILE	2.9
7	2H	116	GLU	2.9
45	2n	16	PHE	2.9
52	1u	10	ARG	2.9
33	2b	135	GLN	2.9
40	1i	122	ALA	2.9
34	2c	152	ILE	2.9
20	2Y	60	PHE	2.9
1	2A	2151	G	2.9
14	2S	37	ALA	2.9
44	1m	4	ILE	2.9
12	2Q	59	ARG	2.9
30	28	46	ARG	2.9
11	2P	118	GLY	2.9
14	2S	58	LEU	2.9
50	2s	79	THR	2.9
11	2P	67	MET	2.9
38	1g	87	VAL	2.9
30	28	2	PRO	2.9
7	2H	138	LYS	2.9
9	2N	83	LYS	2.9
1	1A	2104	G	2.9
7	2H	4	ILE	2.9

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Mol	Chain	Res	Type	RSRZ
40	2i	93	ARG	2.9
40	2i	128	ARG	2.9
40	2i	37	PHE	2.9
34	2c	179	ARG	2.9
45	2n	55	GLY	2.9
8	2l	75	LEU	2.9
40	1i	79	LEU	2.9
49	1r	79	LEU	2.9
1	2A	2171	A	2.9
38	1g	61	VAL	2.9
7	2H	142	GLY	2.9
40	2i	69	GLY	2.9
31	29	1	MET	2.9
33	1b	229	VAL	2.9
40	1i	17	VAL	2.9
40	2i	44	VAL	2.9
45	2n	24	CYS	2.9
44	2m	101	GLN	2.8
32	1a	1000	U	2.8
34	2c	6	HIS	2.8
36	2e	109	ILE	2.8
40	1i	113	LYS	2.8
38	2g	22	LEU	2.8
7	2H	51	ARG	2.8
7	2H	50	VAL	2.8
16	2U	90	VAL	2.8
40	2i	8	GLY	2.8
50	2s	14	HIS	2.8
1	1A	2144	U	2.8
32	1a	1038	C	2.8
34	2c	199	LYS	2.8
34	2c	207	VAL	2.8
21	2Z	142	SER	2.8
33	2b	226	ARG	2.8
35	2d	35	ARG	2.8
38	1g	3	ARG	2.8
41	1j	96	ILE	2.8
7	2H	171	LEU	2.8
34	2c	15	THR	2.8
1	2A	2105	C	2.8
7	2H	55	PRO	2.8
31	29	31	LYS	2.8

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Mol	Chain	Res	Type	RSRZ
38	1g	22	LEU	2.8
41	1j	58	ASP	2.8
1	1A	2184	G	2.8
32	1a	1503	A	2.8
41	1j	41	PRO	2.8
1	2A	2142	C	2.8
7	2H	132	ARG	2.8
12	1Q	5	ARG	2.8
32	1a	1030	C	2.8
35	2d	4	TYR	2.8
45	1n	61	TRP	2.8
40	2i	33	PHE	2.8
41	1j	64	GLU	2.8
40	2i	85	LEU	2.8
34	2c	13	GLY	2.8
42	2k	49	GLY	2.8
29	27	48	LYS	2.8
40	1i	116	LYS	2.8
50	1s	78	ARG	2.8
1	1A	1056	G	2.8
1	1A	2148	G	2.8
1	1A	2152	G	2.8
41	1j	21	GLN	2.8
6	2G	139	LEU	2.8
42	2k	31	THR	2.8
45	2n	14	PRO	2.8
52	1u	22	ARG	2.8
11	2P	136	GLU	2.8
32	2a	1252	A	2.8
51	2t	63	ILE	2.8
1	2A	2179	C	2.8
11	2P	76	LYS	2.8
38	2g	33	ASP	2.7
38	1g	38	LEU	2.7
40	2i	120	ARG	2.7
1	1A	1069	A	2.7
32	2a	1492	A	2.7
41	1j	42	THR	2.7
45	2n	32	SER	2.7
31	29	2	LYS	2.7
41	2j	7	LYS	2.7
33	2b	115	LEU	2.7

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Mol	Chain	Res	Type	RSRZ
34	2c	23	TYR	2.7
40	2i	6	GLY	2.7
45	1n	23	ARG	2.7
32	1a	201	C	2.7
1	2A	2154	G	2.7
32	2a	1033	G	2.7
41	2j	71	LEU	2.7
44	2m	99	ARG	2.7
52	1u	9	ARG	2.7
34	2c	193	TYR	2.7
41	2j	72	VAL	2.7
32	1a	1533	C	2.7
32	2a	1037	C	2.7
40	2i	68	GLY	2.7
37	1f	21	LEU	2.7
34	2c	153	VAL	2.7
1	1A	1070	A	2.7
26	24	67	TYR	2.7
30	28	58	ILE	2.7
32	1a	90	U	2.7
33	2b	41	ILE	2.7
33	2b	214	ILE	2.7
34	2c	17	ASP	2.7
21	2Z	122	ARG	2.7
40	1i	117	HIS	2.7
45	2n	4	LYS	2.7
32	1a	1286	A	2.7
32	2a	204	U	2.7
40	2i	49	PRO	2.7
1	2A	2156	G	2.7
40	1i	108	VAL	2.7
33	1b	11	LEU	2.7
38	2g	59	LEU	2.7
22	20	57	PHE	2.7
7	2H	86	GLU	2.7
7	2H	164	TYR	2.7
41	1j	97	GLU	2.7
30	28	15	LYS	2.7
1	2A	2140	C	2.6
1	2A	2161	C	2.6
33	1b	48	MET	2.6
36	2e	31	LEU	2.6

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Mol	Chain	Res	Type	RSRZ
7	2H	34	GLU	2.6
7	2H	30	LYS	2.6
23	21	26	ARG	2.6
35	2d	47	ARG	2.6
33	2b	228	GLY	2.6
34	1c	15	THR	2.6
40	2i	67	GLY	2.6
47	1p	67	THR	2.6
1	2A	2178	C	2.6
44	1m	106	ASN	2.6
21	2Z	156	LYS	2.6
38	1g	99	LEU	2.6
51	2t	72	LEU	2.6
52	2u	10	ARG	2.6
7	2H	48	GLY	2.6
47	2p	19	ILE	2.6
41	2j	26	ALA	2.6
7	2H	76	VAL	2.6
7	2H	124	GLU	2.6
33	1b	128	GLU	2.6
35	1d	179	GLU	2.6
40	2i	78	LYS	2.6
41	1j	44	VAL	2.6
50	2s	67	VAL	2.6
12	2Q	34	LEU	2.6
37	1f	55	ASP	2.6
32	2a	1236	A	2.6
41	1j	6	ILE	2.6
51	1t	63	ILE	2.6
7	2H	12	PRO	2.6
7	2H	20	ALA	2.6
33	2b	161	ALA	2.6
1	2A	2141	G	2.6
40	2i	91	ASP	2.6
25	23	60	GLU	2.6
42	1k	92	GLU	2.6
30	28	64	TYR	2.6
1	1A	2134	A	2.6
49	1r	39	VAL	2.6
34	2c	33	LEU	2.6
40	2i	113	LYS	2.6
33	2b	97	TRP	2.6

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Mol	Chain	Res	Type	RSRZ
38	1g	42	ILE	2.6
41	2j	27	ALA	2.6
47	1p	17	TYR	2.6
7	2H	114	VAL	2.6
5	2F	181	LEU	2.6
47	2p	6	LEU	2.6
50	2s	6	LYS	2.6
4	2E	148	GLY	2.6
48	1q	7	THR	2.6
6	1G	73	ALA	2.6
51	2t	26	ASN	2.6
1	2A	2177	C	2.6
34	2c	173	VAL	2.6
41	2j	94	VAL	2.6
34	2c	127	ARG	2.6
50	1s	40	ILE	2.5
8	1I	65	ALA	2.5
33	1b	29	ALA	2.5
42	1k	68	ALA	2.5
32	2a	1017	G	2.5
50	2s	43	GLU	2.5
52	1u	18	TYR	2.5
6	2G	160	VAL	2.5
11	2P	115	LEU	2.5
34	2c	120	VAL	2.5
34	2c	195	VAL	2.5
37	1f	61	LEU	2.5
1	1A	888	C	2.5
1	1A	2107	C	2.5
32	2a	1018	C	2.5
40	1i	20	ARG	2.5
40	1i	83	ARG	2.5
40	1i	107	ARG	2.5
40	2i	126	SER	2.5
38	2g	86	GLN	2.5
50	2s	53	ASN	2.5
7	2H	148	ILE	2.5
38	2g	25	ALA	2.5
41	2j	32	ALA	2.5
6	2G	3	LEU	2.5
32	1a	1365	G	2.5
32	2a	1356	G	2.5

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Mol	Chain	Res	Type	RSRZ
33	1b	70	PHE	2.5
1	1A	2794	C	2.5
7	2H	21	PRO	2.5
9	2N	140	VAL	2.5
36	2e	25	ARG	2.5
50	2s	70	LYS	2.5
38	2g	113	GLU	2.5
1	1A	2182	G	2.5
32	1a	1030(A)	G	2.5
32	2a	951	G	2.5
1	1A	2139	C	2.5
7	2H	92	ILE	2.5
35	2d	5	ILE	2.5
40	1i	16	ARG	2.5
44	2m	23	TYR	2.5
51	1t	20	LEU	2.5
1	1A	1026	U	2.5
11	2P	149	GLU	2.5
32	1a	949	A	2.5
32	1a	1363(A)	A	2.5
33	1b	134	GLU	2.5
40	1i	33	PHE	2.5
23	1l	26	ARG	2.5
1	2A	280	C	2.5
32	1a	1033	G	2.5
32	1a	1354	C	2.5
40	2i	52	ALA	2.5
41	1j	4	ILE	2.5
47	2p	7	ALA	2.5
51	2t	28	ALA	2.5
52	1u	2	GLY	2.5
21	2Z	155	LEU	2.5
40	2i	102	LEU	2.5
34	1c	35	GLU	2.5
41	2j	97	GLU	2.5
11	2P	101	VAL	2.5
11	2P	50	ARG	2.5
19	1X	94	GLY	2.5
44	1m	100	GLY	2.5
7	2H	146	ALA	2.5
45	2n	49	HIS	2.5
6	2G	29	TRP	2.5

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Mol	Chain	Res	Type	RSRZ
47	2p	20	VAL	2.5
7	2H	157	TYR	2.5
43	1l	64	TYR	2.5
40	2i	107	ARG	2.5
1	2A	2182	G	2.5
1	2A	2172	U	2.4
11	2P	64	LYS	2.4
41	1j	20	ALA	2.4
45	1n	58	LYS	2.4
45	2n	17	LYS	2.4
8	1I	35	LEU	2.4
1	2A	2126	A	2.4
29	17	46	VAL	2.4
43	2l	18	VAL	2.4
50	2s	35	SER	2.4
41	2j	5	ARG	2.4
44	1m	94	ARG	2.4
51	1t	22	ARG	2.4
35	2d	2	GLY	2.4
31	29	33	LYS	2.4
34	2c	135	LYS	2.4
51	2t	14	LYS	2.4
11	2P	97	PRO	2.4
1	1A	1059	G	2.4
1	1A	1097	U	2.4
1	1A	2123	G	2.4
7	2H	151	ILE	2.4
21	2Z	150	LEU	2.4
28	26	11	LEU	2.4
6	2G	28	VAL	2.4
6	2G	37	VAL	2.4
43	2l	32	PHE	2.4
50	1s	12	ASP	2.4
44	2m	13	LYS	2.4
44	2m	95	GLY	2.4
36	2e	128	PRO	2.4
44	2m	97	PRO	2.4
12	2Q	107	ALA	2.4
30	28	10	ALA	2.4
32	2a	1020	U	2.4
33	2b	102	LEU	2.4
32	1a	1024	G	2.4

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Mol	Chain	Res	Type	RSRZ
40	1i	125	TYR	2.4
40	2i	98	PRO	2.4
28	16	36	LEU	2.4
1	1A	889	C	2.4
41	2j	61	GLU	2.4
7	2H	38	SER	2.4
1	2A	272(A)	U	2.4
9	2N	8	GLN	2.4
45	1n	56	VAL	2.4
34	2c	185	GLY	2.4
32	2a	80	G	2.4
40	1i	93	ARG	2.4
44	2m	92	HIS	2.4
47	1p	66	PRO	2.4
33	2b	139	LYS	2.4
44	1m	78	ILE	2.4
26	24	54	GLY	2.4
34	2c	103	VAL	2.4
51	1t	9	ASN	2.4
38	1g	26	PHE	2.4
30	28	59	LYS	2.4
34	1c	4	LYS	2.4
38	2g	6	ARG	2.4
7	2H	150	ALA	2.4
33	2b	67	THR	2.4
38	2g	24	THR	2.4
33	1b	37	ASN	2.4
45	1n	7	ILE	2.4
34	1c	64	VAL	2.4
34	1c	128	PHE	2.4
40	1i	86	VAL	2.4
45	2n	18	VAL	2.4
1	2A	2119	A	2.4
3	1D	275	LYS	2.4
5	1F	17	ARG	2.4
32	1a	1287	A	2.4
32	2a	1150	U	2.4
51	2t	23	ARG	2.4
20	2Y	5	MET	2.4
34	2c	142	MET	2.4
45	2n	21	TYR	2.4
28	26	41	PRO	2.4

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Mol	Chain	Res	Type	RSRZ
40	2i	3	GLN	2.4
11	2P	3	LEU	2.4
34	2c	200	ALA	2.4
41	1j	48	THR	2.4
49	2r	51	LEU	2.4
1	1A	2190	G	2.4
7	2H	121	ILE	2.4
21	2Z	160	GLY	2.4
32	1a	1224	G	2.4
38	2g	36	LYS	2.4
40	1i	78	LYS	2.4
44	2m	73	GLU	2.4
30	28	63	PRO	2.3
32	1a	345	C	2.3
32	1a	1357	A	2.3
34	2c	28	GLN	2.3
41	2j	37	PRO	2.3
42	2k	57	THR	2.3
50	1s	15	LEU	2.3
9	2N	61	ARG	2.3
33	2b	144	ARG	2.3
35	1d	122	ARG	2.3
36	2e	76	ILE	2.3
45	2n	19	ARG	2.3
51	2t	80	ARG	2.3
12	2Q	104	PHE	2.3
31	29	3	VAL	2.3
33	1b	152	PHE	2.3
51	1t	73	HIS	2.3
11	2P	59	LEU	2.3
45	1n	6	LEU	2.3
45	2n	47	LEU	2.3
1	2A	645	C	2.3
32	2a	1038	C	2.3
41	2j	100	THR	2.3
38	2g	84	ASN	2.3
17	2V	22	VAL	2.3
33	1b	28	PHE	2.3
35	2d	8	VAL	2.3
23	11	2	SER	2.3
32	2a	1353	G	2.3
33	2b	233	SER	2.3

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Mol	Chain	Res	Type	RSRZ
35	1d	38	TYR	2.3
49	1r	40	LEU	2.3
41	2j	87	THR	2.3
1	1A	2136	C	2.3
32	2a	1354	C	2.3
33	2b	223	ILE	2.3
11	2P	83	VAL	2.3
44	1m	98	VAL	2.3
51	2t	29	LYS	2.3
22	20	11	ARG	2.3
33	2b	121	LEU	2.3
41	2j	93	GLY	2.3
45	1n	35	ARG	2.3
1	1A	1063	G	2.3
1	2A	652(U)	G	2.3
32	1a	1032	G	2.3
6	2G	70	VAL	2.3
28	26	5	VAL	2.3
32	1a	152	A	2.3
20	2Y	50	ARG	2.3
40	2i	16	ARG	2.3
6	2G	90	LEU	2.3
7	2H	41	MET	2.3
6	2G	39	ILE	2.3
32	2a	1066	C	2.3
30	28	29	LYS	2.3
32	2a	949	A	2.3
34	1c	34	LEU	2.3
38	1g	86	GLN	2.3
52	2u	17	THR	2.3
1	1A	2150	U	2.3
32	1a	1446	U	2.3
34	1c	151	VAL	2.3
40	1i	41	VAL	2.3
35	2d	18	LYS	2.3
40	2i	80	GLY	2.3
8	2I	12	LEU	2.3
31	29	32	HIS	2.3
32	1a	1034	G	2.3
38	1g	77	SER	2.3
51	1t	13	LEU	2.3
34	2c	50	ALA	2.3

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Mol	Chain	Res	Type	RSRZ
38	2g	152	ALA	2.3
40	2i	55	ALA	2.3
43	2l	69	TYR	2.3
32	1a	975	A	2.3
40	2i	42	ARG	2.3
6	2G	49	ASP	2.3
7	2H	125	VAL	2.3
33	1b	136	VAL	2.3
15	2T	99	LEU	2.2
34	1c	188	LEU	2.2
40	2i	96	LEU	2.2
44	2m	67	GLU	2.2
1	1A	2188	C	2.2
1	2A	2124	G	2.2
32	1a	102	G	2.2
52	2u	5	ASP	2.2
32	2a	1447	A	2.2
37	2f	6	VAL	2.2
41	1j	36	GLY	2.2
33	1b	135	GLN	2.2
21	2Z	5	LEU	2.2
35	2d	115	ARG	2.2
40	1i	119	ALA	2.2
7	2H	100	GLY	2.2
32	2a	1115	C	2.2
34	2c	194	GLY	2.2
41	1j	11	PHE	2.2
1	2A	2149	G	2.2
32	1a	1030(C)	G	2.2
43	2l	43	VAL	2.2
14	2S	110	LEU	2.2
33	2b	10	LEU	2.2
34	2c	72	LYS	2.2
34	2c	101	LEU	2.2
34	2c	188	LEU	2.2
40	2i	50	LEU	2.2
51	1t	62	LEU	2.2
34	1c	78	GLY	2.2
38	2g	34	GLY	2.2
40	1i	100	GLY	2.2
34	2c	206	GLU	2.2
41	1j	38	ILE	2.2

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Mol	Chain	Res	Type	RSRZ
51	1t	68	LYS	2.2
1	2A	2188	C	2.2
38	2g	109	ASN	2.2
1	1A	2168	G	2.2
11	2P	102	ARG	2.2
21	2Z	24	LEU	2.2
34	1c	91	LEU	2.2
46	1o	57	LEU	2.2
32	2a	1001	A	2.2
6	1G	49	ASP	2.2
33	1b	228	GLY	2.2
30	28	21	LYS	2.2
35	2d	38	TYR	2.2
40	2i	11	LYS	2.2
51	1t	21	LYS	2.2
8	2I	4	ILE	2.2
47	1p	2	VAL	2.2
47	1p	53	VAL	2.2
7	1H	2	SER	2.2
7	2H	130	ARG	2.2
45	2n	26	ARG	2.2
45	2n	60	SER	2.2
52	2u	9	ARG	2.2
21	2Z	76	LEU	2.2
34	2c	175	LEU	2.2
44	1m	19	LEU	2.2
1	1A	652(S)	C	2.2
33	2b	13	ALA	2.2
26	14	54	GLY	2.2
40	1i	75	ASP	2.2
32	1a	216	G	2.2
42	2k	90	GLY	2.2
20	2Y	55	TYR	2.2
32	2a	1030(D)	A	2.2
32	2a	1250	A	2.2
38	2g	62	PHE	2.2
12	2Q	102	VAL	2.2
30	28	16	ILE	2.2
33	2b	93	VAL	2.2
34	1c	179	ARG	2.2
33	1b	131	PRO	2.2
38	1g	59	LEU	2.2

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Mol	Chain	Res	Type	RSRZ
50	1s	2	PRO	2.2
51	1t	24	LEU	2.2
7	2H	27	LYS	2.2
32	1a	1223	C	2.2
32	2a	1114	C	2.2
34	2c	148	GLY	2.2
40	1i	52	ALA	2.2
40	2i	30	GLY	2.2
45	1n	20	ALA	2.2
33	1b	137	ARG	2.2
44	2m	94	ARG	2.2
7	2H	134	SER	2.2
33	2b	162	ILE	2.2
1	1A	887	A	2.2
9	2N	68	GLU	2.2
41	2j	39	PRO	2.2
11	2P	82	GLY	2.2
23	2l	28	GLY	2.2
47	1p	64	ALA	2.2
50	2s	68	GLY	2.2
45	1n	22	THR	2.2
34	2c	126	ARG	2.2
7	2H	109	PHE	2.2
32	1a	948	C	2.2
3	2D	38	LYS	2.1
12	2Q	32	TYR	2.1
32	2a	1235	U	2.1
51	1t	26	ASN	2.1
4	2E	150	VAL	2.1
33	1b	201	ILE	2.1
42	2k	29	ILE	2.1
1	2A	2152	G	2.1
32	1a	149	A	2.1
14	2S	20	ARG	2.1
40	2i	13	ALA	2.1
41	2j	86	MET	2.1
7	2H	90	LYS	2.1
1	1A	2803	C	2.1
33	2b	68	ILE	2.1
40	1i	28	VAL	2.1
43	2l	96	VAL	2.1
39	2h	2	LEU	2.1

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Mol	Chain	Res	Type	RSRZ
50	2s	69	HIS	2.1
12	2Q	33	GLY	2.1
40	1i	111	ARG	2.1
7	2H	77	LYS	2.1
35	2d	166	LYS	2.1
41	2j	20	ALA	2.1
44	1m	109	THR	2.1
40	2i	48	GLU	2.1
11	2P	75	ILE	2.1
34	1c	66	VAL	2.1
34	1c	153	VAL	2.1
42	2k	21	ILE	2.1
1	1A	2161	C	2.1
12	2Q	5	ARG	2.1
32	1a	91	C	2.1
32	1a	1358	U	2.1
35	1d	7	PRO	2.1
38	2g	14	PRO	2.1
45	2n	20	ALA	2.1
51	1t	76	ALA	2.1
34	2c	170	GLN	2.1
1	1A	1077	A	2.1
1	1A	2162	G	2.1
32	1a	971	G	2.1
32	1a	1031	G	2.1
32	2a	1003	G	2.1
7	2H	175	LYS	2.1
11	2P	107	LYS	2.1
34	2c	197	GLY	2.1
44	1m	56	LEU	2.1
44	2m	100	GLY	2.1
50	2s	2	PRO	2.1
32	1a	950	U	2.1
32	2a	1219	U	2.1
38	2g	8	GLU	2.1
41	1j	59	SER	2.1
22	20	39	ARG	2.1
35	2d	183	GLY	2.1
38	1g	32	ARG	2.1
34	1c	175	LEU	2.1
40	1i	47	LEU	2.1
40	2i	86	VAL	2.1

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Mol	Chain	Res	Type	RSRZ
41	1j	23	ILE	2.1
42	2k	59	TYR	2.1
44	2m	96	LEU	2.1
32	2a	1044	A	2.1
34	1c	169	ALA	2.1
40	1i	87	GLN	2.1
40	2i	87	GLN	2.1
21	1Z	1	MET	2.1
32	1a	163	C	2.1
32	1a	1352	C	2.1
47	1p	59	TRP	2.1
30	28	48	PHE	2.1
35	1d	24	GLU	2.1
33	1b	81	VAL	2.1
34	1c	134	ILE	2.1
42	1k	14	VAL	2.1
40	1i	36	TYR	2.1
33	2b	132	LYS	2.1
38	2g	39	ALA	2.1
40	1i	127	LYS	2.1
41	2j	57	LYS	2.1
22	20	53	MET	2.1
31	29	35	ARG	2.1
38	2g	10	ARG	2.1
41	2j	51	ARG	2.1
47	1p	48	TRP	2.1
11	2P	91	PHE	2.1
33	2b	57	PHE	2.1
38	2g	26	PHE	2.1
35	1d	23	GLY	2.1
45	1n	55	GLY	2.1
21	1Z	141	VAL	2.1
22	20	63	VAL	2.1
33	2b	164	VAL	2.1
42	1k	80	VAL	2.1
48	1q	5	VAL	2.1
21	2Z	167	PRO	2.1
23	21	68	PRO	2.1
35	2d	46	LYS	2.1
40	2i	73	GLN	2.1
51	2t	55	ILE	2.1
14	2S	92	TYR	2.1

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Mol	Chain	Res	Type	RSRZ
34	1c	160	ALA	2.1
40	1i	128	ARG	2.1
40	1i	64	THR	2.1
1	1A	2506	U	2.0
7	2H	78	GLY	2.1
32	1a	1353	G	2.0
32	2a	1014	A	2.1
32	2a	1094	G	2.0
54	2x	46	G	2.0
12	2Q	63	LYS	2.0
38	2g	99	LEU	2.0
45	1n	11	LYS	2.0
44	2m	7	VAL	2.0
34	2c	184	TYR	2.0
34	2c	201	TYR	2.0
40	1i	45	ALA	2.0
42	1k	117	ASN	2.0
40	2i	75	ASP	2.0
41	2j	36	GLY	2.0
14	2S	57	LYS	2.0
44	1m	115	LYS	2.0
32	1a	1049	U	2.0
50	2s	16	LEU	2.0
1	1A	2062	A	2.0
1	2A	899	A	2.0
1	1A	2157	G	2.0
7	2H	17	VAL	2.0
32	1a	1041	A	2.0
32	2a	1251	A	2.0
33	2b	81	VAL	2.0
53	2v	14	A	2.0
9	2N	85	ILE	2.0
34	1c	57	ILE	2.0
35	2d	70	ILE	2.0
32	2a	91	C	2.0
52	2u	18	TYR	2.0
45	1n	10	ALA	2.0
7	2H	56	SER	2.0
36	2e	29	GLY	2.0
48	2q	100	LYS	2.0
52	1u	11	GLY	2.0
34	2c	34	LEU	2.0

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Mol	Chain	Res	Type	RSRZ
12	2Q	56	ARG	2.0
31	29	20	HIS	2.0
35	1d	170	VAL	2.0
37	1f	90	VAL	2.0
40	2i	111	ARG	2.0
43	2l	99	HIS	2.0
34	1c	68	VAL	2.0
47	1p	75	ARG	2.0
16	2U	62	ILE	2.0
21	2Z	133	ILE	2.0
16	2U	21	ALA	2.0
31	29	24	TYR	2.0
32	1a	1157	A	2.0
32	1a	64	G	2.0
32	2a	1030(C)	G	2.0
32	2a	1039	C	2.0
32	2a	1255	G	2.0
34	1c	80	GLY	2.0
34	1c	189	ALA	2.0
45	2n	9	LYS	2.0
47	1p	39	TYR	2.0
38	1g	82	GLY	2.0
34	2c	162	GLN	2.0
10	2O	1	MET	2.0
35	1d	110	PHE	2.0
25	13	60	GLU	2.0
25	23	26	LEU	2.0
40	1i	42	ARG	2.0
14	2S	85	VAL	2.0
35	2d	56	VAL	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, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
32	2MG	2a	1207	24/25	0.90	0.18	72,84,90,96	0
32	PSU	2a	516	20/21	0.92	0.17	66,76,86,86	0
1	5MU	2A	1915	21/22	0.93	0.15	64,68,74,78	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
32	M2G	2a	966	25/26	0.93	0.24	60,66,80,86	0
32	5MC	2a	967	21/22	0.93	0.23	63,70,78,83	0
1	PSU	2A	1917	20/21	0.93	0.16	52,60,67,75	0
54	4SU	2x	8	20/21	0.93	0.17	69,75,80,82	0
54	PSU	2x	55	20/21	0.93	0.12	68,76,80,83	0
54	PSU	1x	55	20/21	0.94	0.16	49,53,62,66	0
32	2MG	1a	1207	24/25	0.94	0.18	65,76,80,83	0
54	5MC	2x	32	21/22	0.94	0.21	68,73,77,85	0
43	0TD	1l	92	10/11	0.94	0.13	49,54,59,67	0
43	0TD	2l	92	10/11	0.95	0.19	60,63,64,77	0
32	G7M	2a	527	24/25	0.95	0.18	63,68,73,74	0
1	5MU	1A	1915	21/22	0.96	0.17	49,53,63,66	0
1	PSU	1A	1917	20/21	0.96	0.15	39,50,57,60	0
54	5MC	1x	32	21/22	0.96	0.22	43,52,59,64	0
54	5MU	1x	54	21/22	0.96	0.15	53,58,64,70	0
32	PSU	1a	516	20/21	0.96	0.16	60,67,70,71	0
32	4OC	2a	1402	22/23	0.96	0.20	54,60,66,70	0
32	5MC	2a	1404	21/22	0.96	0.20	48,52,57,62	0
1	PSU	2A	1911	20/21	0.96	0.16	57,61,75,76	0
32	G7M	1a	527	24/25	0.96	0.20	45,50,59,65	0
32	M2G	1a	966	25/26	0.96	0.24	41,52,61,66	0
54	5MU	2x	54	21/22	0.96	0.15	70,75,81,84	0
1	OMC	2A	1920	21/22	0.96	0.17	51,56,60,64	0
32	5MC	2a	1407	21/22	0.97	0.20	45,49,53,59	0
32	UR3	2a	1498	21/22	0.97	0.22	44,53,58,63	0
32	MA6	2a	1519	24/25	0.97	0.25	46,56,60,66	0
1	PSU	1A	1911	20/21	0.97	0.19	38,46,51,54	0
54	4SU	1x	8	20/21	0.97	0.19	47,56,64,71	0
32	5MC	2a	1400	21/22	0.97	0.19	64,70,73,75	0
32	5MC	1a	967	21/22	0.97	0.20	44,52,63,66	0
1	OMC	1A	1920	21/22	0.97	0.21	34,43,47,51	0
1	PSU	2A	2605	20/21	0.98	0.20	28,35,38,39	0
32	MA6	1a	1519	24/25	0.98	0.24	34,40,47,50	0
1	5MC	1A	1962	21/22	0.98	0.19	25,33,38,38	0
1	OMU	1A	2552	21/22	0.98	0.20	21,26,31,35	0
1	PSU	1A	2605	20/21	0.98	0.22	20,24,28,33	0
1	5MC	1A	1942	21/22	0.98	0.18	36,40,42,50	0
32	5MC	1a	1400	21/22	0.98	0.19	44,50,53,54	0
32	4OC	1a	1402	22/23	0.98	0.19	39,42,48,58	0
32	5MC	1a	1404	21/22	0.98	0.18	28,35,41,42	0
32	5MC	1a	1407	21/22	0.98	0.20	34,38,42,44	0
32	MA6	1a	1518	24/25	0.98	0.22	34,39,43,44	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
32	MA6	2a	1518	24/25	0.98	0.20	46,56,62,65	0
1	5MU	2A	1939	21/22	0.98	0.19	29,34,38,40	0
1	5MC	2A	1942	21/22	0.98	0.17	42,47,52,59	0
1	5MC	2A	1962	21/22	0.98	0.18	32,42,46,61	0
1	OMG	2A	2251	24/25	0.98	0.20	31,35,41,42	0
1	2MA	2A	2503	23/24	0.98	0.22	20,33,38,42	0
1	OMU	2A	2552	21/22	0.98	0.18	29,36,39,40	0
32	UR3	1a	1498	21/22	0.99	0.21	32,37,41,43	0
1	2MA	1A	2503	23/24	0.99	0.21	16,20,24,28	0
1	5MU	1A	1939	21/22	0.99	0.18	20,24,29,32	0
1	OMG	1A	2251	24/25	0.99	0.20	16,23,27,27	0

6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
55	MG	1A	4041	1/1	0.32	0.57	68,68,68,68	0
58	ZN	24	501	1/1	0.33	0.17	140,140,140,140	0
55	MG	2a	1719	1/1	0.39	0.25	109,109,109,109	0
55	MG	1a	1797	1/1	0.41	1.14	84,84,84,84	0
55	MG	2a	1685	1/1	0.41	0.27	81,81,81,81	0
55	MG	2a	1787	1/1	0.44	0.08	91,91,91,91	0
55	MG	1A	3359	1/1	0.45	1.26	66,66,66,66	0
55	MG	1A	4043	1/1	0.46	0.11	55,55,55,55	0
55	MG	1A	3970	1/1	0.46	0.15	45,45,45,45	0
55	MG	2B	204	1/1	0.47	1.31	93,93,93,93	0
55	MG	2A	3716	1/1	0.49	0.12	67,67,67,67	0
55	MG	1A	3392	1/1	0.49	0.57	64,64,64,64	0
55	MG	1A	3680	1/1	0.50	0.24	67,67,67,67	0
55	MG	2A	3433	1/1	0.52	0.70	66,66,66,66	0
55	MG	1A	3368	1/1	0.54	0.32	70,70,70,70	0
55	MG	2A	3337	1/1	0.56	0.28	71,71,71,71	0
55	MG	1A	3356	1/1	0.57	0.45	76,76,76,76	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
55	MG	2A	3148	1/1	0.57	0.45	80,80,80,80	0
55	MG	1F	307	1/1	0.60	0.57	59,59,59,59	0
55	MG	1a	1655	1/1	0.61	0.38	81,81,81,81	0
55	MG	1a	1786	1/1	0.61	0.18	64,64,64,64	0
55	MG	2A	3702	1/1	0.61	0.19	58,58,58,58	0
55	MG	1a	1632	1/1	0.62	0.14	77,77,77,77	0
55	MG	2a	1786	1/1	0.62	0.38	76,76,76,76	0
55	MG	2A	3603	1/1	0.62	0.13	48,48,48,48	0
55	MG	1a	1692	1/1	0.62	0.34	71,71,71,71	0
55	MG	1A	3462	1/1	0.63	0.55	69,69,69,69	0
55	MG	1a	1723	1/1	0.63	0.16	56,56,56,56	0
55	MG	2A	3194	1/1	0.64	0.26	74,74,74,74	0
55	MG	2A	3262	1/1	0.64	0.52	85,85,85,85	0
55	MG	1E	309	1/1	0.64	0.15	29,29,29,29	0
55	MG	2a	1712	1/1	0.64	0.23	75,75,75,75	0
55	MG	1O	201	1/1	0.65	0.24	64,64,64,64	0
55	MG	1A	3969	1/1	0.65	0.41	63,63,63,63	0
55	MG	1a	1792	1/1	0.66	0.16	66,66,66,66	0
55	MG	2A	3553	1/1	0.66	0.10	77,77,77,77	0
55	MG	1A	3048	1/1	0.66	0.20	43,43,43,43	0
55	MG	1A	3983	1/1	0.67	0.29	67,67,67,67	0
55	MG	1A	3912	1/1	0.67	0.13	65,65,65,65	0
55	MG	2B	202	1/1	0.67	0.19	66,66,66,66	0
55	MG	1A	3297	1/1	0.67	0.25	68,68,68,68	0
55	MG	1A	3347	1/1	0.67	0.23	77,77,77,77	0
55	MG	2A	3434	1/1	0.67	0.15	56,56,56,56	0
55	MG	2A	3065	1/1	0.67	0.23	51,51,51,51	0
55	MG	2A	3587	1/1	0.67	0.13	67,67,67,67	0
55	MG	1E	311	1/1	0.67	0.51	80,80,80,80	0
55	MG	2x	102	1/1	0.67	0.11	71,71,71,71	0
55	MG	2A	3652	1/1	0.67	0.10	63,63,63,63	0
55	MG	1A	3282	1/1	0.68	0.66	70,70,70,70	0
55	MG	2a	1743	1/1	0.68	0.17	63,63,63,63	0
56	K	1A	3482	1/1	0.68	0.37	90,90,90,90	0
55	MG	2A	3117	1/1	0.68	0.30	68,68,68,68	0
55	MG	2a	1691	1/1	0.69	0.07	83,83,83,83	0
55	MG	2a	1693	1/1	0.69	0.19	72,72,72,72	0
55	MG	1A	3488	1/1	0.69	0.22	39,39,39,39	0
55	MG	1A	3916	1/1	0.69	0.23	79,79,79,79	0
55	MG	1A	3936	1/1	0.69	0.13	80,80,80,80	0
55	MG	2A	3580	1/1	0.69	0.20	74,74,74,74	0
55	MG	1A	3388	1/1	0.69	0.24	70,70,70,70	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
55	MG	2B	213	1/1	0.69	0.10	75,75,75,75	0
55	MG	2a	1650	1/1	0.69	0.14	65,65,65,65	0
55	MG	1A	3908	1/1	0.69	0.45	74,74,74,74	0
55	MG	1a	1751	1/1	0.70	0.29	91,91,91,91	0
55	MG	1A	3252	1/1	0.70	0.20	64,64,64,64	0
55	MG	1a	1685	1/1	0.70	0.14	60,60,60,60	0
55	MG	1A	3514	1/1	0.70	1.00	85,85,85,85	0
55	MG	1A	3668	1/1	0.70	0.11	60,60,60,60	0
55	MG	2A	3380	1/1	0.70	0.23	53,53,53,53	0
55	MG	1A	3457	1/1	0.71	0.29	54,54,54,54	0
55	MG	1A	3984	1/1	0.71	0.16	83,83,83,83	0
55	MG	2A	3247	1/1	0.71	0.19	68,68,68,68	0
55	MG	2A	3487	1/1	0.71	0.42	60,60,60,60	0
55	MG	2B	203	1/1	0.71	0.36	78,78,78,78	0
55	MG	2A	3258	1/1	0.71	0.28	67,67,67,67	0
55	MG	2A	3260	1/1	0.71	0.27	68,68,68,68	0
55	MG	2B	214	1/1	0.71	0.09	70,70,70,70	0
55	MG	1a	1680	1/1	0.71	0.19	67,67,67,67	0
55	MG	1R	205	1/1	0.71	0.20	45,45,45,45	0
55	MG	1W	207	1/1	0.72	0.66	47,47,47,47	0
55	MG	2A	3326	1/1	0.72	0.26	67,67,67,67	0
55	MG	1A	3967	1/1	0.72	0.30	70,70,70,70	0
55	MG	1a	1637	1/1	0.72	0.15	69,69,69,69	0
55	MG	2A	3153	1/1	0.72	0.19	68,68,68,68	0
55	MG	1a	1776	1/1	0.72	0.12	72,72,72,72	0
55	MG	2A	3459	1/1	0.72	0.19	50,50,50,50	0
55	MG	1A	3471	1/1	0.72	0.26	83,83,83,83	0
55	MG	2A	3551	1/1	0.72	0.36	70,70,70,70	0
55	MG	1A	3329	1/1	0.72	0.26	63,63,63,63	0
55	MG	1A	3419	1/1	0.72	0.24	51,51,51,51	0
55	MG	1a	1771	1/1	0.73	0.08	70,70,70,70	0
55	MG	1x	103	1/1	0.73	0.24	68,68,68,68	0
55	MG	1B	232	1/1	0.73	0.17	79,79,79,79	0
55	MG	1a	1785	1/1	0.73	0.19	75,75,75,75	0
55	MG	1A	3783	1/1	0.73	0.38	56,56,56,56	0
55	MG	2A	3509	1/1	0.73	0.14	72,72,72,72	0
55	MG	2A	3513	1/1	0.73	0.18	64,64,64,64	0
55	MG	2A	3285	1/1	0.73	0.18	55,55,55,55	0
55	MG	1A	3337	1/1	0.73	0.29	61,61,61,61	0
55	MG	2A	3178	1/1	0.73	0.23	63,63,63,63	0
55	MG	2a	1620	1/1	0.73	0.20	67,67,67,67	0
55	MG	2a	1646	1/1	0.73	0.15	68,68,68,68	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
55	MG	1A	4054	1/1	0.74	0.15	59,59,59,59	0
55	MG	1A	3408	1/1	0.74	0.27	58,58,58,58	0
55	MG	2a	1601	1/1	0.74	0.19	72,72,72,72	0
55	MG	1a	1601	1/1	0.74	0.20	69,69,69,69	0
55	MG	2a	1640	1/1	0.74	0.37	64,64,64,64	0
55	MG	1A	3733	1/1	0.74	0.16	64,64,64,64	0
55	MG	1A	3534	1/1	0.74	0.20	60,60,60,60	0
55	MG	1A	3887	1/1	0.74	0.17	65,65,65,65	0
55	MG	1A	3284	1/1	0.74	0.78	50,50,50,50	0
55	MG	1A	3074	1/1	0.75	0.14	55,55,55,55	0
55	MG	2A	3689	1/1	0.75	0.34	69,69,69,69	0
55	MG	1A	3226	1/1	0.75	0.17	61,61,61,61	0
55	MG	2A	3244	1/1	0.75	0.29	68,68,68,68	0
55	MG	2a	1756	1/1	0.75	0.14	68,68,68,68	0
55	MG	1A	3250	1/1	0.75	0.26	56,56,56,56	0
55	MG	2A	3462	1/1	0.75	0.27	70,70,70,70	0
55	MG	2a	1675	1/1	0.75	0.26	72,72,72,72	0
55	MG	2A	3475	1/1	0.75	0.30	69,69,69,69	0
55	MG	1A	3405	1/1	0.75	0.51	64,64,64,64	0
55	MG	2A	3256	1/1	0.76	0.46	57,57,57,57	0
55	MG	2A	3081	1/1	0.76	0.14	80,80,80,80	0
55	MG	2a	1694	1/1	0.76	0.40	66,66,66,66	0
55	MG	1a	1671	1/1	0.76	0.21	59,59,59,59	0
55	MG	1A	3638	1/1	0.76	0.15	24,24,24,24	0
55	MG	1A	3854	1/1	0.76	0.13	65,65,65,65	0
55	MG	2a	1630	1/1	0.76	0.17	58,58,58,58	0
55	MG	2A	3690	1/1	0.76	0.10	68,68,68,68	0
55	MG	1a	1624	1/1	0.76	0.11	65,65,65,65	0
55	MG	1A	3991	1/1	0.76	0.95	63,63,63,63	0
55	MG	1B	203	1/1	0.76	0.26	56,56,56,56	0
55	MG	1A	4004	1/1	0.76	0.16	55,55,55,55	0
55	MG	1A	3394	1/1	0.77	0.42	49,49,49,49	0
55	MG	1A	3666	1/1	0.77	0.22	53,53,53,53	0
55	MG	1A	3314	1/1	0.77	0.24	63,63,63,63	0
55	MG	2D	306	1/1	0.77	0.42	43,43,43,43	0
55	MG	1a	1659	1/1	0.77	0.11	64,64,64,64	0
55	MG	1A	3387	1/1	0.77	0.75	59,59,59,59	0
55	MG	1A	3249	1/1	0.77	0.19	51,51,51,51	0
55	MG	1A	3928	1/1	0.77	0.14	51,51,51,51	0
55	MG	1A	4024	1/1	0.77	0.17	73,73,73,73	0
55	MG	1A	3782	1/1	0.77	0.28	58,58,58,58	0
55	MG	2A	3535	1/1	0.77	0.25	74,74,74,74	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
55	MG	2A	3545	1/1	0.77	0.23	77,77,77,77	0
55	MG	1a	1735	1/1	0.77	0.10	69,69,69,69	0
55	MG	2A	3228	1/1	0.77	1.79	73,73,73,73	0
55	MG	1a	1750	1/1	0.77	0.11	61,61,61,61	0
55	MG	18	108	1/1	0.77	0.47	72,72,72,72	0
55	MG	2A	3249	1/1	0.77	0.19	63,63,63,63	0
55	MG	1a	1766	1/1	0.77	0.17	74,74,74,74	0
55	MG	1A	3177	1/1	0.77	0.18	48,48,48,48	0
55	MG	1a	1605	1/1	0.77	0.11	63,63,63,63	0
55	MG	1a	1784	1/1	0.77	0.10	65,65,65,65	0
55	MG	2f	202	1/1	0.77	0.18	81,81,81,81	0
55	MG	1a	1610	1/1	0.77	0.13	68,68,68,68	0
55	MG	1A	3968	1/1	0.77	0.13	45,45,45,45	0
55	MG	1a	1787	1/1	0.77	0.17	76,76,76,76	0
55	MG	1A	3835	1/1	0.78	0.21	53,53,53,53	0
55	MG	2A	3151	1/1	0.78	0.17	44,44,44,44	0
55	MG	1A	3841	1/1	0.78	0.12	41,41,41,41	0
55	MG	2A	3167	1/1	0.78	0.31	49,49,49,49	0
55	MG	2A	3175	1/1	0.78	0.29	63,63,63,63	0
55	MG	2A	3273	1/1	0.78	0.16	56,56,56,56	0
55	MG	1A	3780	1/1	0.78	0.18	65,65,65,65	0
55	MG	2A	3311	1/1	0.78	0.38	67,67,67,67	0
55	MG	1a	1669	1/1	0.78	0.18	58,58,58,58	0
55	MG	2a	1778	1/1	0.78	0.50	63,63,63,63	0
55	MG	2A	3198	1/1	0.78	0.20	67,67,67,67	0
55	MG	2A	3085	1/1	0.78	0.21	82,82,82,82	0
55	MG	2A	3240	1/1	0.78	0.20	70,70,70,70	0
55	MG	2A	3093	1/1	0.78	0.15	78,78,78,78	0
55	MG	2A	3682	1/1	0.78	0.20	77,77,77,77	0
55	MG	1A	3879	1/1	0.78	0.16	60,60,60,60	0
55	MG	2A	3468	1/1	0.79	0.29	61,61,61,61	0
55	MG	1a	1631	1/1	0.79	0.15	72,72,72,72	0
55	MG	2B	217	1/1	0.79	0.13	77,77,77,77	0
55	MG	2A	3480	1/1	0.79	0.30	48,48,48,48	0
55	MG	1A	3371	1/1	0.79	0.45	57,57,57,57	0
55	MG	2a	1602	1/1	0.79	0.12	61,61,61,61	0
55	MG	1A	3889	1/1	0.79	0.13	47,47,47,47	0
55	MG	1A	3421	1/1	0.79	0.18	61,61,61,61	0
55	MG	1A	3401	1/1	0.79	0.52	58,58,58,58	0
55	MG	1A	3708	1/1	0.79	0.13	65,65,65,65	0
55	MG	1B	231	1/1	0.79	0.30	77,77,77,77	0
55	MG	2A	3277	1/1	0.79	0.13	62,62,62,62	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
55	MG	2a	1678	1/1	0.79	0.11	55,55,55,55	0
55	MG	1A	3881	1/1	0.79	0.14	54,54,54,54	0
55	MG	2A	3298	1/1	0.79	0.24	64,64,64,64	0
55	MG	1A	3886	1/1	0.79	0.11	47,47,47,47	0
55	MG	2A	3609	1/1	0.79	0.42	77,77,77,77	0
55	MG	2a	1703	1/1	0.79	0.19	65,65,65,65	0
55	MG	2a	1708	1/1	0.79	0.11	72,72,72,72	0
55	MG	2A	3617	1/1	0.79	0.17	63,63,63,63	0
55	MG	1A	3965	1/1	0.79	0.16	52,52,52,52	0
55	MG	2A	3656	1/1	0.79	0.13	41,41,41,41	0
55	MG	1a	1694	1/1	0.79	0.08	76,76,76,76	0
55	MG	1a	1697	1/1	0.79	0.32	48,48,48,48	0
55	MG	2A	3403	1/1	0.79	0.20	55,55,55,55	0
55	MG	2A	3428	1/1	0.79	0.13	56,56,56,56	0
55	MG	2a	1796	1/1	0.79	0.19	65,65,65,65	0
55	MG	2A	3219	1/1	0.79	0.45	41,41,41,41	0
55	MG	2q	201	1/1	0.79	0.17	78,78,78,78	0
55	MG	1l	201	1/1	0.79	0.16	76,76,76,76	0
55	MG	1a	1711	1/1	0.79	0.13	69,69,69,69	0
55	MG	1a	1627	1/1	0.79	0.09	78,78,78,78	0
55	MG	2A	3185	1/1	0.80	0.39	60,60,60,60	0
55	MG	2A	3003	1/1	0.80	0.12	67,67,67,67	0
55	MG	1a	1629	1/1	0.80	0.15	62,62,62,62	0
55	MG	1A	4020	1/1	0.80	0.21	75,75,75,75	0
55	MG	10	104	1/1	0.80	0.23	41,41,41,41	0
55	MG	2A	3710	1/1	0.80	0.12	70,70,70,70	0
55	MG	2A	3315	1/1	0.80	0.10	79,79,79,79	0
55	MG	2A	3527	1/1	0.80	0.18	54,54,54,54	0
55	MG	2A	3229	1/1	0.80	0.19	59,59,59,59	0
55	MG	1A	3531	1/1	0.80	0.20	65,65,65,65	0
55	MG	1A	3260	1/1	0.80	0.17	55,55,55,55	0
55	MG	1a	1658	1/1	0.80	0.30	70,70,70,70	0
55	MG	1A	3607	1/1	0.80	0.16	27,27,27,27	0
55	MG	2a	1753	1/1	0.80	0.15	73,73,73,73	0
55	MG	1A	3636	1/1	0.80	0.17	45,45,45,45	0
55	MG	2a	1763	1/1	0.80	0.13	77,77,77,77	0
55	MG	2Q	203	1/1	0.80	0.55	54,54,54,54	0
55	MG	2a	1785	1/1	0.80	0.08	82,82,82,82	0
55	MG	2A	3589	1/1	0.80	0.10	49,49,49,49	0
55	MG	1A	3348	1/1	0.80	0.17	62,62,62,62	0
55	MG	2a	1605	1/1	0.80	0.13	63,63,63,63	0
55	MG	2a	1613	1/1	0.80	0.08	64,64,64,64	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
55	MG	1B	205	1/1	0.80	0.20	63,63,63,63	0
55	MG	2A	3460	1/1	0.80	0.59	63,63,63,63	0
55	MG	2a	1633	1/1	0.80	0.17	76,76,76,76	0
55	MG	1x	107	1/1	0.80	0.15	67,67,67,67	0
55	MG	2A	3263	1/1	0.81	0.12	60,60,60,60	0
55	MG	2A	3130	1/1	0.81	0.45	77,77,77,77	0
55	MG	1A	3403	1/1	0.81	0.36	59,59,59,59	0
55	MG	1A	3470	1/1	0.81	0.51	73,73,73,73	0
55	MG	2A	3565	1/1	0.81	0.56	48,48,48,48	0
55	MG	2a	1636	1/1	0.81	0.35	72,72,72,72	0
55	MG	2A	3571	1/1	0.81	0.14	62,62,62,62	0
55	MG	1A	3258	1/1	0.81	0.27	50,50,50,50	0
55	MG	2A	3161	1/1	0.81	0.23	51,51,51,51	0
55	MG	1A	3102	1/1	0.81	0.14	57,57,57,57	0
55	MG	2A	3317	1/1	0.81	0.27	59,59,59,59	0
55	MG	1A	3509	1/1	0.81	0.16	66,66,66,66	0
55	MG	2a	1689	1/1	0.81	0.29	79,79,79,79	0
55	MG	1T	202	1/1	0.81	0.37	57,57,57,57	0
55	MG	2A	3623	1/1	0.81	0.15	35,35,35,35	0
55	MG	1V	202	1/1	0.81	0.54	48,48,48,48	0
55	MG	2A	3383	1/1	0.81	0.18	32,32,32,32	0
55	MG	2A	3395	1/1	0.81	0.32	55,55,55,55	0
55	MG	1A	3251	1/1	0.81	0.35	50,50,50,50	0
55	MG	1a	1677	1/1	0.81	0.19	58,58,58,58	0
55	MG	2a	1733	1/1	0.81	0.12	56,56,56,56	0
55	MG	2a	1739	1/1	0.81	0.16	73,73,73,73	0
55	MG	2A	3215	1/1	0.81	0.11	71,71,71,71	0
55	MG	2a	1745	1/1	0.81	0.20	69,69,69,69	0
55	MG	1A	3525	1/1	0.81	0.31	67,67,67,67	0
55	MG	1l	104	1/1	0.81	0.17	40,40,40,40	0
55	MG	1A	3742	1/1	0.81	0.19	45,45,45,45	0
55	MG	1A	3530	1/1	0.81	0.31	55,55,55,55	0
55	MG	1A	3420	1/1	0.81	0.25	68,68,68,68	0
55	MG	1A	3065	1/1	0.81	0.47	37,37,37,37	0
55	MG	2A	3074	1/1	0.81	0.07	71,71,71,71	0
55	MG	2A	3483	1/1	0.81	0.41	70,70,70,70	0
55	MG	1A	3595	1/1	0.81	0.20	60,60,60,60	0
55	MG	2G	201	1/1	0.81	0.13	67,67,67,67	0
55	MG	1a	1734	1/1	0.81	0.08	55,55,55,55	0
55	MG	1A	3288	1/1	0.81	0.27	42,42,42,42	0
58	ZN	14	102	1/1	0.81	0.14	128,128,128,128	0
55	MG	1A	3632	1/1	0.81	0.14	58,58,58,58	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
55	MG	1A	3683	1/1	0.82	0.15	54,54,54,54	0
55	MG	2A	3184	1/1	0.82	0.15	66,66,66,66	0
55	MG	2A	3556	1/1	0.82	0.13	78,78,78,78	0
55	MG	2a	1623	1/1	0.82	0.10	68,68,68,68	0
55	MG	1A	3971	1/1	0.82	0.14	30,30,30,30	0
55	MG	2A	3570	1/1	0.82	0.15	78,78,78,78	0
55	MG	2A	3324	1/1	0.82	0.16	68,68,68,68	0
55	MG	1a	1682	1/1	0.82	0.21	65,65,65,65	0
55	MG	1A	3914	1/1	0.82	0.12	59,59,59,59	0
55	MG	2A	3364	1/1	0.82	0.17	37,37,37,37	0
55	MG	1x	102	1/1	0.82	0.10	64,64,64,64	0
55	MG	1A	3427	1/1	0.82	0.49	61,61,61,61	0
55	MG	1a	1616	1/1	0.82	0.36	50,50,50,50	0
55	MG	1a	1622	1/1	0.82	0.23	57,57,57,57	0
55	MG	2A	3643	1/1	0.82	0.11	59,59,59,59	0
55	MG	2A	3230	1/1	0.82	0.13	57,57,57,57	0
55	MG	1A	3989	1/1	0.82	0.28	49,49,49,49	0
55	MG	2A	3242	1/1	0.82	0.23	71,71,71,71	0
55	MG	2A	3686	1/1	0.82	0.16	59,59,59,59	0
55	MG	2A	3688	1/1	0.82	0.14	63,63,63,63	0
55	MG	1A	3390	1/1	0.82	0.22	56,56,56,56	0
55	MG	1A	4002	1/1	0.82	0.14	51,51,51,51	0
55	MG	1N	201	1/1	0.82	0.21	61,61,61,61	0
55	MG	2A	3704	1/1	0.82	0.12	76,76,76,76	0
55	MG	2A	3463	1/1	0.82	0.23	65,65,65,65	0
55	MG	2A	3715	1/1	0.82	0.23	64,64,64,64	0
55	MG	1a	1746	1/1	0.82	0.09	54,54,54,54	0
55	MG	2a	1759	1/1	0.82	0.21	78,78,78,78	0
55	MG	1A	3257	1/1	0.82	0.29	48,48,48,48	0
55	MG	1A	4017	1/1	0.82	0.16	63,63,63,63	0
55	MG	1A	3953	1/1	0.82	0.22	63,63,63,63	0
55	MG	1A	3468	1/1	0.82	0.17	58,58,58,58	0
55	MG	2A	3489	1/1	0.82	0.16	44,44,44,44	0
55	MG	2A	3505	1/1	0.82	0.15	66,66,66,66	0
55	MG	2D	301	1/1	0.82	0.29	39,39,39,39	0
55	MG	1A	3382	1/1	0.82	0.28	71,71,71,71	0
55	MG	1A	3326	1/1	0.82	0.54	52,52,52,52	0
55	MG	2A	3283	1/1	0.82	0.35	62,62,62,62	0
55	MG	1A	3311	1/1	0.82	0.70	36,36,36,36	0
55	MG	1a	1676	1/1	0.82	0.13	70,70,70,70	0
55	MG	2A	3159	1/1	0.83	0.17	56,56,56,56	0
55	MG	2a	1681	1/1	0.83	0.23	77,77,77,77	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
55	MG	1A	3640	1/1	0.83	0.15	35,35,35,35	0
55	MG	2A	3415	1/1	0.83	0.12	72,72,72,72	0
55	MG	1A	3893	1/1	0.83	0.11	62,62,62,62	0
55	MG	1a	1709	1/1	0.83	0.19	66,66,66,66	0
55	MG	1A	3418	1/1	0.83	0.20	64,64,64,64	0
55	MG	2a	1697	1/1	0.83	0.26	69,69,69,69	0
55	MG	2B	207	1/1	0.83	0.10	69,69,69,69	0
55	MG	2A	3574	1/1	0.83	0.12	54,54,54,54	0
55	MG	1a	1713	1/1	0.83	0.17	71,71,71,71	0
55	MG	1A	3830	1/1	0.83	0.14	38,38,38,38	0
55	MG	1A	3349	1/1	0.83	0.19	50,50,50,50	0
55	MG	2A	3597	1/1	0.83	0.46	79,79,79,79	0
55	MG	1B	212	1/1	0.83	0.26	59,59,59,59	0
55	MG	1A	3171	1/1	0.83	0.28	36,36,36,36	0
55	MG	2a	1749	1/1	0.83	0.35	70,70,70,70	0
55	MG	2A	3307	1/1	0.83	0.21	62,62,62,62	0
55	MG	1A	3853	1/1	0.83	0.09	33,33,33,33	0
55	MG	2A	3634	1/1	0.83	0.10	70,70,70,70	0
55	MG	1A	3478	1/1	0.83	0.33	36,36,36,36	0
55	MG	1A	3290	1/1	0.83	0.45	45,45,45,45	0
55	MG	2a	1782	1/1	0.83	0.08	75,75,75,75	0
55	MG	1a	1768	1/1	0.83	0.07	73,73,73,73	0
55	MG	2A	3498	1/1	0.83	0.10	57,57,57,57	0
55	MG	1a	1614	1/1	0.83	0.09	47,47,47,47	0
55	MG	1A	3315	1/1	0.83	0.13	59,59,59,59	0
55	MG	2a	1797	1/1	0.83	0.17	76,76,76,76	0
55	MG	1G	203	1/1	0.83	0.57	72,72,72,72	0
55	MG	2a	1643	1/1	0.83	0.18	58,58,58,58	0
55	MG	2q	202	1/1	0.83	0.12	81,81,81,81	0
55	MG	2A	3377	1/1	0.83	0.19	31,31,31,31	0
55	MG	1A	3407	1/1	0.83	0.14	56,56,56,56	0
55	MG	2a	1662	1/1	0.83	0.18	58,58,58,58	0
55	MG	1A	3182	1/1	0.83	0.14	34,34,34,34	0
55	MG	2A	3246	1/1	0.84	0.32	68,68,68,68	0
55	MG	1A	3435	1/1	0.84	0.25	40,40,40,40	0
55	MG	1A	3884	1/1	0.84	0.13	43,43,43,43	0
55	MG	1a	1602	1/1	0.84	0.17	63,63,63,63	0
55	MG	1A	3304	1/1	0.84	0.17	56,56,56,56	0
55	MG	2A	3472	1/1	0.84	0.08	87,87,87,87	0
55	MG	1a	1606	1/1	0.84	0.09	62,62,62,62	0
55	MG	1A	3188	1/1	0.84	0.20	58,58,58,58	0
55	MG	1A	3692	1/1	0.84	0.17	53,53,53,53	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
55	MG	2A	3701	1/1	0.84	0.13	62,62,62,62	0
55	MG	1A	3585	1/1	0.84	0.23	35,35,35,35	0
55	MG	1A	4021	1/1	0.84	0.75	96,96,96,96	0
55	MG	2a	1696	1/1	0.84	0.41	62,62,62,62	0
55	MG	1a	1695	1/1	0.84	0.16	57,57,57,57	0
55	MG	1a	1793	1/1	0.84	0.07	59,59,59,59	0
55	MG	1A	3639	1/1	0.84	0.31	60,60,60,60	0
55	MG	1A	4033	1/1	0.84	0.12	54,54,54,54	0
55	MG	2a	1718	1/1	0.84	0.06	58,58,58,58	0
55	MG	2A	3187	1/1	0.84	0.19	57,57,57,57	0
55	MG	1A	3467	1/1	0.84	0.34	52,52,52,52	0
55	MG	2B	205	1/1	0.84	0.24	66,66,66,66	0
55	MG	1A	3859	1/1	0.84	0.23	24,24,24,24	0
55	MG	1A	3977	1/1	0.84	0.23	25,25,25,25	0
55	MG	1x	109	1/1	0.84	0.12	66,66,66,66	0
55	MG	2A	3221	1/1	0.84	0.17	58,58,58,58	0
55	MG	2a	1755	1/1	0.84	0.18	65,65,65,65	0
55	MG	2A	3225	1/1	0.84	0.36	69,69,69,69	0
55	MG	2A	3566	1/1	0.84	0.29	52,52,52,52	0
55	MG	2F	303	1/1	0.84	0.10	71,71,71,71	0
55	MG	1V	208	1/1	0.84	0.14	56,56,56,56	0
55	MG	2A	3036	1/1	0.84	0.14	67,67,67,67	0
55	MG	2a	1783	1/1	0.84	0.17	70,70,70,70	0
55	MG	20	101	1/1	0.84	0.17	71,71,71,71	0
55	MG	1A	3596	1/1	0.84	0.12	35,35,35,35	0
55	MG	2A	3392	1/1	0.84	0.14	32,32,32,32	0
55	MG	2A	3233	1/1	0.84	0.38	60,60,60,60	0
55	MG	1a	1744	1/1	0.84	0.07	47,47,47,47	0
55	MG	2a	1614	1/1	0.84	0.16	64,64,64,64	0
55	MG	2A	3241	1/1	0.84	0.22	55,55,55,55	0
55	MG	2A	3419	1/1	0.84	0.08	69,69,69,69	0
55	MG	1A	3923	1/1	0.84	0.15	29,29,29,29	0
55	MG	1B	210	1/1	0.84	0.28	48,48,48,48	0
55	MG	2A	3245	1/1	0.84	0.16	74,74,74,74	0
55	MG	2A	3628	1/1	0.84	0.15	44,44,44,44	0
55	MG	1A	3336	1/1	0.85	0.17	48,48,48,48	0
55	MG	1B	216	1/1	0.85	0.22	54,54,54,54	0
55	MG	1A	3955	1/1	0.85	0.08	53,53,53,53	0
55	MG	2A	3493	1/1	0.85	0.14	77,77,77,77	0
55	MG	27	103	1/1	0.85	0.21	56,56,56,56	0
55	MG	28	3403	1/1	0.85	0.19	72,72,72,72	0
55	MG	1a	1796	1/1	0.85	0.13	85,85,85,85	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
55	MG	1a	1645	1/1	0.85	0.30	65,65,65,65	0
55	MG	2a	1604	1/1	0.85	0.28	71,71,71,71	0
55	MG	1f	201	1/1	0.85	0.29	61,61,61,61	0
55	MG	1a	1651	1/1	0.85	0.16	64,64,64,64	0
55	MG	1A	3301	1/1	0.85	0.15	38,38,38,38	0
55	MG	1D	310	1/1	0.85	0.17	65,65,65,65	0
55	MG	1A	3466	1/1	0.85	0.44	52,52,52,52	0
55	MG	2A	3257	1/1	0.85	0.35	58,58,58,58	0
55	MG	1a	1663	1/1	0.85	0.16	69,69,69,69	0
55	MG	1A	3262	1/1	0.85	0.17	55,55,55,55	0
55	MG	2A	3558	1/1	0.85	0.32	72,72,72,72	0
55	MG	2A	3560	1/1	0.85	0.14	47,47,47,47	0
55	MG	2A	3032	1/1	0.85	0.11	60,60,60,60	0
55	MG	1A	3039	1/1	0.85	0.13	37,37,37,37	0
55	MG	2A	3044	1/1	0.85	0.19	61,61,61,61	0
55	MG	2a	1664	1/1	0.85	0.24	68,68,68,68	0
55	MG	2a	1673	1/1	0.85	0.14	70,70,70,70	0
55	MG	2A	3055	1/1	0.85	0.09	75,75,75,75	0
55	MG	1F	308	1/1	0.85	0.20	51,51,51,51	0
55	MG	1A	3313	1/1	0.85	0.21	57,57,57,57	0
55	MG	2a	1682	1/1	0.85	0.21	65,65,65,65	0
55	MG	1A	3877	1/1	0.85	0.17	53,53,53,53	0
55	MG	1A	3973	1/1	0.85	0.10	59,59,59,59	0
55	MG	2A	3594	1/1	0.85	0.13	41,41,41,41	0
55	MG	1A	3255	1/1	0.85	0.15	61,61,61,61	0
55	MG	1A	3143	1/1	0.85	0.18	38,38,38,38	0
55	MG	2A	3316	1/1	0.85	0.14	51,51,51,51	0
55	MG	1A	3316	1/1	0.85	0.54	43,43,43,43	0
55	MG	2A	3323	1/1	0.85	0.15	65,65,65,65	0
55	MG	1A	3416	1/1	0.85	0.15	56,56,56,56	0
55	MG	2A	3150	1/1	0.85	0.30	60,60,60,60	0
55	MG	2a	1716	1/1	0.85	0.11	79,79,79,79	0
55	MG	2A	3336	1/1	0.85	0.09	62,62,62,62	0
55	MG	2A	3648	1/1	0.85	0.20	56,56,56,56	0
55	MG	2a	1726	1/1	0.85	0.16	69,69,69,69	0
55	MG	1A	3370	1/1	0.85	0.38	42,42,42,42	0
55	MG	2A	3353	1/1	0.85	0.15	34,34,34,34	0
55	MG	2A	3680	1/1	0.85	0.21	60,60,60,60	0
55	MG	2a	1744	1/1	0.85	0.12	69,69,69,69	0
55	MG	1Y	201	1/1	0.85	0.18	64,64,64,64	0
55	MG	1A	3996	1/1	0.85	0.12	56,56,56,56	0
55	MG	1a	1712	1/1	0.85	0.36	57,57,57,57	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
55	MG	1A	3515	1/1	0.85	0.16	39,39,39,39	0
55	MG	14	101	1/1	0.85	0.18	81,81,81,81	0
55	MG	15	102	1/1	0.85	0.25	40,40,40,40	0
55	MG	1A	3325	1/1	0.85	0.23	60,60,60,60	0
55	MG	1A	3894	1/1	0.85	0.10	19,19,19,19	0
55	MG	2a	1780	1/1	0.85	0.06	69,69,69,69	0
55	MG	1A	3730	1/1	0.85	0.20	17,17,17,17	0
55	MG	1A	3372	1/1	0.85	0.33	65,65,65,65	0
55	MG	1A	3023	1/1	0.85	0.45	66,66,66,66	0
55	MG	2A	3207	1/1	0.85	0.38	58,58,58,58	0
55	MG	1A	3209	1/1	0.85	0.16	51,51,51,51	0
55	MG	2a	1792	1/1	0.85	0.11	70,70,70,70	0
55	MG	1A	3330	1/1	0.85	0.18	45,45,45,45	0
55	MG	1A	3925	1/1	0.85	0.25	62,62,62,62	0
55	MG	2A	3224	1/1	0.85	0.16	65,65,65,65	0
55	MG	1A	3446	1/1	0.85	0.22	53,53,53,53	0
55	MG	1A	3929	1/1	0.85	0.20	49,49,49,49	0
55	MG	2A	3474	1/1	0.85	0.46	70,70,70,70	0
55	MG	1A	3793	1/1	0.85	0.12	52,52,52,52	0
55	MG	2D	302	1/1	0.85	0.35	61,61,61,61	0
55	MG	1A	3945	1/1	0.85	0.10	36,36,36,36	0
55	MG	1a	1688	1/1	0.86	0.20	43,43,43,43	0
55	MG	28	3402	1/1	0.86	0.12	44,44,44,44	0
55	MG	2A	3072	1/1	0.86	0.16	57,57,57,57	0
55	MG	10	102	1/1	0.86	0.84	52,52,52,52	0
55	MG	1A	3115	1/1	0.86	0.20	49,49,49,49	0
55	MG	2A	3275	1/1	0.86	0.58	48,48,48,48	0
55	MG	2A	3554	1/1	0.86	0.14	68,68,68,68	0
55	MG	2A	3084	1/1	0.86	0.21	63,63,63,63	0
55	MG	1A	3511	1/1	0.86	0.19	49,49,49,49	0
55	MG	1A	4026	1/1	0.86	0.20	51,51,51,51	0
55	MG	1A	3451	1/1	0.86	0.16	60,60,60,60	0
55	MG	2A	3304	1/1	0.86	0.11	76,76,76,76	0
55	MG	2A	3306	1/1	0.86	0.35	43,43,43,43	0
55	MG	1A	3309	1/1	0.86	0.17	54,54,54,54	0
55	MG	2a	1638	1/1	0.86	0.16	54,54,54,54	0
55	MG	1A	3646	1/1	0.86	0.37	68,68,68,68	0
55	MG	1A	4050	1/1	0.86	0.16	46,46,46,46	0
55	MG	2a	1644	1/1	0.86	0.21	65,65,65,65	0
55	MG	1A	3650	1/1	0.86	0.15	59,59,59,59	0
55	MG	1A	3957	1/1	0.86	0.15	69,69,69,69	0
55	MG	2A	3593	1/1	0.86	0.18	81,81,81,81	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
55	MG	1A	3353	1/1	0.86	0.51	61,61,61,61	0
55	MG	2a	1669	1/1	0.86	0.18	62,62,62,62	0
55	MG	1A	3528	1/1	0.86	0.21	65,65,65,65	0
55	MG	2A	3599	1/1	0.86	0.12	66,66,66,66	0
55	MG	1A	3328	1/1	0.86	0.14	61,61,61,61	0
55	MG	2A	3605	1/1	0.86	0.17	41,41,41,41	0
55	MG	2A	3608	1/1	0.86	0.18	71,71,71,71	0
55	MG	2A	3172	1/1	0.86	0.62	42,42,42,42	0
55	MG	2A	3612	1/1	0.86	0.14	54,54,54,54	0
55	MG	1a	1620	1/1	0.86	0.12	59,59,59,59	0
55	MG	1A	3130	1/1	0.86	0.23	61,61,61,61	0
55	MG	2A	3624	1/1	0.86	0.21	49,49,49,49	0
55	MG	2A	3182	1/1	0.86	0.16	50,50,50,50	0
55	MG	1a	1623	1/1	0.86	0.10	51,51,51,51	0
55	MG	1A	3289	1/1	0.86	0.18	56,56,56,56	0
55	MG	1A	3560	1/1	0.86	0.11	28,28,28,28	0
55	MG	2A	3387	1/1	0.86	0.16	32,32,32,32	0
55	MG	2A	3193	1/1	0.86	0.10	61,61,61,61	0
55	MG	2A	3673	1/1	0.86	0.34	70,70,70,70	0
55	MG	1A	3561	1/1	0.86	0.17	29,29,29,29	0
55	MG	1a	1630	1/1	0.86	0.12	72,72,72,72	0
55	MG	2A	3408	1/1	0.86	0.19	66,66,66,66	0
55	MG	1E	307	1/1	0.86	0.68	51,51,51,51	0
55	MG	2A	3209	1/1	0.86	0.22	58,58,58,58	0
55	MG	1E	308	1/1	0.86	0.15	48,48,48,48	0
55	MG	2A	3695	1/1	0.86	0.22	62,62,62,62	0
55	MG	1A	3079	1/1	0.86	0.26	54,54,54,54	0
55	MG	2a	1752	1/1	0.86	0.16	65,65,65,65	0
55	MG	1A	3980	1/1	0.86	0.18	39,39,39,39	0
55	MG	2A	3445	1/1	0.86	0.12	62,62,62,62	0
55	MG	2A	3709	1/1	0.86	0.28	55,55,55,55	0
55	MG	1a	1649	1/1	0.86	0.22	59,59,59,59	0
55	MG	2a	1761	1/1	0.86	0.21	87,87,87,87	0
55	MG	1A	3587	1/1	0.86	0.15	36,36,36,36	0
55	MG	2a	1769	1/1	0.86	0.18	52,52,52,52	0
55	MG	1A	3907	1/1	0.86	0.18	58,58,58,58	0
55	MG	1b	301	1/1	0.86	0.06	80,80,80,80	0
55	MG	1A	3748	1/1	0.86	0.21	40,40,40,40	0
55	MG	1A	3272	1/1	0.86	0.11	61,61,61,61	0
55	MG	1a	1660	1/1	0.86	0.18	56,56,56,56	0
55	MG	1N	203	1/1	0.86	0.41	52,52,52,52	0
55	MG	1A	3994	1/1	0.86	0.08	44,44,44,44	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
55	MG	1A	3145	1/1	0.86	0.28	47,47,47,47	0
55	MG	2a	1795	1/1	0.86	0.34	84,84,84,84	0
55	MG	1A	4000	1/1	0.86	0.05	38,38,38,38	0
55	MG	1A	3439	1/1	0.86	0.37	66,66,66,66	0
55	MG	1A	3920	1/1	0.86	0.15	32,32,32,32	0
55	MG	2A	3495	1/1	0.86	0.14	53,53,53,53	0
55	MG	2F	301	1/1	0.86	0.22	47,47,47,47	0
55	MG	2r	101	1/1	0.86	0.10	84,84,84,84	0
55	MG	1A	3497	1/1	0.86	0.18	65,65,65,65	0
55	MG	2A	3048	1/1	0.86	0.25	58,58,58,58	0
55	MG	1A	3805	1/1	0.86	0.09	25,25,25,25	0
55	MG	2A	3060	1/1	0.86	0.23	44,44,44,44	0
55	MG	2A	3191	1/1	0.87	0.20	67,67,67,67	0
55	MG	1A	3278	1/1	0.87	0.64	62,62,62,62	0
55	MG	2a	1635	1/1	0.87	0.21	71,71,71,71	0
55	MG	1A	4028	1/1	0.87	0.14	58,58,58,58	0
55	MG	2A	3196	1/1	0.87	0.18	57,57,57,57	0
55	MG	2A	3197	1/1	0.87	0.21	60,60,60,60	0
55	MG	1X	103	1/1	0.87	0.21	38,38,38,38	0
55	MG	2A	3204	1/1	0.87	0.24	67,67,67,67	0
55	MG	2A	3615	1/1	0.87	0.20	46,46,46,46	0
55	MG	2A	3205	1/1	0.87	0.62	52,52,52,52	0
55	MG	2a	1661	1/1	0.87	0.15	62,62,62,62	0
55	MG	1a	1667	1/1	0.87	0.11	52,52,52,52	0
55	MG	1A	3868	1/1	0.87	0.13	27,27,27,27	0
55	MG	1A	3873	1/1	0.87	0.16	54,54,54,54	0
55	MG	1A	3875	1/1	0.87	0.14	18,18,18,18	0
55	MG	2A	3432	1/1	0.87	0.14	35,35,35,35	0
55	MG	1A	3540	1/1	0.87	0.22	23,23,23,23	0
55	MG	2A	3649	1/1	0.87	0.10	55,55,55,55	0
55	MG	1x	104	1/1	0.87	0.21	65,65,65,65	0
55	MG	1A	3159	1/1	0.87	0.12	40,40,40,40	0
55	MG	2A	3456	1/1	0.87	0.12	36,36,36,36	0
55	MG	1A	3428	1/1	0.87	0.67	49,49,49,49	0
55	MG	18	101	1/1	0.87	0.39	49,49,49,49	0
55	MG	2A	3005	1/1	0.87	0.21	62,62,62,62	0
55	MG	1A	3572	1/1	0.87	0.09	23,23,23,23	0
55	MG	1B	208	1/1	0.87	0.18	81,81,81,81	0
55	MG	1A	3483	1/1	0.87	0.38	45,45,45,45	0
55	MG	2A	3693	1/1	0.87	0.14	51,51,51,51	0
55	MG	1A	3283	1/1	0.87	0.81	56,56,56,56	0
55	MG	2A	3697	1/1	0.87	0.34	60,60,60,60	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
55	MG	1A	3735	1/1	0.87	0.09	62,62,62,62	0
55	MG	1a	1701	1/1	0.87	0.15	51,51,51,51	0
55	MG	1A	3162	1/1	0.87	0.34	31,31,31,31	0
55	MG	1A	3500	1/1	0.87	0.18	45,45,45,45	0
55	MG	1D	304	1/1	0.87	0.23	28,28,28,28	0
55	MG	2a	1740	1/1	0.87	0.17	65,65,65,65	0
55	MG	1A	3771	1/1	0.87	0.17	60,60,60,60	0
55	MG	1A	3445	1/1	0.87	0.33	63,63,63,63	0
55	MG	1A	3990	1/1	0.87	0.23	47,47,47,47	0
55	MG	2a	1746	1/1	0.87	0.15	57,57,57,57	0
55	MG	2A	3092	1/1	0.87	0.10	49,49,49,49	0
55	MG	1A	3628	1/1	0.87	0.07	34,34,34,34	0
55	MG	2A	3101	1/1	0.87	0.16	63,63,63,63	0
55	MG	2A	3518	1/1	0.87	0.19	71,71,71,71	0
55	MG	2A	3524	1/1	0.87	0.17	34,34,34,34	0
55	MG	1A	3069	1/1	0.87	0.32	28,28,28,28	0
55	MG	2A	3118	1/1	0.87	0.40	61,61,61,61	0
55	MG	2A	3542	1/1	0.87	0.09	49,49,49,49	0
55	MG	2a	1768	1/1	0.87	0.14	64,64,64,64	0
55	MG	1A	3005	1/1	0.87	0.17	46,46,46,46	0
55	MG	2D	305	1/1	0.87	0.56	43,43,43,43	0
55	MG	1A	3373	1/1	0.87	0.14	64,64,64,64	0
55	MG	2a	1781	1/1	0.87	0.11	73,73,73,73	0
55	MG	1A	3516	1/1	0.87	0.14	40,40,40,40	0
55	MG	1a	1765	1/1	0.87	0.20	74,74,74,74	0
55	MG	1A	3831	1/1	0.87	0.16	28,28,28,28	0
55	MG	1a	1636	1/1	0.87	0.12	65,65,65,65	0
55	MG	2A	3160	1/1	0.87	0.21	59,59,59,59	0
55	MG	1A	3268	1/1	0.87	0.23	62,62,62,62	0
55	MG	1a	1773	1/1	0.87	0.20	83,83,83,83	0
55	MG	1a	1774	1/1	0.87	0.16	63,63,63,63	0
55	MG	1A	4018	1/1	0.87	0.17	76,76,76,76	0
55	MG	1A	3292	1/1	0.87	0.18	52,52,52,52	0
55	MG	2I	203	1/1	0.87	0.09	64,64,64,64	0
55	MG	1a	1650	1/1	0.87	0.22	63,63,63,63	0
55	MG	1S	203	1/1	0.87	0.11	71,71,71,71	0
55	MG	2a	1606	1/1	0.87	0.26	62,62,62,62	0
55	MG	1A	3324	1/1	0.87	0.17	61,61,61,61	0
55	MG	2A	3590	1/1	0.87	0.18	45,45,45,45	0
55	MG	2A	3186	1/1	0.87	0.21	60,60,60,60	0
55	MG	1A	3230	1/1	0.87	0.52	68,68,68,68	0
55	MG	2I	101	1/1	0.88	0.12	51,51,51,51	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
55	MG	2A	3071	1/1	0.88	0.15	52,52,52,52	0
55	MG	1a	1704	1/1	0.88	0.08	62,62,62,62	0
55	MG	1A	3307	1/1	0.88	0.77	25,25,25,25	0
55	MG	2A	3079	1/1	0.88	0.12	46,46,46,46	0
55	MG	1a	1604	1/1	0.88	0.11	64,64,64,64	0
55	MG	1A	3201	1/1	0.88	0.42	49,49,49,49	0
55	MG	1A	3205	1/1	0.88	0.18	60,60,60,60	0
55	MG	1A	3469	1/1	0.88	0.15	68,68,68,68	0
55	MG	2a	1609	1/1	0.88	0.19	78,78,78,78	0
55	MG	2A	3265	1/1	0.88	0.26	52,52,52,52	0
55	MG	2A	3559	1/1	0.88	0.15	59,59,59,59	0
55	MG	2a	1615	1/1	0.88	0.18	67,67,67,67	0
55	MG	2a	1619	1/1	0.88	0.18	69,69,69,69	0
55	MG	1A	3678	1/1	0.88	0.36	59,59,59,59	0
55	MG	2A	3094	1/1	0.88	0.26	51,51,51,51	0
55	MG	2A	3276	1/1	0.88	0.23	64,64,64,64	0
55	MG	2a	1632	1/1	0.88	0.13	65,65,65,65	0
55	MG	1A	3869	1/1	0.88	0.12	39,39,39,39	0
55	MG	2A	3281	1/1	0.88	0.25	57,57,57,57	0
55	MG	1a	1740	1/1	0.88	0.11	62,62,62,62	0
55	MG	1B	227	1/1	0.88	0.20	69,69,69,69	0
55	MG	2A	3584	1/1	0.88	0.08	54,54,54,54	0
55	MG	2A	3293	1/1	0.88	0.13	54,54,54,54	0
55	MG	2A	3125	1/1	0.88	0.14	50,50,50,50	0
55	MG	1A	3266	1/1	0.88	0.18	52,52,52,52	0
55	MG	1A	3544	1/1	0.88	0.23	40,40,40,40	0
55	MG	2A	3149	1/1	0.88	0.39	66,66,66,66	0
55	MG	2A	3596	1/1	0.88	0.09	69,69,69,69	0
55	MG	1A	3688	1/1	0.88	0.18	54,54,54,54	0
55	MG	2a	1668	1/1	0.88	0.21	57,57,57,57	0
55	MG	1a	1758	1/1	0.88	0.10	57,57,57,57	0
55	MG	1a	1625	1/1	0.88	0.07	71,71,71,71	0
55	MG	2A	3155	1/1	0.88	0.19	55,55,55,55	0
55	MG	2A	3322	1/1	0.88	0.51	58,58,58,58	0
55	MG	1A	3118	1/1	0.88	0.14	37,37,37,37	0
55	MG	1A	3111	1/1	0.88	0.25	39,39,39,39	0
55	MG	1A	3712	1/1	0.88	0.12	41,41,41,41	0
55	MG	1A	3571	1/1	0.88	0.23	54,54,54,54	0
55	MG	1A	3277	1/1	0.88	0.10	46,46,46,46	0
55	MG	1A	3389	1/1	0.88	0.69	56,56,56,56	0
55	MG	1a	1780	1/1	0.88	0.10	63,63,63,63	0
55	MG	2A	3179	1/1	0.88	0.15	59,59,59,59	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
55	MG	2A	3378	1/1	0.88	0.11	46,46,46,46	0
55	MG	1A	3351	1/1	0.88	0.17	51,51,51,51	0
55	MG	1A	3992	1/1	0.88	0.07	35,35,35,35	0
55	MG	1A	3498	1/1	0.88	0.52	60,60,60,60	0
55	MG	2A	3655	1/1	0.88	0.30	57,57,57,57	0
55	MG	1A	3768	1/1	0.88	0.12	39,39,39,39	0
55	MG	2A	3661	1/1	0.88	0.12	61,61,61,61	0
55	MG	2A	3665	1/1	0.88	0.14	54,54,54,54	0
55	MG	2A	3667	1/1	0.88	0.12	67,67,67,67	0
55	MG	1A	3998	1/1	0.88	0.15	54,54,54,54	0
55	MG	2A	3400	1/1	0.88	0.23	73,73,73,73	0
55	MG	2A	3681	1/1	0.88	0.31	54,54,54,54	0
55	MG	1A	3438	1/1	0.88	0.30	67,67,67,67	0
55	MG	1A	3911	1/1	0.88	0.13	65,65,65,65	0
55	MG	1A	3296	1/1	0.88	0.35	44,44,44,44	0
55	MG	1A	4011	1/1	0.88	0.12	39,39,39,39	0
55	MG	2a	1751	1/1	0.88	0.10	64,64,64,64	0
55	MG	1a	1662	1/1	0.88	0.14	57,57,57,57	0
55	MG	1V	207	1/1	0.88	0.59	63,63,63,63	0
55	MG	2A	3199	1/1	0.88	0.13	69,69,69,69	0
55	MG	2A	3202	1/1	0.88	0.20	54,54,54,54	0
55	MG	2A	3443	1/1	0.88	0.14	45,45,45,45	0
55	MG	1A	3614	1/1	0.88	0.30	64,64,64,64	0
55	MG	1A	3080	1/1	0.88	0.16	36,36,36,36	0
55	MG	1A	3357	1/1	0.88	0.23	46,46,46,46	0
55	MG	1A	3280	1/1	0.88	0.29	60,60,60,60	0
55	MG	2A	3211	1/1	0.88	0.25	54,54,54,54	0
55	MG	2a	1779	1/1	0.88	0.23	71,71,71,71	0
55	MG	1A	3817	1/1	0.88	0.19	27,27,27,27	0
55	MG	2A	3216	1/1	0.88	0.06	74,74,74,74	0
55	MG	2A	3217	1/1	0.88	0.21	49,49,49,49	0
55	MG	1A	3829	1/1	0.88	0.23	81,81,81,81	0
55	MG	1A	3360	1/1	0.88	0.81	46,46,46,46	0
55	MG	2A	3008	1/1	0.88	0.18	65,65,65,65	0
55	MG	2A	3028	1/1	0.88	0.17	37,37,37,37	0
55	MG	2a	1789	1/1	0.88	0.12	46,46,46,46	0
55	MG	12	101	1/1	0.88	0.19	49,49,49,49	0
55	MG	2B	215	1/1	0.88	0.16	69,69,69,69	0
55	MG	1A	3168	1/1	0.88	0.21	40,40,40,40	0
55	MG	2A	3042	1/1	0.88	0.14	52,52,52,52	0
55	MG	2f	201	1/1	0.88	0.29	57,57,57,57	0
55	MG	1A	3937	1/1	0.88	0.15	73,73,73,73	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
55	MG	1A	3526	1/1	0.88	0.55	55,55,55,55	0
55	MG	2A	3053	1/1	0.88	0.18	58,58,58,58	0
55	MG	18	103	1/1	0.88	0.49	43,43,43,43	0
55	MG	2A	3059	1/1	0.88	0.17	47,47,47,47	0
55	MG	1A	3951	1/1	0.88	0.13	55,55,55,55	0
55	MG	2A	3523	1/1	0.88	0.19	35,35,35,35	0
55	MG	2W	203	1/1	0.88	0.12	63,63,63,63	0
55	MG	1A	3839	1/1	0.88	0.41	28,28,28,28	0
55	MG	2A	3714	1/1	0.89	0.15	63,63,63,63	0
55	MG	1A	3832	1/1	0.89	0.14	59,59,59,59	0
55	MG	1a	1717	1/1	0.89	0.13	63,63,63,63	0
55	MG	2A	3389	1/1	0.89	0.19	32,32,32,32	0
55	MG	1A	3014	1/1	0.89	0.27	32,32,32,32	0
55	MG	10	101	1/1	0.89	0.46	46,46,46,46	0
55	MG	1A	3327	1/1	0.89	0.36	65,65,65,65	0
55	MG	2B	206	1/1	0.89	0.09	68,68,68,68	0
55	MG	1A	3503	1/1	0.89	0.09	41,41,41,41	0
55	MG	10	105	1/1	0.89	0.17	61,61,61,61	0
55	MG	2A	3409	1/1	0.89	0.08	56,56,56,56	0
55	MG	2A	3411	1/1	0.89	0.06	62,62,62,62	0
55	MG	2A	3173	1/1	0.89	0.13	61,61,61,61	0
55	MG	1A	3507	1/1	0.89	0.23	35,35,35,35	0
55	MG	1A	3425	1/1	0.89	0.15	45,45,45,45	0
55	MG	1A	3856	1/1	0.89	0.08	45,45,45,45	0
55	MG	2A	3180	1/1	0.89	0.22	61,61,61,61	0
55	MG	2E	302	1/1	0.89	0.12	57,57,57,57	0
55	MG	2E	305	1/1	0.89	0.15	38,38,38,38	0
55	MG	1A	3228	1/1	0.89	0.26	48,48,48,48	0
55	MG	2A	3183	1/1	0.89	0.14	62,62,62,62	0
55	MG	1a	1760	1/1	0.89	0.18	48,48,48,48	0
55	MG	1A	3861	1/1	0.89	0.27	53,53,53,53	0
55	MG	2V	202	1/1	0.89	0.17	63,63,63,63	0
55	MG	2A	3457	1/1	0.89	0.18	51,51,51,51	0
55	MG	1A	3642	1/1	0.89	0.13	65,65,65,65	0
55	MG	18	107	1/1	0.89	0.14	38,38,38,38	0
55	MG	2A	3190	1/1	0.89	0.39	61,61,61,61	0
55	MG	1A	3644	1/1	0.89	0.17	43,43,43,43	0
55	MG	1A	3513	1/1	0.89	0.36	74,74,74,74	0
55	MG	1A	3017	1/1	0.89	0.30	47,47,47,47	0
55	MG	1A	4015	1/1	0.89	0.31	53,53,53,53	0
55	MG	1A	3651	1/1	0.89	0.21	45,45,45,45	0
55	MG	1a	1781	1/1	0.89	0.11	65,65,65,65	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
55	MG	1A	3243	1/1	0.89	0.23	45,45,45,45	0
55	MG	1A	3379	1/1	0.89	0.17	61,61,61,61	0
55	MG	2a	1612	1/1	0.89	0.13	54,54,54,54	0
55	MG	1a	1613	1/1	0.89	0.10	70,70,70,70	0
55	MG	1A	3674	1/1	0.89	0.19	17,17,17,17	0
55	MG	1a	1615	1/1	0.89	0.32	56,56,56,56	0
55	MG	2a	1617	1/1	0.89	0.14	74,74,74,74	0
55	MG	2a	1618	1/1	0.89	0.19	61,61,61,61	0
55	MG	1A	3517	1/1	0.89	0.34	68,68,68,68	0
55	MG	1A	4025	1/1	0.89	0.30	62,62,62,62	0
55	MG	1A	3333	1/1	0.89	0.36	45,45,45,45	0
55	MG	2a	1627	1/1	0.89	0.10	75,75,75,75	0
55	MG	1A	3682	1/1	0.89	0.21	41,41,41,41	0
55	MG	1A	4032	1/1	0.89	0.12	39,39,39,39	0
55	MG	1A	3386	1/1	0.89	0.20	64,64,64,64	0
55	MG	2a	1634	1/1	0.89	0.30	62,62,62,62	0
55	MG	2A	3220	1/1	0.89	0.44	57,57,57,57	0
55	MG	1A	4034	1/1	0.89	0.16	63,63,63,63	0
55	MG	1A	3335	1/1	0.89	0.20	40,40,40,40	0
55	MG	1A	3904	1/1	0.89	0.11	50,50,50,50	0
55	MG	2A	3227	1/1	0.89	0.17	74,74,74,74	0
55	MG	1A	3274	1/1	0.89	0.16	61,61,61,61	0
55	MG	1A	3700	1/1	0.89	0.16	40,40,40,40	0
55	MG	1a	1635	1/1	0.89	0.21	59,59,59,59	0
55	MG	1B	201	1/1	0.89	0.22	47,47,47,47	0
55	MG	1A	3910	1/1	0.89	0.17	59,59,59,59	0
55	MG	2A	3014	1/1	0.89	0.12	65,65,65,65	0
55	MG	2A	3024	1/1	0.89	0.21	56,56,56,56	0
55	MG	2A	3564	1/1	0.89	0.15	43,43,43,43	0
55	MG	2a	1672	1/1	0.89	0.10	64,64,64,64	0
55	MG	1A	3179	1/1	0.89	0.26	31,31,31,31	0
55	MG	2A	3030	1/1	0.89	0.22	45,45,45,45	0
55	MG	1A	3460	1/1	0.89	0.16	24,24,24,24	0
55	MG	2A	3034	1/1	0.89	0.16	51,51,51,51	0
55	MG	1A	3723	1/1	0.89	0.14	64,64,64,64	0
55	MG	2a	1684	1/1	0.89	0.10	68,68,68,68	0
55	MG	2A	3575	1/1	0.89	0.22	37,37,37,37	0
55	MG	2A	3255	1/1	0.89	0.30	49,49,49,49	0
55	MG	2A	3582	1/1	0.89	0.36	67,67,67,67	0
55	MG	1A	3727	1/1	0.89	0.16	24,24,24,24	0
55	MG	2A	3043	1/1	0.89	0.10	54,54,54,54	0
55	MG	1a	1653	1/1	0.89	0.10	60,60,60,60	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
55	MG	2A	3046	1/1	0.89	0.12	65,65,65,65	0
55	MG	1A	3535	1/1	0.89	0.14	22,22,22,22	0
55	MG	2A	3049	1/1	0.89	0.21	51,51,51,51	0
55	MG	1B	225	1/1	0.89	0.22	52,52,52,52	0
55	MG	1A	3340	1/1	0.89	0.23	59,59,59,59	0
55	MG	1A	3344	1/1	0.89	0.09	28,28,28,28	0
55	MG	1A	3741	1/1	0.89	0.14	57,57,57,57	0
55	MG	2A	3604	1/1	0.89	0.10	61,61,61,61	0
55	MG	2a	1727	1/1	0.89	0.07	82,82,82,82	0
55	MG	2a	1728	1/1	0.89	0.13	71,71,71,71	0
55	MG	1A	3104	1/1	0.89	0.19	68,68,68,68	0
55	MG	1a	1665	1/1	0.89	0.40	60,60,60,60	0
55	MG	1A	3105	1/1	0.89	0.39	41,41,41,41	0
55	MG	1A	3194	1/1	0.89	0.35	37,37,37,37	0
55	MG	2A	3289	1/1	0.89	0.17	38,38,38,38	0
55	MG	1A	3254	1/1	0.89	0.19	37,37,37,37	0
55	MG	2A	3294	1/1	0.89	0.15	63,63,63,63	0
55	MG	1A	3950	1/1	0.89	0.23	74,74,74,74	0
55	MG	2A	3626	1/1	0.89	0.20	33,33,33,33	0
55	MG	1A	3776	1/1	0.89	0.07	49,49,49,49	0
55	MG	2A	3632	1/1	0.89	0.14	35,35,35,35	0
55	MG	2A	3305	1/1	0.89	0.16	55,55,55,55	0
55	MG	1A	3582	1/1	0.89	0.29	55,55,55,55	0
55	MG	2A	3647	1/1	0.89	0.09	64,64,64,64	0
55	MG	1A	3954	1/1	0.89	0.12	76,76,76,76	0
55	MG	2A	3309	1/1	0.89	0.23	61,61,61,61	0
55	MG	1A	3043	1/1	0.89	0.24	42,42,42,42	0
55	MG	1A	3204	1/1	0.89	0.20	65,65,65,65	0
55	MG	1A	3322	1/1	0.89	0.09	43,43,43,43	0
55	MG	2A	3660	1/1	0.89	0.08	60,60,60,60	0
55	MG	2A	3105	1/1	0.89	0.19	48,48,48,48	0
55	MG	1A	3022	1/1	0.89	0.18	33,33,33,33	0
55	MG	1A	3602	1/1	0.89	0.18	37,37,37,37	0
55	MG	1A	3820	1/1	0.89	0.16	27,27,27,27	0
55	MG	1A	3821	1/1	0.89	0.14	45,45,45,45	0
55	MG	2A	3329	1/1	0.89	0.33	37,37,37,37	0
55	MG	2A	3332	1/1	0.89	0.24	57,57,57,57	0
55	MG	2A	3136	1/1	0.89	0.10	74,74,74,74	0
55	MG	2A	3141	1/1	0.89	0.18	47,47,47,47	0
55	MG	2A	3350	1/1	0.89	0.20	62,62,62,62	0
55	MG	1A	3825	1/1	0.89	0.14	26,26,26,26	0
55	MG	2A	3692	1/1	0.89	0.22	64,64,64,64	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
55	MG	2A	3355	1/1	0.89	0.16	47,47,47,47	0
55	MG	2A	3694	1/1	0.89	0.09	51,51,51,51	0
55	MG	2I	202	1/1	0.89	0.25	60,60,60,60	0
55	MG	2A	3358	1/1	0.89	0.16	71,71,71,71	0
55	MG	1A	3489	1/1	0.89	0.91	33,33,33,33	0
55	MG	2A	3368	1/1	0.89	0.19	42,42,42,42	0
55	MG	2A	3375	1/1	0.89	0.10	34,34,34,34	0
55	MG	2x	101	1/1	0.89	0.21	65,65,65,65	0
55	MG	1A	3116	1/1	0.89	0.23	41,41,41,41	0
55	MG	1A	3616	1/1	0.89	0.15	47,47,47,47	0
55	MG	2A	3152	1/1	0.89	0.11	57,57,57,57	0
55	MG	2A	3712	1/1	0.89	0.17	71,71,71,71	0
55	MG	1Z	302	1/1	0.90	0.20	57,57,57,57	0
55	MG	1A	3458	1/1	0.90	0.16	63,63,63,63	0
55	MG	1a	1699	1/1	0.90	0.75	65,65,65,65	0
55	MG	2A	3533	1/1	0.90	0.16	58,58,58,58	0
55	MG	2A	3073	1/1	0.90	0.15	42,42,42,42	0
55	MG	1A	3338	1/1	0.90	0.25	51,51,51,51	0
55	MG	2A	3250	1/1	0.90	0.20	43,43,43,43	0
55	MG	2A	3076	1/1	0.90	0.23	47,47,47,47	0
55	MG	1A	3791	1/1	0.90	0.15	53,53,53,53	0
55	MG	1A	4019	1/1	0.90	0.15	68,68,68,68	0
55	MG	1I	103	1/1	0.90	0.14	64,64,64,64	0
55	MG	1A	3339	1/1	0.90	0.23	53,53,53,53	0
55	MG	1A	3795	1/1	0.90	0.23	57,57,57,57	0
55	MG	1A	3800	1/1	0.90	0.11	42,42,42,42	0
55	MG	1A	3221	1/1	0.90	0.26	36,36,36,36	0
55	MG	15	106	1/1	0.90	0.48	43,43,43,43	0
55	MG	17	106	1/1	0.90	0.19	49,49,49,49	0
55	MG	2A	3106	1/1	0.90	0.20	49,49,49,49	0
55	MG	2A	3107	1/1	0.90	0.58	43,43,43,43	0
55	MG	2A	3572	1/1	0.90	0.14	53,53,53,53	0
55	MG	2A	3116	1/1	0.90	0.13	69,69,69,69	0
55	MG	1A	3341	1/1	0.90	0.54	65,65,65,65	0
55	MG	2A	3577	1/1	0.90	0.42	55,55,55,55	0
55	MG	1A	3343	1/1	0.90	0.20	39,39,39,39	0
55	MG	2A	3119	1/1	0.90	0.33	41,41,41,41	0
55	MG	1A	3378	1/1	0.90	0.10	58,58,58,58	0
55	MG	1A	3935	1/1	0.90	0.13	63,63,63,63	0
55	MG	2A	3134	1/1	0.90	0.12	55,55,55,55	0
55	MG	2A	3299	1/1	0.90	0.25	64,64,64,64	0
55	MG	2A	3135	1/1	0.90	0.36	58,58,58,58	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
55	MG	2a	1637	1/1	0.90	0.10	65,65,65,65	0
55	MG	1A	3131	1/1	0.90	0.15	43,43,43,43	0
55	MG	2A	3137	1/1	0.90	0.39	66,66,66,66	0
55	MG	2a	1641	1/1	0.90	0.36	56,56,56,56	0
55	MG	1A	3380	1/1	0.90	0.12	65,65,65,65	0
55	MG	1a	1759	1/1	0.90	0.08	63,63,63,63	0
55	MG	1A	3474	1/1	0.90	0.38	37,37,37,37	0
55	MG	1a	1763	1/1	0.90	0.09	59,59,59,59	0
55	MG	1A	4044	1/1	0.90	0.14	73,73,73,73	0
55	MG	1A	3543	1/1	0.90	0.17	55,55,55,55	0
55	MG	1A	3676	1/1	0.90	0.10	37,37,37,37	0
55	MG	1A	3287	1/1	0.90	0.18	42,42,42,42	0
55	MG	2A	3156	1/1	0.90	0.47	49,49,49,49	0
55	MG	2A	3616	1/1	0.90	0.22	55,55,55,55	0
55	MG	1A	3547	1/1	0.90	0.17	14,14,14,14	0
55	MG	2A	3327	1/1	0.90	0.18	58,58,58,58	0
55	MG	2a	1677	1/1	0.90	0.08	70,70,70,70	0
55	MG	1A	3422	1/1	0.90	0.15	54,54,54,54	0
55	MG	1A	3485	1/1	0.90	0.19	20,20,20,20	0
55	MG	2A	3162	1/1	0.90	0.14	55,55,55,55	0
55	MG	2A	3631	1/1	0.90	0.11	50,50,50,50	0
55	MG	2A	3163	1/1	0.90	0.73	43,43,43,43	0
55	MG	2a	1688	1/1	0.90	0.24	50,50,50,50	0
55	MG	2A	3349	1/1	0.90	0.22	34,34,34,34	0
55	MG	2A	3165	1/1	0.90	0.14	59,59,59,59	0
55	MG	1a	1779	1/1	0.90	0.13	69,69,69,69	0
55	MG	2A	3168	1/1	0.90	0.45	37,37,37,37	0
55	MG	2A	3171	1/1	0.90	0.36	39,39,39,39	0
55	MG	2A	3651	1/1	0.90	0.10	74,74,74,74	0
55	MG	2a	1700	1/1	0.90	0.37	61,61,61,61	0
55	MG	1A	3958	1/1	0.90	0.20	48,48,48,48	0
55	MG	1A	3385	1/1	0.90	0.86	52,52,52,52	0
55	MG	2a	1709	1/1	0.90	0.22	66,66,66,66	0
55	MG	1A	3180	1/1	0.90	0.17	50,50,50,50	0
55	MG	1A	3577	1/1	0.90	0.14	29,29,29,29	0
55	MG	1B	226	1/1	0.90	0.15	62,62,62,62	0
55	MG	1A	3133	1/1	0.90	0.14	31,31,31,31	0
55	MG	2a	1721	1/1	0.90	0.16	45,45,45,45	0
55	MG	1A	3430	1/1	0.90	0.32	61,61,61,61	0
55	MG	2A	3668	1/1	0.90	0.42	74,74,74,74	0
55	MG	2A	3669	1/1	0.90	0.22	60,60,60,60	0
55	MG	1A	3240	1/1	0.90	0.18	52,52,52,52	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
55	MG	2A	3676	1/1	0.90	0.34	65,65,65,65	0
55	MG	2A	3679	1/1	0.90	0.25	69,69,69,69	0
55	MG	1B	238	1/1	0.90	0.11	31,31,31,31	0
55	MG	1D	301	1/1	0.90	0.59	43,43,43,43	0
55	MG	1a	1798	1/1	0.90	0.09	74,74,74,74	0
55	MG	1A	3501	1/1	0.90	0.53	40,40,40,40	0
55	MG	2A	3402	1/1	0.90	0.23	64,64,64,64	0
55	MG	1A	3974	1/1	0.90	0.15	49,49,49,49	0
55	MG	1A	3185	1/1	0.90	0.27	32,32,32,32	0
55	MG	1x	101	1/1	0.90	0.35	75,75,75,75	0
55	MG	1a	1641	1/1	0.90	0.12	63,63,63,63	0
55	MG	1A	3978	1/1	0.90	0.11	36,36,36,36	0
55	MG	1a	1647	1/1	0.90	0.18	81,81,81,81	0
55	MG	2A	3423	1/1	0.90	0.14	60,60,60,60	0
55	MG	2a	1762	1/1	0.90	0.18	81,81,81,81	0
55	MG	1A	3295	1/1	0.90	0.34	36,36,36,36	0
55	MG	1A	3443	1/1	0.90	0.29	71,71,71,71	0
55	MG	1A	3015	1/1	0.90	0.16	57,57,57,57	0
55	MG	2A	3203	1/1	0.90	0.22	64,64,64,64	0
55	MG	1A	3985	1/1	0.90	0.11	14,14,14,14	0
55	MG	1A	3986	1/1	0.90	0.11	52,52,52,52	0
55	MG	1A	3988	1/1	0.90	0.24	42,42,42,42	0
55	MG	2A	3208	1/1	0.90	0.41	65,65,65,65	0
55	MG	1A	3512	1/1	0.90	0.15	52,52,52,52	0
55	MG	2B	201	1/1	0.90	0.16	75,75,75,75	0
55	MG	1A	3618	1/1	0.90	0.30	63,63,63,63	0
55	MG	1O	202	1/1	0.90	1.15	56,56,56,56	0
55	MG	1O	205	1/1	0.90	0.26	65,65,65,65	0
55	MG	2A	3033	1/1	0.90	0.32	54,54,54,54	0
55	MG	1A	3758	1/1	0.90	0.15	37,37,37,37	0
55	MG	1A	3888	1/1	0.90	0.09	50,50,50,50	0
55	MG	1T	201	1/1	0.90	0.10	52,52,52,52	0
55	MG	2A	3223	1/1	0.90	0.14	70,70,70,70	0
55	MG	1A	3759	1/1	0.90	0.10	37,37,37,37	0
55	MG	1U	204	1/1	0.90	0.45	61,61,61,61	0
55	MG	1U	205	1/1	0.90	0.52	37,37,37,37	0
55	MG	1A	3892	1/1	0.90	0.11	38,38,38,38	0
55	MG	1A	3764	1/1	0.90	0.15	52,52,52,52	0
55	MG	2A	3497	1/1	0.90	0.22	53,53,53,53	0
55	MG	1A	3622	1/1	0.90	0.21	18,18,18,18	0
55	MG	1A	3320	1/1	0.90	0.12	51,51,51,51	0
55	MG	2x	103	1/1	0.90	0.16	75,75,75,75	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
55	MG	2x	104	1/1	0.90	0.26	69,69,69,69	0
55	MG	1A	3398	1/1	0.90	0.40	54,54,54,54	0
55	MG	1A	3212	1/1	0.90	0.25	32,32,32,32	0
58	ZN	2Y	202	1/1	0.90	0.11	97,97,97,97	0
55	MG	2A	3061	1/1	0.90	0.52	45,45,45,45	0
55	MG	1A	3169	1/1	0.91	0.38	38,38,38,38	0
55	MG	1A	3432	1/1	0.91	0.40	32,32,32,32	0
55	MG	2A	3177	1/1	0.91	0.16	60,60,60,60	0
55	MG	1a	1611	1/1	0.91	0.06	70,70,70,70	0
55	MG	2A	3424	1/1	0.91	0.23	58,58,58,58	0
55	MG	1A	3606	1/1	0.91	0.17	17,17,17,17	0
55	MG	1A	3769	1/1	0.91	0.15	50,50,50,50	0
55	MG	2A	3181	1/1	0.91	0.27	65,65,65,65	0
55	MG	1A	4051	1/1	0.91	0.20	48,48,48,48	0
55	MG	2A	3441	1/1	0.91	0.16	36,36,36,36	0
55	MG	1A	3241	1/1	0.91	0.25	59,59,59,59	0
55	MG	1A	3774	1/1	0.91	0.29	58,58,58,58	0
55	MG	2A	3454	1/1	0.91	0.13	39,39,39,39	0
55	MG	1A	3613	1/1	0.91	0.14	26,26,26,26	0
55	MG	1A	3778	1/1	0.91	0.25	50,50,50,50	0
55	MG	1A	3932	1/1	0.91	0.33	42,42,42,42	0
55	MG	1A	3393	1/1	0.91	0.51	47,47,47,47	0
55	MG	2A	3461	1/1	0.91	0.17	43,43,43,43	0
55	MG	1B	211	1/1	0.91	0.41	56,56,56,56	0
55	MG	2A	3192	1/1	0.91	0.13	62,62,62,62	0
55	MG	2A	3466	1/1	0.91	0.95	46,46,46,46	0
55	MG	2R	201	1/1	0.91	0.21	57,57,57,57	0
55	MG	1A	3365	1/1	0.91	0.17	61,61,61,61	0
55	MG	1B	215	1/1	0.91	0.14	56,56,56,56	0
55	MG	1r	101	1/1	0.91	0.35	69,69,69,69	0
55	MG	1t	201	1/1	0.91	0.21	67,67,67,67	0
55	MG	2A	3476	1/1	0.91	0.11	61,61,61,61	0
55	MG	1A	3504	1/1	0.91	0.24	43,43,43,43	0
55	MG	1A	3938	1/1	0.91	0.20	49,49,49,49	0
55	MG	1A	3440	1/1	0.91	0.10	74,74,74,74	0
55	MG	1A	3948	1/1	0.91	0.24	40,40,40,40	0
55	MG	1B	229	1/1	0.91	0.19	36,36,36,36	0
55	MG	1x	108	1/1	0.91	0.10	61,61,61,61	0
55	MG	1A	3261	1/1	0.91	0.24	46,46,46,46	0
55	MG	2a	1607	1/1	0.91	0.29	75,75,75,75	0
55	MG	1x	110	1/1	0.91	0.12	36,36,36,36	0
55	MG	2A	3503	1/1	0.91	0.07	64,64,64,64	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
55	MG	1a	1642	1/1	0.91	0.11	50,50,50,50	0
55	MG	2A	3506	1/1	0.91	0.14	59,59,59,59	0
55	MG	1A	3400	1/1	0.91	0.39	39,39,39,39	0
55	MG	2A	3510	1/1	0.91	0.28	60,60,60,60	0
55	MG	2A	3512	1/1	0.91	0.22	65,65,65,65	0
55	MG	2A	3213	1/1	0.91	0.35	47,47,47,47	0
55	MG	1A	3952	1/1	0.91	0.12	59,59,59,59	0
55	MG	1A	3219	1/1	0.91	0.20	47,47,47,47	0
55	MG	2A	3018	1/1	0.91	0.29	58,58,58,58	0
55	MG	2a	1629	1/1	0.91	0.14	59,59,59,59	0
55	MG	2A	3020	1/1	0.91	0.50	46,46,46,46	0
55	MG	2A	3022	1/1	0.91	0.11	41,41,41,41	0
55	MG	1A	3803	1/1	0.91	0.14	39,39,39,39	0
55	MG	2A	3536	1/1	0.91	0.13	36,36,36,36	0
55	MG	1A	3450	1/1	0.91	0.79	44,44,44,44	0
55	MG	1A	3810	1/1	0.91	0.51	52,52,52,52	0
55	MG	2A	3548	1/1	0.91	0.15	52,52,52,52	0
55	MG	1a	1654	1/1	0.91	0.24	72,72,72,72	0
55	MG	1A	3813	1/1	0.91	0.06	50,50,50,50	0
55	MG	1a	1656	1/1	0.91	0.18	49,49,49,49	0
55	MG	2a	1642	1/1	0.91	0.12	76,76,76,76	0
55	MG	1A	3961	1/1	0.91	0.64	65,65,65,65	0
55	MG	1A	3402	1/1	0.91	0.21	58,58,58,58	0
55	MG	1A	3454	1/1	0.91	0.39	55,55,55,55	0
55	MG	1a	1661	1/1	0.91	0.14	71,71,71,71	0
55	MG	2a	1655	1/1	0.91	0.15	71,71,71,71	0
55	MG	1A	3264	1/1	0.91	0.23	44,44,44,44	0
55	MG	1F	311	1/1	0.91	0.42	53,53,53,53	0
55	MG	1a	1664	1/1	0.91	0.14	70,70,70,70	0
55	MG	1A	3824	1/1	0.91	0.18	24,24,24,24	0
55	MG	1I	201	1/1	0.91	0.21	71,71,71,71	0
55	MG	2a	1670	1/1	0.91	0.21	57,57,57,57	0
55	MG	2A	3058	1/1	0.91	0.15	52,52,52,52	0
55	MG	1A	3244	1/1	0.91	0.38	51,51,51,51	0
55	MG	1N	202	1/1	0.91	0.38	52,52,52,52	0
55	MG	2a	1676	1/1	0.91	0.13	52,52,52,52	0
55	MG	1a	1672	1/1	0.91	0.13	62,62,62,62	0
55	MG	2A	3578	1/1	0.91	0.16	60,60,60,60	0
55	MG	2A	3062	1/1	0.91	0.41	40,40,40,40	0
55	MG	1A	3523	1/1	0.91	0.22	48,48,48,48	0
55	MG	2A	3067	1/1	0.91	0.60	62,62,62,62	0
55	MG	1A	3406	1/1	0.91	0.13	47,47,47,47	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
55	MG	1A	3046	1/1	0.91	0.10	48,48,48,48	0
55	MG	1A	3464	1/1	0.91	0.23	54,54,54,54	0
55	MG	1a	1684	1/1	0.91	0.19	65,65,65,65	0
55	MG	2A	3268	1/1	0.91	0.13	48,48,48,48	0
55	MG	2A	3272	1/1	0.91	0.15	57,57,57,57	0
55	MG	1A	3465	1/1	0.91	0.12	56,56,56,56	0
55	MG	1A	3836	1/1	0.91	0.19	46,46,46,46	0
55	MG	2A	3602	1/1	0.91	0.11	79,79,79,79	0
55	MG	1A	3669	1/1	0.91	0.20	54,54,54,54	0
55	MG	1A	3672	1/1	0.91	0.11	58,58,58,58	0
55	MG	1A	3843	1/1	0.91	0.15	47,47,47,47	0
55	MG	2A	3091	1/1	0.91	0.21	56,56,56,56	0
55	MG	1A	3004	1/1	0.91	0.12	25,25,25,25	0
55	MG	1A	3532	1/1	0.91	0.21	51,51,51,51	0
55	MG	1A	3412	1/1	0.91	0.20	47,47,47,47	0
55	MG	1A	3345	1/1	0.91	0.71	47,47,47,47	0
55	MG	2a	1723	1/1	0.91	0.07	64,64,64,64	0
55	MG	1a	1708	1/1	0.91	0.13	58,58,58,58	0
55	MG	1A	3536	1/1	0.91	0.16	33,33,33,33	0
55	MG	2A	3303	1/1	0.91	0.26	77,77,77,77	0
55	MG	2A	3625	1/1	0.91	0.19	37,37,37,37	0
55	MG	1a	1710	1/1	0.91	0.06	56,56,56,56	0
55	MG	2A	3109	1/1	0.91	0.33	46,46,46,46	0
55	MG	2a	1742	1/1	0.91	0.07	62,62,62,62	0
55	MG	2A	3112	1/1	0.91	0.29	63,63,63,63	0
55	MG	2A	3115	1/1	0.91	0.22	50,50,50,50	0
55	MG	1A	3273	1/1	0.91	0.21	56,56,56,56	0
55	MG	1A	3685	1/1	0.91	0.18	46,46,46,46	0
55	MG	2A	3313	1/1	0.91	0.16	56,56,56,56	0
55	MG	1Z	301	1/1	0.91	0.09	60,60,60,60	0
55	MG	1A	3687	1/1	0.91	0.11	52,52,52,52	0
55	MG	2A	3122	1/1	0.91	0.29	51,51,51,51	0
55	MG	1a	1718	1/1	0.91	0.16	60,60,60,60	0
55	MG	1A	3197	1/1	0.91	0.19	39,39,39,39	0
55	MG	2A	3132	1/1	0.91	0.20	45,45,45,45	0
55	MG	2A	3657	1/1	0.91	0.11	50,50,50,50	0
55	MG	1a	1724	1/1	0.91	0.08	40,40,40,40	0
55	MG	1a	1728	1/1	0.91	0.16	54,54,54,54	0
55	MG	1a	1733	1/1	0.91	0.09	48,48,48,48	0
55	MG	1A	3384	1/1	0.91	0.33	41,41,41,41	0
55	MG	1A	3878	1/1	0.91	0.11	59,59,59,59	0
55	MG	2A	3142	1/1	0.91	0.26	65,65,65,65	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
55	MG	2A	3341	1/1	0.91	0.12	62,62,62,62	0
55	MG	2A	3145	1/1	0.91	0.14	41,41,41,41	0
55	MG	1A	3694	1/1	0.91	0.18	19,19,19,19	0
55	MG	1A	3546	1/1	0.91	0.18	44,44,44,44	0
55	MG	1A	3276	1/1	0.91	0.35	60,60,60,60	0
55	MG	1A	3709	1/1	0.91	0.10	41,41,41,41	0
55	MG	2A	3685	1/1	0.91	0.15	64,64,64,64	0
55	MG	1A	3211	1/1	0.91	0.09	40,40,40,40	0
55	MG	1a	1752	1/1	0.91	0.12	59,59,59,59	0
55	MG	1A	3479	1/1	0.91	0.10	60,60,60,60	0
55	MG	1A	3480	1/1	0.91	0.23	61,61,61,61	0
55	MG	1A	3424	1/1	0.91	0.19	65,65,65,65	0
55	MG	2e	201	1/1	0.91	0.10	79,79,79,79	0
55	MG	1A	3236	1/1	0.91	0.20	50,50,50,50	0
55	MG	2A	3382	1/1	0.91	0.18	59,59,59,59	0
55	MG	1a	1764	1/1	0.91	0.09	51,51,51,51	0
55	MG	1A	3734	1/1	0.91	0.17	54,54,54,54	0
55	MG	2A	3698	1/1	0.91	0.13	58,58,58,58	0
55	MG	1A	3578	1/1	0.91	0.12	31,31,31,31	0
55	MG	2A	3391	1/1	0.91	0.28	62,62,62,62	0
55	MG	1A	3486	1/1	0.91	0.36	33,33,33,33	0
55	MG	2A	3708	1/1	0.91	0.22	74,74,74,74	0
55	MG	2A	3166	1/1	0.91	0.29	40,40,40,40	0
55	MG	1A	4031	1/1	0.91	0.22	70,70,70,70	0
55	MG	1A	3237	1/1	0.91	0.25	54,54,54,54	0
55	MG	2A	3170	1/1	0.91	0.49	43,43,43,43	0
55	MG	1A	3239	1/1	0.91	0.15	46,46,46,46	0
55	MG	1A	3495	1/1	0.91	0.17	52,52,52,52	0
55	MG	1A	3919	1/1	0.92	0.15	25,25,25,25	0
55	MG	1A	3792	1/1	0.92	0.45	33,33,33,33	0
55	MG	1A	3922	1/1	0.92	0.14	27,27,27,27	0
55	MG	1A	4042	1/1	0.92	0.40	61,61,61,61	0
55	MG	2O	201	1/1	0.92	0.23	54,54,54,54	0
55	MG	2A	3514	1/1	0.92	0.12	57,57,57,57	0
55	MG	2A	3264	1/1	0.92	0.43	57,57,57,57	0
55	MG	1A	3238	1/1	0.92	0.34	49,49,49,49	0
55	MG	2A	3266	1/1	0.92	0.14	75,75,75,75	0
55	MG	1A	3794	1/1	0.92	0.14	43,43,43,43	0
55	MG	1A	3926	1/1	0.92	0.30	52,52,52,52	0
55	MG	1A	3206	1/1	0.92	0.20	44,44,44,44	0
55	MG	1A	3541	1/1	0.92	0.12	57,57,57,57	0
55	MG	1A	3096	1/1	0.92	0.55	40,40,40,40	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
55	MG	2A	3543	1/1	0.92	0.17	64,64,64,64	0
55	MG	2A	3124	1/1	0.92	0.31	54,54,54,54	0
55	MG	2a	1603	1/1	0.92	0.14	58,58,58,58	0
55	MG	1A	3804	1/1	0.92	0.26	34,34,34,34	0
55	MG	1A	3429	1/1	0.92	0.28	57,57,57,57	0
55	MG	1A	3806	1/1	0.92	0.28	31,31,31,31	0
55	MG	2A	3133	1/1	0.92	0.08	35,35,35,35	0
55	MG	1A	3545	1/1	0.92	0.15	41,41,41,41	0
55	MG	2a	1611	1/1	0.92	0.10	58,58,58,58	0
55	MG	1A	3484	1/1	0.92	0.31	32,32,32,32	0
55	MG	2A	3297	1/1	0.92	0.21	29,29,29,29	0
55	MG	1A	3098	1/1	0.92	0.38	49,49,49,49	0
55	MG	1A	3819	1/1	0.92	0.16	26,26,26,26	0
55	MG	1A	3552	1/1	0.92	0.20	28,28,28,28	0
55	MG	1B	221	1/1	0.92	0.09	30,30,30,30	0
55	MG	1A	3431	1/1	0.92	0.32	27,27,27,27	0
55	MG	1A	3242	1/1	0.92	0.16	51,51,51,51	0
55	MG	1A	3355	1/1	0.92	0.21	57,57,57,57	0
55	MG	2a	1626	1/1	0.92	0.33	46,46,46,46	0
55	MG	2A	3308	1/1	0.92	0.19	52,52,52,52	0
55	MG	1A	3827	1/1	0.92	0.11	24,24,24,24	0
55	MG	1a	1788	1/1	0.92	0.15	59,59,59,59	0
55	MG	1B	230	1/1	0.92	0.20	74,74,74,74	0
55	MG	1A	3436	1/1	0.92	0.39	31,31,31,31	0
55	MG	1A	3062	1/1	0.92	0.23	61,61,61,61	0
55	MG	1B	235	1/1	0.92	0.20	67,67,67,67	0
55	MG	1A	3960	1/1	0.92	0.06	35,35,35,35	0
55	MG	1A	3120	1/1	0.92	0.49	30,30,30,30	0
55	MG	1A	3395	1/1	0.92	0.14	50,50,50,50	0
55	MG	2A	3325	1/1	0.92	0.19	60,60,60,60	0
55	MG	1A	3270	1/1	0.92	0.21	40,40,40,40	0
55	MG	1l	202	1/1	0.92	0.14	66,66,66,66	0
55	MG	1m	3001	1/1	0.92	0.08	59,59,59,59	0
55	MG	1a	1646	1/1	0.92	0.68	64,64,64,64	0
55	MG	2A	3335	1/1	0.92	0.25	44,44,44,44	0
55	MG	1E	304	1/1	0.92	0.26	38,38,38,38	0
55	MG	2a	1652	1/1	0.92	0.23	48,48,48,48	0
55	MG	1E	305	1/1	0.92	0.31	49,49,49,49	0
55	MG	2a	1656	1/1	0.92	0.09	68,68,68,68	0
55	MG	1A	3699	1/1	0.92	0.20	26,26,26,26	0
55	MG	1A	3246	1/1	0.92	0.38	37,37,37,37	0
55	MG	1A	3588	1/1	0.92	0.15	35,35,35,35	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
55	MG	2A	3611	1/1	0.92	0.16	61,61,61,61	0
55	MG	2A	3352	1/1	0.92	0.14	50,50,50,50	0
55	MG	1A	3589	1/1	0.92	0.15	39,39,39,39	0
55	MG	1F	303	1/1	0.92	0.14	31,31,31,31	0
55	MG	1F	305	1/1	0.92	0.30	25,25,25,25	0
55	MG	2a	1674	1/1	0.92	0.12	66,66,66,66	0
55	MG	2A	3619	1/1	0.92	0.14	55,55,55,55	0
55	MG	2A	3620	1/1	0.92	0.08	53,53,53,53	0
55	MG	2A	3362	1/1	0.92	0.32	58,58,58,58	0
55	MG	1A	3972	1/1	0.92	0.12	39,39,39,39	0
55	MG	2A	3366	1/1	0.92	0.18	42,42,42,42	0
55	MG	1A	3852	1/1	0.92	0.26	80,80,80,80	0
55	MG	2a	1683	1/1	0.92	0.16	75,75,75,75	0
55	MG	2A	3374	1/1	0.92	0.12	61,61,61,61	0
55	MG	2A	3004	1/1	0.92	0.06	67,67,67,67	0
55	MG	1A	3362	1/1	0.92	0.62	45,45,45,45	0
55	MG	1A	3715	1/1	0.92	0.19	19,19,19,19	0
55	MG	2A	3637	1/1	0.92	0.17	49,49,49,49	0
55	MG	2A	3379	1/1	0.92	0.23	28,28,28,28	0
55	MG	2A	3646	1/1	0.92	0.17	64,64,64,64	0
55	MG	1A	3718	1/1	0.92	0.14	33,33,33,33	0
55	MG	1A	3300	1/1	0.92	0.57	45,45,45,45	0
55	MG	1A	3334	1/1	0.92	0.26	62,62,62,62	0
55	MG	1A	3248	1/1	0.92	0.29	36,36,36,36	0
55	MG	1N	205	1/1	0.92	0.74	54,54,54,54	0
55	MG	2A	3653	1/1	0.92	0.18	39,39,39,39	0
55	MG	2a	1710	1/1	0.92	0.25	51,51,51,51	0
55	MG	2A	3654	1/1	0.92	0.18	55,55,55,55	0
55	MG	2a	1715	1/1	0.92	0.16	62,62,62,62	0
55	MG	1A	3455	1/1	0.92	0.22	34,34,34,34	0
55	MG	1A	3872	1/1	0.92	0.14	54,54,54,54	0
55	MG	2A	3031	1/1	0.92	0.17	28,28,28,28	0
55	MG	1A	3611	1/1	0.92	0.14	43,43,43,43	0
55	MG	1a	1673	1/1	0.92	0.08	56,56,56,56	0
55	MG	1P	206	1/1	0.92	0.68	40,40,40,40	0
55	MG	2A	3404	1/1	0.92	0.20	53,53,53,53	0
55	MG	1A	3075	1/1	0.92	0.23	57,57,57,57	0
55	MG	2A	3041	1/1	0.92	0.38	60,60,60,60	0
55	MG	2a	1734	1/1	0.92	0.12	64,64,64,64	0
55	MG	1A	3225	1/1	0.92	0.17	56,56,56,56	0
55	MG	1A	3002	1/1	0.92	0.28	54,54,54,54	0
55	MG	2A	3416	1/1	0.92	0.11	40,40,40,40	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
55	MG	1A	3374	1/1	0.92	0.34	49,49,49,49	0
55	MG	1A	3749	1/1	0.92	0.26	59,59,59,59	0
55	MG	2A	3047	1/1	0.92	0.19	60,60,60,60	0
55	MG	2A	3425	1/1	0.92	0.17	61,61,61,61	0
55	MG	2A	3426	1/1	0.92	0.05	54,54,54,54	0
55	MG	2A	3687	1/1	0.92	0.26	61,61,61,61	0
55	MG	1A	3756	1/1	0.92	0.12	24,24,24,24	0
55	MG	1A	3621	1/1	0.92	0.15	35,35,35,35	0
55	MG	2A	3052	1/1	0.92	0.17	54,54,54,54	0
55	MG	2A	3210	1/1	0.92	0.17	50,50,50,50	0
55	MG	2A	3438	1/1	0.92	0.10	71,71,71,71	0
55	MG	1A	3310	1/1	0.92	0.81	42,42,42,42	0
55	MG	1A	3417	1/1	0.92	0.40	36,36,36,36	0
55	MG	1W	202	1/1	0.92	0.15	47,47,47,47	0
55	MG	2a	1764	1/1	0.92	0.15	62,62,62,62	0
55	MG	1A	3629	1/1	0.92	0.18	24,24,24,24	0
55	MG	2A	3700	1/1	0.92	0.14	45,45,45,45	0
55	MG	2a	1770	1/1	0.92	0.11	55,55,55,55	0
55	MG	2a	1773	1/1	0.92	0.11	71,71,71,71	0
55	MG	1A	4008	1/1	0.92	0.14	38,38,38,38	0
55	MG	1a	1703	1/1	0.92	0.09	63,63,63,63	0
55	MG	1A	3019	1/1	0.92	0.23	32,32,32,32	0
55	MG	2A	3705	1/1	0.92	0.21	62,62,62,62	0
55	MG	1A	3633	1/1	0.92	0.21	24,24,24,24	0
55	MG	1A	3279	1/1	0.92	0.28	59,59,59,59	0
55	MG	1A	3902	1/1	0.92	0.14	55,55,55,55	0
55	MG	1A	3172	1/1	0.92	0.18	39,39,39,39	0
55	MG	1A	3383	1/1	0.92	0.82	41,41,41,41	0
55	MG	2a	1788	1/1	0.92	0.07	77,77,77,77	0
55	MG	1A	3779	1/1	0.92	0.12	55,55,55,55	0
55	MG	1A	4022	1/1	0.92	0.11	47,47,47,47	0
55	MG	2A	3078	1/1	0.92	0.15	59,59,59,59	0
55	MG	1A	3175	1/1	0.92	0.15	42,42,42,42	0
55	MG	1A	3423	1/1	0.92	0.28	39,39,39,39	0
55	MG	2A	3082	1/1	0.92	0.13	63,63,63,63	0
55	MG	2A	3482	1/1	0.92	0.16	50,50,50,50	0
55	MG	13	102	1/1	0.92	0.18	47,47,47,47	0
55	MG	2A	3486	1/1	0.92	0.26	46,46,46,46	0
55	MG	2B	208	1/1	0.92	0.21	70,70,70,70	0
55	MG	13	103	1/1	0.92	0.12	45,45,45,45	0
55	MG	1a	1732	1/1	0.92	0.09	61,61,61,61	0
55	MG	1A	3473	1/1	0.92	0.36	48,48,48,48	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
55	MG	2t	201	1/1	0.92	0.10	61,61,61,61	0
55	MG	1A	3913	1/1	0.92	0.21	61,61,61,61	0
55	MG	1A	3788	1/1	0.92	0.14	22,22,22,22	0
55	MG	17	104	1/1	0.92	0.24	34,34,34,34	0
55	MG	2A	3102	1/1	0.92	0.42	68,68,68,68	0
55	MG	2A	3104	1/1	0.92	0.56	52,52,52,52	0
55	MG	2E	301	1/1	0.92	0.12	39,39,39,39	0
55	MG	1A	3136	1/1	0.92	0.12	36,36,36,36	0
55	MG	2E	303	1/1	0.92	0.16	30,30,30,30	0
58	ZN	2n	501	1/1	0.92	0.10	90,90,90,90	0
55	MG	1Q	202	1/1	0.93	0.16	33,33,33,33	0
55	MG	1a	1675	1/1	0.93	0.08	63,63,63,63	0
55	MG	2A	3218	1/1	0.93	0.28	58,58,58,58	0
55	MG	1A	3508	1/1	0.93	0.37	62,62,62,62	0
55	MG	1A	3404	1/1	0.93	0.52	40,40,40,40	0
55	MG	1a	1679	1/1	0.93	0.14	56,56,56,56	0
55	MG	1A	3885	1/1	0.93	0.09	61,61,61,61	0
55	MG	1A	3453	1/1	0.93	0.29	41,41,41,41	0
55	MG	1A	3167	1/1	0.93	0.20	54,54,54,54	0
55	MG	2E	306	1/1	0.93	0.11	64,64,64,64	0
55	MG	2A	3494	1/1	0.93	0.10	46,46,46,46	0
55	MG	1A	3366	1/1	0.93	0.28	27,27,27,27	0
55	MG	2A	3496	1/1	0.93	0.10	69,69,69,69	0
55	MG	1a	1686	1/1	0.93	0.14	71,71,71,71	0
55	MG	2A	3054	1/1	0.93	0.24	53,53,53,53	0
55	MG	1a	1687	1/1	0.93	0.12	56,56,56,56	0
55	MG	1U	211	1/1	0.93	0.30	43,43,43,43	0
55	MG	2W	201	1/1	0.93	0.29	67,67,67,67	0
55	MG	2A	3235	1/1	0.93	0.14	64,64,64,64	0
55	MG	2A	3507	1/1	0.93	0.19	58,58,58,58	0
55	MG	2A	3238	1/1	0.93	0.21	58,58,58,58	0
55	MG	25	101	1/1	0.93	0.27	55,55,55,55	0
55	MG	27	101	1/1	0.93	0.28	50,50,50,50	0
55	MG	1U	212	1/1	0.93	0.21	49,49,49,49	0
55	MG	2A	3511	1/1	0.93	0.07	77,77,77,77	0
55	MG	1A	3456	1/1	0.93	0.23	42,42,42,42	0
55	MG	1A	3891	1/1	0.93	0.10	32,32,32,32	0
55	MG	1a	1696	1/1	0.93	0.20	40,40,40,40	0
55	MG	2A	3063	1/1	0.93	0.15	44,44,44,44	0
55	MG	2A	3521	1/1	0.93	0.10	44,44,44,44	0
55	MG	1A	3766	1/1	0.93	0.26	64,64,64,64	0
55	MG	1A	3025	1/1	0.93	0.17	35,35,35,35	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
55	MG	2A	3526	1/1	0.93	0.27	69,69,69,69	0
55	MG	1A	3064	1/1	0.93	0.16	45,45,45,45	0
55	MG	2a	1610	1/1	0.93	0.24	63,63,63,63	0
55	MG	1a	1702	1/1	0.93	0.17	57,57,57,57	0
55	MG	1A	3770	1/1	0.93	0.17	66,66,66,66	0
55	MG	1A	3459	1/1	0.93	0.32	44,44,44,44	0
55	MG	1A	3906	1/1	0.93	0.11	56,56,56,56	0
55	MG	2A	3077	1/1	0.93	0.14	35,35,35,35	0
55	MG	2a	1616	1/1	0.93	0.33	67,67,67,67	0
55	MG	1A	3520	1/1	0.93	0.21	28,28,28,28	0
55	MG	1Z	303	1/1	0.93	0.14	53,53,53,53	0
55	MG	2A	3550	1/1	0.93	0.15	67,67,67,67	0
55	MG	2A	3080	1/1	0.93	0.08	73,73,73,73	0
55	MG	2a	1621	1/1	0.93	0.26	47,47,47,47	0
55	MG	1A	3411	1/1	0.93	0.29	45,45,45,45	0
55	MG	1A	3010	1/1	0.93	0.23	42,42,42,42	0
55	MG	1A	3463	1/1	0.93	0.20	66,66,66,66	0
55	MG	1a	1715	1/1	0.93	0.14	59,59,59,59	0
55	MG	2A	3086	1/1	0.93	0.09	58,58,58,58	0
55	MG	2A	3087	1/1	0.93	0.18	40,40,40,40	0
55	MG	1a	1716	1/1	0.93	0.07	69,69,69,69	0
55	MG	1A	4030	1/1	0.93	0.50	52,52,52,52	0
55	MG	1A	3291	1/1	0.93	0.20	50,50,50,50	0
55	MG	2A	3567	1/1	0.93	0.12	55,55,55,55	0
55	MG	2A	3568	1/1	0.93	0.21	63,63,63,63	0
55	MG	1A	3040	1/1	0.93	0.14	39,39,39,39	0
55	MG	2A	3096	1/1	0.93	0.26	43,43,43,43	0
55	MG	2A	3099	1/1	0.93	0.12	57,57,57,57	0
55	MG	1A	3070	1/1	0.93	0.27	42,42,42,42	0
55	MG	2A	3290	1/1	0.93	0.12	57,57,57,57	0
55	MG	1a	1727	1/1	0.93	0.08	57,57,57,57	0
55	MG	2a	1645	1/1	0.93	0.10	51,51,51,51	0
55	MG	1A	3071	1/1	0.93	0.24	45,45,45,45	0
55	MG	2A	3296	1/1	0.93	0.13	38,38,38,38	0
55	MG	1A	4035	1/1	0.93	0.10	51,51,51,51	0
55	MG	1A	4038	1/1	0.93	0.14	67,67,67,67	0
55	MG	1A	3643	1/1	0.93	0.08	61,61,61,61	0
55	MG	2a	1659	1/1	0.93	0.17	53,53,53,53	0
55	MG	2A	3108	1/1	0.93	0.26	52,52,52,52	0
55	MG	1A	3021	1/1	0.93	0.39	55,55,55,55	0
55	MG	2A	3592	1/1	0.93	0.70	77,77,77,77	0
55	MG	2a	1666	1/1	0.93	0.13	66,66,66,66	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
55	MG	2a	1667	1/1	0.93	0.17	36,36,36,36	0
55	MG	1A	3234	1/1	0.93	0.20	47,47,47,47	0
55	MG	2A	3114	1/1	0.93	0.23	39,39,39,39	0
55	MG	2A	3595	1/1	0.93	0.13	62,62,62,62	0
55	MG	1A	3121	1/1	0.93	0.19	36,36,36,36	0
55	MG	1A	3537	1/1	0.93	0.26	47,47,47,47	0
55	MG	1a	1747	1/1	0.93	0.24	72,72,72,72	0
55	MG	2A	3600	1/1	0.93	0.14	66,66,66,66	0
55	MG	1a	1749	1/1	0.93	0.10	63,63,63,63	0
55	MG	1A	3796	1/1	0.93	0.10	47,47,47,47	0
55	MG	18	105	1/1	0.93	0.66	43,43,43,43	0
55	MG	1A	3657	1/1	0.93	0.14	51,51,51,51	0
55	MG	2A	3607	1/1	0.93	0.14	43,43,43,43	0
55	MG	1a	1753	1/1	0.93	0.09	74,74,74,74	0
55	MG	2A	3318	1/1	0.93	0.44	49,49,49,49	0
55	MG	1a	1754	1/1	0.93	0.23	72,72,72,72	0
55	MG	1A	3665	1/1	0.93	0.06	64,64,64,64	0
55	MG	1A	3930	1/1	0.93	0.22	23,23,23,23	0
55	MG	1A	3539	1/1	0.93	0.11	32,32,32,32	0
55	MG	2a	1692	1/1	0.93	0.12	73,73,73,73	0
55	MG	1A	3667	1/1	0.93	0.19	51,51,51,51	0
55	MG	2A	3618	1/1	0.93	0.13	41,41,41,41	0
55	MG	1A	3302	1/1	0.93	0.21	50,50,50,50	0
55	MG	2A	3328	1/1	0.93	0.24	46,46,46,46	0
55	MG	1A	3303	1/1	0.93	0.35	48,48,48,48	0
55	MG	2A	3330	1/1	0.93	0.10	73,73,73,73	0
55	MG	2a	1705	1/1	0.93	0.27	71,71,71,71	0
55	MG	1a	1607	1/1	0.93	0.40	54,54,54,54	0
55	MG	1a	1767	1/1	0.93	0.13	55,55,55,55	0
55	MG	1a	1608	1/1	0.93	0.14	52,52,52,52	0
55	MG	1A	3123	1/1	0.93	0.15	36,36,36,36	0
55	MG	2a	1714	1/1	0.93	0.12	65,65,65,65	0
55	MG	2A	3339	1/1	0.93	0.10	62,62,62,62	0
55	MG	1a	1772	1/1	0.93	0.13	71,71,71,71	0
55	MG	2A	3342	1/1	0.93	0.29	54,54,54,54	0
55	MG	1B	214	1/1	0.93	0.35	63,63,63,63	0
55	MG	1a	1612	1/1	0.93	0.21	69,69,69,69	0
55	MG	1a	1775	1/1	0.93	0.09	50,50,50,50	0
55	MG	1A	3943	1/1	0.93	0.13	28,28,28,28	0
55	MG	1A	3305	1/1	0.93	0.65	54,54,54,54	0
55	MG	2A	3357	1/1	0.93	0.14	29,29,29,29	0
55	MG	2a	1731	1/1	0.93	0.16	49,49,49,49	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
55	MG	2a	1732	1/1	0.93	0.23	42,42,42,42	0
55	MG	1B	217	1/1	0.93	0.12	45,45,45,45	0
55	MG	2A	3157	1/1	0.93	0.24	49,49,49,49	0
55	MG	2a	1737	1/1	0.93	0.13	60,60,60,60	0
55	MG	1A	3818	1/1	0.93	0.13	20,20,20,20	0
55	MG	1B	222	1/1	0.93	0.11	63,63,63,63	0
55	MG	1a	1621	1/1	0.93	0.08	64,64,64,64	0
55	MG	1B	223	1/1	0.93	0.23	56,56,56,56	0
55	MG	1A	3044	1/1	0.93	0.36	44,44,44,44	0
55	MG	1A	3016	1/1	0.93	0.18	49,49,49,49	0
55	MG	1A	3189	1/1	0.93	0.30	35,35,35,35	0
55	MG	1A	3191	1/1	0.93	0.14	42,42,42,42	0
55	MG	1A	3312	1/1	0.93	0.30	60,60,60,60	0
55	MG	1A	3433	1/1	0.93	0.67	47,47,47,47	0
55	MG	2A	3671	1/1	0.93	0.19	58,58,58,58	0
55	MG	1A	3009	1/1	0.93	0.07	34,34,34,34	0
55	MG	1A	3086	1/1	0.93	0.49	38,38,38,38	0
55	MG	2a	1758	1/1	0.93	0.06	61,61,61,61	0
55	MG	2A	3677	1/1	0.93	0.16	54,54,54,54	0
55	MG	2a	1760	1/1	0.93	0.17	60,60,60,60	0
55	MG	1a	1633	1/1	0.93	0.14	55,55,55,55	0
55	MG	1A	3959	1/1	0.93	0.33	34,34,34,34	0
55	MG	2A	3176	1/1	0.93	0.52	68,68,68,68	0
55	MG	1A	3491	1/1	0.93	0.14	32,32,32,32	0
55	MG	2a	1767	1/1	0.93	0.12	85,85,85,85	0
55	MG	1A	3492	1/1	0.93	0.24	42,42,42,42	0
55	MG	1A	3697	1/1	0.93	0.18	39,39,39,39	0
55	MG	1A	3199	1/1	0.93	0.41	44,44,44,44	0
55	MG	2a	1771	1/1	0.93	0.20	61,61,61,61	0
55	MG	2a	1772	1/1	0.93	0.19	70,70,70,70	0
55	MG	1a	1644	1/1	0.93	0.15	61,61,61,61	0
55	MG	1A	3583	1/1	0.93	0.11	31,31,31,31	0
55	MG	1A	3702	1/1	0.93	0.15	29,29,29,29	0
55	MG	2A	3691	1/1	0.93	0.14	63,63,63,63	0
55	MG	1A	3703	1/1	0.93	0.13	18,18,18,18	0
55	MG	1A	3851	1/1	0.93	0.47	39,39,39,39	0
55	MG	1A	3087	1/1	0.93	0.13	39,39,39,39	0
55	MG	1A	3586	1/1	0.93	0.14	33,33,33,33	0
55	MG	2A	3188	1/1	0.93	0.25	48,48,48,48	0
55	MG	1a	1652	1/1	0.93	0.19	78,78,78,78	0
55	MG	2A	3002	1/1	0.93	0.28	42,42,42,42	0
55	MG	1A	3399	1/1	0.93	0.63	43,43,43,43	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
55	MG	1A	3050	1/1	0.93	0.42	59,59,59,59	0
55	MG	2a	1793	1/1	0.93	0.23	81,81,81,81	0
55	MG	1A	3155	1/1	0.93	0.10	36,36,36,36	0
55	MG	2A	3195	1/1	0.93	0.15	68,68,68,68	0
55	MG	2A	3006	1/1	0.93	0.14	60,60,60,60	0
55	MG	1A	3590	1/1	0.93	0.12	35,35,35,35	0
55	MG	2A	3010	1/1	0.93	0.09	34,34,34,34	0
55	MG	1A	3594	1/1	0.93	0.20	14,14,14,14	0
55	MG	2A	3200	1/1	0.93	0.31	51,51,51,51	0
55	MG	2A	3453	1/1	0.93	0.13	45,45,45,45	0
55	MG	2l	204	1/1	0.93	0.12	64,64,64,64	0
55	MG	1G	204	1/1	0.93	0.22	61,61,61,61	0
55	MG	1A	3502	1/1	0.93	0.10	44,44,44,44	0
55	MG	1A	3870	1/1	0.93	0.15	50,50,50,50	0
55	MG	1A	3053	1/1	0.93	0.16	27,27,27,27	0
55	MG	2A	3206	1/1	0.93	0.22	60,60,60,60	0
55	MG	1A	3601	1/1	0.93	0.17	19,19,19,19	0
55	MG	1A	3447	1/1	0.93	0.17	44,44,44,44	0
55	MG	1A	3876	1/1	0.93	0.18	27,27,27,27	0
55	MG	1A	3604	1/1	0.93	0.14	14,14,14,14	0
55	MG	2B	211	1/1	0.93	0.09	76,76,76,76	0
55	MG	1A	3059	1/1	0.93	0.16	30,30,30,30	0
55	MG	1P	201	1/1	0.93	0.28	30,30,30,30	0
55	MG	1A	3746	1/1	0.93	0.21	51,51,51,51	0
55	MG	1A	3496	1/1	0.94	0.17	42,42,42,42	0
55	MG	2A	3420	1/1	0.94	0.24	38,38,38,38	0
55	MG	1A	3855	1/1	0.94	0.19	42,42,42,42	0
55	MG	1A	3551	1/1	0.94	0.10	39,39,39,39	0
55	MG	1x	111	1/1	0.94	0.17	62,62,62,62	0
55	MG	1A	3743	1/1	0.94	0.10	31,31,31,31	0
55	MG	2A	3189	1/1	0.94	0.20	46,46,46,46	0
55	MG	1F	302	1/1	0.94	0.48	35,35,35,35	0
55	MG	1A	3745	1/1	0.94	0.14	48,48,48,48	0
55	MG	1A	3866	1/1	0.94	0.09	52,52,52,52	0
55	MG	2A	3435	1/1	0.94	0.22	39,39,39,39	0
55	MG	2A	3437	1/1	0.94	0.22	48,48,48,48	0
55	MG	1A	3641	1/1	0.94	0.11	45,45,45,45	0
55	MG	2A	3440	1/1	0.94	0.17	27,27,27,27	0
55	MG	1A	3110	1/1	0.94	0.28	43,43,43,43	0
55	MG	2A	3442	1/1	0.94	0.11	59,59,59,59	0
55	MG	1F	309	1/1	0.94	0.25	33,33,33,33	0
55	MG	2A	3444	1/1	0.94	0.10	30,30,30,30	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
55	MG	2A	3013	1/1	0.94	0.38	37,37,37,37	0
55	MG	2D	303	1/1	0.94	0.34	48,48,48,48	0
55	MG	2A	3452	1/1	0.94	0.34	41,41,41,41	0
55	MG	1A	3557	1/1	0.94	0.23	52,52,52,52	0
55	MG	2A	3017	1/1	0.94	0.12	33,33,33,33	0
55	MG	1G	201	1/1	0.94	0.14	39,39,39,39	0
55	MG	1G	202	1/1	0.94	0.15	48,48,48,48	0
55	MG	2E	304	1/1	0.94	0.14	53,53,53,53	0
55	MG	1A	3375	1/1	0.94	0.17	45,45,45,45	0
55	MG	1A	3409	1/1	0.94	0.33	37,37,37,37	0
55	MG	2A	3025	1/1	0.94	0.24	47,47,47,47	0
55	MG	1A	3874	1/1	0.94	0.06	44,44,44,44	0
55	MG	1A	3648	1/1	0.94	0.15	57,57,57,57	0
55	MG	1A	3761	1/1	0.94	0.18	48,48,48,48	0
55	MG	1A	3762	1/1	0.94	0.35	49,49,49,49	0
55	MG	2Q	204	1/1	0.94	0.15	59,59,59,59	0
55	MG	1N	204	1/1	0.94	0.18	49,49,49,49	0
55	MG	2T	201	1/1	0.94	0.17	62,62,62,62	0
55	MG	2V	201	1/1	0.94	0.51	48,48,48,48	0
55	MG	2A	3473	1/1	0.94	0.34	68,68,68,68	0
55	MG	1A	3565	1/1	0.94	0.21	61,61,61,61	0
55	MG	1A	3570	1/1	0.94	0.12	37,37,37,37	0
55	MG	2A	3212	1/1	0.94	0.25	67,67,67,67	0
55	MG	2A	3478	1/1	0.94	0.26	59,59,59,59	0
55	MG	2A	3039	1/1	0.94	0.12	45,45,45,45	0
55	MG	2A	3481	1/1	0.94	0.24	69,69,69,69	0
55	MG	1A	3880	1/1	0.94	0.11	40,40,40,40	0
55	MG	1O	203	1/1	0.94	0.17	48,48,48,48	0
55	MG	1O	204	1/1	0.94	0.20	47,47,47,47	0
55	MG	1A	3652	1/1	0.94	0.21	45,45,45,45	0
55	MG	2A	3045	1/1	0.94	0.17	55,55,55,55	0
55	MG	2A	3492	1/1	0.94	0.21	63,63,63,63	0
55	MG	1a	1678	1/1	0.94	0.17	52,52,52,52	0
55	MG	1A	3882	1/1	0.94	0.12	72,72,72,72	0
55	MG	2A	3222	1/1	0.94	0.43	72,72,72,72	0
55	MG	1A	3993	1/1	0.94	0.10	29,29,29,29	0
55	MG	1A	3210	1/1	0.94	0.43	45,45,45,45	0
55	MG	2A	3050	1/1	0.94	0.16	51,51,51,51	0
55	MG	2A	3500	1/1	0.94	0.11	45,45,45,45	0
55	MG	2A	3501	1/1	0.94	0.13	56,56,56,56	0
55	MG	2A	3502	1/1	0.94	0.14	61,61,61,61	0
55	MG	1a	1683	1/1	0.94	0.31	73,73,73,73	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
55	MG	1Q	203	1/1	0.94	0.20	41,41,41,41	0
55	MG	1A	3091	1/1	0.94	0.48	38,38,38,38	0
55	MG	1A	3413	1/1	0.94	0.24	67,67,67,67	0
55	MG	2A	3231	1/1	0.94	0.10	75,75,75,75	0
55	MG	2A	3056	1/1	0.94	0.11	48,48,48,48	0
55	MG	2A	3057	1/1	0.94	0.18	35,35,35,35	0
55	MG	2A	3236	1/1	0.94	0.34	52,52,52,52	0
55	MG	1A	3095	1/1	0.94	0.36	35,35,35,35	0
55	MG	1A	3058	1/1	0.94	0.29	55,55,55,55	0
55	MG	2A	3517	1/1	0.94	0.10	77,77,77,77	0
55	MG	2a	1628	1/1	0.94	0.15	69,69,69,69	0
55	MG	1a	1689	1/1	0.94	0.23	44,44,44,44	0
55	MG	2A	3520	1/1	0.94	0.13	59,59,59,59	0
55	MG	2a	1631	1/1	0.94	0.12	67,67,67,67	0
55	MG	1U	203	1/1	0.94	0.42	40,40,40,40	0
55	MG	1A	3147	1/1	0.94	0.31	38,38,38,38	0
55	MG	1A	3670	1/1	0.94	0.09	58,58,58,58	0
55	MG	1U	206	1/1	0.94	0.20	42,42,42,42	0
55	MG	2A	3066	1/1	0.94	0.17	52,52,52,52	0
55	MG	1U	208	1/1	0.94	0.39	37,37,37,37	0
55	MG	2A	3070	1/1	0.94	0.14	48,48,48,48	0
55	MG	2a	1639	1/1	0.94	0.46	68,68,68,68	0
55	MG	2A	3252	1/1	0.94	0.32	48,48,48,48	0
55	MG	2A	3537	1/1	0.94	0.15	47,47,47,47	0
55	MG	2A	3540	1/1	0.94	0.28	58,58,58,58	0
55	MG	2A	3253	1/1	0.94	0.22	59,59,59,59	0
55	MG	1A	3671	1/1	0.94	0.17	49,49,49,49	0
55	MG	1A	4014	1/1	0.94	0.21	54,54,54,54	0
55	MG	1A	3781	1/1	0.94	0.15	50,50,50,50	0
55	MG	1V	206	1/1	0.94	0.22	40,40,40,40	0
55	MG	1A	3222	1/1	0.94	0.08	44,44,44,44	0
55	MG	2a	1654	1/1	0.94	0.10	62,62,62,62	0
55	MG	2A	3552	1/1	0.94	0.12	45,45,45,45	0
55	MG	1a	1705	1/1	0.94	0.14	53,53,53,53	0
55	MG	2a	1657	1/1	0.94	0.12	52,52,52,52	0
55	MG	1A	3895	1/1	0.94	0.26	54,54,54,54	0
55	MG	1A	3901	1/1	0.94	0.23	45,45,45,45	0
55	MG	2A	3557	1/1	0.94	0.18	52,52,52,52	0
55	MG	1W	206	1/1	0.94	0.18	24,24,24,24	0
55	MG	2a	1665	1/1	0.94	0.08	72,72,72,72	0
55	MG	1A	3461	1/1	0.94	0.41	48,48,48,48	0
55	MG	1X	102	1/1	0.94	0.62	36,36,36,36	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
55	MG	2A	3562	1/1	0.94	0.13	52,52,52,52	0
55	MG	2A	3269	1/1	0.94	0.24	39,39,39,39	0
55	MG	2A	3271	1/1	0.94	0.19	56,56,56,56	0
55	MG	1A	3903	1/1	0.94	0.10	57,57,57,57	0
55	MG	1a	1714	1/1	0.94	0.28	47,47,47,47	0
55	MG	2A	3274	1/1	0.94	0.21	63,63,63,63	0
55	MG	1X	105	1/1	0.94	0.17	40,40,40,40	0
55	MG	1A	3281	1/1	0.94	0.11	41,41,41,41	0
55	MG	2A	3090	1/1	0.94	0.08	43,43,43,43	0
55	MG	2A	3280	1/1	0.94	0.09	67,67,67,67	0
55	MG	1A	4023	1/1	0.94	0.21	40,40,40,40	0
55	MG	2A	3282	1/1	0.94	0.08	58,58,58,58	0
55	MG	1A	3905	1/1	0.94	0.18	54,54,54,54	0
55	MG	1A	3677	1/1	0.94	0.16	18,18,18,18	0
55	MG	2A	3581	1/1	0.94	0.17	67,67,67,67	0
55	MG	2A	3286	1/1	0.94	0.23	52,52,52,52	0
55	MG	2A	3583	1/1	0.94	0.14	46,46,46,46	0
55	MG	1A	3028	1/1	0.94	0.56	28,28,28,28	0
55	MG	2A	3585	1/1	0.94	0.05	71,71,71,71	0
55	MG	1A	3157	1/1	0.94	0.11	35,35,35,35	0
55	MG	2A	3292	1/1	0.94	0.33	65,65,65,65	0
55	MG	1A	3909	1/1	0.94	0.12	31,31,31,31	0
55	MG	1a	1729	1/1	0.94	0.18	54,54,54,54	0
55	MG	1A	3350	1/1	0.94	0.20	33,33,33,33	0
55	MG	2a	1701	1/1	0.94	0.39	58,58,58,58	0
55	MG	2a	1702	1/1	0.94	0.15	66,66,66,66	0
55	MG	10	107	1/1	0.94	0.11	54,54,54,54	0
55	MG	1A	3253	1/1	0.94	0.31	65,65,65,65	0
55	MG	2a	1706	1/1	0.94	0.17	56,56,56,56	0
55	MG	1A	3227	1/1	0.94	0.12	55,55,55,55	0
55	MG	1a	1738	1/1	0.94	0.13	45,45,45,45	0
55	MG	1A	3391	1/1	0.94	0.13	49,49,49,49	0
55	MG	1A	3119	1/1	0.94	0.38	24,24,24,24	0
55	MG	1a	1745	1/1	0.94	0.10	48,48,48,48	0
55	MG	1A	3915	1/1	0.94	0.20	60,60,60,60	0
55	MG	1A	3691	1/1	0.94	0.18	9,9,9,9	0
55	MG	2a	1717	1/1	0.94	0.17	66,66,66,66	0
55	MG	1A	3917	1/1	0.94	0.16	51,51,51,51	0
55	MG	1A	3918	1/1	0.94	0.19	17,17,17,17	0
55	MG	1A	3161	1/1	0.94	0.15	30,30,30,30	0
55	MG	1A	4045	1/1	0.94	0.10	51,51,51,51	0
55	MG	1A	4046	1/1	0.94	0.25	41,41,41,41	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
55	MG	2A	3123	1/1	0.94	0.24	65,65,65,65	0
55	MG	2A	3613	1/1	0.94	0.17	62,62,62,62	0
55	MG	2a	1729	1/1	0.94	0.10	74,74,74,74	0
55	MG	1A	4048	1/1	0.94	0.11	47,47,47,47	0
55	MG	2A	3320	1/1	0.94	0.21	49,49,49,49	0
55	MG	1A	3231	1/1	0.94	0.16	43,43,43,43	0
55	MG	2A	3126	1/1	0.94	0.24	40,40,40,40	0
55	MG	2a	1735	1/1	0.94	0.14	61,61,61,61	0
55	MG	2A	3127	1/1	0.94	0.39	56,56,56,56	0
55	MG	2a	1738	1/1	0.94	0.13	59,59,59,59	0
55	MG	1A	3472	1/1	0.94	0.67	35,35,35,35	0
55	MG	2A	3131	1/1	0.94	0.14	47,47,47,47	0
55	MG	1A	3259	1/1	0.94	0.34	40,40,40,40	0
55	MG	1A	3814	1/1	0.94	0.13	31,31,31,31	0
55	MG	1A	3815	1/1	0.94	0.06	37,37,37,37	0
55	MG	1B	204	1/1	0.94	0.21	36,36,36,36	0
55	MG	2A	3331	1/1	0.94	0.09	48,48,48,48	0
55	MG	2a	1748	1/1	0.94	0.23	73,73,73,73	0
55	MG	1A	3396	1/1	0.94	0.17	55,55,55,55	0
55	MG	2a	1750	1/1	0.94	0.11	68,68,68,68	0
55	MG	1B	206	1/1	0.94	0.12	42,42,42,42	0
55	MG	2A	3138	1/1	0.94	0.11	68,68,68,68	0
55	MG	2A	3639	1/1	0.94	0.11	58,58,58,58	0
55	MG	2A	3640	1/1	0.94	0.15	38,38,38,38	0
55	MG	1A	3397	1/1	0.94	0.14	37,37,37,37	0
55	MG	1B	209	1/1	0.94	0.15	48,48,48,48	0
55	MG	1a	1609	1/1	0.94	0.17	31,31,31,31	0
55	MG	2A	3146	1/1	0.94	0.37	59,59,59,59	0
55	MG	2A	3343	1/1	0.94	0.22	30,30,30,30	0
55	MG	1A	3233	1/1	0.94	0.12	20,20,20,20	0
55	MG	1A	3704	1/1	0.94	0.07	63,63,63,63	0
55	MG	2A	3351	1/1	0.94	0.12	54,54,54,54	0
55	MG	1A	3099	1/1	0.94	0.38	31,31,31,31	0
55	MG	1A	3437	1/1	0.94	0.19	43,43,43,43	0
55	MG	1A	3082	1/1	0.94	0.27	29,29,29,29	0
55	MG	2A	3356	1/1	0.94	0.11	44,44,44,44	0
55	MG	1A	3067	1/1	0.94	0.24	30,30,30,30	0
55	MG	1A	3625	1/1	0.94	0.07	63,63,63,63	0
55	MG	2A	3359	1/1	0.94	0.16	67,67,67,67	0
55	MG	2a	1774	1/1	0.94	0.10	61,61,61,61	0
55	MG	2a	1777	1/1	0.94	0.08	77,77,77,77	0
55	MG	2A	3666	1/1	0.94	0.17	47,47,47,47	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
55	MG	1a	1618	1/1	0.94	0.22	64,64,64,64	0
55	MG	1A	3720	1/1	0.94	0.12	40,40,40,40	0
55	MG	1A	3721	1/1	0.94	0.18	39,39,39,39	0
55	MG	1A	3299	1/1	0.94	0.20	20,20,20,20	0
55	MG	2A	3672	1/1	0.94	0.15	56,56,56,56	0
55	MG	2A	3370	1/1	0.94	0.08	41,41,41,41	0
55	MG	2A	3371	1/1	0.94	0.20	30,30,30,30	0
55	MG	2A	3372	1/1	0.94	0.20	40,40,40,40	0
55	MG	2A	3678	1/1	0.94	0.13	67,67,67,67	0
55	MG	1A	3125	1/1	0.94	0.31	33,33,33,33	0
55	MG	2a	1790	1/1	0.94	0.22	51,51,51,51	0
55	MG	1A	3729	1/1	0.94	0.18	21,21,21,21	0
55	MG	1A	3444	1/1	0.94	0.22	58,58,58,58	0
55	MG	2A	3164	1/1	0.94	0.72	55,55,55,55	0
55	MG	1a	1795	1/1	0.94	0.18	56,56,56,56	0
55	MG	1B	228	1/1	0.94	0.13	35,35,35,35	0
55	MG	1a	1628	1/1	0.94	0.13	54,54,54,54	0
55	MG	1A	3731	1/1	0.94	0.15	44,44,44,44	0
55	MG	1A	3170	1/1	0.94	0.59	43,43,43,43	0
55	MG	2j	201	1/1	0.94	0.14	86,86,86,86	0
55	MG	2k	201	1/1	0.94	0.11	63,63,63,63	0
55	MG	1A	3845	1/1	0.94	0.47	37,37,37,37	0
55	MG	1A	3847	1/1	0.94	0.14	30,30,30,30	0
55	MG	1A	3850	1/1	0.94	0.20	41,41,41,41	0
55	MG	2A	3394	1/1	0.94	0.21	41,41,41,41	0
55	MG	2A	3174	1/1	0.94	0.29	55,55,55,55	0
55	MG	1A	3038	1/1	0.94	0.21	34,34,34,34	0
55	MG	1A	3106	1/1	0.94	0.13	38,38,38,38	0
55	MG	1D	303	1/1	0.94	0.12	19,19,19,19	0
55	MG	1v	101	1/1	0.94	0.11	65,65,65,65	0
55	MG	2A	3406	1/1	0.94	0.13	50,50,50,50	0
55	MG	1A	3962	1/1	0.94	0.12	43,43,43,43	0
55	MG	1A	3964	1/1	0.94	0.16	38,38,38,38	0
57	T8B	1A	4052	44/44	0.94	0.20	48,53,59,65	0
57	T8B	2A	3717	44/44	0.94	0.18	58,66,71,76	0
55	MG	1a	1643	1/1	0.94	0.14	52,52,52,52	0
58	ZN	1n	102	1/1	0.94	0.09	71,71,71,71	0
55	MG	1A	3739	1/1	0.94	0.16	24,24,24,24	0
55	MG	1A	3966	1/1	0.94	0.10	47,47,47,47	0
55	MG	2A	3418	1/1	0.94	0.30	70,70,70,70	0
55	MG	1A	3713	1/1	0.95	0.13	41,41,41,41	0
55	MG	10	103	1/1	0.95	0.15	48,48,48,48	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
55	MG	1A	3183	1/1	0.95	0.37	27,27,27,27	0
55	MG	1A	3036	1/1	0.95	0.50	36,36,36,36	0
55	MG	2P	201	1/1	0.95	0.42	59,59,59,59	0
55	MG	10	106	1/1	0.95	0.13	53,53,53,53	0
55	MG	1a	1720	1/1	0.95	0.10	66,66,66,66	0
55	MG	1a	1721	1/1	0.95	0.12	47,47,47,47	0
55	MG	2R	202	1/1	0.95	0.16	47,47,47,47	0
55	MG	1A	3933	1/1	0.95	0.16	16,16,16,16	0
55	MG	2T	202	1/1	0.95	0.13	38,38,38,38	0
55	MG	11	102	1/1	0.95	0.09	41,41,41,41	0
55	MG	1A	3160	1/1	0.95	0.16	19,19,19,19	0
55	MG	1A	3363	1/1	0.95	0.36	33,33,33,33	0
55	MG	1A	3626	1/1	0.95	0.15	25,25,25,25	0
55	MG	2A	3267	1/1	0.95	0.29	43,43,43,43	0
55	MG	12	102	1/1	0.95	0.26	43,43,43,43	0
55	MG	1B	207	1/1	0.95	0.45	45,45,45,45	0
55	MG	1A	3364	1/1	0.95	0.27	34,34,34,34	0
55	MG	1A	3939	1/1	0.95	0.15	27,27,27,27	0
55	MG	1a	1736	1/1	0.95	0.10	71,71,71,71	0
55	MG	2A	3516	1/1	0.95	0.17	22,22,22,22	0
55	MG	1A	3940	1/1	0.95	0.12	21,21,21,21	0
55	MG	2A	3095	1/1	0.95	0.13	35,35,35,35	0
55	MG	2A	3519	1/1	0.95	0.36	61,61,61,61	0
55	MG	1a	1739	1/1	0.95	0.14	57,57,57,57	0
55	MG	15	103	1/1	0.95	0.43	41,41,41,41	0
55	MG	1a	1741	1/1	0.95	0.15	75,75,75,75	0
55	MG	1a	1743	1/1	0.95	0.08	56,56,56,56	0
55	MG	2A	3525	1/1	0.95	0.19	49,49,49,49	0
55	MG	1A	3542	1/1	0.95	0.18	24,24,24,24	0
55	MG	15	107	1/1	0.95	0.08	66,66,66,66	0
55	MG	2A	3529	1/1	0.95	0.20	60,60,60,60	0
55	MG	2A	3284	1/1	0.95	0.70	44,44,44,44	0
55	MG	1A	3837	1/1	0.95	0.20	31,31,31,31	0
55	MG	1A	3630	1/1	0.95	0.16	30,30,30,30	0
55	MG	1a	1748	1/1	0.95	0.12	52,52,52,52	0
55	MG	2A	3538	1/1	0.95	0.18	56,56,56,56	0
55	MG	1A	3949	1/1	0.95	0.16	51,51,51,51	0
55	MG	2A	3541	1/1	0.95	0.19	69,69,69,69	0
55	MG	2A	3110	1/1	0.95	0.07	64,64,64,64	0
55	MG	1A	3441	1/1	0.95	0.18	66,66,66,66	0
55	MG	2a	1622	1/1	0.95	0.26	63,63,63,63	0
55	MG	2A	3544	1/1	0.95	0.26	49,49,49,49	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
55	MG	1A	3001	1/1	0.95	0.07	39,39,39,39	0
55	MG	2A	3546	1/1	0.95	0.12	58,58,58,58	0
55	MG	2A	3547	1/1	0.95	0.16	54,54,54,54	0
55	MG	2A	3295	1/1	0.95	0.14	55,55,55,55	0
55	MG	18	106	1/1	0.95	0.12	49,49,49,49	0
55	MG	1B	219	1/1	0.95	0.12	45,45,45,45	0
55	MG	1B	220	1/1	0.95	0.15	42,42,42,42	0
55	MG	1A	3190	1/1	0.95	0.07	76,76,76,76	0
55	MG	2A	3300	1/1	0.95	0.16	67,67,67,67	0
55	MG	2A	3301	1/1	0.95	0.08	62,62,62,62	0
55	MG	1A	3637	1/1	0.95	0.13	27,27,27,27	0
55	MG	2A	3121	1/1	0.95	0.20	63,63,63,63	0
55	MG	1A	3737	1/1	0.95	0.12	25,25,25,25	0
55	MG	1A	3018	1/1	0.95	0.14	20,20,20,20	0
55	MG	1A	3956	1/1	0.95	0.07	47,47,47,47	0
55	MG	1A	3369	1/1	0.95	0.38	39,39,39,39	0
55	MG	1A	3192	1/1	0.95	0.10	68,68,68,68	0
55	MG	2A	3310	1/1	0.95	0.21	44,44,44,44	0
55	MG	1A	3332	1/1	0.95	0.12	48,48,48,48	0
55	MG	2A	3128	1/1	0.95	0.08	65,65,65,65	0
55	MG	1A	3164	1/1	0.95	0.12	34,34,34,34	0
55	MG	1a	1769	1/1	0.95	0.07	56,56,56,56	0
55	MG	2a	1651	1/1	0.95	0.09	51,51,51,51	0
55	MG	1A	3195	1/1	0.95	0.26	58,58,58,58	0
55	MG	1A	3857	1/1	0.95	0.07	53,53,53,53	0
55	MG	2A	3319	1/1	0.95	0.27	59,59,59,59	0
55	MG	1B	233	1/1	0.95	0.11	60,60,60,60	0
55	MG	1B	234	1/1	0.95	0.15	60,60,60,60	0
55	MG	1A	3858	1/1	0.95	0.08	49,49,49,49	0
55	MG	2a	1660	1/1	0.95	0.14	69,69,69,69	0
55	MG	1B	236	1/1	0.95	0.14	71,71,71,71	0
55	MG	1A	3747	1/1	0.95	0.20	55,55,55,55	0
55	MG	1A	3265	1/1	0.95	0.25	42,42,42,42	0
55	MG	1A	3863	1/1	0.95	0.13	38,38,38,38	0
55	MG	1a	1782	1/1	0.95	0.17	66,66,66,66	0
55	MG	2A	3586	1/1	0.95	0.06	61,61,61,61	0
55	MG	1a	1783	1/1	0.95	0.10	42,42,42,42	0
55	MG	2A	3147	1/1	0.95	0.16	52,52,52,52	0
55	MG	1A	3564	1/1	0.95	0.18	18,18,18,18	0
55	MG	2a	1671	1/1	0.95	0.10	61,61,61,61	0
55	MG	1D	306	1/1	0.95	0.34	27,27,27,27	0
55	MG	1D	307	1/1	0.95	0.29	39,39,39,39	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
55	MG	1A	3751	1/1	0.95	0.13	35,35,35,35	0
55	MG	1a	1626	1/1	0.95	0.12	47,47,47,47	0
55	MG	1E	302	1/1	0.95	0.46	34,34,34,34	0
55	MG	2A	3154	1/1	0.95	0.20	38,38,38,38	0
55	MG	1E	303	1/1	0.95	0.40	32,32,32,32	0
55	MG	2a	1679	1/1	0.95	0.30	59,59,59,59	0
55	MG	2a	1680	1/1	0.95	0.23	51,51,51,51	0
55	MG	1a	1794	1/1	0.95	0.08	78,78,78,78	0
55	MG	2A	3601	1/1	0.95	0.07	57,57,57,57	0
55	MG	2A	3345	1/1	0.95	0.32	39,39,39,39	0
55	MG	1A	3196	1/1	0.95	0.28	31,31,31,31	0
55	MG	2A	3158	1/1	0.95	0.22	54,54,54,54	0
55	MG	2a	1686	1/1	0.95	0.25	63,63,63,63	0
55	MG	1A	3567	1/1	0.95	0.14	24,24,24,24	0
55	MG	1A	3569	1/1	0.95	0.09	40,40,40,40	0
55	MG	1A	3165	1/1	0.95	0.36	36,36,36,36	0
55	MG	1A	3653	1/1	0.95	0.13	45,45,45,45	0
55	MG	1e	201	1/1	0.95	0.13	76,76,76,76	0
55	MG	1a	1634	1/1	0.95	0.20	46,46,46,46	0
55	MG	1A	3763	1/1	0.95	0.13	60,60,60,60	0
55	MG	2A	3614	1/1	0.95	0.11	62,62,62,62	0
55	MG	1E	312	1/1	0.95	0.41	39,39,39,39	0
55	MG	2A	3360	1/1	0.95	0.14	56,56,56,56	0
55	MG	1A	3655	1/1	0.95	0.12	62,62,62,62	0
55	MG	1m	3002	1/1	0.95	0.11	65,65,65,65	0
55	MG	1p	101	1/1	0.95	0.10	65,65,65,65	0
55	MG	1a	1639	1/1	0.95	0.14	47,47,47,47	0
55	MG	2A	3621	1/1	0.95	0.35	74,74,74,74	0
55	MG	1A	3166	1/1	0.95	0.46	34,34,34,34	0
55	MG	1A	3981	1/1	0.95	0.09	33,33,33,33	0
55	MG	2a	1711	1/1	0.95	0.17	48,48,48,48	0
55	MG	1A	3658	1/1	0.95	0.09	66,66,66,66	0
55	MG	1A	3006	1/1	0.95	0.14	29,29,29,29	0
55	MG	1A	3575	1/1	0.95	0.17	75,75,75,75	0
55	MG	2A	3629	1/1	0.95	0.16	27,27,27,27	0
55	MG	1A	3381	1/1	0.95	0.33	33,33,33,33	0
55	MG	1A	3773	1/1	0.95	0.10	37,37,37,37	0
55	MG	1A	3109	1/1	0.95	0.37	28,28,28,28	0
55	MG	2A	3636	1/1	0.95	0.16	44,44,44,44	0
55	MG	1A	3510	1/1	0.95	0.21	53,53,53,53	0
55	MG	2a	1724	1/1	0.95	0.18	49,49,49,49	0
55	MG	2a	1725	1/1	0.95	0.15	63,63,63,63	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
55	MG	2A	3381	1/1	0.95	0.23	59,59,59,59	0
55	MG	1A	3089	1/1	0.95	0.32	35,35,35,35	0
55	MG	2A	3641	1/1	0.95	0.15	43,43,43,43	0
55	MG	1A	3012	1/1	0.95	0.63	26,26,26,26	0
55	MG	2A	3386	1/1	0.95	0.17	37,37,37,37	0
55	MG	1x	113	1/1	0.95	0.10	75,75,75,75	0
55	MG	2A	3388	1/1	0.95	0.11	42,42,42,42	0
55	MG	1x	114	1/1	0.95	0.40	53,53,53,53	0
55	MG	2A	3001	1/1	0.95	0.29	57,57,57,57	0
55	MG	1A	3141	1/1	0.95	0.20	21,21,21,21	0
55	MG	1A	3030	1/1	0.95	0.08	37,37,37,37	0
55	MG	1A	3890	1/1	0.95	0.10	53,53,53,53	0
55	MG	1A	3060	1/1	0.95	0.37	35,35,35,35	0
55	MG	1A	3045	1/1	0.95	0.10	30,30,30,30	0
55	MG	2A	3007	1/1	0.95	0.15	37,37,37,37	0
55	MG	1A	3426	1/1	0.95	0.36	45,45,45,45	0
55	MG	1A	3593	1/1	0.95	0.13	14,14,14,14	0
55	MG	2A	3662	1/1	0.95	0.10	47,47,47,47	0
55	MG	2A	3407	1/1	0.95	0.19	40,40,40,40	0
55	MG	2A	3012	1/1	0.95	0.50	43,43,43,43	0
55	MG	1A	3154	1/1	0.95	0.34	48,48,48,48	0
55	MG	1A	4009	1/1	0.95	0.12	55,55,55,55	0
55	MG	2A	3016	1/1	0.95	0.24	60,60,60,60	0
55	MG	1A	3900	1/1	0.95	0.18	46,46,46,46	0
55	MG	2a	1754	1/1	0.95	0.30	60,60,60,60	0
55	MG	1A	3522	1/1	0.95	0.24	44,44,44,44	0
55	MG	1P	205	1/1	0.95	0.43	31,31,31,31	0
55	MG	2a	1757	1/1	0.95	0.13	57,57,57,57	0
55	MG	2A	3201	1/1	0.95	0.18	66,66,66,66	0
55	MG	2A	3421	1/1	0.95	0.28	63,63,63,63	0
55	MG	2A	3422	1/1	0.95	0.35	54,54,54,54	0
55	MG	1a	1666	1/1	0.95	0.12	55,55,55,55	0
55	MG	1A	3063	1/1	0.95	0.52	33,33,33,33	0
55	MG	1Q	201	1/1	0.95	0.61	40,40,40,40	0
55	MG	1A	3598	1/1	0.95	0.13	20,20,20,20	0
55	MG	1A	3599	1/1	0.95	0.13	24,24,24,24	0
55	MG	1Q	204	1/1	0.95	0.11	64,64,64,64	0
55	MG	1R	202	1/1	0.95	0.49	50,50,50,50	0
55	MG	1A	3798	1/1	0.95	0.11	66,66,66,66	0
55	MG	1S	202	1/1	0.95	0.14	45,45,45,45	0
55	MG	1A	3799	1/1	0.95	0.14	21,21,21,21	0
55	MG	1A	3100	1/1	0.95	0.31	30,30,30,30	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
55	MG	2A	3439	1/1	0.95	0.15	47,47,47,47	0
55	MG	2a	1775	1/1	0.95	0.19	59,59,59,59	0
55	MG	1A	3802	1/1	0.95	0.29	31,31,31,31	0
55	MG	2A	3214	1/1	0.95	0.15	49,49,49,49	0
55	MG	1a	1681	1/1	0.95	0.19	46,46,46,46	0
55	MG	1A	3223	1/1	0.95	0.17	47,47,47,47	0
55	MG	1A	3603	1/1	0.95	0.11	36,36,36,36	0
55	MG	1A	3696	1/1	0.95	0.15	21,21,21,21	0
55	MG	2A	3448	1/1	0.95	0.14	33,33,33,33	0
55	MG	2A	3449	1/1	0.95	0.17	50,50,50,50	0
55	MG	1A	3527	1/1	0.95	0.23	32,32,32,32	0
55	MG	1U	207	1/1	0.95	0.26	33,33,33,33	0
55	MG	1A	3807	1/1	0.95	0.34	39,39,39,39	0
55	MG	2A	3455	1/1	0.95	0.11	32,32,32,32	0
55	MG	1A	4029	1/1	0.95	0.59	49,49,49,49	0
55	MG	1A	3698	1/1	0.95	0.11	21,21,21,21	0
55	MG	2A	3713	1/1	0.95	0.19	61,61,61,61	0
55	MG	1U	213	1/1	0.95	0.20	47,47,47,47	0
55	MG	1a	1693	1/1	0.95	0.26	48,48,48,48	0
55	MG	1A	3812	1/1	0.95	0.36	39,39,39,39	0
55	MG	1A	3318	1/1	0.95	0.48	30,30,30,30	0
55	MG	1A	3285	1/1	0.95	0.27	49,49,49,49	0
55	MG	1A	3609	1/1	0.95	0.13	21,21,21,21	0
55	MG	2A	3467	1/1	0.95	0.09	37,37,37,37	0
55	MG	1A	3816	1/1	0.95	0.12	57,57,57,57	0
55	MG	2A	3469	1/1	0.95	0.24	71,71,71,71	0
55	MG	2A	3471	1/1	0.95	0.15	64,64,64,64	0
55	MG	1W	204	1/1	0.95	0.21	31,31,31,31	0
55	MG	2A	3234	1/1	0.95	0.11	45,45,45,45	0
55	MG	1A	4037	1/1	0.95	0.15	47,47,47,47	0
55	MG	1A	3286	1/1	0.95	0.48	39,39,39,39	0
55	MG	1A	3921	1/1	0.95	0.15	18,18,18,18	0
55	MG	1A	3477	1/1	0.95	0.52	36,36,36,36	0
55	MG	2A	3064	1/1	0.95	0.18	29,29,29,29	0
55	MG	1A	3707	1/1	0.95	0.09	38,38,38,38	0
55	MG	2A	3243	1/1	0.95	0.11	62,62,62,62	0
55	MG	1A	3924	1/1	0.95	0.36	51,51,51,51	0
55	MG	2A	3485	1/1	0.95	0.18	61,61,61,61	0
55	MG	1A	3434	1/1	0.95	0.50	35,35,35,35	0
55	MG	2A	3068	1/1	0.95	0.31	59,59,59,59	0
55	MG	1A	3615	1/1	0.95	0.18	21,21,21,21	0
55	MG	2A	3491	1/1	0.95	0.23	67,67,67,67	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
55	MG	1A	3927	1/1	0.95	0.25	43,43,43,43	0
58	ZN	26	501	1/1	0.95	0.14	66,66,66,66	0
55	MG	1A	3358	1/1	0.95	0.41	31,31,31,31	0
55	MG	1A	3346	1/1	0.96	0.34	50,50,50,50	0
55	MG	2Q	201	1/1	0.96	0.12	46,46,46,46	0
55	MG	1A	3134	1/1	0.96	0.52	39,39,39,39	0
55	MG	1A	3181	1/1	0.96	0.35	31,31,31,31	0
55	MG	2A	3287	1/1	0.96	0.23	45,45,45,45	0
55	MG	2A	3515	1/1	0.96	0.08	63,63,63,63	0
55	MG	2A	3288	1/1	0.96	0.15	63,63,63,63	0
55	MG	1A	3550	1/1	0.96	0.14	35,35,35,35	0
55	MG	1A	3656	1/1	0.96	0.12	54,54,54,54	0
55	MG	2A	3291	1/1	0.96	0.17	42,42,42,42	0
55	MG	1A	3072	1/1	0.96	0.10	51,51,51,51	0
55	MG	2W	202	1/1	0.96	0.33	38,38,38,38	0
55	MG	1A	3784	1/1	0.96	0.19	13,13,13,13	0
55	MG	1A	3785	1/1	0.96	0.19	39,39,39,39	0
55	MG	17	101	1/1	0.96	0.15	30,30,30,30	0
55	MG	23	101	1/1	0.96	0.26	52,52,52,52	0
55	MG	1A	3787	1/1	0.96	0.09	49,49,49,49	0
55	MG	17	105	1/1	0.96	0.17	41,41,41,41	0
55	MG	27	102	1/1	0.96	0.17	54,54,54,54	0
55	MG	1A	3137	1/1	0.96	0.24	35,35,35,35	0
55	MG	28	3401	1/1	0.96	0.15	58,58,58,58	0
55	MG	1A	3556	1/1	0.96	0.12	61,61,61,61	0
55	MG	2A	3532	1/1	0.96	0.05	66,66,66,66	0
55	MG	1a	1761	1/1	0.96	0.09	46,46,46,46	0
55	MG	1a	1762	1/1	0.96	0.13	62,62,62,62	0
55	MG	2A	3302	1/1	0.96	0.14	63,63,63,63	0
55	MG	1A	3042	1/1	0.96	0.18	19,19,19,19	0
55	MG	1A	3558	1/1	0.96	0.15	14,14,14,14	0
55	MG	2A	3539	1/1	0.96	0.13	36,36,36,36	0
55	MG	1B	213	1/1	0.96	0.19	55,55,55,55	0
55	MG	2a	1608	1/1	0.96	0.07	75,75,75,75	0
55	MG	1A	3103	1/1	0.96	0.11	27,27,27,27	0
55	MG	1A	3476	1/1	0.96	0.25	32,32,32,32	0
55	MG	1A	3144	1/1	0.96	0.18	60,60,60,60	0
55	MG	1A	3415	1/1	0.96	0.24	30,30,30,30	0
55	MG	2A	3129	1/1	0.96	0.43	54,54,54,54	0
55	MG	1A	3566	1/1	0.96	0.20	22,22,22,22	0
55	MG	1A	3673	1/1	0.96	0.13	42,42,42,42	0
55	MG	1A	3034	1/1	0.96	0.28	61,61,61,61	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
55	MG	2A	3549	1/1	0.96	0.06	43,43,43,43	0
55	MG	1A	3675	1/1	0.96	0.34	32,32,32,32	0
55	MG	1A	3931	1/1	0.96	0.09	13,13,13,13	0
55	MG	1A	3298	1/1	0.96	0.13	43,43,43,43	0
55	MG	1a	1777	1/1	0.96	0.06	46,46,46,46	0
55	MG	1A	3481	1/1	0.96	0.37	49,49,49,49	0
55	MG	2A	3555	1/1	0.96	0.20	52,52,52,52	0
55	MG	2A	3321	1/1	0.96	0.61	49,49,49,49	0
55	MG	1A	3146	1/1	0.96	0.22	47,47,47,47	0
55	MG	2A	3140	1/1	0.96	0.18	33,33,33,33	0
55	MG	1A	3679	1/1	0.96	0.14	45,45,45,45	0
55	MG	1A	3809	1/1	0.96	0.44	34,34,34,34	0
55	MG	1A	3247	1/1	0.96	0.19	37,37,37,37	0
55	MG	1A	3574	1/1	0.96	0.26	53,53,53,53	0
55	MG	1A	3077	1/1	0.96	0.13	29,29,29,29	0
55	MG	1A	3684	1/1	0.96	0.10	35,35,35,35	0
55	MG	1a	1619	1/1	0.96	0.29	64,64,64,64	0
55	MG	1A	3944	1/1	0.96	0.11	21,21,21,21	0
55	MG	1a	1789	1/1	0.96	0.20	63,63,63,63	0
55	MG	1A	3361	1/1	0.96	0.32	35,35,35,35	0
55	MG	1A	3148	1/1	0.96	0.36	33,33,33,33	0
55	MG	1A	3580	1/1	0.96	0.11	29,29,29,29	0
55	MG	1A	3689	1/1	0.96	0.14	47,47,47,47	0
55	MG	2A	3576	1/1	0.96	0.14	27,27,27,27	0
55	MG	1A	3690	1/1	0.96	0.13	53,53,53,53	0
55	MG	1A	3581	1/1	0.96	0.14	52,52,52,52	0
55	MG	2A	3579	1/1	0.96	0.13	67,67,67,67	0
55	MG	1A	3150	1/1	0.96	0.10	41,41,41,41	0
55	MG	2a	1648	1/1	0.96	0.23	60,60,60,60	0
55	MG	2A	3344	1/1	0.96	0.13	22,22,22,22	0
55	MG	1A	3823	1/1	0.96	0.11	35,35,35,35	0
55	MG	1D	309	1/1	0.96	0.45	26,26,26,26	0
55	MG	2a	1653	1/1	0.96	0.08	58,58,58,58	0
55	MG	1A	3035	1/1	0.96	0.06	23,23,23,23	0
55	MG	1A	3695	1/1	0.96	0.12	34,34,34,34	0
55	MG	1A	3027	1/1	0.96	0.35	29,29,29,29	0
55	MG	1A	3828	1/1	0.96	0.18	24,24,24,24	0
55	MG	1A	3493	1/1	0.96	0.18	38,38,38,38	0
55	MG	1A	3494	1/1	0.96	0.14	53,53,53,53	0
55	MG	2A	3591	1/1	0.96	0.18	49,49,49,49	0
55	MG	1A	3306	1/1	0.96	0.56	19,19,19,19	0
55	MG	2a	1663	1/1	0.96	0.20	54,54,54,54	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
55	MG	1A	3156	1/1	0.96	0.10	33,33,33,33	0
55	MG	2A	3169	1/1	0.96	0.33	39,39,39,39	0
55	MG	1A	3701	1/1	0.96	0.16	25,25,25,25	0
55	MG	1a	1640	1/1	0.96	0.08	64,64,64,64	0
55	MG	1A	3200	1/1	0.96	0.29	52,52,52,52	0
55	MG	2A	3598	1/1	0.96	0.09	42,42,42,42	0
55	MG	1F	301	1/1	0.96	0.40	38,38,38,38	0
55	MG	2A	3367	1/1	0.96	0.17	41,41,41,41	0
55	MG	1A	3592	1/1	0.96	0.19	21,21,21,21	0
55	MG	1x	105	1/1	0.96	0.26	67,67,67,67	0
55	MG	1A	3838	1/1	0.96	0.17	38,38,38,38	0
55	MG	1F	304	1/1	0.96	0.10	31,31,31,31	0
55	MG	1A	3020	1/1	0.96	0.10	16,16,16,16	0
55	MG	2A	3606	1/1	0.96	0.23	41,41,41,41	0
55	MG	1A	3203	1/1	0.96	0.30	40,40,40,40	0
55	MG	1A	3158	1/1	0.96	0.15	32,32,32,32	0
55	MG	1A	3026	1/1	0.96	0.53	34,34,34,34	0
55	MG	1F	310	1/1	0.96	0.11	50,50,50,50	0
55	MG	1A	3710	1/1	0.96	0.15	25,25,25,25	0
55	MG	1A	3849	1/1	0.96	0.18	20,20,20,20	0
55	MG	1A	3113	1/1	0.96	0.17	14,14,14,14	0
55	MG	1A	3975	1/1	0.96	0.13	35,35,35,35	0
55	MG	2A	3384	1/1	0.96	0.20	49,49,49,49	0
55	MG	2A	3385	1/1	0.96	0.14	29,29,29,29	0
55	MG	1A	3208	1/1	0.96	0.23	33,33,33,33	0
55	MG	1a	1657	1/1	0.96	0.15	47,47,47,47	0
55	MG	1A	3506	1/1	0.96	0.07	51,51,51,51	0
55	MG	1A	3376	1/1	0.96	0.17	47,47,47,47	0
55	MG	1A	3377	1/1	0.96	0.49	40,40,40,40	0
55	MG	2a	1695	1/1	0.96	0.25	50,50,50,50	0
55	MG	1A	3982	1/1	0.96	0.19	16,16,16,16	0
55	MG	1A	3114	1/1	0.96	0.14	42,42,42,42	0
55	MG	1A	3605	1/1	0.96	0.20	26,26,26,26	0
55	MG	2A	3398	1/1	0.96	0.19	43,43,43,43	0
55	MG	2A	3399	1/1	0.96	0.10	61,61,61,61	0
55	MG	1N	206	1/1	0.96	0.20	43,43,43,43	0
55	MG	2a	1704	1/1	0.96	0.19	54,54,54,54	0
55	MG	1A	3725	1/1	0.96	0.13	48,48,48,48	0
55	MG	1A	3317	1/1	0.96	0.14	31,31,31,31	0
55	MG	2A	3635	1/1	0.96	0.11	43,43,43,43	0
55	MG	1A	3728	1/1	0.96	0.18	18,18,18,18	0
55	MG	2A	3405	1/1	0.96	0.16	53,53,53,53	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
55	MG	1A	3263	1/1	0.96	0.12	48,48,48,48	0
55	MG	2A	3023	1/1	0.96	0.24	42,42,42,42	0
55	MG	1A	3862	1/1	0.96	0.17	50,50,50,50	0
55	MG	2A	3642	1/1	0.96	0.13	37,37,37,37	0
55	MG	1A	3319	1/1	0.96	0.36	39,39,39,39	0
55	MG	2A	3644	1/1	0.96	0.19	35,35,35,35	0
55	MG	2A	3026	1/1	0.96	0.16	45,45,45,45	0
55	MG	1P	202	1/1	0.96	0.42	45,45,45,45	0
55	MG	2A	3029	1/1	0.96	0.11	53,53,53,53	0
55	MG	2a	1722	1/1	0.96	0.16	49,49,49,49	0
55	MG	1P	203	1/1	0.96	0.45	36,36,36,36	0
55	MG	1A	3865	1/1	0.96	0.16	57,57,57,57	0
55	MG	1A	3033	1/1	0.96	0.51	28,28,28,28	0
55	MG	1A	3732	1/1	0.96	0.12	45,45,45,45	0
55	MG	1A	3442	1/1	0.96	0.11	72,72,72,72	0
55	MG	2A	3035	1/1	0.96	0.15	44,44,44,44	0
55	MG	1A	3163	1/1	0.96	0.07	45,45,45,45	0
55	MG	2A	3037	1/1	0.96	0.14	54,54,54,54	0
55	MG	2A	3658	1/1	0.96	0.10	40,40,40,40	0
55	MG	1A	3871	1/1	0.96	0.12	40,40,40,40	0
55	MG	1R	201	1/1	0.96	0.13	33,33,33,33	0
55	MG	2A	3429	1/1	0.96	0.14	52,52,52,52	0
55	MG	2A	3664	1/1	0.96	0.12	56,56,56,56	0
55	MG	2A	3431	1/1	0.96	0.17	26,26,26,26	0
55	MG	1A	3088	1/1	0.96	0.26	30,30,30,30	0
55	MG	1R	203	1/1	0.96	0.71	41,41,41,41	0
55	MG	1R	204	1/1	0.96	0.26	29,29,29,29	0
55	MG	1A	3736	1/1	0.96	0.09	23,23,23,23	0
55	MG	1A	4005	1/1	0.96	0.17	30,30,30,30	0
55	MG	1A	3213	1/1	0.96	0.26	19,19,19,19	0
55	MG	1A	3269	1/1	0.96	0.65	33,33,33,33	0
55	MG	2A	3674	1/1	0.96	0.17	52,52,52,52	0
55	MG	2A	3675	1/1	0.96	0.20	36,36,36,36	0
55	MG	1a	1691	1/1	0.96	0.10	49,49,49,49	0
55	MG	1A	4010	1/1	0.96	0.22	39,39,39,39	0
55	MG	2A	3051	1/1	0.96	0.15	43,43,43,43	0
55	MG	2A	3226	1/1	0.96	0.34	35,35,35,35	0
55	MG	1U	201	1/1	0.96	0.38	33,33,33,33	0
55	MG	1A	3214	1/1	0.96	0.22	35,35,35,35	0
55	MG	2A	3446	1/1	0.96	0.32	38,38,38,38	0
55	MG	2A	3683	1/1	0.96	0.14	46,46,46,46	0
55	MG	2A	3684	1/1	0.96	0.13	74,74,74,74	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
55	MG	1A	4013	1/1	0.96	0.16	53,53,53,53	0
55	MG	1A	3449	1/1	0.96	0.62	32,32,32,32	0
55	MG	2A	3451	1/1	0.96	0.12	36,36,36,36	0
55	MG	1A	3623	1/1	0.96	0.20	14,14,14,14	0
55	MG	1a	1698	1/1	0.96	0.19	66,66,66,66	0
55	MG	1A	3624	1/1	0.96	0.13	21,21,21,21	0
55	MG	1A	3524	1/1	0.96	0.17	31,31,31,31	0
55	MG	1U	210	1/1	0.96	0.68	36,36,36,36	0
55	MG	2A	3237	1/1	0.96	0.19	62,62,62,62	0
55	MG	2A	3458	1/1	0.96	0.24	32,32,32,32	0
55	MG	1A	3271	1/1	0.96	0.17	43,43,43,43	0
55	MG	2A	3239	1/1	0.96	0.08	57,57,57,57	0
55	MG	1A	3216	1/1	0.96	0.43	25,25,25,25	0
55	MG	1A	3883	1/1	0.96	0.15	58,58,58,58	0
55	MG	1a	1707	1/1	0.96	0.15	64,64,64,64	0
55	MG	1A	3218	1/1	0.96	0.31	39,39,39,39	0
55	MG	1V	205	1/1	0.96	0.18	49,49,49,49	0
55	MG	1A	3331	1/1	0.96	0.29	43,43,43,43	0
55	MG	2A	3706	1/1	0.96	0.12	69,69,69,69	0
55	MG	2A	3707	1/1	0.96	0.15	59,59,59,59	0
55	MG	1A	3752	1/1	0.96	0.14	37,37,37,37	0
55	MG	2A	3470	1/1	0.96	0.29	49,49,49,49	0
55	MG	2a	1784	1/1	0.96	0.17	52,52,52,52	0
55	MG	2A	3069	1/1	0.96	0.39	43,43,43,43	0
55	MG	2A	3248	1/1	0.96	0.30	36,36,36,36	0
55	MG	1A	3755	1/1	0.96	0.29	31,31,31,31	0
55	MG	1A	3066	1/1	0.96	0.13	35,35,35,35	0
55	MG	1A	3757	1/1	0.96	0.12	34,34,34,34	0
55	MG	1A	3090	1/1	0.96	0.15	42,42,42,42	0
55	MG	2A	3718	1/1	0.96	0.24	59,59,59,59	0
55	MG	2A	3254	1/1	0.96	0.30	34,34,34,34	0
55	MG	2a	1794	1/1	0.96	0.19	67,67,67,67	0
55	MG	1A	3634	1/1	0.96	0.15	17,17,17,17	0
55	MG	1A	3051	1/1	0.96	0.35	50,50,50,50	0
55	MG	1A	3094	1/1	0.96	0.32	48,48,48,48	0
55	MG	1X	104	1/1	0.96	0.16	39,39,39,39	0
55	MG	2A	3484	1/1	0.96	0.17	42,42,42,42	0
55	MG	1A	3068	1/1	0.96	0.35	26,26,26,26	0
55	MG	1X	106	1/1	0.96	0.15	49,49,49,49	0
55	MG	1A	3124	1/1	0.96	0.32	32,32,32,32	0
55	MG	2A	3488	1/1	0.96	0.43	39,39,39,39	0
55	MG	1A	3899	1/1	0.96	0.17	43,43,43,43	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
55	MG	1A	4036	1/1	0.96	0.15	53,53,53,53	0
55	MG	1A	3765	1/1	0.96	0.14	52,52,52,52	0
55	MG	1a	1730	1/1	0.96	0.10	36,36,36,36	0
55	MG	1A	3041	1/1	0.96	0.24	30,30,30,30	0
55	MG	1A	3767	1/1	0.96	0.30	37,37,37,37	0
55	MG	2A	3270	1/1	0.96	0.54	55,55,55,55	0
55	MG	1A	3538	1/1	0.96	0.20	25,25,25,25	0
55	MG	1A	3128	1/1	0.96	0.24	27,27,27,27	0
55	MG	1A	3173	1/1	0.96	0.08	50,50,50,50	0
55	MG	2x	105	1/1	0.96	0.10	70,70,70,70	0
55	MG	1A	3097	1/1	0.96	0.39	38,38,38,38	0
56	K	2A	3278	1/1	0.96	0.32	73,73,73,73	0
55	MG	1A	3176	1/1	0.96	0.52	38,38,38,38	0
55	MG	1A	4047	1/1	0.96	0.20	54,54,54,54	0
55	MG	2A	3097	1/1	0.96	0.19	52,52,52,52	0
55	MG	1A	3054	1/1	0.96	0.16	14,14,14,14	0
55	MG	2F	302	1/1	0.96	0.09	57,57,57,57	0
55	MG	2A	3100	1/1	0.96	0.20	53,53,53,53	0
55	MG	1A	4049	1/1	0.96	0.18	21,21,21,21	0
55	MG	1A	3056	1/1	0.96	0.45	28,28,28,28	0
55	MG	1A	3107	1/1	0.97	0.16	49,49,49,49	0
55	MG	1A	3129	1/1	0.97	0.11	44,44,44,44	0
55	MG	1A	4016	1/1	0.97	0.14	42,42,42,42	0
55	MG	1A	3654	1/1	0.97	0.14	27,27,27,27	0
55	MG	1G	205	1/1	0.97	0.09	56,56,56,56	0
55	MG	1A	3354	1/1	0.97	0.12	52,52,52,52	0
55	MG	1A	3529	1/1	0.97	0.29	52,52,52,52	0
55	MG	2A	3083	1/1	0.97	0.11	28,28,28,28	0
55	MG	1A	3822	1/1	0.97	0.17	49,49,49,49	0
55	MG	1A	3092	1/1	0.97	0.29	31,31,31,31	0
55	MG	1A	3093	1/1	0.97	0.18	33,33,33,33	0
55	MG	1A	3659	1/1	0.97	0.15	49,49,49,49	0
55	MG	2A	3413	1/1	0.97	0.17	34,34,34,34	0
55	MG	2a	1625	1/1	0.97	0.34	52,52,52,52	0
55	MG	2A	3088	1/1	0.97	0.34	65,65,65,65	0
55	MG	2A	3089	1/1	0.97	0.08	59,59,59,59	0
55	MG	2A	3417	1/1	0.97	0.10	51,51,51,51	0
55	MG	1A	3660	1/1	0.97	0.23	49,49,49,49	0
55	MG	1A	3132	1/1	0.97	0.31	40,40,40,40	0
55	MG	1A	3744	1/1	0.97	0.14	40,40,40,40	0
55	MG	1A	4027	1/1	0.97	0.16	46,46,46,46	0
55	MG	1A	3533	1/1	0.97	0.12	50,50,50,50	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
55	MG	1A	3013	1/1	0.97	0.14	29,29,29,29	0
55	MG	2A	3610	1/1	0.97	0.19	61,61,61,61	0
55	MG	1A	3061	1/1	0.97	0.19	26,26,26,26	0
55	MG	1A	3833	1/1	0.97	0.18	36,36,36,36	0
55	MG	1A	3834	1/1	0.97	0.06	59,59,59,59	0
55	MG	2A	3427	1/1	0.97	0.11	32,32,32,32	0
55	MG	1a	1778	1/1	0.97	0.14	57,57,57,57	0
55	MG	2A	3251	1/1	0.97	0.30	57,57,57,57	0
55	MG	1P	204	1/1	0.97	0.36	25,25,25,25	0
55	MG	1A	3487	1/1	0.97	0.51	41,41,41,41	0
55	MG	2A	3103	1/1	0.97	0.15	45,45,45,45	0
55	MG	1A	3275	1/1	0.97	0.21	32,32,32,32	0
55	MG	1A	3750	1/1	0.97	0.92	30,30,30,30	0
55	MG	2a	1647	1/1	0.97	0.10	51,51,51,51	0
55	MG	2A	3622	1/1	0.97	0.13	49,49,49,49	0
55	MG	2a	1649	1/1	0.97	0.06	58,58,58,58	0
55	MG	1A	3135	1/1	0.97	0.48	33,33,33,33	0
55	MG	1A	3600	1/1	0.97	0.12	19,19,19,19	0
55	MG	2A	3259	1/1	0.97	0.17	49,49,49,49	0
55	MG	1A	3840	1/1	0.97	0.13	52,52,52,52	0
55	MG	2A	3261	1/1	0.97	0.15	46,46,46,46	0
55	MG	1Q	205	1/1	0.97	0.26	45,45,45,45	0
55	MG	2A	3630	1/1	0.97	0.14	57,57,57,57	0
55	MG	1Q	206	1/1	0.97	0.10	46,46,46,46	0
55	MG	2a	1658	1/1	0.97	0.08	61,61,61,61	0
55	MG	1A	4039	1/1	0.97	0.12	52,52,52,52	0
55	MG	1A	4040	1/1	0.97	0.19	32,32,32,32	0
55	MG	1a	1791	1/1	0.97	0.21	49,49,49,49	0
55	MG	1A	3753	1/1	0.97	0.11	24,24,24,24	0
55	MG	1A	3934	1/1	0.97	0.06	39,39,39,39	0
55	MG	2A	3638	1/1	0.97	0.05	63,63,63,63	0
55	MG	2A	3450	1/1	0.97	0.23	53,53,53,53	0
55	MG	1A	3754	1/1	0.97	0.10	29,29,29,29	0
55	MG	1A	3844	1/1	0.97	0.25	44,44,44,44	0
55	MG	1A	3198	1/1	0.97	0.12	30,30,30,30	0
55	MG	1A	3846	1/1	0.97	0.51	33,33,33,33	0
55	MG	1A	3052	1/1	0.97	0.26	33,33,33,33	0
55	MG	1A	3083	1/1	0.97	0.20	30,30,30,30	0
55	MG	1d	3201	1/1	0.97	0.18	56,56,56,56	0
55	MG	1A	3942	1/1	0.97	0.20	26,26,26,26	0
55	MG	1A	3139	1/1	0.97	0.21	28,28,28,28	0
55	MG	2A	3650	1/1	0.97	0.15	26,26,26,26	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
55	MG	1A	3084	1/1	0.97	0.15	26,26,26,26	0
55	MG	1A	4053	1/1	0.97	0.17	57,57,57,57	0
55	MG	1A	3142	1/1	0.97	0.12	34,34,34,34	0
55	MG	1A	3947	1/1	0.97	0.12	27,27,27,27	0
55	MG	2A	3464	1/1	0.97	0.08	45,45,45,45	0
55	MG	2A	3465	1/1	0.97	0.15	64,64,64,64	0
55	MG	1A	3117	1/1	0.97	0.46	24,24,24,24	0
55	MG	1A	3085	1/1	0.97	0.45	32,32,32,32	0
55	MG	1A	3610	1/1	0.97	0.16	24,24,24,24	0
55	MG	1A	3207	1/1	0.97	0.39	44,44,44,44	0
55	MG	1a	1670	1/1	0.97	0.14	49,49,49,49	0
55	MG	2a	1687	1/1	0.97	0.10	52,52,52,52	0
55	MG	2A	3663	1/1	0.97	0.12	47,47,47,47	0
55	MG	1V	201	1/1	0.97	0.38	19,19,19,19	0
55	MG	1A	3612	1/1	0.97	0.14	53,53,53,53	0
55	MG	2A	3139	1/1	0.97	0.09	55,55,55,55	0
55	MG	1V	203	1/1	0.97	0.42	35,35,35,35	0
55	MG	1a	1674	1/1	0.97	0.32	61,61,61,61	0
55	MG	1x	106	1/1	0.97	0.10	53,53,53,53	0
55	MG	2A	3670	1/1	0.97	0.10	55,55,55,55	0
55	MG	2A	3143	1/1	0.97	0.33	61,61,61,61	0
55	MG	2a	1698	1/1	0.97	0.35	53,53,53,53	0
55	MG	2A	3479	1/1	0.97	0.14	29,29,29,29	0
55	MG	2A	3144	1/1	0.97	0.15	49,49,49,49	0
55	MG	1V	204	1/1	0.97	0.38	31,31,31,31	0
55	MG	1A	3549	1/1	0.97	0.15	34,34,34,34	0
55	MG	1A	3031	1/1	0.97	0.23	24,24,24,24	0
55	MG	1A	3032	1/1	0.97	0.72	36,36,36,36	0
55	MG	1A	3008	1/1	0.97	0.13	21,21,21,21	0
55	MG	2a	1707	1/1	0.97	0.33	57,57,57,57	0
55	MG	1x	112	1/1	0.97	0.12	68,68,68,68	0
55	MG	1W	201	1/1	0.97	0.27	45,45,45,45	0
55	MG	1A	3553	1/1	0.97	0.14	27,27,27,27	0
55	MG	1x	115	1/1	0.97	0.20	54,54,54,54	0
55	MG	2A	3490	1/1	0.97	0.12	63,63,63,63	0
55	MG	1A	3619	1/1	0.97	0.10	28,28,28,28	0
55	MG	1A	3555	1/1	0.97	0.12	40,40,40,40	0
55	MG	1A	3775	1/1	0.97	0.18	43,43,43,43	0
55	MG	1X	101	1/1	0.97	0.21	28,28,28,28	0
55	MG	1A	3693	1/1	0.97	0.21	37,37,37,37	0
55	MG	1A	3777	1/1	0.97	0.08	55,55,55,55	0
55	MG	1B	218	1/1	0.97	0.16	42,42,42,42	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
55	MG	2A	3314	1/1	0.97	0.36	64,64,64,64	0
55	MG	1A	3007	1/1	0.97	0.15	22,22,22,22	0
55	MG	2A	3009	1/1	0.97	0.08	50,50,50,50	0
55	MG	1A	3505	1/1	0.97	0.40	30,30,30,30	0
55	MG	2A	3011	1/1	0.97	0.13	45,45,45,45	0
55	MG	2A	3696	1/1	0.97	0.32	48,48,48,48	0
55	MG	2A	3504	1/1	0.97	0.13	35,35,35,35	0
55	MG	1A	3149	1/1	0.97	0.52	35,35,35,35	0
55	MG	1A	3029	1/1	0.97	0.50	30,30,30,30	0
55	MG	1A	3151	1/1	0.97	0.32	32,32,32,32	0
55	MG	2A	3015	1/1	0.97	0.21	32,32,32,32	0
55	MG	1B	224	1/1	0.97	0.14	59,59,59,59	0
55	MG	1A	3627	1/1	0.97	0.14	37,37,37,37	0
55	MG	2a	1736	1/1	0.97	0.06	80,80,80,80	0
55	MG	1A	3562	1/1	0.97	0.11	16,16,16,16	0
55	MG	1A	3563	1/1	0.97	0.10	25,25,25,25	0
55	MG	2A	3021	1/1	0.97	0.19	47,47,47,47	0
55	MG	1A	3786	1/1	0.97	0.12	61,61,61,61	0
55	MG	1A	3215	1/1	0.97	0.66	39,39,39,39	0
55	MG	1A	3256	1/1	0.97	0.13	57,57,57,57	0
55	MG	1A	3789	1/1	0.97	0.15	22,22,22,22	0
55	MG	1A	3976	1/1	0.97	0.19	25,25,25,25	0
55	MG	2A	3333	1/1	0.97	0.16	45,45,45,45	0
55	MG	2a	1747	1/1	0.97	0.12	53,53,53,53	0
55	MG	2A	3334	1/1	0.97	0.21	34,34,34,34	0
55	MG	2A	3522	1/1	0.97	0.13	33,33,33,33	0
55	MG	2A	3027	1/1	0.97	0.33	46,46,46,46	0
55	MG	1A	3152	1/1	0.97	0.53	21,21,21,21	0
55	MG	1A	3705	1/1	0.97	0.15	20,20,20,20	0
55	MG	1A	3979	1/1	0.97	0.14	38,38,38,38	0
55	MG	1A	3706	1/1	0.97	0.17	13,13,13,13	0
55	MG	2A	3528	1/1	0.97	0.14	61,61,61,61	0
55	MG	1A	3153	1/1	0.97	0.42	32,32,32,32	0
55	MG	2A	3530	1/1	0.97	0.12	49,49,49,49	0
55	MG	2B	210	1/1	0.97	0.11	69,69,69,69	0
55	MG	2A	3531	1/1	0.97	0.13	60,60,60,60	0
55	MG	2B	212	1/1	0.97	0.13	69,69,69,69	0
55	MG	1A	3635	1/1	0.97	0.10	14,14,14,14	0
55	MG	1D	302	1/1	0.97	0.18	28,28,28,28	0
55	MG	15	101	1/1	0.97	0.33	27,27,27,27	0
55	MG	2B	216	1/1	0.97	0.23	68,68,68,68	0
55	MG	2A	3348	1/1	0.97	0.11	49,49,49,49	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
55	MG	1A	3078	1/1	0.97	0.28	50,50,50,50	0
55	MG	1A	3797	1/1	0.97	0.17	42,42,42,42	0
55	MG	2A	3038	1/1	0.97	0.19	45,45,45,45	0
55	MG	2D	304	1/1	0.97	0.14	34,34,34,34	0
55	MG	15	105	1/1	0.97	0.32	31,31,31,31	0
55	MG	1A	3220	1/1	0.97	0.13	29,29,29,29	0
55	MG	2D	307	1/1	0.97	0.12	57,57,57,57	0
55	MG	2A	3354	1/1	0.97	0.39	51,51,51,51	0
55	MG	1A	3184	1/1	0.97	0.36	27,27,27,27	0
55	MG	1D	308	1/1	0.97	0.17	45,45,45,45	0
55	MG	17	102	1/1	0.97	0.12	33,33,33,33	0
55	MG	1a	1722	1/1	0.97	0.11	57,57,57,57	0
55	MG	1A	3987	1/1	0.97	0.28	63,63,63,63	0
55	MG	1A	3126	1/1	0.97	0.44	35,35,35,35	0
55	MG	2A	3361	1/1	0.97	0.16	39,39,39,39	0
55	MG	1a	1725	1/1	0.97	0.19	34,34,34,34	0
55	MG	1D	311	1/1	0.97	0.21	38,38,38,38	0
55	MG	2N	201	1/1	0.97	0.10	57,57,57,57	0
55	MG	2A	3365	1/1	0.97	0.16	44,44,44,44	0
55	MG	1E	301	1/1	0.97	0.41	35,35,35,35	0
55	MG	1A	3186	1/1	0.97	0.25	45,45,45,45	0
55	MG	2Q	202	1/1	0.97	0.33	45,45,45,45	0
55	MG	18	104	1/1	0.97	0.39	32,32,32,32	0
55	MG	2A	3369	1/1	0.97	0.14	31,31,31,31	0
55	MG	1a	1731	1/1	0.97	0.19	32,32,32,32	0
55	MG	1A	3518	1/1	0.97	0.07	39,39,39,39	0
55	MG	1A	3719	1/1	0.97	0.11	39,39,39,39	0
55	MG	2A	3373	1/1	0.97	0.22	44,44,44,44	0
55	MG	2A	3561	1/1	0.97	0.06	64,64,64,64	0
55	MG	1A	3896	1/1	0.97	0.09	56,56,56,56	0
55	MG	1A	3897	1/1	0.97	0.13	45,45,45,45	0
55	MG	1A	3898	1/1	0.97	0.19	20,20,20,20	0
55	MG	1A	3519	1/1	0.97	0.14	24,24,24,24	0
55	MG	2I	201	1/1	0.97	0.45	59,59,59,59	0
55	MG	2Y	201	1/1	0.97	0.23	53,53,53,53	0
55	MG	2Z	301	1/1	0.97	0.10	71,71,71,71	0
55	MG	1A	3997	1/1	0.97	0.15	43,43,43,43	0
55	MG	1A	3224	1/1	0.97	0.18	37,37,37,37	0
55	MG	2A	3569	1/1	0.97	0.18	50,50,50,50	0
55	MG	1A	3999	1/1	0.97	0.22	12,12,12,12	0
55	MG	1a	1742	1/1	0.97	0.17	68,68,68,68	0
55	MG	1A	3187	1/1	0.97	0.22	65,65,65,65	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
55	MG	2A	3573	1/1	0.97	0.07	52,52,52,52	0
55	MG	1A	3808	1/1	0.97	0.32	37,37,37,37	0
55	MG	1A	3724	1/1	0.97	0.19	46,46,46,46	0
55	MG	1A	3645	1/1	0.97	0.05	58,58,58,58	0
55	MG	1F	306	1/1	0.97	0.27	31,31,31,31	0
55	MG	1A	3127	1/1	0.97	0.26	16,16,16,16	0
55	MG	1A	3647	1/1	0.97	0.11	13,13,13,13	0
55	MG	2A	3390	1/1	0.97	0.16	54,54,54,54	0
58	ZN	1Y	203	1/1	0.97	0.13	85,85,85,85	0
55	MG	1A	3267	1/1	0.97	0.47	40,40,40,40	0
55	MG	1A	3308	1/1	0.97	0.45	25,25,25,25	0
55	MG	2A	3393	1/1	0.97	0.10	64,64,64,64	0
55	MG	1A	3584	1/1	0.97	0.12	42,42,42,42	0
58	ZN	25	102	1/1	0.97	0.17	66,66,66,66	0
55	MG	1a	1617	1/1	0.97	0.09	51,51,51,51	0
58	ZN	29	501	1/1	0.97	0.08	69,69,69,69	0
55	MG	2A	3396	1/1	0.97	0.12	32,32,32,32	0
55	MG	1n	101	1/1	0.98	0.17	67,67,67,67	0
55	MG	1A	3452	1/1	0.98	0.32	39,39,39,39	0
55	MG	1A	3811	1/1	0.98	0.27	28,28,28,28	0
55	MG	1A	3597	1/1	0.98	0.10	32,32,32,32	0
55	MG	2A	3397	1/1	0.98	0.10	30,30,30,30	0
55	MG	2A	3633	1/1	0.98	0.22	31,31,31,31	0
55	MG	1A	3946	1/1	0.98	0.09	27,27,27,27	0
55	MG	1D	305	1/1	0.98	0.21	26,26,26,26	0
55	MG	1A	3294	1/1	0.98	0.12	42,42,42,42	0
55	MG	2A	3401	1/1	0.98	0.20	22,22,22,22	0
55	MG	1A	3521	1/1	0.98	0.06	47,47,47,47	0
55	MG	1A	3367	1/1	0.98	0.21	50,50,50,50	0
55	MG	2U	201	1/1	0.98	0.36	49,49,49,49	0
55	MG	1A	3559	1/1	0.98	0.06	38,38,38,38	0
55	MG	1a	1719	1/1	0.98	0.15	71,71,71,71	0
55	MG	1A	3057	1/1	0.98	0.12	9,9,9,9	0
55	MG	2a	1713	1/1	0.98	0.05	75,75,75,75	0
55	MG	1A	3649	1/1	0.98	0.08	40,40,40,40	0
55	MG	1A	3342	1/1	0.98	0.35	44,44,44,44	0
55	MG	2A	3645	1/1	0.98	0.13	22,22,22,22	0
55	MG	1A	3760	1/1	0.98	0.11	55,55,55,55	0
55	MG	2A	3410	1/1	0.98	0.23	67,67,67,67	0
55	MG	1A	3490	1/1	0.98	0.61	35,35,35,35	0
55	MG	2a	1720	1/1	0.98	0.07	62,62,62,62	0
55	MG	2A	3412	1/1	0.98	0.25	47,47,47,47	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
55	MG	1A	3122	1/1	0.98	0.16	44,44,44,44	0
55	MG	2A	3414	1/1	0.98	0.10	33,33,33,33	0
55	MG	1a	1726	1/1	0.98	0.10	40,40,40,40	0
55	MG	1A	3235	1/1	0.98	0.17	57,57,57,57	0
55	MG	2A	3534	1/1	0.98	0.17	41,41,41,41	0
55	MG	2A	3098	1/1	0.98	0.15	57,57,57,57	0
55	MG	1W	203	1/1	0.98	0.29	35,35,35,35	0
55	MG	1A	3112	1/1	0.98	0.29	39,39,39,39	0
55	MG	2a	1730	1/1	0.98	0.18	64,64,64,64	0
55	MG	1W	205	1/1	0.98	0.40	43,43,43,43	0
55	MG	2A	3659	1/1	0.98	0.23	36,36,36,36	0
55	MG	1A	3608	1/1	0.98	0.10	18,18,18,18	0
55	MG	1A	3826	1/1	0.98	0.12	22,22,22,22	0
55	MG	1E	310	1/1	0.98	0.17	14,14,14,14	0
55	MG	1A	3321	1/1	0.98	0.27	47,47,47,47	0
55	MG	1A	3217	1/1	0.98	0.40	29,29,29,29	0
55	MG	2A	3312	1/1	0.98	0.08	47,47,47,47	0
55	MG	1A	3568	1/1	0.98	0.11	54,54,54,54	0
55	MG	1A	3711	1/1	0.98	0.18	19,19,19,19	0
55	MG	2a	1741	1/1	0.98	0.13	62,62,62,62	0
55	MG	1A	3323	1/1	0.98	0.07	48,48,48,48	0
55	MG	2A	3430	1/1	0.98	0.09	58,58,58,58	0
55	MG	1A	3081	1/1	0.98	0.16	26,26,26,26	0
55	MG	2A	3111	1/1	0.98	0.23	29,29,29,29	0
55	MG	1Y	202	1/1	0.98	0.34	46,46,46,46	0
55	MG	1A	3772	1/1	0.98	0.10	37,37,37,37	0
55	MG	1A	3714	1/1	0.98	0.09	44,44,44,44	0
55	MG	2A	3436	1/1	0.98	0.20	36,36,36,36	0
55	MG	1A	3661	1/1	0.98	0.17	42,42,42,42	0
55	MG	1A	3716	1/1	0.98	0.10	60,60,60,60	0
55	MG	1A	3662	1/1	0.98	0.08	47,47,47,47	0
55	MG	1A	3663	1/1	0.98	0.14	26,26,26,26	0
55	MG	2A	3019	1/1	0.98	0.11	28,28,28,28	0
55	MG	1A	3202	1/1	0.98	0.10	58,58,58,58	0
55	MG	1A	3047	1/1	0.98	0.16	27,27,27,27	0
55	MG	1A	3573	1/1	0.98	0.09	17,17,17,17	0
55	MG	2A	3563	1/1	0.98	0.18	39,39,39,39	0
55	MG	1A	3842	1/1	0.98	0.12	38,38,38,38	0
55	MG	11	101	1/1	0.98	0.64	33,33,33,33	0
55	MG	1A	3617	1/1	0.98	0.11	30,30,30,30	0
55	MG	1A	3352	1/1	0.98	0.45	30,30,30,30	0
55	MG	1a	1755	1/1	0.98	0.09	47,47,47,47	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
55	MG	1a	1756	1/1	0.98	0.06	63,63,63,63	0
55	MG	2a	1765	1/1	0.98	0.12	76,76,76,76	0
55	MG	2a	1766	1/1	0.98	0.10	63,63,63,63	0
55	MG	1A	3726	1/1	0.98	0.18	45,45,45,45	0
55	MG	2A	3232	1/1	0.98	0.15	35,35,35,35	0
55	MG	1A	3174	1/1	0.98	0.28	37,37,37,37	0
55	MG	1A	3620	1/1	0.98	0.19	20,20,20,20	0
55	MG	2A	3340	1/1	0.98	0.12	48,48,48,48	0
55	MG	13	101	1/1	0.98	0.16	30,30,30,30	0
55	MG	1A	3848	1/1	0.98	0.15	22,22,22,22	0
55	MG	1A	3576	1/1	0.98	0.17	20,20,20,20	0
55	MG	2A	3699	1/1	0.98	0.28	61,61,61,61	0
55	MG	2a	1776	1/1	0.98	0.10	67,67,67,67	0
55	MG	1a	1668	1/1	0.98	0.24	52,52,52,52	0
55	MG	1A	3076	1/1	0.98	0.22	38,38,38,38	0
55	MG	2A	3346	1/1	0.98	0.18	34,34,34,34	0
55	MG	2A	3347	1/1	0.98	0.08	56,56,56,56	0
55	MG	1A	3055	1/1	0.98	0.28	27,27,27,27	0
55	MG	1A	3579	1/1	0.98	0.10	25,25,25,25	0
55	MG	1A	3790	1/1	0.98	0.23	40,40,40,40	0
55	MG	2A	3040	1/1	0.98	0.10	32,32,32,32	0
55	MG	1A	3410	1/1	0.98	0.26	49,49,49,49	0
55	MG	1A	3140	1/1	0.98	0.18	35,35,35,35	0
55	MG	2A	3711	1/1	0.98	0.13	40,40,40,40	0
55	MG	1A	3245	1/1	0.98	0.56	35,35,35,35	0
55	MG	16	101	1/1	0.98	0.21	47,47,47,47	0
55	MG	1A	3178	1/1	0.98	0.41	29,29,29,29	0
55	MG	2a	1791	1/1	0.98	0.14	56,56,56,56	0
55	MG	1A	3414	1/1	0.98	0.32	30,30,30,30	0
55	MG	17	103	1/1	0.98	0.21	30,30,30,30	0
55	MG	1A	3738	1/1	0.98	0.09	38,38,38,38	0
55	MG	1A	3995	1/1	0.98	0.05	36,36,36,36	0
55	MG	1A	3860	1/1	0.98	0.12	31,31,31,31	0
55	MG	1A	3475	1/1	0.98	0.59	35,35,35,35	0
55	MG	18	102	1/1	0.98	0.74	38,38,38,38	0
55	MG	1A	3740	1/1	0.98	0.66	29,29,29,29	0
55	MG	1A	3193	1/1	0.98	0.52	47,47,47,47	0
55	MG	1A	3864	1/1	0.98	0.10	10,10,10,10	0
55	MG	1A	4001	1/1	0.98	0.15	22,22,22,22	0
55	MG	2B	209	1/1	0.98	0.09	60,60,60,60	0
55	MG	1A	3049	1/1	0.98	0.23	34,34,34,34	0
55	MG	1a	1690	1/1	0.98	0.11	46,46,46,46	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
55	MG	1A	4003	1/1	0.98	0.16	19,19,19,19	0
55	MG	1Q	207	1/1	0.98	0.25	34,34,34,34	0
55	MG	1a	1790	1/1	0.98	0.11	57,57,57,57	0
55	MG	1A	3801	1/1	0.98	0.24	37,37,37,37	0
55	MG	1A	3867	1/1	0.98	0.12	17,17,17,17	0
55	MG	1A	4006	1/1	0.98	0.18	20,20,20,20	0
55	MG	1A	4007	1/1	0.98	0.09	57,57,57,57	0
55	MG	1A	3108	1/1	0.98	0.26	27,27,27,27	0
55	MG	1A	3229	1/1	0.98	0.16	28,28,28,28	0
55	MG	1A	3448	1/1	0.98	0.30	41,41,41,41	0
55	MG	1A	3591	1/1	0.98	0.12	28,28,28,28	0
55	MG	1A	4012	1/1	0.98	0.18	35,35,35,35	0
55	MG	1A	3073	1/1	0.98	0.16	20,20,20,20	0
55	MG	1U	202	1/1	0.98	0.61	52,52,52,52	0
55	MG	1A	3101	1/1	0.98	0.51	35,35,35,35	0
55	MG	1a	1706	1/1	0.98	0.14	37,37,37,37	0
58	ZN	19	501	1/1	0.98	0.17	43,43,43,43	0
55	MG	2A	3279	1/1	0.98	0.24	15,15,15,15	0
55	MG	2a	1690	1/1	0.98	0.08	64,64,64,64	0
55	MG	2A	3075	1/1	0.98	0.29	44,44,44,44	0
55	MG	1A	3293	1/1	0.98	0.16	45,45,45,45	0
55	MG	1B	237	1/1	0.98	0.09	38,38,38,38	0
55	MG	2A	3508	1/1	0.98	0.16	46,46,46,46	0
55	MG	1A	3554	1/1	0.98	0.21	22,22,22,22	0
55	MG	1A	3138	1/1	0.99	0.22	25,25,25,25	0
55	MG	1A	3722	1/1	0.99	0.16	15,15,15,15	0
55	MG	1A	3631	1/1	0.99	0.16	23,23,23,23	0
55	MG	2A	3338	1/1	0.99	0.14	60,60,60,60	0
55	MG	1E	313	1/1	0.99	0.12	52,52,52,52	0
55	MG	1A	3003	1/1	0.99	0.12	20,20,20,20	0
55	MG	1a	1757	1/1	0.99	0.13	60,60,60,60	0
55	MG	1A	3011	1/1	0.99	0.12	24,24,24,24	0
55	MG	1A	3024	1/1	0.99	0.20	21,21,21,21	0
55	MG	2A	3376	1/1	0.99	0.19	38,38,38,38	0
55	MG	2A	3477	1/1	0.99	0.06	70,70,70,70	0
55	MG	1A	3963	1/1	0.99	0.13	19,19,19,19	0
55	MG	1U	209	1/1	0.99	0.35	30,30,30,30	0
55	MG	2A	3588	1/1	0.99	0.13	50,50,50,50	0
55	MG	1A	3681	1/1	0.99	0.10	30,30,30,30	0
55	MG	2A	3703	1/1	0.99	0.12	52,52,52,52	0
55	MG	2A	3627	1/1	0.99	0.15	44,44,44,44	0
55	MG	1a	1638	1/1	0.99	0.12	48,48,48,48	0

Continued on next page...

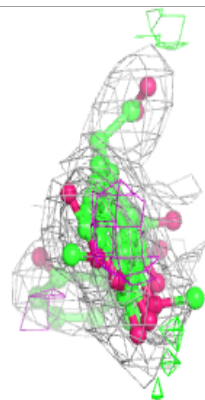
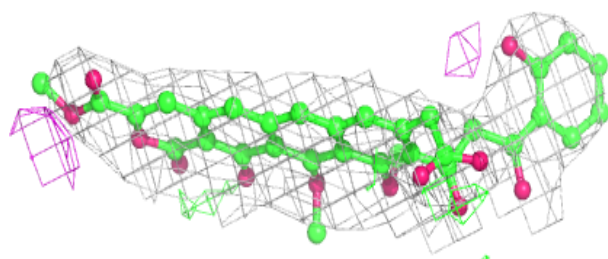
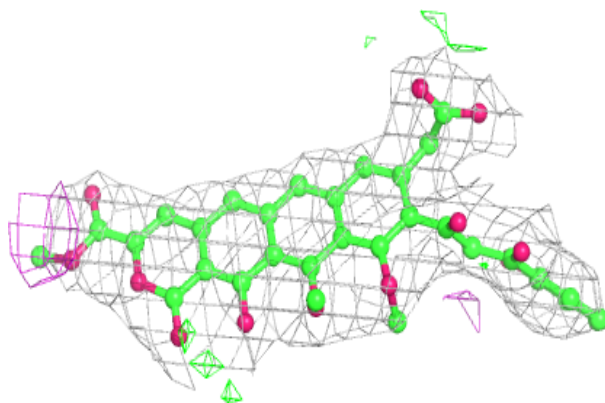
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
55	MG	2A	3447	1/1	0.99	0.14	52,52,52,52	0
55	MG	1a	1737	1/1	0.99	0.10	48,48,48,48	0
55	MG	1B	202	1/1	0.99	0.23	44,44,44,44	0
55	MG	1A	3232	1/1	0.99	0.15	31,31,31,31	0
55	MG	1A	3037	1/1	0.99	0.25	33,33,33,33	0
55	MG	1A	3717	1/1	0.99	0.17	35,35,35,35	0
55	MG	1A	3548	1/1	0.99	0.17	10,10,10,10	0
55	MG	1a	1770	1/1	0.99	0.09	48,48,48,48	0
55	MG	2A	3113	1/1	0.99	0.22	41,41,41,41	0
55	MG	1S	201	1/1	0.99	0.23	49,49,49,49	0
55	MG	1E	306	1/1	0.99	0.11	31,31,31,31	0
55	MG	1A	3499	1/1	0.99	0.15	40,40,40,40	0
55	MG	1A	3941	1/1	0.99	0.09	23,23,23,23	0
55	MG	1a	1648	1/1	0.99	0.08	68,68,68,68	0
55	MG	1a	1603	1/1	0.99	0.09	65,65,65,65	0
58	ZN	16	102	1/1	0.99	0.19	39,39,39,39	0
55	MG	2a	1699	1/1	0.99	0.26	48,48,48,48	0
55	MG	2A	3120	1/1	0.99	0.19	33,33,33,33	0
55	MG	2A	3363	1/1	0.99	0.10	39,39,39,39	0
55	MG	2A	3499	1/1	0.99	0.11	59,59,59,59	0
55	MG	15	104	1/1	0.99	0.59	27,27,27,27	0
55	MG	1A	3686	1/1	0.99	0.10	23,23,23,23	0
55	MG	2a	1624	1/1	0.99	0.16	57,57,57,57	0
55	MG	1a	1700	1/1	0.99	0.28	44,44,44,44	0
59	SF4	1d	3202	8/8	0.99	0.17	58,70,78,85	0
59	SF4	2d	501	8/8	0.99	0.14	68,75,83,84	0
58	ZN	15	108	1/1	1.00	0.18	43,43,43,43	0
55	MG	1A	3664	1/1	1.00	0.15	18,18,18,18	0

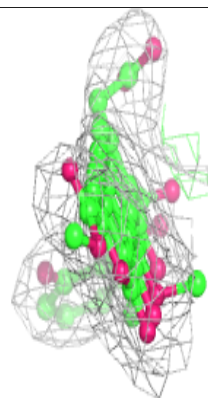
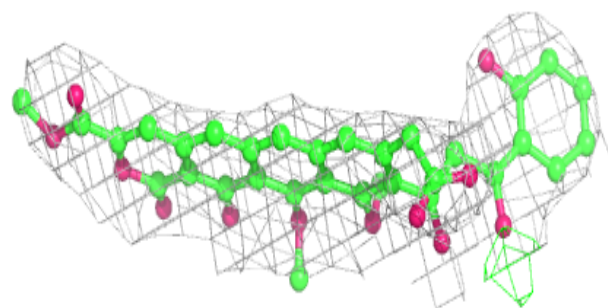
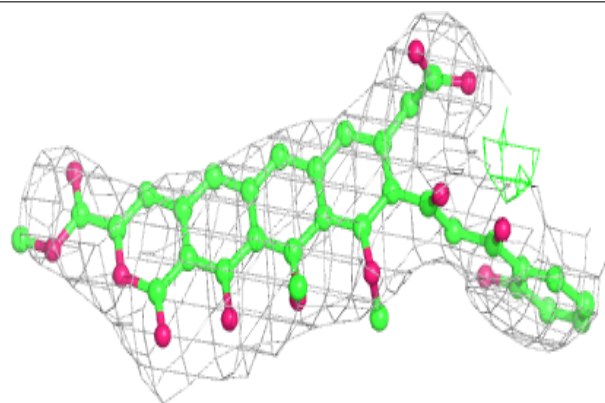
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around T8B 1A 4052:

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

**Electron density around T8B 2A 3717:**

$2mF_o-DF_c$ (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.